Machine learning theory

Regression

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Introduction

1. Let $\mathcal{X}$ denote the input space and $\mathcal{Y}$ a measurable subset of $\mathbb{R}$ and $\mathcal{D}$ be a distribution over $\mathcal{X} \times \mathcal{Y}$.
2. Learner receives sample $S = \{(x_1, y_m), \ldots, (x_m, y_m)\} \in (\mathcal{X} \times \mathcal{Y})^m$ drawn i.i.d. according to $\mathcal{D}$.
3. Let $L : \mathcal{X} \times \mathcal{Y} \mapsto \mathbb{R}_+$ be the loss function used to measure the magnitude of error.
4. The most used loss function is
   - L_2 defined as $L(y, y') = |y' - y|^2$ for all $y, y' \in \mathcal{Y}$.
   - L_p defined as $L(y, y') = |y' - y|^p$ for all $p \geq 1$ and $y, y' \in \mathcal{Y}$.

The regression problem is defined as

Definition (Regression problem)

Given a hypothesis set $H = \{h : \mathcal{X} \mapsto \mathcal{Y} \mid h \in H\}$, regression problem consists of using labeled sample S to find a hypothesis $h \in H$ with small generalization error $\mathbf{R}(h)$ respect to target f:

$$\mathbf{R}(h) = \mathop{\mathbb{E}}_{(x,y)\sim\mathcal{D}}[L(h(x), y)]$$

The empirical loss or error of $h \in H$ is denoted by

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

If $L(y, y) \leq M$ for all $y, y' \in \mathcal{Y}$, problem is called bounded regression problem.

Generalization bounds

Theorem (Generalization bounds for finite hypothesis sets)

Let $L \leq M$ be a bounded loss function and the hypothesis set H is finite. Then, for any $\delta > 0$, with probability at least $(1-\delta)$, the following inequality holds for all $h \in H$

$$\mathbf{R}(h) \leq \hat{\mathbf{R}}(h) + M\sqrt{\frac{\log|H| + \log\frac{1}{\delta}}{2m}}.$$

Proof (Generalization bounds for finite hypothesis sets).

By Hoeffding's inequality, since $L \in [0, M]$, for any $h \in H$, the following holds

$$\mathbb{P}\left[\mathbf{R}(h) - \hat{\mathbf{R}}(h) > \epsilon\right] \leq \exp\left(-2\frac{m\epsilon^2}{M^2}\right).$$

Thus, by the union bound, we can write

$$\begin{aligned}\mathbb{P}\left[\exists h \in H \;\middle|\; \mathbf{R}(h) - \hat{\mathbf{R}}(h) > \epsilon\right] &\leq \sum_{h\in H} \mathbb{P}\left[\mathbf{R}(h) - \hat{\mathbf{R}}(h) > \epsilon\right] \\ &\leq |H| \exp\left(-2\frac{m\epsilon^2}{M^2}\right).\end{aligned}$$

Setting the right-hand side to be equal to δ, the theorem will proved. □

Theorem (Rademacher complexity of μ-Lipschitz loss functions)

Let $L \leq M$ be a bounded loss function such that for any fixed $y' \in \mathcal{Y}$, $L(y, y')$ is μ-Lipschitz for some $\mu > 0$. Then for any sample $S = \{(x_1, y_m), \ldots, (x_m, y_m)\}$, the upper bound of the Rademacher complexity of the family $\mathcal{G} = \{(x, y) \mapsto L(h(x), y) \mid h \in H\}$ is

$$\hat{\mathcal{R}}(\mathcal{G}) \leq \mu \hat{\mathcal{R}}(H).$$

Lemma (Talagrand's Lemma (special case))

Let ϕ be a μ-Lipschitz function from $\mathbb{R}$ to $\mathbb{R}$ and $\sigma_1, \ldots, \sigma_m$ be Rademacher random variables. Then, for any hypothesis set H of real-valued functions, the following inequality holds:

$$\hat{\mathcal{R}}(\phi \circ H) \leq \mu \hat{\mathcal{R}}(H).$$

Proof (Rademacher complexity of μ-Lipschitz loss functions).

Since for any fixed y_i, $L(y, y')$ is μ-Lipschitz for some $\mu > 0$, by Talagrand's Lemma, we can write

$$\begin{aligned}\hat{\mathcal{R}}(\mathcal{G}) &= \frac{1}{m}\mathop{\mathbb{E}}_{\sigma}\left[\sum_{i=1}^{m}\sigma_i L(h(x_i), y_i)\right]\\ &\leq \frac{1}{m}\mathop{\mathbb{E}}_{\sigma}\left[\sum_{i=1}^{m}\sigma_i \mu h(x_i)\right]\\ &= \mu\hat{\mathcal{R}}(H).\end{aligned}$$

□

Theorem (Rademacher complexity of L_p loss functions)

Let $p \geq 1$ and $\mathcal{G} = \{\mathbf{x} \mapsto |h(x) - f(x)|^p \mid h \in H\}$ and $|h(x) - f(x)| \leq M$ for all $x \in \mathcal{X}$ and $h \in H$. Then for any sample $S = \{(x_1, y_m), \ldots, (x_m, y_m)\}$, the following inequality holds

$$\hat{\mathcal{R}}(\mathcal{G}) \leq pM^{p-1}\hat{\mathcal{R}}(H).$$

Proof (Rademacher complexity of L_p loss functions).

