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,

$$\widehat{\mathfrak{R}}_S(H_p) \leq pM^{p-1}\widehat{\mathfrak{R}}_S(H).$$

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.

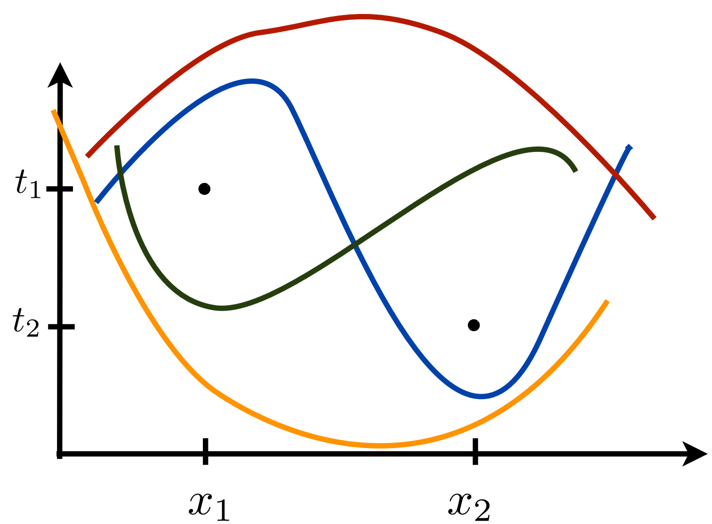
Notes

- 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

$$\left| \left\{ \begin{bmatrix} \operatorname{sgn}\left(g(x_1) - t_1\right) \\ \vdots \\ \operatorname{sgn}\left(g(x_m) - t_m\right) \end{bmatrix} : g \in G \right\} \right| = 2^m.$$

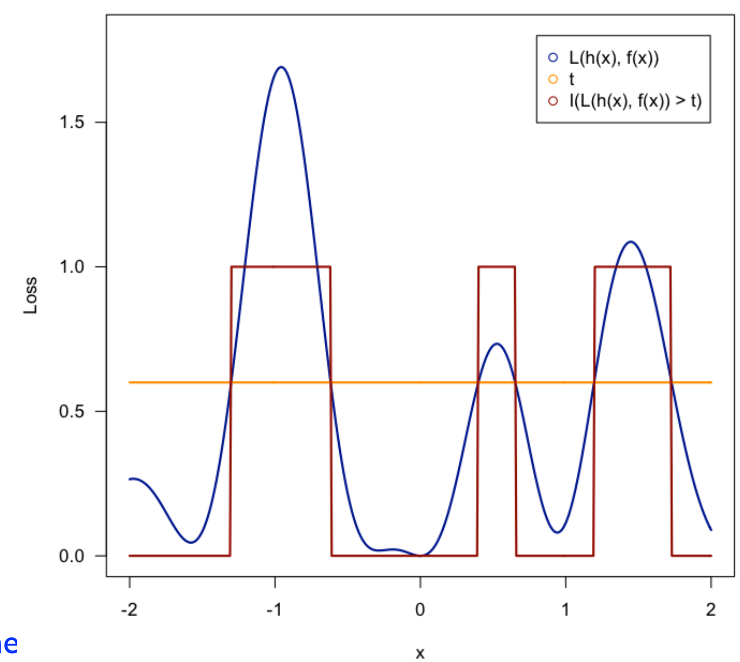


Pseudo-Dimension

(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.

Bound in terms of Pdim

- The right-hand side is bounded by the VC-dimension of the family

$$\mathcal{C} = \Big\{(x, y) \mapsto \mathbb{I}\big(L(h(x), y) > t\big) : h \in \mathcal{H},\ t \in \mathbb{R}\Big\}.$$

- To bound the VC-dimension of this family, consider the augmented real-valued class

$$\mathcal{G}' = \big\{(x, y) \mapsto L(h(x), y) - t : h \in \mathcal{H},\ t \in \mathbb{R}\big\}.$$

- Define $\mathcal{G} = \{(x, y) \mapsto L(h(x), y) : h \in \mathcal{H}\}$. Then, we have

$$\mathrm{VCdim}(\mathcal{C}) \leq \mathrm{Pdim}(\mathcal{G}') \leq \mathrm{Pdim}(\mathcal{G}) + 1.$$

Generalization Bound - Pdim

- **Theorem**: Let H be a family of real-valued functions. Assume that $\text{Pdim}(\{L(h,f)\colon h \in H\}) = d < \infty$ and that the loss L is bounded by M. Then, for any $\delta > 0$, with probability at least $1-\delta$, for any $h \in H$,

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

- **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.

