Foundations of Machine Learning
Convex Optimization

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Convex Optimization

Convexity

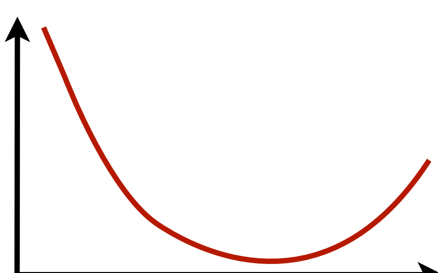
- Definition: $X \subseteq \mathbb{R}^N$ is said to be convex if for any two points $x, y \in X$ the segment $[x, y]$ lies in X:

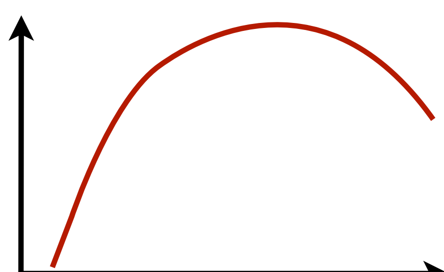
$$\{\alpha x + (1-\alpha)y, 0 \leq \alpha \leq 1\} \subseteq X.$$

- Definition: let X be a convex set. A function $f\colon X \to \mathbb{R}$ is said to be convex if for all $x, y \in X$ and $\alpha \in [0,1]$,

$$f(\alpha x + (1-\alpha)y) \leq \alpha f(x) + (1-\alpha)f(y).$$

With a strict inequality, f is said to be strictly convex. f is said to be concave when $-f$ is convex.

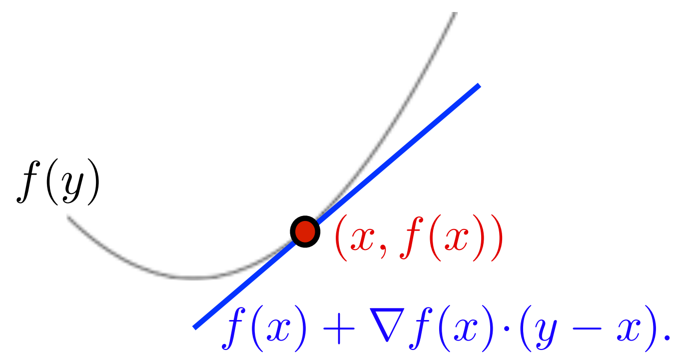




Properties of Convex Functions

- **Theorem**: let f be a differentiable function. Then, f is convex iff $\mathrm{dom}(f)$ is convex and

$$\forall x, y \in \mathrm{dom}(f), \;\; f(y) - f(x) \geq \nabla f(x) \cdot (y - x).$$



- **Theorem**: let f be a twice differentiable function. Then, f is convex iff its Hessian is positive semi-definite:

$$\forall x \in \mathrm{dom}(f), \;\; \nabla^2 f(x) \succeq 0.$$

Constrained Optimization Problem

- Problem: Let $X \subseteq \mathbb{R}^N$ and $f, g_i : X \to \mathbb{R}$, $i \in [1, m]$. A constrained optimization problem has the form:

$$\min_{\mathbf{x} \in X} \quad f(\mathbf{x})$$
$$\text{subject to:} \quad g_i(\mathbf{x}) \leq 0, i \in [1, m].$$

- Definition: The Lagrange function or Lagrangian associated to this problem is the function defined by:

$$\forall \mathbf{x} \in X, \forall \boldsymbol{\alpha} \geq 0, L(\mathbf{x}, \boldsymbol{\alpha}) = f(\mathbf{x}) + \sum_{i=1}^{m} \alpha_i g_i(x).$$

α_is are called Lagrange or dual variables.

Sufficient Condition

(Lagrange, 1797)

- **Theorem**: Let P be a constrained optimization problem over $X = \mathbb{R}^N$. If $(\mathbf{x}^*, \boldsymbol{\alpha}^*)$ is a saddle point, that is $\forall \mathbf{x} \in \mathbb{R}^N, \forall \boldsymbol{\alpha} \geq 0,\ L(\mathbf{x}^*, \boldsymbol{\alpha}) \leq L(\mathbf{x}^*, \boldsymbol{\alpha}^*) \leq L(\mathbf{x}, \boldsymbol{\alpha}^*)$, then it is a solution of P.

- **Proof**: By the first inequality,

$$\forall \boldsymbol{\alpha} \geq 0, L(\mathbf{x}^*, \boldsymbol{\alpha}) \leq L(\mathbf{x}^*, \boldsymbol{\alpha}^*) \Rightarrow \forall \boldsymbol{\alpha} \geq 0, \boldsymbol{\alpha} \cdot g(\mathbf{x}^*) \leq \boldsymbol{\alpha}^* \cdot g(\mathbf{x}^*)$$

$$(\text{use } \alpha \to +\infty \text{ then } \alpha \to 0) \Rightarrow \boxed{g(\mathbf{x}^*) \leq 0 \wedge \boldsymbol{\alpha}^* \cdot g(\mathbf{x}^*) = 0.}$$

  - In view of that, the second inequality gives

$$\forall \mathbf{x}, L(\mathbf{x}^*, \boldsymbol{\alpha}^*) \leq L(\mathbf{x}, \boldsymbol{\alpha}^*) \Rightarrow \forall \mathbf{x}, f(\mathbf{x}^*) \leq f(\mathbf{x}) + \boldsymbol{\alpha}^* \cdot g(\mathbf{x}).$$

Thus, for all x such that $g(x) \leq 0$, $\boxed{f(\mathbf{x}^*) \leq f(\mathbf{x}).}$

Constraint Qualification

- Definition: Assume that $\mathbf{int}\, X \neq \emptyset$. Then, the following is the strong constraint qualification or Slater's condition:

$$\exists\, \overline{\mathbf{x}} \in \mathbf{int}\, X\colon\ g(\overline{\mathbf{x}}) < 0.$$

- Definition: Assume that $\mathbf{int}\, X \neq \emptyset$. Then, the following is the weak constraint qualification or Slater's condition:

$$\exists\, \overline{\mathbf{x}} \in \mathbf{int}\, X\colon\ \forall i \in [1, m], \big(g_i(\overline{\mathbf{x}}) < 0\big) \vee \big(g_i(\overline{\mathbf{x}}) = 0 \wedge g_i \text{ affine}\big).$$

Necessary Conditions

- Theorem: Assume that f and g_i , $i \in [1, m]$, are convex functions and that Slater's condition holds. If $\mathbf{x}$ is a solution of the constrained optimization problem, then there exists $\alpha \geq 0$ such that $(\mathbf{x}, \boldsymbol{\alpha})$ is a saddle point of the Lagrangian.
- Theorem: Assume that f and g_i , $i \in [1, m]$, are convex differentiable functions and that the weak Slater's condition holds. If $\mathbf{x}$ is a solution of the constrained optimization problem, then there exists $\alpha \geq 0$ such that $(\mathbf{x}, \boldsymbol{\alpha})$ is a saddle point of the Lagrangian.

Kuhn-Tucker's Theorem

(Karush 1939; Kuhn-Tucker, 1951)

- **Theorem**: Assume that $f, g_i \colon X \to \mathbb{R}, i \in [1, m]$ are convex and differentiable and that the constraints are qualified. Then $\overline{\mathbf{x}}$ is a solution of the constrained program iff there exist $\overline{\boldsymbol{\alpha}} \geq 0$ such that:

$$\left.\begin{aligned}
&\nabla_{\mathbf{x}} L(\overline{\mathbf{x}}, \overline{\boldsymbol{\alpha}}) = \nabla_{\mathbf{x}} f(\overline{\mathbf{x}}) + \overline{\boldsymbol{\alpha}} \cdot \nabla_{\mathbf{x}} g(\overline{\mathbf{x}}) = 0 \\
&\nabla_{\boldsymbol{\alpha}} L(\overline{\mathbf{x}}, \overline{\boldsymbol{\alpha}}) = g(\overline{\mathbf{x}}) \leq 0 \\
&\overline{\boldsymbol{\alpha}} \cdot g(\overline{\mathbf{x}}) = \sum_{i=1}^{m} \overline{\boldsymbol{\alpha}}_i g_i(\overline{\mathbf{x}}) = 0 \,.
\end{aligned}\right\} \quad \text{KKT conditions}$$

- **Note**: Last two conditions equivalent to

$$\big(g(\overline{\mathbf{x}}) \leq 0\big) \wedge \big(\underbrace{\forall i \in [1, m], \bar{\alpha}_i g_i(\overline{\mathbf{x}}) = 0}_{\text{complementary conditions}}\big).$$

- Since the constraints are qualified, if $\overline{\mathbf{x}}$ is solution, then there exists $\overline{\boldsymbol{\alpha}}$ such that $(\overline{\mathbf{x}}, \overline{\boldsymbol{\alpha}})$ is a saddle point. In that case, the three conditions are verified (for the 3rd condition see proof of sufficient condition slide).
- Conversely, assume that the conditions are verified. Then, for any $\mathbf{x}$ such that $g(\mathbf{x}) < 0$,

$$
\begin{aligned}
f(\mathbf{x}) - f(\overline{\mathbf{x}}) &\geq \nabla_{\mathbf{x}} f(\overline{\mathbf{x}}) \cdot (\mathbf{x} - \overline{\mathbf{x}}) && \text{(convexity of } f\text{)} \\
&= -\sum_{i=1}^{m} \overline{\boldsymbol{\alpha}}_i \nabla_{\mathbf{x}} g_i(\overline{\mathbf{x}}) \cdot (\mathbf{x} - \overline{\mathbf{x}}) && \text{(first condition)} \\
&\geq -\sum_{i=1}^{m} \overline{\boldsymbol{\alpha}}_i [g_i(\mathbf{x}) - g_i(\overline{\mathbf{x}})] && \text{(convexity of } g_i\text{s)} \\
&= -\sum_{i=1}^{m} \overline{\boldsymbol{\alpha}}_i g_i(\mathbf{x}) \geq 0, && \text{(third condition)}
\end{aligned}
$$

Primal and Dual Problems

- Primal problem:

$$\min_{\mathbf{x} \in X} \quad f(\mathbf{x})$$
$$\text{subject to: } \quad g(\mathbf{x}) \leq 0.$$

- Dual problem:

$$\max_{\boldsymbol{\alpha}} \inf_{\mathbf{x} \in X} \quad L(\mathbf{x}, \boldsymbol{\alpha})$$
$$\text{subject to: } \quad \boldsymbol{\alpha} \geq 0.$$

Equivalent problems when constraints qualified.

Foundations of Machine Learning
Introduction to ML

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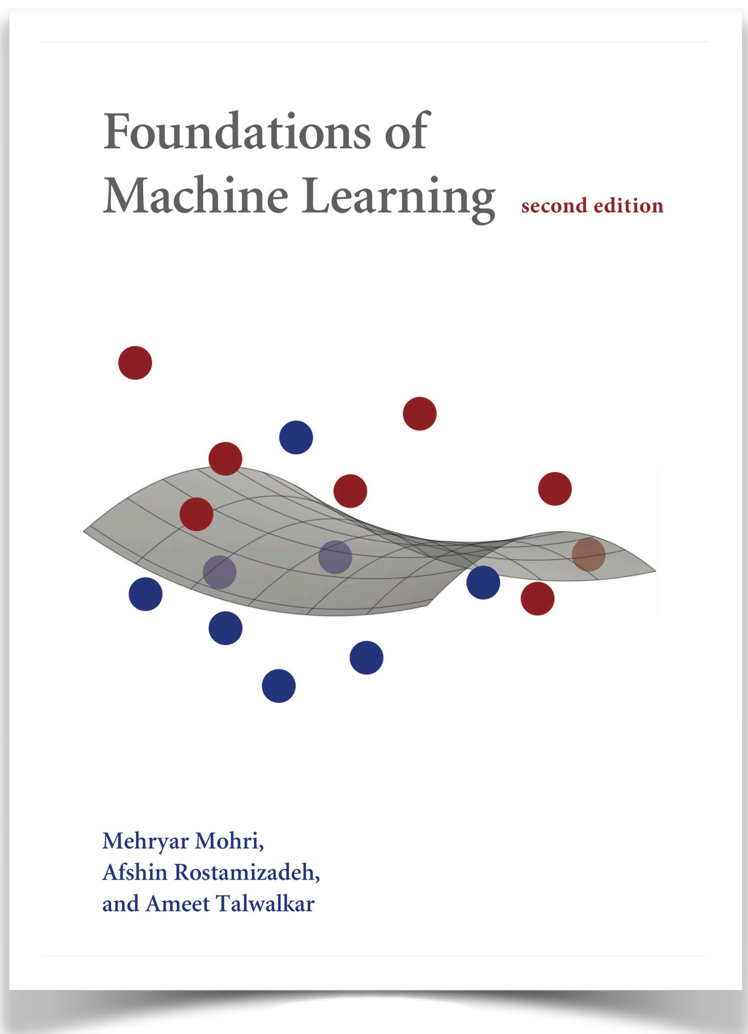
Logistics

- Prerequisites: basics in linear algebra, probability, and analysis of algorithms.
- Workload: about 3-4 homework assignments + project.
- Mailing list: join as soon as possible.

Course Material

- Textbook



- Slides: course web page.

  https://cs.nyu.edu/~mohri/ml24/

This Lecture

- Basic definitions and concepts.
- Introduction to the problem of learning.
- Probability tools.

Machine Learning

- Definition: computational methods using experience to improve performance.
- Experience: → data-driven task, thus statistics, probability, and optimization.
- Computer science: learning algorithms, analysis of complexity, theoretical guarantees.
- Example: use document word counts to predict its topic.

Examples of Learning Tasks

- Text: document classification, spam detection.
- Language: NLP tasks (e.g., morphological analysis, POS tagging, context-free parsing, dependency parsing).
- Speech: recognition, synthesis, verification.
- Image: annotation, face recognition, OCR, handwriting recognition.
- Games (e.g., chess, backgammon, go).
- Unassisted control of vehicles (robots, car).
- Medical diagnosis, fraud detection, network intrusion.

Some Broad ML Tasks

- Classification: assign a category to each item (e.g., document classification).
- Regression: predict a real value for each item (prediction of stock values, economic variables).
- Ranking: order items according to some criterion (relevant web pages returned by a search engine).
- Clustering: partition data into ‘homogenous’ regions (analysis of very large data sets).
- Dimensionality reduction: find lower-dimensional manifold preserving some properties of the data.

General Objectives of ML

- Theoretical questions:
  - what can be learned, under what conditions?
  - are there learning guarantees?
  - analysis of learning algorithms.
- Algorithms:
  - more efficient and more accurate algorithms.
  - deal with large-scale problems.
  - handle a variety of different learning problems.

This Course

- Theoretical foundations:
  - learning guarantees.
  - analysis of algorithms.
- Algorithms:
  - main mathematically well-studied algorithms.
  - discussion of their extensions.
- Applications:
  - illustration of their use.

Topics

- Probability tools, concentration inequalities.
- PAC learning model, Rademacher complexity, VC-dimension, generalization bounds.
- Support vector machines (SVMs), margin bounds, kernel methods.
- Ensemble methods, boosting.
- Logistic regression and conditional maximum entropy models.
- On-line learning, weighted majority algorithm, Perceptron algorithm, mistake bounds.
- Regression, generalization, algorithms.
- Ranking, generalization, algorithms.
- Reinforcement learning, MDPs, bandit problems and algorithm.

Definitions and Terminology

- Example: item, instance of the data used.
- Features: attributes associated to an item, often represented as a vector (e.g., word counts).
- Labels: category (classification) or real value (regression) associated to an item.
- Data:
  - training data (typically labeled).
  - test data (labeled but labels not seen).
  - validation data (labeled, for tuning parameters).

General Learning Scenarios

- Settings:
  - batch: learner receives full (training) sample, which he uses to make predictions for unseen points.
  - on-line: learner receives one sample at a time and makes a prediction for that sample.
- Queries:
  - active: the learner can request the label of a point.
  - passive: the learner receives labeled points.

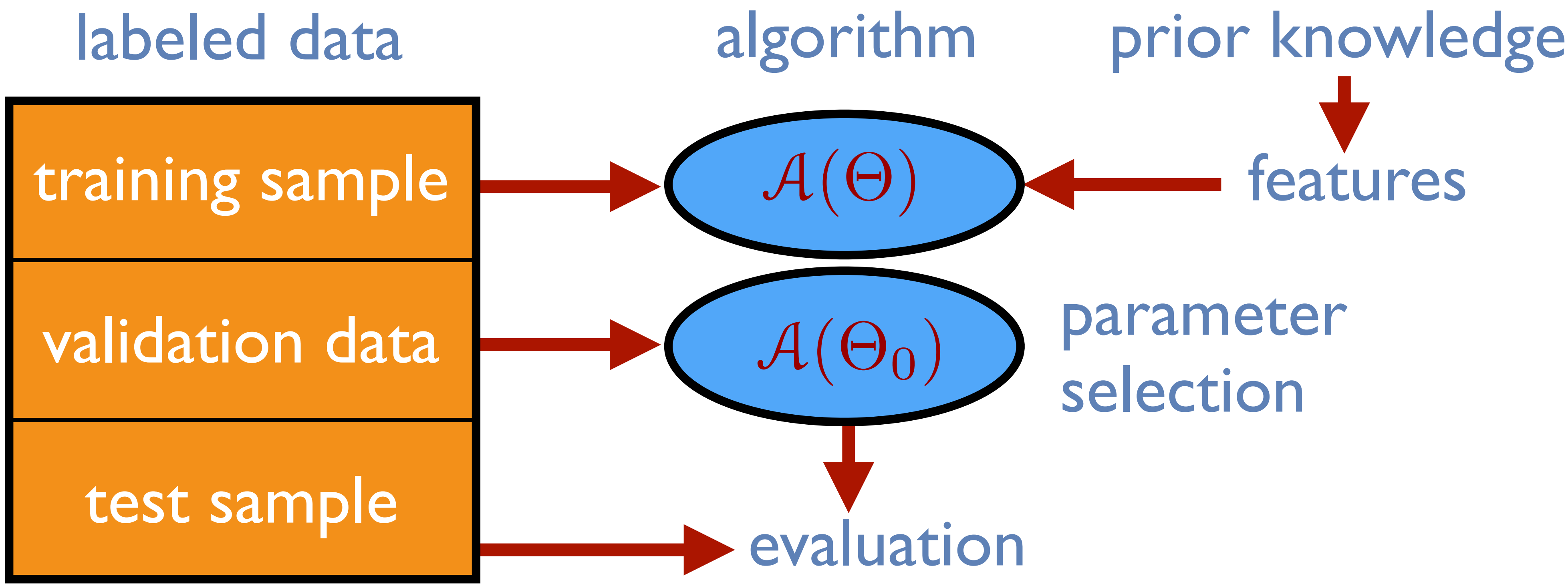
Standard Batch Scenarios

- Unsupervised learning: no labeled data.
- Supervised learning: uses labeled data for prediction on unseen points.
- Semi-supervised learning: uses labeled and unlabeled data for prediction on unseen points.
- Transduction: uses labeled and unlabeled data for prediction on seen points.

Example - SPAM Detection

- Problem: classify each e-mail message as SPAM or non-SPAM (binary classification problem).
- Potential data: large collection of SPAM and non-SPAM messages (labeled examples).

Learning Stages



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Definitions

- Spaces: input space X, output space Y.
- Loss function: $L\colon Y \times Y \to \mathbb{R}$.
  - $L(\widehat{y}, y)$: cost of predicting $\widehat{y}$ instead of y.
  - binary classification: 0-1 loss, $L(y, y') = 1_{y \neq y'}$.
  - regression: $Y \subseteq \mathbb{R}$, $l(y, y') = (y' - y)^2$.
- Hypothesis set: $H \subseteq Y^X$, subset of functions out of which the learner selects his hypothesis.
  - depends on features.
  - represents prior knowledge about task.

Supervised Learning Set-Up

- Training data: sample S of size m drawn i.i.d. from $X \times Y$ according to distribution D:

$$S = ((x_1, y_1), \ldots, (x_m, y_m)).$$

- Problem: find hypothesis $h \in H$ with small generalization error.
  - deterministic case: output label deterministic function of input, $y = f(x)$.
  - stochastic case: output probabilistic function of input.

Errors ⇒ They are essentially probabilities

- Generalization error: for $h \in H$, it is defined by

$$R(h) = \mathop{\mathrm{E}}_{(x,y)\sim D}[L(h(x), y)].$$ true error

(we don't have access to D)

- Empirical error: for $h \in H$ and sample S, it is

$$\widehat{R}(h) = \frac{1}{m} \sum_{i=1}^{m} L(h(x_i), y_i).$$

- Bayes error:

$$R^\star = \inf_{\substack{h \\ h \text{ measurable}}} R(h).$$ The absolute best error

  - in deterministic case, $R^\star = 0$.

Noise

- Noise:
  - in binary classification, for any $x \in X$,

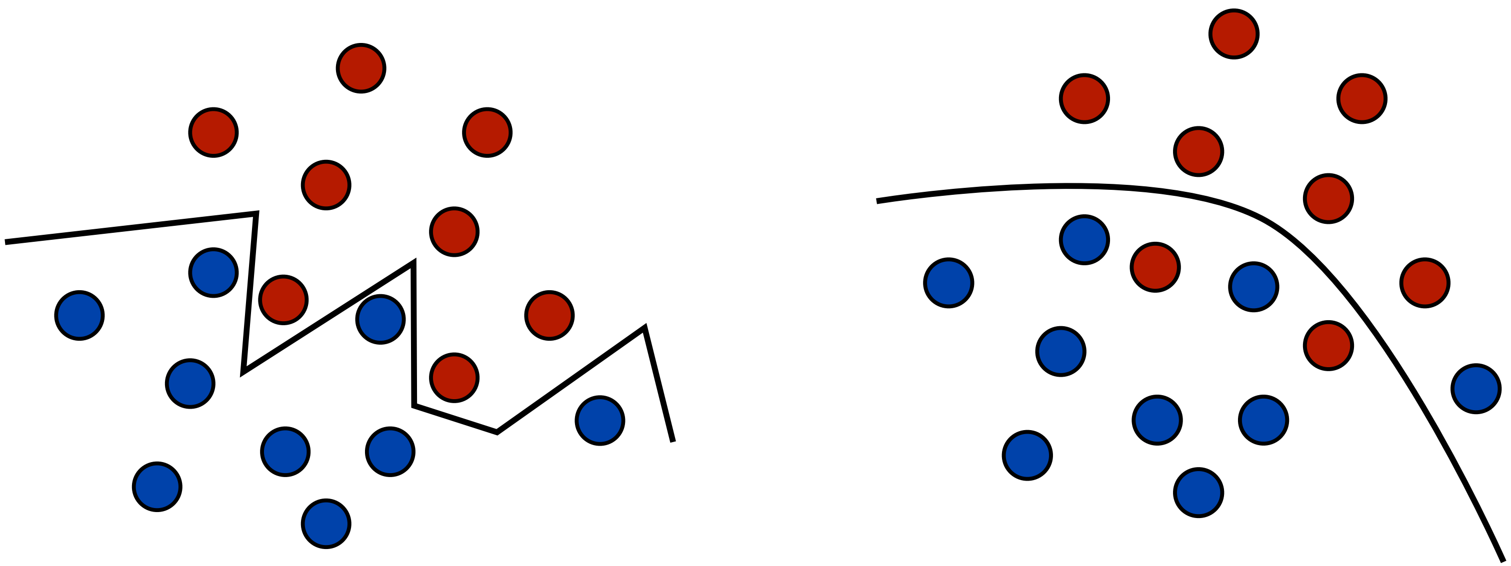
prob.

$$\text{noise}(x) = \min\{\Pr[1|x], \Pr[0|x]\}.$$

  - observe that $\text{E}[\text{noise}(x)] = R^*$.

what you suffer anyway
as you will pick the max

Learning ≠ Fitting



Notion of simplicity/complexity.

→ How do we define complexity?

Generalization

(Heart)

- Observations:
  - the best hypothesis on the sample may not be the best overall.
  - generalization is not memorization.
  - complex rules (very complex separation surfaces) can be poor predictors.
  - trade-off: complexity of hypothesis set vs sample size (underfitting/overfitting).

Model Selection

- General equality: for any $h \in H$,

best in class H

$$R(h) - R^* = \underbrace{[R(h) \overset{\geqslant}{-} R(h^*)]}_{\text{estimation}} + \underbrace{[R(h^*) - R^*]}_{\text{approximation}}.$$

- Approximation: not a random variable, only depends on H.
- Estimation: only term we can hope to bound.
- How should we choose H?

Empirical Risk Minimization

- Select hypothesis set H.
- Find hypothesis $h \in H$ minimizing empirical error:

$$h = \operatorname*{argmin}_{h \in H} \widehat{R}(h).$$

  - but H may be too complex.
  - the sample size may not be large enough.

Generalization Bounds

- Definition: upper bound on $\Pr\left[\sup_{h\in H} |R(h) - \widehat{R}(h)| > \epsilon\right]$.
- Bound on estimation error for hypothesis h_0 given by ERM:

$$\begin{aligned} R(h_0) - R(h^*) &= R(h_0) - \widehat{R}(h_0) + \widehat{R}(h_0) - R(h^*) \\ &\leq R(h_0) - \widehat{R}(h_0) + \widehat{R}(h^*) - R(h^*) \\ &\leq 2 \sup_{h\in H} |R(h) - \widehat{R}(h)|. \end{aligned}$$

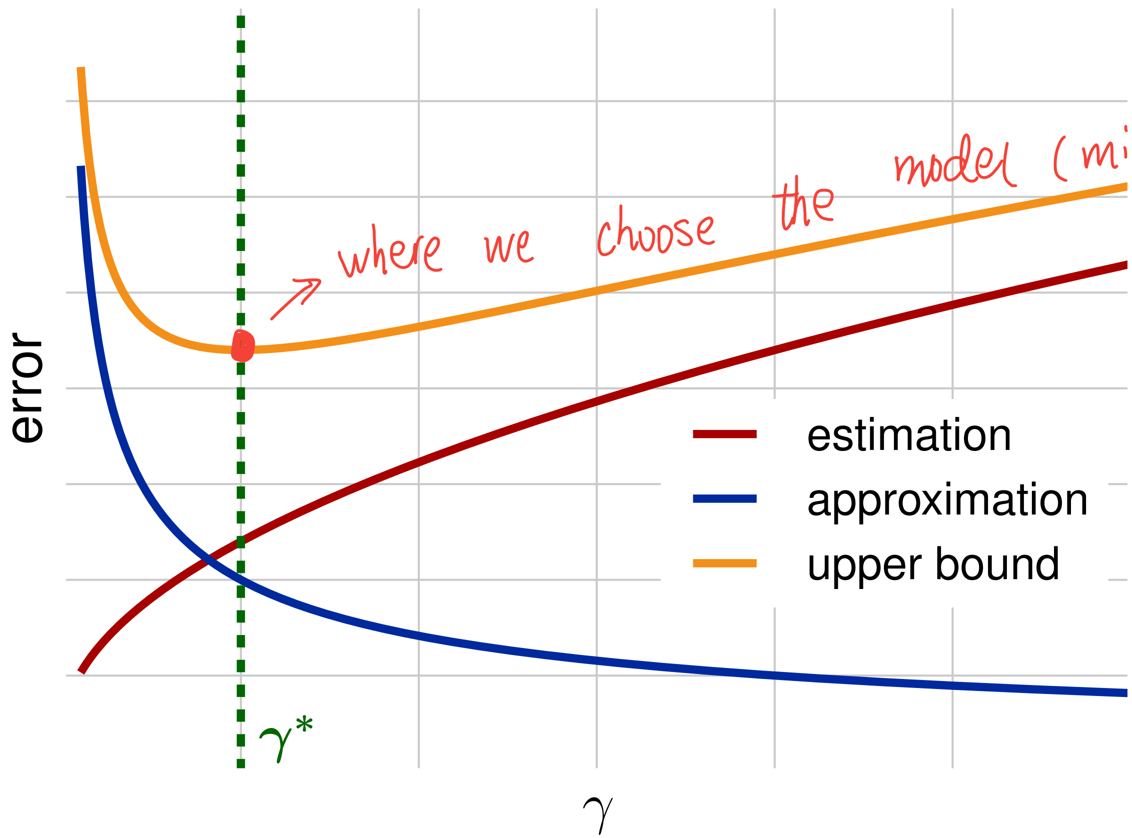
h_0 is best for $\widehat{R}$

h^* is best for R

for infinite dataset, h_0 could be h^*

→ How should we choose H? (model selection problem)

Model Selection



where we choose the model (min of orange, which is esti. + approx.)

$$\mathcal{H} = \bigcup_{\gamma \in \Gamma} \mathcal{H}_\gamma.$$

how complex $\mathcal{H}_\gamma$ is (e.g. degree)

Structural Risk Minimization

(Vapnik, 1995)

- Principle: consider an infinite sequence of hypothesis sets ordered for inclusion,

$$H_1 \subset H_2 \subset \cdots \subset H_n \subset \cdots$$

sample size

$$h = \operatorname*{argmin}_{h \in H_n, n \in \mathbb{N}} \widehat{R}(h) + \textbf{penalty}(H_n, m).$$

in particular, regularization

- strong theoretical guarantees.
- typically computationally hard.

General Algorithm Families

- Empirical risk minimization (ERM):

$$h = \operatorname*{argmin}_{h \in H} \widehat{R}(h).$$

- Structural risk minimization (SRM): $H_n \subseteq H_{n+1}$,

$$h = \operatorname*{argmin}_{h \in H_n, n \in \mathbb{N}} \widehat{R}(h) + \textbf{penalty}(H_n, m).$$

→ penalizing the complexity

- Regularization-based algorithms: $\lambda \geq 0$,

$$h = \operatorname*{argmin}_{h \in H} \widehat{R}(h) + \lambda \|h\|^2.$$

(can be viewed as a smooth version of SRM)

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- Basic definitions and concepts.
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Basic Properties

- Union bound: $\Pr[A \vee B] \leq \Pr[A] + \Pr[B]$.

??

- Inversion: if $\Pr[X \geq \epsilon] \leq f(\epsilon)$, then, for any $\delta > 0$, with probability at least $1 - \delta$, $X \leq f^{-1}(\delta)$.

- Jensen's inequality: if f is convex, $f(\mathrm{E}[X]) \leq \mathrm{E}[f(X)]$.

- Expectation: if $X \geq 0$, $\mathrm{E}[X] = \int_0^{+\infty} \Pr[X > t]\, dt$.

Basic Inequalities

- Markov's inequality: if $X \geq 0$ and $\epsilon > 0$, then

$$\Pr[X \geq \epsilon] \leq \frac{\mathrm{E}[X]}{\epsilon}.$$

- Chebyshev's inequality: for any $\epsilon > 0$,

Var(X)

$$\Pr[|X - \mathrm{E}[X]| \geq \epsilon] \leq \frac{\sigma_X^2}{\epsilon^2}.$$

Hoeffding's Inequality

- Theorem: Let $X_1, \ldots, X_m$ be indep. rand. variables with the same expectation μ and $X_i \in [a, b]$, ($a < b$). Then, for any $\epsilon > 0$, the following inequalities hold:

$$\Pr\left[\mu - \frac{1}{m}\sum_{i=1}^{m} X_i > \epsilon\right] \leq \exp\left(-\frac{2m\epsilon^2}{(b-a)^2}\right)$$

$$\Pr\left[\frac{1}{m}\sum_{i=1}^{m} X_i - \mu > \epsilon\right] \leq \exp\left(-\frac{2m\epsilon^2}{(b-a)^2}\right).$$

Hope: as long as the same size m is large enough,
we can estimate the expectation μ.

McDiarmid's Inequality

(McDiarmid, 1989)

- **Theorem**: let $X_1, \ldots, X_m$ be independent random variables taking values in U and $f: U^m \to \mathbb{R}$ a function verifying for all $i \in [1, m]$,

$$\sup_{x_1,\ldots,x_m,x_i'} |f(x_1,\ldots,x_i,\ldots,x_m) - f(x_1,\ldots,x_i',\ldots,x_m)| \leq c_i.$$

best: $c_i \in (\frac{1}{m^2}, \frac{1}{m})$

"Lipschitz condition"

we would like it to be dependent on m

if it's $\frac{1}{m}$, it's Hoffding's thm.

Then, for all $\epsilon > 0$,

$$\Pr\Big[\big|f(X_1,\ldots,X_m) - \mathrm{E}[f(X_1,\ldots,X_m)]\big| > \epsilon\Big] \leq 2\exp\left(-\frac{2\epsilon^2}{\sum_{i=1}^m c_i^2}\right).$$

Rmk. Hoffding's thm. is the special example for McDiamid's Ineq. by taking f to be the average function

Appendix

Markov's Inequality

- Theorem: let X be a non-negative random variable with $\mathrm{E}[X] < \infty$, then, for all $t > 0$,

$$\Pr[X \geq t\mathrm{E}[X]] \leq \frac{1}{t}.$$

- Proof:

$$\begin{aligned}
\Pr[X \geq t\,\mathrm{E}[X]] &= \sum_{x \geq t\mathrm{E}[X]} \Pr[X = x] \\
&\leq \sum_{x \geq t\,\mathrm{E}[X]} \Pr[X = x] \frac{x}{t\,\mathrm{E}[X]} \\
&\leq \sum_{x} \Pr[X = x] \frac{x}{t\,\mathrm{E}[X]} \\
&= \mathrm{E}\left[\frac{X}{t\,\mathrm{E}[X]}\right] = \frac{1}{t}.
\end{aligned}$$

Chebyshev's Inequality

- Theorem: let X be a random variable with $\mathrm{Var}[X] < \infty$, then, for all $t > 0$,

$$\Pr[|X - \mathrm{E}[X]| \geq t\sigma_X] \leq \frac{1}{t^2}.$$

- Proof: Observe that

$$\Pr[|X - \mathrm{E}[X]| \geq t\sigma_X] = \Pr[(X - \mathrm{E}[X])^2 \geq t^2\sigma_X^2].$$

The result follows Markov's inequality.

Weak Law of Large Numbers

- Theorem: let $(X_n)_{n\in\mathbb{N}}$ be a sequence of independent random variables with the same mean μ and variance $\sigma^2 < \infty$ and let $\overline{X}_n = \frac{1}{n}\sum_{i=1}^{n} X_i$, then, for any $\epsilon > 0$,

$$\lim_{n\to\infty} \Pr[|\overline{X}_n - \mu| \geq \epsilon] = 0.$$

- Proof: Since the variables are independent,

$$\mathrm{Var}[\overline{X}_n] = \sum_{i=1}^{n} \mathrm{Var}\left[\frac{X_i}{n}\right] = \frac{n\sigma^2}{n^2} = \frac{\sigma^2}{n}.$$

- Thus, by Chebyshev's inequality,

$$\Pr[|\overline{X}_n - \mu| \geq \epsilon] \leq \frac{\sigma^2}{n\epsilon^2}.$$

Concentration Inequalities

- Some general tools for error analysis and bounds:
  - Hoeffding's inequality (additive).
  - Chernoff bounds (multiplicative).
  - McDiarmid's inequality (more general).

Hoeffding's Inequality

- Corollary: for any $\epsilon > 0$, any distribution D and any hypothesis $h \colon X \to \{0, 1\}$, the following inequalities hold:

$$\Pr[\widehat{R}(h) - R(h) \geq \epsilon] \leq e^{-2m\epsilon^2}$$
$$\Pr[\widehat{R}(h) - R(h) \leq -\epsilon] \leq e^{-2m\epsilon^2}.$$

- Proof: follows directly Hoeffding's theorem.

- Combining these one-sided inequalities yields

$$\Pr\left[\left|\widehat{R}(h) - R(h)\right| \geq \epsilon\right] \leq 2e^{-2m\epsilon^2}.$$

Chernoff's Inequality

- Theorem: for any $\epsilon > 0$, any distribution D and any hypothesis $h\colon X \to \{0,1\}$, the following inequalities hold:

$$\Pr[\widehat{R}(h) \geq (1+\epsilon)R(h)] \leq e^{-m\,R(h)\,\epsilon^2/3}$$

$$\Pr[\widehat{R}(h) \leq (1-\epsilon)R(h)] \leq e^{-m\,R(h)\,\epsilon^2/2}.$$

- Proof: proof based on Chernoff's bounding technique.

McDiarmid's Inequality

(McDiarmid, 1989)

- Theorem: let $X_1, \ldots, X_m$ be independent random variables taking values in U and $f\colon U^m \to \mathbb{R}$ a function verifying for all $i \in [1, m]$,

$$\sup_{x_1,\ldots,x_m,x'_i} \left|f(x_1,\ldots,x_i,\ldots,x_m) - f(x_1,\ldots,x'_i,\ldots,x_m)\right| \leq c_i.$$

Then, for all $\epsilon > 0$,

$$\Pr\Big[\big|f(X_1,\ldots,X_m) - \mathrm{E}[f(X_1,\ldots,X_m)]\big| > \epsilon\Big] \leq 2\exp\left(-\frac{2\epsilon^2}{\sum_{i=1}^m c_i^2}\right).$$

- Comments:
  - Proof: uses Hoeffding's lemma.
  - Hoeffding's inequality is a special case of McDiarmid's with

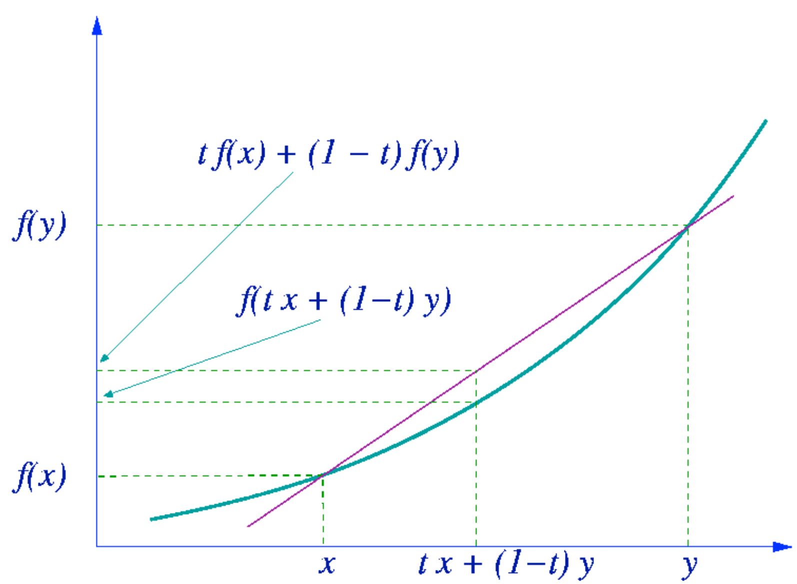
$$f(x_1, \ldots, x_m) = \frac{1}{m} \sum_{i=1}^{m} x_i \quad \text{and} \quad c_i = \frac{|b_i - a_i|}{m}.$$

Jensen's Inequality

- Theorem: let X be a random variable and f a measurable convex function. Then,

$$f(\mathrm{E}[X]) \leq \mathrm{E}[f(X)].$$

- Proof: definition of convexity, continuity of convex functions, and density of finite distributions.



Foundations of Machine Learning

Learning with Finite Hypothesis Sets

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Motivation

- Some computational learning questions
  - What can be learned efficiently?
  - What is inherently hard to learn?
  - A general model of learning?
- Complexity
  - Computational complexity: time and space.
  - Sample complexity: amount of training data needed to learn successfully.
  - Mistake bounds: number of mistakes before learning successfully.

This lecture

- PAC Model
- Sample complexity, finite *H*, consistent case
- Sample complexity, finite *H*, inconsistent case

Definitions and Notation

- X: set of all possible instances or examples, e.g., the set of all men and women characterized by their height and weight.

→ we start with binary classification

- $c \colon X \to \{0, 1\}$: the target concept to learn; can be identified with its support $\{x \in X \colon c(x) = 1\}$.

(≠0)

- C: concept class, a set of target concepts c.
- D: target distribution, a fixed probability distribution over X. Training and test examples are drawn according to D.

Definitions and Notation

- S : training sample.
- H : set of concept hypotheses, e.g., the set of all linear classifiers.
- The learning algorithm receives sample S and selects a hypothesis h_S from H approximating c .

Errors

- True error or generalization error of h with respect to the target concept c and distribution D:

$$R(h) = \Pr_{x \sim D}[h(x) \neq c(x)] = \mathop{\mathrm{E}}_{x \sim D}[1_{h(x) \neq c(x)}].$$

- Empirical error: average error of h on the training sample S drawn according to distribution D,

$$\widehat{R}_S(h) = \Pr_{x \sim \widehat{D}}[h(x) \neq c(x)] = \mathop{\mathrm{E}}_{x \sim \widehat{D}}[1_{h(x) \neq c(x)}] = \frac{1}{m} \sum_{i=1}^{m} 1_{h(x_i) \neq c(x_i)}.$$

empirical distribution

- Note: $R(h) = \mathop{\mathrm{E}}_{S \sim D^m}\left[\widehat{R}_S(h)\right].$

PAC Model

(Valiant, 1984)

- PAC learning: Probably Approximately Correct learning.

  $\varepsilon \rightarrow$ error
  $\delta \rightarrow$ prob.

- Definition: concept class C is PAC-learnable if there exists a learning algorithm L such that:
  - for all $c \in C, \epsilon > 0, \delta > 0$, and all distributions D,

D is indep. of L

$$\Pr_{S \sim D^m}[R(h_S) \leq \epsilon] \geq 1 - \delta,$$

(very strict on L as D itself is indep.)

  - for samples S of size $m = poly(1/\epsilon, 1/\delta)$ for a fixed polynomial.

Remarks

- Concept class C is known to the algorithm.
- Distribution-free model: no assumption on D.
- Both training and test examples drawn $\sim D$.
  (may be not the same D)
- Probably: confidence $1-\delta$.
- Approximately correct: accuracy $1-\epsilon$.
- Efficient PAC-learning: L runs in time $poly(1/\epsilon, 1/\delta)$.
- What about the cost of the representation of $c \in C$?

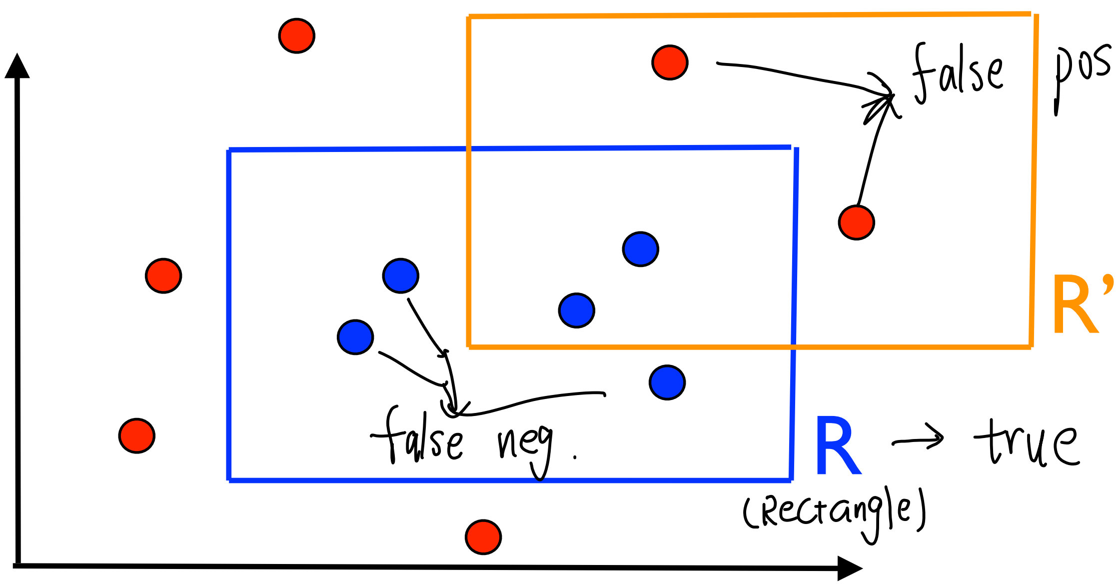
PAC Model - New Definition

- Computational representation:
  - cost for $x \in X$ in $O(n)$.
  - cost for $c \in C$ in $O(size(c))$.
- Extension: running time.

$$O(poly(1/\epsilon, 1/\delta)) \longrightarrow O(poly(1/\epsilon, 1/\delta, n, size(c))).$$

Example - Rectangle Learning

- Problem: learn unknown axis-aligned rectangle R using as small a labeled sample as possible.



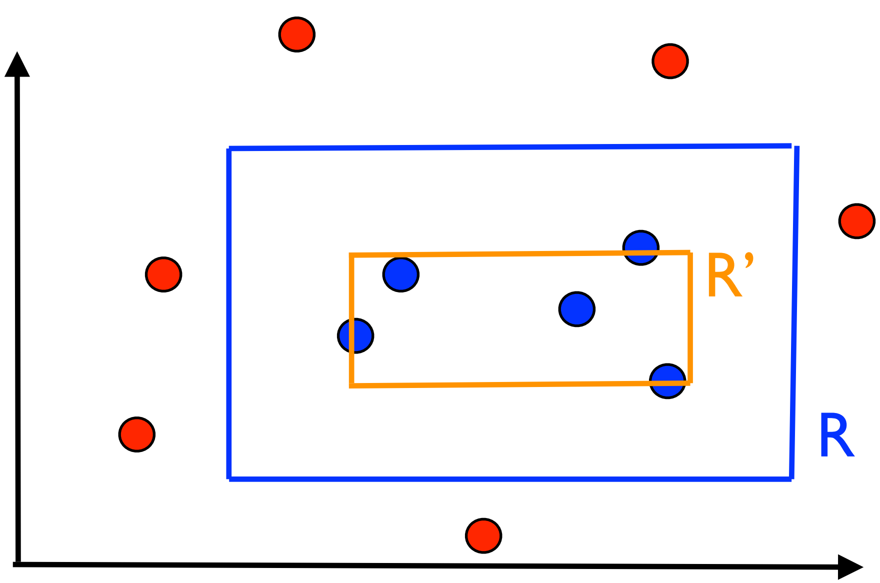
R' → concept that L selects out

R → true concept

- Hypothesis: rectangle R'. In general, there may be false positive and false negative points.

Example - Rectangle Learning

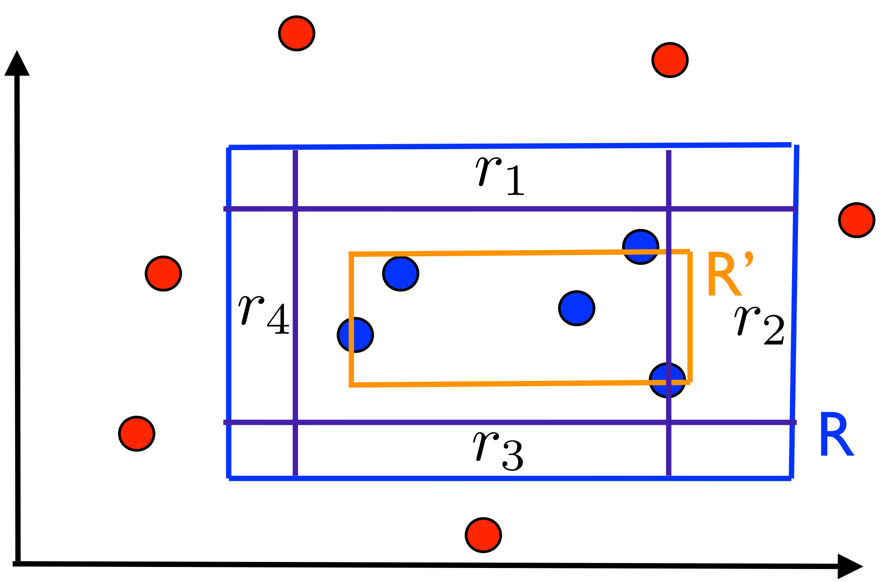
- Simple method: choose tightest consistent rectangle R' for a large enough sample. How large a sample? Is this class PAC-learnable?



- What is the probability that $R(\mathrm{R}') > \epsilon$?

Example - Rectangle Learning

- Fix $\epsilon > 0$ and assume $\Pr_D[\mathrm{R}] > \epsilon$ (otherwise the result is trivial).
- Let r_1, r_2, r_3, r_4 be four smallest rectangles along the sides of R such that $\Pr_D[r_i] \geq \frac{\epsilon}{4}$.



$$\mathrm{R} = [l, r] \times [b, t]$$
$$r_4 = [l, s_4] \times [b, t]$$
$$s_4 = \inf\{s \colon \Pr\left[[l, s] \times [b, t]\right] \geq \tfrac{\epsilon}{4}\}$$
$$\Pr_D\left[[l, s_4[\times [b, t]\right] < \tfrac{\epsilon}{4}$$

Example - Rectangle Learning

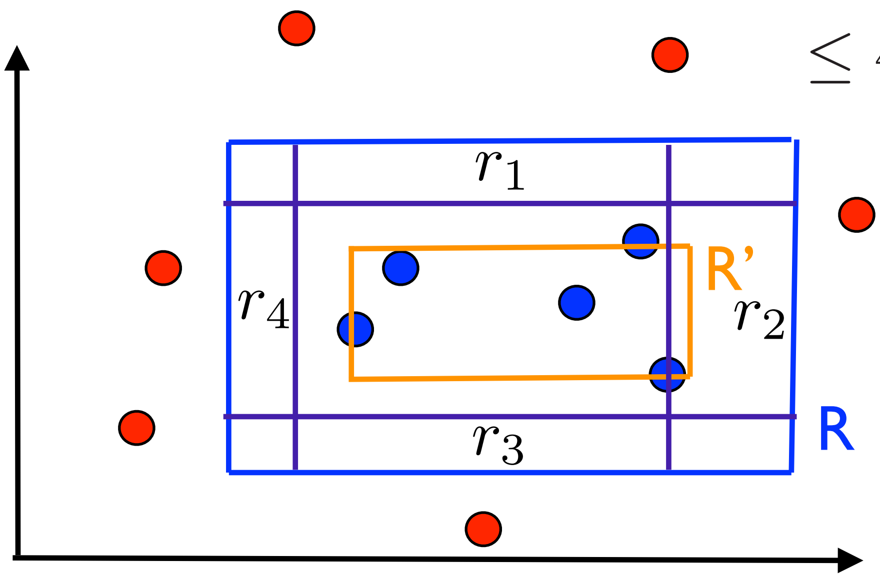
- Errors can only occur in $\mathsf{R}-\mathsf{R}'$. Thus (geometry),

  $R(\mathsf{R}') > \epsilon \Rightarrow \mathsf{R}'$ misses at least one region r_i.

- Therefore, $\Pr[R(\mathsf{R}') > \epsilon] \leq \Pr[\cup_{i=1}^4 \{\mathsf{R}' \text{ misses } r_i\}]$

$$\leq \sum_{i=1}^4 \Pr[\{\mathsf{R}' \text{ misses } r_i\}]$$

$$\leq 4(1-\tfrac{\epsilon}{4})^m \leq 4e^{-\frac{m\epsilon}{4}}.$$



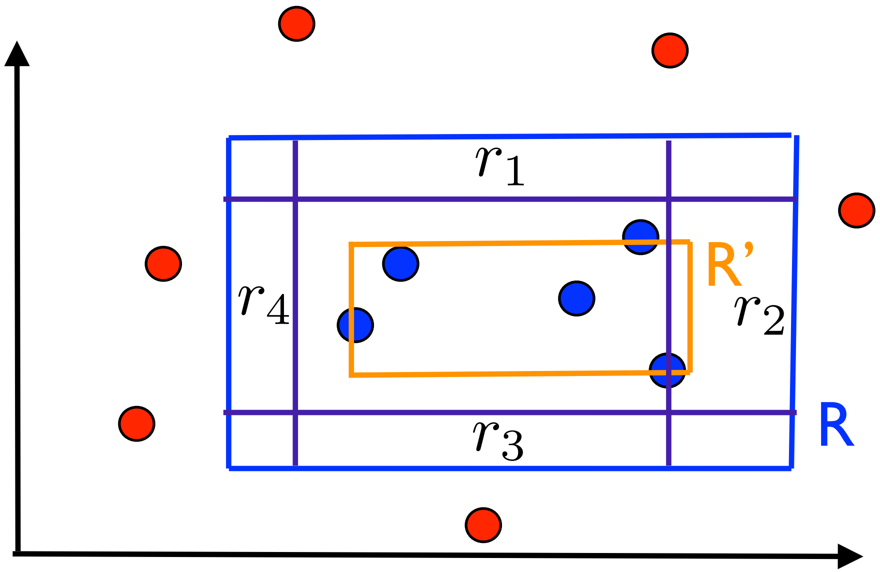
Example - Rectangle Learning

- Set $\delta > 0$ to match the upper bound:

$$4e^{-\frac{m\epsilon}{4}} \leq \delta \Leftrightarrow m \geq \frac{4}{\epsilon} \log \frac{4}{\delta}.$$

- Then, for $m \geq \frac{4}{\epsilon} \log \frac{4}{\delta}$, with probability at least $1 - \delta$,

$$R(\mathsf{R}') \leq \epsilon.$$



Notes

- Infinite hypothesis set, but simple proof.
- Does this proof readily apply to other similar concepts classes?
- Geometric properties:
  - key in this proof.
  - in general non-trivial to extend to other classes, e.g., non-concentric circles (see HW2, 2006).

→ Need for more general proof and results.

This lecture

- PAC Model
- Sample complexity, finite H, consistent case
- Sample complexity, finite H, inconsistent case

Learning Bound for Finite H - Consistent Case

- **Theorem**: let H be a finite set of functions from X to $\{0, 1\}$ and L an algorithm that for any target concept $c \in H$ and sample S returns a consistent hypothesis h_S: $\widehat{R}_S(h_S) = 0$. Then, for any $\delta > 0$, with probability at least $1 - \delta$,

Generalization Bounds

$$R(h_S) \leq \frac{1}{m}\left(\log |H| + \log \frac{1}{\delta}\right).$$

$\Updownarrow$ two identical forms of the ineq.

$\Leftrightarrow$ for $\forall \varepsilon, \delta > 0$, $\mathbb{P}_{S \sim D^m}[R(h_S) \leq \varepsilon] \geq 1 - \delta$ holds if

$m \geq \frac{1}{\varepsilon}\left(\log |H| + \log \frac{1}{\delta}\right)$ Sample Complexity Bounds

$\Updownarrow$

$\varepsilon \leq \frac{1}{m}\left(\log |H| + \log \frac{1}{\delta}\right)$

Learning Bound for Finite H - Consistent Case

as we consider $\mathcal{Y} = \{0, 1\}$

$$\mathbb{P}_{\underset{(\text{sum})}{x \sim D}}\big(\underbrace{h(x) \neq c(x)}_{\text{a condition } x \text{ should satisfy}}\big) > \varepsilon$$

$$= \mathbb{E}_{x \sim D} 1_{\{h(x) \neq c(x)\}}$$

- **Proof**: for any $\epsilon > 0$, define $H_\epsilon = \{h \in H : R(h) > \epsilon\}$. We want to prove that, with high probability, if h_S is consistent, then it has low error:

$$\underbrace{\mathbb{P}\Big[\widehat{R}_S(h_S) = 0 \overset{\text{the ERM algorithm}}{\Rightarrow} R(h_S) \leq \epsilon\Big] \geq 1 - \delta}_{\text{the inequality we want}} \Leftrightarrow \mathbb{P}\Big[\widehat{R}_S(h_S) = 0 \wedge R(h_S) > \epsilon\Big] \leq \delta$$

$$\Leftrightarrow \underbrace{\mathbb{P}\Big[\widehat{R}_S(h_S) = 0 \wedge h_S \in H_\epsilon\Big]}_{(*)} \leq \delta.$$

instead of finding specific h_S, we bound on $\forall h$ s.t. $\widehat{R}_S(h) = 0$

$$(*) \leq \mathbb{P}\Big[\exists h \in H : \widehat{R}_S(h) = 0 \wedge h \in H_\epsilon\Big]$$

$$= \mathbb{P}\Big[\exists h \in H_\epsilon : \widehat{R}_S(h) = 0\Big]$$

$$= \mathbb{P}\Big[\widehat{R}_S(h_1) = 0 \vee \ldots \vee \widehat{R}_S(h_{|H_\epsilon|}) = 0\Big]$$

$$\leq \sum_{h \in H_\epsilon} \mathbb{P}\Big[\widehat{R}_S(h) = 0\Big]$$

$$\leq \sum_{h \in H_\epsilon} (1 - \epsilon)^m \leq |H|(1 - \epsilon)^m \leq \underbrace{|H|e^{-m\epsilon}}_{\text{take it as } \delta}.$$

Rmk. $\overset{R(h) =}{\mathbb{P}_{x \sim D}}\big(h(x) \neq c(x)\big) > \varepsilon$ means the sum of prob. of pick $x \sim D$ which makes false prediction is greater than ε,

hence $\mathbb{P}_{h \in H_\varepsilon}[\underbrace{\widehat{R}_S(h) = 0}_{\text{taking consistent } m \text{ points from } D \text{ points}}] \leq (1-\varepsilon)^m$ (missing all inconsisten

where S is a sample of size m

Remarks

(we have a uniform bound actually)

(one way to choose h_S)

$\exists$ solution for ERM $= 0$

- The algorithm can be ERM if problem realizable.
- Error bound linear in $\frac{1}{m}$ and only logarithmic in $\frac{1}{\delta}$.
- $\log_2 |H|$ is the number of bits used for the representation of H.
- Bound is loose for large $|H|$.
- Uninformative for infinite $|H|$.

Conjunctions of Boolean Literals

- Example for $n=6$.
- Algorithm: start with $x_1 \wedge \overline{x}_1 \wedge \cdots \wedge x_n \wedge \overline{x}_n$ and rule out literals incompatible with positive examples.