Let $\phi_p : x \mapsto |x|^p$, then $\mathcal{G} = \{\phi_p \circ h \mid h \in H'\}$ where $H' = \{\mathbf{x} \mapsto h(x) - f(x) \mid h \in H\}$. Since ϕ_p is pM^{p-1}-Lipschitz over $[-M, M]$, we can apply Talagrand's Lemma,

$$\hat{\mathcal{R}}(\mathcal{G}) \leq pM^{p-1}\hat{\mathcal{R}}(H').$$

Now, $\hat{\mathcal{R}}(H')$ can be expressed as

$$\begin{aligned}
\hat{\mathcal{R}}(H') &= \frac{1}{m}\mathop{\mathbb{E}}_{\sigma}\left[\sup_{h\in H}\sum_{i=1}^{m}(\sigma_i h(\mathbf{x}_i) + \sigma_i f(\mathbf{x}_i))\right] \\
&= \frac{1}{m}\mathop{\mathbb{E}}_{\sigma}\left[\sup_{h\in H}\sum_{i=1}^{m}\sigma_i h(\mathbf{x}_i)\right] + \frac{1}{m}\mathop{\mathbb{E}}_{\sigma}\left[\sum_{i=1}^{m}\sigma_i f(\mathbf{x}_i)\right] = \hat{\mathcal{R}}(H).
\end{aligned}$$

Since $\mathbb{E}_\sigma\left[\sum_{i=1}^{m}\sigma_i f(\mathbf{x}_i)\right] = \sum_{i=1}^{m}\mathbb{E}_\sigma[\sigma_i]\, f(\mathbf{x}_i) = 0.$ □

Theorem (Rademacher complexity regression bounds)

Let $0 \leq L \leq M$ be a bounded loss function such that for any fixed $y' \in \mathcal{Y}$, $L(y, y')$ is μ-Lipschitz for some $\mu > 0$. Then,

$$\mathop{\mathbb{E}}_{(x,y)\sim\mathcal{D}}[L(h(x), y)] \leq \frac{1}{m}\sum_{i=1}^{m} L(h(x_i), y_i) + 2\mu\mathcal{R}_m(H) + M\sqrt{\frac{\log\frac{1}{\delta}}{2m}}$$

$$\mathop{\mathbb{E}}_{(x,y)\sim\mathcal{D}}[L(h(x), y)] \leq \frac{1}{m}\sum_{i=1}^{m} L(h(x_i), y_i) + 2\mu\hat{\mathcal{R}}(H) + 3M\sqrt{\frac{\log\frac{1}{\delta}}{2m}}.$$

Proof (Rademacher complexity of μ-Lipschitz loss functions).

Since for any fixed y_i, $L(y, y')$ is μ-Lipschitz for some $\mu > 0$, by Talagrand's Lemma, we can write

$$\begin{aligned}\hat{\mathcal{R}}(\mathcal{G}) &= \frac{1}{m}\mathop{\mathbb{E}}_{\sigma}\left[\sum_{i=1}^{m}\sigma_i L(h(x_i), y_i)\right] \\ &\leq \frac{1}{m}\mathop{\mathbb{E}}_{\sigma}\left[\sum_{i=1}^{m}\sigma_i \mu h(x_i)\right] \\ &= \mu\hat{\mathcal{R}}(H).\end{aligned}$$

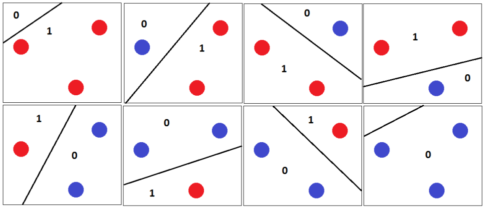
Combining this inequality with general Rademacher complexity learning bound completes proof. □

Pseudo-dimension bounds

1. VC dimension is a measure of complexity of a hypothesis set.

Definition (VC-dimension)

The Vapnik-Chervonenkis (VC) dimension of H, denoted as $VC(H)$, is the cardinality d of the largest set S shattered by H. If arbitrarily large finite sets can be shattered by H, then $VC(H) = \infty$.



2. We define shattering for families of real-valued functions.
3. Let $\mathcal{G}$ be a family of loss functions associated to some hypothesis set H, where

$$\mathcal{G} = \{z = (x, y) \mapsto L(h(x), y) \mid h \in H\}$$

Definition (Shattering)

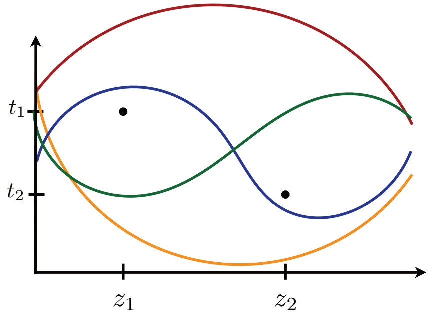
Let $\mathcal{G}$ be a family of functions from a set $\mathcal{Z}$ to $\mathbb{R}$. A set $\{z_1, \ldots, z_m\} \in (\mathcal{X} \times \mathcal{Y})$ is said to be shattered by $\mathcal{G}$ if there exists $t_1, \ldots, t_m \in \mathbb{R}$ such that

$$\left| \left\{ \begin{bmatrix} \operatorname{sgn}\left(g(z_1) - t_1\right) \\ \operatorname{sgn}\left(g(z_2) - t_2\right) \\ \vdots \\ \operatorname{sgn}\left(g(z_m) - t_m\right) \end{bmatrix} \middle| \; g \in \mathcal{G} \right\} \right| = 2^m$$

When they exist, the threshold values $t_1, \ldots, t_m$ are said to witness the shattering.

In other words, S is shattered by $\mathcal{G}$, if there are real numbers $t_1, \ldots, t_m$ such that for $b \in \{0, 1\}^m$, there is a function $g_b \in \mathcal{G}$ with $\operatorname{sgn}\left(g_b(\mathbf{x}_i) - t_i\right) = b_i$ for all $1 \leq i \leq m$.

1. Thus, $\{z_1, \ldots, z_m\}$ is shattered if for some witnesses $t_1, \ldots, t_m$, the family of functions $\mathcal{G}$ is rich enough to contain a function going
   - above a subset A of the set of points $\mathcal{J} = \{(z_i, t_i) \mid 1 \leq i \leq m\}$ and
   - below the others $\mathcal{J} - A$, for any choice of the subset A.