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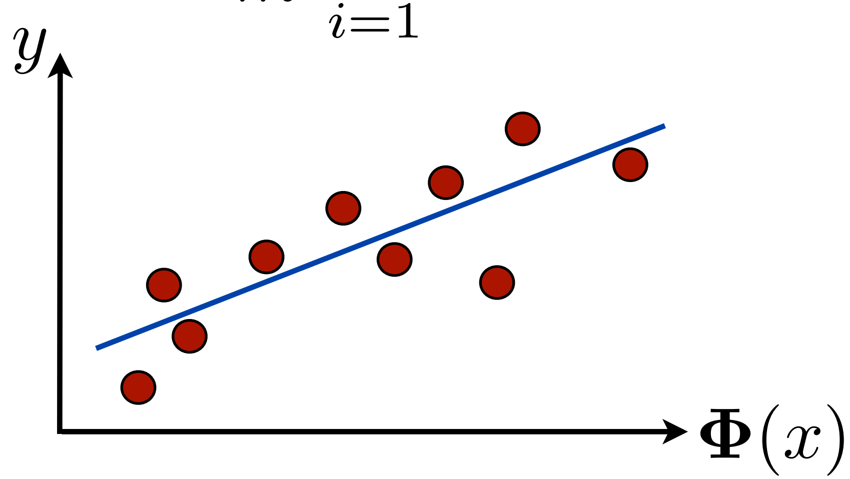
Linear Regression

- Feature mapping $\mathbf{\Phi}: X \to \mathbb{R}^N$.
- 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 $F(\mathbf{W}) = \frac{1}{m}\|\mathbf{X}^\top \mathbf{W} - \mathbf{Y}\|^2$,
$\mathbf{X} = \left[\begin{smallmatrix}\Phi(x_1) & \dots & \Phi(x_m)\\ 1 & \dots & 1\end{smallmatrix}\right] \in \mathbb{R}^{(N+1)\times m}$

$$\text{with } \mathbf{X}^\top = \begin{bmatrix}\mathbf{\Phi}(x_1)^\top & 1\\ \vdots & \\ \mathbf{\Phi}(x_m)^\top & 1\end{bmatrix} \quad \mathbf{W} = \begin{bmatrix} w_1\\ \vdots\\ w_N\\ b\end{bmatrix} \quad \mathbf{Y} = \begin{bmatrix} y_1\\ \vdots\\ y_m\end{bmatrix}.$$

- 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 $K: X \times X \to \mathbb{R}$ be a PDS kernel and let $\Phi: X \to \mathbb{H}$ be a feature mapping associated to K. Let $H = \left\{ \mathbf{x} \mapsto \mathbf{w} \cdot \Phi(x) : \|\mathbf{w}\|_{\mathbb{H}} \leq \Lambda \right\}$. 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:

$$\nabla_{\mathbf{w}} L = -\sum_{i=1}^{m} \alpha_i' \mathbf{\Phi}(x_i) + 2\lambda \mathbf{w} = 0 \iff \boxed{\mathbf{w} = \frac{1}{2\lambda} \sum_{i=1}^{m} \alpha_i' \mathbf{\Phi}(x_i).}$$

$$\nabla_{\xi_i} L = 2\xi_i - \alpha_i' = 0 \iff \boxed{\xi_i = \alpha_i'/2.}$$

$$\boxed{\begin{aligned} &\forall i \in [1, m], \alpha_i'(y_i - \xi_i - \mathbf{w} \cdot \mathbf{\Phi}(x_i)) = 0 \\ &\lambda(\|\mathbf{w}\|^2 - \Lambda^2) = 0. \end{aligned}}$$