0	1	1	0	1	1	+
0	1	1	1	1	1	+
0	0	1	1	0	1	-
0	1	1	1	1	1	+
1	0	0	1	1	0	-
0	1	0	0	1	1	+
0	1	?	?	1	1	

$\rightarrow \overline{x}_1 \wedge x_2 \wedge x_5 \wedge x_6.$

Intersections

Conjunctions of Boolean Literals

- **Problem**: learning class C_n of conjunctions of boolean literals with at most n variables (e.g., for $n=3$, $x_1 \wedge \overline{x_2} \wedge x_3$).

- **Algorithm**: choose h consistent with S.
  - Since $|H|=|C_n|=3^n$, sample complexity:

$$m \geq \frac{1}{\epsilon}((\log 3)\, n + \log \frac{1}{\delta}).$$

$\delta = .02, \epsilon = .1, n = 10, m \geq 149.$

  - Computational complexity: polynomial, since algorithmic cost per training example is in $O(n)$.

This lecture

① deterministic: $\exists! f: \mathcal{X} \to \mathcal{Y}$ (each x_i has prob 1 relating to label y_i)

② consistent: $\exists h \in H$ s.t. $\hat{R}(h) = 0$.

② is stricter than ① as even if deterministic, we still might not achieve consistency.

- PAC Model
- Sample complexity, finite *H*, consistent case
- Sample complexity, finite *H*, inconsistent case

Inconsistent Case

- No $h \in H$ is a consistent hypothesis.
- The typical case in practice: difficult problems, complex concept class.
- But, inconsistent hypotheses with a small number of errors on the training set can be useful.
- Need a more powerful tool: Hoeffding's inequality.

Hoeffding's Inequality

- Corollary: for any $\epsilon > 0$ and any hypothesis $h : X \to \{0, 1\}$ the following inequalities holds:

$$\Pr[R(h) - \widehat{R}(h) \geq \epsilon] \leq e^{-2m\epsilon^2}$$
$$\Pr[\widehat{R}(h) - R(h) \geq \epsilon] \leq e^{-2m\epsilon^2}.$$

- Combining these one-sided inequalities yields

$$\Pr[|R(h) - \widehat{R}(h)| \geq \epsilon] \leq 2e^{-2m\epsilon^2}.$$

Application to Learning Algorithm?

- Can we apply that bound to the hypothesis h_S returned by our learning algorithm when training on sample S?

- No, because h_S is not a fixed hypothesis, it depends on the training sample. Note also that $\underbrace{\mathrm{E}[\widehat{R}(h_S)]}_{\text{a R.V. depending on } S}$ is not a simple quantity such as $R(h_S)$.

- Instead, we need a bound that holds simultaneously for all hypotheses $h \in H$, a uniform convergence bound.

Generalization Bound - Finite H

- **Theorem**: let H be a finite hypothesis set, then, for any $\delta > 0$, with probability at least $1 - \delta$,

$$\forall h \in H,\ R(h) \leq \widehat{R}_S(h) + \sqrt{\frac{\log|H| + \log\frac{2}{\delta}}{2m}}.$$

- **Proof**: By the union bound,

We still derive a union bound.

$$\Pr\left[\max_{h\in H}\left|R(h) - \widehat{R}_S(h)\right| > \epsilon\right]$$
$$= \Pr\left[\left|R(h_1) - \widehat{R}_S(h_1)\right| > \epsilon \vee \ldots \vee \left|R(h_{|H|}) - \widehat{R}_S(h_{|H|})\right| > \epsilon\right]$$
$$\leq \sum_{h\in H} \Pr\left[\left|R(h) - \widehat{R}_S(h)\right| > \epsilon\right]$$
$$\leq 2|H|\exp(-2m\epsilon^2).$$

Remarks

- Thus, for a finite hypothesis set, whp,

$$\forall h \in H, R(h) \leq \widehat{R}_S(h) + O\left(\sqrt{\frac{\log |H|}{m}}\right).$$

- Error bound in $O(\frac{1}{\sqrt{m}})$ (quadratically worse).
- $\log_2 |H|$ can be interpreted as the number of bits needed to encode H.
- Occam's Razor principle (theologian William of Occam): "plurality should not be posited without necessity".

There is a trade of between reducing $\widehat{R}(h)$ and controlling m.

Occam's Razor

- Principle formulated by controversial theologian William of Occam: "plurality should not be posited without necessity", rephrased as "the simplest explanation is best";
  - invoked in a variety of contexts, e.g., syntax. Kolmogorov complexity can be viewed as the corresponding framework in information theory.
  - here, to minimize true error, choose the most parsimonious explanation (smallest $|H|$). choose simplest hypothsis set.
  - we will see later other applications of this principle.

Lecture Summary

- C is PAC-learnable if $\exists L, \forall c \in C, \forall \epsilon, \delta > 0, m = P\left(\frac{1}{\epsilon}, \frac{1}{\delta}\right)$,
$$\Pr_{S \sim D^m}[R(h_S) \leq \epsilon] \geq 1 - \delta.$$
- Learning bound, finite H consistent case:
$$R(h) \leq \frac{1}{m}\left(\log|H| + \log\frac{1}{\delta}\right).$$
- Learning bound, finite H inconsistent case:
$$R(h) \leq \widehat{R}_S(h) + \sqrt{\frac{\log|H| + \log\frac{2}{\delta}}{2m}}.$$
- How do we deal with infinite hypothesis sets?

References

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Appendix

Universal Concept Class

- Problem: each $x \in X$ defined by n boolean features. Let C be the set of all subsets of X.
- Question: is C PAC-learnable?
- Sample complexity: H must contain C. Thus,

$$|H| \geq |C| = 2^{(2^n)}.$$

The bound gives $m = \frac{1}{\epsilon}((\log 2)\, 2^n + \log \frac{1}{\delta})$.

- It can be proved that C is not PAC-learnable, it requires an exponential sample size.

k-Term DNF Formulae

- Definition: expressions of the form $T_1 \vee \cdots \vee T_k$ with each term T_i conjunctions of boolean literals with at most n variables.

- Problem: learning *k*-term DNF formulae.

- Sample complexity: $|H| = |C| = 3^{nk}$. Thus, polynomial sample complexity $\frac{1}{\epsilon}\big((\log 3)\, nk + \log \frac{1}{\delta}\big)$.

- Time complexity: intractable if $RP \neq NP$: the class is then not efficiently PAC-learnable (proof by reduction from graph 3-coloring). But, a strictly larger class is!

k-CNF Expressions

- Definition: expressions $T_1 \wedge \cdots \wedge T_j$ of arbitrary length j with each term T_i a disjunction of at most k boolean attributes.

- Algorithm: reduce problem to that of learning conjunctions of boolean literals. $(2n)^k$ new variables:

$$(u_1, \ldots, u_k) \rightarrow Y_{u_1, \ldots, u_k}.$$

  - the transformation is a bijection;
  - effect of the transformation on the distribution is not an issue: PAC-learning allows any distribution D.

k-Term DNF Terms and *k*-CNF Expressions

- Observation: any *k*-term DNF formula can be written as a *k*-CNF expression. By associativity,

$$\bigvee_{i=1}^{k} u_{i,1} \wedge \cdots \wedge u_{i,n_i} = \bigwedge_{j_1 \in [1,n_1],\ldots,j_k \in [1,n_k]} u_{1,j_1} \vee \cdots \vee u_{k,j_k}.$$

  - Example: $(u_1 \wedge u_2 \wedge u_3) \vee (v_1 \wedge v_2 \wedge v_3) = \bigwedge_{i,j=1}^{3} (u_i \vee v_j)$.
  - But, in general converting a *k*-CNF (equiv. to a *k*-term DNF) to a *k*-term DNF is intractable.
- Key aspects of PAC-learning definition:
  - cost of representation of concept c.
  - choice of hypothesis set H.

Foundations of Machine Learning

Learning with Infinite Hypothesis Sets

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Motivation

- With an infinite hypothesis set H, the error bounds of the previous lecture are not informative.
- Is efficient learning from a finite sample possible when H is infinite?
- Our example of axis-aligned rectangles shows that it is possible.
- Can we reduce the infinite case to a finite set? Project over finite samples?
- Are there useful measures of complexity for infinite hypothesis sets?

This lecture

- Rademacher complexity
- Growth Function
- VC dimension
- Lower bound

Empirical Rademacher Complexity

- Definition:
  - G family of functions mapping from set Z to $[a, b]$.
  - sample $S = (z_1, \ldots, z_m)$.
  - σ_is (Rademacher variables): independent uniform random variables taking values in $\{-1, +1\}$.

$$\widehat{\mathfrak{R}}_S(G) = \operatorname*{E}_{\boldsymbol{\sigma}}\left[\sup_{g \in G} \underbrace{\frac{1}{m} \begin{bmatrix} \sigma_1 \\ \vdots \\ \sigma_m \end{bmatrix} \cdot \begin{bmatrix} g(z_1) \\ \vdots \\ g(z_m) \end{bmatrix}}_{\text{correlation with random noise}}\right] = \operatorname*{E}_{\boldsymbol{\sigma}}\left[\sup_{g \in G} \frac{1}{m} \sum_{i=1}^{m} \sigma_i g(z_i)\right].$$

Rademacher Complexity

- Definitions: let G be a family of functions mapping from Z to $[a, b]$.
  - Empirical Rademacher complexity of G:

$$\widehat{\mathfrak{R}}_S(G) = \operatorname*{E}_{\sigma}\left[\sup_{g \in G} \frac{1}{m} \sum_{i=1}^{m} \sigma_i g(z_i)\right],$$

where σ_is are independent uniform random variables taking values in $\{-1, +1\}$ and $S = (z_1, \ldots, z_m)$.

  - Rademacher complexity of G:

$$\mathfrak{R}_m(G) = \operatorname*{E}_{S \sim D^m}[\widehat{\mathfrak{R}}_S(G)].$$

Rademacher Complexity Bound

(Koltchinskii and Panchenko, 2002)

- **Theorem**: Let G be a family of functions mapping from Z to $[0, 1]$. Then, for any $\delta > 0$, with probability at least $1-\delta$, the following holds for all $g \in G$:

$$\mathrm{E}[g(z)] \leq \frac{1}{m}\sum_{i=1}^{m} g(z_i) + 2\mathfrak{R}_m(G) + \sqrt{\frac{\log\frac{1}{\delta}}{2m}}.$$

$$\mathrm{E}[g(z)] \leq \frac{1}{m}\sum_{i=1}^{m} g(z_i) + 2\widehat{\mathfrak{R}}_S(G) + 3\sqrt{\frac{\log\frac{2}{\delta}}{2m}}.$$

- **Proof**: Apply McDiarmid's inequality to

$$\Phi(S) = \sup_{g \in G} \mathrm{E}[g] - \widehat{\mathrm{E}}_S[g].$$

- Changing one point of S changes $\Phi(S)$ by at most $\frac{1}{m}$.

$$\begin{aligned}\Phi(S') - \Phi(S) &= \sup_{g \in G}\{\mathrm{E}[g] - \widehat{\mathrm{E}}_{S'}[g]\} - \sup_{g \in G}\{\mathrm{E}[g] - \widehat{\mathrm{E}}_S[g]\} \\ &\leq \sup_{g \in G}\{\{\mathrm{E}[g] - \widehat{\mathrm{E}}_{S'}[g]\} - \{\mathrm{E}[g] - \widehat{\mathrm{E}}_S[g]\}\} \\ &= \sup_{g \in G}\{\widehat{\mathrm{E}}_S[g] - \widehat{\mathrm{E}}_{S'}[g]\} = \sup_{g \in G} \frac{1}{m}(g(z_m) - g(z'_m)) \leq \frac{1}{m}.\end{aligned}$$

- Thus, by McDiarmid's inequality, with probability at least $1 - \frac{\delta}{2}$

$$\Phi(S) \leq \mathop{\mathrm{E}}_S[\Phi(S)] + \sqrt{\frac{\log \frac{2}{\delta}}{2m}}.$$

- We are left with bounding the expectation.

- Series of observations:

$$\begin{aligned}
\mathop{\mathrm{E}}_{S}[\Phi(S)] &= \mathop{\mathrm{E}}_{S}\Big[\sup_{g\in G} \mathrm{E}[g] - \widehat{\mathrm{E}}_S(g)\Big] \\
&= \mathop{\mathrm{E}}_{S}\Big[\sup_{g\in G} \mathop{\mathrm{E}}_{S'}[\widehat{\mathrm{E}}_{S'}(g) - \widehat{\mathrm{E}}_S(g)]\Big] \\
\text{(sub-add. of sup)} &\leq \mathop{\mathrm{E}}_{S,S'}\Big[\sup_{g\in G} \widehat{\mathrm{E}}_{S'}(g) - \widehat{\mathrm{E}}_S(g)\Big] \\
&= \mathop{\mathrm{E}}_{S,S'}\Big[\sup_{g\in G} \frac{1}{m}\sum_{i=1}^{m}(g(z'_i) - g(z_i))\Big] \\
\text{(swap } z_i \text{ and } z'_i\text{)} &= \mathop{\mathrm{E}}_{\sigma,S,S'}\Big[\sup_{g\in G} \frac{1}{m}\sum_{i=1}^{m}\sigma_i(g(z'_i) - g(z_i))\Big] \\
\text{(sub-additiv. of sup)} &\leq \mathop{\mathrm{E}}_{\sigma,S'}\Big[\sup_{g\in G} \frac{1}{m}\sum_{i=1}^{m}\sigma_i g(z'_i)\Big] + \mathop{\mathrm{E}}_{\sigma,S}\Big[\sup_{g\in G} \frac{1}{m}\sum_{i=1}^{m}-\sigma_i g(z_i)\Big] \\
&= 2\mathop{\mathrm{E}}_{\sigma,S}\Big[\sup_{g\in G} \frac{1}{m}\sum_{i=1}^{m}\sigma_i g(z_i)\Big] = 2\mathfrak{R}_m(G).
\end{aligned}$$

- Now, changing one point of S makes $\widehat{\mathfrak{R}}_S(G)$ vary by at most $\frac{1}{m}$. Thus, again by McDiarmid's inequality, with probability at least $1-\frac{\delta}{2}$,

$$\mathfrak{R}_m(G) \leq \widehat{\mathfrak{R}}_{\mathcal{S}}(G) + \sqrt{\frac{\log\frac{2}{\delta}}{2m}}.$$

- Thus, by the union bound, with probability at least $1-\delta$,

$$\Phi(S) \leq 2\widehat{\mathfrak{R}}_S(G) + 3\sqrt{\frac{\log\frac{2}{\delta}}{2m}}.$$

Loss Functions - Hypothesis Set

- Proposition: Let H be a family of functions taking values in $\{-1, +1\}$, G the family of zero-one loss functions of H: $G = \big\{(x, y) \mapsto 1_{h(x) \neq y} \colon h \in H\big\}$. Then,

$$\mathfrak{R}_m(G) = \frac{1}{2}\mathfrak{R}_m(H).$$

- Proof:

$$\begin{aligned}
\mathfrak{R}_m(G) &= \mathop{\mathrm{E}}_{S,\sigma}\Big[\sup_{h \in H} \frac{1}{m}\sum_{i=1}^m \sigma_i 1_{h(x_i) \neq y_i}\Big] \\
&= \mathop{\mathrm{E}}_{S,\sigma}\Big[\sup_{h \in H} \frac{1}{m}\sum_{i=1}^m \sigma_i \frac{1}{2}(1 - y_i h(x_i))\Big] \\
&= \underbrace{\frac{1}{2}\mathop{\mathrm{E}}_{S,\sigma}\Big[\sup_{h \in H} \frac{1}{m}\sum_{i=1}^m \sigma_i\Big]}_{=0} + \frac{1}{2}\mathop{\mathrm{E}}_{S,\sigma}\Big[\sup_{h \in H} \frac{1}{m}\sum_{i=1}^m -\sigma_i y_i h(x_i)\Big] \\
&= \frac{1}{2}\mathop{\mathrm{E}}_{S,\sigma}\Big[\sup_{h \in H} \frac{1}{m}\sum_{i=1}^m \sigma_i h(x_i)\Big].
\end{aligned}$$

Generalization Bounds - Rademacher

- Corollary: Let H be a family of functions taking values in $\{-1, +1\}$. Then, for any $\delta > 0$, with probability at least $1 - \delta$, for any $h \in H$,

$$R(h) \leq \widehat{R}(h) + \mathfrak{R}_m(H) + \sqrt{\frac{\log \frac{1}{\delta}}{2m}}.$$

$$R(h) \leq \widehat{R}(h) + \widehat{\mathfrak{R}}_S(H) + 3\sqrt{\frac{\log \frac{2}{\delta}}{2m}}.$$

Remarks

- First bound distribution-dependent, second data-dependent bound, which makes them attractive.
- But, how do we compute the empirical Rademacher complexity?
- Computing $\mathrm{E}_\sigma[\sup_{h\in H} \frac{1}{m}\sum_{i=1}^m \sigma_i h(x_i)]$ requires solving ERM problems, typically computationally hard.
- Relation with combinatorial measures easier to compute?

This lecture

- Rademacher complexity
- Growth Function
- VC dimension
- Lower bound

Growth Function

- Definition: the growth function $\Pi_H \colon \mathbb{N} \to \mathbb{N}$ for a hypothesis set H is defined by

$$\forall m \in \mathbb{N},\ \Pi_H(m) = \max_{\{x_1,\ldots,x_m\} \subseteq X} \Big| \big\{ \big(h(x_1), \ldots, h(x_m)\big) \colon h \in H \big\} \Big|.$$

- Thus, $\Pi_H(m)$ is the maximum number of ways m points can be classified using H.

Massart's Lemma

(Massart, 2000)

- **Theorem**: Let $A \subseteq \mathbb{R}^m$ be a finite set, with $R = \max_{x \in A} \|x\|_2$, then, the following holds:

$$\mathop{\mathrm{E}}_{\sigma}\left[\frac{1}{m}\sup_{x\in A}\sum_{i=1}^{m}\sigma_i x_i\right] \leq \frac{R\sqrt{2\log|A|}}{m}.$$

- **Proof**:

$$\begin{aligned}
\exp\left(t \mathop{\mathrm{E}}_{\sigma}\left[\sup_{x\in A}\sum_{i=1}^{m}\sigma_i x_i\right]\right) &\leq \mathop{\mathrm{E}}_{\sigma}\left(\exp\left[t\sup_{x\in A}\sum_{i=1}^{m}\sigma_i x_i\right]\right) \quad \text{(Jensen's ineq.)}\\
&= \mathop{\mathrm{E}}_{\sigma}\left(\sup_{x\in A}\exp\left[t\sum_{i=1}^{m}\sigma_i x_i\right]\right)\\
&\leq \sum_{x\in A}\mathop{\mathrm{E}}_{\sigma}\left(\exp\left[t\sum_{i=1}^{m}\sigma_i x_i\right]\right) = \sum_{x\in A}\prod_{i=1}^{m}\mathop{\mathrm{E}}_{\sigma}\left(\exp\left[t\sigma_i x_i\right]\right)\\
\text{(Hoeffding's ineq.)} &\leq \sum_{x\in A}\left(\exp\left[\frac{\sum_{i=1}^{m} t^2(2|x_i|)^2}{8}\right]\right) \leq |A|e^{\frac{t^2R^2}{2}}.
\end{aligned}$$

- Taking the log yields:

$$\mathop{\mathrm{E}}_{\sigma}\left[\sup_{x \in A} \sum_{i=1}^{m} \sigma_i x_i\right] \leq \frac{\log |A|}{t} + \frac{tR^2}{2}.$$

- Minimizing the bound by choosing $t = \frac{\sqrt{2 \log |A|}}{R}$ gives

$$\mathop{\mathrm{E}}_{\sigma}\left[\sup_{x \in A} \sum_{i=1}^{m} \sigma_i x_i\right] \leq R\sqrt{2 \log |A|}.$$

Growth Function Bound on Rad. Complexity

- **Corollary**: Let G be a family of functions taking values in $\{-1, +1\}$, then the following holds:

$$\mathfrak{R}_m(G) \leq \sqrt{\frac{2 \log \Pi_G(m)}{m}}.$$

- **Proof**:

$$\begin{aligned}
\widehat{\mathfrak{R}}_S(G) &= \mathop{\mathrm{E}}_{\sigma}\left[\sup_{g \in G} \frac{1}{m} \begin{bmatrix} \sigma_1 \\ \vdots \\ \sigma_m \end{bmatrix} \cdot \begin{bmatrix} g(z_1) \\ \vdots \\ g(z_m) \end{bmatrix}\right] \\
&\leq \frac{\sqrt{m}\sqrt{2 \log |\{(g(z_1), \ldots, g(z_m)) \colon g \in G\}|}}{m} \qquad \text{(Massart's Lemma)} \\
&\leq \frac{\sqrt{m}\sqrt{2 \log \Pi_G(m)}}{m} = \sqrt{\frac{2 \log \Pi_G(m)}{m}}.
\end{aligned}$$

Generalization Bound - Growth Function

- Corollary: Let H be a family of functions taking values in $\{-1,+1\}$. Then, for any $\delta>0$, with probability at least $1-\delta$, for any $h \in H$,

$$R(h) \leq \widehat{R}(h) + \sqrt{\frac{2\log \Pi_H(m)}{m}} + \sqrt{\frac{\log \frac{1}{\delta}}{2m}}.$$

- But, how do we compute the growth function? Relationship with the VC-dimension (Vapnik-Chervonenkis dimension).

This lecture

- Rademacher complexity
- Growth Function
- VC dimension
- Lower bound

VC Dimension

(Vapnik & Chervonenkis, 1968-1971; Vapnik, 1982, 1995, 1998)

- Definition: the VC-dimension of a hypothesis set H is defined by

$$\mathrm{VCdim}(H) = \max\{m \colon \Pi_H(m) = 2^m\}.$$

- Thus, the VC-dimension is the size of the largest set that can be fully shattered by H.

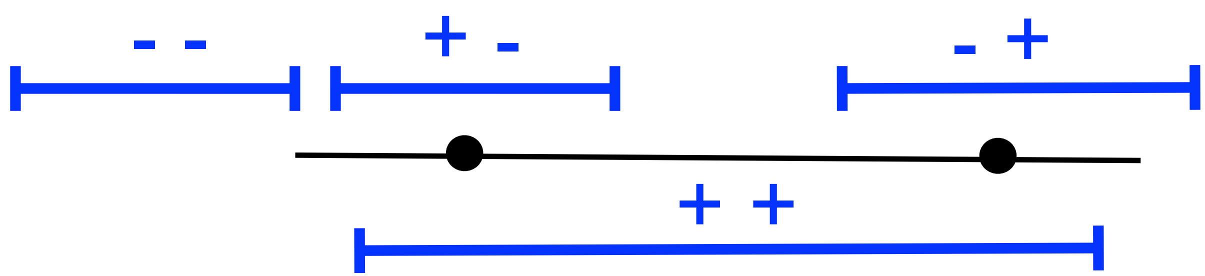
- Purely combinatorial notion.

Examples

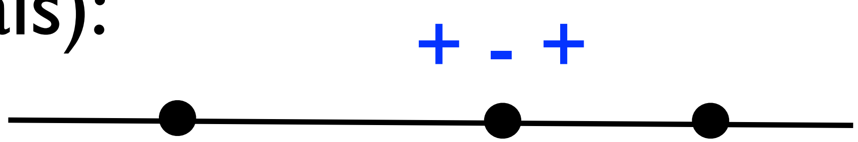
- In the following, we determine the VC dimension for several hypothesis sets.
- To give a lower bound d for $\mathrm{VCdim}(H)$, it suffices to show that a set S of cardinality d can be shattered by H.
- To give an upper bound, we need to prove that no set S of cardinality $d+1$ can be shattered by H, which is typically more difficult.

Intervals of The Real Line

- **Observations:**
  - Any set of two points can be shattered by four intervals



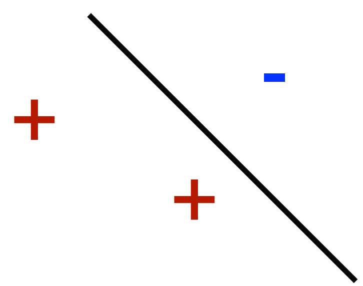
  - No set of three points can be shattered since the following dichotomy "+ - +" is not realizable (by definition of intervals):



  - Thus, $\mathrm{VCdim}(\text{intervals in } \mathbb{R}) = 2$.

Hyperplanes

- Observations:
  - Any three non-collinear points can be shattered:

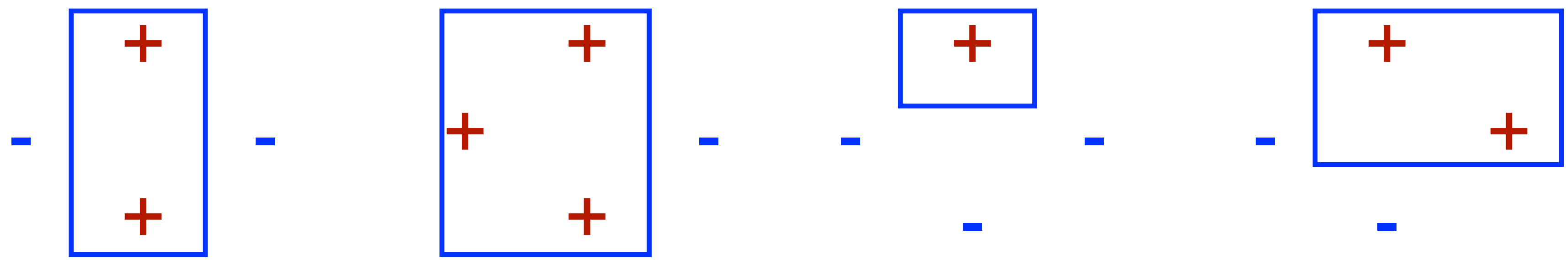


  - Unrealizable dichotomies for four points:

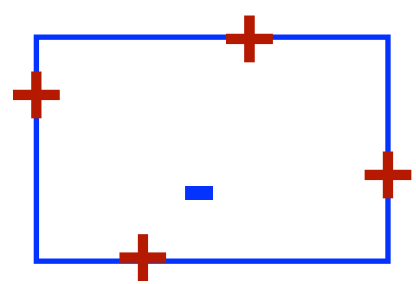
  - Thus, $\mathrm{VCdim}(\text{hyperplanes in } \mathbb{R}^d) = d+1$.

Axis-Aligned Rectangles in the Plane

- **Observations:**
  - The following four points can be shattered:



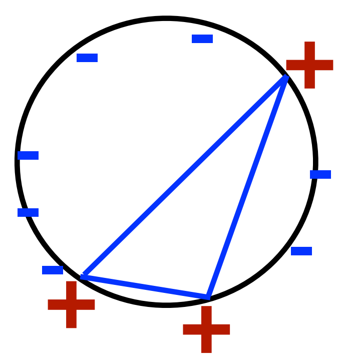
  - No set of five points can be shattered: label negatively the point that is not near the sides.



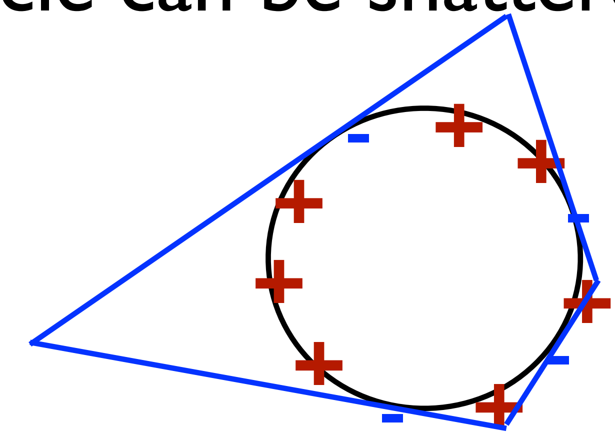
  - Thus, $\text{VCdim}(\text{axis-aligned rectangles}) = 4$.

Convex Polygons in the Plane

- Observations:
  - $2d+1$ points on a circle can be shattered by a *d*-gon:



|positive points| < |negative points|

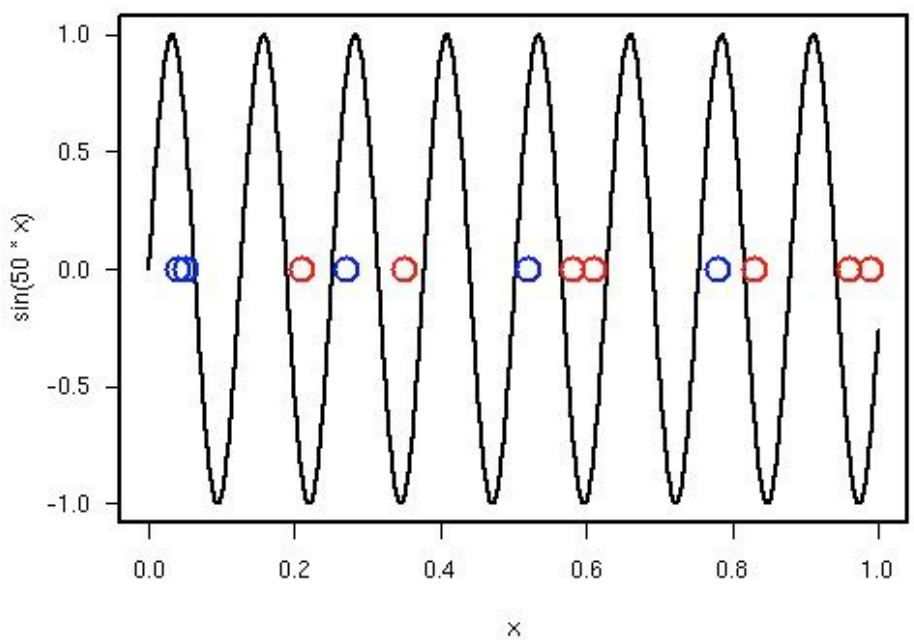


|positive points| > |negative points|

  - It can be shown that choosing the points on the circle maximizes the number of possible dichotomies. Thus, $\mathrm{VCdim}(\text{convex } d\text{-gons}) = 2d+1$. Also, $\mathrm{VCdim}(\text{convex polygons}) = +\infty$.

Sine Functions

- Observations:
  - Any finite set of points on the real line can be shattered by $\{t \mapsto \sin(\omega t) \colon \omega \in \mathbb{R}\}$.
  - Thus, $\text{VCdim}(\text{sine functions}) = +\infty$.



Sauer's Lemma

(Vapnik & Chervonenkis, 1968-1971; Sauer, 1972)

- **Theorem**: let H be a hypothesis set with $\mathrm{VCdim}(H) = d$ then, for all $m \in \mathbb{N}$,

$$\Pi_H(m) \leq \sum_{i=0}^{d} \binom{m}{i}.$$

- **Proof**: the proof is by induction on $m+d$. The statement clearly holds for $m=1$ and $d=0$ or $d=1$. Assume that it holds for $(m-1, d-1)$ and $(m-1, d)$.
  - Fix a set $S = \{x_1, \ldots, x_m\}$ with $\Pi_H(m)$ dichotomies and let $G = H_{|S}$ be the set of concepts H induces by restriction to S.

- Consider the following families over $S' = \{x_1, \ldots, x_{m-1}\}$:

$$G_1 = G_{|S'} \quad G_2 = \{g' \subseteq S' \colon (g' \in G) \wedge (g' \cup \{x_m\} \in G)\}.$$

x_1	x_2	$\cdots$	x_{m-1}	x_m
1	1	0	1	0
1	1	0	1	1
0	1	1	1	1
1	0	0	1	0
1	0	0	0	1
$\cdots$	$\cdots$	$\cdots$	$\cdots$	$\cdots$

- Observe that $|G_1| + |G_2| = |G|$.

- Since $\mathrm{VCdim}(G_1) \leq d$, by the induction hypothesis,

$$|G_1| \leq \Pi_{G_1}(m-1) \leq \sum_{i=0}^{d} \binom{m-1}{i}.$$

- By definition of G_2, if a set $Z \subseteq S'$ is shattered by G_2, then the set $Z \cup \{x_m\}$ is shattered by G. Thus,

$$\mathrm{VCdim}(G_2) \leq \mathrm{VCdim}(G) - 1 = d - 1$$

and by the induction hypothesis,

$$|G_2| \leq \Pi_{G_2}(m-1) \leq \sum_{i=0}^{d-1} \binom{m-1}{i}.$$

- Thus, $|G| \leq \sum_{i=0}^{d} \binom{m-1}{i} + \sum_{i=0}^{d-1} \binom{m-1}{i}$
$= \sum_{i=0}^{d} \binom{m-1}{i} + \binom{m-1}{i-1} = \sum_{i=0}^{d} \binom{m}{i}$.

Sauer's Lemma - Consequence

- **Corollary**: let H be a hypothesis set with $\mathrm{VCdim}(H) = d$ then, for all $m \geq d$,

$$\Pi_H(m) \leq \left(\frac{em}{d}\right)^d = O(m^d).$$

- **Proof**:

$$\begin{aligned}
\sum_{i=0}^{d} \binom{m}{i} &\leq \sum_{i=0}^{d} \binom{m}{i} \left(\frac{m}{d}\right)^{d-i} \\
&\leq \sum_{i=0}^{m} \binom{m}{i} \left(\frac{m}{d}\right)^{d-i} \\
&= \left(\frac{m}{d}\right)^{d} \sum_{i=0}^{m} \binom{m}{i} \left(\frac{d}{m}\right)^{i} \\
&= \left(\frac{m}{d}\right)^{d} \left(1 + \frac{d}{m}\right)^{m} \leq \left(\frac{m}{d}\right)^{d} e^{d}.
\end{aligned}$$

Remarks

- Remarkable property of growth function:
  - either $\mathrm{VCdim}(H) = d < +\infty$ and $\Pi_H(m) = O(m^d)$
  - or $\mathrm{VCdim}(H) = +\infty$ and $\Pi_H(m) = 2^m$.

Generalization Bound - VC Dimension

- **Corollary**: Let H be a family of functions taking values in $\{-1,+1\}$ with VC dimension d. Then, for any $\delta > 0$, with probability at least $1-\delta$, for any $h \in H$,

$$R(h) \leq \widehat{R}(h) + \sqrt{\frac{2d \log \frac{em}{d}}{m}} + \sqrt{\frac{\log \frac{1}{\delta}}{2m}}.$$

- **Proof**: Corollary combined with Sauer's lemma.
- **Note**: The general form of the result is

$$R(h) \leq \widehat{R}(h) + O\left(\sqrt{\frac{\log(m/d)}{(m/d)}}\right).$$

Comparison - Standard VC Bound

(Vapnik & Chervonenkis, 1971; Vapnik, 1982)

- **Theorem**: Let H be a family of functions taking values in $\{-1, +1\}$ with VC dimension d. Then, for any $\delta > 0$, with probability at least $1 - \delta$, for any $h \in H$,

$$R(h) \leq \widehat{R}(h) + \sqrt{\frac{8d \log \frac{2em}{d} + 8 \log \frac{4}{\delta}}{m}}.$$

- **Proof**: Derived from growth function bound

$$\Pr\left[\left|R(h) - \widehat{R}(h)\right| > \epsilon\right] \leq 4\Pi_H(2m) \exp\left(-\frac{m\epsilon^2}{8}\right).$$

This lecture

- Rademacher complexity
- Growth Function
- VC dimension
- Lower bound

VCDim Lower Bound - Realizable Case

(Ehrenfeucht et al., 1988)

- Theorem: let H be a hypothesis set with VC-dimension $d > 1$. Then, for any learning algorithm L,

$$\exists D, \exists f \in H, \ \Pr_{S \sim D^m}\left[R_D(h_S, f) > \frac{d-1}{32m}\right] \geq 1/100.$$

- Proof: choose D such that L can do no better than tossing a coin for some points.
    - Let $X = \{x_0, x_1, \ldots, x_{d-1}\}$ be a set fully shattered. For any $\epsilon > 0$, define D with support X by

$$\Pr_D[x_0] = 1 - 8\epsilon \quad \text{and} \quad \forall i \in [1, d-1], \Pr_D[x_i] = \frac{8\epsilon}{d-1}.$$

- We can assume without loss of generality that L makes no error on x_0.
- For a sample S, let $\overline{S}$ denote the set of its elements falling in $X_1 = \{x_1, \ldots, x_{d-1}\}$ and let $\mathcal{S}$ be the set of samples of size m with at most $(d-1)/2$ points in X_1.
- Fix a sample $S \in \mathcal{S}$. Using $|X - \overline{S}| \geq (d-1)/2$,

$$
\begin{aligned}
\mathop{\mathrm{E}}_{f \sim U}[R_D(h_S, f)] &= \sum_f \sum_{x \in X} 1_{h(x) \neq f(x)} \Pr[x] \Pr[f] \\
&\geq \sum_f \sum_{x \notin \overline{S}} 1_{h(x) \neq f(x)} \Pr[x] \Pr[f] \\
&= \sum_{x \notin \overline{S}} \Big(\sum_f 1_{h(x) \neq f(x)} \Pr[f] \Big) \Pr[x] \\
&= \frac{1}{2} \sum_{x \notin \overline{S}} \Pr[x] \geq \frac{1}{2} \frac{d-1}{2} \frac{8\epsilon}{d-1} = 2\epsilon.
\end{aligned}
$$

- Since the inequality holds for all $S \in \mathcal{S}$, it also holds in expectation: $\mathrm{E}_{S, f \sim U}[R_D(h_S, f)] \geq 2\epsilon$. This implies that there exists a labeling f_0 such that $\mathrm{E}_S[R_D(h_S, f_0)] \geq 2\epsilon$.
- Since $\Pr_D[X - \{x_0\}] \leq 8\epsilon$, we also have $R_D(h_S, f_0) \leq 8\epsilon$. Thus,

$$2\epsilon \leq \mathop{\mathrm{E}}_{S}[R_D(h_S, f_0)] \leq 8\epsilon \mathop{\Pr}_{S \in \mathcal{S}}[R_D(h_S, f_0) \geq \epsilon] + (1 - \mathop{\Pr}_{S \in \mathcal{S}}[R_D(h_S, f_0) \geq \epsilon])\epsilon.$$

- Collecting terms in $\mathop{\Pr}_{S \in \mathcal{S}}[R_D(h_S, f_0) \geq \epsilon]$, we obtain:

$$\mathop{\Pr}_{S \in \mathcal{S}}[R_D(h_S, f_0) \geq \epsilon] \geq \frac{1}{7\epsilon}(2\epsilon - \epsilon) = \frac{1}{7}.$$

- Thus, the probability over all samples S (not necessarily in $\mathcal{S}$) can be lower bounded as

$$\mathop{\Pr}_{S}[R_D(h_S, f_0) \geq \epsilon] \geq \mathop{\Pr}_{S \in \mathcal{S}}[R_D(h_S, f_0) \geq \epsilon] \Pr[\mathcal{S}] \geq \frac{1}{7} \Pr[\mathcal{S}].$$

- This leads us to seeking a lower bound for $\Pr[\mathcal{S}]$. The probability that more than $(d-1)/2$ points be drawn in a sample of size m verifies the Chernoff bound for any $\gamma > 0$:

$$1 - \Pr[\mathcal{S}] = \Pr[S_m \geq 8\epsilon m(1+\gamma)] \leq e^{-8\epsilon m \frac{\gamma^2}{3}}.$$

- Thus, for $\epsilon = (d-1)/(32m)$ and $\gamma = 1$,

$$\Pr[S_m \geq \tfrac{d-1}{2}] \leq e^{-(d-1)/12} \leq e^{-1/12} \leq 1 - 7\delta,$$

for $\delta \leq .01$. Thus, $\Pr[\mathcal{S}] \geq 7\delta$ and

$$\Pr_S[R_D(h_S, f_0) \geq \epsilon] \geq \delta.$$

Agnostic PAC Model

- Definition: concept class C is PAC-learnable if there exists a learning algorithm L such that:
  - for all $c \in C, \epsilon > 0, \delta > 0$, and all distributions D,

$$\Pr_{S \sim D}\left[R(h_S) - \inf_{h \in H} R(h) \leq \epsilon\right] \geq 1 - \delta,$$

  - for samples S of size $m = poly(1/\epsilon, 1/\delta)$ for a fixed polynomial.

VCDim Lower Bound - Non-Realizable Case

(Anthony and Bartlett, 1999)

- Theorem: let H be a hypothesis set with VC dimension $d > 1$. Then, for any learning algorithm L,

$\exists D$ over $X \times \{0, 1\}$,

$$\Pr_{S \sim D^m}\left[R_D(h_S) - \inf_{h \in H} R_D(h) > \sqrt{\frac{d}{320m}}\right] \geq 1/64.$$

- Equivalently, for any learning algorithm, the sample complexity verifies

$$m \geq \frac{d}{320\epsilon^2}.$$

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Foundations of Machine Learning
Support Vector Machines

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Binary Classification Problem

- Training data: sample drawn i.i.d. from set $X \subseteq \mathbb{R}^N$ according to some distribution D,

$$S = ((x_1, y_1), \ldots, (x_m, y_m)) \in X \times \{-1, +1\}.$$

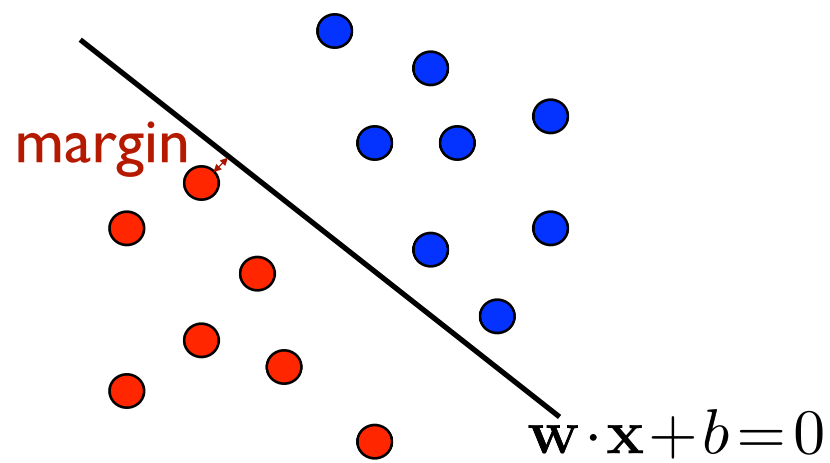
- Problem: find hypothesis $h : X \mapsto \{-1, +1\}$ in H (classifier) with small generalization error $R(h)$.
    - choice of hypothesis set H : learning guarantees of previous lecture.

      → linear classification (hyperplanes) if dimension N is not too large.

This Lecture

- Support Vector Machines - separable case
- Support Vector Machines - non-separable case
- Margin guarantees

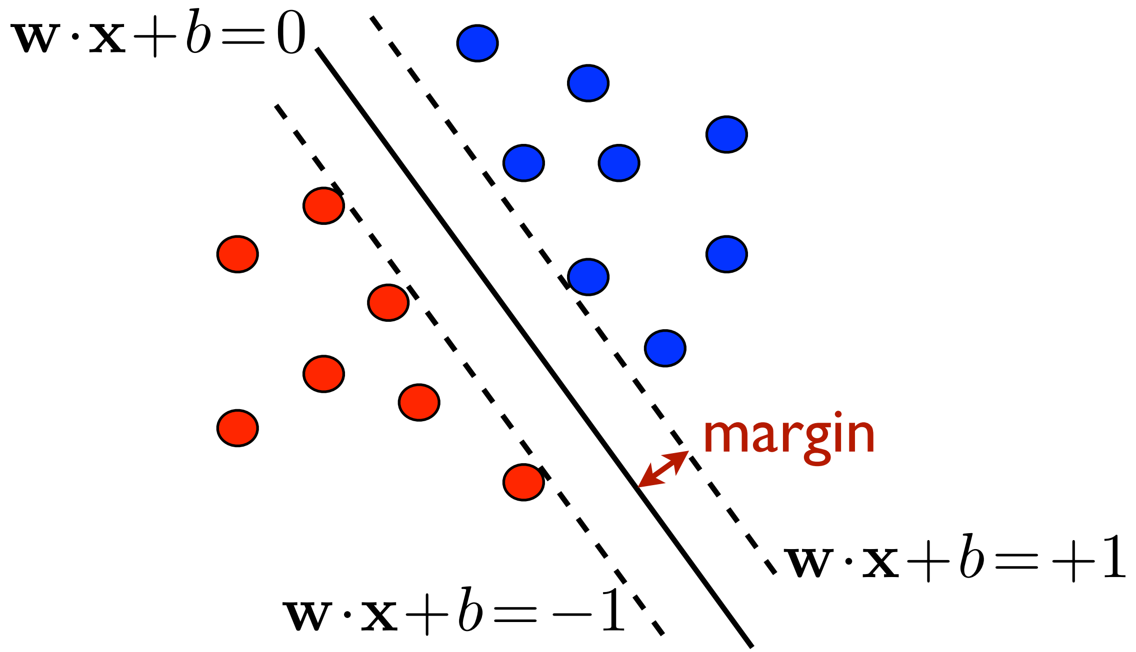
Linear Separation



- classifiers: $H=\{\mathbf{x}\mapsto \text{sgn}(\mathbf{w}\cdot\mathbf{x}+b) : \mathbf{w}\in\mathbb{R}^N, b\in\mathbb{R}\}$.
- geometric margin: $\rho = \min_{i\in[1,m]} \frac{|\mathbf{w}\cdot\mathbf{x}_i+b|}{\|\mathbf{w}\|}$.
- which separating hyperplane?

Optimal Hyperplane: Max. Margin

(Vapnik and Chervonenkis, 1965)



$$\rho = \max_{\mathbf{w},b\,:\,y_i(\mathbf{w}\cdot\mathbf{x}_i+b)\geq 0} \; \min_{i\in[1,m]} \frac{|\mathbf{w}\cdot\mathbf{x}_i + b|}{\|\mathbf{w}\|}.$$

Maximum Margin

$$
\begin{aligned}
\rho &= \max_{\mathbf{w},b\colon\, y_i(\mathbf{w}\cdot\mathbf{x}_i+b)\geq 0} \ \min_{i\in[1,m]} \frac{|\mathbf{w}\cdot\mathbf{x}_i+b|}{\|\mathbf{w}\|} \\
&= \max_{\substack{\mathbf{w},b\colon\, y_i(\mathbf{w}\cdot\mathbf{x}_i+b)\geq 0\\ \min_{i\in[1,m]} |\mathbf{w}\cdot\mathbf{x}_i+b|=1}} \ \min_{i\in[1,m]} \frac{|\mathbf{w}\cdot\mathbf{x}_i+b|}{\|\mathbf{w}\|} \qquad \text{(scale-invariance)} \\
&= \max_{\substack{\mathbf{w},b\colon\, y_i(\mathbf{w}\cdot\mathbf{x}_i+b)\geq 0\\ \min_{i\in[1,m]} |\mathbf{w}\cdot\mathbf{x}_i+b|=1}} \frac{1}{\|\mathbf{w}\|} \\
&= \max_{\mathbf{w},b\colon\, y_i(\mathbf{w}\cdot\mathbf{x}_i+b)\geq 1} \frac{1}{\|\mathbf{w}\|}. \qquad \text{(min. reached)}
\end{aligned}
$$

Optimization Problem

- Constrained optimization:

$$\min_{\mathbf{w},b} \ \frac{1}{2}\|\mathbf{w}\|^2$$
$$\text{subject to } \ y_i(\mathbf{w}\cdot\mathbf{x}_i + b) \geq 1, i \in [1, m].$$

- Properties:
  - Convex optimization.
  - Unique solution for linearly separable sample.

Optimal Hyperplane Equations

- Lagrangian: for all $\mathbf{w}, b, \alpha_i \geq 0$,

$$L(\mathbf{w}, b, \alpha) = \frac{1}{2}\|\mathbf{w}\|^2 - \sum_{i=1}^{m} \alpha_i [y_i(\mathbf{w} \cdot \mathbf{x}_i + b) - 1].$$

- KKT conditions:

$$\nabla_{\mathbf{w}} L = \mathbf{w} - \sum_{i=1}^{m} \alpha_i y_i \mathbf{x}_i = 0 \iff \boxed{\mathbf{w} = \sum_{i=1}^{m} \alpha_i y_i \mathbf{x}_i .}$$

$$\nabla_b L = -\sum_{i=1}^{m} \alpha_i y_i = 0 \iff \boxed{\sum_{i=1}^{m} \alpha_i y_i = 0.}$$

$$\boxed{\forall i \in [1, m],\ \alpha_i [y_i(\mathbf{w} \cdot \mathbf{x}_i + b) - 1] = 0.}$$

Support Vectors

- Complementarity conditions:

$$\alpha_i[y_i(\mathbf{w} \cdot \mathbf{x}_i + b) - 1] = 0 \implies \alpha_i = 0 \vee y_i(\mathbf{w} \cdot \mathbf{x}_i + b) = 1.$$

- Support vectors: vectors $\mathbf{x}_i$ such that

$$\alpha_i \neq 0 \wedge y_i(\mathbf{w} \cdot \mathbf{x}_i + b) = 1.$$

  - Note: support vectors are not unique.

Moving to The Dual

- Plugging in the expression of $\mathbf{w}$ in L gives:

$$L = \underbrace{\frac{1}{2}\left\|\sum_{i=1}^{m}\alpha_i y_i \mathbf{x}_i\right\|^2 - \sum_{i,j=1}^{m}\alpha_i\alpha_j y_i y_j(\mathbf{x}_i\cdot\mathbf{x}_j)}_{-\frac{1}{2}\sum_{i,j=1}^{m}\alpha_i\alpha_j y_i y_j(\mathbf{x}_i\cdot\mathbf{x}_j)} - \underbrace{\sum_{i=1}^{m}\alpha_i y_i b}_{0} + \sum_{i=1}^{m}\alpha_i.$$

- Thus,

$$L = \sum_{i=1}^{m}\alpha_i - \frac{1}{2}\sum_{i,j=1}^{m}\alpha_i\alpha_j y_i y_j(\mathbf{x}_i\cdot\mathbf{x}_j).$$

Equivalent Dual Opt. Problem

- Constrained optimization:

$$\max_{\alpha} \sum_{i=1}^{m} \alpha_i - \frac{1}{2} \sum_{i,j=1}^{m} \alpha_i \alpha_j y_i y_j (\mathbf{x}_i \cdot \mathbf{x}_j)$$

$$\text{subject to: } \alpha_i \geq 0 \wedge \sum_{i=1}^{m} \alpha_i y_i = 0, i \in [1, m].$$

- Solution:

$$h(x) = \operatorname{sgn}\Big(\sum_{i=1}^{m} \alpha_i y_i (\mathbf{x}_i \cdot \mathbf{x}) + b \Big),$$

with $b = y_i - \sum_{j=1}^{m} \alpha_j y_j (\mathbf{x}_j \cdot \mathbf{x}_i)$ for any SV $\mathbf{x}_i$.

Leave-One-Out Error

- **Definition**: let h_S be the hypothesis output by learning algorithm L after receiving sample S of size m. Then, the leave-one-out error of L over S is:

$$\widehat{R}_{\text{loo}}(L) = \frac{1}{m} \sum_{i=1}^{m} 1_{h_{S-\{x_i\}}(x_i) \neq f(x_i)}.$$

- **Property**: unbiased estimate of expected error of hypothesis trained on sample of size $m-1$,

$$\boxed{\mathop{\mathrm{E}}_{S \sim D^m}[\widehat{R}_{\text{loo}}(L)]} = \frac{1}{m} \sum_{i=1}^{m} \mathop{\mathrm{E}}_{S}[1_{h_{S-\{x_i\}}(x_i) \neq f(x_i)}] = \mathop{\mathrm{E}}_{S}[1_{h_{S-\{x\}}(x) \neq f(x)}]$$

$$= \mathop{\mathrm{E}}_{S' \sim D^{m-1}}[\mathop{\mathrm{E}}_{x \sim D}[1_{h_{S'}(x) \neq f(x)}]] \boxed{= \mathop{\mathrm{E}}_{S' \sim D^{m-1}}[R(h_{S'})]}.$$

Leave-One-Out Analysis

- **Theorem**: let h_S be the optimal hyperplane for a sample S and let $N_{\rm SV}(S)$ be the number of support vectors defining h_S. Then,

$$\mathop{\rm E}_{S \sim D^m}[R(h_S)] \leq \mathop{\rm E}_{S \sim D^{m+1}}\left[\frac{N_{\rm SV}(S)}{m+1}\right].$$

- **Proof**: Let $S \sim D^{m+1}$ be a sample linearly separable and let $x \in S$. If $h_{S-\{x\}}$ misclassifies x, then x must be a SV for h_S. Thus,

$$\widehat{R}_{\rm loo}(\text{opt.-hyp.}) \leq \frac{N_{\rm SV}(S)}{m+1}.$$

Notes

- Bound on expectation of error only, not the probability of error.
- Argument based on sparsity (number of support vectors). We will see later other arguments in support of the optimal hyperplanes based on the concept of margin.

This Lecture

- Support Vector Machines - separable case
- Support Vector Machines - non-separable case
- Margin guarantees

Support Vector Machines

(Cortes and Vapnik, 1995)

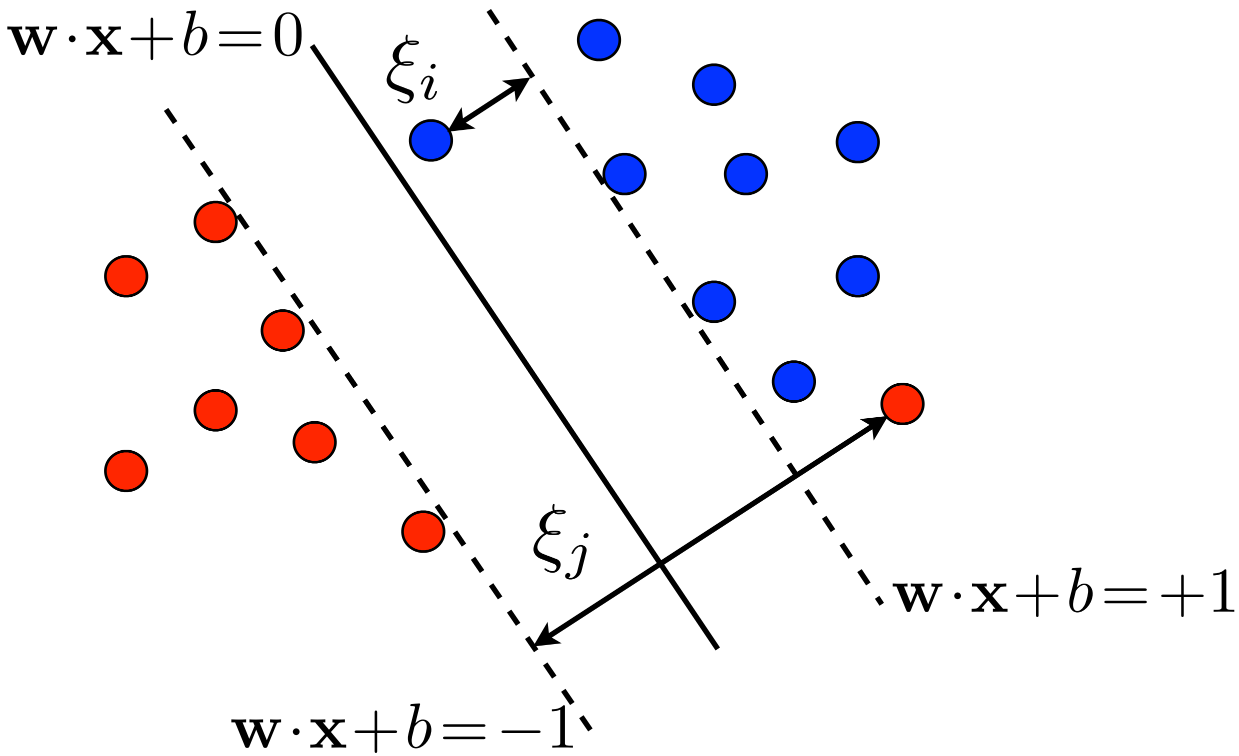
- Problem: data often not linearly separable in practice. For any hyperplane, there exists $\mathbf{x}_i$ such that

$$y_i \left[\mathbf{w} \cdot \mathbf{x}_i + b\right] \not\geq 1.$$

- Idea: relax constraints using slack variables $\xi_i \geq 0$

$$y_i \left[\mathbf{w} \cdot \mathbf{x}_i + b\right] \geq 1 - \xi_i.$$

Soft-Margin Hyperplanes



- Support vectors: points along the margin or outliers.
- Soft margin: $\rho = 1/\|\mathbf{w}\|$.

Optimization Problem

(Cortes and Vapnik, 1995)

- Constrained optimization:

$$\min_{\mathbf{w},b,\xi} \quad \frac{1}{2}\|\mathbf{w}\|^2 + C\sum_{i=1}^{m}\xi_i$$

$$\text{subject to} \quad y_i(\mathbf{w}\cdot\mathbf{x}_i + b) \geq 1 - \xi_i \;\wedge\; \xi_i \geq 0, i \in [1, m].$$

- Properties:
  - $C \geq 0$ trade-off parameter.
  - Convex optimization.
  - Unique solution.

Notes

- Parameter C: trade-off between maximizing margin and minimizing training error. How do we determine C?
- The general problem of determining a hyperplane minimizing the error on the training set is NP-complete (as a function of the dimension).
- Other convex functions of the slack variables could be used: this choice and a similar one with squared slack variables lead to a convenient formulation and solution.