2. For any $g \in \mathcal{G}$, let B_g be the indicator function of the region below or on the graph of g, that is

$$B_g(\mathbf{x}, y) = \operatorname{sgn}(g(\mathbf{x}) - y).$$

3. Let $B_{\mathcal{G}} = \{B_g \mid g \in \mathcal{G}\}$.

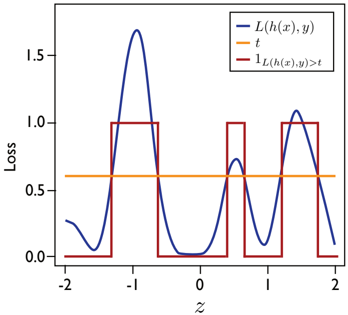
1. The notion of shattering naturally leads to definition of pseudo-dimension.

Definition (Pseudo-dimension)

Let $\mathcal{G}$ be a family of functions from $\mathcal{Z}$ to $\mathbb{R}$. Then, the pseudo-dimension of $\mathcal{G}$, denoted by $Pdim(\mathcal{G})$, is the size of the largest set shattered by $\mathcal{G}$. If no such maximum exists, then $Pdim(\mathcal{G}) = \infty$.

2. $Pdim(\mathcal{G})$ coincides with VC of the corresponding thresholded functions mapping $\mathcal{X}$ to $\{0, 1\}$.

$$Pdim(\mathcal{G}) = VC\left(\{(x, t) \mapsto \mathbb{I}\left[(g(x) - t) > 0\right] \mid g \in \mathcal{G}\}\right)$$



Theorem (Composition with non-decreasing function)

Suppose $\mathcal{G}$ is a class of real-valued functions and $\sigma : \mathbb{R} \mapsto \mathbb{R}$ is a non-decreasing function. Define $\sigma(\mathcal{G}) = \{\sigma \circ g \mid g \in \mathcal{G}\}$. Then

$$Pdim(\sigma(\mathcal{G})) \leq Pdim(\mathcal{G}).$$

Proof (Pseudo-dimension of hyperplanes).

1. For $d \leq Pdim(\sigma(\mathcal{G}))$, suppose set $\left\{\sigma \circ g_b \;\middle|\; b \in \{0,1\}^d\right\} \subseteq \sigma(\mathcal{G})$ shatters a set $\{\mathbf{x}_1, \ldots, \mathbf{x}_d\} \subseteq \mathcal{X}$ witnessed by $(t_1, \ldots, t_d)$.
2. By suitably relabeling g_b, for all $\{0,1\}^d$ and $1 \leq i \leq d$, we have $\text{sgn}\left(\sigma(g_b(\mathbf{x}_i)) - t_i\right) = b_i$.
3. For all $1 \leq i \leq d$, take $y_i = \min\left\{g_b(\mathbf{x}_i) \;\middle|\; \sigma(g_b(\mathbf{x}_i)) \geq t_i, b \in \{0,1\}^d\right\}$.
4. Since σ is non-decreasing, it is straightforward to verify that $\text{sgn}\left(g_b(\mathbf{x}_i) - t_i\right) = b_i$ for all $\{0,1\}^d$ and $1 \leq i \leq d$

□

A class $\mathcal{G}$ of real-valued functions is **a vector space** if for all $g_1, g_2 \in \mathcal{G}$ and any numbers $\lambda, \mu \in \mathbb{R}$, we have $\lambda g_1 + \mu g_2 \in \mathcal{G}$.

Theorem (Pseudo-dimension of vector spaces)

If $\mathcal{G}$ is a vector space of real-valued functions, then $Pdim(\mathcal{G}) = dim(\mathcal{G})$.

Theorem (VC-dimension of vector spaces)

Let F be a vector space of real-valued functions, g is a real-valued function, and $H = \{sgn(f+g) \mid f \in F\}$. Then $VCdim(H) = dim(F)$.

Proof (Pseudo-dimension of vector spaces).

1. If $B_{\mathcal{G}}$ be class of **below the graph** indicator functions, then $Pdim(\mathcal{G}) = VC(B_{\mathcal{G}})$.
2. But $B_{\mathcal{G}} = \{(\mathbf{x}, y) \mapsto \text{sgn}\left(g(\mathbf{x}) - y\right) \mid g \in \mathcal{G}\}$.
3. Hence, functions $B_{\mathcal{G}}$ are of the form $\text{sgn}\left(g_1 + g_2\right)$, where
   - $g_1 = g$ is a function from vector space
   - g_2 is the fixed function $g_2(\mathbf{x}, y) = -y$.
4. Then, Theorem (VC-dimension of vector spaces) shows that $Pdim(\mathcal{G}) = dim(\mathcal{G})$.

□

Functions that map into some bounded range are not vector space.

Corollary

If $\mathcal{G}$ is a subset of a vector space $\mathcal{G}'$ of real valued functions then $Pdim(\mathcal{G}) \leq dim(\mathcal{G}')$

Theorem (Pseudo-dimension of hyperplanes)

Let $\mathcal{G} = \{\mathbf{x} \mapsto \langle \mathbf{w}, \mathbf{x} \rangle + b \mid \mathbf{w} \in \mathbb{R}^n, b \in \mathbb{R}\}$ be the class of hyperplanes in $\mathbb{R}^n$, then $Pdim(\mathcal{G}) = n + 1$.

Pseudo-dimension of hyperplanes.

1. It is easy to check that $\mathcal{G}$ is a vector space.
2. Let g_i be the ith coordinate projection $f_i(\mathbf{x}) = x_i$ for all $1 \leq i \leq n$ and $\mathbf{1}$ be identity-1 function. Then $B = \{g_1, \ldots, g_n, \mathbf{1}\}$ is basis of $\mathcal{G}$.
3. Hence, from Theorem (Pseudo-dimension of vector spaces), we obtain $Pdim(\mathcal{G}) = n + 1$

□

A polynomial transformation of $\mathbb{R}^n$ is $g(\mathbf{x}) = w_0 + w_1\phi_1(\mathbf{x}) + w_2\phi_2(\mathbf{x}) + \ldots + w_k\phi_k(\mathbf{x})$ for $\mathbf{x} \in \mathbb{R}^n$, where k is an integer and for each $1 \leq i \leq k$, function $\phi_i(\mathbf{x})$ is defined as

$$\phi_i(\mathbf{x}) = \prod_{j=1}^{n} x_j^{r_{ij}}$$

for some nonnegative integers r_{ij} and $r_i = r_{i1} + r_{i2} + \ldots + r_{in}$ and the degree of g as $r = \max_i r_i$.