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:

$$h(x) = \sum_{i=1}^{m} \alpha_i \mathbf{\Phi}(\mathbf{x}_i) \cdot \mathbf{\Phi}(x),$$

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
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Support Vector Regression

(Vapnik, 1995)

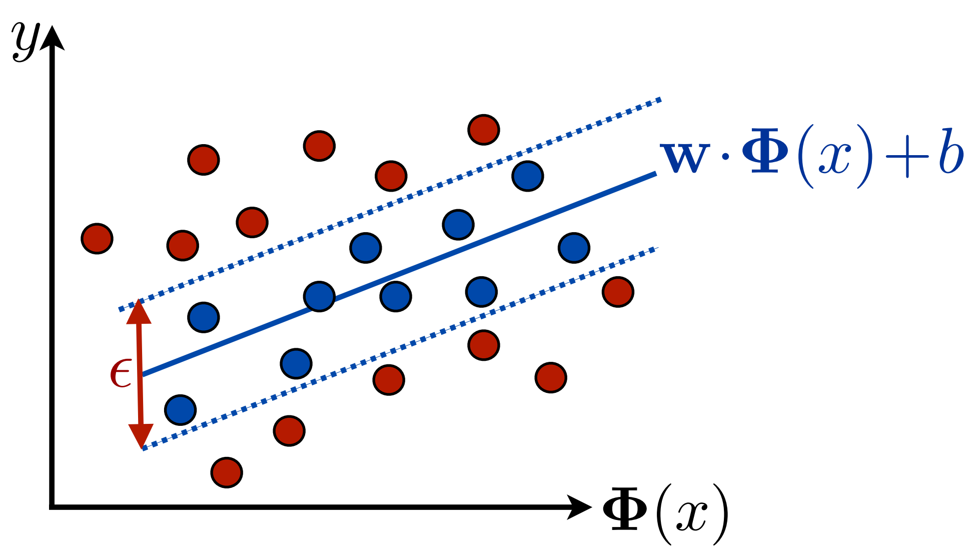
- Hypothesis set:

$$\{x \mapsto \mathbf{w} \cdot \mathbf{\Phi}(x) + b \colon \mathbf{w} \in \mathbb{R}^N, b \in \mathbb{R}\}.$$

- 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:

$$h(x) = \sum_{i=1}^{m} (\alpha'_i - \alpha_i) K(\mathbf{x}_i, \mathbf{x}) + b$$

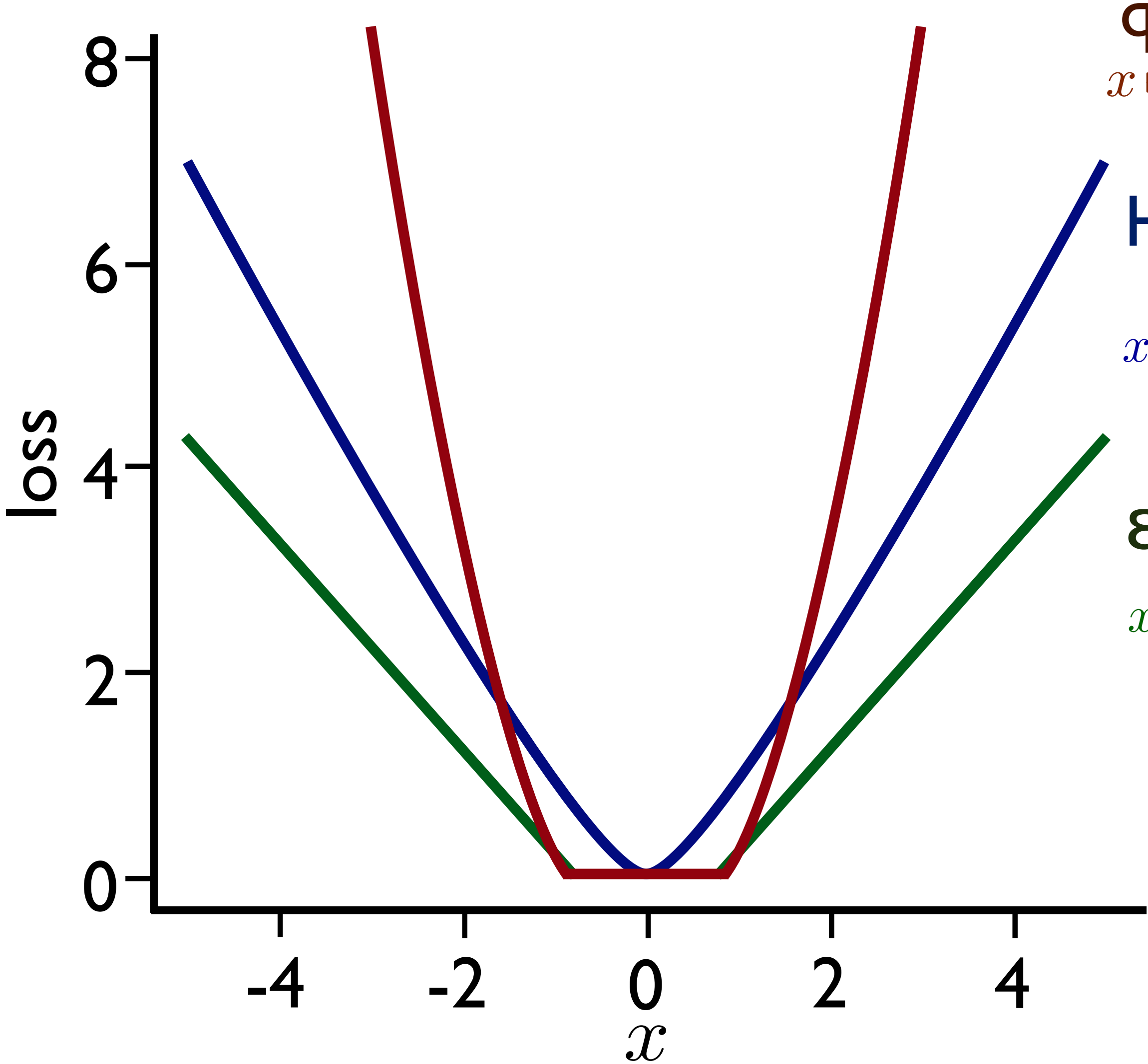
with $b = \begin{cases} -\sum_{i=1}^m (\alpha'_j - \alpha_j) K(x_j, x_i) + y_i + \epsilon & \text{when } 0 < \alpha_i < C \\ -\sum_{i=1}^m (\alpha'_j - \alpha_j) K(x_j, x_i) + y_i - \epsilon & \text{when } 0 < \alpha'_i < C. \end{cases}$

- 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 $\Phi: X \to H$ be a feature mapping associated to K. Let $H = \{\mathbf{x} \mapsto \mathbf{w} \cdot \Phi(x) : \|\mathbf{w}\|_H \leq \Lambda\}$. 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)

$\textsc{WidrowHoff}(\mathbf{w}_0)$

$\quad \mathbf{w}_1 \leftarrow \mathbf{w}_0 \qquad \triangleright \text{typically } \mathbf{w}_0 = \mathbf{0}$

$\quad$ **for** $t \leftarrow 1$ **to** T **do**

$\qquad \textsc{Receive}(\mathbf{x}_t)$

$\qquad \widehat{y}_t \leftarrow \mathbf{w}_t \cdot \mathbf{x}_t$

$\qquad \textsc{Receive}(y_t)$

$\qquad \mathbf{w}_{t+1} \leftarrow \mathbf{w}_t + 2\eta(\mathbf{w}_t \cdot \mathbf{x}_t - y_t)\mathbf{x}_t \qquad \triangleright\, \eta > 0$

$\quad$ **return** $\mathbf{w}_{T+1}$

Dual On-Line SVR

(Vijayakumar and Wu, 1988)

$(b = 0)$

$\textsc{DualSVR}()$

$\boldsymbol{\alpha} \leftarrow \mathbf{0}$

$\boldsymbol{\alpha}' \leftarrow \mathbf{0}$

for $t \leftarrow 1$ **to** T **do**

$\quad \textsc{Receive}(x_t)$

$\quad \widehat{y}_t \leftarrow \sum_{s=1}^{T} (\alpha'_s - \alpha_s) K(x_s, x_t)$