SVM - Equivalent Problem

- **Optimization:**

$$\min_{\mathbf{w},b} \quad \frac{1}{2}\|\mathbf{w}\|^2 + C\sum_{i=1}^{m}\Big(1 - y_i(\mathbf{w}\cdot\mathbf{x}_i + b)\Big)_+.$$

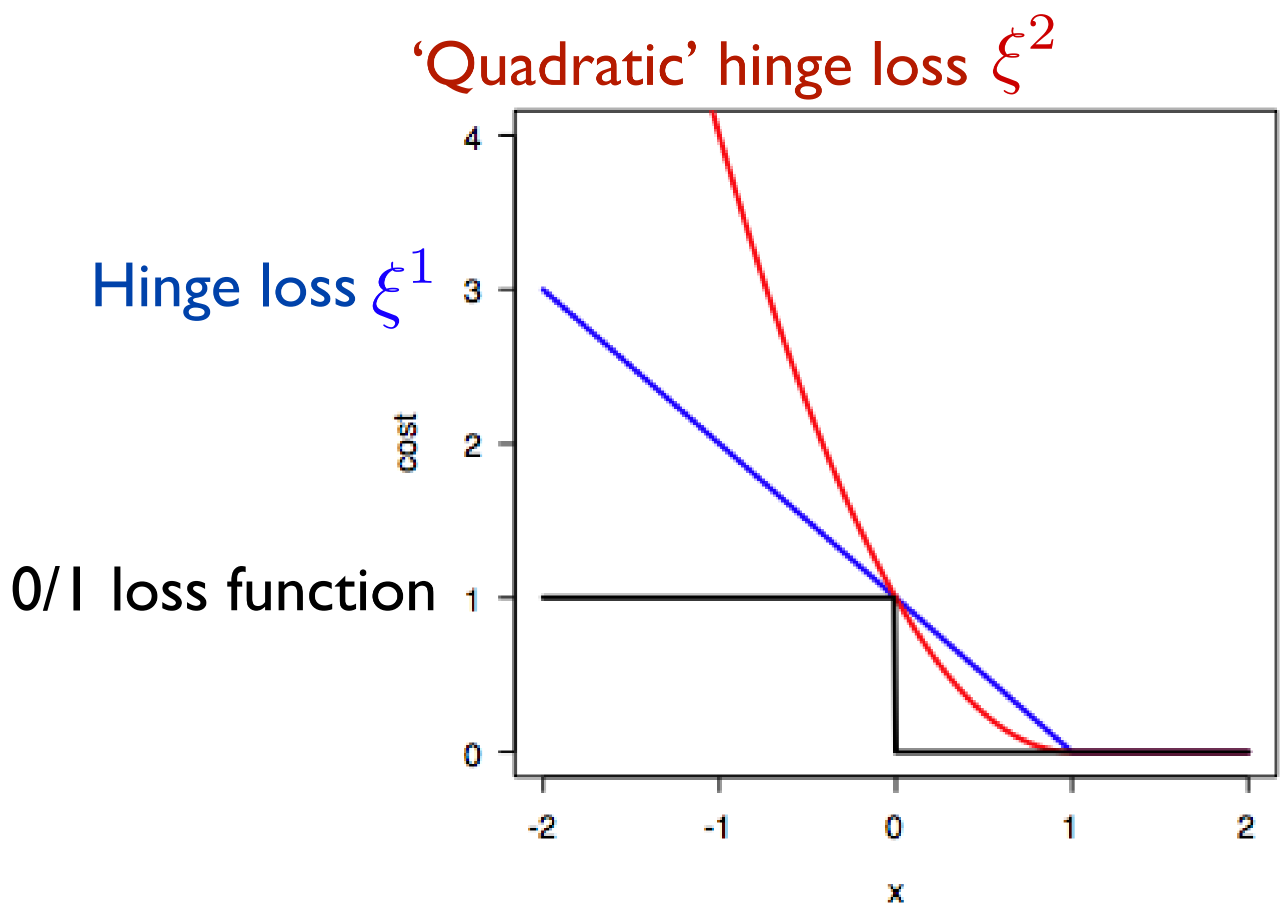
- **Loss functions:**
  - hinge loss:

$$L(h(x), y) = (1 - yh(x))_+.$$

  - quadratic hinge loss:

$$L(h(x), y) = (1 - yh(x))_+^2.$$

Hinge Loss


'Quadratic' hinge loss ξ^2
Hinge loss ξ^1
0/1 loss function
cost
x
4
3
2
1
0
-2
-1
0
1
2

SVMs Equations

- Lagrangian: for all $\mathbf{w}, b, \alpha_i \geq 0, \beta_i \geq 0,$

$$L(\mathbf{w}, b, \boldsymbol{\xi}, \boldsymbol{\alpha}, \boldsymbol{\beta}) = \frac{1}{2}\|\mathbf{w}\|^2 + C\sum_{i=1}^m \xi_i - \sum_{i=1}^m \alpha_i[y_i(\mathbf{w}\cdot\mathbf{x}_i + b) - 1 + \xi_i] - \sum_{i=1}^m \beta_i \xi_i\,.$$

- KKT conditions:

$$\nabla_w L = \mathbf{w} - \sum_{i=1}^m \alpha_i y_i \mathbf{x}_i = 0 \iff \boxed{\mathbf{w} = \sum_{i=1}^m \alpha_i y_i \mathbf{x}_i.}$$

$$\nabla_b L = -\sum_{i=1}^m \alpha_i y_i = 0 \iff \boxed{\sum_{i=1}^m \alpha_i y_i = 0.}$$

$$\nabla_{\xi_i} L = C - \alpha_i - \beta_i = 0 \iff \boxed{\alpha_i + \beta_i = C.}$$

$$\boxed{\begin{aligned} &\forall i \in [1, m],\ \alpha_i[y_i(\mathbf{w}\cdot\mathbf{x}_i + b) - 1 + \xi_i] = 0 \\ &\qquad\qquad \beta_i \xi_i = 0. \end{aligned}}$$

Support Vectors

- Complementarity conditions:

$$\alpha_i[y_i(\mathbf{w} \cdot \mathbf{x}_i + b) - 1 + \xi_i] = 0 \implies \alpha_i = 0 \vee y_i(\mathbf{w} \cdot \mathbf{x}_i + b) = 1 - \xi_i.$$

- Support vectors: vectors $\mathbf{x}_i$ such that

$$\alpha_i \neq 0 \wedge y_i(\mathbf{w} \cdot \mathbf{x}_i + b) = 1 - \xi_i.$$

  - Note: support vectors are not unique.

Moving to The Dual

- Plugging in the expression of w in L gives:

$$L = \underbrace{\frac{1}{2}\Big\|\sum_{i=1}^m \alpha_i y_i \mathbf{x}_i\Big\|^2 - \sum_{i,j=1}^m \alpha_i \alpha_j y_i y_j (\mathbf{x}_i \cdot \mathbf{x}_j)}_{-\frac{1}{2}\sum_{i,j=1}^m \alpha_i \alpha_j y_i y_j (\mathbf{x}_i \cdot \mathbf{x}_j)} - \underbrace{\sum_{i=1}^m \alpha_i y_i b}_{0} + \sum_{i=1}^m \alpha_i.$$

- Thus,

$$L = \sum_{i=1}^m \alpha_i - \frac{1}{2}\sum_{i,j=1}^m \alpha_i \alpha_j y_i y_j (\mathbf{x}_i \cdot \mathbf{x}_j).$$

- The condition $\beta_i \geq 0$ is equivalent to $\alpha_i \leq C$.

Dual Optimization Problem

- Constrained optimization:

$$\max_{\alpha} \sum_{i=1}^{m} \alpha_i - \frac{1}{2} \sum_{i,j=1}^{m} \alpha_i \alpha_j y_i y_j (\mathbf{x}_i \cdot \mathbf{x}_j)$$

$$\text{subject to: } 0 \leq \alpha_i \boxed{\leq C} \wedge \sum_{i=1}^{m} \alpha_i y_i = 0, i \in [1, m].$$

- Solution:

$$h(x) = \operatorname{sgn}\Big(\sum_{i=1}^{m} \alpha_i y_i (\mathbf{x}_i \cdot \mathbf{x}) + b \Big),$$

with $b = y_i - \sum_{j=1}^{m} \alpha_j y_j (\mathbf{x}_j \cdot \mathbf{x}_i)$ for any $\mathbf{x}_i$ with $0 < \alpha_i \boxed{< C.}$

This Lecture

- Support Vector Machines - separable case
- Support Vector Machines - non-separable case
- Margin guarantees

High-Dimension

- Learning guarantees: for hyperplanes in dimension N with probability at least $1-\delta$,

$$R(h) \leq \widehat{R}(h) + \sqrt{\frac{2(N+1)\log\frac{em}{N+1}}{m}} + \sqrt{\frac{\log\frac{1}{\delta}}{2m}}.$$

  - bound is uninformative for $N \gg m$.
  - but SVMs have been remarkably successful in high-dimension.
  - can we provide a theoretical justification?
  - analysis of underlying scoring function.

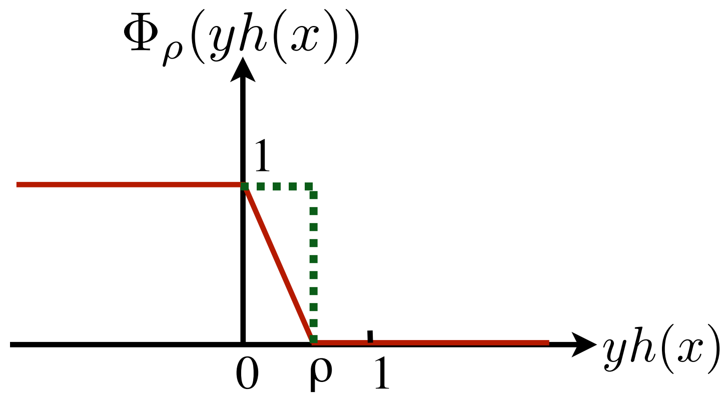
Confidence Margin

- Definition: the confidence margin of a real-valued function h at $(x, y) \in X \times Y$ is $\rho_h(x, y) = yh(x)$.
  - interpreted as the hypothesis' confidence in prediction.
  - if correctly classified coincides with $|h(x)|$.
  - relationship with geometric margin for linear functions $h \colon \mathbf{x} \mapsto \mathbf{w} \cdot \mathbf{x} + b$: for x in the sample,

$$|\rho_h(x, y)| \geq \rho_{\text{geom}} \|\mathbf{w}\|.$$

Confidence Margin Loss

- **Definition**: for any confidence margin parameter $\rho > 0$ the ρ-margin loss function Φ_ρ is defined by



- For a sample $S = (x_1, \ldots, x_m)$ and real-valued hypothesis h, the empirical margin loss is

$$\widehat{R}_\rho(h) = \frac{1}{m} \sum_{i=1}^{m} \Phi_\rho(y_i h(x_i)) \leq \boxed{\frac{1}{m} \sum_{i=1}^{m} 1_{y_i h(x_i) < \rho}}.$$

General Margin Bound

- **Theorem**: Let H be a set of real-valued functions. Fix $\rho > 0$. For any $\delta > 0$, with probability at least $1-\delta$, the following holds for all $h \in H$:

$$R(h) \leq \widehat{R}_\rho(h) + \frac{2}{\rho}\mathfrak{R}_m(H) + \sqrt{\frac{\log \frac{1}{\delta}}{2m}}$$

$$R(h) \leq \widehat{R}_\rho(h) + \frac{2}{\rho}\widehat{\mathfrak{R}}_S(H) + 3\sqrt{\frac{\log \frac{2}{\delta}}{2m}}.$$

- **Proof**: Let $\widetilde{H} = \{z = (x, y) \mapsto yh(x) : h \in H\}$. Consider the family of functions taking values in $[0, 1]$:

$$\widetilde{\mathcal{H}} = \{\Phi_\rho \circ f : f \in \widetilde{H}\}.$$

- By the theorem of Lecture 3, with probability at least $1-\delta$, for all $g \in \widetilde{\mathcal{H}}$,

$$\mathrm{E}[g(z)] \leq \frac{1}{m}\sum_{i=1}^{m} g(z_i) + 2\mathfrak{R}_m(\widetilde{\mathcal{H}}) + \sqrt{\frac{\log\frac{1}{\delta}}{2m}}.$$

- Thus,

$$\mathrm{E}[\Phi_\rho(yh(x))] \leq \widehat{R}_\rho(h) + 2\mathfrak{R}_m\big(\Phi_\rho \circ \widetilde{H}\big) + \sqrt{\frac{\log\frac{1}{\delta}}{2m}}.$$

- Since Φ_ρ is $\frac{1}{\rho}$ - Lipschitz, by Talagrand's lemma,

$$\mathfrak{R}_m\big(\Phi_\rho \circ \widetilde{H}\big) \leq \frac{1}{\rho}\mathfrak{R}_m(\widetilde{H}) = \frac{1}{\rho m}\mathop{\mathrm{E}}_{\sigma,S}\Big[\sup_{h\in H}\sum_{i=1}^{m}\sigma_i y_i h(x_i)\Big] = \frac{1}{\rho}\mathfrak{R}_m\big(H\big).$$

- Since $1_{yh(x)<0} \leq \Phi_\rho(yh(x))$, this shows the first statement, and similarly the second one.

Rademacher Complexity of Linear Hypotheses

- **Theorem**: Let $S \subseteq \{x \colon \|\mathbf{x}\| \leq R\}$ be a sample of size m and let $H = \{\mathbf{x} \mapsto \mathbf{w} \cdot \mathbf{x} \colon \|\mathbf{w}\| \leq \Lambda\}$. Then,

$$\widehat{\mathfrak{R}}_S(H) \leq \sqrt{\frac{R^2 \Lambda^2}{m}}.$$

- **Proof**:

$$\begin{aligned}
\widehat{\mathfrak{R}}_S(H) &= \frac{1}{m} \operatorname*{E}_{\sigma} \left[\sup_{\|\mathbf{w}\| \leq \Lambda} \sum_{i=1}^{m} \sigma_i \mathbf{w} \cdot \mathbf{x}_i \right] = \frac{1}{m} \operatorname*{E}_{\sigma} \left[\sup_{\|\mathbf{w}\| \leq \Lambda} \mathbf{w} \cdot \sum_{i=1}^{m} \sigma_i \mathbf{x}_i \right] \\
&\leq \frac{\Lambda}{m} \operatorname*{E}_{\sigma} \left[\left\| \sum_{i=1}^{m} \sigma_i \mathbf{x}_i \right\| \right] \leq \frac{\Lambda}{m} \left[\operatorname*{E}_{\sigma} \left[\left\| \sum_{i=1}^{m} \sigma_i \mathbf{x}_i \right\|^2 \right] \right]^{1/2} \\
&\leq \frac{\Lambda}{m} \left[\operatorname*{E}_{\sigma} \left[\sum_{i=1}^{m} \|\mathbf{x}_i\|^2 \right] \right]^{1/2} \leq \frac{\Lambda \sqrt{m R^2}}{m} = \sqrt{\frac{R^2 \Lambda^2}{m}}.
\end{aligned}$$

Margin Bound - Linear Classifiers

- **Corollary**: Let $\rho > 0$ and $H = \{\mathbf{x} \mapsto \mathbf{w} \cdot \mathbf{x} \colon \|\mathbf{w}\| \leq \Lambda\}$. Assume that $X \subseteq \{\mathbf{x} \colon \|\mathbf{x}\| \leq R\}$. Then, for any $\delta > 0$, with probability at least $1 - \delta$, for any $h \in H$,

$$R(h) \leq \widehat{R}_\rho(h) + 2\sqrt{\frac{R^2\Lambda^2/\rho^2}{m}} + 3\sqrt{\frac{\log \frac{2}{\delta}}{2m}}.$$

- **Proof**: Follows directly general margin bound and bound on $\widehat{\mathfrak{R}}_S(H)$ for linear classifiers.
  - Finer relative deviation margin bounds (Cortes, MM, Suresh; ICML 2021).

High-Dimensional Feature Space

- Observations:
  - generalization bound does not depend on the dimension but on the margin.
  - this suggests seeking a large-margin hyperplane in a higher-dimensional feature space.
- Computational problems:
  - taking dot products in a high-dimensional feature space can be very costly.
  - solution based on kernels (next lecture).

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Appendix

Saddle Point

- Let $(\mathbf{w}^*, b^*, \alpha^*)$ be the saddle point of the Langrangian. Multiplying both sides of the equation giving b^* by $\alpha_i^* y_i$ and taking the sum leads to:

$$\sum_{i=1}^{m} \alpha_i^* y_i b = \sum_{i=1}^{m} \alpha_i^* y_i^2 - \sum_{i,j=1}^{m} \alpha_i^* \alpha_j^* y_i y_j (\mathbf{x}_i \cdot \mathbf{x}_j).$$

- Using $y_i^2 = 1$, $\sum_{i=1}^{m} \alpha_i^* y_i = 0$, and $\mathbf{w}^* = \sum_{i=1}^{m} \alpha_i^* y_i \mathbf{x}_i$ yields

$$0 = \sum_{i=1}^{m} \alpha_i^* - \|\mathbf{w}^*\|^2.$$

- Thus, the margin is also given by:

$$\boxed{\rho^2 = \frac{1}{\|\mathbf{w}^*\|_2^2} = \frac{1}{\|\alpha^*\|_1}.}$$

Talagrand's Contraction Lemma

(Ledoux and Talagrand, 1991; pp. 112-114)

- **Theorem**: Let $\Phi\colon \mathbb{R} \to \mathbb{R}$ be an L-Lipschitz function. Then, for any hypothesis set H of real-valued functions,

$$\widehat{\mathfrak{R}}_S(\Phi \circ H) \leq L\, \widehat{\mathfrak{R}}_S(H).$$

- **Proof**: fix sample $S = (x_1, \ldots, x_m)$. By definition,

$$\begin{aligned}
\mathfrak{R}_S(\Phi \circ H) &= \frac{1}{m} \mathop{\mathrm{E}}_{\boldsymbol{\sigma}} \left[\sup_{h \in H} \sum_{i=1}^{m} \sigma_i (\Phi \circ h)(x_i) \right] \\
&= \frac{1}{m} \mathop{\mathrm{E}}_{\sigma_1, \ldots, \sigma_{m-1}} \left[\mathop{\mathrm{E}}_{\sigma_m} \left[\sup_{h \in H} u_{m-1}(h) + \sigma_m (\Phi \circ h)(x_m) \right] \right],
\end{aligned}$$

with $u_{m-1}(h) = \sum_{i=1}^{m-1} \sigma_i (\Phi \circ h)(x_i)$.

Talagrand's Contraction Lemma

- Now, assuming that the suprema are reached, there exist $h_1, h_2 \in H$ such that

$$
\begin{aligned}
&\mathop{\mathrm{E}}_{\sigma_m}\left[\sup_{h\in H} u_{m-1}(h) + \sigma_m(\Phi \circ h)(x_m)\right]\Big] \\
&= \frac{1}{2}[u_{m-1}(h_1) + (\Phi \circ h_1)(x_m)] + \frac{1}{2}[u_{m-1}(h_2) - (\Phi \circ h_2)(x_m)] \\
&\leq \frac{1}{2}[u_{m-1}(h_1) + u_{m-1}(h_2) + sL(h_1(x_m) - h_2(x_m))] \\
&= \frac{1}{2}[u_{m-1}(h_1) + sLh_1(x_m)] + \frac{1}{2}[u_{m-1}(h_2) - sLh_2(x_m)] \\
&\leq \mathop{\mathrm{E}}_{\sigma_m}\left[\sup_{h\in H} u_{m-1}(h) + \sigma_m L h(x_m)\right],
\end{aligned}
$$

where $s = \mathrm{sgn}(h_1(x_m) - h_2(x_m))$.

Talagrand's Contraction Lemma

- When the suprema are not reached, the same can be shown modulo ϵ, followed by $\epsilon \to 0$.
- Proceeding similarly for other σ_is directly leads to the result.

VC Dimension of Canonical Hyperplanes

- **Theorem**: Let $S \subseteq \{\mathbf{x} : \|\mathbf{x}\| \leq R\}$. Then, the VC dimension d of the set of canonical hyperplanes $\{x \mapsto \text{sgn}(\mathbf{w} \cdot \mathbf{x}) \colon \min_{x \in S} |\mathbf{w} \cdot \mathbf{x}| = 1 \wedge \|\mathbf{w}\| \leq \Lambda\}$ verifies

$$d \leq R^2 \Lambda^2.$$

- **Proof**: Let $\{\mathbf{x}_1, \ldots, \mathbf{x}_d\}$ be a set fully shattered. Then, for all $\mathbf{y} \in \{-1, +1\}^d$, there exists $\mathbf{w}$ such

$$\forall i \in [1, d], 1 \leq y_i(\mathbf{w} \cdot \mathbf{x}_i).$$

- Summing up the inequalities gives

$$d \leq \mathbf{w} \cdot \sum_{i=1}^{d} y_i \mathbf{x}_i \leq \|\mathbf{w}\| \|\sum_{i=1}^{d} y_i \mathbf{x}_i\| \leq \Lambda \|\sum_{i=1}^{d} y_i \mathbf{x}_i\|.$$

- Taking the expectation over $\mathbf{y} \sim U$ (uniform) yields

$$d \leq \Lambda \operatorname*{E}_{\mathbf{y}\sim U}[\|\sum_{i=1}^{d} y_i \mathbf{x}_i\|] \leq \Lambda \Big[\operatorname*{E}_{\mathbf{y}\sim U}[\|\sum_{i=1}^{d} y_i \mathbf{x}_i\|^2] \Big]^{1/2} \text{ (Jensen's ineq.)}$$

$$= \Lambda \Big[\sum_{i,j=1}^{d} \mathrm{E}[y_i y_j](\mathbf{x}_i \cdot \mathbf{x}_j) \Big]^{1/2}$$

$$= \Lambda \Big[\sum_{i=1}^{d} (\mathbf{x}_i \cdot \mathbf{x}_i) \Big]^{1/2} \leq \Lambda \big[dR^2 \big]^{1/2} = \Lambda R \sqrt{d}.$$

- Thus, $\sqrt{d} \leq \Lambda R$.

Foundations of Machine Learning
Kernel Methods

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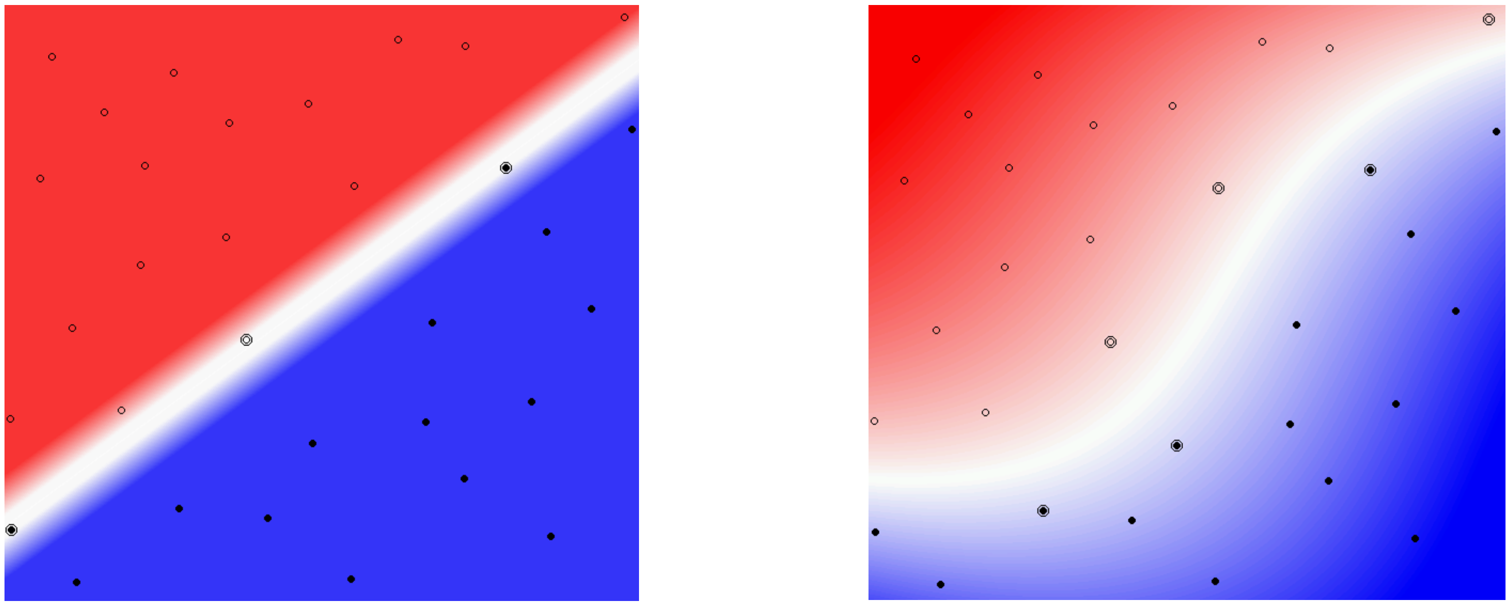
Motivation

- Efficient computation of inner products in high dimension.
- Non-linear decision boundary.
- Non-vectorial inputs.
- Flexible selection of more complex features.

This Lecture

- Kernels
- Kernel-based algorithms
- Closure properties
- Sequence Kernels
- Negative kernels

Non-Linear Separation



- Linear separation impossible in most problems.
- Non-linear mapping from input space to high-dimensional feature space: $\Phi\colon X \to F$.
- Generalization ability: independent of $\dim(F)$, depends only on margin and sample size.

Kernel Methods

- Idea:
  - Define $K: X \times X \to \mathbb{R}$, called kernel, such that:
  $$\Phi(x) \cdot \Phi(y) = K(x, y).$$
  - K often interpreted as a similarity measure.
- Benefits:
  - Efficiency: K is often more efficient to compute than Φ and the dot product.
  - Flexibility: K can be chosen arbitrarily so long as the existence of Φ is guaranteed (PDS condition or Mercer's condition).

PDS Condition

- **Definition**: a kernel $K\colon X \times X \to \mathbb{R}$ is positive definite symmetric (PDS) if for any $\{x_1, \ldots, x_m\} \subseteq X$, the matrix $\mathbf{K} = [K(x_i, x_j)]_{ij} \in \mathbb{R}^{m \times m}$ is symmetric positive semi-definite (SPSD).
- $\mathbf{K}$ SPSD if symmetric and one of the 2 equiv. cond.'s:
  - its eigenvalues are non-negative.
  - for any $\mathbf{c} \in \mathbb{R}^{m \times 1}$, $\mathbf{c}^\top \mathbf{K} \mathbf{c} = \sum_{i,j=1}^{m} c_i c_j K(x_i, x_j) \geq 0.$
- **Terminology**: PDS for kernels, SPSD for kernel matrices (see (Berg et al., 1984)).

Example - Polynomial Kernels

- **Definition:**

$$\forall x, y \in \mathbb{R}^N, \;\; K(x, y) = (x \cdot y + c)^d, \quad c > 0.$$

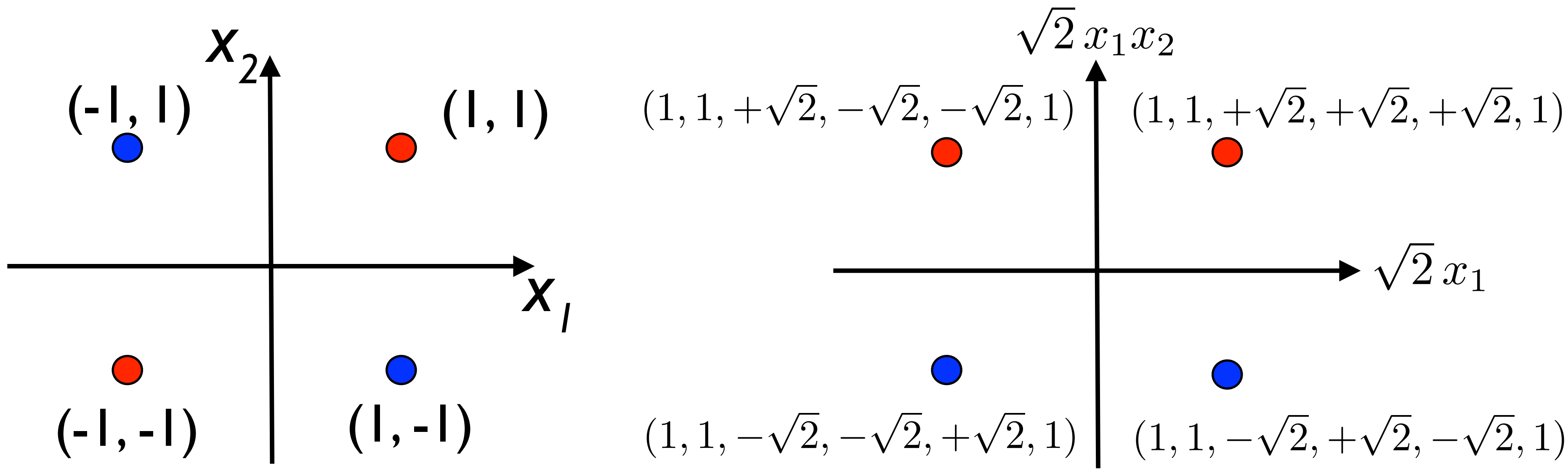
- **Example:** for $N = 2$ and $d = 2$,

$$K(x, y) = (x_1 y_1 + x_2 y_2 + c)^2$$

$$= \begin{bmatrix} x_1^2 \\ x_2^2 \\ \sqrt{2}\, x_1 x_2 \\ \sqrt{2c}\, x_1 \\ \sqrt{2c}\, x_2 \\ c \end{bmatrix} \cdot \begin{bmatrix} y_1^2 \\ y_2^2 \\ \sqrt{2}\, y_1 y_2 \\ \sqrt{2c}\, y_1 \\ \sqrt{2c}\, y_2 \\ c \end{bmatrix}.$$

XOR Problem

- Use second-degree polynomial kernel with $c = 1$:



Linearly non-separable

Linearly separable by $x_1 x_2 = 0.$

Normalized Kernels

- **Definition**: the normalized kernel K' associated to a kernel K is defined by

$$\forall x, x' \in \mathcal{X}, \; K'(x, x') = \begin{cases} 0 & \text{if } (K(x,x) = 0) \vee (K(x',x') = 0) \\ \frac{K(x,x')}{\sqrt{K(x,x)K(x',x')}} & \text{otherwise.} \end{cases}$$

- If K is PDS, then K' is PDS:

$$\sum_{i,j=1}^{m} \frac{c_i c_j K(x_i, x_j)}{\sqrt{K(x_i,x_i)K(x_j,x_j)}} = \sum_{i,j=1}^{m} \frac{c_i c_j \langle \Phi(x_i), \Phi(x_j) \rangle}{\|\Phi(x_i)\|_H \, \|\Phi(x_j)\|_{\mathbb{H}}} = \left\| \sum_{i=1}^{m} \frac{c_i \Phi(x_i)}{\|\Phi(x_i)\|_H} \right\|_{\mathbb{H}}^2 \geq 0.$$

- By definition, for all x with $K(x,x) \neq 0$,

$$K'(x, x) = 1.$$

Other Standard PDS Kernels

- Gaussian kernels:

$$K(x, y) = \exp\left(-\frac{||x-y||^2}{2\sigma^2}\right), \ \sigma \neq 0.$$

  - Normalized kernel of $(\mathbf{x}, \mathbf{x}') \mapsto \exp\left(\frac{\mathbf{x} \cdot \mathbf{x}'}{\sigma^2}\right)$.

- Sigmoid Kernels:

$$K(x, y) = \tanh(a(x \cdot y) + b), \ a, b \geq 0.$$

Reproducing Kernel Hilbert Space

(Aronszajn, 1950)

- Theorem: Let $K\colon X \times X \to \mathbb{R}$ be a PDS kernel. Then, there exists a Hilbert space H and a mapping Φ from X to H such that

$$\forall x, y \in X, \;\; K(x, y) = \Phi(x) \cdot \Phi(y).$$

- Proof: For any $x \in X$, define $\Phi(x)\colon X \to \mathbb{R}^X$ as follows:

$$\forall y \in X, \;\; \Phi(x)(y) = K(x, y).$$

  - Let $H_0 = \Big\{ \sum_{i \in I} a_i \Phi(x_i) \colon a_i \in \mathbb{R}, x_i \in X, \mathrm{card}(I) < \infty \Big\}.$
  - We are going to define an inner product $\langle \cdot, \cdot \rangle$ on H_0.

- Definition: for any $f = \sum_{i \in I} a_i \Phi(x_i)$, $g = \sum_{j \in J} b_j \Phi(y_j)$,

$$\langle f, g \rangle = \sum_{i \in I, j \in J} a_i b_j K(x_i, y_j) = \sum_{j \in J} b_j f(y_j) = \sum_{i \in I} a_i g(x_i).$$

- $\langle \cdot, \cdot \rangle$ does not depend on representations of f and g.
- $\langle \cdot, \cdot \rangle$ is bilinear and symmetric.
- $\langle \cdot, \cdot \rangle$ is positive semi-definite since K is PDS: for any f,

$$\langle f, f \rangle = \sum_{i, j \in I} a_i a_j K(x_i, x_j) \geq 0.$$

- note: for any $f_1, \ldots, f_m$ and $c_1, \ldots, c_m$,

$$\sum_{i,j=1}^{m} c_i c_j \langle f_i, f_j \rangle = \Big\langle \sum_{i=1}^{m} c_i f_i, \sum_{j=1}^{m} c_j f_j \Big\rangle \geq 0.$$

$\longrightarrow$ $\langle \cdot, \cdot \rangle$ is a PDS kernel on H_0.

- $\langle \cdot, \cdot \rangle$ is definite:
  - first, Cauchy-Schwarz inequality for PDS kernels. If K is PDS, $\mathbf{M} = \begin{pmatrix} K(x,x) & K(x,y) \\ K(y,x) & K(y,y) \end{pmatrix}$ is SPSD for all $x, y \in X$. In particular, the product of its eigenvalues, $\det(\mathbf{M})$ is non-negative:

$$\det(\mathbf{M}) = K(x,x)K(y,y) - K(x,y)^2 \geq 0.$$

  - since $\langle \cdot, \cdot \rangle$ is a PDS kernel, for any $f \in H_0$ and $x \in X$,

$$\langle f, \Phi(x) \rangle^2 \leq \langle f, f \rangle \langle \Phi(x), \Phi(x) \rangle.$$

  - observe the reproducing property of $\langle \cdot, \cdot \rangle$:

$$\forall f \in H_0, \forall x \in X, \ \ f(x) = \sum_{i \in I} a_i K(x_i, x) = \langle f, \Phi(x) \rangle.$$

  - Thus, $[f(x)]^2 \leq \langle f, f \rangle K(x,x)$ for all $x \in X$, which shows the definiteness of $\langle \cdot, \cdot \rangle$.

- Thus, $\langle \cdot, \cdot \rangle$ defines an inner product on H_0, which thereby becomes a pre-Hilbert space.
- H_0 can be completed to form a Hilbert space H in which it is dense.

Notes:

- H is called the reproducing kernel Hilbert space (RKHS) associated to K.
- A Hilbert space such that there exists $\Phi: X \to H$ with $K(x, y) = \Phi(x) \cdot \Phi(y)$ for all $x, y \in X$ is also called a feature space associated to K. Φ is called a feature mapping.
- Feature spaces associated to K are in general not unique.

This Lecture

- Kernels
- Kernel-based algorithms
- Closure properties
- Sequence Kernels
- Negative kernels

SVMs with PDS Kernels

(Boser, Guyon, and Vapnik, 1992)

- Constrained optimization:

$$\max_{\alpha} \sum_{i=1}^{m} \alpha_i - \frac{1}{2} \sum_{i,j=1}^{m} \alpha_i \alpha_j y_i y_j K(x_i, x_j)$$

$\Phi(x_i) \cdot \Phi(x_j)$

$$\text{subject to: } 0 \leq \alpha_i \leq C \wedge \sum_{i=1}^{m} \alpha_i y_i = 0, i \in [1, m].$$

- Solution:

$$h(x) = \operatorname{sgn}\Big(\sum_{i=1}^{m} \alpha_i y_i K(x_i, x) + b \Big),$$

with $b = y_i - \sum_{j=1}^{m} \alpha_j y_j K(x_j, x_i)$ for any x_i with $0 < \alpha_i < C.$

Rad. Complexity of Kernel-Based Hypotheses

- **Theorem**: Let $K\colon X \times X \to \mathbb{R}$ be a PDS kernel and let $\Phi: X \to \mathbb{H}$ be a feature mapping associated to K. Let $S \subseteq \{x : K(x,x) \leq R^2\}$ be a sample of size m, and let $H = \{\mathbf{x} \mapsto \mathbf{w} \cdot \Phi(x) : \|\mathbf{w}\|_{\mathbb{H}} \leq \Lambda\}$. Then,

$$\widehat{\mathfrak{R}}_S(H) \leq \frac{\Lambda\sqrt{\mathrm{Tr}[\mathbf{K}]}}{m} \leq \sqrt{\frac{R^2\Lambda^2}{m}}.$$

- **Proof**: $\widehat{\mathfrak{R}}_S(H) = \frac{1}{m}\mathop{\mathrm{E}}_{\sigma}\Big[\sup_{\|\mathbf{w}\|\leq\Lambda} \mathbf{w} \cdot \sum_{i=1}^m \sigma_i \Phi(x_i)\Big] \leq \frac{\Lambda}{m}\mathop{\mathrm{E}}_{\sigma}\Big[\Big\|\sum_{i=1}^m \sigma_i \Phi(x_i)\Big\|\Big]$

$$\text{(Jensen's ineq.)} \leq \frac{\Lambda}{m}\bigg[\mathop{\mathrm{E}}_{\sigma}\Big[\Big\|\sum_{i=1}^m \sigma_i \Phi(x_i)\Big\|^2\Big]\bigg]^{1/2} \leq \frac{\Lambda}{m}\bigg[\mathop{\mathrm{E}}_{\sigma}\Big[\sum_{i=1}^m \|\Phi(x_i)\|^2\Big]\bigg]^{1/2}$$

$$= \frac{\Lambda}{m}\bigg[\mathop{\mathrm{E}}_{\sigma}\Big[\sum_{i=1}^m K(x_i, x_i)\Big]\bigg]^{1/2} = \frac{\Lambda\sqrt{\mathrm{Tr}[\mathbf{K}]}}{m} \leq \sqrt{\frac{R^2\Lambda^2}{m}}.$$

Generalization: Representer Theorem

(Kimeldorf and Wahba, 1971)

- **Theorem**: Let $K\colon X \times X \to \mathbb{R}$ be a PDS kernel with H the corresponding RKHS. Then, for any non-decreasing function $G\colon \mathbb{R} \to \mathbb{R}$ and any $L\colon \mathbb{R}^m \to \mathbb{R} \cup \{+\infty\}$ problem

$$\operatorname*{argmin}_{h \in H} F(h) = \operatorname*{argmin}_{h \in H} \; G(\|h\|_H) + L\big(h(x_1), \ldots, h(x_m)\big)$$

admits a solution of the form $h^* = \sum_{i=1}^{m} \alpha_i K(x_i, \cdot)$.

If G is further assumed to be increasing, then any solution has this form.

- Proof: let $H_1 = \text{span}(\{K(x_i, \cdot) : i \in [1, m]\})$. Any $h \in H$ admits the decomposition $h = h_1 + h^\perp$ according to $H = H_1 \oplus H_1^\perp$.
  - Since G is non-decreasing,
  $$G(\|h_1\|_H) \leq G\Big(\sqrt{\|h_1\|_H^2 + \|h^\perp\|_H^2}\Big) = G(\|h\|_H).$$
  - By the reproducing property, for all $i \in [1, m]$,
  $$h(x_i) = \langle h, K(x_i, \cdot)\rangle = \langle h_1, K(x_i, \cdot)\rangle = h_1(x_i).$$
  - Thus, $L\big(h(x_1), \ldots, h(x_m)\big) = L\big(h_1(x_1), \ldots, h_1(x_m)\big)$ and $F(h_1) \leq F(h)$.
  - If G is increasing, then $F(h_1) < F(h)$ when $h^\perp \neq 0$ and any solution of the optimization problem must be in H_1.

Kernel-Based Algorithms

- PDS kernels used to extend a variety of algorithms in classification and other areas:
  - regression.
  - ranking.
  - dimensionality reduction.
  - clustering.
- But, how do we define PDS kernels?

This Lecture

- Kernels
- Kernel-based algorithms
- Closure properties
- Sequence Kernels
- Negative kernels

Closure Properties of PDS Kernels

- Theorem: Positive definite symmetric (PDS) kernels are closed under:
  - sum,
  - product,
  - tensor product,
  - pointwise limit,
  - composition with a power series with non-negative coefficients.

Closure Properties - Proof

- **Proof**: closure under sum:

$$\mathbf{c}^\top \mathbf{K}\mathbf{c} \geq 0 \wedge \mathbf{c}^\top \mathbf{K}'\mathbf{c} \geq 0 \Rightarrow \mathbf{c}^\top (\mathbf{K} + \mathbf{K}')\mathbf{c} \geq 0.$$

  - closure under product: $\mathbf{K} = \mathbf{M}\mathbf{M}^\top$,

$$\begin{aligned}
\sum_{i,j=1}^{m} c_i c_j (\mathbf{K}_{ij}\mathbf{K}'_{ij}) &= \sum_{i,j=1}^{m} c_i c_j \left(\left[\sum_{k=1}^{m} \mathbf{M}_{ik}\mathbf{M}_{jk} \right] \mathbf{K}'_{ij} \right) \\
&= \sum_{k=1}^{m} \left[\sum_{i,j=1}^{m} c_i c_j \mathbf{M}_{ik}\mathbf{M}_{jk}\mathbf{K}'_{ij} \right] \\
&= \sum_{k=1}^{m} \begin{bmatrix} c_1\mathbf{M}_{1k} \\ \cdots \\ c_m\mathbf{M}_{mk} \end{bmatrix}^\top \mathbf{K}' \begin{bmatrix} c_1\mathbf{M}_{1k} \\ \cdots \\ c_m\mathbf{M}_{mk} \end{bmatrix} \geq 0.
\end{aligned}$$

- Closure under tensor product:
  - definition: for all $x_1, x_2, y_1, y_2 \in X$,

$$(K_1 \otimes K_2)(x_1, y_1, x_2, y_2) = K_1(x_1, x_2) K_2(y_1, y_2).$$

  - thus, PDS kernel as product of the kernels

$$(x_1, y_1, x_2, y_2) \to K_1(x_1, x_2) \quad (x_1, y_1, x_2, y_2) \to K_2(y_1, y_2).$$

- Closure under pointwise limit: if for all $x, y \in X$,

$$\lim_{n \to \infty} K_n(x, y) = K(x, y),$$

Then, $(\forall n, \mathbf{c}^\top \mathbf{K}_n \mathbf{c} \geq 0) \Rightarrow \lim_{n \to \infty} \mathbf{c}^\top \mathbf{K}_n \mathbf{c} = \mathbf{c}^\top \mathbf{K} \mathbf{c} \geq 0.$

- Closure under composition with power series:
  - assumptions: K PDS kernel with $|K(x, y)| < \rho$ for all $x, y \in X$ and $f(x) = \sum_{n=0}^{\infty} a_n x^n, a_n \geq 0$ power series with radius of convergence ρ.
  - $f \circ K$ is a PDS kernel since K^n is PDS by closure under product, $\sum_{n=0}^{N} a_n K^n$ is PDS by closure under sum, and closure under pointwise limit.
- Example: for any PDS kernel K, $\exp(K)$ is PDS.

This Lecture

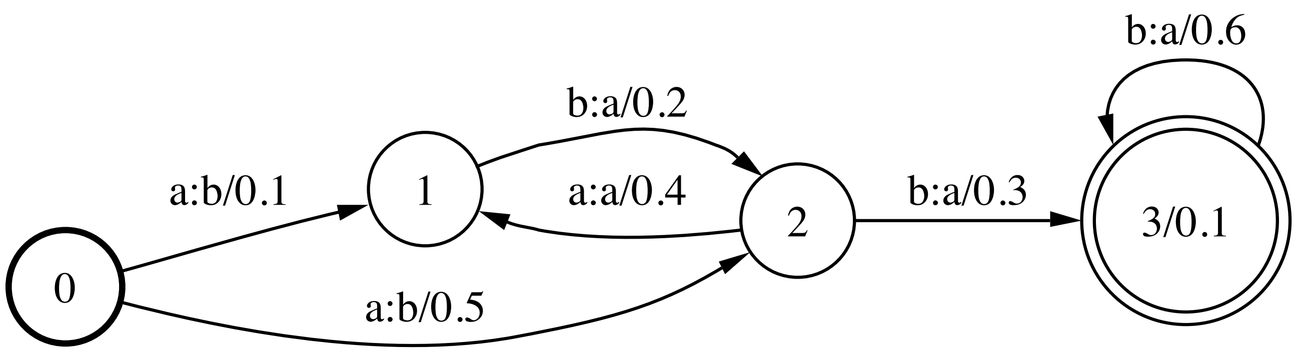
- Kernels
- Kernel-based algorithms
- Closure properties
- Sequence Kernels
- Negative kernels

Sequence Kernels

- Definition: Kernels defined over pairs of strings.
  - Motivation: computational biology, text and speech classification.
  - Idea: two sequences are related when they share some common substrings or subsequences.
  - Example: bigram kernel;

$$K(x, y) = \sum_{\text{bigram } u} \text{count}_x(u) \times \text{count}_y(u).$$

Weighted Transducers



$T(x, y) =$ Sum of the weights of all accepting paths with input x and output y.

$$T(abb, baa) = .1 \times .2 \times .3 \times .1 + .5 \times .3 \times .6 \times .1$$

Rational Kernels over Strings

(Cortes et al., 2004)

- Definition: a kernel $K:\Sigma^*\times\Sigma^*\rightarrow\mathbb{R}$ is rational if $K=T$ for some weighted transducer T.

- Definition: let $T_1:\Sigma^*\times\Delta^*\rightarrow\mathbb{R}$ and $T_2:\Delta^*\times\Omega^*\rightarrow\mathbb{R}$ be two weighted transducers. Then, the composition of T_1 and T_2 is defined for all $x\in\Sigma^*, y\in\Omega^*$ by

$$(T_1\circ T_2)(x,y)=\sum_{z\in\Delta^*} T_1(x,z)\ T_2(z,y).$$

- Definition: the inverse of a transducer $T:\Sigma^*\times\Delta^*\rightarrow\mathbb{R}$ is the transducer $T^{-1}:\Delta^*\times\Sigma^*\rightarrow\mathbb{R}$ obtained from T by swapping input and output labels.

PDS Rational Kernels
General Construction

- **Theorem**: for any weighted transducer $T\colon \Sigma^* \times \Sigma^* \to \mathbb{R}$, the function $K = T \circ T^{-1}$ is a PDS rational kernel.

- **Proof**: by definition, for all $x, y \in \Sigma^*$,

$$K(x, y) = \sum_{z \in \Delta^*} T(x, z)\, T(y, z).$$

  - K is pointwise limit of $(K_n)_{n \geq 0}$ defined by

$$\forall x, y \in \Sigma^*, \;\; K_n(x, y) = \sum_{|z| \leq n} T(x, z)\, T(y, z).$$

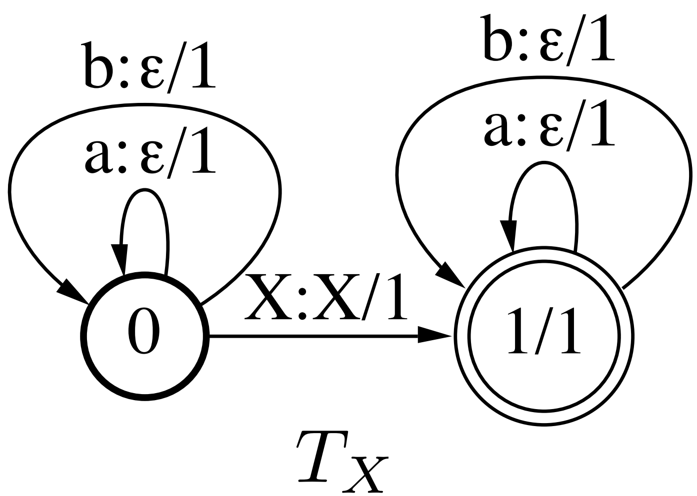
  - K_n is PDS since for any sample $(x_1, \ldots, x_m)$,

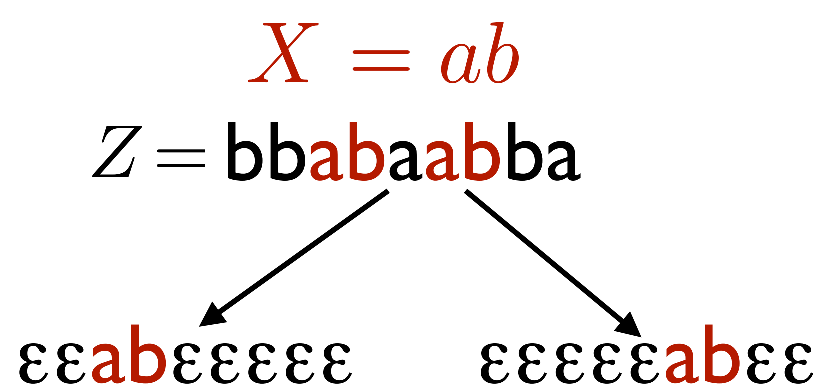
$$\mathbf{K}_n = \mathbf{A}\mathbf{A}^\top \text{ with } \mathbf{A} = (K_n(x_i, z_j))_{\substack{i \in [1, m] \\ j \in [1, N]}}.$$

PDS Sequence Kernels

- PDS sequences kernels in computational biology, text classification, other applications:
  - special instances of PDS rational kernels.
  - PDS rational kernels easy to define and modify.
  - single general algorithm for their computation: composition + shortest-distance computation.
  - no need for a specific 'dynamic-programming' algorithm and proof for each kernel instance.
  - general sub-family: based on counting transducers.

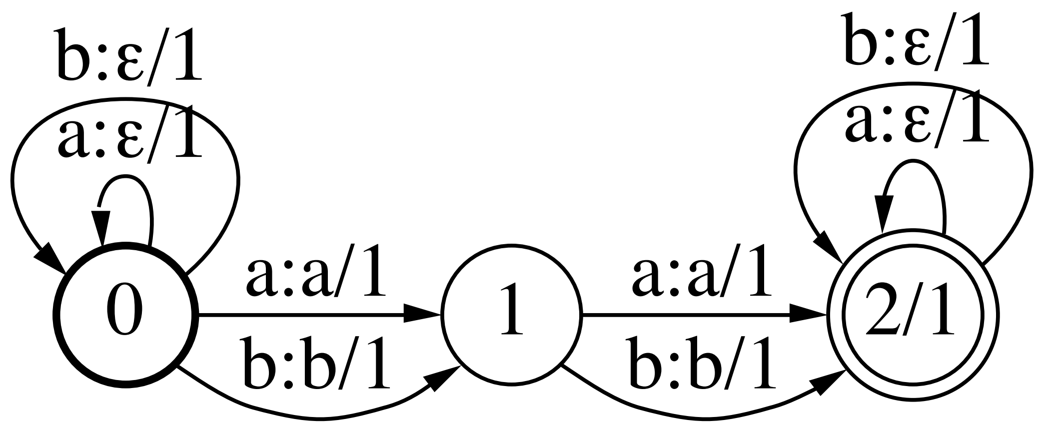
Counting Transducers





- X may be a string or an automaton representing a regular expression.
- Counts of Z in X: sum of the weights of accepting paths of $Z \circ T_X$.

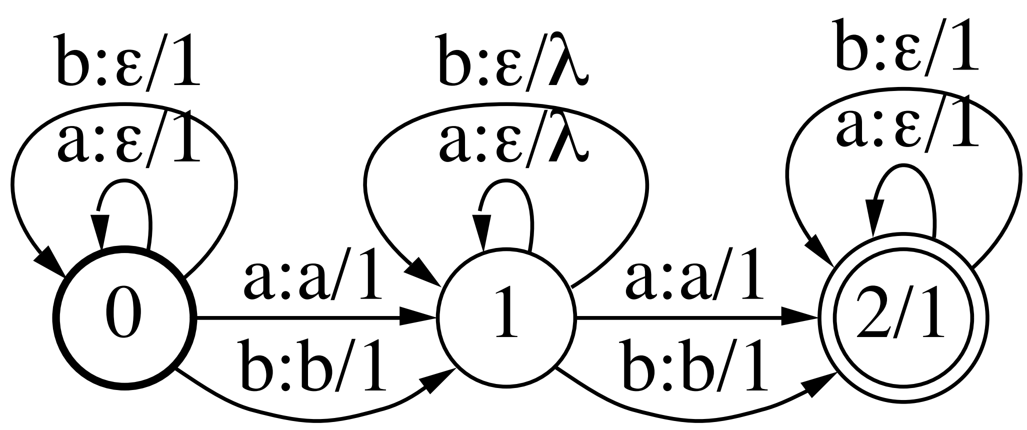
Transducer Counting Bigrams



T_{bigram}

Counts of Z given by $Z \circ T_{\text{bigram}} \circ ab$.

Transducer Counting Gappy Bigrams



$T_{\text{gappy bigram}}$

Counts of Z given by $Z \circ T_{\text{gappy bigram}} \circ ab$,
gap penalty $\lambda \in (0, 1)$.

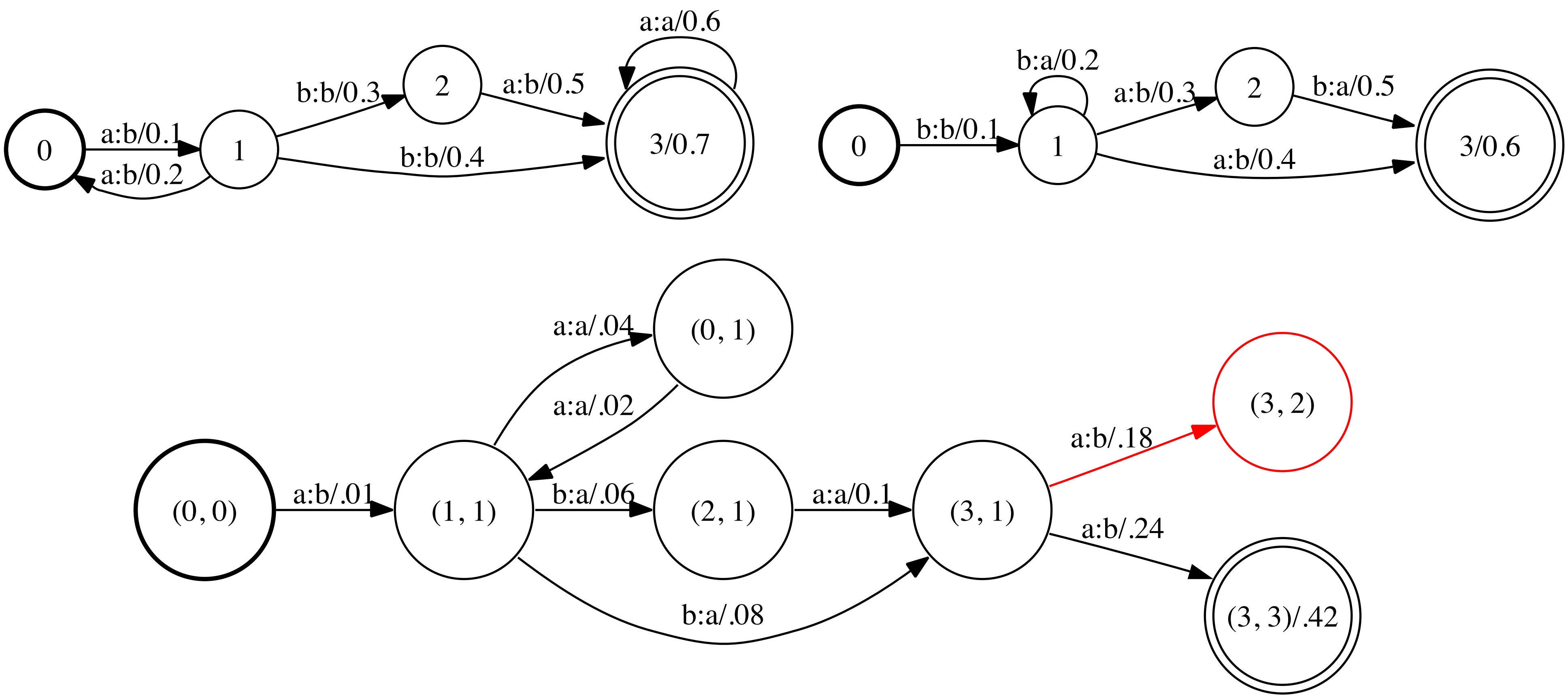
Composition

- Theorem: the composition of two weighted transducer is also a weighted transducer.
- Proof: constructive proof based on composition algorithm.
  - states identified with pairs.
  - ϵ-free case: transitions defined by

$$E = \biguplus_{\substack{(q_1, a, b, w_1, q_2) \in E_1 \\ (q_1', b, c, w_2, q_2') \in E_2}} \left\{ \Big((q_1, q_1'), a, c, w_1 \times w_2, (q_2, q_2') \Big) \right\}.$$

  - general case: use of intermediate ϵ-filter.

Composition Algorithm
ε-Free Case

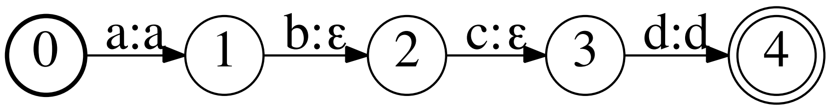


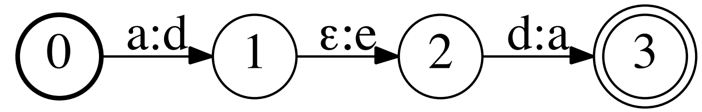
Complexity: $O(|T_1|\,|T_2|)$ in general, linear in some cases.