Theorem (Pseudo-dimension of polynomial transformation)

If $\mathcal{G}$ is a class of all polynomial transformations on $\mathbb{R}^n$ of degree at most r, then $Pdim(\mathcal{G}) = \binom{n+r}{r}$.

Theorem (Pseudo-dimension of all polynomial transformations)

Let $\mathcal{G}$ be class of all polynomial transformations on $\{0,1\}^n$ of degree at most r, then $Pdim(\mathcal{G}) = \sum_{i=0}^{r} \binom{n}{i}$.

Homework: Prove the above Theorems.

Theorem (Generalization bound for bounded regression)

Let H be a family of real-valued functions and $\mathcal{G} = \{z = (\mathbf{x}, y) \mapsto L(h(x), y) \mid h \in H\}$ be a family of loss functions associated to a hypothesis set H. Assume that $Pdim(\mathcal{G}) = d$ and loss function L is non-negative and bounded by M. Then, for any $\delta > 0$, with probability at least $(1 - \delta)$ over the choice of an i.i.d. sample S of size m drawn from $\mathcal{D}^m$, the following inequality holds for all $h \in H$

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

Proof (Generalization bound for bounded regression).

Homework: Prove this Theorem. □

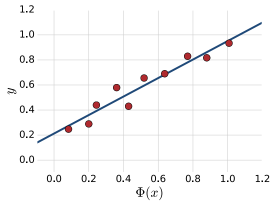
Regression algorithms

Regression algorithms

Linear regression

1. Let $\Phi : \mathcal{X} \mapsto \mathbb{R}^n$ and $H = \{h : \mathbf{x} \mapsto \langle \mathbf{w}, \Phi(\mathbf{x}) \rangle + b \mid \mathbf{w} \in \mathbb{R}^n, b \in \mathbb{R}\}$.
2. Given sample S, the problem is to find a $h \in H$ such that

$$h = \min_{\mathbf{w},b} \hat{\mathbf{R}}(h) = \min_{\mathbf{w},b} \frac{1}{m} \sum_{i=1}^{m} \left(\langle \mathbf{w}, \Phi(x_i) \rangle + b - y_i\right)^2$$



3. Define data matrix $\mathbf{X} = \begin{bmatrix} \Phi(\mathbf{x}_1) & \phi(\mathbf{x}_2) & \dots & \phi(\mathbf{x}_m) \\ 1 & 1 & \dots & 1 \end{bmatrix}$.
4. Let $\mathbf{w} = (w_1, \dots, w_n, b)^T$ and $\mathbf{y} = (y_1, \dots, y_m)^T$ be weight and target vectors.
5. By setting $\nabla \hat{\mathbf{R}}(h) = 0$, we obtain

$$\mathbf{w} = (\mathbf{X}\mathbf{X}^T)^{\dagger}\mathbf{X}\mathbf{y}$$

6. When $\mathbf{X}\mathbf{X}^T$ is invertible, this problem has a unique solution; otherwise there are several solutions.

Theorem

Let $K : \mathcal{X} \times \mathcal{X} \mapsto \mathbb{R}$ be a PDS kernel, $\Phi : \mathcal{X} \mapsto \mathbb{H}$ a feature mapping associated to K, and $H = \{\mathbf{x} \mapsto \langle \mathbf{w}, \Phi(\mathbf{x})\rangle \mid \|\mathbf{w}\|_{\mathbb{H}} \leq \Lambda\}$. Assume that there exists $r > 0$ suh that $K(\mathbf{x}, \mathbf{x}) \leq r^2$ and $M > 0$ such that $|h(\mathbf{x}) - y| < M$ for all $(\mathbf{x}, y \in \mathcal{X} \times \mathcal{Y})$. Then for any $\delta > 0$, with probability at least $(1 - \delta)$, each of the following inequalities holds for all $h \in H$.

$$\mathbf{R}(h) \leq \hat{\mathbf{R}}(h) + 4M\sqrt{\frac{r^2\Lambda^2}{m}} + M^2\sqrt{\frac{\log \frac{1}{\delta}}{2m}}$$

$$\mathbf{R}(h) \leq \hat{\mathbf{R}}(h) + \frac{4M\Lambda\sqrt{\mathrm{Tr}\left[\mathbf{K}\right]}}{m} + 3M^2\sqrt{\frac{\log \frac{2}{\delta}}{2m}}$$

Proof.

1. By the bound on the empirical Rademacher complexity of kernel-based hypotheses, the following holds for any sample S of size m:

$$\hat{\mathcal{R}}(H) \leq \frac{\Lambda\sqrt{\mathrm{Tr}\left[K\right]}}{m} \leq \sqrt{\frac{r^2\Lambda^2}{m}}$$

2. This implies that $\mathcal{R}_m(h) \leq \sqrt{\frac{r^2\Lambda^2}{m}}$.
3. Combining these inequalities with the bounds of Theorem Rademacher complexity regression bounds, the Theorem will be proved.

□

Regression algorithms

Kernel ridge regression

1. The following bound suggests minimizing a trade-off between empirical squared loss and norm of the weight vector.

$$\mathbf{R}(h) \leq \hat{\mathbf{R}}(h) + 4M\sqrt{\frac{r^2\Lambda^2}{m}} + M^2\sqrt{\frac{\log\frac{1}{\delta}}{2m}}$$

2. Kernel ridge regression is defined by minimization of an objective function

$$\begin{aligned}\min_{\mathbf{w}} F(\mathbf{w}) &= \min_{\mathbf{w}} \left[\lambda \|\mathbf{w}\|^2 + \sum_{i=1}^{m} (\langle \mathbf{w}, \Phi(\mathbf{x}_i)\rangle - y_i)^2\right] \\ &= \min_{\mathbf{w}} \left[\lambda \|\mathbf{w}\|^2 + \left\|\mathbf{\Phi}^T\mathbf{w} - \mathbf{y}\right\|^2\right]\end{aligned}$$

3. By setting $\nabla F(\mathbf{w}) = 0$, we obtain $\mathbf{w} = (\mathbf{\Phi}\mathbf{\Phi}^T + \lambda\mathbf{I})^{-1}\mathbf{\Phi}\mathbf{y}$.