$\quad \textsc{Receive}(y_t)$

$\quad \alpha'_{t+1} \leftarrow \alpha'_t + \min(\max(\eta(y_t - \widehat{y}_t - \epsilon), -\alpha'_t), C - \alpha'_t)$

$\quad \alpha_{t+1} \leftarrow \alpha_t + \min(\max(\eta(\widehat{y}_t - y_t - \epsilon), -\alpha_t), C - \alpha_t)$

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)

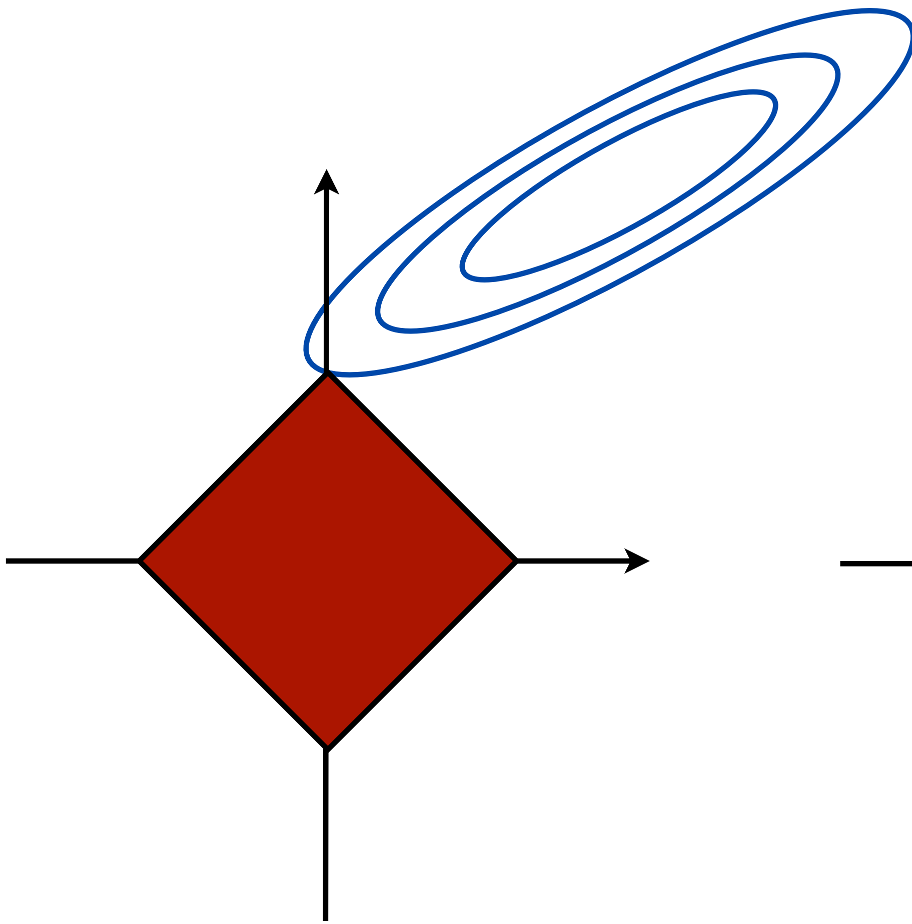
- Optimization problem: 'least absolute shrinkage and selection operator'.

$$\min_{\mathbf{w}} F(\mathbf{w}, b) = \lambda \|\mathbf{w}\|_1 + \sum_{i=1}^{m} (\mathbf{w} \cdot \mathbf{x}_i + b - y_i)^2 \,,$$