Redundant ε-Paths Problem

(MM, Pereira, and Riley, 1996; Pereira and Riley, 1997)

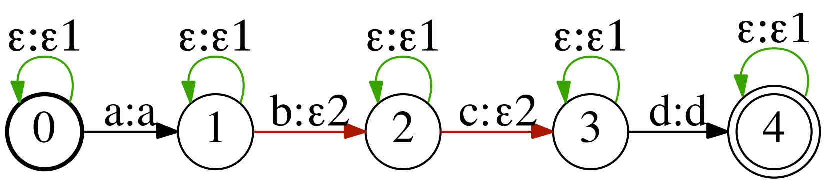
T_1

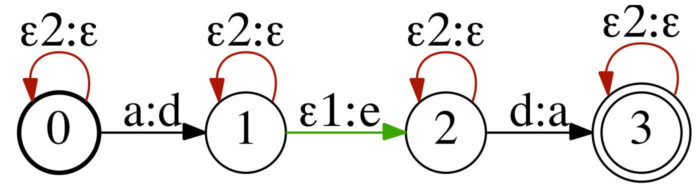




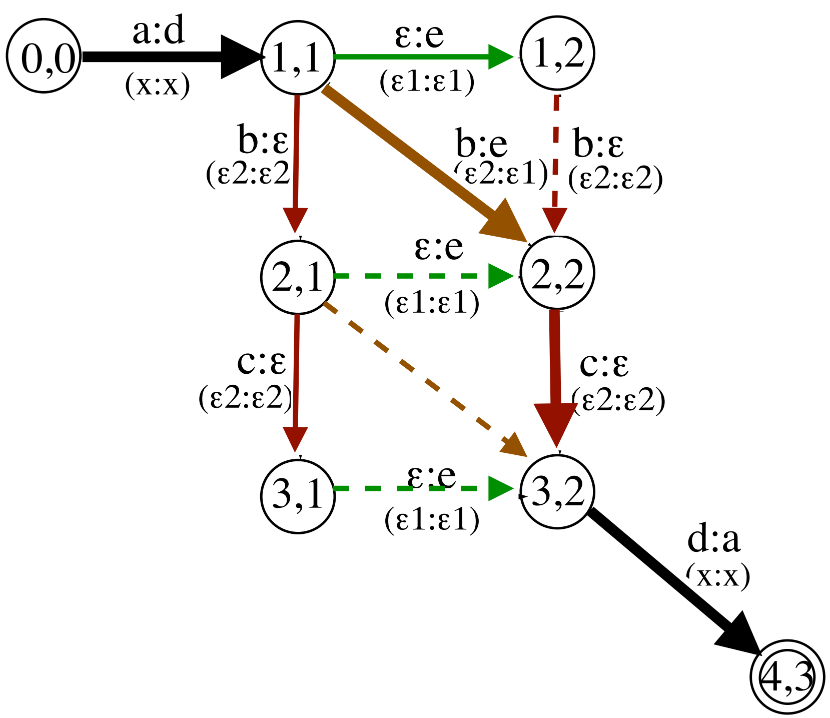
T_2

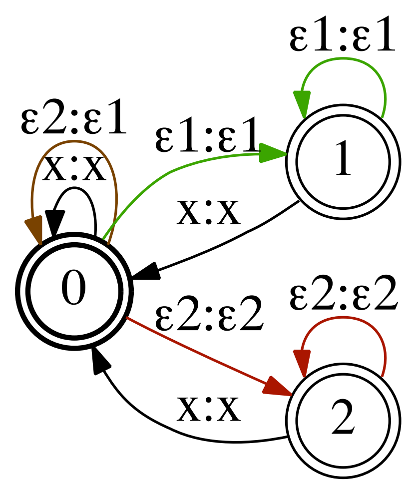
$\widetilde{T}_1$





$\widetilde{T}_2$





F

$$T = \widetilde{T}_1 \circ F \circ \widetilde{T}_2.$$

Kernels for Other Discrete Structures

- Similarly, PDS kernels can be defined on other discrete structures:
  - Images,
  - graphs,
  - parse trees,
  - automata,
  - weighted automata.

This Lecture

- Kernels
- Kernel-based algorithms
- Closure properties
- Sequence Kernels
- Negative kernels

Questions

- Gaussian kernels have the form $\exp(-d^2)$ where d is a metric.
  - for what other functions d does $\exp(-d^2)$ define a PDS kernel?
  - what other PDS kernels can we construct from a metric in a Hilbert space?

Negative Definite Kernels

(Schoenberg, 1938)

- Definition: A function $K\colon X \times X \to \mathbb{R}$ is said to be a negative definite symmetric (NDS) kernel if it is symmetric and if for all $\{x_1, \ldots, x_m\} \subseteq X$ and $\mathbf{c} \in \mathbb{R}^{m\times 1}$ with $\mathbf{1}^\top \mathbf{c} = 0$,

$$\mathbf{c}^\top \mathbf{K} \mathbf{c} \leq 0.$$

- Clearly, if K is PDS, then $-K$ is NDS, but the converse does not hold in general.

Examples

- The squared distance $||x-y||^2$ in a Hilbert space H defines an NDS kernel. If $\sum_{i=1}^m c_i = 0$,

$$\begin{aligned}
\sum_{i,j=1}^m c_i c_j ||\mathbf{x}_i - \mathbf{x}_j||^2 &= \sum_{i,j=1}^m c_i c_j (\mathbf{x}_i - \mathbf{x}_j) \cdot (\mathbf{x}_i - \mathbf{x}_j) \\
&= \sum_{i,j=1}^m c_i c_j (\|\mathbf{x}_i\|^2 + \|\mathbf{x}_j\|^2 - 2\mathbf{x}_i \cdot \mathbf{x}_j) \\
&= \sum_{i,j=1}^m c_i c_j (\|\mathbf{x}_i\|^2 + \|\mathbf{x}_j\|^2) - 2 \sum_{i=1}^m c_i \mathbf{x}_i \cdot \sum_{j=1}^m c_j \mathbf{x}_j \\
&\leq \sum_{i,j=1}^m c_i c_j (\|\mathbf{x}_i\|^2 + \|\mathbf{x}_j\|^2) \\
&= \sum_{j=1}^m c_j \Big(\sum_{i=1}^m c_i (\|\mathbf{x}_i\|^2 \Big) + \sum_{i=1}^m c_i \Big(\sum_{j=1}^m c_j \|\mathbf{x}_j\|^2 \Big) = 0.
\end{aligned}$$

NDS Kernels - Property

(Schoenberg, 1938)

- **Theorem**: Let $K\colon X \times X \to \mathbb{R}$ be an NDS kernel such that for all $x, y \in X$, $K(x, y) = 0$ iff $x = y$. Then, there exists a Hilbert space H and a mapping $\Phi\colon X \to H$ such that

$$\forall x, y \in X, \;\; K(x, y) = \|\Phi(x) - \Phi(y)\|^2.$$

Thus, under the hypothesis of the theorem, $\sqrt{K}$ defines a metric.

PDS and NDS Kernels

(Schoenberg, 1938)

- Theorem: let $K\colon X \times X \to \mathbb{R}$ be a symmetric kernel, then:
  - K is NDS iff $\exp(-tK)$ is a PDS kernel for all $t > 0$.
  - Let K' be defined for any x_0 by

$$K'(x, y) = K(x, x_0) + K(y, x_0) - K(x, y) - K(x_0, x_0)$$

for all $x, y \in X$. Then, K is NDS iff K' is PDS.

Example

- The kernel defined by $K(x, y) = \exp(-t||x - y||^2)$ is PDS for all $t > 0$ since $||x - y||^2$ is NDS.
- The kernel $\exp(-|x - y|^p)$ is not PDS for $p > 2$. Otherwise, for any $t > 0$, $\{x_1, \ldots, x_m\} \subseteq X$ and $\mathbf{c} \in \mathbb{R}^{m \times 1}$

$$\sum_{i,j=1}^{m} c_i c_j e^{-t|x_i - x_j|^p} = \sum_{i,j=1}^{m} c_i c_j e^{-|t^{1/p} x_i - t^{1/p} x_j|^p} \geq 0.$$

- This would imply that $|x - y|^p$ is NDS for $p > 2$, but that cannot be (see past homework assignments).

Conclusion

- PDS kernels:
  - rich mathematical theory and foundation.
  - general idea for extending many linear algorithms to non-linear prediction.
  - flexible method: any PDS kernel can be used.
  - widely used in modern algorithms and applications.
  - can we further learn a PDS kernel and a hypothesis based on that kernel from labeled data? (see tutorial: http://www.cs.nyu.edu/~mohri/icml2011-tutorial/).

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Appendix

Mercer's Condition

(Mercer, 1909)

- **Theorem**: Let $X \times X$ be a compact subset of $\mathbb{R}^N$ and let $K : X \times X \to \mathbb{R}$ be in $L_\infty(X \times X)$ and symmetric. Then, K admits a uniformly convergent expansion

$$K(x, y) = \sum_{n=0}^{\infty} a_n \phi_n(x) \phi_n(y), \text{ with } a_n > 0,$$

iff for any function c in $L_2(X)$,

$$\int\int_{X \times X} c(x)c(y)K(x, y)dxdy \geq 0.$$

SVMs with PDS Kernels

- Constrained optimization:

Hadamard product

$$\max_{\boldsymbol{\alpha}} 2\, \mathbf{1}^\top \boldsymbol{\alpha} - (\boldsymbol{\alpha} \circ \mathbf{y})^\top \mathbf{K} (\boldsymbol{\alpha} \circ \mathbf{y})$$

$$\text{subject to: } \mathbf{0} \leq \boldsymbol{\alpha} \leq \mathbf{C} \wedge \boldsymbol{\alpha}^\top \mathbf{y} = 0.$$

- Solution:

$$h = \operatorname{sgn}\Big(\sum_{i=1}^{m} \alpha_i y_i K(x_i, \cdot) + b \Big),$$

with $b = y_i - (\boldsymbol{\alpha} \circ \mathbf{y})^\top \mathbf{K} \mathbf{e}_i$ for any x_i with $0 < \alpha_i < C.$

Foundations of Machine Learning
Boosting

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Weak Learning

(Kearns and Valiant, 1994)

- Definition: concept class C is weakly PAC-learnable if there exists a (weak) learning algorithm L and $\gamma > 0$ such that:
  - for all $\delta > 0$, for all $c \in C$ and all distributions D,

$$\Pr_{S \sim D}\left[R(h_S) \leq \frac{1}{2} - \gamma\right] \geq 1 - \delta,$$

  - for samples S of size $m = poly(1/\delta)$ for a fixed polynomial.

Boosting Ideas

- Finding simple relatively accurate base classifiers often not hard $\longleftarrow$ weak learner.
- Main ideas:
  - use weak learner to create a strong learner.
  - combine base classifiers returned by weak learner (ensemble method).
- But, how should the base classifiers be combined?

AdaBoost

(Freund and Schapire, 1997)

$H \subseteq \{-1,+1\}^X$.

$\textsc{AdaBoost}(S=((x_1,y_1),\ldots,(x_m,y_m)))$

$\textbf{for } i \leftarrow 1 \textbf{ to } m \textbf{ do}$
$\quad D_1(i) \leftarrow \frac{1}{m}$
$\textbf{for } t \leftarrow 1 \textbf{ to } T \textbf{ do}$
$\quad h_t \leftarrow \text{base classifier in } H \text{ with small error } \epsilon_t = \Pr_{i \sim D_t}[h_t(x_i) \neq y_i]$
$\quad \alpha_t \leftarrow \frac{1}{2} \log \frac{1-\epsilon_t}{\epsilon_t}$
$\quad Z_t \leftarrow 2[\epsilon_t(1-\epsilon_t)]^{\frac{1}{2}} \quad \triangleright \text{ normalization factor}$
$\quad \textbf{for } i \leftarrow 1 \textbf{ to } m \textbf{ do}$
$\quad\quad D_{t+1}(i) \leftarrow \frac{D_t(i)\exp(-\alpha_t y_i h_t(x_i))}{Z_t}$
$\quad f_t \leftarrow \sum_{s=1}^{t} \alpha_s h_s$
$\textbf{return } h = \operatorname{sgn}(f_T)$

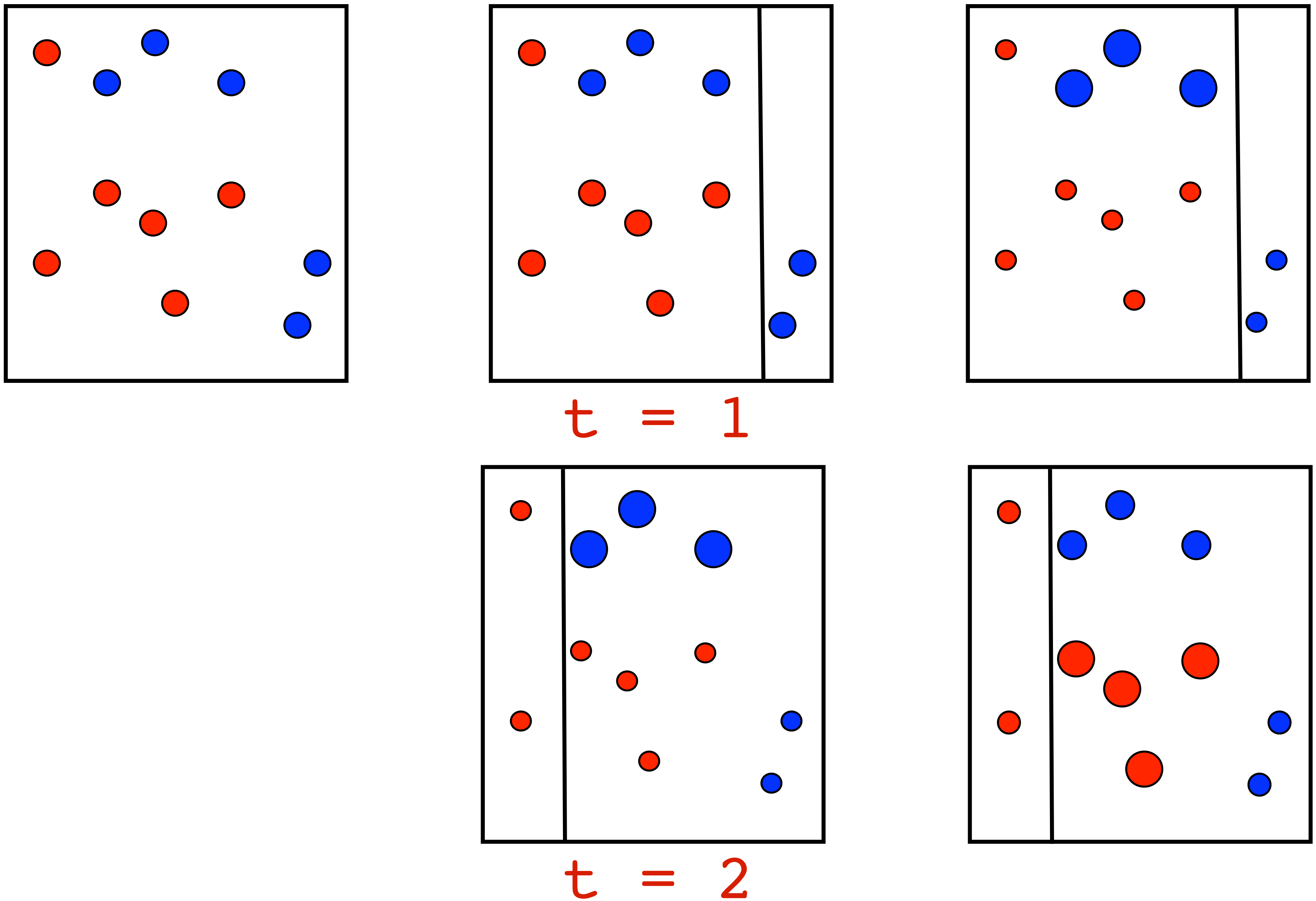
Notes

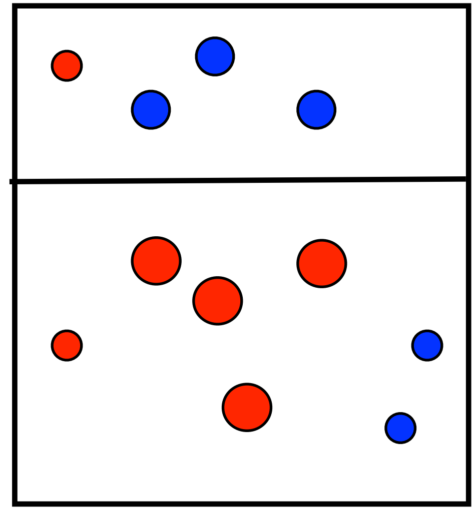
- Distributions D_t over training sample:
  - originally uniform.
  - at each round, the weight of a misclassified example is increased.
  - observation: $D_{t+1}(i) = \frac{e^{-y_i f_t(x_i)}}{m \prod_{s=1}^t Z_s}$, since

$$D_{t+1}(i) = \frac{D_t(i) e^{-\alpha_t y_i h_t(x_i)}}{Z_t} = \frac{D_{t-1}(i) e^{-\alpha_{t-1} y_i h_{t-1}(x_i)} e^{-\alpha_t y_i h_t(x_i)}}{Z_{t-1} Z_t} = \frac{1}{m} \frac{e^{-y_i \sum_{s=1}^t \alpha_s h_s(x_i)}}{\prod_{s=1}^t Z_s}.$$

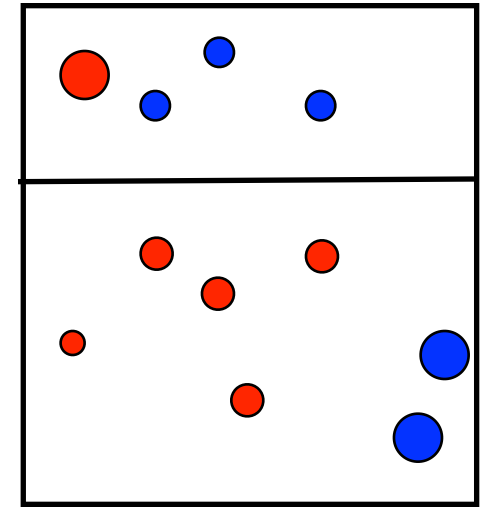
- Weight assigned to base classifier h_t: α_t directly depends on the accuracy of h_t at round t .

Illustration

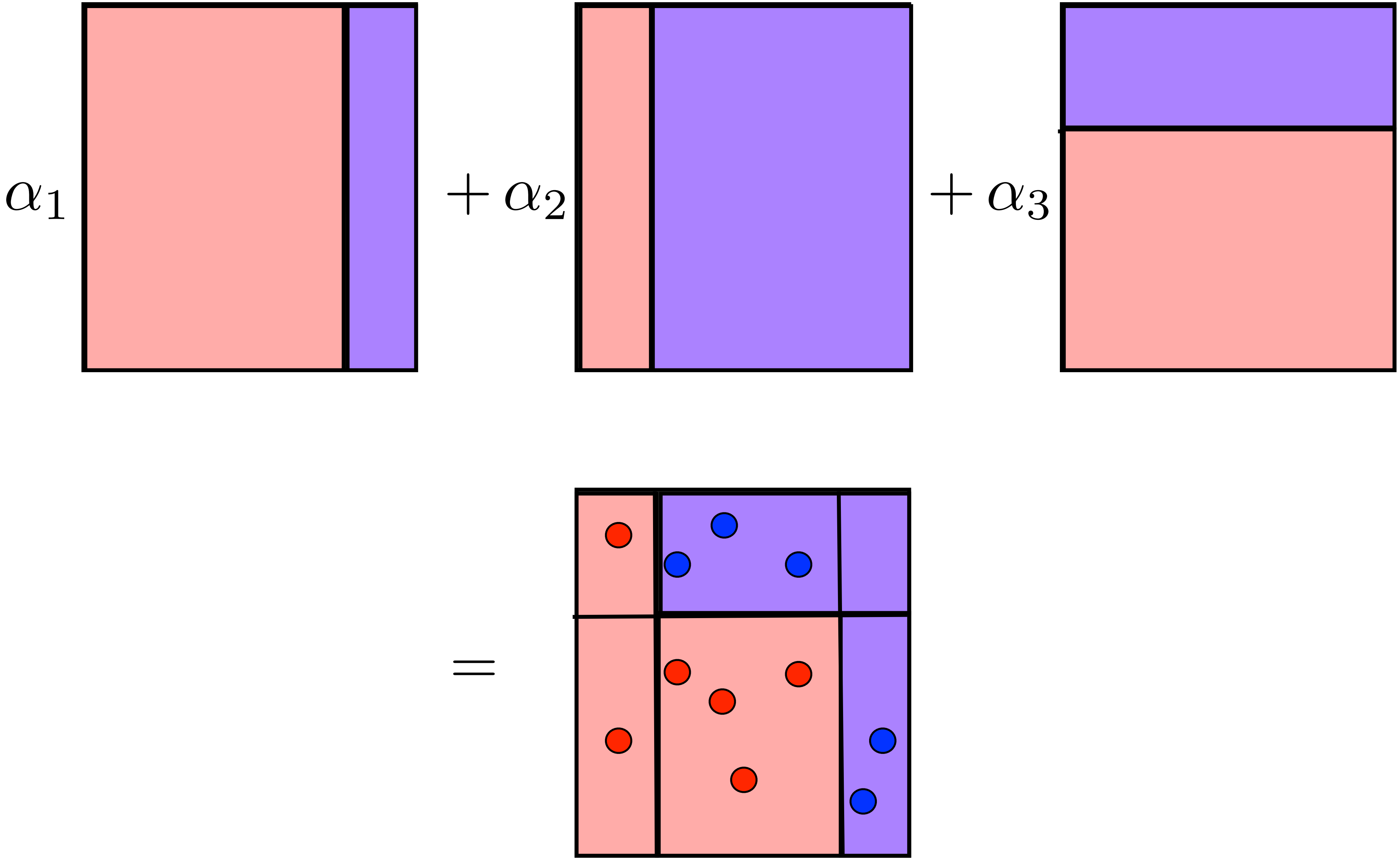




t = 3



. . .   . . .


α_1
$+\,\alpha_2$
$+\,\alpha_3$
$=$

Bound on Empirical Error

(Freund and Schapire, 1997)

- Theorem: The empirical error of the classifier output by AdaBoost verifies:

$$\widehat{R}(h) \leq \exp\left[-2\sum_{t=1}^{T}\left(\frac{1}{2}-\epsilon_t\right)^2\right].$$

  - If further for all $t \in [1, T]$, $\gamma \leq \left(\frac{1}{2} - \epsilon_t\right)$, then

$$\widehat{R}(h) \leq \exp(-2\gamma^2 T).$$

  - γ does not need to be known in advance: adaptive boosting.

- Proof: Since, as we saw, $D_{t+1}(i) = \frac{e^{-y_i f_t(x_i)}}{m \prod_{s=1}^{t} Z_s}$,

$$\widehat{R}(h) = \frac{1}{m} \sum_{i=1}^{m} 1_{y_i f(x_i) \leq 0} \leq \frac{1}{m} \sum_{i=1}^{m} \exp(-y_i f(x_i))$$

$$\leq \frac{1}{m} \sum_{i=1}^{m} \left[m \prod_{t=1}^{T} Z_t \right] D_{T+1}(i) = \prod_{t=1}^{T} Z_t.$$

- Now, since Z_t is a normalization factor,

$$\begin{aligned} Z_t &= \sum_{i=1}^{m} D_t(i) e^{-\alpha_t y_i h_t(x_i)} \\ &= \sum_{i: y_i h_t(x_i) \geq 0} D_t(i) e^{-\alpha_t} + \sum_{i: y_i h_t(x_i) < 0} D_t(i) e^{\alpha_t} \\ &= (1 - \epsilon_t) e^{-\alpha_t} + \epsilon_t e^{\alpha_t} \\ &= (1 - \epsilon_t) \sqrt{\frac{\epsilon_t}{1 - \epsilon_t}} + \epsilon_t \sqrt{\frac{1 - \epsilon_t}{\epsilon_t}} = 2\sqrt{\epsilon_t (1 - \epsilon_t)}. \end{aligned}$$

- Thus,

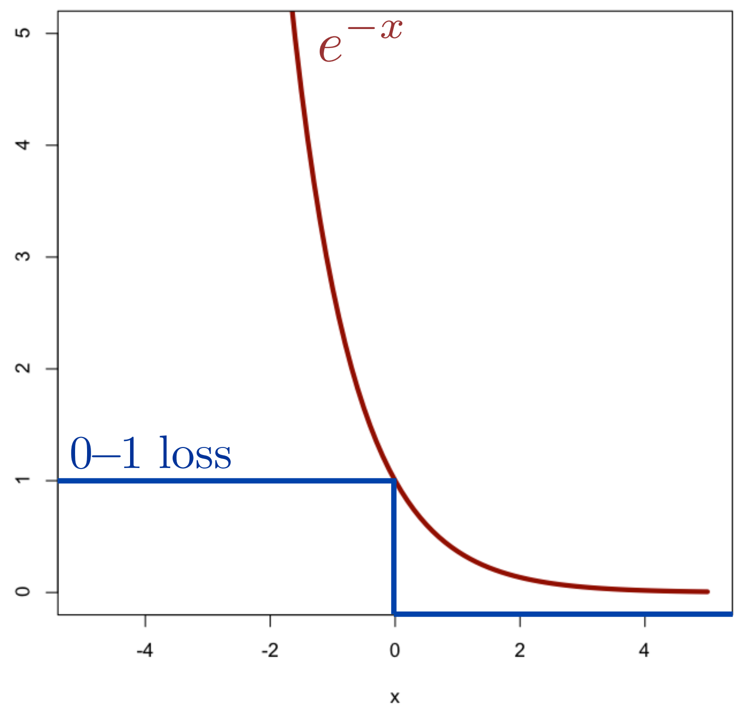
$$\prod_{t=1}^{T} Z_t = \prod_{t=1}^{T} 2\sqrt{\epsilon_t(1-\epsilon_t)} = \prod_{t=1}^{T} \sqrt{1 - 4\Big(\frac{1}{2} - \epsilon_t\Big)^2}$$
$$\leq \prod_{t=1}^{T} \exp\Big[-2\Big(\frac{1}{2} - \epsilon_t\Big)^2\Big] = \exp\Big[-2\sum_{t=1}^{T}\Big(\frac{1}{2} - \epsilon_t\Big)^2\Big].$$

- Notes:
  - α_t minimizer of $\alpha \mapsto (1-\epsilon_t)e^{-\alpha} + \epsilon_t e^{\alpha}$.
  - since $(1-\epsilon_t)e^{-\alpha_t} = \epsilon_t e^{\alpha_t}$, at each round, AdaBoost assigns the same probability mass to correctly classified and misclassified instances.
  - for base classifiers $x \mapsto [-1, +1]$, α_t can be similarly chosen to minimize Z_t.

AdaBoost = Coordinate Descent

- Objective Function: convex and differentiable.

$$F(\bar{\boldsymbol{\alpha}}) = \frac{1}{m}\sum_{i=1}^{m} e^{-y_i f(x_i)} = \frac{1}{m}\sum_{i=1}^{m} e^{-y_i \sum_{j=1}^{N} \bar{\alpha}_j h_j(x_i)}.$$



- Direction: unit vector $\mathbf{e}_k$ with best directional derivative:

$$F'(\bar{\boldsymbol{\alpha}}_{t-1}, \mathbf{e}_k) = \lim_{\eta \to 0} \frac{F(\bar{\boldsymbol{\alpha}}_{t-1} + \eta \mathbf{e}_k) - F(\bar{\boldsymbol{\alpha}}_{t-1})}{\eta}.$$

- Since $F(\bar{\boldsymbol{\alpha}}_{t-1} + \eta \mathbf{e}_k) = \frac{1}{m} \sum_{i=1}^{m} e^{-y_i \sum_{j=1}^{N} \bar{\alpha}_{t-1,j} h_j(x_i) - \eta y_i h_k(x_i)}$,

$$\begin{aligned}
F'(\bar{\boldsymbol{\alpha}}_{t-1}, \mathbf{e}_k) &= -\frac{1}{m} \sum_{i=1}^{m} y_i h_k(x_i) e^{-y_i \sum_{j=1}^{N} \bar{\alpha}_{t-1,j} h_j(x_i)} \\
&= -\frac{1}{m} \sum_{i=1}^{m} y_i h_k(x_i) \bar{D}_t(i) \bar{Z}_t \\
&= -\left[\sum_{i=1}^{m} \bar{D}_t(i) 1_{y_i h_k(x_i) = +1} - \sum_{i=1}^{m} \bar{D}_t(i) 1_{y_i h_k(x_i) = -1} \right] \frac{\bar{Z}_t}{m} \\
&= -\left[(1 - \bar{\epsilon}_{t,k}) - \bar{\epsilon}_{t,k} \right] \frac{\bar{Z}_t}{m} = \left[\boxed{2\bar{\epsilon}_{t,k} - 1} \right] \frac{\bar{Z}_t}{m}.
\end{aligned}$$

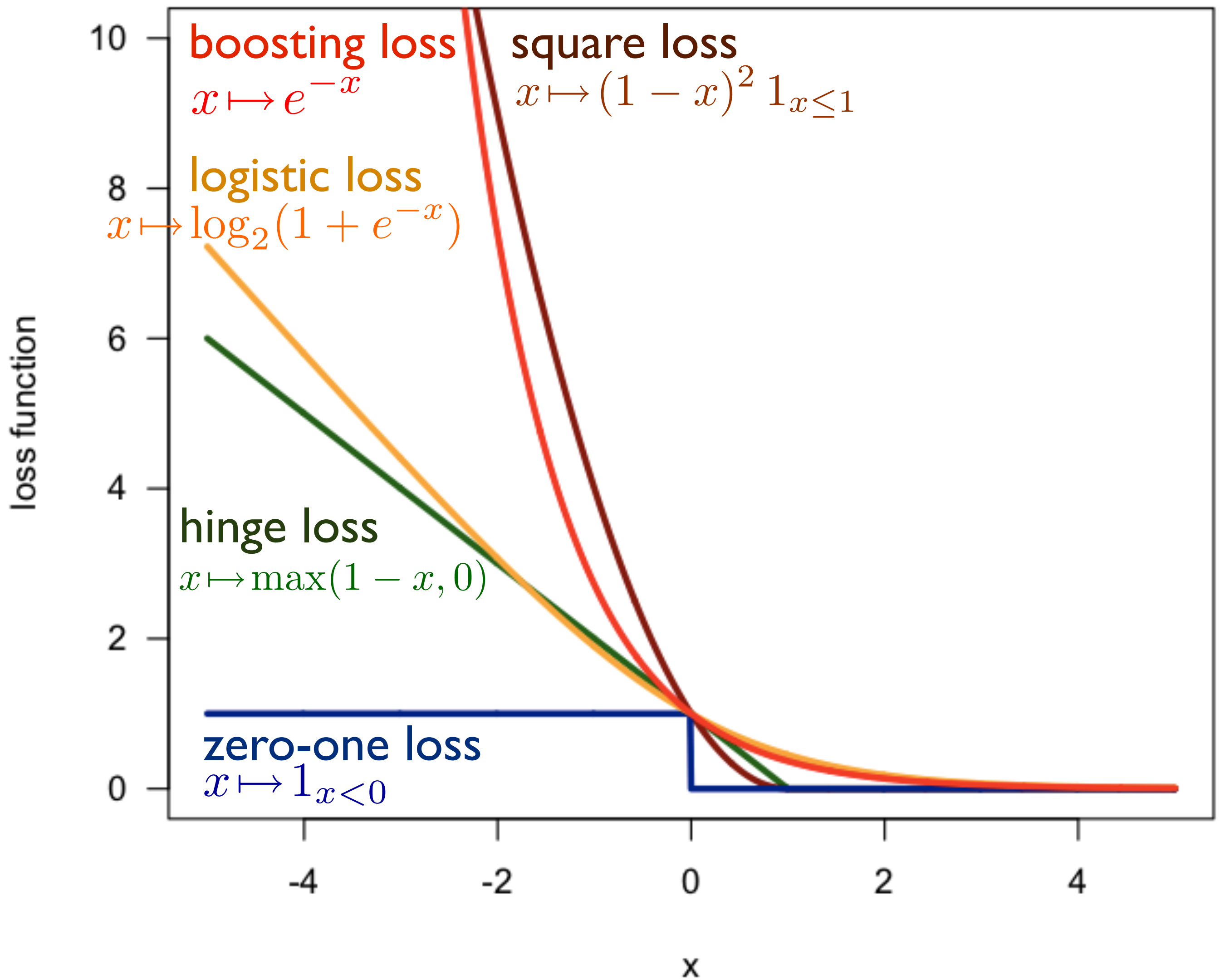
Thus, direction corresponding to base classifier with smallest error.

- **Step size**: η chosen to minimize $F(\bar{\boldsymbol{\alpha}}_{t-1} + \eta\, \mathbf{e}_k)$;

$$\begin{aligned}
\frac{dF(\bar{\boldsymbol{\alpha}}_{t-1} + \eta \mathbf{e}_k)}{d\eta} = 0 &\Leftrightarrow -\sum_{i=1}^{m} y_i h_k(x_i) e^{-y_i \sum_{j=1}^{N} \bar{\alpha}_{t-1,j} h_j(x_i)} e^{-\eta y_i h_k(x_i)} = 0 \\
&\Leftrightarrow -\sum_{i=1}^{m} y_i h_k(x_i) \bar{D}_t(i) \bar{Z}_t e^{-\eta y_i h_k(x_i)} = 0 \\
&\Leftrightarrow -\sum_{i=1}^{m} y_i h_k(x_i) \bar{D}_t(i) e^{-\eta y_i h_k(x_i)} = 0 \\
&\Leftrightarrow -\left[(1 - \bar{\epsilon}_{t,k}) e^{-\eta} - \bar{\epsilon}_{t,k} e^{\eta}\right] = 0 \\
&\Leftrightarrow \boxed{\eta = \frac{1}{2} \log \frac{1 - \bar{\epsilon}_{t,k}}{\bar{\epsilon}_{t,k}}.}
\end{aligned}$$

Thus, step size matches base classifier weight of AdaBoost.

Alternative Loss Functions



Standard Use in Practice

- Base learners: decision trees, quite often just decision stumps (trees of depth one).
- Boosting stumps:
  - data in $\mathbb{R}^N$, e.g., $N = 2$, $(\text{height}(x), \text{weight}(x))$.
  - associate a stump to each component.
  - pre-sort each component: $O(Nm \log m)$.
  - at each round, find best component and threshold.
  - total complexity: $O((m \log m)N + mNT)$.
  - stumps not weak learners: think XOR example!

Overfitting?

- Assume that $\mathrm{VCdim}(H) = d$ and for a fixed T, define

$$\mathcal{F}_T = \left\{ \mathrm{sgn}\left(\sum_{t=1}^{T} \alpha_t h_t - b \right) : \alpha_t, b \in \mathbb{R}, h_t \in H \right\}.$$

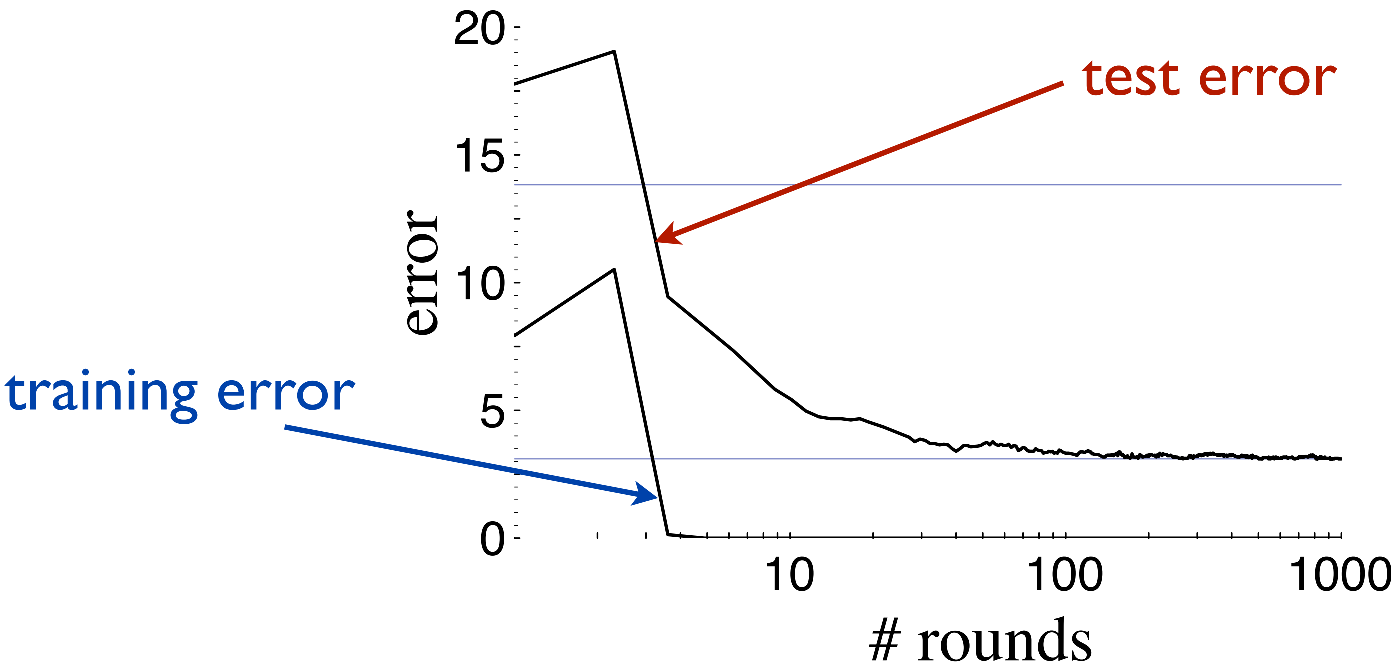
- $\mathcal{F}_T$ can form a very rich family of classifiers. It can be shown (Freund and Schapire, 1997) that:

$$\mathrm{VCdim}(\mathcal{F}_T) \leq 2(d+1)(T+1)\log_2((T+1)e).$$

- This suggests that AdaBoost could overfit for large values of T, and that is in fact observed in some cases, but in various others it is not!

Empirical Observations

- Several empirical observations (not all): AdaBoost does not seem to overfit, furthermore:



C4.5 decision trees (Schapire et al., 1998).

Rademacher Complexity of Convex Hulls

- **Theorem**: Let H be a set of functions mapping from X to $\mathbb{R}$. Let the convex hull of H be defined as

$$\text{conv}(H) = \{\sum_{k=1}^{p} \mu_k h_k : p \geq 1, \mu_k \geq 0, \sum_{k=1}^{p} \mu_k \leq 1, h_k \in H\}.$$

  Then, for any sample S, $\widehat{\mathfrak{R}}_S(\text{conv}(H)) = \widehat{\mathfrak{R}}_S(H)$.

- **Proof**: $\widehat{\mathfrak{R}}_S(\text{conv}(H)) = \dfrac{1}{m} \underset{\sigma}{\text{E}} \left[\sup_{h_k \in H, \boldsymbol{\mu} \geq 0, \|\boldsymbol{\mu}\|_1 \leq 1} \sum_{i=1}^{m} \sigma_i \sum_{k=1}^{p} \mu_k h_k(x_i) \right]$

$$= \frac{1}{m} \underset{\sigma}{\text{E}} \left[\sup_{h_k \in H} \sup_{\boldsymbol{\mu} \geq 0, \|\boldsymbol{\mu}\|_1 \leq 1} \sum_{k=1}^{p} \mu_k \Big(\sum_{i=1}^{m} \sigma_i h_k(x_i) \Big) \right]$$

$$= \frac{1}{m} \underset{\sigma}{\text{E}} \left[\sup_{h_k \in H} \max_{k \in [1,p]} \Big(\sum_{i=1}^{m} \sigma_i h_k(x_i) \Big) \right]$$

$$= \frac{1}{m} \underset{\sigma}{\text{E}} \left[\sup_{h \in H} \sum_{i=1}^{m} \sigma_i h(x_i) \right] = \widehat{\mathfrak{R}}_S(H).$$

Margin Bound - Ensemble Methods

(Koltchinskii and Panchenko, 2002)

- Corollary: Let H be a set of real-valued functions. Fix $\rho > 0$. For any $\delta > 0$, with probability at least $1-\delta$, the following holds for all $h \in \operatorname{conv}(H)$:

$$R(h) \leq \widehat{R}_\rho(h) + \frac{2}{\rho}\mathfrak{R}_m(H) + \sqrt{\frac{\log \frac{1}{\delta}}{2m}}$$

$$R(h) \leq \widehat{R}_\rho(h) + \frac{2}{\rho}\widehat{\mathfrak{R}}_S(H) + 3\sqrt{\frac{\log \frac{2}{\delta}}{2m}}.$$

- Proof: Direct consequence of margin bound of Lecture 4 and $\widehat{\mathfrak{R}}_S(\operatorname{conv}(H)) = \widehat{\mathfrak{R}}_S(H)$.

Margin Bound - Ensemble Methods

(Koltchinskii and Panchenko, 2002); see also (Schapire et al., 1998)

- **Corollary**: Let H be a family of functions taking values in $\{-1, +1\}$ with VC dimension d. Fix $\rho > 0$. For any $\delta > 0$, with probability at least $1 - \delta$, the following holds for all $h \in \mathrm{conv}(H)$:

$$R(h) \leq \widehat{R}_\rho(h) + \frac{2}{\rho}\sqrt{\frac{2d \log \frac{em}{d}}{m}} + \sqrt{\frac{\log \frac{1}{\delta}}{2m}}.$$

- **Proof**: Follows directly previous corollary and VC dimension bound on Rademacher complexity (see lecture 3).

Notes

- All of these bounds can be generalized to hold uniformly for all $\rho \in (0, 1)$, at the cost of an additional term $\sqrt{\frac{\log \log_2 \frac{2}{\rho}}{m}}$ and other minor constant factor changes (Koltchinskii and Panchenko, 2002).
- For AdaBoost, the bound applies to the functions
$$x \mapsto \frac{f(x)}{\|\boldsymbol{\alpha}\|_1} = \frac{\sum_{t=1}^T \alpha_t h_t(x)}{\|\boldsymbol{\alpha}\|_1} \in \operatorname{conv}(H).$$
- Note that T does not appear in the bound.

Margin Distribution

- **Theorem**: For any $\rho > 0$, the following holds:

$$\widehat{\Pr}\left[\frac{yf(x)}{\|\boldsymbol{\alpha}\|_1} \leq \rho\right] \leq 2^T \prod_{t=1}^{T} \sqrt{\epsilon_t^{1-\rho}(1-\epsilon_t)^{1+\rho}}.$$

- **Proof**: Using the identity $D_{t+1}(i) = \frac{e^{-y_i f(x_i)}}{m \prod_{t=1}^T Z_t}$,

$$\begin{aligned}
\frac{1}{m}\sum_{i=1}^{m} 1_{y_i f(x_i) - \|\boldsymbol{\alpha}\|_1 \rho \leq 0} &\leq \frac{1}{m}\sum_{i=1}^{m} \exp(-y_i f(x_i) + \|\boldsymbol{\alpha}\|_1 \rho) \\
&= \frac{1}{m}\sum_{i=1}^{m} e^{\|\boldsymbol{\alpha}\|_1 \rho}\left[m \prod_{t=1}^{T} Z_t\right] D_{T+1}(i) \\
&= e^{\|\boldsymbol{\alpha}\|_1 \rho} \prod_{t=1}^{T} Z_t = 2^T \prod_{t=1}^{T} \left[\sqrt{\tfrac{1-\epsilon_t}{\epsilon_t}}\right]^{\rho} \sqrt{\epsilon_t(1-\epsilon_t)}.
\end{aligned}$$

Notes

- If for all $t \in [1, T]$, $\gamma \leq (\frac{1}{2} - \epsilon_t)$, then the upper bound can be bounded by

$$\widehat{\Pr}\left[\frac{yf(x)}{\|\boldsymbol{\alpha}\|_1} \leq \rho\right] \leq \left[(1-2\gamma)^{1-\rho}(1+2\gamma)^{1+\rho}\right]^{T/2}.$$

  For $\rho < \gamma$, $(1-2\gamma)^{1-\rho}(1+2\gamma)^{1+\rho} < 1$ and the bound decreases exponentially in T.

- For the bound to be convergent: $\rho \gg O(1/\sqrt{m})$, thus $\gamma \gg O(1/\sqrt{m})$ is roughly the condition on the edge value.

L1-Geometric Margin

- Definition: the L_1-margin $\rho_f(x)$ of a linear function $f = \sum_{t=1}^{T} \alpha_t h_t$ with $\boldsymbol{\alpha} \neq 0$ at a point $x \in \mathcal{X}$ is defined by

$$\rho_f(x) = \frac{|f(x)|}{\|\boldsymbol{\alpha}\|_1} = \frac{|\sum_{t=1}^{T} \alpha_t h_t(x)|}{\|\boldsymbol{\alpha}\|_1} = \frac{\big|\boldsymbol{\alpha} \cdot \mathbf{h}(x)\big|}{\|\boldsymbol{\alpha}\|_1}.$$

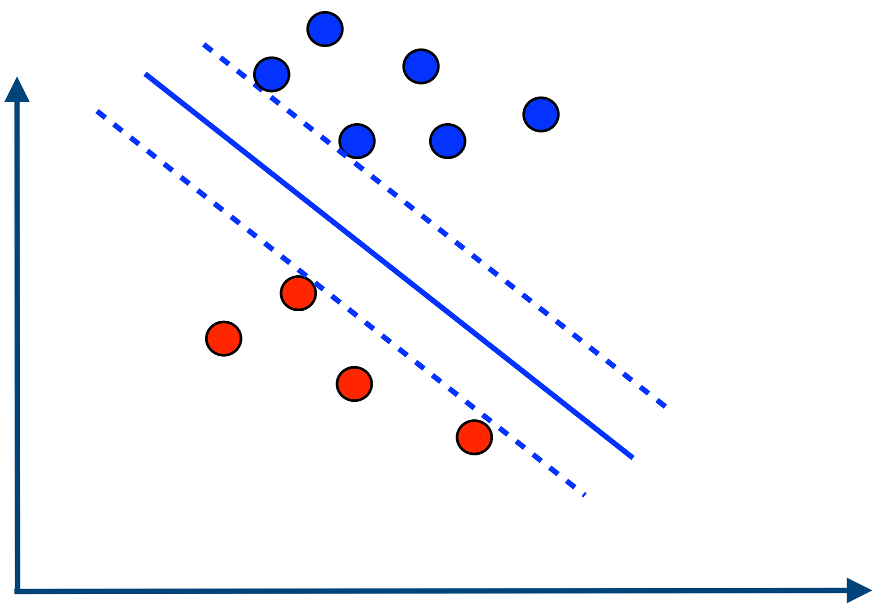
  - the L_1-margin of f over a sample $S = (x_1, \ldots, x_m)$ is its minimum margin at points in that sample:

$$\rho_f = \min_{i \in [1,m]} \rho_f(x_i) = \min_{i \in [1,m]} \frac{\big|\boldsymbol{\alpha} \cdot \mathbf{h}(x_i)\big|}{\|\boldsymbol{\alpha}\|_1}.$$

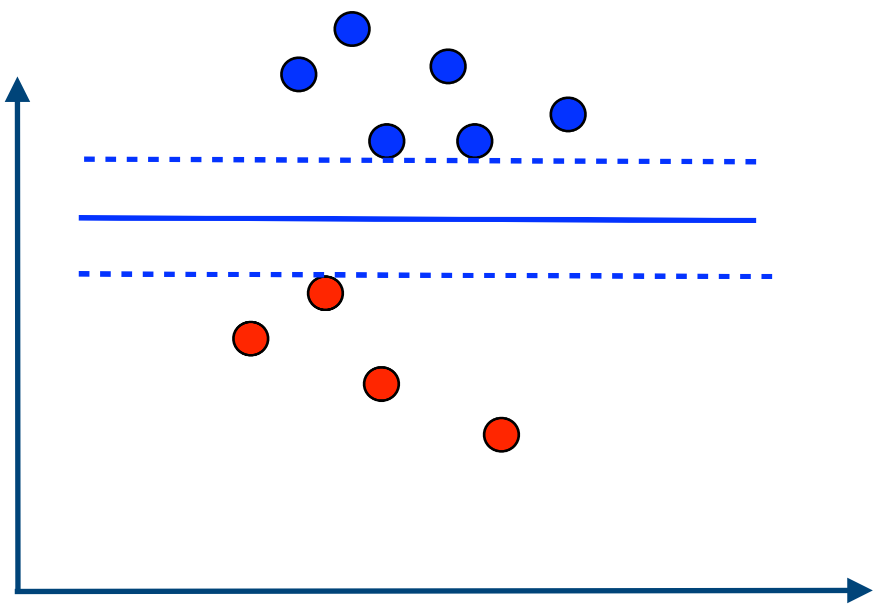
SVM vs AdaBoost

	SVM	AdaBoost
features or base hypotheses	$\mathbf{\Phi}(x) = \begin{bmatrix} \Phi_1(x) \\ \vdots \\ \Phi_N(x) \end{bmatrix}$	$\mathbf{h}(x) = \begin{bmatrix} h_1(x) \\ \vdots \\ h_N(x) \end{bmatrix}$
predictor	$x \mapsto \mathbf{w} \cdot \mathbf{\Phi}(x)$	$x \mapsto \boldsymbol{\alpha} \cdot \mathbf{h}(x)$
geom. margin	$\frac{\lvert \mathbf{w} \cdot \mathbf{\Phi}(x) \rvert}{\lVert \mathbf{w} \rVert_2} = d_2(\mathbf{\Phi}(x), \text{hyperpl.})$	$\frac{\lvert \boldsymbol{\alpha} \cdot \mathbf{h}(x) \rvert}{\lVert \boldsymbol{\alpha} \rVert_1} = d_\infty(\mathbf{h}(x), \text{hyperpl.})$
conf. margin	$y(\mathbf{w} \cdot \mathbf{\Phi}(x))$	$y(\boldsymbol{\alpha} \cdot \mathbf{h}(x))$
regularization	$\lVert \mathbf{w} \rVert_2$	$\lVert \boldsymbol{\alpha} \rVert_1$ (L1-AB)

Maximum-Margin Solutions



Norm $\|\cdot\|_2$.



Norm $\|\cdot\|_\infty$.

But, Does AdaBoost Maximize the Margin?

- No: AdaBoost may converge to a margin that is significantly below the maximum margin (Rudin et al., 2004) (e.g., 1/3 instead of 3/8)!
- Lower bound: AdaBoost can achieve asymptotically a margin that is at least $\frac{\rho_{\max}}{2}$ if the data is separable and some conditions on the base learners hold (Rätsch and Warmuth, 2002).
- Several boosting-type margin-maximization algorithms: but, performance in practice not clear or not reported.

AdaBoost's Weak Learning Condition

- Definition: the edge of a base classifier h_t for a distribution D over the training sample is

$$\gamma(t) = \frac{1}{2} - \epsilon_t = \frac{1}{2} \sum_{i=1}^{m} y_i h_t(x_i) D(i).$$

- Condition: there exists $\gamma > 0$ for any distribution D over the training sample and any base classifier

$$\gamma(t) \geq \gamma.$$

Zero-Sum Games

- Definition:
  - payoff matrix $\mathbf{M} = (\mathbf{M}_{ij}) \in \mathbb{R}^{m \times n}$.
  - m possible actions (pure strategy) for row player.
  - n possible actions for column player.
  - $\mathbf{M}_{ij}$ payoff for row player ($=$ loss for column player) when row plays i, column plays j.
- Example:

	rock	paper	scissors
rock	0	-1	1
paper	1	0	-1
scissors	-1	1	0

Mixed Strategies

(von Neumann, 1928)

- Definition: player row selects a distribution $\mathbf{p}$ over the rows, player column a distribution $\mathbf{q}$ over columns. The expected payoff for row is

$$\mathop{\mathrm{E}}_{\substack{i \sim p \\ j \sim q}}[\mathbf{M}_{ij}] = \sum_{i=1}^{m} \sum_{j=1}^{n} p_i \mathbf{M}_{ij} q_j = \mathbf{p}^\top \mathbf{M} \mathbf{q}.$$

- von Neumann's minimax theorem:

$$\max_{\mathbf{p}} \min_{\mathbf{q}} \mathbf{p}^\top \mathbf{M} \mathbf{q} = \min_{\mathbf{q}} \max_{\mathbf{p}} \mathbf{p}^\top \mathbf{M} \mathbf{q}.$$

  - equivalent form:

$$\max_{\mathbf{p}} \min_{j \in [1,n]} \mathbf{p}^\top \mathbf{M} \mathbf{e}_j = \min_{\mathbf{q}} \max_{i \in [1,m]} \mathbf{e}_i^\top \mathbf{M} \mathbf{q}.$$

John von Neumann (1903 - 1957)

AdaBoost and Game Theory

- Game:
  - Player A: selects point x_i, $i \in [1, m]$.
  - Player B: selects base hypothesis h_t, $t \in [1, T]$.
  - Payoff matrix $\mathbf{M} \in \{-1, +1\}^{m \times T}$: $\mathbf{M}_{it} = y_i h_t(x_i)$.
- von Neumann's theorem: assume finite H.

$$2\gamma^* = \min_D \max_{h \in H} \sum_{i=1}^m D(i) y_i h(x_i) = \max_{\boldsymbol{\alpha}} \min_{i \in [1,m]} y_i \sum_{t=1}^T \frac{\alpha_t h_t(x_i)}{\|\boldsymbol{\alpha}\|_1} = \rho^*.$$

Consequences

- Weak learning condition $\Longrightarrow$ non-zero margin.
  - thus, possible to search for non-zero margin.
  - AdaBoost $=$ (suboptimal) search for corresponding α; achieves at least half of the maximum margin.
- Weak learning $=$ strong condition:
  - the condition implies linear separability with margin $2\gamma^* > 0$.

Linear Programming Problem

- Maximizing the margin:

$$\rho = \max_{\boldsymbol{\alpha}} \min_{i \in [1,m]} y_i \frac{(\boldsymbol{\alpha} \cdot \mathbf{x}_i)}{||\alpha||_1}.$$

- This is equivalent to the following convex optimization LP problem:

$$\max_{\boldsymbol{\alpha}} \rho$$

$$\text{subject to : } y_i(\boldsymbol{\alpha} \cdot \mathbf{x}_i) \geq \rho$$

$$\|\boldsymbol{\alpha}\|_1 = 1.$$

- Note that:

$$\frac{|\boldsymbol{\alpha} \cdot \mathbf{x}|}{\|\boldsymbol{\alpha}\|_1} = \|\mathbf{x} - H\|_\infty, \text{ with } H = \{\mathbf{x} \colon \boldsymbol{\alpha} \cdot \mathbf{x} = 0\}.$$

Advantages of AdaBoost

- Simple: straightforward implementation.
- Efficient: complexity $O(mNT)$ for stumps:
  - when N and T are not too large, the algorithm is quite fast.
- Theoretical guarantees: but still many questions.
  - AdaBoost not designed to maximize margin.
  - regularized versions of AdaBoost.

Outliers

- AdaBoost assigns larger weights to harder examples.
- Application:
  - Detecting mislabeled examples.
  - Dealing with noisy data: regularization based on the average weight assigned to a point (soft margin idea for boosting) (Meir and Rätsch, 2003).

Weaker Aspects

- Parameters:
  - need to determine T, the number of rounds of boosting: stopping criterion.
  - need to determine base learners: risk of overfitting or low margins.
- Noise: severely damages the accuracy of Adaboost (Dietterich, 2000).

Other Boosting Algorithms

- arc-gv (Breiman, 1996): designed to maximize the margin, but outperformed by AdaBoost in experiments (Reyzin and Schapire, 2006).
- L1-regularized AdaBoost (Raetsch et al., 2001): outperfoms AdaBoost in experiments (Cortes et al., 2014).
- DeepBoost (Cortes et al., 2014): more favorable learning guarantees, outperforms both AdaBoost and L1-regularized AdaBoost in experiments.

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Foundations of Machine Learning

Maximum Entropy Models, Logistic Regression

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Motivation

- Probabilistic models:
  - density estimation.
  - classification.

This Lecture

- Notions of information theory.
- Introduction to density estimation.
- Maxent models.
- Conditional Maxent models.

Entropy

(Shannon, 1948)

- Definition: the entropy of a discrete random variable X with probability mass distribution $\mathsf{p}(x) = \Pr[X = x]$ is

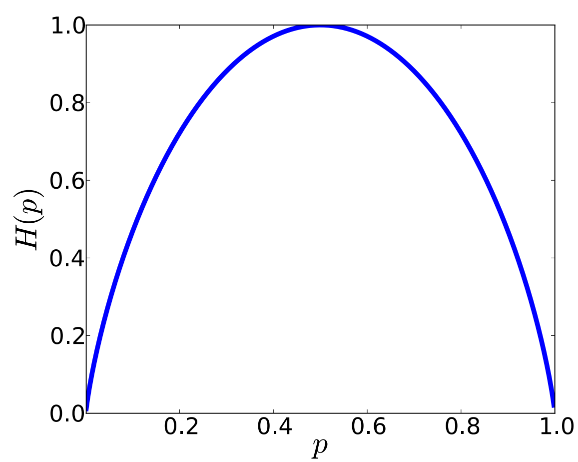
$$H(X) = -\mathrm{E}[\log \mathsf{p}(X)] = -\sum_{x \in X} \mathsf{p}(x) \log \mathsf{p}(x).$$

- Properties:
  - $H(X) \geq 0$.
  - measure of uncertainty of X.
  - maximal for uniform distribution. For a finite support, by Jensen's inequality:

$$H(X) = \mathrm{E}\left[\log \frac{1}{\mathsf{p}(X)}\right] \leq \log \mathrm{E}\left[\frac{1}{\mathsf{p}(X)}\right] = \log N.$$

Entropy

- Base of logarithm: not critical; for base 2, $-\log_2(\mathsf{p}(x))$ is the number of bits needed to represent $\mathsf{p}(x)$.
- Definition and notation: the entropy of a distribution p is defined by the same quantity and denoted by $H(\mathsf{p})$.
- Special case of Rényi entropy (Rényi, 1961).
- Binary entropy: $H(\mathsf{p}) = -\mathsf{p}\log\mathsf{p} - (1-\mathsf{p})\log(1-\mathsf{p})$.