1. An alternative formulation of kernel ridge regression is

$$\min_{\mathbf{w}} \left\| \mathbf{\Phi}^T \mathbf{w} - \mathbf{y} \right\|^2 \text{ subject to } \|\mathbf{w}\|^2 \leq \Lambda^2$$

$$\min_{\mathbf{w}} \sum_{i=1}^{m} \xi_i^2 \text{ subject to } (\|\mathbf{w}\|^2 \leq \Lambda^2) \wedge (\forall i \in \{1, \ldots, m\}, \xi_i = y_i - \langle \mathbf{w}, \Phi(\mathbf{x}_i) \rangle)$$

2. By using the Lagrangian method, we obtain

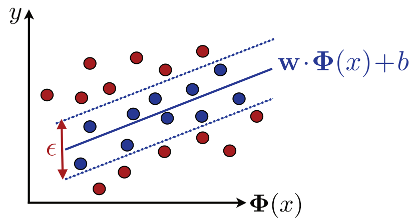
$$\mathbf{w} = \mathbf{\Phi} \left(\mathbf{K} + \lambda \mathbf{I} \right)^{-1} \mathbf{y}.$$

3. Note that $(\mathbf{K} + \lambda \mathbf{I})^{-1}$ is invertible.
4. Therefore, the dual optimization problem as well as the primal optimization problem has a closed-form solution.

Regression algorithms

Support vector regression

1. Support vector regression (SVR) algorithm is inspired by SVM algorithm.
2. The main idea of SVR consists of fitting a tube of width $\epsilon > 0$ to the data.



3. This defines two sets of points:
   - points falling inside the tube, which are ϵ-close to the predicted function, not penalized,
   - points falling outside the tube are penalized based on their distance to the predicted function.
4. This is similar to the penalization used by SVMs in classification.
5. Using a hypothesis set of linear functions $H = \{\mathbf{x} \mapsto \langle \mathbf{w}, \Phi(\mathbf{x}) \rangle + b \mid \mathbf{w} \in \mathbb{R}^n, b \in \mathbb{R}\}$, where Φ is the feature mapping corresponding some PDS kernel K.

1. The optimization problem for SVR is

$$\min_{\mathbf{w},b} \left[\frac{1}{2}\lambda \left\| \mathbf{w} \right\|^2 + C \sum_{i=1}^{m} \left| y_i - (\langle \mathbf{w}, \Phi(\mathbf{x}_i) \rangle + b) \right|_\epsilon \right]$$

where $|.|_\epsilon$ denotes ϵ-insensitive loss

$$\forall y, y' \in \mathcal{Y}, \quad |y' - y|_\epsilon = \max\left(0, |y' - y| - \epsilon\right)$$

2. The use of ϵ-insensitive loss leads to sparse solutions with a relatively small number of support vectors.

1. Using slack variables $\xi_i \geq 0$ and $\xi'_i \geq 0$ for $1 \leq i \leq m$, the problem becomes

$$\min_{\mathbf{w},b,\xi,\xi'} \left[\frac{1}{2}\lambda \|\mathbf{w}\|^2 + C\sum_{i=1}^{m}\left(\xi_i + \xi'_i\right)\right]$$

$$\text{subject to } \left(\langle \mathbf{w}, \Phi(\mathbf{x}_i)\rangle + b\right) - y_i \leq \epsilon + \xi_i$$

$$y_i - \left(\langle \mathbf{w}, \Phi(\mathbf{x}_i)\rangle + b\right) \leq \epsilon + \xi'_i$$

$$\xi_i \geq 0, \quad \xi'_i \geq 0, \quad \forall i, 1 \leq i \leq m$$

2. This is a convex quadratic program (QP) with affine constraints.
3. By introducing Lagrangian and applying KKT conditions, the problem will be solved.
4. Let $\mathcal{D}$ be the distribution according to which sample points are drawn.
5. Let $\hat{\mathcal{D}}$ the empirical distribution defined by a training sample of size m.

Theorem (Generalization bounds of SVR)

Let $K : \mathcal{X} \times \mathcal{X} \mapsto \mathbb{R}$ be a PDS kernel, $\Phi : \mathcal{X} \mapsto \mathbb{H}$ a feature mapping associated to K, and $H = \{\mathbf{x} \mapsto \langle \mathbf{w}, \Phi(\mathbf{x})\rangle \mid \|\mathbf{w}\|_{\mathbb{H}} \leq \Lambda\}$. Assume that there exists $r > 0$ suh that $K(\mathbf{x}, \mathbf{x}) \leq r^2$ and $M > 0$ such that $|h(\mathbf{x}) - y| < M$ for all $(\mathbf{x}, y \in \mathcal{X} \times \mathcal{Y})$. Then for any $\delta > 0$, with probability at least $(1 - \delta)$, each of the following inequalities holds for all $h \in H$.