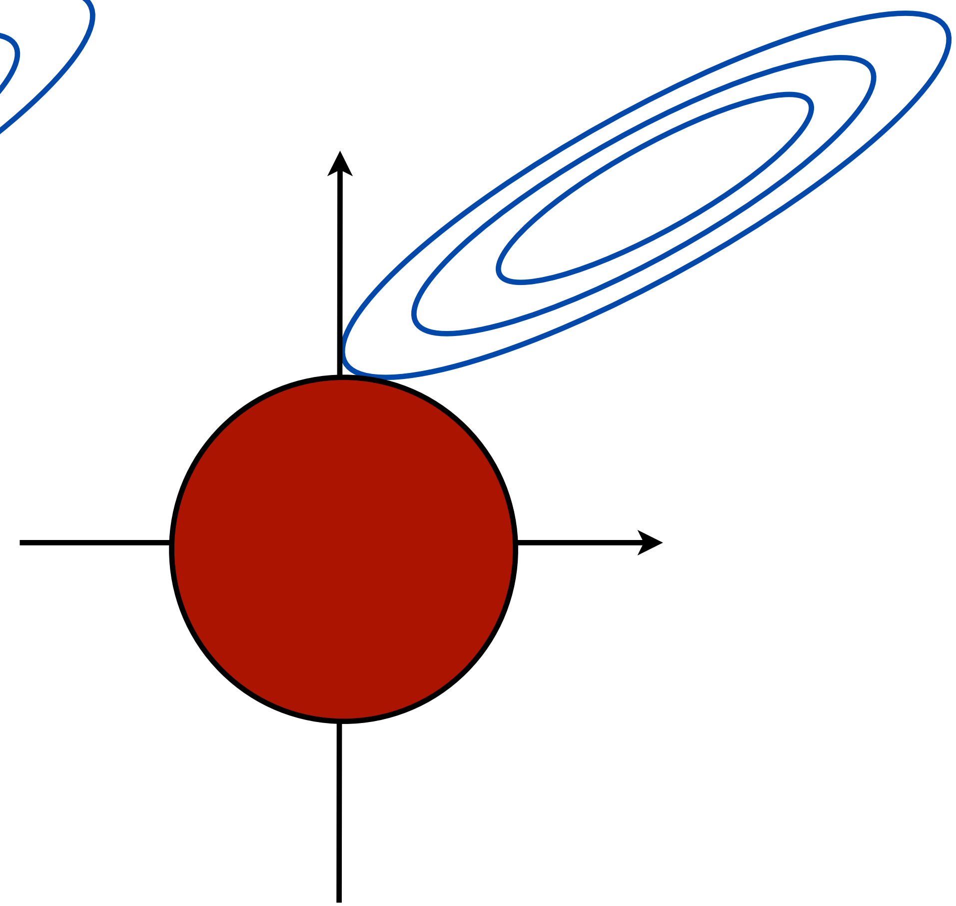
  where $\lambda \geq 0$ is a (regularization) parameter.

- 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:

$$
\begin{aligned}
\widehat{\mathfrak{R}}_S(H) &= \frac{1}{m} \operatorname*{E}_{\boldsymbol{\sigma}} \left[\sup_{\|\mathbf{w}\|_1 \leq \Lambda_1} \sum_{i=1}^{m} \sigma_i \mathbf{w} \cdot \mathbf{x}_i \right] \\
&= \frac{\Lambda_1}{m} \operatorname*{E}_{\boldsymbol{\sigma}} \left[\left\| \sum_{i=1}^{m} \sigma_i \mathbf{x}_i \right\|_\infty \right] && \text{(by definition of the dual norm)} \\
&= \frac{\Lambda_1}{m} \operatorname*{E}_{\boldsymbol{\sigma}} \left[\max_{j \in [1,N]} \left| \sum_{i=1}^{m} \sigma_i x_{ij} \right| \right] && \text{(by definition of } \| \cdot \|_\infty\text{)} \\
&= \frac{\Lambda_1}{m} \operatorname*{E}_{\boldsymbol{\sigma}} \left[\max_{j \in [1,N]} \max_{s \in \{-1,+1\}} s \sum_{i=1}^{m} \sigma_i x_{ij} \right] && \text{(by definition of } | \cdot |\text{)} \\
&= \frac{\Lambda_1}{m} \operatorname*{E}_{\boldsymbol{\sigma}} \left[\sup_{\mathbf{z} \in A} \sum_{i=1}^{m} \sigma_i z_i \right] \leq r_\infty \Lambda_1 \sqrt{\frac{2 \log(2N)}{m}}. && \text{(Massart's lemma)}
\end{aligned}
$$

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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