Relative Entropy

(Shannon, 1948; Kullback and Leibler, 1951)

- Definition: the relative entropy (or Kullback-Leibler divergence) between two distributions p and q (discrete case) is

$$D(\mathsf{p} \parallel \mathsf{q}) = \mathrm{E}_{\mathsf{p}}\left[\log \frac{\mathsf{p}(X)}{\mathsf{q}(X)}\right] = \sum_{x \in \mathcal{X}} \mathsf{p}(x) \log \frac{\mathsf{p}(x)}{\mathsf{q}(x)},$$

with $0 \log \frac{0}{\mathsf{q}} = 0$ and $\mathsf{p} \log \frac{\mathsf{p}}{0} = +\infty.$

- Properties:
  - asymmetric: in general, $D(\mathsf{p} \parallel \mathsf{q}) \neq D(\mathsf{q} \parallel \mathsf{p})$ for $\mathsf{p} \neq \mathsf{q}$.
  - non-negative: $D(\mathsf{p} \parallel \mathsf{q}) \geq 0$ for all p and q.
  - definite: $(D(\mathsf{p} \parallel \mathsf{q}) = 0) \Rightarrow (\mathsf{p} = \mathsf{q})$.

Non-Negativity of Rel. Entropy

- By the concavity of log and Jensen's inequality,

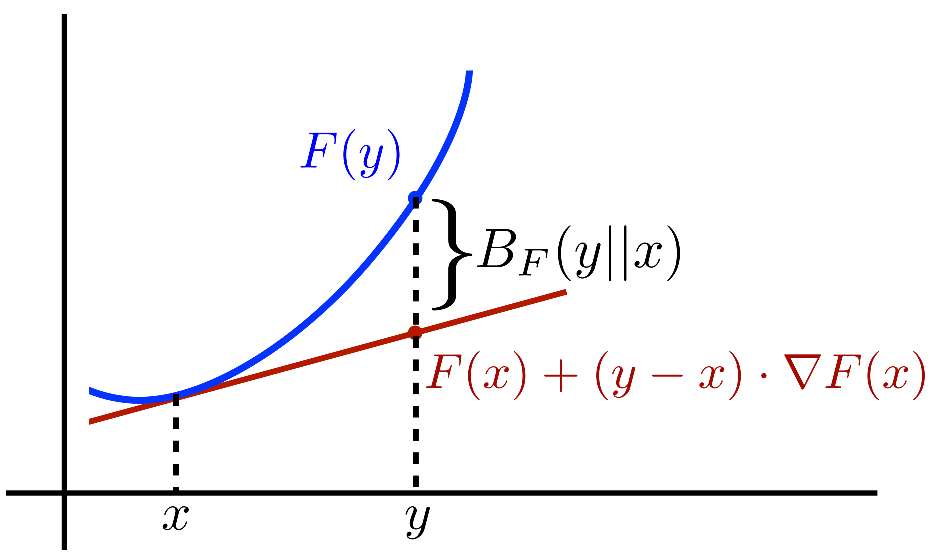
$$
\begin{aligned}
-D(\mathsf{p} \parallel \mathsf{q}) &= \sum_{x:\ \mathsf{p}(x)>0} \mathsf{p}(x) \log\left(\frac{\mathsf{q}(x)}{\mathsf{p}(x)}\right) \\
&\leq \log\left(\sum_{x:\ \mathsf{p}(x)>0} \mathsf{p}(x)\frac{\mathsf{q}(x)}{\mathsf{p}(x)}\right) \\
&= \log\left(\sum_{x:\ \mathsf{p}(x)>0} \mathsf{q}(x)\right) \leq \log(1) = 0.
\end{aligned}
$$

Bregman Divergence

(Bregman, 1967)

- Definition: let F be a convex and differentiable function defined over a convex set C in a Hilbert space $\mathbb{H}$. Then, the Bregman divergence B_F associated to F is defined by

$$B_F(x \parallel y) = F(x) - F(y) - \langle \nabla F(y), x - y \rangle .$$



Bregman Divergence

- Examples:

	$B_F(x \parallel y)$	$F(x)$
Squared L_2-distance	$\|\mathbf{x} - \mathbf{y}\|^2$	$\|\mathbf{x}\|^2$
Mahalanobis distance	$(\mathbf{x} - \mathbf{y})^\top \mathbf{K}^{-1}(\mathbf{x} - \mathbf{y})$	$\mathbf{x}^\top \mathbf{K}^{-1} \mathbf{x}$
Unnormalized relative entropy	$\widetilde{D}(\mathbf{x} \parallel \mathbf{y})$	$\sum_{i \in I} x_i \log x_i - x_i$

  - note: relative entropy not a Bregman divergence since not defined over an open set; but, on the simplex, coincides with unnormalized relative entropy

$$\widetilde{D}(\mathsf{p} \parallel \mathsf{q}) = \sum_{x \in \mathcal{X}} \mathsf{p}(x) \log \left[\frac{\mathsf{p}(x)}{\mathsf{q}(x)} \right] + \big(\mathsf{q}(x) - \mathsf{p}(x) \big).$$

Conditional Relative Entropy

- Definition: let p and q be two probability distributions over $\mathcal{X} \times \mathcal{Y}$. Then, the conditional relative entropy of p and q with respect to distribution r over $\mathcal{X}$ is defined by

$$\begin{aligned}\underset{X\sim\mathsf{r}}{\mathrm{E}}\Big[D\big(\mathsf{p}(\cdot|X)\parallel\mathsf{q}(\cdot|X)\big)\Big] &= \sum_{x\in\mathcal{X}}\mathsf{r}(x)\sum_{y\in\mathcal{Y}}\mathsf{p}(y|x)\log\frac{\mathsf{p}(y|x)}{\mathsf{q}(y|x)}\\ &= D(\widetilde{\mathsf{p}}\parallel\widetilde{\mathsf{q}}),\end{aligned}$$

  with $\widetilde{\mathsf{p}}(x,y)=\mathsf{r}(x)\mathsf{p}(y|x)$, $\widetilde{\mathsf{q}}(x,y)=\mathsf{r}(x)\mathsf{q}(y|x)$, and the conventions $0\log 0=0$, $0\log\frac{0}{0}=0$, and $\mathsf{p}\log\frac{\mathsf{p}}{0}=+\infty$.

  - note: the definition of conditional relative entropy is not intrinsic, it depends on a third distribution r.

This Lecture

- Notions of information theory.
- Introduction to density estimation.
- Maxent models.
- Conditional Maxent models.

Density Estimation Problem

- Training data: sample S of size m drawn i.i.d. from set $\mathcal{X}$ according to some distribution $\mathcal{D}$,

$$S = (x_1, \ldots, x_m).$$

- Problem: find distribution p out of hypothesis set $\mathcal{P}$ that best estimates $\mathcal{D}$.

Maximum Likelihood Solution

- Maximum Likelihood principle: select distribution $\mathsf{p} \in \mathcal{P}$ maximizing likelihood of observed sample S,

$$\begin{aligned}
\mathsf{p}_{\mathrm{ML}} &= \operatorname*{argmax}_{\mathsf{p}\in\mathcal{P}} \Pr[S|\mathsf{p}] \\
&= \operatorname*{argmax}_{\mathsf{p}\in\mathcal{P}} \prod_{i=1}^{m} \mathsf{p}(x_i) \\
&= \operatorname*{argmax}_{\mathsf{p}\in\mathcal{P}} \sum_{i=1}^{m} \log \mathsf{p}(x_i).
\end{aligned}$$

Relative Entropy Formulation

- Lemma: let $\widehat{\mathsf{p}}_S$ be the empirical distribution for sample S, then

$$\mathsf{p}_{\mathrm{ML}} = \operatorname*{argmin}_{\mathsf{p} \in \mathcal{P}} D(\widehat{\mathsf{p}}_S \parallel \mathsf{p}).$$

- Proof:

$$\begin{aligned}
D(\widehat{\mathsf{p}}_S \parallel \mathsf{p}) &= \sum_x \widehat{\mathsf{p}}_S(x) \log \widehat{\mathsf{p}}_S(x) - \sum_x \widehat{\mathsf{p}}_S(x) \log \mathsf{p}(x) \\
&= -H(\widehat{\mathsf{p}}_S) - \sum_x \frac{\sum_{i=1}^m 1_{x=x_i}}{m} \log \mathsf{p}(x) \\
&= -H(\widehat{\mathsf{p}}_S) - \sum_{i=1}^m \sum_x \frac{1_{x=x_i}}{m} \log \mathsf{p}(x) \\
&= -H(\widehat{\mathsf{p}}_S) - \sum_{i=1}^m \frac{\log \mathsf{p}(x_i)}{m}.
\end{aligned}$$

Maximum a Posteriori (MAP)

- Maximum a Posteriori principle: select distribution $\mathsf{p} \in \mathcal{P}$ that is the most likely, given the observed sample S and assuming a prior distribution $\Pr[\mathsf{p}]$ over $\mathcal{P}$,

$$\begin{aligned}
\mathsf{p}_{\mathrm{MAP}} &= \operatorname*{argmax}_{\mathsf{p} \in \mathcal{P}} \Pr[\mathsf{p}|S] \\
&= \operatorname*{argmax}_{\mathsf{p} \in \mathcal{P}} \frac{\Pr[S|\mathsf{p}] \Pr[\mathsf{p}]}{\Pr[S]} \\
&= \operatorname*{argmax}_{\mathsf{p} \in \mathcal{P}} \Pr[S|\mathsf{p}] \Pr[\mathsf{p}].
\end{aligned}$$

  - note: for a uniform prior, ML = MAP.

This Lecture

- Notions of information theory.
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Density Estimation + Features

- Training data: sample S of size m drawn i.i.d. from set $\mathcal{X}$ according to some distribution $\mathcal{D}$,

$$S = (x_1, \ldots, x_m).$$

- Features: associated to elements of $\mathcal{X}$,

$$\begin{aligned} \mathbf{\Phi} \colon \mathcal{X} &\to \mathbb{R}^N \\ x &\mapsto \mathbf{\Phi}(x) = \begin{bmatrix} \Phi_1(x) \\ \vdots \\ \Phi_N(x) \end{bmatrix}. \end{aligned}$$

- Problem: find distribution p out of hypothesis set $\mathcal{P}$ that best estimates $\mathcal{D}$.
  - for simplicity, in what follows, $\mathcal{X}$ is assumed to be finite.

Features

- Feature functions Φ_j assumed to be in H and $\|\mathbf{\Phi}\|_\infty \leq \Lambda$.
- Examples of H:
  - family of threshold functions $\{\mathbf{x} \mapsto 1_{x_i \leq \theta} \colon \mathbf{x} \in \mathbb{R}^N, \theta \in \mathbb{R}\}$ defined over N variables.
  - functions defined via decision trees with larger depths.
  - k-degree monomials of the original features.
  - zero-one features (often used in NLP, e.g., presence/absence of a word or POS tag).

Maximum Entropy Principle

(E. T. Jaynes, 1957, 1983)

- Idea: empirical feature vector average close to expectation. For any $\delta > 0$, with probability at least $1 - \delta$

$$\left\| \underset{x \sim \mathcal{D}}{\mathrm{E}}[\mathbf{\Phi}(x)] - \underset{x \sim \widehat{\mathcal{D}}}{\mathrm{E}}[\mathbf{\Phi}(x)] \right\|_\infty \leq 2\mathfrak{R}_m(H) + \Lambda \sqrt{\frac{\log \frac{2}{\delta}}{2m}},$$

- Maxent principle: find distribution p that is closest to a prior distribution p_0 (typically uniform distribution) while verifying $\left\| \mathrm{E}_{x \sim \mathsf{p}}[\mathbf{\Phi}(x)] - \mathrm{E}_{x \sim \widehat{\mathcal{D}}}[\mathbf{\Phi}(x)] \right\|_\infty \leq \beta$.
- Closeness is measured using relative entropy.
  - note: no set $\mathcal{P}$ needed to be specified.

Maxent Formulation

- Optimization problem:

$$\min_{\mathsf{p} \in \Delta} D(\mathsf{p} \parallel \mathsf{p}_0)$$

$$\text{subject to: } \Big\| \mathop{\mathrm{E}}_{x \sim \mathsf{p}}[\mathbf{\Phi}(x)] - \mathop{\mathrm{E}}_{x \sim S}[\mathbf{\Phi}(x)] \Big\|_\infty \leq \beta.$$

  - convex optimization problem, unique solution.
  - $\beta = 0$: standard Maxent (or unregularized Maxent).
  - $\beta > 0$: regularized Maxent.

Relation with Entropy

- Relationship with entropy: for a uniform prior p_0,

$$
\begin{aligned}
D(\mathsf{p} \parallel \mathsf{p}_0) &= \sum_{x \in \mathcal{X}} \mathsf{p}(x) \log \frac{\mathsf{p}(x)}{\mathsf{p}_0(x)} \\
&= -\sum_{x \in \mathcal{X}} \mathsf{p}(x) \log \mathsf{p}_0(x) + \sum_{x \in \mathcal{X}} \mathsf{p}(x) \log \mathsf{p}(x) \\
&= \log |\mathcal{X}| - H(\mathsf{p}).
\end{aligned}
$$

Maxent Problem

- Optimization: convex optimization problem.

$$
\begin{aligned}
\min_{\mathsf{p}} \quad & \sum_{x \in \mathcal{X}} \mathsf{p}(x) \log \mathsf{p}(x) \\
\text{subject to:} \quad & \mathsf{p}(x) \geq 0, \forall x \in \mathcal{X} \\
& \sum_{x \in \mathcal{X}} \mathsf{p}(x) = 1 \\
& \left| \sum_{x \in \mathcal{X}} \mathsf{p}(x) \Phi_j(x) - \frac{1}{m} \sum_{i=1}^{m} \Phi_j(x_i) \right| \leq \beta, \forall j \in [1, N].
\end{aligned}
$$

Gibbs Distributions

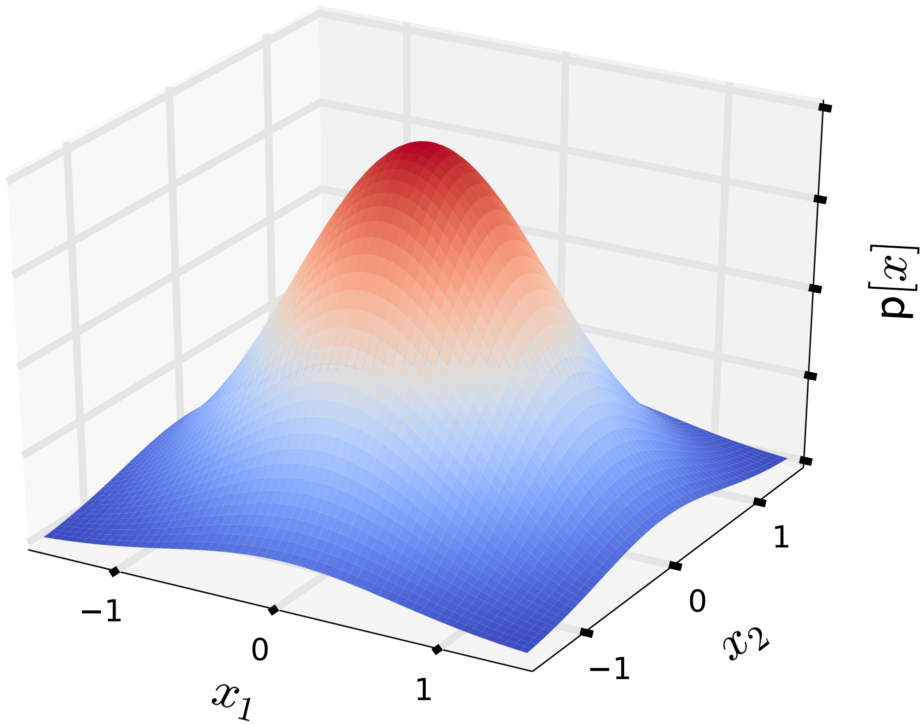
- Gibbs distributions: set $\mathcal{Q}$ of distributions $p_{\mathbf{w}}$ with $\mathbf{w} \in \mathbb{R}^N$,

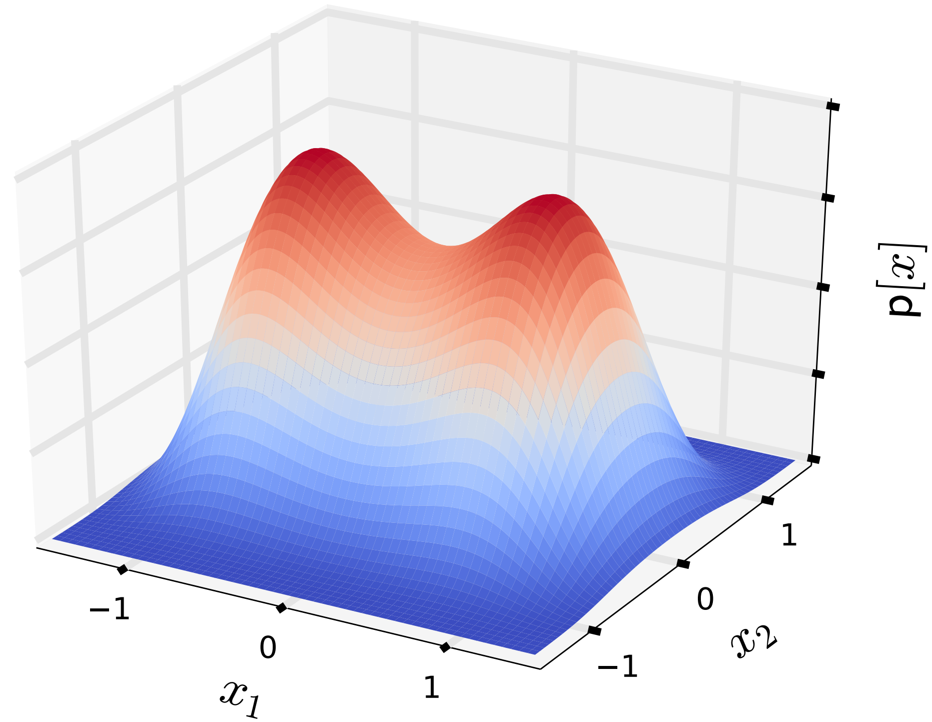
$$\mathsf{p}_{\mathbf{w}}[x] = \frac{\mathsf{p}_0[x] \exp\big(\mathbf{w} \cdot \mathbf{\Phi}(x)\big)}{Z} = \frac{\mathsf{p}_0[x] \exp\big(\sum_{j=1}^N w_j \Phi_j(x)\big)}{Z},$$

with $Z = \sum_x \mathsf{p}_0[x] \exp\big(\mathbf{w} \cdot \mathbf{\Phi}(x)\big)$.

- Rich family:
  - for linear and quadratic features: includes Gaussians and other distributions with non-PSD quadratic forms in exponents.
  - for higher-degree polynomials of raw features: more complex multi-modal distributions.

Examples





$$\mathsf{p}[(x_1, x_2)] = \frac{e^{-(x_1^2+x_2^2)}}{Z}.$$

$$\mathsf{p}[(x_1, x_2)] = \frac{e^{-(x_1^4+x_2^4)+x_1^2-x_2^2}}{Z}.$$

Dual Problems

- Regularized Maxent problem:

$$\min_{\mathsf{p}} F(\mathsf{p}) = \overline{D}(\mathsf{p} \parallel \mathsf{p}_0) + I_C(\mathop{\mathrm{E}}_{\mathsf{p}}[\mathbf{\Phi}]),$$

$$\text{with } \begin{cases} \overline{D}(\mathsf{p} \parallel \mathsf{p}_0) = D(\mathsf{p} \parallel \mathsf{p}_0) \text{ if } \mathsf{p} \in \Delta, +\infty \text{ otherwise;} \\ C = \left\{\mathbf{u} \colon \|\mathbf{u} - \mathop{\mathrm{E}}_{S}[\mathbf{\Phi}]\|_\infty \leq \beta\right\}; \\ I_C(x) = 0 \text{ if } x \in C,\ I_C(x) = +\infty \text{ otherwise.} \end{cases}$$

- Regularized Maximum Likelihood problem with Gibbs distributions:

$$\sup_{\mathbf{w}} G(\mathbf{w}) = \frac{1}{m}\sum_{i=1}^{m} \log\left[\frac{\mathsf{p}_{\mathbf{w}}[x_i]}{\mathsf{p}_0[x_i]}\right] - \beta\|\mathbf{w}\|_1.$$

Duality Theorem

(Della Pietra et al., 1997; Dudík et al., 2007; Cortes et al., 2015)

- Theorem: the regularized Maxent and ML with Gibbs distributions problems are equivalent,

$$\sup_{\mathbf{w}\in\mathbb{R}^N} G(\mathbf{w}) = \min_{\mathsf{p}} F(\mathsf{p}).$$

  - furthemore, let $\mathsf{p}^* = \operatorname*{argmin}_{\mathsf{p}} F(\mathsf{p})$, then, for any $\epsilon > 0$,

$$\Big(\big|G(\mathbf{w}) - \sup_{\mathbf{w}\in\mathbb{R}^N} G(\mathbf{w})\big| < \epsilon\Big) \Rightarrow \Big(D(\mathsf{p}^* \,\|\, \mathsf{p}_{\mathbf{w}}) \leq \epsilon\Big).$$

Notes

- Maxent formulation:
  - no explicit restriction to a family of distributions $\mathcal{P}$.
  - but solution coincides with regularized ML with a specific family $\mathcal{P}$!
  - more general Bregman divergence-based formulation.

L_1-Regularized Maxent

(Kazama and Tsujii, 2003)

- Optimization problem:

$$\inf_{\mathbf{w}\in\mathbb{R}^N} \beta\|\mathbf{w}\|_1 - \frac{1}{m}\sum_{i=1}^{m} \log \mathsf{p}_{\mathbf{w}}[x_i].$$

$$\text{where } \mathsf{p}_{\mathbf{w}}[x] = \frac{1}{Z}\exp\big(\mathbf{w}\cdot\mathbf{\Phi}(x)\big).$$

- Bayesian interpretation: equivalent to MAP with Laplacian prior $q_{\text{prior}}(\mathbf{w})$ (Williams, 1994),

$$\max_{\mathbf{w}} \log\Big(\prod_{i=1}^{m} \mathsf{p}_{\mathbf{w}}[x_i]\, \mathsf{q}_{\text{prior}}(\mathbf{w})\Big)$$

$$\text{with } q_{\text{prior}}(\mathbf{w}) = \prod_{j=1}^{N} \frac{\beta_j}{2}\exp(-\beta_j|w_j|).$$

Generalization Guarantee

(Dudík et al., 2007)

- Notation: $\mathcal{L}_{\mathcal{D}}(\mathbf{w}) = \underset{x \sim \mathcal{D}}{\mathrm{E}}[-\log \mathsf{p}_{\mathbf{w}}[x]]$, $\mathcal{L}_S(\mathbf{w}) = \underset{x \sim S}{\mathrm{E}}[-\log \mathsf{p}_{\mathbf{w}}[x]]$.
- Theorem: Fix $\delta > 0$. Let $\widehat{\mathbf{w}}$ be the solution of the L1-reg. Maxent problem for $\beta = 2\mathfrak{R}_m(H) + \Lambda\sqrt{\log(\frac{2}{\delta})/2m}$. Then, with probability at least $1 - \delta$,

$$\mathcal{L}_{\mathcal{D}}(\widehat{\mathbf{w}}) \leq \inf_{\mathbf{w}} \mathcal{L}_{\mathcal{D}}(\mathbf{w}) + 2\|\mathbf{w}\|_1 \left[2\mathfrak{R}_m(H) + \Lambda\sqrt{\frac{\log \frac{2}{\delta}}{2m}}\right].$$

Proof

- By Hölder's inequality and the concentration bound for average feature vectors,

$$\begin{aligned}
\mathcal{L}_{\mathcal{D}}(\widehat{\mathbf{w}}) - \mathcal{L}_S(\widehat{\mathbf{w}}) &= \widehat{\mathbf{w}} \cdot \big[\mathop{\mathrm{E}}_{S}[\mathbf{\Phi}] - \mathop{\mathrm{E}}_{\mathcal{D}}[\mathbf{\Phi}]\big] \\
&\leq \|\widehat{\mathbf{w}}\|_1 \, \big\| \mathop{\mathrm{E}}_{S}[\mathbf{\Phi}] - \mathop{\mathrm{E}}_{\mathcal{D}}[\mathbf{\Phi}] \big\|_\infty \leq \beta \|\widehat{\mathbf{w}}\|_1.
\end{aligned}$$

- Since $\widehat{\mathbf{w}}$ is a minimizer,

$$\begin{aligned}
\mathcal{L}_{\mathcal{D}}(\widehat{\mathbf{w}}) - \mathcal{L}_{\mathcal{D}}(\mathbf{w}) &= \mathcal{L}_{\mathcal{D}}(\widehat{\mathbf{w}}) - \mathcal{L}_S(\widehat{\mathbf{w}}) + \mathcal{L}_S(\widehat{\mathbf{w}}) - \mathcal{L}_{\mathcal{D}}(\mathbf{w}) \\
&\leq \beta \|\widehat{\mathbf{w}}\|_1 + \mathcal{L}_S(\widehat{\mathbf{w}}) - \mathcal{L}_{\mathcal{D}}(\mathbf{w}) \\
&\leq \beta \|\mathbf{w}\|_1 + \mathcal{L}_S(\mathbf{w}) - \mathcal{L}_{\mathcal{D}}(\mathbf{w}) \leq 2\beta \|\mathbf{w}\|_1. \\
&\qquad\qquad (\widehat{\mathbf{w}} \text{ minimizer of } \beta\|\mathbf{w}\|_1 + \mathcal{L}_S(\mathbf{w}))
\end{aligned}$$

L_2-Regularized Maxent

(Chen and Rosenfeld, 2000; Lebanon and Lafferty, 2001)

- Different relaxations:
  - L_1 constraints:

$$\forall j \in [1, N], \quad \left| \mathop{\mathrm{E}}_{x \sim p}[\Phi_j(x)] - \mathop{\mathrm{E}}_{x \sim \widehat{p}}[\Phi_j(x)] \right| \leq \beta_j.$$

  - L_2 constraints:

$$\left\| \mathop{\mathrm{E}}_{x \sim p}[\mathbf{\Phi}(x)] - \mathop{\mathrm{E}}_{x \sim \widehat{p}}[\mathbf{\Phi}(x)] \right\|_2 \leq B.$$

L_2-Regularized Maxent

- Optimization problem:

$$\inf_{\mathbf{w}\in\mathbb{R}^N} \beta\|\mathbf{w}\|_2^2 - \frac{1}{m}\sum_{i=1}^{m}\log \mathsf{p}_{\mathbf{w}}[x_i].$$

$$\text{where } \mathsf{p}_{\mathbf{w}}[x] = \frac{1}{Z}\exp\big(\mathbf{w}\cdot\mathbf{\Phi}(x)\big).$$

- Bayesian interpretation: equivalent to MAP with Gaussian prior $q_{\text{prior}}(\mathbf{w})$ (Goodman, 2004),

$$\max_{\mathbf{w}} \ \log\Big(\prod_{i=1}^{m}\mathsf{p}_{\mathbf{w}}[x_i]\,\mathsf{q}_{\text{prior}}(\mathbf{w})\Big)$$

$$\text{with } \mathsf{q}_{\text{prior}}(\mathbf{w}) = \prod_{j=1}^{N}\frac{1}{\sqrt{2\pi\sigma^2}}e^{-\frac{w_j^2}{2\sigma^2}}.$$

This Lecture

- Notions of information theory.
- Introduction to density estimation.
- Maxent models.
- Conditional Maxent models.

Conditional Maxent Models

- Maxent models for conditional probabilities:
  - conditional probability modeling each class.
  - use in multi-class classification.
  - can use different features for each class.
  - a.k.a. multinomial logistic regression.
  - logistic regression: special case of two classes.

Problem

- Data: sample drawn i.i.d. according to some distribution D,

$$S = ((x_1, y_1), \ldots, (x_m, y_m)) \in (\mathcal{X} \times \mathcal{Y})^m.$$

  - $\mathcal{Y} = \{1, \ldots, k\}$, or $\mathcal{Y} = \{0, 1\}^k$ in multi-label case.

- Features: mapping $\mathbf{\Phi}\colon \mathcal{X} \times \mathcal{Y} \to \mathbb{R}^N$.

- Problem: find accurate conditional probability models $\Pr[\cdot \mid x]$, $x \in \mathcal{X}$, based on $\mathbf{\Phi}$.

Conditional Maxent Principle

(Berger et al., 1996; Cortes et al., 2015)

- Idea: empirical feature vector average close to expectation. For any $\delta > 0$, with probability at least $1 - \delta$,
$$\left\| \mathop{\mathrm{E}}_{\substack{x \sim \widehat{\mathsf{p}} \\ y \sim \mathcal{D}[\cdot|x]}} [\mathbf{\Phi}(x, y)] - \mathop{\mathrm{E}}_{\substack{x \sim \widehat{\mathsf{p}} \\ y \sim \widehat{\mathsf{p}}[\cdot|x]}} [\mathbf{\Phi}(x, y)] \right\|_{\infty} \leq 2\mathfrak{R}_m(H) + \sqrt{\frac{\log \frac{2}{\delta}}{2m}}.$$
- Maxent principle: find conditional distributions $\mathsf{p}[\cdot|x]$ that are closest to priors $\mathsf{p}_0[\cdot|x]$ (typically uniform distributions) while verifying $\left\| \mathrm{E}_{\substack{x \sim \widehat{\mathsf{p}} \\ y \sim \mathsf{p}[\cdot|x]}} [\mathbf{\Phi}(x, y)] - \mathrm{E}_{\substack{x \sim \widehat{\mathsf{p}} \\ y \sim \widehat{\mathsf{p}}[\cdot|x]}} [\mathbf{\Phi}(x, y)] \right\|_{\infty} \leq \beta$.
- Closeness is measured using conditional relative entropy based on $\widehat{\mathsf{p}}$.

Cond. Maxent Formulation

(Berger et al., 1996; Cortes et al., 2015)

- Optimization problem: find distribution p solution of

$$\min_{\mathsf{p}[\cdot|x] \in \Delta} \sum_{x \in \mathcal{X}} \widehat{\mathsf{p}}[x] \, D\big(\mathsf{p}[\cdot|x] \parallel \mathsf{p}_0[\cdot|x]\big)$$

$$\text{s.t.} \left\| \mathop{\mathrm{E}}_{x \sim \widehat{\mathsf{p}}} \left[\mathop{\mathrm{E}}_{y \sim \mathsf{p}[\cdot|x]} [\mathbf{\Phi}(x, y)] \right] - \mathop{\mathrm{E}}_{(x,y) \sim S} [\mathbf{\Phi}(x, y)] \right\|_\infty \leq \beta.$$

  - convex optimization problem, unique solution.
  - $\beta = 0$: unregularized conditional Maxent.
  - $\beta > 0$: regularized conditional Maxent.

Dual Problems

- Regularized conditional Maxent problem:

$$\widetilde{F}(\mathsf{p}) = \mathop{\mathrm{E}}_{x \sim \widehat{p}} \Big[\overline{D}\big(\mathsf{p}[\cdot|x] \parallel \mathsf{p}_0[\cdot|x]\big) + I_\Delta\big(\mathsf{p}[\cdot|x]\big) \Big] + I_C\Big(\mathop{\mathrm{E}}_{\substack{x \sim \widehat{\mathsf{p}} \\ y \sim \mathsf{p}[\cdot|x]}} [\mathbf{\Phi}] \Big).$$

- Regularized Maximum Likelihood problem with conditional Gibbs distributions:

$$\widetilde{G}(\mathbf{w}) = \frac{1}{m} \sum_{i=1}^{m} \log \left[\frac{\mathsf{p}_{\mathbf{w}}[y_i|x_i]}{\mathsf{p}_0[y_i|x_i]} \right] - \beta \|\mathbf{w}\|_1 ,$$

where $\forall (x, y) \in \mathcal{X} \times \mathcal{Y}$,

$$\mathsf{p}_{\mathbf{w}}[y|x] = \frac{\mathsf{p}_0[y|x] \exp\big(\mathbf{w} \cdot \mathbf{\Phi}(x, y)\big)}{Z(x)}$$

$$Z(x) = \sum_{y \in \mathcal{Y}} \mathsf{p}_0[y|x] \exp(\mathbf{w} \cdot \mathbf{\Phi}(x, y)).$$

Duality Theorem

(Cortes et al., 2015)

- Theorem: the regularized conditional Maxent and ML with conditional Gibbs distributions problems are equivalent,

$$\sup_{\mathbf{w} \in \mathbb{R}^N} \widetilde{G}(\mathbf{w}) = \min_{\mathsf{p}} \widetilde{F}(\mathsf{p}).$$

  - furthemore, let $\mathsf{p}^* = \operatorname*{argmin}_{\mathsf{p}} \widetilde{F}(\mathsf{p})$, then, for any $\epsilon > 0$,

$$\Big(|\widetilde{G}(\mathbf{w}) - \sup_{\mathbf{w} \in \mathbb{R}^N} \widetilde{G}(\mathbf{w})| < \epsilon\Big) \Rightarrow \operatorname*{E}_{x \sim \widehat{p}}\Big[D\big(\mathsf{p}^*[\cdot|x] \parallel \mathsf{p}_{\mathbf{w}}[\cdot|x]\big)\Big] \leq \epsilon.$$

Regularized Cond. Maxent

(Berger et al., 1996; Cortes et al., 2015)

- Optimization problem: convex optimizations, regularization parameter $\lambda \geq 0$.

$$\min_{\mathbf{w} \in \mathbb{R}^N} \quad \lambda \|\mathbf{w}\|_1 - \frac{1}{m} \sum_{i=1}^{m} \log \mathsf{p}_{\mathbf{w}}[y_i | x_i]$$

$$\text{or} \quad \min_{\mathbf{w} \in \mathbb{R}^N} \quad \lambda \|\mathbf{w}\|_2^2 - \frac{1}{m} \sum_{i=1}^{m} \log \mathsf{p}_{\mathbf{w}}[y_i | x_i],$$

where $\forall (x, y) \in \mathcal{X} \times \mathcal{Y}$,

$$\mathsf{p}_{\mathbf{w}}[y|x] = \frac{\exp(\mathbf{w} \cdot \mathbf{\Phi}(x, y))}{Z(x)}$$

$$Z(x) = \sum_{y \in \mathcal{Y}} \exp(\mathbf{w} \cdot \mathbf{\Phi}(x, y)).$$

More Explicit Forms

- Optimization problem: multinomial logistic loss.

$$\min_{\mathbf{w}\in\mathbb{R}^N} \begin{cases} \lambda\|\mathbf{w}\|_1 \\ \lambda\|\mathbf{w}\|_2^2 \end{cases} + \frac{1}{m}\sum_{i=1}^{m} \log\left[\sum_{y\in\mathcal{Y}} \exp\Big(\mathbf{w}\cdot\mathbf{\Phi}(x_i, y) - \mathbf{w}\cdot\mathbf{\Phi}(x_i, y_i)\Big)\right].$$

$$\min_{\mathbf{w}\in\mathbb{R}^N} \begin{cases} \lambda\|\mathbf{w}\|_1 \\ \lambda\|\mathbf{w}\|_2^2 \end{cases} - \mathbf{w}\cdot\frac{1}{m}\sum_{i=1}^{m}\mathbf{\Phi}(x_i, y_i) + \frac{1}{m}\sum_{i=1}^{m} \log\left[\sum_{y\in\mathcal{Y}} e^{\mathbf{w}\cdot\mathbf{\Phi}(x_i, y)}\right].$$

Related Problem

- Optimization problem: log-sum-exp replaced by max.

$$\min_{\mathbf{w}\in\mathbb{R}^N} \begin{cases} \lambda\|\mathbf{w}\|_1 \\ \lambda\|\mathbf{w}\|_2^2 \end{cases} + \frac{1}{m}\sum_{i=1}^{m} \underbrace{\max_{y\in\mathcal{Y}}\Big(\mathbf{w}\cdot\mathbf{\Phi}(x_i,y) - \mathbf{w}\cdot\mathbf{\Phi}(x_i,y_i)\Big)}_{-\rho_{\mathbf{w}}(x_i,y_i)}.$$

Common Feature Choice

- Multi-class features:

$$\mathbf{\Phi}(x,y) = \begin{bmatrix} 0 \\ \vdots \\ 0 \\ \mathbf{\Gamma}(x) \\ 0 \\ \vdots \\ 0 \end{bmatrix} \quad \mathbf{w} = \begin{bmatrix} \mathbf{w}_1 \\ \vdots \\ \mathbf{w}_{y-1} \\ \mathbf{w}_y \\ \mathbf{w}_{y+1} \\ \vdots \\ \mathbf{w}_{|\mathcal{Y}|} \end{bmatrix} \longrightarrow \mathbf{w} \cdot \mathbf{\Phi}(x,y) = \mathbf{w}_y \cdot \mathbf{\Gamma}(x).$$

- L_2-regularized cond. maxent optimization:

$$\min_{\mathbf{w} \in \mathbb{R}^N} \lambda \sum_{y \in \mathcal{Y}} \|\mathbf{w}_y\|_2^2 + \frac{1}{m} \sum_{i=1}^{m} \log \left[\sum_{y \in \mathcal{Y}} \exp\Big(\mathbf{w}_y \cdot \mathbf{\Gamma}(x_i) - \mathbf{w}_{y_i} \cdot \mathbf{\Gamma}(x_i)\Big) \right].$$

Prediction

- Prediction with $\mathsf{p}_{\mathbf{w}}[y|x] = \frac{\exp(\mathbf{w}\cdot\mathbf{\Phi}(x,y))}{Z(x)}$:

$$\widehat{y}(x) = \operatorname{argmax}_{y \in \mathcal{Y}} \mathsf{p}_{\mathbf{w}}[y|x] = \operatorname{argmax}_{y \in \mathcal{Y}} \mathbf{w} \cdot \mathbf{\Phi}(x, y).$$

Binary Classification

- Simpler expression:

$$\begin{aligned}
&\sum_{y \in \mathcal{Y}} \exp\Big(\mathbf{w} \cdot \mathbf{\Phi}(x_i, y) - \mathbf{w} \cdot \mathbf{\Phi}(x_i, y_i)\Big) \\
&= e^{\mathbf{w} \cdot \mathbf{\Phi}(x_i, +1) - \mathbf{w} \cdot \mathbf{\Phi}(x_i, y_i)} + e^{\mathbf{w} \cdot \mathbf{\Phi}(x_i, -1) - \mathbf{w} \cdot \mathbf{\Phi}(x_i, y_i)} \\
&= 1 + e^{-y_i \mathbf{w} \cdot [\mathbf{\Phi}(x_i, +1) - \mathbf{\Phi}(x_i, -1)]} \\
&= 1 + e^{-y_i \mathbf{w} \cdot \mathbf{\Psi}(x_i)},
\end{aligned}$$

with $\mathbf{\Psi}(x) = \mathbf{\Phi}(x, +1) - \mathbf{\Phi}(x, -1)$.

Logistic Regression

(Berkson, 1944)

- Binary case of conditional Maxent.
- Optimization problem: regularized logistic loss.

$$\min_{\mathbf{w}\in\mathbb{R}^N} \begin{Bmatrix} \lambda\|\mathbf{w}\|_1 \\ \lambda\|\mathbf{w}\|_2^2 \end{Bmatrix} + \frac{1}{m}\sum_{i=1}^{m} \log\left[1 + e^{-y_i \mathbf{w}\cdot\boldsymbol{\Psi}(x_i)}\right].$$

  - convex optimization.
  - variety of solutions: SGD, coordinate descent, etc.
  - coordinate descent: similar to AdaBoost with logistic loss $\phi(-u) = \log_2(1 + e^{-u}) \geq 1_{u \leq 0}$ instead of exponential loss.

Generalization Bound

- Theorem: assume that $\pm\Phi_j \in H$ for all $j \in [1, N]$. Then, for any $\delta > 0$, with probability at least $1 - \delta$ over the draw of a sample S of size m, for all $f : x \mapsto \mathbf{w} \cdot \Phi(x)$,

$$R(f) \leq \frac{1}{m} \sum_{i=1}^{m} \log_{u_0}\left(1 + e^{-y_i \mathbf{w} \cdot \Phi(x_i)}\right) + 4\|\mathbf{w}\|_1 \mathfrak{R}_m(H)$$

$$+ \sqrt{\frac{\log \log_2 2\|\mathbf{w}\|_1}{m}} + \sqrt{\frac{\log \frac{2}{\delta}}{m}},$$

where $u_0 = 1 + \frac{1}{e}$.

Proof

- Proof: by the learning bound for convex ensembles holding uniformly for all ρ, with probability at least $1-\delta$, for all f and $\rho > 0$,
$$R(f) \leq \frac{1}{m}\sum_{i=1}^{m} 1_{\frac{y_i \mathbf{w}\cdot\Phi(x_i)}{\rho\|\mathbf{w}\|_1} - 1 \leq 0} + \frac{4}{\rho}\mathfrak{R}_m(H) + \sqrt{\frac{\log\log_2 \frac{2}{\rho}}{m}} + \sqrt{\frac{\log \frac{2}{\delta}}{m}}.$$

- Choosing $\rho = \frac{1}{\|\mathbf{w}\|_1}$ and using $1_{u \leq 1} \leq \log_{u_0}(1+e^{-u})$ yields immediately the learning bound of the theorem.

Logistic Regression

(Berkson, 1944)

- Logistic model:

$$\Pr[y=+1 \mid x] = \frac{e^{\mathbf{w}\cdot\mathbf{\Phi}(x,+1)}}{Z(x)},$$

where $Z(x) = e^{\mathbf{w}\cdot\mathbf{\Phi}(x,+1)} + e^{\mathbf{w}\cdot\mathbf{\Phi}(x,-1)}$

- Properties:
  - linear decision rule, sign of log-odds ratio:

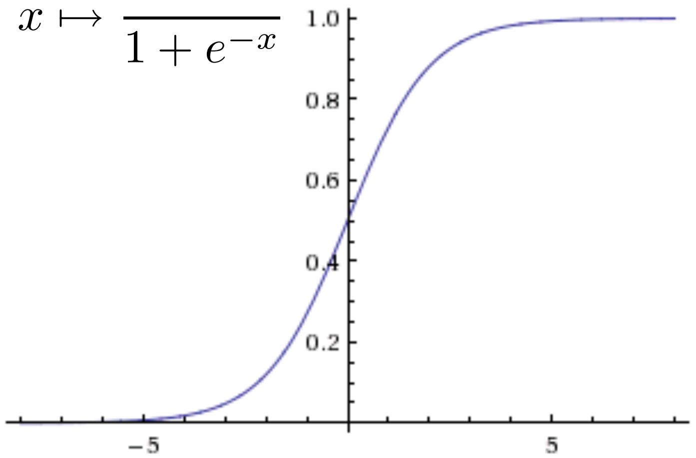
$$\log \frac{\Pr[y=+1 \mid x]}{\Pr[y=-1 \mid x]} = \mathbf{w} \cdot \big(\mathbf{\Phi}(x,+1) - \mathbf{\Phi}(x,-1)\big) = \mathbf{w} \cdot \mathbf{\Psi}(x).$$

  - logistic form:

$$\Pr[y=+1 \mid x] = \frac{1}{1 + e^{-\mathbf{w}\cdot[\mathbf{\Phi}(x,+1)-\mathbf{\Phi}(x,-1)]}} = \frac{1}{1 + e^{-\mathbf{w}\cdot\mathbf{\Psi}(x)}}.$$

Logistic/Sigmoid Function

$$f\colon x \mapsto \frac{1}{1+e^{-x}}$$



$$\Pr[y=+1 \mid x] = f\big(\mathbf{w} \cdot \mathbf{\Psi}(x)\big).$$

Applications

- Natural language processing (Berger et al., 1996; Rosenfeld, 1996; Pietra et al., 1997; Malouf, 2002; Manning and Klein, 2003; Mann et al., 2009; Ratnaparkhi, 2010).
- Species habitat modeling (Phillips et al., 2004, 2006; Dudík et al., 2007; Elith et al, 2011).
- Computer vision (Jeon and Manmatha, 2004).

Extensions

- Extensive theoretical study of alternative regularizations: (Dudík et al., 2007) (see also (Altun and Smola, 2006) though some proofs unclear).
- Maxent models with other Bregman divergences (see for example (Altun and Smola, 2006)).
- Structural Maxent models (Cortes et al., 2015):
  - extension to the case of multiple feature families.
  - empirically outperform Maxent and L1-Maxent.
  - conditional structural Maxent: coincide with deep boosting using the logistic loss.

Conclusion

- Logistic regression/maxent models:
  - theoretical foundation.
  - natural solution when probabilites are required.
  - widely used for density estimation/classification.
  - often very effective in practice.
  - distributed optimization solutions.
  - no natural non-linear L1-version (use of kernels).
  - connections with boosting.
  - connections with neural networks.

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Foundations of Machine Learning
On-Line Learning

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Motivation

- PAC learning:
  - distribution fixed over time (training and test).
  - IID assumption.
- On-line learning:
  - no distributional assumption.
  - worst-case analysis (adversarial).
  - mixed training and test.
  - Performance measure: mistake model, regret.

This Lecture

- Prediction with expert advice
- Linear classification

General On-Line Setting

- For $t=1$ to T do
  - receive instance $x_t \in X$.
  - predict $\widehat{y}_t \in Y$.
  - receive label $y_t \in Y$.
  - incur loss $L(\widehat{y}_t, y_t)$.
- Classification: $Y = \{0, 1\}, L(y, y') = |y' - y|$.
- Regression: $Y \subseteq \mathbb{R}, L(y, y') = (y' - y)^2$.
- Objective: minimize total loss $\sum_{t=1}^{T} L(\widehat{y}_t, y_t)$.

Prediction with Expert Advice

- For $t = 1$ to T do
  - receive instance $x_t \in X$ and advice $y_{t,i} \in Y, i \in [1, N]$.
  - predict $\widehat{y}_t \in Y$.
  - receive label $y_t \in Y$.
  - incur loss $L(\widehat{y}_t, y_t)$.
- Objective: minimize regret, i.e., difference of total loss incurred and that of best expert.

$$\text{Regret}(T) = \sum_{t=1}^{T} L(\widehat{y}_t, y_t) - \min_{i=1}^{N} \sum_{t=1}^{T} L(y_{t,i}, y_t).$$

Mistake Bound Model

- Definition: the maximum number of mistakes a learning algorithm L makes to learn c is defined by

$$M_L(c) = \max_{x_1, \ldots, x_T} |\text{mistakes}(L, c)|.$$

- Definition: for any concept class C the maximum number of mistakes a learning algorithm L makes is

$$M_L(C) = \max_{c \in C} M_L(c).$$

A mistake bound is a bound M on $M_L(C)$.

Halving Algorithm

see (Mitchell, 1997)

$\textsc{Halving}(H)$

$H_1 \leftarrow H$

for $t \leftarrow 1$ **to** T **do**

  $\textsc{Receive}(x_t)$

  $\widehat{y}_t \leftarrow \textsc{MajorityVote}(H_t, x_t)$

  $\textsc{Receive}(y_t)$

  if $\widehat{y}_t \neq y_t$ **then**

    $H_{t+1} \leftarrow \{c \in H_t \colon c(x_t) = y_t\}$

return H_{T+1}

Halving Algorithm - Bound

(Littlestone, 1988)

- Theorem: Let H be a finite hypothesis set, then

$$M_{Halving(H)} \leq \log_2 |H|.$$

- Proof: At each mistake, the hypothesis set is reduced at least by half.

VC Dimension Lower Bound

(Littlestone, 1988)

- Theorem: Let $\text{opt}(H)$ be the optimal mistake bound for H. Then,

$$\text{VCdim}(H) \leq \text{opt}(H) \leq M_{Halving(H)} \leq \log_2 |H|.$$

- Proof: for a fully shattered set, form a complete binary tree of the mistakes with height $\text{VCdim}(H)$.

Weighted Majority Algorithm

(Littlestone and Warmuth, 1988)

$\textsc{Weighted-Majority}(N \text{ experts})$ $\quad\triangleright\quad y_t, y_{t,i} \in \{0, 1\}.$

$\quad\quad\quad\quad\quad\quad\quad\quad\quad\quad\quad\quad\quad\quad\quad\quad\quad\quad\quad\quad\quad\quad\;\; \beta \in [0, 1).$

for $i \leftarrow 1$ **to** N **do**
    $w_{1,i} \leftarrow 1$
for $t \leftarrow 1$ **to** T **do**
    $\textsc{Receive}(x_t)$
    $\widehat{y}_t \leftarrow 1_{\sum_{y_{t,i}=1}^{N} w_t \geq \sum_{y_{t,i}=0}^{N} w_t}$ $\quad\triangleright$ weighted majority vot
    $\textsc{Receive}(y_t)$
    if $\widehat{y}_t \neq y_t$ **then**
        for $i \leftarrow 1$ **to** N **do**
            if $(y_{t,i} \neq y_t)$ **then**
                $w_{t+1,i} \leftarrow \beta w_{t,i}$
            else $w_{t+1,i} \leftarrow w_{t,i}$
return $\mathbf{w}_{T+1}$

Weighted Majority - Bound

- Theorem: Let m_t be the number of mistakes made by the WM algorithm till time t and m_t^* that of the best expert. Then, for all t,

$$\boxed{m_t \leq \frac{\log N + m_t^* \log \frac{1}{\beta}}{\log \frac{2}{1+\beta}}.}$$

  - Thus, $m_t \leq O(\log N) + \text{constant} \times \text{best expert}.$
  - Realizable case: $m_t \leq O(\log N).$
  - Halving algorithm: $\beta = 0$.

Weighted Majority - Proof

- Potential: $\Phi_t = \sum_{i=1}^{N} w_{t,i}$.
- Upper bound: after each error,

$$\Phi_{t+1} \leq \left[\tfrac{1}{2} + \tfrac{1}{2} \times \beta\right] \Phi_t = \left[\frac{1+\beta}{2}\right] \Phi_t.$$

Thus, $\Phi_t \leq \left[\frac{1+\beta}{2}\right]^{m_t} N.$

- Lower bound: for any expert i, $\Phi_t \geq w_{t,i} = \beta^{m_{t,i}}$.
- Comparison: $\beta^{m_t^*} \leq \left[\frac{1+\beta}{2}\right]^{m_t} N$

$$\Rightarrow m_t^* \log \beta \leq \log N + m_t \log \left[\frac{1+\beta}{2}\right]$$

$$\Rightarrow m_t \log \left[\frac{2}{1+\beta}\right] \leq \log N + m_t^* \log \frac{1}{\beta}.$$

Weighted Majority - Notes

- Advantage: remarkable bound requiring no assumption.
- Disadvantage: no deterministic algorithm can achieve a regret $R_T = o(T)$ with the binary loss.
  - better guarantee with randomized WM.
  - better guarantee for WM with convex losses.

Exponential Weighted Average

total loss incurred by expert i up to time t

- **Algorithm**:
  - weight update: $w_{t+1,i} \leftarrow w_{t,i}\, e^{-\eta L(y_{t,i}, y_t)} = e^{-\eta L_{t,i}}$.
  - prediction: $\widehat{y}_t = \frac{\sum_{i=1}^N w_{t,i} y_{t,i}}{\sum_{i=1}^N w_{t,i}}$.
- **Theorem**: assume that L is convex in its first argument and takes values in $[0,1]$. Then, for any $\eta > 0$ and any sequence $y_1, \ldots, y_T \in Y$, the regret at T satisfies

$$\text{Regret}(T) \leq \frac{\log N}{\eta} + \frac{\eta T}{8}.$$

For $\eta = \sqrt{8 \log N / T}$,

$$\boxed{\text{Regret}(T) \leq \sqrt{(T/2) \log N}}.$$

Exponential Weighted Avg - Proof

- **Potential:** $\Phi_t = \log \sum_{i=1}^N w_{t,i}.$
- **Upper bound:**

$$\begin{aligned}
\Phi_t - \Phi_{t-1} &= \log \frac{\sum_{i=1}^N w_{t-1,i}\, e^{-\eta L(y_{t,i}, y_t)}}{\sum_{i=1}^N w_{t-1,i}} \\
&= \log \Big(\operatorname*{E}_{w_{t-1}} [e^{-\eta L(y_{t,i}, y_t)}] \Big) \\
&= \log \left(\operatorname*{E}_{w_{t-1}} \left[\exp \left(-\eta \Big(L(y_{t,i}, y_t) - \operatorname*{E}_{w_{t-1}} [L(y_{t,i}, y_t)] \Big) - \eta \operatorname*{E}_{w_{t-1}} [L(y_{t,i}, y_t)] \right) \right] \right) \\
&\leq -\eta \operatorname*{E}_{w_{t-1}} [L(y_{t,i}, y_t)] + \frac{\eta^2}{8} \quad \text{(Hoeffding's ineq.)} \\
&\leq -\eta L(\operatorname*{E}_{w_{t-1}} [y_{t,i}], y_t) + \frac{\eta^2}{8} \quad \text{(convexity of first arg. of } L) \\
&= -\eta L(\widehat{y}_t, y_t) + \frac{\eta^2}{8}.
\end{aligned}$$

Exponential Weighted Avg - Proof

- Upper bound: summing up the inequalities yields

$$\Phi_T - \Phi_0 \leq -\eta \sum_{t=1}^{T} L(\widehat{y}_t, y_t) + \frac{\eta^2 T}{8}.$$

- Lower bound:

$$\begin{aligned}\Phi_T - \Phi_0 = \log \sum_{i=1}^{N} e^{-\eta L_{T,i}} - \log N &\geq \log \max_{i=1}^{N} e^{-\eta L_{T,i}} - \log N \\ &= -\eta \min_{i=1}^{N} L_{T,i} - \log N.\end{aligned}$$

- Comparison:

$$-\eta \min_{i=1}^{N} L_{T,i} - \log N \leq -\eta \sum_{t=1}^{T} L(\widehat{y}_t, y_t) + \frac{\eta^2 T}{8}$$

$$\Rightarrow \sum_{t=1}^{T} L(\widehat{y}_t, y_t) - \min_{i=1}^{N} L_{T,i} \leq \frac{\log N}{\eta} + \frac{\eta T}{8}.$$

Exponential Weighted Avg - Notes

- Advantage: bound on regret per bound is of the form $\frac{R_T}{T} = O\Big(\sqrt{\frac{\log(N)}{T}}\Big)$.
- Disadvantage: choice of η requires knowledge of horizon T.

Doubling Trick

- Idea: divide time into periods $[2^k, 2^{k+1}-1]$ of length 2^k with $k=0, \ldots, n$, $T \geq 2^n - 1$, and choose $\eta_k = \sqrt{\frac{8 \log N}{2^k}}$ in each period.

- Theorem: with the same assumptions as before, for any T, the following holds:

$$\boxed{\text{Regret}(T) \leq \frac{\sqrt{2}}{\sqrt{2}-1} \sqrt{(T/2) \log N} + \sqrt{\log N/2}.}$$

Doubling Trick - Proof

- By the previous theorem, for any $I_k = [2^k, 2^{k+1} - 1]$,

$$L_{I_k} - \min_{i=1}^{N} L_{I_k,i} \leq \sqrt{2^k/2 \, \log N}.$$

Thus, $L_T = \sum_{k=0}^{n} L_{I_k} \leq \sum_{k=0}^{n} \min_{i=1}^{N} L_{I_k,i} + \sum_{k=0}^{n} \sqrt{2^k \, (\log N)/2}$

$$\leq \min_{i=1}^{N} L_{T,i} + \sum_{k=0}^{n} 2^{\frac{k}{2}} \sqrt{(\log N)/2}.$$

with

$$\sum_{i=0}^{n} 2^{\frac{k}{2}} = \frac{\sqrt{2}^{n+1} - 1}{\sqrt{2} - 1} = \frac{2^{(n+1)/2} - 1}{\sqrt{2} - 1} \leq \frac{\sqrt{2}\sqrt{T+1} - 1}{\sqrt{2} - 1} \leq \frac{\sqrt{2}(\sqrt{T} + 1) - 1}{\sqrt{2} - 1} \leq \frac{\sqrt{2}\sqrt{T}}{\sqrt{2} - 1} + 1.$$

Notes

- Doubling trick used in a variety of other contexts and proofs.
- More general method, learning parameter function of time: $\eta_t = \sqrt{(8 \log N)/t}$. Constant factor improvement:

$$\boxed{\text{Regret}(T) \leq 2\sqrt{(T/2)\log N} + \sqrt{(1/8)\log N}.}$$

This Lecture

- Prediction with expert advice
- Linear classification

Perceptron Algorithm

(Rosenblatt, 1958)

Perceptron($\mathbf{w}_0$)

$\mathbf{w}_1 \leftarrow \mathbf{w}_0$ $\quad \triangleright$ typically $\mathbf{w}_0 = \mathbf{0}$

for $t \leftarrow 1$ **to** T **do**

  Receive($\mathbf{x}_t$)

  $\widehat{y}_t \leftarrow \operatorname{sgn}(\mathbf{w}_t \cdot \mathbf{x}_t)$

  Receive(y_t)

  if $(\widehat{y}_t \neq y_t)$ **then**

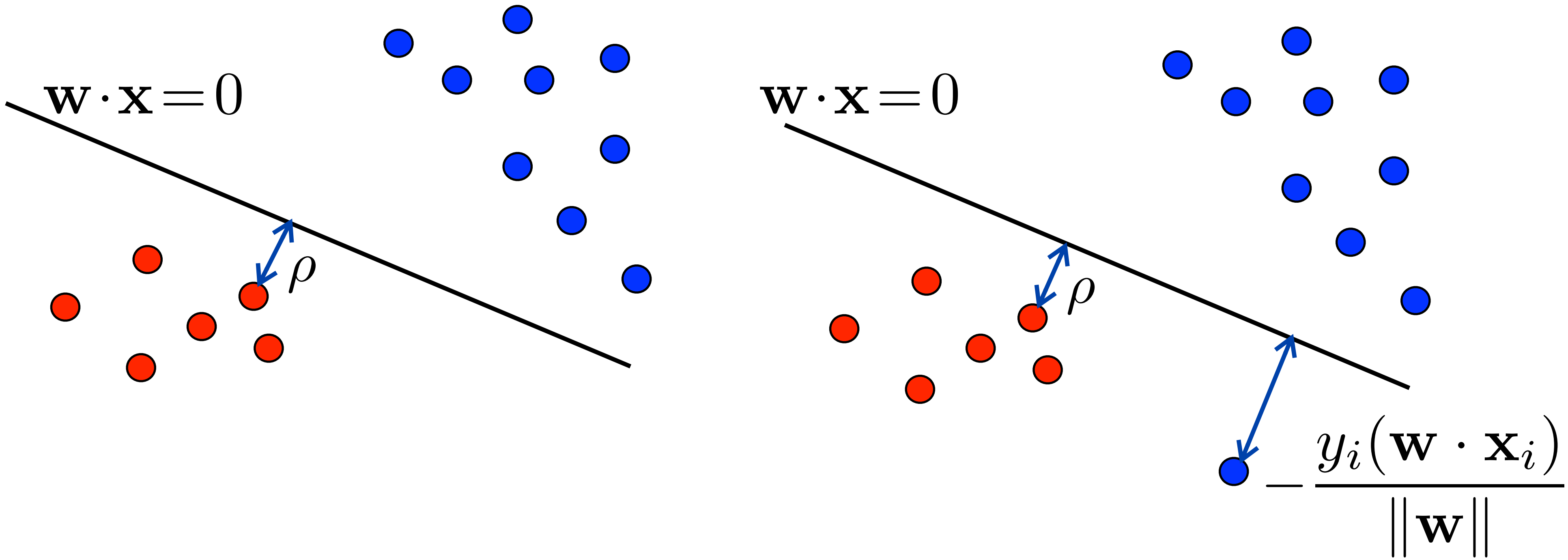
    $\mathbf{w}_{t+1} \leftarrow \mathbf{w}_t + y_t \mathbf{x}_t$ $\quad \triangleright$ more generally $\eta y_t \mathbf{x}_t, \eta > 0$

  else $\mathbf{w}_{t+1} \leftarrow \mathbf{w}_t$

return $\mathbf{w}_{T+1}$

Separating Hyperplane

- Margin and errors



Perceptron = Stochastic Gradient Descent

- **Objective function**: convex but not differentiable.

$$F(\mathbf{w}) = \frac{1}{T}\sum_{t=1}^{T} \max\Big(0, -y_t(\mathbf{w}\cdot\mathbf{x}_t)\Big) = \operatorname*{E}_{\mathbf{x}\sim\widehat{D}}[f(\mathbf{w},\mathbf{x})]$$

with $f(\mathbf{w},\mathbf{x}) = \max\big(0, -y(\mathbf{w}\cdot\mathbf{x})\big)$.