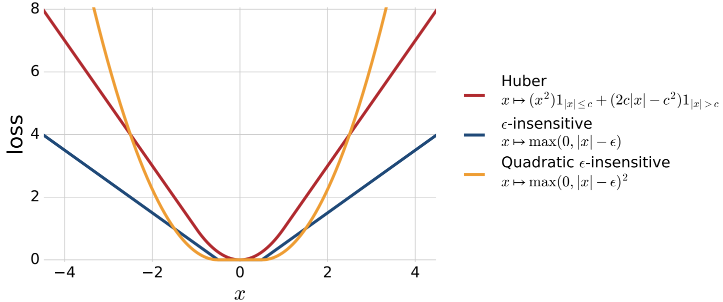
$$\underset{(\mathbf{x},y)\sim\mathcal{D}}{\mathbb{E}}\left[|h(\mathbf{x}) - y|_\epsilon\right] \leq \underset{(\mathbf{x},y)\sim\hat{\mathcal{D}}}{\mathbb{E}}\left[|h(\mathbf{x}) - y|_\epsilon\right] + 2\sqrt{\frac{r^2\Lambda^2}{m}} + M\sqrt{\frac{\log\frac{1}{\delta}}{2m}}$$

$$\underset{(\mathbf{x},y)\sim\mathcal{D}}{\mathbb{E}}\left[|h(\mathbf{x}) - y|_\epsilon\right] \leq \underset{(\mathbf{x},y)\sim\hat{\mathcal{D}}}{\mathbb{E}}\left[|h(\mathbf{x}) - y|_\epsilon\right] + \frac{2\Lambda\sqrt{\mathrm{Tr}\left[\mathbf{K}\right]}}{m} + 3M\sqrt{\frac{\log\frac{2}{\delta}}{2m}}$$

Proof (Generalization bounds of SVR).

Since for any $y' \in \mathcal{Y}$, the function $y \mapsto |y - y'|_\epsilon$ is 1-Lipschitz, the result follows Theorem Rademacher complexity regression bounds and the bound on the empirical Rademacher complexity of H. □

1. Alternative convex loss functions can be used to define regression algorithms.



2. SVR admits several advantages
   - SVR algorithm is based on solid theoretical guarantees,
   - The solution returned SVR is sparse
   - SVR allows a natural use of PDS kernels
   - SVR also admits favorable stability properties.
3. SVR also admits several disadvantages
   - SVR requires the selection of two parameters, C and ϵ, which are determined by cross-validation.
   - may be computationally expensive when dealing with large training sets.

Regression algorithms

Least absolute shrinkage and selection operator (Lasso)

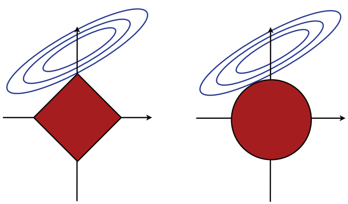
1. The optimization problem for Lasso is defined as

$$\min_{\mathbf{w},b} F(\mathbf{w}) = \min_{\mathbf{w},b} \left[\lambda \|\mathbf{w}\|_1 + C \sum_{i=1}^{m} \left(\langle \mathbf{w}, \mathbf{x}_i \rangle + b - y_i \right)^2 \right]$$

2. This is a **convex optimization problem**, because
   - $\|\mathbf{w}\|_1$ is convex as with all norms
   - the empirical error term is convex
3. Hence, the optimization problem can be written as

$$\min_{\mathbf{w},b} \left[\sum_{i=1}^{m} \left(\langle \mathbf{w}, \mathbf{x}_i \rangle + b - y_i \right)^2 \right] \text{ subject to } \|\mathbf{w}\|_1 \leq \Lambda_1$$

4. The L_1 norm constraint is that it leads to a **sparse solution $\mathbf{w}$**.



Theorem (Bounds of $\hat{\mathcal{R}}(H)$ of Lasso)

Let $\mathcal{X} \subseteq \mathbb{R}^n$ and let $S = \{(\mathbf{x}_1, y_1), \ldots, (\mathbf{x}_m, y_m)\} \in (\mathcal{X} \times \mathcal{Y})^m$ be sample of size m. Assume that for all $1 \leq i \leq m$, $\|\mathbf{x}_i\|_\infty \leq r_\infty$ for some $r_\infty > 0$, and let $H = \{\mathbf{x} \mapsto \langle \mathbf{w}, \mathbf{x} \rangle \mid \|\mathbf{w}\|_1 \leq \Lambda_1\}$. Then, the empirical Rademacher complexity of H can be bounded as follows

$$\hat{\mathcal{R}}(H) \leq \sqrt{\frac{2r_\infty^2 \Lambda_1^2 \log(2n)}{m}}$$

Definition (Dual norms)

Let $\|.\|$ be a norm on $\mathbb{R}^n$. Then, dual norm $\|.\|_*$ associated to $\|.\|$ is defined by

$$\forall \mathbf{y} \in \mathbb{R}^n, \quad \|\mathbf{y}\|_* = \sup_{\|\mathbf{x}\|=1} |\langle \mathbf{y}, \mathbf{x} \rangle|$$

For any $p, q \geq 1$ that are conjugate $(\frac{1}{p} + \frac{1}{q} = 1)$, L_p and L_q norms are dual norms. In particular, L_2 is dual norm of L_2, and L_1 is dual norm of L_∞ norm.

Proof (Bounds of $\hat{\mathcal{R}}(H)$ of Lasso)

1. For any $1 \leq i \leq m$, we denote by x_{ij}, the jth component of $\mathbf{x}_i$.

$$\hat{\mathcal{R}}(H) = \frac{1}{m} \mathop{\mathbb{E}}_{\sigma} \left[\sup_{\|\mathbf{w}\|_1 \leq \Lambda_1} \sum_{i=1}^{m} \sigma_i \langle \mathbf{w}, \mathbf{x}_i \rangle \right]$$

$$= \frac{\Lambda_1}{m} \mathop{\mathbb{E}}_{\sigma} \left[\left\| \sum_{i=1}^{m} \sigma_i \mathbf{x}_i \right\|_\infty \right] \quad \text{(by definition of the dual norm)}$$

$$= \frac{\Lambda_1}{m} \mathop{\mathbb{E}}_{\sigma} \left[\max_{j \in \{1,\ldots,n\}} \left| \sum_{i=1}^{m} \sigma_i x_{ij} \right| \right] \quad \text{(by definition of } \|.\|_\infty\text{)}$$

$$= \frac{\Lambda_1}{m} \mathop{\mathbb{E}}_{\sigma} \left[\max_{j \in \{1,\ldots,n\}} \max_{s \in \{-1,+1\}} s \sum_{i=1}^{m} \sigma_i x_{ij} \right] \quad \text{(by definition of } \|.\|_\infty\text{)}$$

$$= \frac{\Lambda_1}{m} \mathop{\mathbb{E}}_{\sigma} \left[\sup_{\mathbf{z} \in A} \sum_{i=1}^{m} \sigma_i z_i \right].$$

where A is set of n vectors $\{s(x_{1j}, \ldots, x_{mj}) \mid j \in \{1, \ldots, n\}, s \in \{-1, +1\}\}$.

Proof (Bounds of $\hat{\mathcal{R}}(H)$ of Lasso).

2. For any $\mathbf{z} \in A$, we have $\|\mathbf{z}\|_2 \leq \sqrt{mr_\infty^2} = r_\infty\sqrt{m}$.
3. Thus by Massart's Lemma, since A contains at most $2n$ elements, the following inequality holds:

$$\hat{\mathcal{R}}(H) \leq \Lambda_1 r_\infty \sqrt{m}\frac{2\log(2n)}{m} = \Lambda_1 r_\infty \sqrt{\frac{2\log(2n)}{m}}.$$

□

1. This bounds depends on dimension n is only logarithmic, which suggests that using very high-dimensional feature spaces does not significantly affect generalization.
2. By combining of Theorem (Bounds of $\hat{\mathcal{R}}(H)$ of Lasso) and Rademacher generalization bound, we can prove the following Theorem.

Theorem (Rademacher complexity of linear hypotheses with bounded L_1 norm)

Let $\mathcal{X} \subseteq \mathbb{R}^n$ and $H = \{\mathbf{x}_1 \mapsto \langle \mathbf{w}, \mathbf{x} \rangle \mid \|\mathbf{w}\|_1 \leq \Lambda_1\}$. Let also $S = \{(\mathbf{x}_1, y_1), \ldots, (\mathbf{x}_m, y_m)\} \in (\mathcal{X} \times \mathcal{Y})^m$ be sample of size m. Assume that there exists $r_\infty > 0$ such that for all $\mathbf{x} \in \mathcal{X}$, $\|\mathbf{x}_i\|_\infty \leq r_\infty$ and $M > 0$ such that $|h(\mathbf{x}) - y| \leq M$ for all $(\mathbf{x}, y) \in \mathcal{X} \times \mathcal{Y}$. Then, for any $\delta > 0$, with probability at least $(1 - \delta)$, each of the following inequality holds for $h \in H$

$$\mathbf{R}(h) \leq \hat{\mathbf{R}}(h) + 2 r_\infty \Lambda_1 M \sqrt{\frac{2\log(2n)}{m}} + M^2 \sqrt{\frac{\log \frac{1}{\delta}}{2m}}$$

1. Ridge regression and Lasso have same form as the right-hand side of this generalization bound.
2. Lasso has several advantages:
   - It benefits from strong theoretical guarantees and returns a sparse solution.
   - The sparsity of the solution is also computationally attractive (inner product).
   - The algorithm's sparsity can also be used for feature selection.
3. The main drawbacks are: usability of kernel and closed-form solution.

Regression algorithms

Online regression algorithms

Online regression algorithms

1. The regression algorithms admit natural online versions.
2. These algorithms are useful when we have very large data sets, where a batch solution can be computationally expensive.

Online linear regression

> Initialize $\mathbf{w}_1$.
> **for** $t \leftarrow 1, 2, \ldots, T$ **do**.
>   Receive $\mathbf{x}_t \in \mathbb{R}^n$.
>   Predict $\hat{y}_t = \langle \mathbf{w}_t, \mathbf{x}_t \rangle$.
>   Observe true label $y_t = h^*(\mathbf{x}_t)$.
>   Compute the loss $L(\hat{y}_t, y_t)$. s
>   Update $\mathbf{w}_{t+1}$.
> **end for**

Widrow-Hoff algorithm

1. Widrow-Hoff algorithm uses stochastic gradient descent technique to linear regression objective function.
2. At each round, the weight vector is augmented with a quantity that depends on the prediction error $(\langle \mathbf{w}_t, \mathbf{x}_t \rangle - y_t)$.

WidrowHoff regression

```
function WidrowHoff(w_0)
    Initialize w_1 ← w_0.                                   ▷ typically w_0 = 0.
    for t ← 1, 2, ..., T do.
        Receive x_t ∈ ℝ^n.
        Predict ŷ_t = ⟨w_t, x_t⟩.
        Observe true label y_t = h*(x_t).
        Compute the loss L(ŷ_t, y_t).
        Update w_{t+1} ← w_t − 2η(⟨w_t, x_t⟩ − y_t) x_t.     ▷ learning rate η > 0.
    end for
    return w_{T+1}
end function
```

1. There are two motivations for the update rule in Widrow-Hoff.
2. The first motivation is that
   - The loss function is defined as
   $$L(\mathbf{w}, \mathbf{x}, y) = (\langle \mathbf{w}, \mathbf{x} \rangle - y)^2$$
   - To minimize the loss function, move in the direction of the negative gradient
   $$\nabla_{\mathbf{w}} L(\mathbf{w}, \mathbf{x}, y) = 2\left(\langle \mathbf{w}, \mathbf{x} \rangle - y\right)\mathbf{x}$$
   - This gives the following update rule
   $$\mathbf{w}_{t+1} \leftarrow \mathbf{w}_t - \eta \nabla_{\mathbf{w}} L(\mathbf{w}_t, \mathbf{x}_t, y_t)$$
3. The second motivation is that we have two goals:
   - We want loss of $\mathbf{w}_{t+1}$ on $(\mathbf{x}_t, y_t)$ be small, which means we want to minimize $(\langle \mathbf{w}_{t+1}, \mathbf{x}_t \rangle - y_t)^2$.
   - We don't want $\mathbf{w}_{t+1}$ be too far from $\mathbf{w}_t$, ie. we don't want $\|\mathbf{w}_t - \mathbf{w}_{t+1}\|$ be too big.