- **Stochastic gradient**: for each $\mathbf{x}_t$, the update is

$$\mathbf{w}_{t+1} \leftarrow \begin{cases} \mathbf{w}_t - \eta\nabla_{\mathbf{w}} f(\mathbf{w}_t, \mathbf{x}_t) & \text{if differentiable} \\ \mathbf{w}_t & \text{otherwise,} \end{cases}$$

where $\eta > 0$ is a learning rate parameter.

- **Here**:

$$\mathbf{w}_{t+1} \leftarrow \begin{cases} \mathbf{w}_t + \eta y_t \mathbf{x}_t & \text{if } y_t(\mathbf{w}_t\cdot\mathbf{x}_t) < 0 \\ \mathbf{w}_t & \text{otherwise.} \end{cases}$$

Perceptron Algorithm - Bound

(Novikoff, 1962)

- Theorem: Assume that $\|x_t\| \leq R$ for all $t \in [1, T]$ and that for some $\rho > 0$ and $\mathbf{v} \in \mathbb{R}^N$, for all $t \in [1, T]$,

$$\rho \leq \frac{y_t(\mathbf{v} \cdot \mathbf{x}_t)}{\|\mathbf{v}\|}.$$

  Then, the number of mistakes made by the perceptron algorithm is bounded by $\boxed{R^2/\rho^2}$.

- Proof: Let I be the set of ts at which there is an update and let M be the total number of updates.

- Summing up the assumption inequalities gives:

$$
\begin{aligned}
M\rho &\leq \frac{\mathbf{v} \cdot \sum_{t \in I} y_t \mathbf{x}_t}{\|\mathbf{v}\|} \\
&= \frac{\mathbf{v} \cdot \sum_{t \in I} (\mathbf{w}_{t+1} - \mathbf{w}_t)}{\|\mathbf{v}\|} && \text{(definition of updates)} \\
&= \frac{\mathbf{v} \cdot \mathbf{w}_{T+1}}{\|\mathbf{v}\|} \\
&\leq \|\mathbf{w}_{T+1}\| && \text{(Cauchy-Schwarz ineq.)} \\
&= \|\mathbf{w}_{t_m} + y_{t_m} \mathbf{x}_{t_m}\| && (t_m \text{ largest } t \text{ in } I) \\
&= \Big[\|\mathbf{w}_{t_m}\|^2 + \|\mathbf{x}_{t_m}\|^2 + 2 \underbrace{y_{t_m} \mathbf{w}_{t_m} \cdot \mathbf{x}_{t_m}}_{\leq 0}\Big]^{1/2} \\
&\leq \Big[\|\mathbf{w}_{t_m}\|^2 + R^2\Big]^{1/2} \\
&\leq \Big[M R^2\Big]^{1/2} = \sqrt{M} R. && \text{(applying the same to previous } t\text{s in } I)
\end{aligned}
$$

- Notes:
  - bound independent of dimension and tight.
  - convergence can be slow for small margin, it can be in $\Omega(2^N)$.
  - among the many variants: voted perceptron algorithm. Predict according to

$$\operatorname{sign}\Big(\big(\sum_{t \in I} c_t \mathbf{w}_t\big) \cdot \mathbf{x}\Big),$$

    where c_t is the number of iterations $\mathbf{w}_t$ survives.
  - $\{x_t : t \in I\}$ are the support vectors for the perceptron algorithm.
  - non-separable case: does not converge.

Perceptron - Leave-One-Out Analysis

- Theorem: Let h_S be the hypothesis returned by the perceptron algorithm for sample $S=(x_1,\ldots,x_T)\sim D$ and let $M(S)$ be the number of updates defining h_S. Then,

$$\mathop{\mathrm{E}}_{S\sim D^m}[R(h_S)] \leq \mathop{\mathrm{E}}_{S\sim D^{m+1}}\left[\frac{\min(M(S), R^2_{m+1}/\rho^2_{m+1})}{m+1}\right].$$

- Proof: Let $S\sim D^{m+1}$ be a sample linearly separable and let $\mathbf{x}\in S$. If $h_{S-\{\mathbf{x}\}}$ misclassifies $\mathbf{x}$, then $\mathbf{x}$ must be a 'support vector' for h_S (update at $\mathbf{x}$). Thus,

$$\widehat{R}_{\mathrm{loo}}(\mathrm{perceptron}) \leq \frac{M(S)}{m+1}.$$

Perceptron - Non-Separable Bound

(MM and Rostamizadeh, 2013)

- Theorem: let I denote the set of rounds at which the Perceptron algorithm makes an update when processing $\mathbf{x}_1, \ldots, \mathbf{x}_T$ and let $M_T = |I|$. Then,

$$\boxed{M_T \leq \inf_{\rho > 0, \|\mathbf{u}\|_2 \leq 1} \left[\sqrt{L_\rho(\mathbf{u})} + \frac{R}{\rho} \right]^2},$$

where $R = \max_{t \in I} \|\mathbf{x}_t\|$

$$L_\rho(\mathbf{u}) = \sum_{t \in I} \left(1 - \frac{y_t(\mathbf{u} \cdot \mathbf{x}_t)}{\rho}\right)_+.$$

- Proof: for any t, $1-\frac{y_t(\mathbf{u}\cdot\mathbf{x}_t)}{\rho} \leq \big(1-\frac{y_t(\mathbf{u}\cdot\mathbf{x}_t)}{\rho}\big)_+$, summing up these inequalities for $t \in I$ yields:

$$\begin{aligned} M_T &\leq \sum_{t\in I}\left(1-\frac{y_t(\mathbf{u}\cdot\mathbf{x}_t)}{\rho}\right)_+ + \sum_{t\in I}\frac{y_t(\mathbf{u}\cdot\mathbf{x}_t)}{\rho} \\ &\leq L_\rho(\mathbf{u}) + \frac{\sqrt{M_T}R}{\rho}, \end{aligned}$$

  by upper-bounding $\sum_{t\in I}(y_t\mathbf{u}\cdot\mathbf{x}_t)$ as in the proof for the separable case.

- solving the second-degree inequality

$$M_T \leq L_\rho(\mathbf{u}) + \frac{\sqrt{M_T}R}{\rho},$$

  gives $\sqrt{M_T} \leq \dfrac{\frac{R}{\rho}+\sqrt{\frac{R^2}{\rho^2}+4L_\rho(\mathbf{u})}}{2} \leq \dfrac{R}{\rho}+\sqrt{L_\rho(\mathbf{u})}.$

Non-Separable Case - L2 Bound

(Freund and Schapire, 1998; MM and Rostamizadeh, 2013)

- **Theorem**: let I denote the set of rounds at which the Perceptron algorithm makes an update when processing $\mathbf{x}_1, \ldots, \mathbf{x}_T$ and let $M_T = |I|$. Then,

$$M_T \leq \inf_{\rho>0, \|u\|_2 \leq 1} \left[\frac{\|\mathbf{L}_\rho(\mathbf{u})\|_2}{2} + \sqrt{\frac{\|\mathbf{L}_\rho(\mathbf{u})\|_2^2}{4} + \frac{\sqrt{\sum_{t \in I} \|\mathbf{x}_t\|^2}}{\rho}} \right]^2.$$

  - when $\|\mathbf{x}_t\| \leq R$ for all $t \in I$, this implies

$$\boxed{M_T \leq \inf_{\rho>0, \|u\|_2 \leq 1} \left(\frac{R}{\rho} + \|\mathbf{L}_\rho(\mathbf{u})\|_2 \right)^2},$$

where $\mathbf{L}_\rho(\mathbf{u}) = \left[\left(1 - \frac{y_t(\mathbf{u} \cdot \mathbf{x}_t)}{\rho}\right)_+ \right]_{t \in I}$.

- Proof: Reduce problem to separable case in higher dimension. Let $l_t = \left(1 - \frac{y_t \mathbf{u}\cdot\mathbf{x}_t}{\rho}\right)_+ 1_{t \in I}$, for $t \in [1, T]$.
  - Mapping (similar to trivial mapping):

$$\mathbf{x}_t = \begin{bmatrix} x_{t,1} \\ \vdots \\ x_{t,N} \end{bmatrix} \rightarrow \mathbf{x}'_t = \begin{array}{r} \\ \\ \\ \\ \\ \\ (N+t)\text{th component} \\ \\ \\ \\ \end{array} \begin{bmatrix} x_{t,1} \\ \vdots \\ x_{t,N} \\ 0 \\ \vdots \\ 0 \\ \Delta \\ 0 \\ \vdots \\ 0 \end{bmatrix} \qquad \mathbf{u} \rightarrow \mathbf{u}' = \begin{bmatrix} \frac{u_1}{Z} \\ \vdots \\ \frac{u_N}{Z} \\ \frac{y_1 \rho l_1}{\Delta Z} \\ \vdots \\ \frac{y_T \rho l_T}{\Delta Z} \end{bmatrix}$$

$$\|\mathbf{u}'\| = 1 \implies Z = \sqrt{1 + \frac{\rho^2 \|\mathbf{L}_\rho(\mathbf{u})\|^2}{\Delta^2}}.$$

- Observe that the Perceptron algorithm makes the same predictions and makes updates at the same rounds when processing $\mathbf{x}'_1, \ldots, \mathbf{x}'_T$.
- For any $t \in I$,

$$
\begin{aligned}
y_t(\mathbf{u}' \cdot \mathbf{x}'_t) &= y_t\Big(\frac{\mathbf{u} \cdot \mathbf{x}_t}{Z} + \Delta \frac{y_t \rho l_t}{Z\Delta}\Big) \\
&= \frac{y_t \mathbf{u} \cdot \mathbf{x}_t}{Z} + \frac{\rho l_t}{Z} \\
&= \frac{1}{Z}\big(y_t \mathbf{u} \cdot \mathbf{x}_t + [\rho - y_t(\mathbf{u} \cdot \mathbf{x}_t)]_+\big) \geq \frac{\rho}{Z}.
\end{aligned}
$$

- Summing up and using the proof in the separable case yields:

$$
M_T \frac{\rho}{Z} \leq \sum_{t \in I} y_t(\mathbf{u}' \cdot \mathbf{x}'_t) \leq \sqrt{\sum_{t \in I} \|\mathbf{x}'_t\|^2}.
$$

- The inequality can be rewritten as

$$M_T^2 \leq \Big(\frac{1}{\rho^2}+\frac{\|\mathbf{L}_\rho(\mathbf{u})\|^2}{\Delta^2}\Big)\Big(r^2+M_T\Delta^2\Big)=\frac{r^2}{\rho^2}+\frac{r^2\|\mathbf{L}_\rho(\mathbf{u})\|^2}{\Delta^2}+\frac{M_T\Delta^2}{\rho^2}+M_T\|\,\mathbf{L}_\rho(\mathbf{u})\|^2_2;$$

where $r=\sqrt{\sum_{t\in I}\|\mathbf{x}_t\|^2}$.

- Selecting Δ to minimize the bound gives $\Delta^2=\frac{\rho\|\mathbf{L}_\rho(\mathbf{u})\|_2 r}{\sqrt{M_T}}$ and leads to

$$M_T^2 \leq \frac{r^2}{\rho^2}+2\frac{\sqrt{M_T}\|\mathbf{L}_\rho(\mathbf{u})\|r}{\rho}+M_T\|\mathbf{L}_\rho(\mathbf{u})\|^2=(\tfrac{r}{\rho}+\sqrt{M_T}\|\mathbf{L}_\rho(\mathbf{u})\|_2)^2.$$

- Solving the second-degree inequality

$$M_T-\sqrt{M_T}\|\,\mathbf{L}_\rho(\mathbf{u})\|_2-\frac{r}{\rho}\leq 0$$

yields directly the first statement. The second one results from replacing r with $\sqrt{M_T}R$.

Dual Perceptron Algorithm

$\textsc{Dual-Perceptron}(\boldsymbol{\alpha}^0)$

$\boldsymbol{\alpha} \leftarrow \boldsymbol{\alpha}^0 \qquad \triangleright$ typically $\boldsymbol{\alpha}^0 = \mathbf{0}$
for $t \leftarrow 1$ **to** T **do**
  $\textsc{Receive}(\mathbf{x}_t)$
  $\widehat{y}_t \leftarrow \text{sgn}(\sum_{s=1}^{T} \alpha_s y_s (\mathbf{x}_s \cdot \mathbf{x}_t))$
  $\textsc{Receive}(y_t)$
  if $(\widehat{y}_t \neq y_t)$ **then**
    $\alpha_t \leftarrow \alpha_t + 1$
return $\boldsymbol{\alpha}$

Kernel Perceptron Algorithm

(Aizerman et al., 1964)

K PDS kernel.

$\textsc{Kernel-Perceptron}(\boldsymbol{\alpha}^0)$

$\boldsymbol{\alpha} \leftarrow \boldsymbol{\alpha}^0 \qquad \triangleright$ typically $\boldsymbol{\alpha}^0 = \mathbf{0}$

for $t \leftarrow 1$ **to** T **do**

  $\textsc{Receive}(x_t)$

  $\widehat{y}_t \leftarrow \operatorname{sgn}(\sum_{s=1}^{T} \alpha_s y_s K(x_s, x_t))$

  $\textsc{Receive}(y_t)$

  if $(\widehat{y}_t \neq y_t)$ **then**

    $\alpha_t \leftarrow \alpha_t + 1$

return $\boldsymbol{\alpha}$

Winnow Algorithm

(Littlestone, 1988)

$\textsc{Winnow}(\eta)$

$w_1 \leftarrow \mathbf{1}/N$
for $t \leftarrow 1$ **to** T **do**
  $\textsc{Receive}(\mathbf{x}_t)$
  $\widehat{y}_t \leftarrow \operatorname{sgn}(\mathbf{w}_t \cdot \mathbf{x}_t)$ $\quad\triangleright\quad y_t \in \{-1, +1\}$
  $\textsc{Receive}(y_t)$
  if $(\widehat{y}_t \neq y_t)$ **then**
    $Z_t \leftarrow \sum_{i=1}^{N} w_{t,i} \exp(\eta y_t x_{t,i})$
    for $i \leftarrow 1$ **to** N **do**
      $w_{t+1,i} \leftarrow \dfrac{w_{t,i} \exp(\eta y_t x_{t,i})}{Z_t}$
  else $\mathbf{w}_{t+1} \leftarrow \mathbf{w}_t$
return $\mathbf{w}_{T+1}$

Notes

- Winnow $=$ weighted majority:
  - for $y_{t,i} = x_{t,i} \in \{-1, +1\}$, $\operatorname{sgn}(\mathbf{w}_t \cdot \mathbf{x}_t)$ coincides with the majority vote.
  - multiplying by e^{η} or $e^{-\eta}$ the weight of correct or incorrect experts, is equivalent to multiplying by $\beta = e^{-2\eta}$ the weight of incorrect ones.
- Relationships with other algorithms: e.g., boosting and Perceptron (Winnow and Perceptron can be viewed as special instances of a general family).

Winnow Algorithm - Bound

- **Theorem**: Assume that $\|x_t\|_\infty \leq R_\infty$ for all $t \in [1, T]$ and that for some $\rho_\infty > 0$ and $\mathbf{v} \in \mathbb{R}^N$, $\mathbf{v} \geq 0$ for all $t \in [1, T]$,

$$\rho_\infty \leq \frac{y_t(\mathbf{v} \cdot \mathbf{x}_t)}{\|\mathbf{v}\|_1}.$$

  Then, the number of mistakes made by the Winnow algorithm is bounded by $\boxed{2\left(R_\infty^2/\rho_\infty^2\right)\log N}$.

- **Proof**: Let I be the set of ts at which there is an update and let M be the total number of updates.

Notes

- Comparison with perceptron bound:
  - dual norms: norms for $\mathbf{x}_t$ and $\mathbf{v}$.
  - similar bounds with different norms.
  - each advantageous in different cases:
    - Winnow bound favorable when a sparse set of experts can predict well. For example, if $\mathbf{v} = \mathbf{e}_1$ and $\mathbf{x}_t \in \{\pm 1\}^N$, $\log N$ vs N.
    - Perceptron favorable in opposite situation.

Winnow Algorithm - Bound

- **Potential:** $\Phi_t = \sum_{i=1}^{N} \frac{v_i}{\|\mathbf{v}\|} \log \frac{v_i/\|\mathbf{v}\|}{w_{t,i}}$. (relative entropy)
- **Upper bound:** for each t in I,

$$\begin{aligned}
\Phi_{t+1} - \Phi_t &= \sum_{i=1}^{N} \frac{v_i}{\|\mathbf{v}\|_1} \log \frac{w_{t,i}}{w_{t+1,i}} \\
&= \sum_{i=1}^{N} \frac{v_i}{\|\mathbf{v}\|_1} \log \frac{Z_t}{\exp(\eta y_t x_{t,i})} \\
&= \log Z_t - \eta \sum_{i=1}^{N} \frac{v_i}{\|\mathbf{v}\|_1} y_t x_{t,i} \\
&\leq \log \Big[\sum_{i=1}^{N} w_{t,i} \exp(\eta y_t x_{t,i}) \Big] - \eta \rho_\infty \\
&= \log \mathop{\mathrm{E}}_{\mathbf{w}_t} \Big[\exp(\eta y_t x_t) \Big] - \eta \rho_\infty \\
\text{(Hoeffding)} &\leq \log \Big[\exp(\eta^2 (2R_\infty)^2/8) \Big] + \underbrace{\eta y_t \mathbf{w}_t \cdot \mathbf{x}_t}_{\leq 0} - \eta \rho_\infty \\
&\leq \eta^2 R_\infty^2/2 - \eta \rho_\infty .
\end{aligned}$$

Winnow Algorithm - Bound

- **Upper bound:** summing up the inequalities yields

$$\Phi_{T+1} - \Phi_1 \leq M(\eta^2 R_\infty^2/2 - \eta\rho_\infty).$$

- **Lower bound:** note that

$$\Phi_1 = \sum_{i=1}^N \frac{v_i}{\|\mathbf{v}\|_1} \log \frac{v_i/\|\mathbf{v}\|_1}{1/N} = \log N + \sum_{i=1}^N \frac{v_i}{\|\mathbf{v}\|_1} \log \frac{v_i}{\|\mathbf{v}\|_1} \leq \log N$$

and for all $t, \Phi_t \geq 0$ (property of relative entropy).

Thus, $\Phi_{T+1} - \Phi_1 \geq 0 - \log N = -\log N.$

- **Comparison:** $-\log N \leq M(\eta^2 R_\infty^2/2 - \eta\rho_\infty)$. For $\eta = \frac{\rho_\infty}{R_\infty^2}$ we obtain

$$M \leq 2 \log N \frac{R_\infty^2}{\rho_\infty^2}.$$

Conclusion

- On-line learning:
  - wide and fast-growing literature.
  - many related topics, e.g., game theory, text compression, convex optimization.
  - online to batch bounds and techniques.
  - online version of batch algorithms, e.g., regression algorithms (see regression lecture).

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Appendix

SVMs - Leave-One-Out Analysis

(Vapnik, 1995)

- **Theorem**: let h_S be the optimal hyperplane for a sample S and let $N_{\mathrm{SV}}(S)$ be the number of support vectors defining h_S. Then,

$$\mathop{\mathrm{E}}_{S \sim D^m}[R(h_S)] \leq \mathop{\mathrm{E}}_{S \sim D^{m+1}}\left[\frac{\min(N_{\mathrm{SV}}(S), R^2_{m+1}/\rho^2_{m+1})}{m+1}\right].$$

- **Proof**: one part proven in lecture 4. The other part due to $\alpha_i \geq 1/R^2_{m+1}$ for $\mathbf{x}_i$ misclassified by SVMs.

Comparison

- Bounds on expected error, not high probability statements.
- Leave-one-out bounds not sufficient to distinguish SVMs and perceptron algorithm. Note however:
  - same maximum margin ρ_{m+1} can be used in both.
  - but different radius R_{m+1} of support vectors.
- Difference: margin distribution.

Foundations of Machine Learning
Ranking

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Motivation

- Very large data sets:
  - too large to display or process.
  - limited resources, need priorities.
  - $\longrightarrow$ ranking more desirable than classification.
- Applications:
  - search engines, information extraction.
  - decision making, auctions, fraud detection.
- Can we learn to predict ranking accurately?

Related Problem

- Rank aggregation: given n candidates and k voters each giving a ranking of the candidates, find ordering as close as possible to these.
  - closeness measured in number of pairwise misrankings.
  - problem NP-hard even for $k=4$ (Dwork et al., 2001).

This Talk

- Score-based ranking
- Preference-based ranking

Score-Based Setting

- Single stage: learning algorithm
  - receives labeled sample of pairwise preferences;
  - returns scoring function $h\colon U \rightarrow \mathbb{R}$.
- Drawbacks:
  - h induces a linear ordering for full set U.
  - does not match a query-based scenario.
- Advantages:
  - efficient algorithms.
  - good theory: VC bounds, margin bounds, stability bounds (FISS 03, RCMS 05, AN 05, AGHHR 05, CMR 07).

Score-Based Ranking

- **Training data**: sample of i.i.d. labeled pairs drawn from $U \times U$ according to some distribution D,

$$S = \Big((x_1, x'_1, y_1), \ldots, (x_m, x'_m, y_m)\Big) \in U \times U \times \{-1, 0, +1\},$$

with $y_i = \begin{cases} +1 & \text{if } x'_i >_{\text{pref}} x_i \\ 0 & \text{if } x_i =_{\text{pref}} x'_i \text{ or no information} \\ -1 & \text{if } x'_i <_{\text{pref}} x_i. \end{cases}$

- **Problem**: find hypothesis $h : U \to \mathbb{R}$ in H with small generalization error

$$R(h) = \Pr_{(x,x') \sim D} \Big[(f(x, x') \neq 0) \wedge (f(x, x')\big(h(x') - h(x)\big) \leq 0) \Big].$$

Notes

- Empirical error:

$$\widehat{R}(h) = \frac{1}{m} \sum_{i=1}^{m} 1_{(y_i \neq 0) \wedge (y_i(h(x'_i) - h(x_i)) \leq 0)} \,.$$

- The relation $x \,\mathcal{R}\, x' \Leftrightarrow f(x, x') = 1$ may be non-transitive (needs not even be anti-symmetric).
- Problem different from classification.

Distributional Assumptions

- Distribution over points: m points (literature).
  - labels for pairs.
  - $\longrightarrow$ squared number of examples $O(m^2)$.
  - dependency issue.
- Distribution over pairs: m pairs.
  - label for each pair received.
  - independence assumption.
  - same (linear) number of examples.

Confidence Margin in Ranking

- Labels assumed to be in $\{+1, -1\}$.
- Empirical margin loss for ranking: for $\rho > 0$,

$$\widehat{R}_\rho(h) = \frac{1}{m} \sum_{i=1}^{m} \Phi_\rho\Big(y_i\big(h(x'_i) - h(x_i)\big)\Big).$$

$$\widehat{R}_\rho(h) \leq \frac{1}{m} \sum_{i=1}^{m} 1_{y_i[h(x'_i) - h(x_i)] \leq \rho}.$$

Marginal Rademacher Complexities

- Distributions:
  - D_1 marginal distribution with respect to the first element of the pairs;
  - D_2 marginal distribution with respect to second element of the pairs.
- Samples: $S_1 = \big((x_1, y_1), \ldots, (x_m, y_m)\big)$
  $S_2 = \big((x'_1, y_1), \ldots, (x'_m, y_m)\big).$
- Marginal Rademacher complexities:

$$\mathfrak{R}_m^{D_1}(H) = \mathrm{E}[\widehat{\mathfrak{R}}_{S_1}(H)] \qquad \mathfrak{R}_m^{D_2}(H) = \mathrm{E}[\widehat{\mathfrak{R}}_{S_2}(H)].$$

Ranking Margin Bound

(Boyd, Cortes, MM, and Radovanovich 2012; MM, Rostamizadeh, and Talwalkar, 2012)

- Theorem: let H be a family of real-valued functions. Fix $\rho > 0$, then, for any $\delta > 0$, with probability at least $1-\delta$ over the choice of a sample of size m, the following holds for all $h \in H$:

$$R(h) \leq \widehat{R}_\rho(h) + \frac{2}{\rho}\Big(\mathfrak{R}_m^{D_1}(H) + \mathfrak{R}_m^{D_2}(H)\Big) + \sqrt{\frac{\log \frac{1}{\delta}}{2m}}.$$

Proof

- **Define:** $\widetilde{\mathcal{H}} = \{z = ((x, x'), y) \mapsto y[h(x') - h(x)] \colon h \in \mathcal{H}\}$. Then, by the general margin bound, with probability at least $1-\delta$,

$$\mathbb{E}\left[\Phi_\rho(y[h(x') - h(x)])\right] \leq \widehat{R}_{S,\rho}(h) + 2\mathfrak{R}_m\big(\Phi_\rho \circ \widetilde{\mathcal{H}}\big) + \sqrt{\frac{\log \frac{1}{\delta}}{2m}}.$$

- We have $\mathfrak{R}_m(\Phi_\rho \circ \widehat{\mathcal{H}}) \leq \frac{1}{\rho}\mathfrak{R}_m(\widehat{\mathcal{H}})$ and

$$\begin{aligned}
\mathfrak{R}_m(\widetilde{\mathcal{H}}) &= \frac{1}{m} \mathop{\mathbb{E}}_{S,\sigma}\left[\sup_{h \in \mathcal{H}} \sum_{i=1}^m \sigma_i y_i (h(x'_i) - h(x_i))\right] \\
&= \frac{1}{m} \mathop{\mathbb{E}}_{S,\sigma}\left[\sup_{h \in \mathcal{H}} \sum_{i=1}^m \sigma_i (h(x'_i) - h(x_i))\right] && (y_i\sigma_i \text{ and } \sigma_i\text{: same distrib.}) \\
&\leq \frac{1}{m} \mathop{\mathbb{E}}_{S,\sigma}\left[\sup_{h \in \mathcal{H}} \sum_{i=1}^m \sigma_i h(x'_i) + \sup_{h \in \mathcal{H}} \sum_{i=1}^m \sigma_i h(x_i)\right] && (\text{by sub-additivity of sup}) \\
&= \mathop{\mathbb{E}}_{S}\left[\mathfrak{R}_{S_2}(\mathcal{H}) + \mathfrak{R}_{S_1}(\mathcal{H})\right] && (\text{definition of } S_1 \text{ and } S_2).
\end{aligned}$$

Ranking with SVMs

see for example (Joachims, 2002)

- Optimization problem: application of SVMs.

$$\min_{\mathbf{w},\boldsymbol{\xi}} \frac{1}{2}\|\mathbf{w}\|^2 + C\sum_{i=1}^{m}\xi_i$$

$$\text{subject to: } y_i\Big[\mathbf{w}\cdot\big(\boldsymbol{\Phi}(x_i')-\boldsymbol{\Phi}(x_i)\big)\Big] \geq 1-\xi_i$$

$$\xi_i \geq 0, \quad \forall i \in [1,m].$$

- Decision function:

$$h\colon x \mapsto \mathbf{w}\cdot\boldsymbol{\Phi}(x)+b.$$

Notes

- The algorithm coincides with SVMs using feature mapping

$$(x, x') \mapsto \mathbf{\Psi}(x, x') = \mathbf{\Phi}(x') - \mathbf{\Phi}(x).$$

- Can be used with kernels:

$$\begin{aligned} K'((x_i, x'_i), (x_j, x'_j)) &= \mathbf{\Psi}(x_i, x'_i) \cdot \mathbf{\Psi}(x_j, x'_j) \\ &= K(x_i, x_j) + K(x'_i, x'_j) - K(x'_i, x_j) - K(x_i, x'_j). \end{aligned}$$

- Algorithm directly based on margin bound.

Boosting for Ranking

- Use weak ranking algorithm and create stronger ranking algorithm.
- Ensemble method: combine base rankers returned by weak ranking algorithm.
- Finding simple relatively accurate base rankers often not hard.
- How should base rankers be combined?

CD RankBoost

(Freund et al., 2003; Rudin et al., 2005)

$$H \subseteq \{0,1\}^X. \epsilon_t^0 + \epsilon_t^+ + \epsilon_t^- = 1, \epsilon_t^s(h) = \Pr_{(x,x')\sim D_t}\Big[\operatorname{sgn}\big(f(x,x')(h(x')-h(x))\big) = s\Big].$$

$\textsc{RankBoost}(S = ((x_1, x_1', y_1) \ldots, (x_m, x_m', y_m)))$

$$
\begin{array}{l}
\textbf{for } i \leftarrow 1 \textbf{ to } m \textbf{ do}\\
\qquad D_1(x_i, x_i') \leftarrow \frac{1}{m}\\
\textbf{for } t \leftarrow 1 \textbf{ to } T \textbf{ do}\\
\qquad h_t \leftarrow \text{base ranker in } H \text{ with smallest } \epsilon_t^- - \epsilon_t^+ = -\operatorname{E}_{i\sim D_t}\Big[y_i\big(h_t(x_i') - h_t(x_i)\big)\Big]\\
\qquad \alpha_t \leftarrow \frac{1}{2}\log\frac{\epsilon_t^+}{\epsilon_t^-}\\
\qquad Z_t \leftarrow \epsilon_t^0 + 2[\epsilon_t^+ \epsilon_t^-]^{\frac{1}{2}} \qquad \triangleright \text{normalization factor}\\
\qquad \textbf{for } i \leftarrow 1 \textbf{ to } m \textbf{ do}\\
\qquad\qquad D_{t+1}(x_i, x_i') \leftarrow \frac{D_t(x_i, x_i')\exp\Big[-\alpha_t y_i\Big(h_t(x_i') - h_t(x_i)\Big)\Big]}{Z_t}\\
\varphi_T \leftarrow \sum_{t=1}^T \alpha_t h_t\\
\textbf{return } \varphi_T
\end{array}
$$

Notes

- Distributions D_t over pairs of sample points:
  - originally uniform.
  - at each round, the weight of a misclassified example is increased.
  - observation: $D_{t+1}(x, x') = \frac{e^{-y[\varphi_t(x') - \varphi_t(x)]}}{|S| \prod_{s=1}^t Z_s}$, since

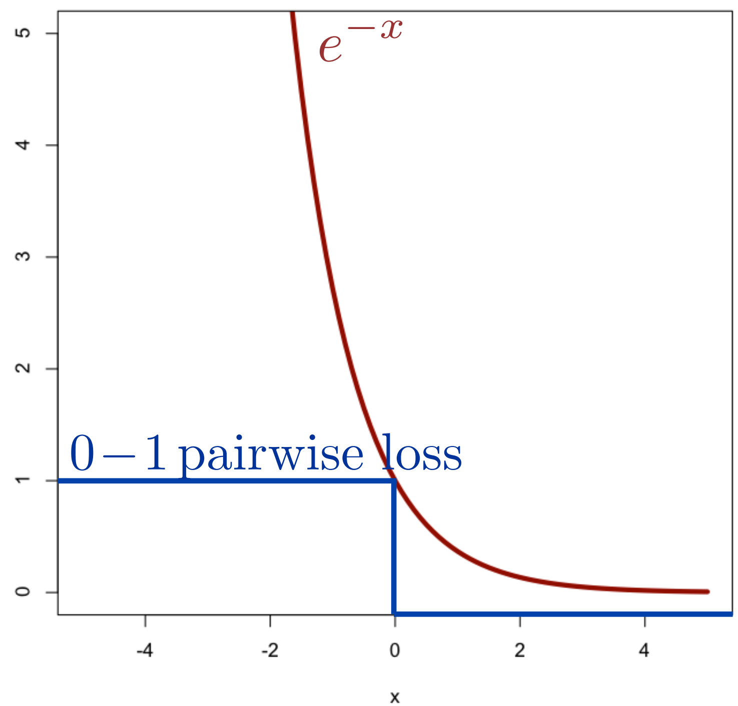
$$D_{t+1}(x, x') = \frac{D_t(x, x') e^{-y\alpha_t[h_t(x') - h_t(x)]}}{Z_t} = \frac{1}{|S|} \frac{e^{-y \sum_{s=1}^t \alpha_s [h_s(x') - h_s(x)]}}{\prod_{s=1}^t Z_s}.$$

- weight assigned to base classifier h_t: α_t directly depends on the accuracy of h_t at round t .

Coordinate Descent RankBoost

- **Objective Function**: convex and differentiable.

$$F(\boldsymbol{\alpha}) = \sum_{(x,x',y)\in S} e^{-y[\varphi_T(x')-\varphi_T(x)]} = \sum_{(x,x',y)\in S} \exp\Big(-y\sum_{t=1}^{T}\alpha_t[h_t(x')-h_t(x)]\Big).$$



- Direction: unit vector $\mathbf{e}_t$ with

$$\mathbf{e}_t = \operatorname*{argmin}_t \left.\frac{dF(\boldsymbol{\alpha} + \eta\mathbf{e}_t)}{d\eta}\right|_{\eta=0}.$$

- Since $F(\boldsymbol{\alpha} + \eta\mathbf{e}_t) = \sum_{(x,x',y)\in S} e^{-y\sum_{s=1}^T \alpha_s[h_s(x')-h_s(x)]} e^{-y\eta[h_t(x')-h_t(x)]}$,

$$\begin{aligned}
\left.\frac{dF(\alpha + \eta e_t)}{d\eta}\right|_{\eta=0} &= -\sum_{(x,x',y)\in S} y[h_t(x') - h_t(x)] \exp\Big[-y\sum_{s=1}^T \alpha_s[h_s(x') - h_s(x)]\Big] \\
&= -\sum_{(x,x',y)\in S} y[h_t(x') - h_t(x)] D_{T+1}(x,x')\Big[m\prod_{s=1}^T Z_s\Big] \\
&= \boxed{-[\epsilon_t^+ - \epsilon_t^-]}\Big[m\prod_{s=1}^T Z_s\Big].
\end{aligned}$$

Thus, direction corresponding to base classifier selected by the algorithm.

- **Step size**: obtained via

$$\frac{dF(\boldsymbol{\alpha} + \eta \mathbf{e}_t)}{d\eta} = 0$$

$$\Leftrightarrow -\sum_{(x,x',y)\in S} y[h_t(x') - h_t(x)] \exp\Big[-y\sum_{s=1}^{T} \alpha_s [h_s(x') - h_s(x)]\Big] e^{-y[h_t(x')-h_t(x)]\eta} = 0$$

$$\Leftrightarrow -\sum_{(x,x',y)\in S} y[h_t(x') - h_t(x)] D_{T+1}(x,x') \Big[m \prod_{s=1}^{T} Z_s \Big] e^{-y[h_t(x')-h_t(x)]\eta} = 0$$

$$\Leftrightarrow -\sum_{(x,x',y)\in S} y[h_t(x') - h_t(x)] D_{T+1}(x,x') e^{-y[h_t(x')-h_t(x)]\eta} = 0$$

$$\Leftrightarrow -[\epsilon_t^+ e^{-\eta} - \epsilon_t^- e^{\eta}] = 0$$

$$\Leftrightarrow \boxed{\eta = \frac{1}{2}\log\frac{\epsilon_t^+}{\epsilon_t^-}}.$$

Thus, step size matches base classifier weight used in algorithm.

Bipartite Ranking

- Training data:
  - sample of negative points drawn according to D_-
$$S_- = (x_1, \ldots, x_m) \in U.$$
  - sample of positive points drawn according to D_+
$$S_+ = (x'_1, \ldots, x'_{m'}) \in U.$$

- Problem: find hypothesis $h \colon U \to \mathbb{R}$ in H with small generalization error

$$R_D(h) = \Pr_{x \sim D_-, x' \sim D_+} \Big[h(x') < h(x) \Big].$$

Properties

- Connection between AdaBoost and RankBoost (Cortes & MM, 04; Rudin et al., 05).
  - if constant base ranker used.
  - relationship between objective functions.
- More efficient algorithm in this special case (Freund et al., 2003).
- Bipartite ranking results typically reported in terms of AUC.

AdaBoost and CD RankBoost

- Objective functions: comparison.

$$
\begin{aligned}
F_{\text{Ada}}(\boldsymbol{\alpha}) &= \sum_{x_i \in S_- \cup S_+} \exp\left(-y_i f(x_i)\right) \\
&= \sum_{x_i \in S_-} \exp\left(+f(x_i)\right) + \sum_{x_i \in S_+} \exp\left(-f(x_i)\right) \\
&= F_-(\alpha) + F_+(\alpha).
\end{aligned}
$$

$$
\begin{aligned}
F_{\text{Rank}}(\boldsymbol{\alpha}) &= \sum_{(i,j) \in S_- \times S_+} \exp\Big(-\left[f(x_j) - f(x_i)\right]\Big) \\
&= \sum_{(i,j) \in S_- \times S_+} \exp\left(+f(x_i)\right) \exp\left(-f(x_j)\right) \\
&= F_-(\alpha) F_+(\alpha).
\end{aligned}
$$

AdaBoost and CD RankBoost

(Rudin et al., 2005)

- **Property:** AdaBoost (non-separable case).
  - constant base learner $h=1$ $\longrightarrow$ equal contribution of positive and negative points (in the limit).
  - consequence: AdaBoost asymptotically achieves optimum of CD RankBoost objective.
- **Observations:** if $F_+(\boldsymbol{\alpha}) = F_-(\boldsymbol{\alpha})$,

$$\begin{aligned} d(F_{\text{Rank}}) &= F_+ d(F_-) + F_- d(F_+) \\ &= F_+ \big(d(F_-) + d(F_+) \big) \\ &= F_+ d(F_{\text{Ada}}). \end{aligned}$$

Bipartite RankBoost - Efficiency

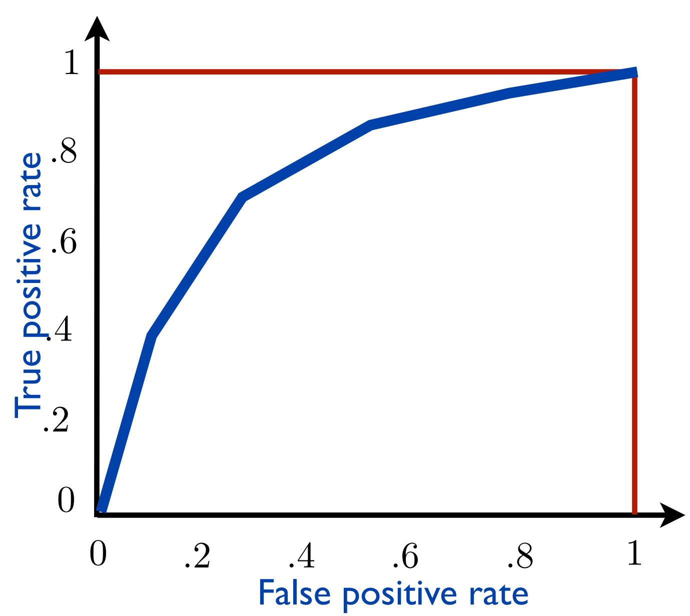
- Decomposition of distribution: for $(x, x') \in (S_-, S_+)$,
$$D(x, x') = D_-(x) D_+(x').$$
- Thus,
$$\begin{aligned} D_{t+1}(x, x') &= \frac{D_t(x, x') e^{-\alpha_t [h_t(x') - h_t(x)]}}{Z_t} \\ &= \frac{D_{t,-}(x) e^{\alpha_t h_t(x)}}{Z_{t,-}} \frac{D_{t,+}(x') e^{-\alpha_t h_t(x')}}{Z_{t,+}}, \end{aligned}$$

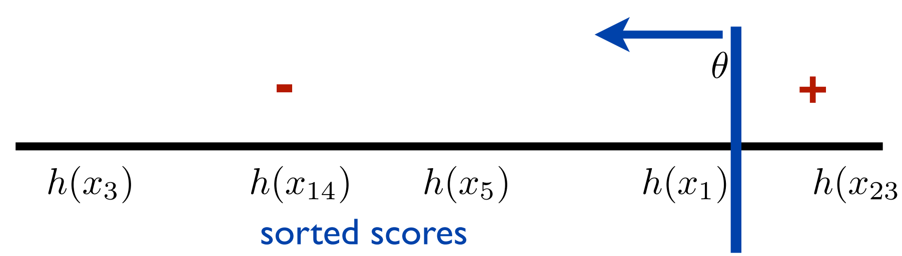
with $Z_{t,-} = \sum_{x \in S_-} D_{t,-}(x) e^{\alpha_t h_t(x)} \quad Z_{t,+} = \sum_{x' \in S_+} D_{t,+}(x') e^{-\alpha_t h_t(x')}.$

ROC Curve

(Egan, 1975)

- Definition: the receiver operating characteristic (ROC) curve is a plot of the true positive rate (TP) vs. false positive rate (FP).
  - TP: % positive points correctly labeled positive.
  - FP: % negative points incorrectly labeled positive.

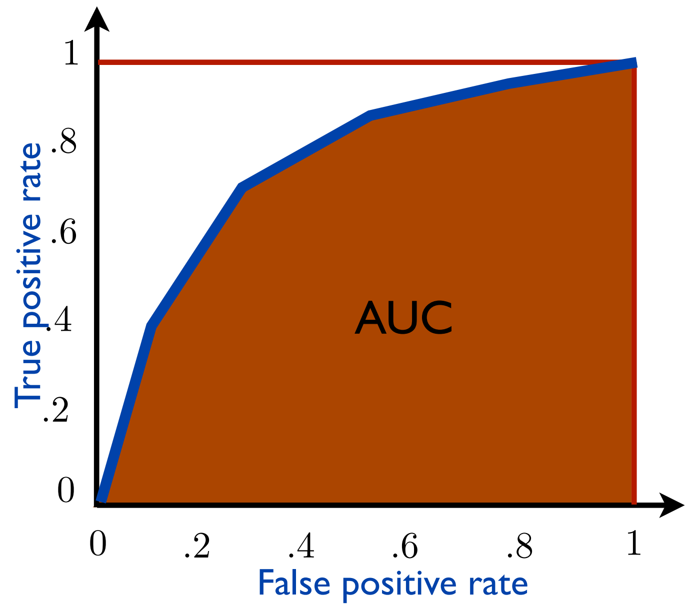




Area under the ROC Curve (AUC)

(Hanley and McNeil, 1982)

- Definition: the AUC is the area under the ROC curve. Measure of ranking quality.



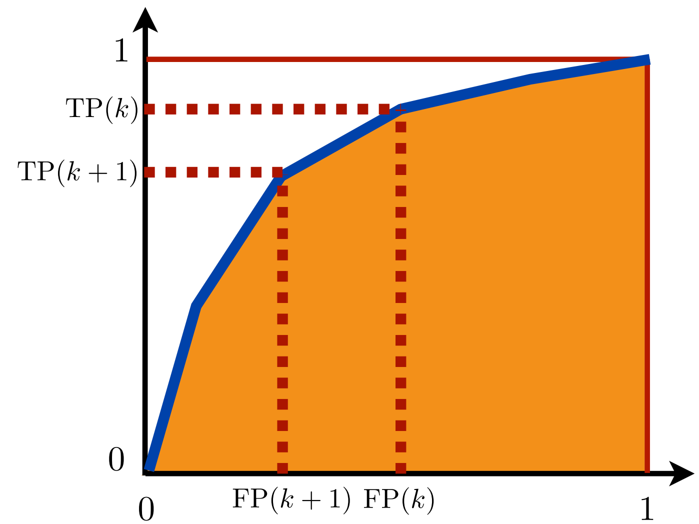
- Equivalently,

$$\mathrm{AUC}(h) = \frac{1}{m_- m_+} \sum_{i=1}^{m_-} \sum_{j=1}^{m_+} 1_{h(x_i) < h(x'_j)} = \Pr_{\substack{x \sim \widehat{D}_- \\ x' \sim \widehat{D}_+}} [h(x') > h(x)]$$

$$= 1 - \widehat{R}(h).$$

Proof

$$\begin{aligned}
\mathrm{AUC} &= \sum_{k=1}^{m-1} \frac{[\mathrm{TP}(k)+\mathrm{TP}(k+1)][\mathrm{FP}(k)-\mathrm{FP}(k+1)]}{2} && \text{(trapezoid area)}\\
&= \sum_{k=1}^{m-1} \frac{\sum_{l=k+1}^{m} 1_{y_l=+1} + \frac{1}{2} 1_{y_k=+1}}{m_+} \frac{1_{y_k=-1}}{m_-}\\
&= \frac{1}{m_+ m_-} \sum_{k=1}^{m-1} \sum_{l=k+1}^{m} 1_{y_l=+1} 1_{y_k=-1} && (1_{y_k=+1} 1_{y_k=-1} = 0)\\
&= \frac{1}{m_+ m_-} \sum_{k=1}^{m} \sum_{l=1}^{m} 1_{y_k=-1} 1_{y_l=+1} 1_{k<l}\\
&= \frac{1}{m_- m_+} \sum_{i=1}^{m_-} \sum_{j=1}^{m_+} 1_{h(x_i)<h(x'_j)}.
\end{aligned}$$



$$\mathrm{TP}(k) = \frac{\sum_{i=k}^{m} 1_{y_i=+1}}{m_+}$$

$$\mathrm{FP}(k) = \frac{\sum_{i=k}^{m} 1_{y_i=-1}}{m_-}$$

This Talk

- Score-based ranking
- Preference-based ranking

Preference-Based Setting

- Definitions:
  - U: universe, full set of objects.
  - V: finite query subset to rank, $V \subseteq U$.
  - τ^*: target ranking for V (random variable).
- Two stages: can be viewed as a reduction.
  - learn preference function $h \colon U \times U \to [0, 1]$.
  - given V, use h to determine ranking σ of V.
- Running-time: measured in terms of |calls to h|.

Preference-Based Ranking Problem

- Training data: pairs (V, τ^*) sampled i.i.d. according to D:

$$(V_1, \tau_1^*), (V_2, \tau_2^*), \ldots, (V_m, \tau_m^*) \qquad V_i \subseteq U.$$

subsets ranked by different labelers.

learn classifier

preference function $h \colon U \times U \to [0, 1]$.

- Problem: for any query set $V \subseteq U$, use h to return ranking σ_h close to target τ^* with small average error

$$R(h, \sigma) = \mathop{\mathrm{E}}_{(V,\tau^*)\sim D}[L(\sigma_{h,V}, \tau^*)].$$

Preference Function

- $h(u, v)$ close to 1 when u preferred to v, close to 0 otherwise. For the analysis, $h(u, v) \in \{0, 1\}$.
- Assumed pairwise consistent:
$$h(u, v) + h(v, u) = 1.$$
- May be non-transitive, e.g., we may have
$$h(u, v) = h(v, w) = h(w, u) = 1.$$
- Output of classifier or 'black-box'.

Loss Functions

(for fixed (V, τ^*))

- Preference loss:

$$L(h, \tau^*) = \frac{2}{n(n-1)} \sum_{u \neq v} h(u, v)\tau^*(v, u).$$

- Ranking loss:

$$L(\sigma, \tau^*) = \frac{2}{n(n-1)} \sum_{u \neq v} \sigma(u, v)\tau^*(v, u).$$

(Weak) Regret

- Preference regret:

$$\mathcal{R}'_{class}(h) = \mathop{\mathbb{E}}_{V,\tau^*}\left[L(h_{|V}, \tau^*)\right] - \mathop{\mathbb{E}}_{V}\left[\min_{\tilde{h}} \mathop{\mathbb{E}}_{\tau^*|V}\left[L(\tilde{h}, \tau^*)\right]\right].$$

- Ranking regret:

$$\mathcal{R}'_{rank}(A) = \mathop{\mathbb{E}}_{V,\tau^*,s}\left[L(A_s(V), \tau^*)\right] - \mathop{\mathbb{E}}_{V}\left[\min_{\tilde{\sigma}\in S(V)} \mathop{\mathbb{E}}_{\tau^*|V}\left[L(\tilde{\sigma}, \tau^*)\right]\right].$$

Deterministic Algorithm

(Balcan et al., 07)

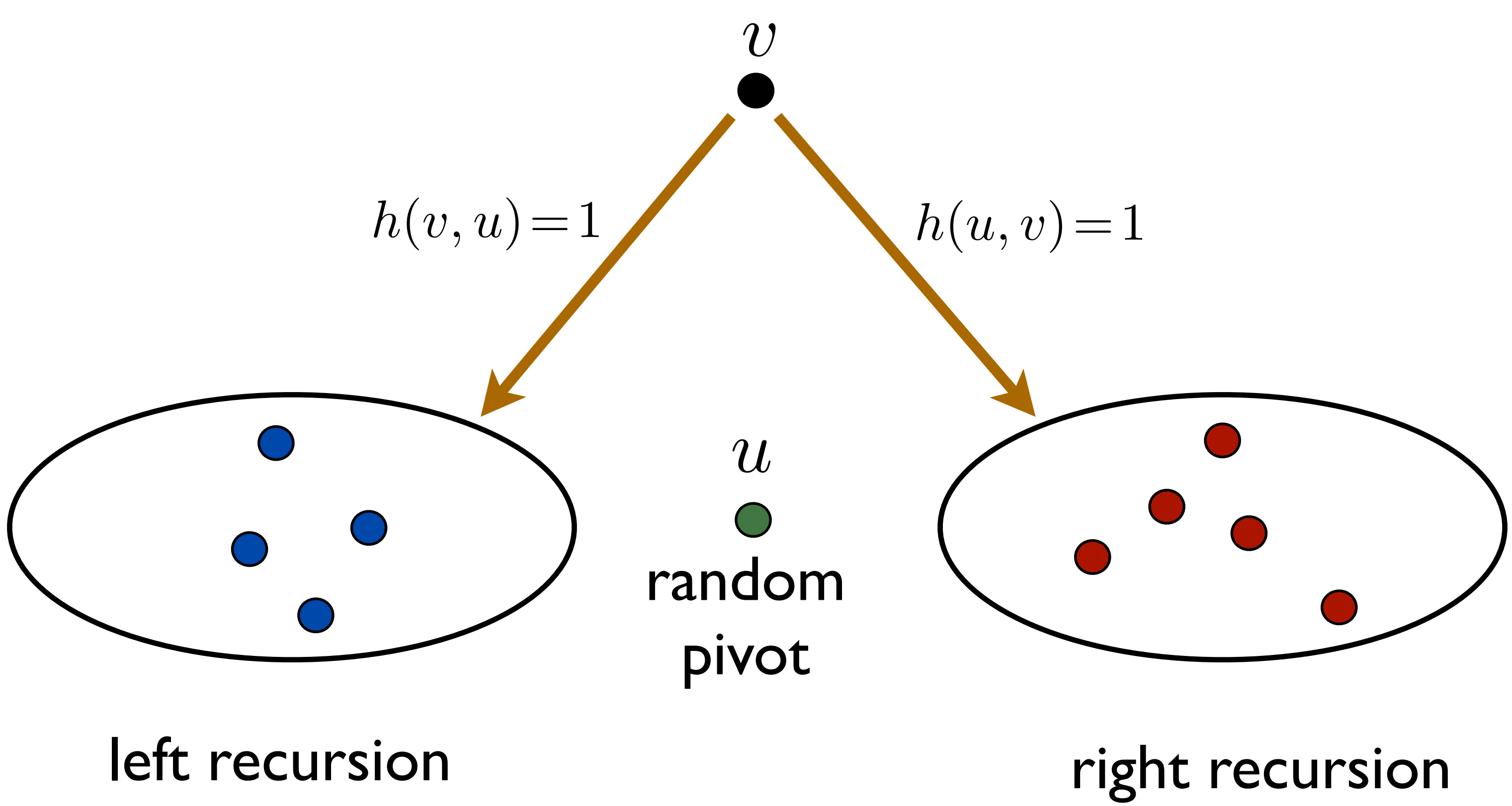
- Stage one: standard classification. Learn preference function $h : U \times U \to [0, 1]$.
- Stage two: sort-by-degree using comparison function h.
  - sort by number of points ranked below.
  - quadratic time complexity $O(n^2)$.

Randomized Algorithm

(Ailon & MM, 08)

- Stage one: standard classification. Learn preference function $h\colon U\times U\to[0,1]$.
- Stage two: randomized QuickSort (Hoare, 61) using h as comparison function.
  - comparison function non-transitive unlike textbook description.
  - but, time complexity shown to be $O(n\log n)$ in general.

Randomized QS



Deterministic Algo. - Bipartite Case

$(V = V_+ \cup V_-)$ (Balcan et al., 07)

- Bounds: for deterministic sort-by-degree algorithm
  - expected loss:

$$\mathop{\mathrm{E}}_{V,\tau^*}[L(A(V), \tau^*)] \leq 2 \mathop{\mathrm{E}}_{V,\tau^*}[L(h, \tau^*)].$$

  - regret:

$$\mathcal{R}'_{rank}(A(V)) \leq 2\, \mathcal{R}'_{class}(h).$$

- Time complexity: $\Omega(|V|^2)$.

Randomized Algo. - Bipartite Case

$(V = V_+ \cup V_-)$ (Ailon & MM, 08)

- Bounds: for randomized QuickSort.
  - expected loss (equality):

$$\mathop{\mathrm{E}}_{V,\tau^*,s}[L(Q_s^h(V), \tau^*)] = \mathop{\mathrm{E}}_{V,\tau^*}[L(h, \tau^*)].$$

  - regret:

$$\mathcal{R}'_{rank}(Q_s^h(\cdot)) \leq \mathcal{R}'_{class}(h) \quad .$$

- Time complexity:
  - full set: $O(n \log n)$.
  - top *k*: $O(n + k \log k)$.

Proof Ideas

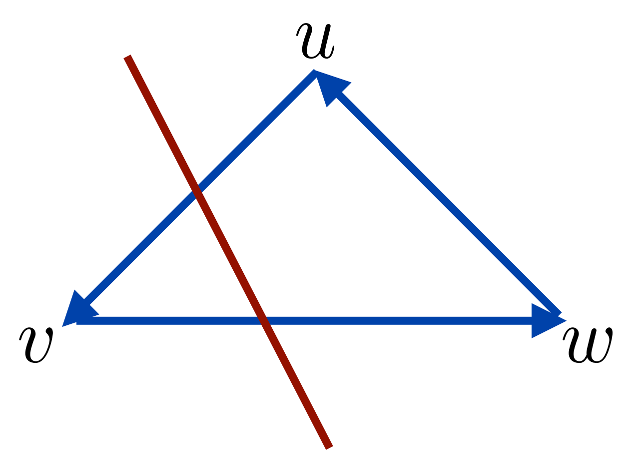
- QuickSort decomposition:

$$p_{uv} + \frac{1}{3} \sum_{w \notin \{u,v\}} p_{uvw} \Big(h(u,w)h(w,v) + h(v,w)h(w,u) \Big) = 1.$$

- Bipartite property:

$$\tau^*(u,v) + \tau^*(v,w) + \tau^*(w,u) =$$

$$\tau^*(v,u) + \tau^*(w,v) + \tau^*(u,w).$$



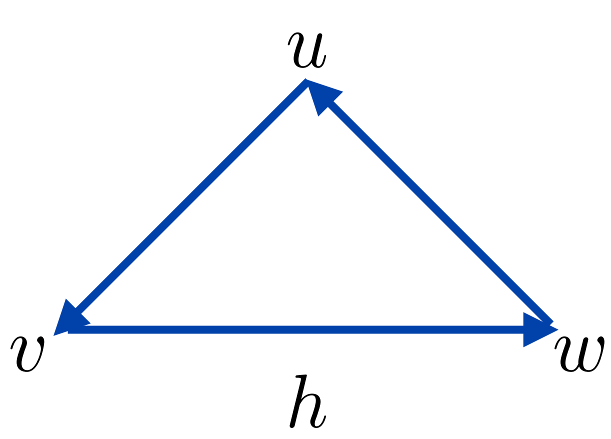
Lower Bound

- **Theorem**: for any deterministic algorithm A, there is a bipartite distribution for which

$$\mathcal{R}_{rank}(A) \geq 2\,\mathcal{R}_{class}(h).$$

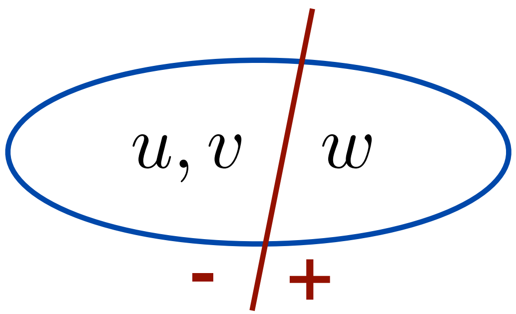
  - thus, factor of 2 $=$ best in deterministic case.
  - randomization necessary for better bound.
- **Proof**: take simple case $U = V = \{u, v, w\}$ and assume that h induces a cycle.
  - up to symmetry, A returns

    u, v, w or w, v, u.

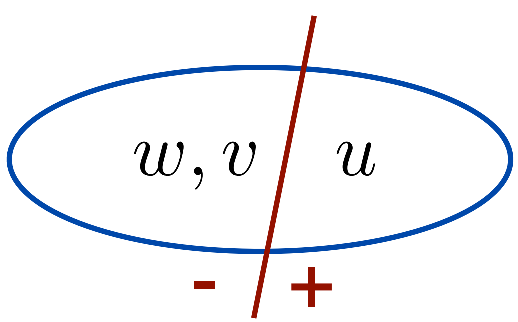


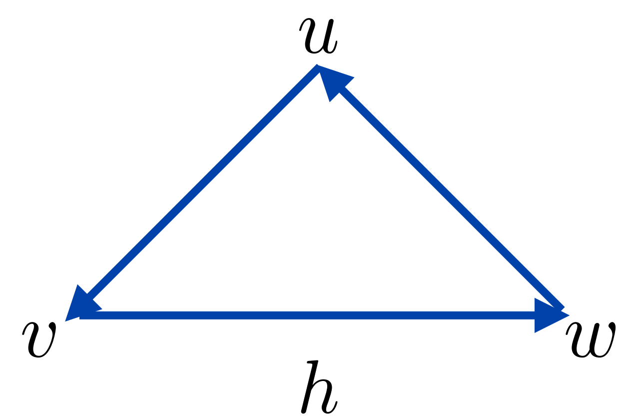
Lower Bound

- If A returns u, v, w, then choose τ^* as:



- If A returns w, v, u, then choose τ^* as:





$$L[h, \tau^*] = \frac{1}{3};$$

$$L[A, \tau^*] = \frac{2}{3}.$$

Guarantees - General Case

- Loss bound for QuickSort:

$$\underset{V,\tau^*,s}{\mathrm{E}}[L(Q_s^h(V),\tau^*)] \leq 2 \underset{V,\tau^*}{\mathrm{E}}[L(h,\tau^*)].$$

- Comparison with optimal ranking (see (CSS 99)):

$$\mathrm{E}_s[L(Q_s^h(V),\sigma_{optimal})] \leq 2\,L(h,\sigma_{optimal})$$

$$\mathrm{E}_s[L(h,Q_s^h(V))] \leq 3\,L(h,\sigma_{optimal}),$$

where $\sigma_{optimal} = \underset{\sigma}{\operatorname{argmin}}\, L(h,\sigma).$

Weight Function

- Generalization:

$$\tau^*(u,v) = \sigma^*(u,v)\,\omega(\sigma^*(u),\sigma^*(v)).$$

- Properties: needed for all previous results to hold,
  - symmetry: $\omega(i,j) = \omega(j,i)$ for all i,j.
  - monotonicity: $\omega(i,j), \omega(j,k) \leq \omega(i,k)$ for $i < j < k$.
  - triangle inequality: $\omega(i,j) \leq \omega(i,k) + \omega(k,j)$ for all triplets i,j,k.

Weight Function - Examples

- Kemeny: $w(i,j) = 1, \ \forall i, j.$
- Top-*k*: $w(i,j) = \begin{cases} 1 & \text{if } i \leq k \text{ or } j \leq k; \\ 0 & \text{otherwise.} \end{cases}$
- Bipartite: $w(i,j) = \begin{cases} 1 & \text{if } i \leq k \text{ and } j > k; \\ 0 & \text{otherwise.} \end{cases}$
- *k*-partite: can be defined similarly.

(Strong) Regret Definitions

- Ranking regret:

$$\mathcal{R}_{rank}(A) = \mathop{\mathrm{E}}_{V,\tau^*,s}[L(A_s(V), \tau^*)] - \min_{\tilde{\sigma}} \mathop{\mathrm{E}}_{V,\tau^*}[L(\tilde{\sigma}_{|V}, \tau^*)].$$

- Preference regret:

$$\mathcal{R}_{class}(h) = \mathop{\mathrm{E}}_{V,\tau^*}[L(h_{|V}, \tau^*)] - \min_{\tilde{h}} \mathop{\mathrm{E}}_{V,\tau^*}[L(\tilde{h}_{|V}, \tau^*)].$$

- All previous regret results hold if for $V_1, V_2 \supseteq \{u, v\}$,

$$\mathop{\mathrm{E}}_{\tau^*|V_1}[\tau^*(u, v)] = \mathop{\mathrm{E}}_{\tau^*|V_2}[\tau^*(u, v)]$$

for all u, v (pairwise independence on irrelevant alternatives).

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Foundations of Machine Learning
Multi-Class Classification

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Motivation

- Real-world problems often have multiple classes: text, speech, image, biological sequences.
- Algorithms studied so far: designed for binary classification problems.
- How do we design multi-class classification algorithms?
  - can the algorithms used for binary classification be generalized to multi-class classification?
  - can we reduce multi-class classification to binary classification?

Multi-Class Classification Problem

- Training data: sample drawn i.i.d. from set X according to some distribution D,

$$S=((x_1,y_1),\ldots,(x_m,y_m))\in X\times Y,$$

  - mono-label case: $\mathrm{Card}(Y)=k$.
  - multi-label case: $Y=\{-1,+1\}^k$.

- Problem: find classifier $h\colon X\to Y$ in H with small generalization error,
  - mono-label case: $R(h)=\mathrm{E}_{x\sim D}[1_{h(x)\neq f(x)}]$.
  - multi-label case: $R(h)=\mathrm{E}_{x\sim D}\left[\frac{1}{k}\sum_{l=1}^{k}1_{[h(x)]_l\neq[f(x)]_l}\right]$.

Notes

- In most tasks considered, number of classes $k \leq 100$.
- For k large, problem often not treated as a multi-class classification problem (ranking or density estimation, e.g., automatic speech recognition).
- Computational efficiency issues arise for larger ks.
- In general, classes not balanced.

Multi-Class Classification - Margin

- Hypothesis set H:
  - functions $h\colon X \times Y \to \mathbb{R}$.
  - label returned: $x \mapsto \operatorname*{argmax}_{y \in Y} h(x, y)$.
- Margin:
  - $\rho_h(x, y) = h(x, y) - \max_{y' \neq y} h(x, y')$.
  - error: $1_{\rho_h(x,y) \leq 0} \leq \Phi_\rho(\rho_h(x, y))$.
  - empirical margin loss:

$$\widehat{R}_\rho(h) = \frac{1}{m} \sum_{i=1}^{m} \Phi_\rho(\rho_h(x_i, y_i)).$$

Multi-Class Margin Bound

(MM et al. 2012; Kuznetsov, MM, and Syed, 2014)

- Theorem: let $H \subseteq \mathbb{R}^{X \times Y}$ with $Y = \{1, \ldots, k\}$. Fix $\rho > 0$. Then, for any $\delta > 0$, with probability at least $1 - \delta$, the following multi-class classification bound holds for all $h \in H$:

$$R(h) \leq \widehat{R}_\rho(h) + \frac{4k}{\rho} \mathfrak{R}_m(\Pi_1(H)) + \sqrt{\frac{\log \frac{1}{\delta}}{2m}},$$

with $\Pi_1(H) = \{x \mapsto h(x, y) \colon y \in Y, h \in H\}$.

Kernel-Based Hypotheses

- Hypothesis set $H_{K,p}$:
  - $\mathbf{\Phi}$ feature mapping associated to PDS kernel K.
  - functions $(x, y) \mapsto \mathbf{w}_y \cdot \mathbf{\Phi}(x)$, $y \in \{1, \ldots, k\}$.
  - label returned: $x \mapsto \underset{y \in \{1,\ldots,k\}}{\operatorname{argmax}} \; \mathbf{w}_y \cdot \mathbf{\Phi}(x)$.
  - for any $p \geq 1$,

$$H_{K,p} = \{(x, y) \in X \times [1, k] \mapsto \mathbf{w}_y \cdot \mathbf{\Phi}(x) \colon \mathbf{W} = (\mathbf{w}_1, \ldots, \mathbf{w}_k)^\top, \|\mathbf{W}\|_{\mathbb{H},p} \leq \Lambda\}.$$

$$\mathfrak{R}_m(\Pi_1(\mathcal{H}_{K,p})) \leq \sqrt{\frac{r^2 \Lambda^2}{m}}.$$

Multi-Class Margin Bound - Kernels

(MM et al. 2012)

- Theorem: let $K\colon X \times X \to \mathbb{R}$ be a PDS kernel and let $\Phi\colon X \to \mathbb{H}$ be a feature mapping associated to K. Fix $\rho > 0$. Then, for any $\delta > 0$, with probability at least $1 - \delta$, the following multiclass bound holds for all $h \in H_{K,p}$:

$$R(h) \leq \widehat{R}_\rho(h) + 4k\sqrt{\frac{r^2\Lambda^2}{\rho^2 m}} + \sqrt{\frac{\log \frac{1}{\delta}}{2m}},$$

where $r^2 = \sup_{x \in X} K(x, x)$.

Approaches

- Single classifier:
  - Multi-class SVMs.
  - AdaBoost.MH.
  - Conditional Maxent.
  - Decision trees.
- Combination of binary classifiers:
  - One-vs-all.
  - One-vs-one.
  - Error-correcting codes.

Multi-Class SVMs

(Weston and Watkins, 1999; Crammer and Singer, 2001)

- Optimization problem:

$$\min_{\mathbf{w},\boldsymbol{\xi}} \frac{1}{2}\sum_{l=1}^{k} \|\mathbf{w}_l\|^2 + C\sum_{i=1}^{m} \xi_i$$

$$\text{subject to: } \mathbf{w}_{y_i}\cdot\mathbf{x}_i + \delta_{y_i,l} \geq \mathbf{w}_l\cdot\mathbf{x}_i + 1 - \xi_i$$

$$\xi_i \geq 0, (i,l)\in[1,m]\times Y.$$

- Decision function:

$$h\colon x \mapsto \operatorname*{argmax}_{l\in Y}\,(\mathbf{w}_l\cdot\mathbf{x}).$$

Notes

- Directly based on generalization bounds.
- Comparison with (Weston and Watkins, 1999): single slack variable per point, maximum of slack variables (penalty for worst class):
$$\sum_{l=1}^{k} \xi_{il} \rightarrow \max_{l=1}^{k} \xi_{il}.$$
- PDS kernel instead of inner product
- Optimization: complex constraints, mk-size problem.
  - specific solution based on decomposition into m disjoint sets of constraints (Crammer and Singer, 2001).

Dual Formulation

- Optimization problem: $\boldsymbol{\alpha}_i$ ith row of matrix $\boldsymbol{\alpha} \in \mathbb{R}^{m \times k}$.

$$\max_{\boldsymbol{\alpha}=[\alpha_{ij}]} \sum_{i=1}^{m} \boldsymbol{\alpha}_i \cdot \mathbf{e}_{y_i} - \frac{1}{2} \sum_{i=1}^{m} (\boldsymbol{\alpha}_i \cdot \boldsymbol{\alpha}_j)(\mathbf{x}_i \cdot \mathbf{x}_j)$$

$$\text{subject to: } \forall i \in [1, m], (0 \leq \alpha_{iy_i} \leq C) \wedge (\forall j \neq y_i, \alpha_{ij} \leq 0) \wedge (\boldsymbol{\alpha}_i \cdot \mathbf{1} = 0).$$

- Decision function:

$$h(x) = \operatorname*{argmax}_{l \in [1, k]} \Big(\sum_{i=1}^{m} \alpha_{il} (\mathbf{x}_i \cdot \mathbf{x}) \Big).$$

AdaBoost

(Schapire and Singer, 2000)

- Training data (multi-label case):

$$(x_1, y_1), \ldots, (x_m, y_m) \in X \times \{-1, 1\}^k.$$

- Reduction to binary classification:
  - each example leads to k binary examples:

$$(x_i, y_i) \rightarrow ((x_i, 1), y_i[1]), \ldots, ((x_i, k), y_i[k]), i \in [1, m].$$

  - apply AdaBoost to the resulting problem.
  - choice of α_t.

- Computational cost: mk distribution updates at each round.

AdaBoost.MH

$H \subseteq (\{-1,+1\}^k)^{(X \times Y)}$.

$\textsc{AdaBoost.MH}(S=((x_1,y_1),\ldots,(x_m,y_m)))$

for $i \leftarrow 1$ **to** m **do**
    for $l \leftarrow 1$ **to** k **do**
        $D_1(i,l) \leftarrow \frac{1}{mk}$
for $t \leftarrow 1$ **to** T **do**
    $h_t \leftarrow$ base classifier in H with small error $\epsilon_t = \Pr_{D_t}[h_t(x_i,l) \neq y_i[l]]$
    $\alpha_t \leftarrow$ choose $\quad \triangleright$ to minimize Z_t
    $Z_t \leftarrow \sum_{i,l} D_t(i,l) \exp(-\alpha_t y_i[l] h_t(x_i,l))$
    for $i \leftarrow 1$ **to** m **do**
        for $l \leftarrow 1$ **to** k **do**
            $D_{t+1}(i,l) \leftarrow \frac{D_t(i,l)\exp(-\alpha_t y_i[l] h_t(x_i,l))}{Z_t}$
$f_T \leftarrow \sum_{t=1}^{T} \alpha_t h_t$
return $h_T = \mathrm{sgn}(f_T)$

Bound on Empirical Error

- **Theorem**: The empirical error of the classifier output by AdaBoost.MH verifies:

$$\widehat{R}(h) \leq \prod_{t=1}^{T} Z_t.$$

- **Proof**: similar to the proof for AdaBoost.
- **Choice of α_t**:
  - for $H \subseteq (\{-1, +1\}^k)^{X \times Y}$, as for AdaBoost, $\alpha_t = \frac{1}{2} \log \frac{1-\epsilon_t}{\epsilon_t}$.
  - for $H \subseteq ([-1, 1]^k)^{X \times Y}$, same choice: minimize upper bound.
  - other cases: numerical/approximation method.

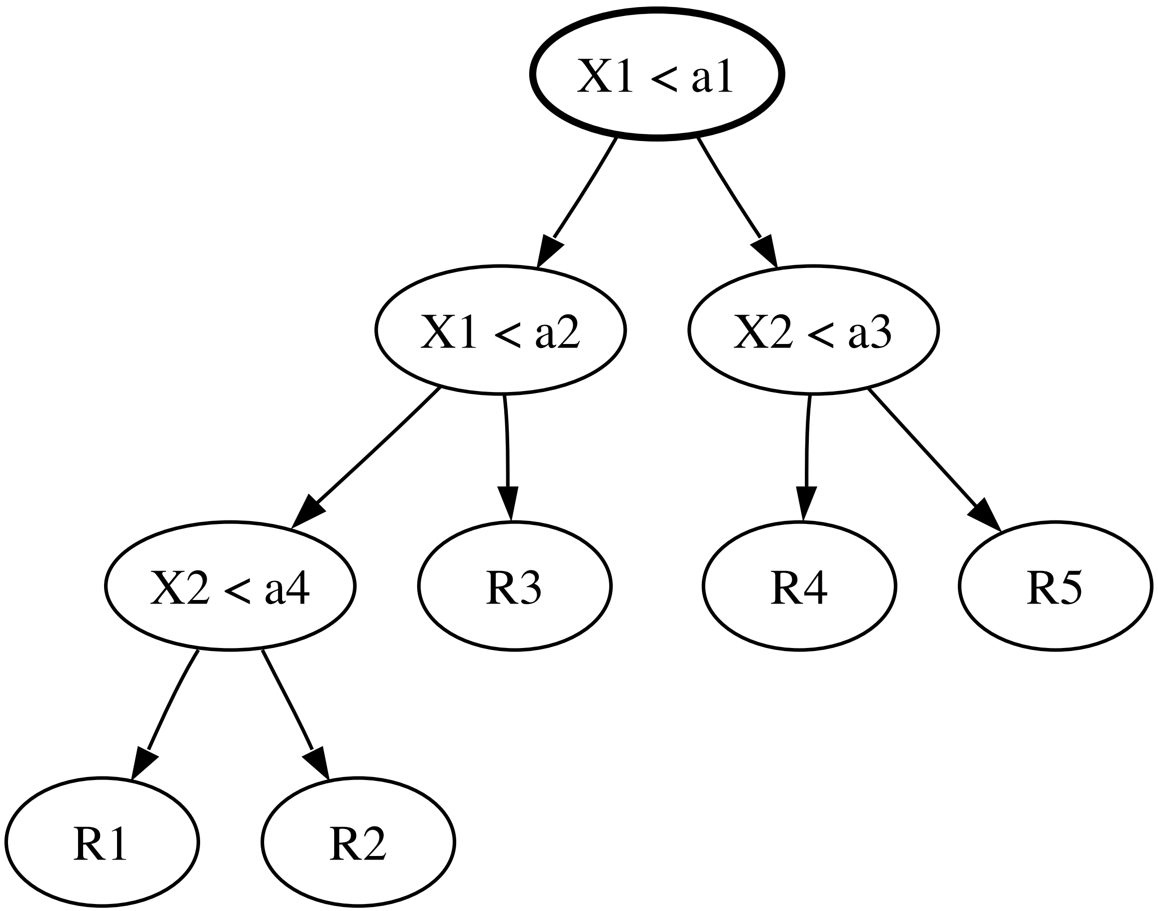
Notes

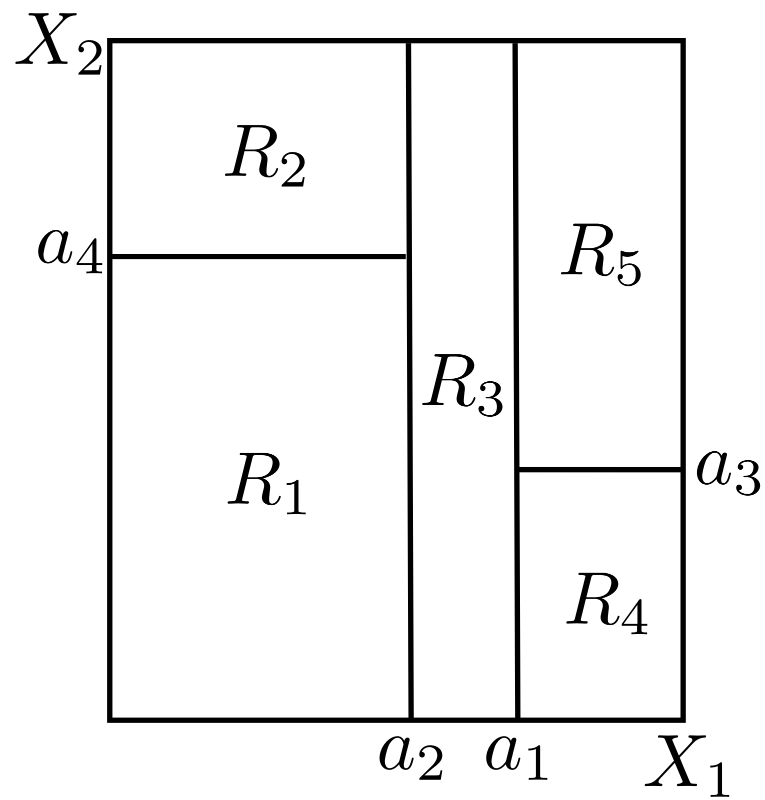
- Objective function:

$$F(\boldsymbol{\alpha}) = \sum_{i=1}^{m} \sum_{l=1}^{k} e^{-y_i[l] f_n(x_i, l)} = \sum_{i=1}^{m} \sum_{l=1}^{k} e^{-y_i[l] \sum_{t=1}^{n} \alpha_t h_t(x_i, l)}.$$

- All comments and analysis given for AdaBoost apply here.
- Alternative: Adaboost.MR, which coincides with a special case of RankBoost (ranking lecture).

Decision Trees





Different Types of Questions

- Decision trees
  - $X \in \{\text{blue}, \text{white}, \text{red}\}$: categorical questions.
  - $X \leq a$: continuous variables.
- Binary space partition (BSP) trees:
  - $\sum_{i=1}^{n} \alpha_i X_i \leq a$: partitioning with convex polyhedral regions.
- Sphere trees:
  - $||X - a_0|| \leq a$: partitioning with pieces of spheres.

Hypotheses

- In each region R_t,
  - classification: majority vote - ties broken arbitrarily,

$$\widehat{y}_t = \operatorname*{argmax}_{y \in Y} \left|\{x_i \in R_t \colon i \in [1, m], y_i = y\}\right|.$$

  - regression: average value,

$$\widehat{y}_t = \frac{1}{|S \cap R_t|} \sum_{\substack{x_i \in R_t \\ i \in [1,m]}} y_i \,.$$

- Form of hypotheses:

$$h \colon x \mapsto \sum_t \widehat{y}_t 1_{x \in R_t} \,.$$

Training

- **Problem**: general problem of determining partition with minimum empirical error is NP-hard.
- **Heuristics**: greedy algorithm.
    - for all $j \in [1, N]$, $\theta \in \mathbb{R}$, $R^+(j,\theta) = \{x_i \in R \colon x_i[j] \geq \theta, i \in [1, m]\}$
      $R^-(j,\theta) = \{x_i \in R \colon x_i[j] < \theta, i \in [1, m]\}$.

$\textsc{Decision-Trees}(S = ((x_1, y_1), \ldots, (x_m, y_m)))$

$P \leftarrow \{S\}$ $\triangleright$ initial partition
for each region $R \in P$ such that $\mathrm{Pred}(R)$ **do**
  $(j, \theta) \leftarrow \mathrm{argmin}_{(j,\theta)}\ \mathrm{error}(R^-(j,\theta)) + \mathrm{error}(R^+(j,\theta))$
  $P \leftarrow P - R \cup \{R^-(j,\theta), R^+(j,\theta)\}$
return P

Splitting/Stopping Criteria

- Problem: larger trees overfit training sample.
- Conservative splitting:
  - split node only if loss reduced by some fixed value $\eta > 0$.
  - issue: seemingly bad split dominating useful splits.
- Grow-then-prune technique (CART):
  - grow very large tree, $\mathrm{Pred}(R)$: $|R| > |n_0|$.
  - prune tree based on: $F(T) = \widehat{\mathrm{Loss}}(T) + \alpha |T|$, $\alpha \geq 0$ parameter determined by cross-validation.

Decision Tree Tools

- Most commonly used tools for learning decision trees:
  - CART (classification and regression tree) (Breiman et al., 1984).
  - C4.5 (Quinlan, 1986, 1993) and C5.0 (RuleQuest Research) a commercial system.
- Differences: minor between latest versions.

Approaches

- Single classifier:
  - SVM-type algorithm.
  - AdaBoost-type algorithm.
  - Conditional Maxent.
  - Decision trees.
- Combination of binary classifiers:
  - One-vs-all.
  - One-vs-one.
  - Error-correcting codes.

One-vs-All

- Technique:
  - for each class $l \in Y$ learn binary classifier $h_l = \operatorname{sgn}(f_l)$.
  - combine binary classifiers via voting mechanism, typically majority vote: $h \colon x \mapsto \operatorname*{argmax}_{l \in Y} f_l(x)$.
- Problem: poor justification (in general).
  - calibration: classifier scores not comparable.
  - nevertheless: simple and frequently used in practice, computational advantages in some cases.

One-vs-One

- Technique:
  - for each pair $(l, l') \in Y, l \neq l'$ learn binary classifier $h_{ll'} : X \to \{0, 1\}$.
  - combine binary classifiers via majority vote:
$$h(x) = \underset{l' \in Y}{\operatorname{argmax}} \left|\{l : h_{ll'}(x) = 1\}\right|.$$
- Problem:
  - computational: train $k(k-1)/2$ binary classifiers.
  - overfitting: size of training sample could become small for a given pair.

Computational Comparison

	Training	Testing
One-vs-all	$O(kB_{\text{train}}(m))$ $O(km^\alpha)$	$O(kB_{\text{test}})$
One-vs-one	$O(k^2 B_{\text{train}}(m/k))$ (on average) $O(k^{2-\alpha} m^\alpha)$	$O(k^2 B_{\text{test}})$ *smaller* N_{SV} *per* B

Time complexity for SVMs, α less than 3.

Error-Correcting Code Approach

(Dietterich and Bakiri, 1995)

- Idea:
  - assign F-long binary code word to each class:

    $$\longrightarrow \mathbf{M} = [\mathbf{M}_{lj}] \in \{0, 1\}^{[1,k]\times[1,F]}.$$

  - learn binary classifier $f_j \colon X \to \{0, 1\}$ for each column. Example x in class l labeled with M_{lj}.
  - classifier output: $\Big(\mathbf{f}(x) = \big(f_1(x), \ldots, f_F(x)\big)\Big)$,

$$h \colon x \mapsto \operatorname*{argmin}_{l \in Y} d_{\text{Hamming}}\Big(\mathbf{M}_l, \mathbf{f}(x)\Big).$$

Illustration

- 8 classes, code-length: 6.

codes

classes

	1	2	3	4	5	6
1	0	0	0	1	0	0
2	1	0	0	0	0	0
3	0	1	1	0	1	0
4	1	1	0	0	0	0
5	1	1	0	0	1	0
6	0	0	1	1	0	1
7	0	0	1	0	0	0
8	0	1	0	1	0	0

$f_1(x)$	$f_2(x)$	$f_3(x)$	$f_4(x)$	$f_5(x)$	$f_6(x)$
0	1	1	0	1	1

new example x

Error-Correcting Codes - Design

- Main ideas:
  - independent columns: otherwise no effective discrimination.
  - distance between rows: if the minimal Hamming distance between rows is d, then the multi-class can correct $\left\lfloor \frac{d-1}{2} \right\rfloor$ (classification) errors.
  - columns may correspond to features selected for the task.
  - one-vs-all and one-vs-one (with ternary codes) are special cases.

Extensions

(Allwein et al., 2000)

- Matrix entries in $\{-1, 0, +1\}$:
  - examples marked with 0 disregarded during training.
  - $\longrightarrow$ one-vs-one becomes also a special case.
- Margin loss L: function of $yf(x)$, e.g., hinge loss.
  - Hamming loss:

$$h(x) = \operatorname*{argmin}_{l \in \{1,\ldots,k\}} \sum_{j=1}^{F} \frac{1 - \operatorname{sgn}\big(\mathbf{M}_{lj} f_j(x)\big)}{2}.$$

  - Margin loss:

$$h(x) = \operatorname*{argmin}_{l \in \{1,\ldots,k\}} \sum_{j=1}^{F} L\big(\mathbf{M}_{lj} f_j(x)\big).$$

Applications

- One-vs-all approach is the most widely used combination method.
- No clear empirical evidence of the superiority of other approaches (Rifkin and Klautau, 2004).
  - except perhaps on small data sets with relatively large error rate.
- Large structured multi-class problems: often treated as ranking problems (see ranking lecture).

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Foundations of Machine Learning
Regression

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Regression Problem

- Training data: sample drawn i.i.d. from set X according to some distribution D,

$$S=((x_1,y_1),\ldots,(x_m,y_m))\in X\times Y,$$

  with $Y\subseteq\mathbb{R}$ is a measurable subset.

- Loss function: $L\colon Y\times Y\to\mathbb{R}_+$ a measure of closeness, typically $L(y,y')=(y'-y)^2$ or $L(y,y')=|y'-y|^p$ for some $p\geq 1$.

- Problem: find hypothesis $h\colon X\to\mathbb{R}$ in H with small generalization error with respect to target f

$$R_D(h)=\mathop{\mathrm{E}}_{x\sim D}\Big[L\big(h(x),f(x)\big)\Big].$$

Notes

- Empirical error:

$$\widehat{R}_D(h) = \frac{1}{m}\sum_{i=1}^{m} L\big(h(x_i), y_i\big).$$

- In much of what follows:
  - $Y = \mathbb{R}$ or $Y = [-M, M]$ for some $M > 0$.
  - $L(y, y') = (y' - y)^2 \longrightarrow$ mean squared error.

This Lecture

- Generalization bounds
- Linear regression
- Kernel ridge regression
- Support vector regression
- Lasso

Generalization Bound - Finite H

- Theorem: let H be a finite hypothesis set, and assume that L is bounded by M. Then, for any $\delta > 0$, with probability at least $1-\delta$,

$$\forall h \in H, R(h) \leq \widehat{R}(h) + M\sqrt{\frac{\log|H| + \log\frac{2}{\delta}}{2m}}.$$

- Proof: By the union bound,

$$\Pr\left[\sup_{h\in H}\left|R(h)-\widehat{R}(h)\right|>\epsilon\right] \leq \sum_{h\in H}\Pr\left[\left|R(h)-\widehat{R}(h)\right|>\epsilon\right].$$

By Hoeffding's bound, for a fixed h,

$$\Pr\left[\left|R(h)-\widehat{R}(h)\right|>\epsilon\right] \leq 2e^{-\frac{2m\epsilon^2}{M^2}}.$$

Rademacher Complexity of Lp Loss

- Theorem: Let $p \geq 1$, $H_p = \{x \mapsto |h(x) - f(x)|^p \colon h \in H\}$. Assume that $\sup_{x \in X, h \in H} |h(x) - f(x)| \leq M$. Then, for any sample S of size m,

$$\widehat{\mathfrak{R}}_S(H_p) \leq p M^{p-1} \widehat{\mathfrak{R}}_S(H).$$

Proof

- Proof: Let $H' = \{x \mapsto h(x) - f(x) \colon h \in H\}$. Then, observe that $H_p = \{\phi \circ h \colon h \in H'\}$ with $\phi \colon x \mapsto |x|^p$.
  - ϕ is pM^{p-1} - Lipschitz over $[-M, M]$, thus
  $$\widehat{\mathfrak{R}}_S(H_p) \leq pM^{p-1} \widehat{\mathfrak{R}}_S(H').$$
  - Next, observe that:
  $$\begin{aligned}\widehat{\mathfrak{R}}_S(H') &= \frac{1}{m} \operatorname*{E}_{\boldsymbol{\sigma}} \Big[\sup_{h \in H} \sum_{i=1}^{m} \sigma_i h(x_i) + \sigma_i f(x_i) \Big] \\ &= \frac{1}{m} \operatorname*{E}_{\boldsymbol{\sigma}} \Big[\sup_{h \in H} \sum_{i=1}^{m} \sigma_i h(x_i) \Big] + \operatorname*{E}_{\boldsymbol{\sigma}} \Big[\sum_{i=1}^{m} \sigma_i f(x_i) \Big] = \widehat{\mathfrak{R}}_S(H).\end{aligned}$$

Rad. Complexity Regression Bound

- **Theorem**: Let $p \geq 1$ and assume that $\|h - f\|_\infty \leq M$ for all $h \in H$. Then, for any $\delta > 0$, with probability at least $1-\delta$, for all $h \in H$,

$$\mathrm{E}\Big[\big|h(x) - f(x)\big|^p\Big] \leq \frac{1}{m}\sum_{i=1}^{m}\big|h(x_i) - f(x_i)\big|^p + 2pM^{p-1}\mathfrak{R}_m(H) + M^p\sqrt{\frac{\log\frac{1}{\delta}}{2m}}.$$

$$\mathrm{E}\Big[\big|h(x) - f(x)\big|^p\Big] \leq \frac{1}{m}\sum_{i=1}^{m}\big|h(x_i) - f(x_i)\big|^p + 2pM^{p-1}\widehat{\mathfrak{R}}_S(H) + 3M^p\sqrt{\frac{\log\frac{2}{\delta}}{2m}}.$$

- **Proof**: Follows directly bound on Rademacher complexity and general Rademacher bound.

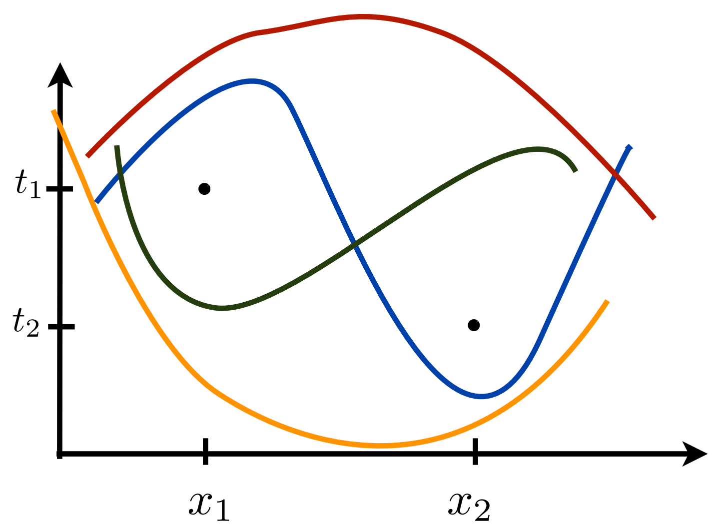
Notes

- As discussed for binary classification:
  - estimating the Rademacher complexity can be computationally hard for some Hs.
  - can we come up instead with a combinatorial measure that is easier to compute?

Shattering

- Definition: Let G be a family of functions mapping from X to $\mathbb{R}$. $A = \{x_1, \ldots, x_m\}$ is shattered by G if there exist $t_1, \ldots, t_m \in \mathbb{R}$ such that

$$\left| \left\{ \begin{bmatrix} \operatorname{sgn}\left(g(x_1) - t_1\right) \\ \vdots \\ \operatorname{sgn}\left(g(x_m) - t_m\right) \end{bmatrix} : g \in G \right\} \right| = 2^m.$$

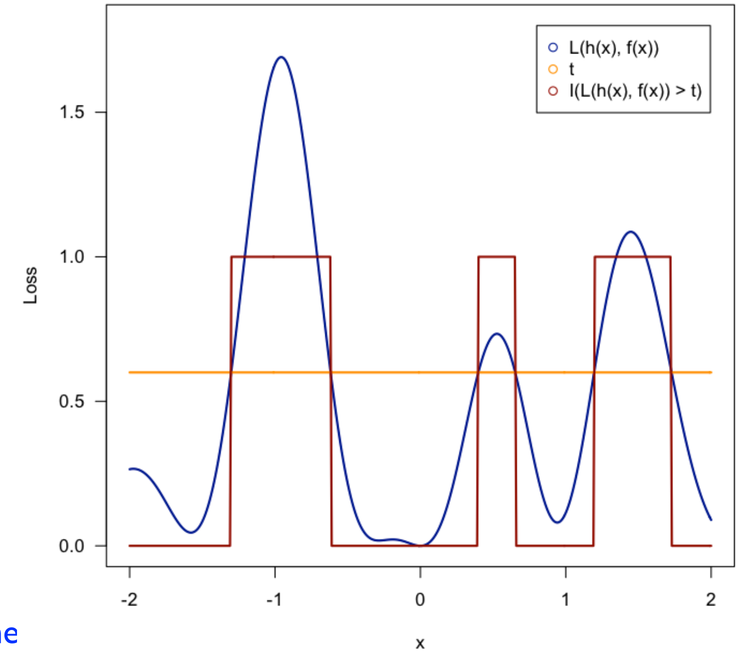


Pseudo-Dimension

(Pollard, 1984)

- **Definition**: Let G be a family of functions mapping from X to $\mathbb{R}$. The pseudo-dimension of G, $\mathrm{Pdim}(G)$, is the size of the largest set shattered by G.
- **Definition** (equivalent, see also (Vapnik, 1995)):

$$\mathrm{Pdim}(G) = \mathrm{VCdim}\Big(\big\{(x,t) \mapsto 1_{(g(x)-t)>0} \colon g \in G\big\}\Big).$$



Pseudo-Dimension - Properties

- Theorem: Pseudo-dimension of hyperplanes.

$$\mathrm{Pdim}(\mathbf{x} \mapsto \mathbf{w} \cdot \mathbf{x} + b \colon \mathbf{w} \in \mathbb{R}^N, b \in \mathbb{R}) = N + 1.$$

- Theorem: Pseudo-dimension of a vector space of real-valued functions H:

$$\mathrm{Pdim}(H) = \dim(H).$$

Generalization Bounds

Classification ⟶ Regression

- **Lemma** (Lebesgue integral): for $f \geq 0$ measurable,

$$\mathop{\mathrm{E}}_{D}[f(x)] = \int_0^\infty \Pr_{D}[f(x) > t]\,dt.$$

- Assume that the loss function L is bounded by M.

$$\begin{aligned}
|R(h) - \widehat{R}(h)| &= \left| \int_0^M \Big(\Pr_{x\sim D}[L(h(x), f(x)) > t] - \Pr_{x\sim S}[L(h(x), f(x)) > t] \Big)\, dt \right| \\
&\leq M \sup_{t\in[0,M]} \left| \Pr_{x\sim D}[L(h(x), f(x)) > t] - \Pr_{x\sim S}[L(h(x), f(x)) > t] \right| \\
&= M \sup_{t\in[0,M]} \left| \mathop{\mathrm{E}}_{x\sim D}[1_{L(h(x),f(x))>t}] - \mathop{\mathrm{E}}_{x\sim S}[1_{L(h(x),f(x))>t}] \right|.
\end{aligned}$$

$$\Pr\left[\sup_{h\in H} |R(h) - \widehat{R}(h)| > \epsilon\right] \boxed{\leq \Pr\left[\sup_{\substack{h\in H\\ t\in[0,M]}} \left| R(1_{L(h,f)>t}) - \widehat{R}(1_{L(h,f)>t}) \right| > \frac{\epsilon}{M}\right]}.$$

Standard classification generalization bound.

Generalization Bound - Pdim

- **Theorem**: Let H be a family of real-valued functions. Assume that $\mathrm{Pdim}(\{L(h,f)\colon h \in H\}) = d < \infty$ and that the loss L is bounded by M. Then, for any $\delta > 0$, with probability at least $1-\delta$, for any $h \in H$,

$$R(h) \leq \widehat{R}(h) + M\sqrt{\frac{2d \log \frac{em}{d}}{m}} + M\sqrt{\frac{\log \frac{1}{\delta}}{2m}}.$$

- **Proof**: follows observation of previous slide and VCDim bound for indicator functions of lecture 3.

Notes

- Pdim bounds in unbounded case modulo assumptions: existence of an envelope function or moment assumptions.
- Other relevant capacity measures:
  - covering numbers.
  - packing numbers.
  - fat-shattering dimension.

This Lecture

- Generalization bounds
- Linear regression
- Kernel ridge regression
- Support vector regression
- Lasso

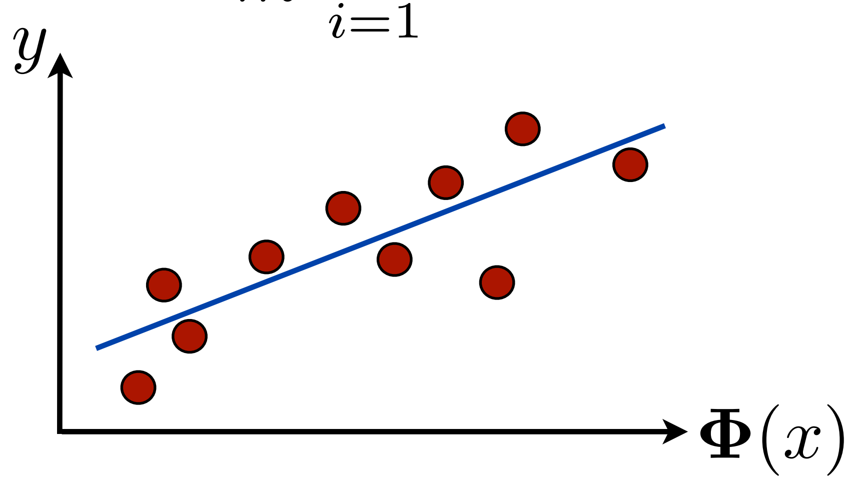
Linear Regression

- Feature mapping $\mathbf{\Phi}\colon X \to \mathbb{R}^N$.
- Hypothesis set: linear functions.

$$\{x \mapsto \mathbf{w} \cdot \mathbf{\Phi}(x) + b\colon \mathbf{w} \in \mathbb{R}^N, b \in \mathbb{R}\}.$$

- Optimization problem: empirical risk minimization.

$$\min_{\mathbf{w}, b} F(\mathbf{w}, b) = \frac{1}{m} \sum_{i=1}^{m} (\mathbf{w} \cdot \mathbf{\Phi}(x_i) + b - y_i)^2 .$$



Linear Regression - Solution

- Rewrite objective function as $F(\mathbf{W}) = \frac{1}{m}\|\mathbf{X}^\top \mathbf{W} - \mathbf{Y}\|^2$, $\mathbf{X} = \left[\begin{smallmatrix} \Phi(x_1) & \ldots & \Phi(x_m) \\ 1 & \ldots & 1 \end{smallmatrix}\right] \in \mathbb{R}^{(N+1)\times m}$

$$\text{with } \mathbf{X}^\top = \begin{bmatrix} \mathbf{\Phi}(x_1)^\top & 1 \\ \vdots & \\ \mathbf{\Phi}(x_m)^\top & 1 \end{bmatrix} \quad \mathbf{W} = \begin{bmatrix} w_1 \\ \vdots \\ w_N \\ b \end{bmatrix} \quad \mathbf{Y} = \begin{bmatrix} y_1 \\ \vdots \\ y_m \end{bmatrix}.$$

- Convex and differentiable function.

$$\nabla F(\mathbf{W}) = \frac{2}{m}\mathbf{X}(\mathbf{X}^\top \mathbf{W} - \mathbf{Y}).$$

$$\nabla F(\mathbf{W}) = 0 \Leftrightarrow \mathbf{X}(\mathbf{X}^\top \mathbf{W} - \mathbf{Y}) = 0 \Leftrightarrow \mathbf{X}\mathbf{X}^\top \mathbf{W} = \mathbf{X}\mathbf{Y}.$$

Linear Regression - Solution

- Solution:

$$\mathbf{W} = \begin{cases} (\mathbf{X}\mathbf{X}^\top)^{-1}\mathbf{X}\mathbf{Y} & \text{if } \mathbf{X}\mathbf{X}^\top \text{ invertible.} \\ (\mathbf{X}\mathbf{X}^\top)^{\dagger}\mathbf{X}\mathbf{Y} & \text{in general.} \end{cases}$$

  - Computational complexity: $O(mN + N^3)$ if matrix inversion in $O(N^3)$.
  - Poor guarantees in general, no regularization.
  - For output labels in $\mathbb{R}^p$, $p > 1$, solve p distinct linear regression problems.

This Lecture

- Generalization bounds
- Linear regression
- Kernel ridge regression
- Support vector regression
- Lasso

Mean Square Bound - Kernel-Based Hypotheses

- **Theorem:** Let $K\colon X \times X \to \mathbb{R}$ be a PDS kernel and let $\Phi\colon X \to \mathbb{H}$ be a feature mapping associated to K. Let $H = \left\{\mathbf{x} \mapsto \mathbf{w} \cdot \Phi(x) \colon \|\mathbf{w}\|_{\mathbb{H}} \leq \Lambda\right\}$. Assume $K(x, x) \leq R^2$ and $|f(x)| \leq \Lambda R$ for all $x \in X$. Then, for any $\delta > 0$, with probability at least $1 - \delta$, for any $h \in H$,

$$R(h) \leq \widehat{R}(h) + \frac{8R^2\Lambda^2}{\sqrt{m}}\left(1 + \frac{1}{2}\sqrt{\frac{\log\frac{1}{\delta}}{2}}\right)$$

$$R(h) \leq \widehat{R}(h) + \frac{8R^2\Lambda^2}{\sqrt{m}}\left(\sqrt{\frac{\mathrm{Tr}[\mathbf{K}]}{mR^2}} + \frac{3}{4}\sqrt{\frac{\log\frac{2}{\delta}}{2}}\right).$$

Mean Square Bound - Kernel-Based Hypotheses

- Proof: direct application of the Rademacher Complexity Regression Bound (this lecture) and bound on the Rademacher complexity of kernel-based hypotheses (lecture 5):

$$\widehat{\mathfrak{R}}_S(H) \leq \frac{\Lambda\sqrt{\mathrm{Tr}[\mathbf{K}]}}{m} \leq \sqrt{\frac{R^2\Lambda^2}{m}}.$$

Ridge Regression

(Hoerl and Kennard, 1970)

- Optimization problem:

$$\min_{\mathbf{w}} F(\mathbf{w}, b) = \lambda \|\mathbf{w}\|^2 + \sum_{i=1}^{m} \left(\mathbf{w} \cdot \mathbf{\Phi}(x_i) + b - y_i\right)^2,$$

where $\lambda \geq 0$ is a (regularization) parameter.

  - directly based on generalization bound.
  - generalization of linear regression.
  - closed-form solution.
  - can be used with kernels.

Ridge Regression - Solution

- Assume $b=0$: often constant feature used (but not equivalent to the use of original offset!).
- Rewrite objective function as

$$F(\mathbf{W}) = \lambda\|\mathbf{W}\|^2 + \|\mathbf{X}^\top\mathbf{W} - \mathbf{Y}\|^2.$$

- Convex and diferentiable function.

$$\nabla F(\mathbf{W}) = 2\lambda\mathbf{W} + 2\mathbf{X}(\mathbf{X}^\top\mathbf{W} - \mathbf{Y}).$$

$$\nabla F(\mathbf{W}) = 0 \Leftrightarrow (\mathbf{X}\mathbf{X}^\top + \lambda\mathbf{I})\mathbf{W} = \mathbf{X}\mathbf{Y}.$$

- Solution: $$\boxed{\mathbf{W} = \underbrace{(\mathbf{X}\mathbf{X}^\top + \lambda\mathbf{I})}_{\text{always invertible.}}{}^{-1}\mathbf{X}\mathbf{Y}}.$$

Ridge Regression - Equivalent Formulations

- Optimization problem:

$$\min_{\mathbf{w}, b} \sum_{i=1}^{m} (\mathbf{w} \cdot \mathbf{\Phi}(x_i) + b - y_i)^2$$

$$\text{subject to: } \|\mathbf{w}\|^2 \leq \Lambda^2.$$

- Optimization problem:

$$\min_{\mathbf{w}, b} \sum_{i=1}^{m} \xi_i^2$$

$$\text{subject to: } \xi_i = \mathbf{w} \cdot \mathbf{\Phi}(x_i) + b - y_i$$

$$\|\mathbf{w}\|^2 \leq \Lambda^2.$$

Ridge Regression Equations

- **Lagrangian**: assume $b = 0$. For all $\xi, \mathbf{w}, \boldsymbol{\alpha}', \lambda \geq 0$,

$$L(\xi, \mathbf{w}, \boldsymbol{\alpha}', \lambda) = \sum_{i=1}^{m} \xi_i^2 + \sum_{i=1}^{m} \alpha_i'(y_i - \xi_i - \mathbf{w} \cdot \mathbf{\Phi}(x_i)) + \lambda(\|\mathbf{w}\|^2 - \Lambda^2).$$

- **KKT conditions**:

$$\nabla_{\mathbf{w}} L = -\sum_{i=1}^{m} \alpha_i' \mathbf{\Phi}(x_i) + 2\lambda \mathbf{w} = 0 \iff \boxed{\mathbf{w} = \frac{1}{2\lambda} \sum_{i=1}^{m} \alpha_i' \mathbf{\Phi}(x_i).}$$

$$\nabla_{\xi_i} L = 2\xi_i - \alpha_i' = 0 \iff \boxed{\xi_i = \alpha_i'/2.}$$

$$\boxed{\begin{array}{l} \forall i \in [1, m], \alpha_i'(y_i - \xi_i - \mathbf{w} \cdot \mathbf{\Phi}(x_i)) = 0 \\ \lambda(\|\mathbf{w}\|^2 - \Lambda^2) = 0. \end{array}}$$

Moving to The Dual

- Plugging in the expression of $\mathbf{w}$ and ξ_is gives

$$L = \sum_{i=1}^{m} \frac{{\alpha'_i}^2}{4} + \sum_{i=1}^{m} \alpha'_i y_i - \sum_{i=1}^{m} \frac{{\alpha'_i}^2}{2} - \frac{1}{2\lambda} \sum_{i,j=1}^{m} \alpha'_i \alpha'_j \mathbf{\Phi}(x_i)^\top \mathbf{\Phi}(x_j) + \lambda \Big(\frac{1}{4\lambda^2} \| \sum_{i=1}^{m} \alpha'_i \mathbf{\Phi}(x_i) \|^2 - \Lambda^2 \Big).$$

- Thus,

$$\begin{aligned} L &= -\frac{1}{4} \sum_{i=1}^{m} {\alpha'_i}^2 + \sum_{i=1}^{m} \alpha'_i y_i - \frac{1}{4\lambda} \sum_{i,j=1}^{m} \alpha'_i \alpha'_j \mathbf{\Phi}(x_i)^\top \mathbf{\Phi}(x_j) - \lambda \Lambda^2 \\ &= -\lambda \sum_{i=1}^{m} \alpha_i^2 + 2 \sum_{i=1}^{m} \alpha_i y_i - \sum_{i,j=1}^{m} \alpha_i \alpha_j \mathbf{\Phi}(x_i)^\top \mathbf{\Phi}(x_j) - \lambda \Lambda^2, \end{aligned}$$

with $\alpha'_i = 2\lambda\alpha_i$.

RR - Dual Optimization Problem

- Optimization problem:

$$\max_{\boldsymbol{\alpha} \in \mathbb{R}^m} -\lambda \boldsymbol{\alpha}^\top \boldsymbol{\alpha} + 2\boldsymbol{\alpha}^\top \mathbf{y} - \boldsymbol{\alpha}^\top (\mathbf{X}^\top \mathbf{X}) \boldsymbol{\alpha}$$

or $$\max_{\boldsymbol{\alpha} \in \mathbb{R}^m} -\boldsymbol{\alpha}^\top (\mathbf{X}^\top \mathbf{X} + \lambda \mathbf{I}) \boldsymbol{\alpha} + 2\boldsymbol{\alpha}^\top \mathbf{y}.$$

- Solution:

$$h(x) = \sum_{i=1}^{m} \alpha_i \boldsymbol{\Phi}(\mathbf{x}_i) \cdot \boldsymbol{\Phi}(x),$$

with $\boldsymbol{\alpha} = (\mathbf{X}^\top \mathbf{X} + \lambda \mathbf{I})^{-1} \mathbf{y}.$

Direct Dual Solution

- Lemma: The following matrix identity always holds.

$$(\mathbf{X}\mathbf{X}^\top + \lambda\mathbf{I})^{-1}\mathbf{X} = \mathbf{X}(\mathbf{X}^\top\mathbf{X} + \lambda\mathbf{I})^{-1}.$$

- Proof: Observe that $(\mathbf{X}\mathbf{X}^\top + \lambda\mathbf{I})\mathbf{X} = \mathbf{X}(\mathbf{X}^\top\mathbf{X} + \lambda\mathbf{I})$. Left-multiplying by $(\mathbf{X}\mathbf{X}^\top + \lambda\mathbf{I})^{-1}$ and right-multiplying by $(\mathbf{X}^\top\mathbf{X} + \lambda\mathbf{I})^{-1}$ yields the statement.

- Dual solution: $\boldsymbol{\alpha}$ such that

$$\mathbf{W} = \sum_{i=1}^m \alpha_i K(x_i, \cdot) = \sum_{i=1}^m \alpha_i \mathbf{\Phi}(x_i) = \mathbf{X}\boxed{\boldsymbol{\alpha}}.$$

By lemma, $\mathbf{W} = (\mathbf{X}\mathbf{X}^\top + \lambda\mathbf{I})^{-1}\mathbf{X}\mathbf{Y} = \mathbf{X}\boxed{(\mathbf{X}^\top\mathbf{X} + \lambda\mathbf{I})^{-1}\mathbf{Y}}$.

This gives $\boxed{\boldsymbol{\alpha} = (\mathbf{X}^\top\mathbf{X} + \lambda\mathbf{I})^{-1}\mathbf{Y}}$.

Computational Complexity

	Solution	Prediction
Primal	$O(mN^2 + N^3)$	$O(N)$
Dual	$O(\kappa m^2 + m^3)$	$O(\kappa m)$

Kernel Ridge Regression

(Saunders et al., 1998)

- Optimization problem:

$$\max_{\boldsymbol{\alpha} \in \mathbb{R}^m} -\lambda \boldsymbol{\alpha}^\top \boldsymbol{\alpha} + 2\boldsymbol{\alpha}^\top \mathbf{y} - \boldsymbol{\alpha}^\top \mathbf{K} \boldsymbol{\alpha}$$

or $$\max_{\boldsymbol{\alpha} \in \mathbb{R}^m} -\boldsymbol{\alpha}^\top (\mathbf{K} + \lambda \mathbf{I}) \boldsymbol{\alpha} + 2\boldsymbol{\alpha}^\top \mathbf{y}.$$

- Solution:

$$h(x) = \sum_{i=1}^{m} \alpha_i K(x_i, x),$$

with $$\boldsymbol{\alpha} = (\mathbf{K} + \lambda \mathbf{I})^{-1} \mathbf{y}.$$

Notes

- Advantages:
  - strong theoretical guarantees.
  - generalization to outputs in $\mathbb{R}^p$: single matrix inversion (Cortes et al., 2007).
  - use of kernels.
- Disadvantages:
  - solution not sparse.
  - training time for large matrices: low-rank approximations of kernel matrix, e.g., Nyström approx., partial Cholesky decomposition.

This Lecture

- Generalization bounds
- Linear regression
- Kernel ridge regression
- Support vector regression
- Lasso

Support Vector Regression

(Vapnik, 1995)

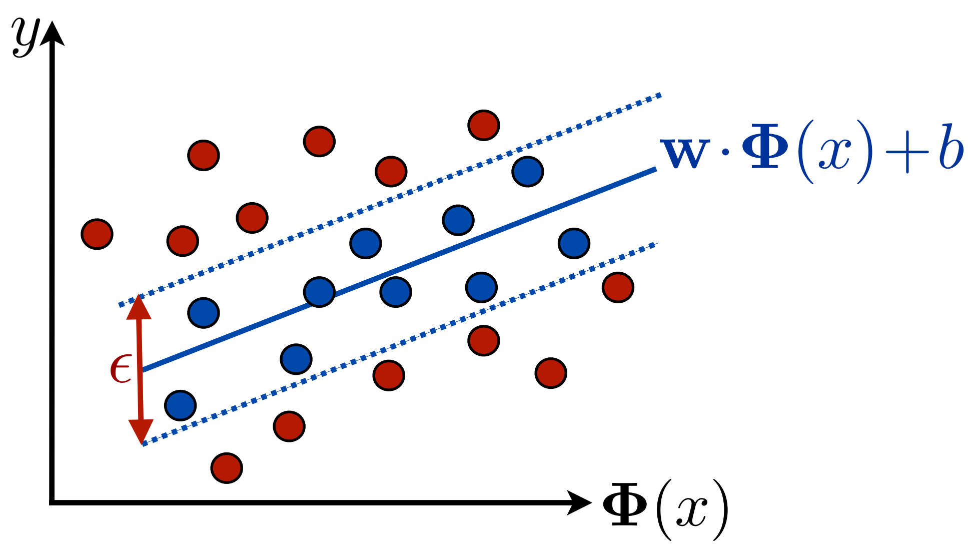
- Hypothesis set:

$$\{x \mapsto \mathbf{w} \cdot \mathbf{\Phi}(x) + b \colon \mathbf{w} \in \mathbb{R}^N, b \in \mathbb{R}\}.$$

- Loss function: ϵ-insensitive loss.

$$L(y, y') = |y' - y|_\epsilon = \max(0, |y' - y| - \epsilon).$$

Fit 'tube' with width ϵ to data.



Support Vector Regression (SVR)

(Vapnik, 1995)

- Optimization problem: similar to that of SVM.

$$\frac{1}{2}\|\mathbf{w}\|^2 + C\sum_{i=1}^{m} \big|y_i - (\mathbf{w} \cdot \mathbf{\Phi}(x_i) + b)\big|_{\epsilon}.$$

- Equivalent formulation:

$$\min_{\mathbf{w},\boldsymbol{\xi},\boldsymbol{\xi}'} \ \frac{1}{2}\|\mathbf{w}\|^2 + C\sum_{i=1}^{m}(\xi_i + \xi_i')$$

$$\begin{aligned}\text{subject to } & (\mathbf{w} \cdot \mathbf{\Phi}(x_i) + b) - y_i \leq \epsilon + \xi_i \\ & y_i - (\mathbf{w} \cdot \mathbf{\Phi}(x_i) + b) \leq \epsilon + \xi_i' \\ & \xi_i \geq 0, \xi_i' \geq 0.\end{aligned}$$

SVR - Dual Optimization Problem

- Optimization problem:

$$\max_{\boldsymbol{\alpha},\boldsymbol{\alpha}'} \; -\epsilon(\boldsymbol{\alpha}'+\boldsymbol{\alpha})^\top\mathbf{1}+(\boldsymbol{\alpha}'-\boldsymbol{\alpha})^\top\mathbf{y}-\frac{1}{2}(\boldsymbol{\alpha}'-\boldsymbol{\alpha})^\top\mathbf{K}(\boldsymbol{\alpha}'-\boldsymbol{\alpha})$$

$$\text{subject to: } (\mathbf{0}\leq\boldsymbol{\alpha}\leq\mathbf{C})\wedge(\mathbf{0}\leq\boldsymbol{\alpha}'\leq\mathbf{C})\wedge((\boldsymbol{\alpha}'-\boldsymbol{\alpha})^\top\mathbf{1}=0)\,.$$

- Solution:

$$h(x)=\sum_{i=1}^{m}(\alpha'_i-\alpha_i)K(\mathbf{x}_i,\mathbf{x})+b$$

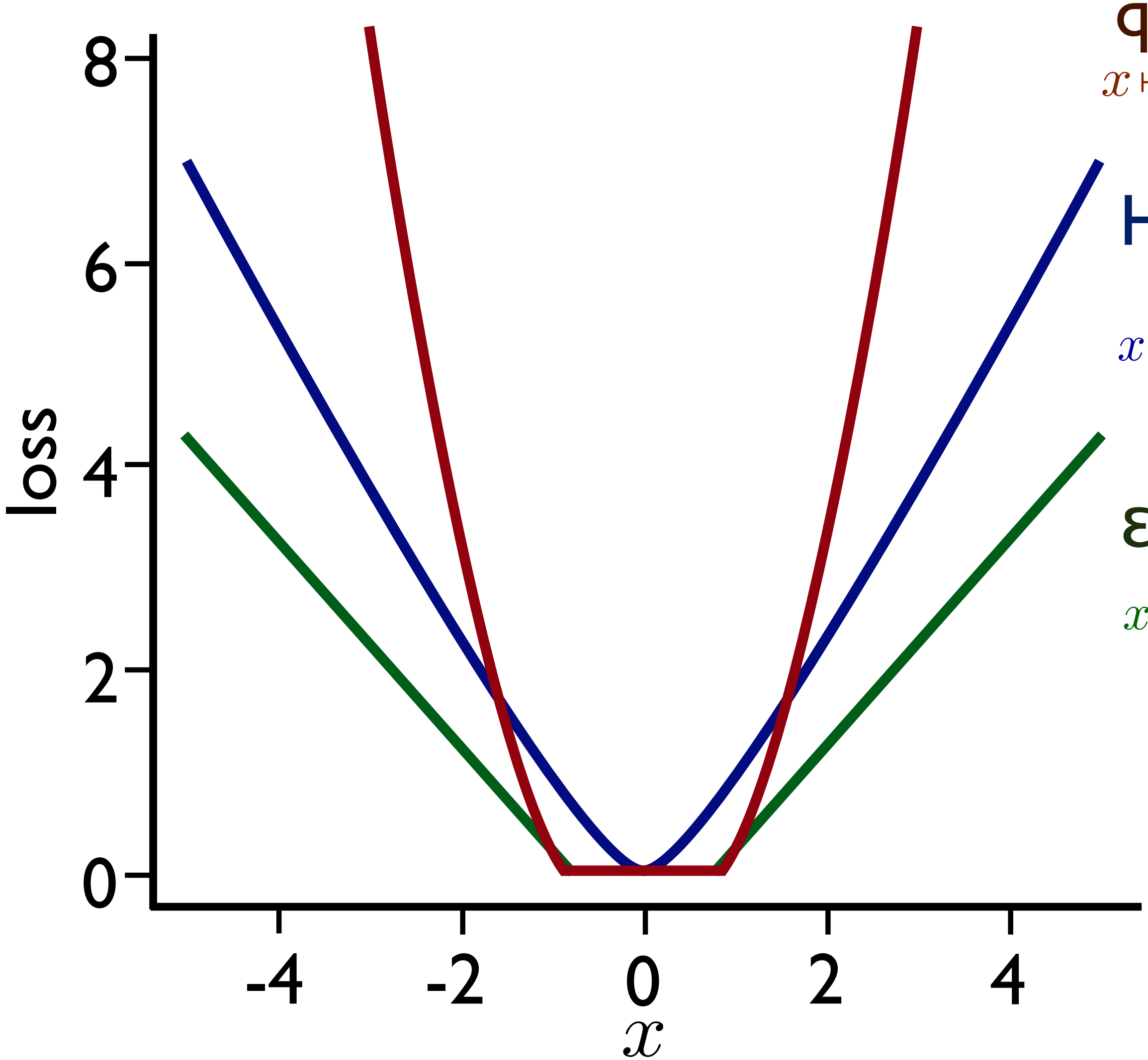
with $b=\begin{cases}-\sum_{i=1}^m(\alpha'_j-\alpha_j)K(x_j,x_i)+y_i+\epsilon & \text{when } 0<\alpha_i<C\\ -\sum_{i=1}^m(\alpha'_j-\alpha_j)K(x_j,x_i)+y_i-\epsilon & \text{when } 0<\alpha'_i<C.\end{cases}$

- Support vectors: points strictly outside the tube.

Notes

- Advantages:
  - strong theoretical guarantees (for that loss).
  - sparser solution.
  - use of kernels.
- Disadvantages:
  - selection of two parameters: C and ϵ. Heuristics:
    - search C near maximum y, ϵ near average difference of ys, measure of no. of SVs.
  - large matrices: low-rank approximations of kernel matrix.

Alternative Loss Functions



quadratic ε-insensitive

$$x \mapsto \max(0, |x| - \epsilon)^2$$

Huber

$$x \mapsto \begin{cases} x^2 & \text{if } |x| \leq c \\ 2c|x| - c^2 & \text{otherwise.} \end{cases}$$

ε-insensitive

$$x \mapsto \max(0, |x| - \epsilon)$$

SVR - Quadratic Loss

- Optimization problem:

$$\max_{\boldsymbol{\alpha},\boldsymbol{\alpha}'} \; -\epsilon(\boldsymbol{\alpha}'+\boldsymbol{\alpha})^\top \mathbf{1} + (\boldsymbol{\alpha}'-\boldsymbol{\alpha})^\top \mathbf{y} - \frac{1}{2}(\boldsymbol{\alpha}'-\boldsymbol{\alpha})^\top \left(\mathbf{K}+\frac{1}{C}\mathbf{I}\right)(\boldsymbol{\alpha}'-\boldsymbol{\alpha})$$

$$\text{subject to: } (\boldsymbol{\alpha} \geq \mathbf{0}) \wedge (\boldsymbol{\alpha} \geq \mathbf{0}) \wedge (\boldsymbol{\alpha}'-\boldsymbol{\alpha})^\top \mathbf{1} = 0) \,.$$

- Solution:

$$h(x) = \sum_{i=1}^{m} (\alpha'_i - \alpha_i) K(\mathbf{x}_i, \mathbf{x}) + b$$

with $b = \begin{cases} -\sum_{i=1}^{m} (\alpha'_j - \alpha_j) K(x_j, x_i) + y_i + \epsilon & \text{when } 0 < \alpha_i \wedge \xi_i = 0 \\ -\sum_{i=1}^{m} (\alpha'_j - \alpha_j) K(x_j, x_i) + y_i - \epsilon & \text{when } 0 < \alpha'_i \wedge \xi'_i = 0. \end{cases}$

- Support vectors: points strictly outside the tube.
- For $\epsilon = 0$, coincides with KRR.

ε-Insensitive Bound - Kernel-Based Hypotheses

- Theorem: Let $K\colon X \times X \to \mathbb{R}$ be a PDS kernel and let $\Phi\colon X \to H$ be a feature mapping associated to K. Let $H = \{\mathbf{x} \mapsto \mathbf{w} \cdot \Phi(x) \colon \|\mathbf{w}\|_H \leq \Lambda\}$. Assume $K(x, x) \leq R^2$ and $|f(x)| \leq \Gamma R$ for all $x \in X$. Then, for any $\delta > 0$, with probability at least $1 - \delta$, for any $h \in H$,

$$\mathrm{E}[|h(x) - f(x)|_\epsilon] \leq \widehat{\mathrm{E}}[|h(x) - f(x)|_\epsilon] + \frac{R\Lambda}{\sqrt{m}}\left[2 + \left(\frac{\Gamma}{\Lambda} + 1\right)\sqrt{\frac{\log \frac{1}{\delta}}{2}}\right].$$

$$\mathrm{E}[|h(x)-f(x)|_\epsilon] \leq \widehat{\mathrm{E}}[|h(x)-f(x)|_\epsilon]+\frac{\Lambda R}{\sqrt{m}}\left[2\sqrt{\frac{\mathrm{Tr}[\mathbf{K}]/R^2}{m}}+3\left(\frac{\Gamma}{\Lambda} + 1\right)\sqrt{\frac{\log \frac{2}{\delta}}{2}}\right].$$

ε-Insensitive Bound - Kernel-Based Hypotheses

- Proof: Let $H_\epsilon = \{x \mapsto |h(x) - f(x)|_\epsilon : h \in H\}$ and let H' be defined by $H' = \{x \mapsto h(x) - f(x) : h \in H\}$.
  - The function $\Phi_\epsilon : x \mapsto |x|_\epsilon$ is 1-Lipschitz and $\Phi_\epsilon(0) = 0$. Thus, by the contraction lemma,
  $$\widehat{\mathfrak{R}}_S(H_\epsilon) \leq \widehat{\mathfrak{R}}_S(H').$$
  - Since $\widehat{\mathfrak{R}}_S(H') = \widehat{\mathfrak{R}}_S(H)$ (see proof for Rademacher Complexity of L_p Loss), this shows that $\widehat{\mathfrak{R}}_S(H_\epsilon) \leq \widehat{\mathfrak{R}}_S(H)$.
  - The rest is a direct application of the Rademacher Complexity Regression Bound (this lecture).

On-line Regression

- On-line version of batch algorithms:
  - stochastic gradient descent.
  - primal or dual.
- Examples:
  - Mean squared error function: Widrow-Hoff (or LMS) algorithm (Widrow and Hoff, 1995).
  - SVR ε-insensitive (dual) linear or quadratic function: on-line SVR.

Widrow-Hoff

(Widrow and Hoff, 1988)

$\textsc{WidrowHoff}(\mathbf{w}_0)$

$\mathbf{w}_1 \leftarrow \mathbf{w}_0 \qquad \triangleright$ typically $\mathbf{w}_0 = \mathbf{0}$

for $t \leftarrow 1$ **to** T **do**

$\quad \textsc{Receive}(\mathbf{x}_t)$

$\quad \widehat{y}_t \leftarrow \mathbf{w}_t \cdot \mathbf{x}_t$

$\quad \textsc{Receive}(y_t)$

$\quad \mathbf{w}_{t+1} \leftarrow \mathbf{w}_t + 2\eta(\mathbf{w}_t \cdot \mathbf{x}_t - y_t)\mathbf{x}_t \qquad \triangleright\, \eta > 0$

return $\mathbf{w}_{T+1}$

Dual On-Line SVR

$(b=0)$ (Vijayakumar and Wu, 1988)

$\textsc{DualSVR}()$

$\boldsymbol{\alpha} \leftarrow \mathbf{0}$
$\boldsymbol{\alpha}' \leftarrow \mathbf{0}$
for $t \leftarrow 1$ **to** T **do**
  $\textsc{Receive}(x_t)$
  $\widehat{y}_t \leftarrow \sum_{s=1}^{T} (\alpha'_s - \alpha_s) K(x_s, x_t)$
  $\textsc{Receive}(y_t)$
  $\alpha'_{t+1} \leftarrow \alpha'_t + \min(\max(\eta(y_t - \widehat{y}_t - \epsilon), -\alpha'_t), C - \alpha'_t)$
  $\alpha_{t+1} \leftarrow \alpha_t + \min(\max(\eta(\widehat{y}_t - y_t - \epsilon), -\alpha_t), C - \alpha_t)$
return $\sum_{t=1}^{T} \alpha_t K(x_t, \cdot)$

This Lecture

- Generalization bounds
- Linear regression
- Kernel ridge regression
- Support vector regression
- Lasso

LASSO

(Tibshirani, 1996)

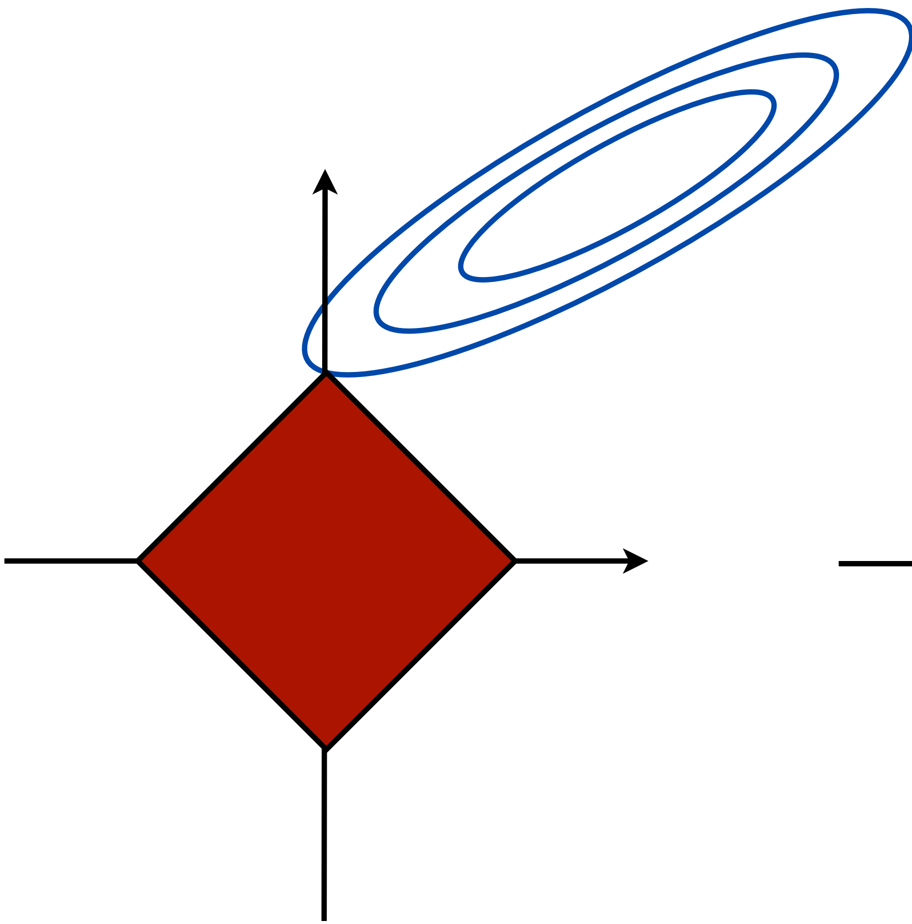
- Optimization problem: 'least absolute shrinkage and selection operator'.

$$\min_{\mathbf{w}} F(\mathbf{w}, b) = \lambda \|\mathbf{w}\|_1 + \sum_{i=1}^{m} (\mathbf{w} \cdot \mathbf{x}_i + b - y_i)^2 \,,$$

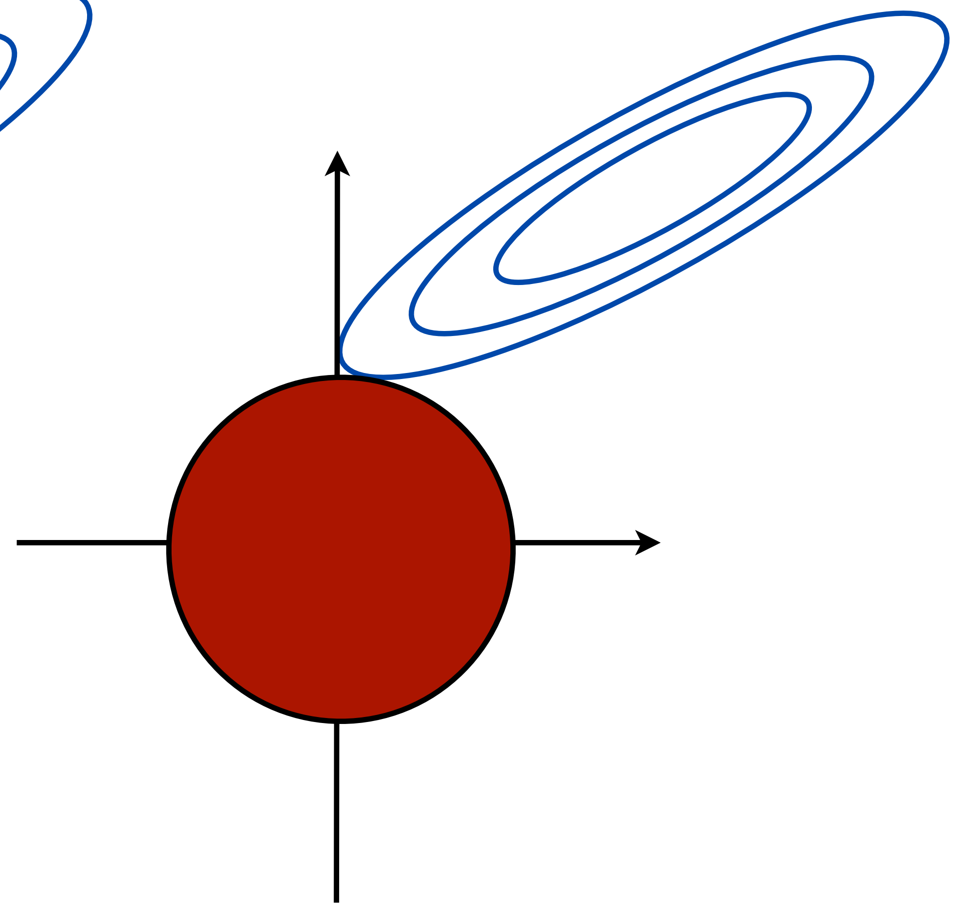
  where $\lambda \geq 0$ is a (regularization) parameter.

- Solution: equiv. convex quadratic program (QP).
  - general: standard QP solvers.
  - specific algorithm: LARS (least angle regression procedure), entire path of solutions.

Sparsity of L1 regularization



L1 regularization



L2 regularization

Sparsity Guarantee

- Rademacher complexity of L1-norm bounded linear hypotheses:

$$
\begin{aligned}
\widehat{\mathfrak{R}}_S(H) &= \frac{1}{m} \operatorname*{E}_{\boldsymbol{\sigma}} \left[\sup_{\|\mathbf{w}\|_1 \le \Lambda_1} \sum_{i=1}^m \sigma_i \mathbf{w} \cdot \mathbf{x}_i \right] \\
&= \frac{\Lambda_1}{m} \operatorname*{E}_{\boldsymbol{\sigma}} \left[\left\| \sum_{i=1}^m \sigma_i \mathbf{x}_i \right\|_\infty \right] && \text{(by definition of the dual norm)} \\
&= \frac{\Lambda_1}{m} \operatorname*{E}_{\boldsymbol{\sigma}} \left[\max_{j \in [1,N]} \left| \sum_{i=1}^m \sigma_i x_{ij} \right| \right] && \text{(by definition of } \| \cdot \|_\infty) \\
&= \frac{\Lambda_1}{m} \operatorname*{E}_{\boldsymbol{\sigma}} \left[\max_{j \in [1,N]} \max_{s \in \{-1,+1\}} s \sum_{i=1}^m \sigma_i x_{ij} \right] && \text{(by definition of } | \cdot |) \\
&= \frac{\Lambda_1}{m} \operatorname*{E}_{\boldsymbol{\sigma}} \left[\sup_{\mathbf{z} \in A} \sum_{i=1}^m \sigma_i z_i \right] \le r_\infty \Lambda_1 \sqrt{\frac{2 \log(2N)}{m}}. && \text{(Massart's lemma)}
\end{aligned}
$$

Notes

- Advantages:
  - theoretical guarantees.
  - sparse solution.
  - feature selection.
- Drawbacks:
  - no natural use of kernels.
  - no closed-form solution (not necessary, but can be convenient for theoretical analysis).

Regression

- Many other families of algorithms: including
  - neural networks.
  - decision trees (see multi-class lecture).
  - boosting trees for regression.

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Foundations of Machine Learning
Reinforcement Learning

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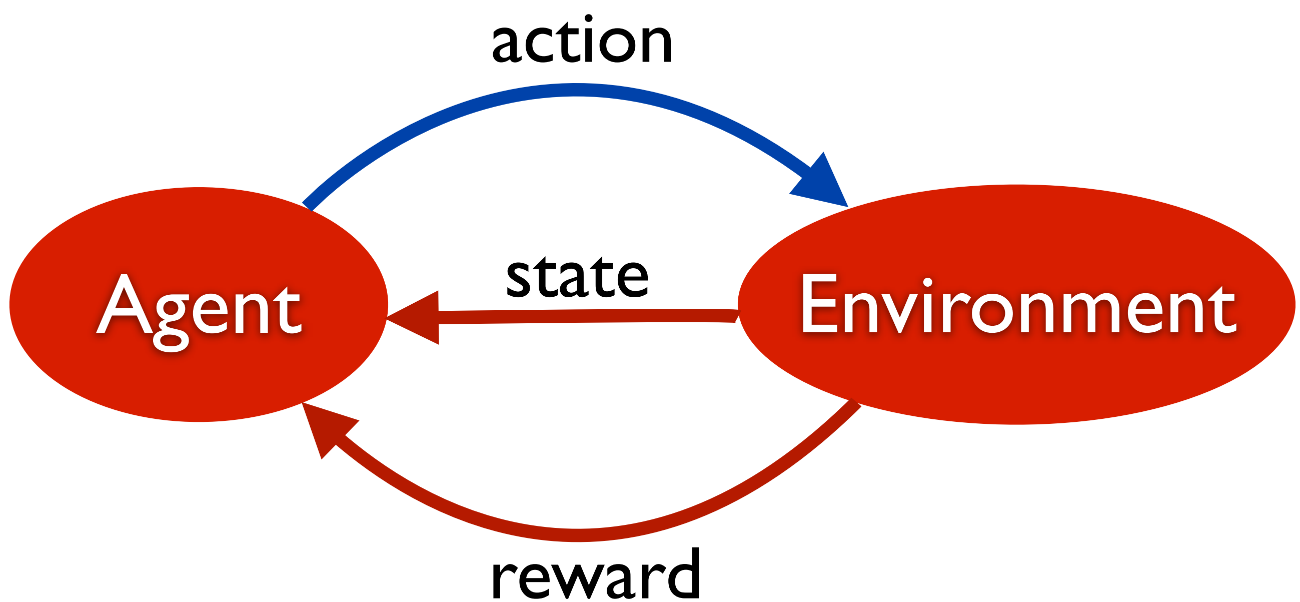
Reinforcement Learning

- Agent exploring environment.
- Interactions with environment:



- Problem: find action policy that maximizes cumulative reward over the course of interactions.

Key Features

- Contrast with supervised learning:
  - no explicit labeled training data.
  - distribution defined by actions taken.
- Delayed rewards or penalties.
- RL trade-off:
  - exploration (of unknown states and actions) to gain more reward information; vs.
  - exploitation (of known information) to optimize reward.

Applications

- Robot control e.g., Robocup Soccer Teams (Stone et al., 1999), helicopter flight, autonomous driving.
- Board games, e.g., TD-Gammon (Tesauro, 1995), Go (Silver et al., 2016).
- Elevator scheduling (Crites and Barto, 1996).
- Ads placement, patient treatment.
- Telecommunications.
- Inventory management.
- Dynamic radio channel assignment.

This Lecture

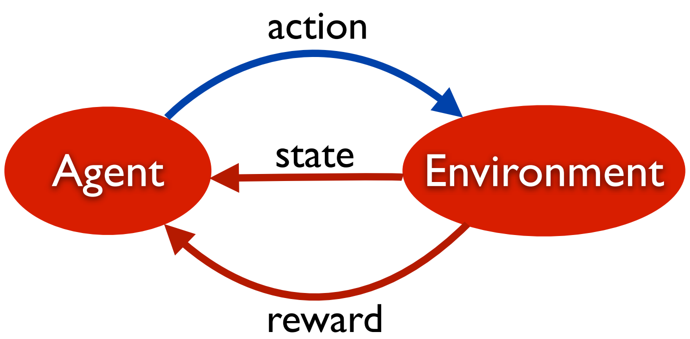
- Markov Decision Processes (MDPs)
- Planning
- Learning
- Multi-armed bandit problem

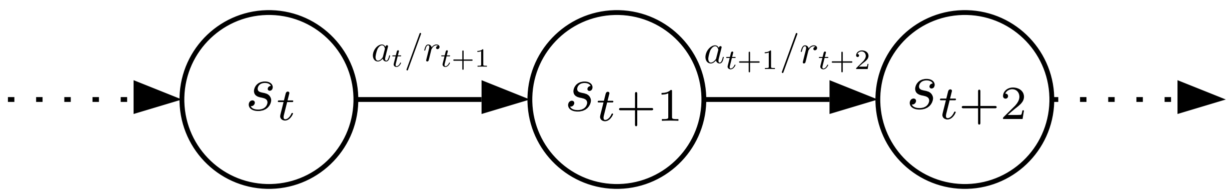
Markov Decision Process (MDP)

- Definition: a Markov Decision Process is defined by:
  - a set of decision epochs $\{0, \ldots, T\}$.
  - a set of states S, possibly infinite.
  - a start state or initial state s_0;
  - a set of actions A, possibly infinite.
  - a transition probability $\Pr[s'|s, a]$: distribution over destination states $s' = \delta(s, a)$.
  - a reward probability $\Pr[r'|s, a]$: distribution over rewards returned $r' = r(s, a)$.

Model

- State observed at time t : $s_t \in S$.
- Action taken at time t : $a_t \in A$.
- State reached $s_{t+1} = \delta(s_t, a_t)$.
- Reward received: $r_{t+1} = r(s_t, a_t)$.

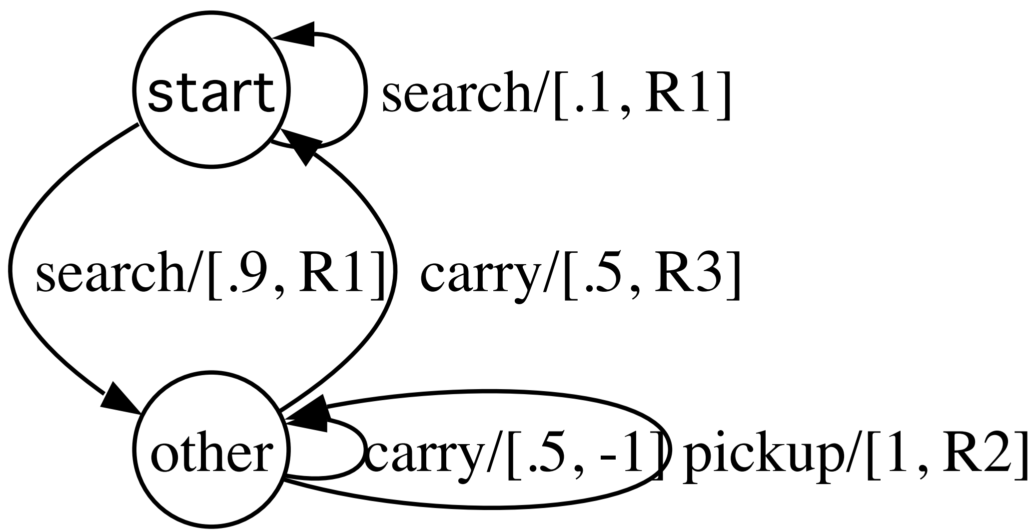




MDPs - Properties

- Finite MDPs: A and S finite sets.
- Finite horizon when $T < \infty$.
- Reward $r(s, a)$: often deterministic function.

Example - Robot Picking up Balls



Policy

- **Definition**: a policy is a mapping $\pi\colon S \to A$.
- **Objective**: find policy π maximizing expected return.
  - finite horizon return: $\sum_{t=0}^{T-1} r\big(s_t, \pi(s_t)\big)$.
  - infinite horizon return: $\sum_{t=0}^{+\infty} \gamma^t r\big(s_t, \pi(s_t)\big)$.
- **Theorem**: for any finite MDP, there exists an optimal policy (for any start state).

Policy Value

- **Definition**: the value of a policy π at state s is
  - finite horizon:

$$V_\pi(s) = \mathrm{E}\left[\sum_{t=0}^{T-1} r\big(s_t, \pi(s_t)\big) \,\Big|\, s_0 = s\right].$$

  - infinite horizon: discount factor $\gamma \in [0, 1)$,

$$V_\pi(s) = \mathrm{E}\left[\sum_{t=0}^{+\infty} \gamma^t r\big(s_t, \pi(s_t)\big) \,\Big|\, s_0 = s\right].$$

- **Problem**: find policy π with maximum value for all states.

Policy Evaluation

- Analysis of policy value:

$$
\begin{aligned}
V_\pi(s) &= \mathrm{E}\left[\sum_{t=0}^{+\infty} \gamma^t r\big(s_t, \pi(s_t)\big) \,\Big|\, s_0 = s\right]. \\
&= \mathrm{E}[r(s, \pi(s))] + \gamma\, \mathrm{E}\left[\sum_{t=0}^{+\infty} \gamma^t r\big(s_{t+1}, \pi(s_{t+1})\big) \,\Big|\, s_0 = s\right] \\
&= \mathrm{E}[r(s, \pi(s)] + \gamma\, \mathrm{E}[V_\pi(\delta(s, \pi(s)))].
\end{aligned}
$$

- Bellman equations (system of linear equations):

$$
\boxed{V_\pi(s) = \mathrm{E}[r(s, \pi(s)] + \gamma \sum_{s'} \Pr[s'|s, \pi(s)] V_\pi(s').}
$$

Bellman Equation - Existence and Uniqueness

- Notation:
  - transition probability matrix $\mathbf{P}_{s,s'} = \Pr[s'|s, \pi(s)]$.
  - value column matrix $\mathbf{V} = V_\pi(s)$.
  - expected reward column matrix: $\mathbf{R} = \mathrm{E}[r(s, \pi(s)]$.
- Theorem: for a finite MDP, Bellman's equation admits a unique solution given by

$$\mathbf{V}_0 = (\mathbf{I} - \gamma \mathbf{P})^{-1} \mathbf{R}.$$

Bellman Equation - Existence and Uniqueness

- Proof: Bellman's equation rewritten as

$$\mathbf{V} = \mathbf{R} + \gamma \mathbf{P}\mathbf{V}.$$

  - $\mathbf{P}$ is a stochastic matrix, thus,

$$\|\mathbf{P}\|_\infty = \max_s \sum_{s'} |\mathbf{P}_{ss'}| = \max_s \sum_{s'} \Pr[s'|s, \pi(s)] = 1.$$

  - This implies that $\|\gamma \mathbf{P}\|_\infty = \gamma < 1$. The eigenvalues of $\gamma \mathrm{P}$ are all less than one and $(\mathbf{I} - \gamma \mathbf{P})$ is invertible.

- Notes: general shortest distance problem (MM, 2002).

Optimal Policy

- Definition: policy π^* with maximal value for all states $s \in S$.
  - value of π^* (optimal value):
$$\forall s \in S, V_{\pi^*}(s) = \max_{\pi} V_{\pi}(s).$$
  - optimal state-action value function: expected return for taking action a at state s and then following optimal policy.
$$\begin{aligned} Q^*(s,a) &= \mathrm{E}[r(s,a)] + \gamma\, \mathrm{E}[V^*(\delta(s,a))] \\ &= \mathrm{E}[r(s,a)] + \gamma \sum_{s' \in S} \Pr[s' \mid s,a] V^*(s'). \end{aligned}$$

Optimal Values - Bellman Equations

- Property: the following equalities hold:

$$\forall s \in S,\ V^*(s) = \max_{a \in A} Q^*(s, a).$$

- Proof: by definition, for all s, $V^*(s) \leq \max_{a \in A} Q^*(s, a)$.
  - If for some s we had $V^*(s) < \max_{a \in A} Q^*(s, a)$, then maximizing action would define a better policy.

- Thus,

$$\boxed{V^*(s) = \max_{a \in A} \Big\{ \mathrm{E}[r(s, a)] + \gamma \sum_{s' \in S} \Pr[s'|s, a] V^*(s') \Big\}.}$$

This Lecture

- Markov Decision Processes (MDPs)
- Planning
- Learning
- Multi-armed bandit problem

Known Model

- Setting: environment model known.
- Problem: find optimal policy.
- Algorithms:
  - value iteration.
  - policy iteration.
  - linear programming.

Value Iteration Algorithm

$$\mathbf{\Phi}(\mathbf{V})(s) = \max_{a \in A} \Big\{ \mathrm{E}[r(s,a)] + \gamma \sum_{s' \in S} \Pr[s'|s,a] V(s') \Big\}.$$

$$\mathbf{\Phi}(\mathbf{V}) = \max_{\pi} \{ \mathbf{R}_\pi + \gamma \mathbf{P}_\pi \mathbf{V} \}.$$

$\textsc{ValueIteration}(\mathbf{V}_0)$

1 $\quad \mathbf{V} \leftarrow \mathbf{V}_0 \quad \triangleright\, \mathbf{V}_0$ arbitrary value

2 $\quad$ **while** $\|\mathbf{V} - \mathbf{\Phi}(\mathbf{V})\| \geq \frac{(1-\gamma)\epsilon}{\gamma}$ **do**

3 $\qquad\quad \mathbf{V} \leftarrow \mathbf{\Phi}(\mathbf{V})$

4 $\quad$ **return** $\mathbf{\Phi}(\mathbf{V})$

VI Algorithm - Convergence

- Theorem: for any initial value $\mathbf{V}_0$, the sequence defined by $\mathbf{V}_{n+1} = \mathbf{\Phi}(\mathbf{V}_n)$ converge to $\mathbf{V}^*$.
- Proof: we show that $\mathbf{\Phi}$ is γ-contracting for $\|\cdot\|_\infty$

→ existence and uniqueness of fixed point for $\mathbf{\Phi}$.

  - for any $s \in S$, let $a^*(s)$ be the maximizing action defining $\mathbf{\Phi}(\mathbf{V})(s)$. Then, for $s \in S$ and any $\mathbf{U}$,

$$\begin{aligned}
\mathbf{\Phi}(\mathbf{V})(s) - \mathbf{\Phi}(\mathbf{U})(s) &\leq \mathbf{\Phi}(\mathbf{V})(s) - \Big(\mathrm{E}[r(s, a^*(s))] + \gamma \sum_{s' \in S} \Pr[s' \mid s, a^*(s)] \mathbf{U}(s') \Big) \\
&= \gamma \sum_{s' \in S} \Pr[s' | s, a^*(s)] [\mathbf{V}(s') - \mathbf{U}(s')] \\
&\leq \gamma \sum_{s' \in S} \Pr[s' | s, a^*(s)] \|\mathbf{V} - \mathbf{U}\|_\infty = \gamma \|\mathbf{V} - \mathbf{U}\|_\infty .
\end{aligned}$$

Complexity and Optimality

- **Complexity**: convergence in $O(\log \frac{1}{\epsilon})$. Observe that

$$\|\mathbf{V}_{n+1} - \mathbf{V}_n\|_\infty \leq \gamma \|\mathbf{V}_n - \mathbf{V}_{n-1}\|_\infty \leq \gamma^n \|\mathbf{\Phi}(\mathbf{V}_0) - \mathbf{V}_0\|_\infty.$$

Thus, $\gamma^n \|\mathbf{\Phi}(\mathbf{V}_0) - \mathbf{V}_0\|_\infty \leq \dfrac{(1-\gamma)\epsilon}{\gamma} \Rightarrow n = O\Big(\log \dfrac{1}{\epsilon}\Big).$

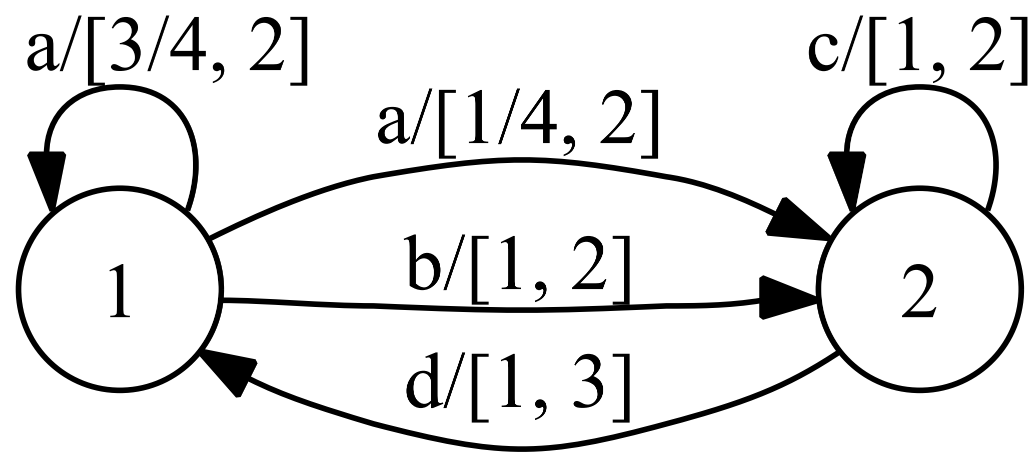
- ϵ**-Optimality**: let $\mathbf{V}_{n+1}$ be the value returned. Then,

$$\begin{aligned}\|\mathbf{V}^* - \mathbf{V}_{n+1}\|_\infty &\leq \|\mathbf{V}^* - \mathbf{\Phi}(\mathbf{V}_{n+1})\|_\infty + \|\mathbf{\Phi}(\mathbf{V}_{n+1}) - \mathbf{V}_{n+1}\|_\infty \\ &\leq \gamma \|\mathbf{V}^* - \mathbf{V}_{n+1}\|_\infty + \gamma \|\mathbf{V}_{n+1} - \mathbf{V}_n\|_\infty.\end{aligned}$$

Thus,

$$\|\mathbf{V}^* - \mathbf{V}_{n+1}\|_\infty \leq \frac{\gamma}{1-\gamma} \|\mathbf{V}_{n+1} - \mathbf{V}_n\|_\infty \leq \epsilon.$$

VI Algorithm - Example



$$\mathbf{V}_{n+1}(1) = \max\left\{2 + \gamma\Big(\frac{3}{4}\mathbf{V}_n(1) + \frac{1}{4}\mathbf{V}_n(2)\Big), 2 + \gamma\mathbf{V}_n(2)\right\}$$

$$\mathbf{V}_{n+1}(2) = \max\left\{3 + \gamma\mathbf{V}_n(1), 2 + \gamma\mathbf{V}_n(2)\right\}.$$

For $\mathbf{V}_0(1) = -1, \mathbf{V}_0(2) = 1, \gamma = 1/2$, $\mathbf{V}_1(1) = \mathbf{V}_1(2) = 5/2.$

But, $\mathbf{V}^*(1) = 14/3, \mathbf{V}^*(2) = 16/3.$

Policy Iteration Algorithm

PolicyIteration(π_0)

$\pi \leftarrow \pi_0$ $\quad \triangleright$ π_0 arbitrary policy
$\pi' \leftarrow$ NIL
while $(\pi \neq \pi')$ **do**
  $\mathbf{V} \leftarrow \mathbf{V}_\pi$ $\quad \triangleright$ policy evaluation: solve $(\mathbf{I} - \gamma \mathbf{P}_\pi)\mathbf{V} = \mathbf{R}_\pi$.
  $\pi' \leftarrow \pi$
  $\pi \leftarrow \operatorname{argmax}_\pi \{\mathbf{R}_\pi + \gamma \mathbf{P}_\pi \mathbf{V}\}$ $\quad \triangleright$ greedy policy improvement.
return π

PI Algorithm - Convergence

- **Theorem**: let $(\mathbf{V}_n)_{n \in \mathbb{N}}$ be the sequence of policy values computed by the algorithm, then,

$$\mathbf{V}_n \leq \mathbf{V}_{n+1} \leq \mathbf{V}^*.$$

- **Proof**: let π_{n+1} be the policy improvement at the nth iteration, then, by definition,

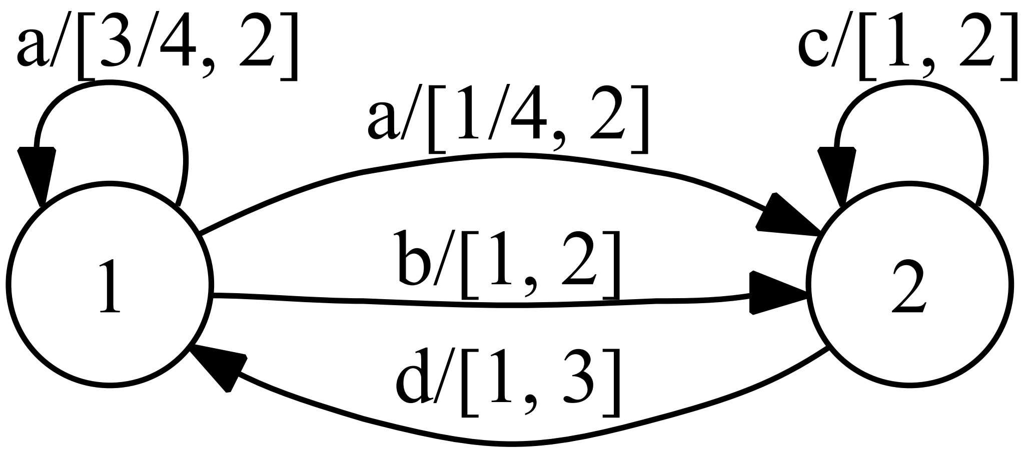
$$\mathbf{R}_{\pi_{n+1}} + \gamma \mathbf{P}_{\pi_{n+1}} \mathbf{V}_n \geq \mathbf{R}_{\pi_n} + \gamma \mathbf{P}_{\pi_n} \mathbf{V}_n = \mathbf{V}_n.$$

  - therefore, $\mathbf{R}_{\pi_{n+1}} \geq (\mathbf{I} - \gamma \mathbf{P}_{\pi_{n+1}}) \mathbf{V}_n$.
  - note that $(\mathbf{I} - \gamma \mathbf{P}_{\pi_{n+1}})^{-1}$ preserves ordering:
    $\mathbf{X} \geq \mathbf{0} \Rightarrow (\mathbf{I} - \gamma \mathbf{P}_{\pi_{n+1}})^{-1} \mathbf{X} = \sum_{k=0}^{\infty} (\gamma \mathbf{P}_{\pi_{n+1}})^k \mathbf{X} \geq \mathbf{0}$.
  - thus, $\mathbf{V}_{n+1} = (\mathbf{I} - \gamma \mathbf{P}_{\pi_{n+1}})^{-1} \mathbf{R}_{\pi_{n+1}} \geq \mathbf{V}_n$.

Notes

- Two consecutive policy values can be equal only at last iteration.
- The total number of possible policies is $|A|^{|S|}$, thus, this is the maximal possible number of iterations.
  - best upper bound known $O(\frac{|A|^{|S|}}{|S|})$.

PI Algorithm - Example



Initial policy: $\pi_0(1) = b, \pi_0(2) = c.$

Evaluation: $V_{\pi_0}(1) = 1 + \gamma V_{\pi_0}(2)$

$$V_{\pi_0}(2) = 2 + \gamma V_{\pi_0}(2).$$

Thus, $V_{\pi_0}(1) = \dfrac{1+\gamma}{1-\gamma} \quad V_{\pi_0}(2) = \dfrac{2}{1-\gamma}.$

VI and PI Algorithms - Comparison

- Theorem: let $(\mathbf{U}_n)_{n\in\mathbb{N}}$ be the sequence of policy values generated by the VI algorithm, and $(\mathbf{V}_n)_{n\in\mathbb{N}}$ the one generated by the PI algorithm. If $\mathbf{U}_0 = \mathbf{V}_0$, then,
$$\forall n \in \mathbb{N}, \; \mathbf{U}_n \leq \mathbf{V}_n \leq \mathbf{V}^*.$$
- Proof: we first show that $\mathbf{\Phi}$ is monotonic. Let $\mathbf{U}$ and $\mathbf{V}$ be such that $\mathbf{U} \leq \mathbf{V}$ and let π be the policy such that $\mathbf{\Phi}(\mathbf{U}) = \mathbf{R}_\pi + \gamma \mathbf{P}_\pi \mathbf{U}$. Then,

$$\mathbf{\Phi}(\mathbf{U}) \leq \mathbf{R}_\pi + \gamma \mathbf{P}_\pi \mathbf{V} \leq \max_{\pi'} \{\mathbf{R}'_\pi + \gamma \mathbf{P}'_\pi \mathbf{V}\} = \mathbf{\Phi}(\mathbf{V}).$$

VI and PI Algorithms - Comparison

- The proof is by induction on n. Assume $\mathbf{U}_n \leq \mathbf{V}_n$, then, by the monotonicity of $\mathbf{\Phi}$,

$$\mathbf{U}_{n+1} = \mathbf{\Phi}(\mathbf{U}_n) \leq \mathbf{\Phi}(\mathbf{V}_n) = \max_{\pi}\{\mathbf{R}_\pi + \gamma \mathbf{P}_\pi \mathbf{V}_n\}.$$

- Let π_{n+1} be the maximizing policy:

$$\pi_{n+1} = \operatorname*{argmax}_{\pi}\{\mathbf{R}_\pi + \gamma \mathbf{P}_\pi \mathbf{V}_n\}.$$

- Then,

$$\mathbf{\Phi}(\mathbf{V}_n) = \mathbf{R}_{\pi_{n+1}} + \gamma \mathbf{P}_{\pi_{n+1}} \mathbf{V}_n \leq \mathbf{R}_{\pi_{n+1}} + \gamma \mathbf{P}_{\pi_{n+1}} \mathbf{V}_{n+1} = \mathbf{V}_{n+1}.$$

Notes

- The PI algorithm converges in a smaller number of iterations than the VI algorithm due to the optimal policy.
- But, each iteration of the PI algorithm requires computing a policy value, i.e., solving a system of linear equations, which is more expensive to compute that an iteration of the VI algorithm.

Primal Linear Program

- LP formulation: choose $\alpha(s) > 0$, with $\sum_s \alpha(s) = 1$.

$$\min_{\mathbf{V}} \quad \sum_{s \in S} \alpha(s) V(s)$$

$$\text{subject to} \quad \forall s \in S, \forall a \in A, V(s) \geq \mathrm{E}[r(s,a)] + \gamma \sum_{s' \in S} \Pr[s'|s,a] V(s').$$

- Parameters:
  - number rows: $|S||A|$.
  - number of columns: $|S|$.

Dual Linear Program

- LP formulation:

$$\max_{\mathbf{x}} \quad \sum_{s \in S, a \in A} \mathrm{E}[r(s,a)]\, x(s,a)$$

$$\text{subject to} \quad \forall s \in S, \sum_{a \in A} x(s',a) = \alpha(s') + \gamma \sum_{s \in S, a \in A} \Pr[s'|s,a]\, x(s',a)$$

$$\forall s \in S, \forall a \in A, x(s,a) \geq 0.$$

- Parameters: more favorable number of rows.
  - number rows: $|S|$.
  - number of columns: $|S||A|$.

This Lecture

- Markov Decision Processes (MDPs)
- Planning
- Learning
- Multi-armed bandit problem

Problem

- Unknown model:
  - transition and reward probabilities not known.
  - realistic scenario in many practical problems, e.g., robot control.
- Training information: sequence of immediate rewards based on actions taken.
- Learning approches:
  - model-free: learn policy directly.
  - model-based: learn model, use it to learn policy.

Learning Approaches

- Two broad families:
  - model-based approaches: use samples based on interactions to learn P and r explicitly; next, use value iteration to learn policy.
  - model-free approaches: do not seek to learn model; instead, use samples to learn Q function; policy readily derived from Q.

Problem

- How do we estimate reward and transition probabilities?
  - use equations derived for policy value and Q-functions.
  - but, equations given in terms of some expectations.
  - $\longrightarrow$ instance of a stochastic approximation problem.

Stochastic Approximation

- Problem: find solution of $\mathbf{x} = H(\mathbf{x})$ with $\mathbf{x} \in \mathbb{R}^N$ while
  - $H(\mathbf{x})$ cannot be computed, e.g., H not accessible;
  - i.i.d. sample of noisy observations $H(\mathbf{x}_i) + \mathbf{w}_i$, available, $i \in [1, m]$, with $\mathrm{E}[\mathbf{w}] = 0$.
- Idea: algorithm based on iterative technique:

$$\begin{aligned}\mathbf{x}_{t+1} &= (1 - \alpha_t)\mathbf{x}_t + \alpha_t[H(\mathbf{x}_t) + \mathbf{w}_t] \\ &= \mathbf{x}_t + \alpha_t[H(\mathbf{x}_t) + \mathbf{w}_t - \mathbf{x}_t].\end{aligned}$$

  - more generally $\mathbf{x}_{t+1} = \mathbf{x}_t + \alpha_t D(\mathbf{x}_t, \mathbf{w}_t)$.

Mean Estimation

- Theorem: Let X be a random variable taking values in $[0, 1]$ and let $x_0, \ldots, x_m$ be i.i.d. values of X. Define the sequence $(\mu_m)_{m \in \mathbb{N}}$ by

$$\mu_{m+1} = (1 - \alpha_m)\mu_m + \alpha_m x_m \quad \text{with } \mu_0 = x_0.$$

Then, for $\alpha_m \in [0, 1]$, with $\sum_{m \geq 0} \alpha_m = +\infty$ and $\sum_{m \geq 0} \alpha_m^2 < +\infty$,

$$\boxed{\mu_m \xrightarrow{\text{a.s}} \mathrm{E}[X].}$$

Proof

- Proof: By the independence assumption, for $m \geq 0$,

$$\begin{aligned}\mathrm{Var}[\mu_{m+1}] &= (1-\alpha_m)^2 \mathrm{Var}[\mu_m] + \alpha_m^2 \mathrm{Var}[x_m] \\ &\leq (1-\alpha_m)\mathrm{Var}[\mu_m] + \alpha_m^2.\end{aligned}$$

  - We have $\alpha_m \to 0$ since $\sum_{m \geq 0} \alpha_m^2 < +\infty$.
  - Let $\epsilon > 0$ and suppose there exists $N \in \mathbb{N}$ such that for all $m \geq N$, $\mathrm{Var}[\mu_m] \geq \epsilon$. Then, for $m \geq N$,

$$\mathrm{Var}[\mu_{m+1}] \leq \mathrm{Var}[\mu_m] - \alpha_m \epsilon + \alpha_m^2,$$

which implies $\mathrm{Var}[\mu_{m+N}] \leq \underbrace{\mathrm{Var}[\mu_N] - \epsilon \sum_{n=N}^{m+N} \alpha_n + \sum_{n=N}^{m+N} \alpha_n^2}_{\to -\infty \text{ when } m \to \infty}$,

contradicting $\mathrm{Var}[\mu_{m+N}] \geq 0$.

Mean Estimation

- Thus, for all $N \in \mathbb{N}$ there exists $m_0 \geq N$ such that $\mathrm{Var}[\mu_{m_0}] < \epsilon$. Choose N large enough so that $\forall m \geq N, \alpha_m \leq \epsilon$. Then,
$$\mathrm{Var}[\mu_{m_0+1}] \leq (1 - \alpha_{m_0})\epsilon + \epsilon\alpha_{m_0} = \epsilon.$$
- Therefore, $\mu_m \leq \epsilon$ for all $m \geq m_0$ (L_2 convergence).

Notes

- special case: $\alpha_m = \frac{1}{m}$.
  - Strong law of large numbers.
- Connection with stochastic approximation.

TD(0) Algorithm

- Idea: recall Bellman's linear equations giving V

$$\begin{aligned} V_\pi(s) &= \mathrm{E}[r(s,\pi(s)] + \gamma \sum_{s'} \Pr[s'|s,\pi(s)]V_\pi(s') \\ &= \mathop{\mathrm{E}}_{s'}\big[r(s,\pi(s)) + \gamma V_\pi(s')|s\big]. \end{aligned}$$

- Algorithm: temporal difference (TD).
  - sample new state s'.
  - update: α depends on number of visits of s.

$$\begin{aligned} V(s) &\leftarrow (1-\alpha)V(s) + \alpha[r(s,\pi(s)) + \gamma V(s')] \\ &= V(s) + \alpha[\underbrace{r(s,\pi(s)) + \gamma V(s') - V(s)}_{\text{temporal difference of } V \text{ values}}]. \end{aligned}$$

TD(0) Algorithm

TD(0)()

$\mathbf{V} \leftarrow \mathbf{V}_0$ ▷ initialization.
for $t \leftarrow 0$ **to** T **do**
  $s \leftarrow \textsc{SelectState}()$
  for each step of epoch t **do**
    $r' \leftarrow \textsc{Reward}(s, \pi(s))$
    $s' \leftarrow \textsc{NextState}(\pi, s)$
    $V(s) \leftarrow (1 - \alpha)V(s) + \alpha[r' + \gamma V(s')]$
    $s \leftarrow s'$
return $\mathbf{V}$

Q-Learning Algorithm

- Idea: assume deterministic rewards.

$$\begin{aligned} Q^*(s, a) &= \mathrm{E}[r(s, a)] + \gamma \sum_{s' \in S} \Pr[s' \mid s, a] V^*(s') \\ &= \mathop{\mathrm{E}}_{s'}[r(s, a) + \gamma \max_{a \in A} Q^*(s', a)] \end{aligned}$$

- Algorithm: $\alpha \in [0, 1]$ depends on number of visits.
  - sample new state s'.
  - update:

$$Q(s, a) \leftarrow (1 - \alpha) Q(s, a) + \alpha[r(s, a) + \gamma \max_{a' \in A} Q(s', a')].$$

Q-Learning Algorithm

(Watkins, 1989; Watkins and Dayan 1992)

Q-LEARNING(π)

$Q \leftarrow Q_0$ $\quad \triangleright$ initialization, e.g., $Q_0 = 0$.
for $t \leftarrow 0$ **to** T **do**
  $s \leftarrow$ SELECTSTATE()
  for each step of epoch t **do**
    $a \leftarrow$ SELECTACTION(π, s) $\triangleright$ policy π derived from Q, e.g., ϵ-greedy.
    $r' \leftarrow$ REWARD(s, a)
    $s' \leftarrow$ NEXTSTATE(s, a)
    $Q(s, a) \leftarrow Q(s, a) + \alpha\big[r' + \gamma \max_{a'} Q(s', a') - Q(s, a)\big]$
    $s \leftarrow s'$
return Q

Notes

- Can be viewed as a stochastic formulation of the value iteration algorithm.
- Convergence for any policy so long as states and actions visited infinitely often and parameter chosen as in mean estimation theorem.
- How to choose the action at each iteration? Maximize reward? Explore other actions?
- Q-learning is an off-policy method: no control over the policy; estimates and evaluates policy using experience from following different policy.

Policies

- Epsilon-greedy strategy:
  - with probability $1-\epsilon$ greedy action from s ;
  - with probability ϵ random action.
- Epoch-dependent strategy (Boltzmann exploration):

$$p_t(a|s,Q) = \frac{e^{\frac{Q(s,a)}{\tau_t}}}{\sum_{a' \in A} e^{\frac{Q(s,a')}{\tau_t}}},$$

  - $\tau_t \rightarrow 0$: greedy selection.
  - larger τ_t : random action.

Convergence of Q-Learning

- Theorem: consider a finite MDP. Assume that for all $s \in S$ and $a \in A$, $\sum_{t=0}^{\infty} \alpha_t(s,a) = \infty, \sum_{t=0}^{\infty} \alpha_t^2(s,a) < \infty$ with $\alpha_t(s,a) \in [0,1]$. Then, the Q-learning algorithm converges to the optimal value Q^* (with probability one).
    - note: the conditions on $\alpha_t(s,a)$ impose that each state-action pair is visited infinitely many times.

This Lecture

- Markov Decision Processes (MDPs)
- Planning
- Learning
- Multi-armed bandit problem

Multi-Armed Bandit Problem

(Robbins, 1952)

- Problem: gambler must decide which arm of a N-slot machine to pull to maximize his total reward in a series of trials.
  - stochastic setting: N lever reward distributions.
  - adversarial setting: reward selected by adversary aware of all the past.

Applications

- Clinical trials.
- Adaptive routing.
- Ads placement on pages.
- Games.

Multi-Armed Bandit Game

- For $t = 1$ to T do
  - adversary determines outcome $y_t \in Y$.
  - player selects probability distribution p_t and pulls lever $I_t \in \{1, \ldots, N\}$, $I_t \sim p_t$.
  - player incurs loss $L(I_t, y_t)$ (adversary is informed of p_t and I_t.
- Objective: minimize regret

$$\text{Regret}(T) = \sum_{t=1}^{T} L(I_t, y_t) - \min_{i=1,\ldots,N} \sum_{t=1}^{T} L(i, y_t).$$

Notes

- Player is informed only of the loss (or reward) corresponding to his own action.
- Adversary knows past but not action selected.
- Stochastic setting: loss $(L(1, y_t), \ldots, L(N, y_t))$ drawn according to some distribution $D = D_1 \otimes \cdots \otimes D_N$. Regret definition modified by taking expectations.
- Exploration/Exploitation trade-off: playing the best arm found so far versus seeking to find an arm with a better payoff.

Notes

- Equivalent views:
  - special case of learning with partial information.
  - one-state MDP learning problem.
- Simple strategy: ϵ-greedy: play arm with best empirical reward with probability $1-\epsilon_t$, random arm with probability ϵ_t.

Exponentially Weighted Average

- **Algorithm**: Exp3, defined for $\eta, \gamma > 0$ by

$$p_{i,t} = (1-\gamma) \frac{\exp\big(-\eta \sum_{s=1}^{t-1} \widehat{l}_{i,t}\big)}{\sum_{i=1}^{N} \exp\big(-\eta \sum_{s=1}^{t-1} \widehat{l}_{i,t}\big)} + \frac{\gamma}{N},$$

with $\forall i \in [1, N]$, $\widehat{l}_{i,t} = \frac{L(I_t, y_t)}{p_{I_t, t}} 1_{I_t = i}$.

- **Guarantee**: expected regret of

$$O(\sqrt{NT \log N}).$$

Exponentially Weighted Average

- Proof: similar to the one for the Exponentially Weighted Average with the additional observation that:

$$\mathrm{E}[\widehat{l}_{i,t}] = \sum_{i=1}^{N} p_{i,t} \frac{L(I_t, y_t)}{p_{I_t,t}} 1_{I_t = i} = L(i, y_t).$$

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