1. Combining these two goals, we compute $\mathbf{w}_{t+1}$ by solving the following optimization problem

$$\mathbf{w}_{t+1} = \arg\min \left(\langle \mathbf{w}_{t+1}, \mathbf{x}_t \rangle - y_t\right)^2 + \|\mathbf{w}_{t+1} - \mathbf{w}_t\|$$

2. Take the gradient of this equation, and make it equal to zero. We obtain

$$\mathbf{w}_{t+1} = \mathbf{w}_t - 2\eta \left(\langle \mathbf{w}_{t+1}, \mathbf{x}_t \rangle - y_t\right) \mathbf{x}_t$$

3. Approximating $\mathbf{w}_{t+1}$ by $\mathbf{w}_t$ on right-hand side gives updating rule of Widrow-Hoff algorithm.
4. Let $L_A = \sum_{t=1}^{T} (\hat{y}_t - y_t)$ be loss of algorithm A.
5. Let $L_{\mathbf{u}} = \sum_{t=1}^{T} (\langle \mathbf{u}, \mathbf{x}_t \rangle - y_t)$ be loss of another regressor denoted by $\mathbf{u} \in \mathbb{R}^n$.
6. We upper bound loss of Widrow-Hoff algorithm in terms of loss of the best vector.

Lemma (Bounds on potential function of Widrow-Hoff algorithm)

Let $\Phi_t = \|\mathbf{w}_t - \mathbf{u}\|_2^2$ *be the potential function, then we have*

$$\Phi_{t+1} - \Phi_t \leq -\eta l_t^2 + \frac{\eta}{1-\eta} g_t^2$$

where

$$l_t = (\hat{y}_t - y) = \langle \mathbf{w}_t, \mathbf{x}_t \rangle - y_t$$
$$g_t = \langle \mathbf{u}_t, \mathbf{x}_t \rangle - y_t$$

So that l_t^2 *denotes the learners loss at round* t*, and* g_t^2 *is* $\mathbf{u}$*'s loss at round* t*.*

Proof (Bounds on potential function of Widrow-Hoff algorithm).

1. Let $\Delta_t = \eta\left(\langle \mathbf{w}_t, \mathbf{x}_t\rangle - y_t\right)\mathbf{x}_t = \eta l_t \mathbf{x}_t$ (update to the weight vector). Then, we have

$$\begin{aligned}
\Phi_{t+1} - \Phi_t &= \|\mathbf{w}_{t+1} - \mathbf{u}\|_2^2 - \|\mathbf{w}_t - \mathbf{u}\|_2^2 \\
&= \|\mathbf{w}_t - \mathbf{u} - \Delta_t\|_2^2 - \|\mathbf{w}_t - \mathbf{u}\|_2^2 \\
&= \|\mathbf{w}_t - \mathbf{u}\|_2^2 - 2\left\langle (\mathbf{w}_t - \mathbf{u}), \Delta_t\right\rangle + \|\Delta_t\|_2^2 - \|\mathbf{w}_t - \mathbf{u}\|_2^2 \\
&= -2\eta l_t \left\langle \mathbf{x}_t, (\mathbf{w}_t - \mathbf{u})\right\rangle + \eta^2 l_t^2 \|\mathbf{x}_t\|_2^2 \\
&\leq -2\eta l_t \left(\langle \mathbf{x}_t, \mathbf{w}_t\rangle - \langle \mathbf{u}, \mathbf{x}_t\rangle\right) + \eta^2 l_t^2 && \text{(since } \|\mathbf{x}_t\|_2^2 \leq 1\text{)} \\
&= -2\eta l_t \left[(\langle \mathbf{w}_t, \mathbf{x}_t\rangle - y_t) - (\langle \mathbf{u}, \mathbf{x}_t\rangle - y_t)\right] + \eta^2 l_t^2 \\
&= -2\eta l_t(l_t - g_t) + \eta^2 l_t^2 = -2\eta l_t^2 + 2\eta l_t g_t + \eta^2 l_t^2 \\
&\leq -2\eta l_t^2 + 2\eta\left(\frac{l_t^2(1-\eta) + g_t^2/(1-\eta)}{2}\right) + \eta^2 l_t^2 && \text{(by AM-GM)} \\
&= -\eta l_t^2 + \left(\frac{\eta}{1-\eta}\right) g_t^2
\end{aligned}$$

Proof (Bounds on potential function of Widrow-Hoff algorithm).

2. Arithmetic mean-geometric mean inequality (AM-GM) states:
   for any set of non-negative real numbers, arithmetic mean of the set is greater than or equal to geometric mean of the set.
3. It states for any real numbers $x_1, \ldots, x_n \geq 0$, we have $\frac{x_1 + \ldots + x_n}{n} \geq \sqrt[n]{x_1 x_2 \ldots x_n}$.
4. For reals $a = l_t^2(1-\eta) \geq 0$ and $b = \dfrac{g_t^2}{1-\eta} \geq 0$, AM-GM is $\sqrt{ab} \leq \dfrac{a+b}{2}$.

□

Theorem (Upper bound of loss Widrow-Hoff algorithm)

Assume that for all rounds t we have $\|\mathbf{x}_t\|_2^2 \leq 1$, then we have

$$L_{WH} \leq \min_{\mathbf{u} \in \mathbb{R}^n} \left[\frac{L_{\mathbf{u}}}{1-\eta} + \frac{\|\mathbf{u}\|_2^2}{\eta} \right]$$

where L_{WH} denotes the loss of Widrow-Hoff algorithm.

Proof (Upperbound of loss Widrow-Hoff algorithm).

1. Let $\sum_{t=1}^{T} (\Phi_{t+1} - \Phi_t) = \Phi_{T+1} - \Phi_1$.
2. By setting $\mathbf{w}_1 = 0$ and observation that $\Phi_t \geq 0$, we obtain

$$-\|u\|_2^2 = -\Phi_1 \leq \Phi_{T+1} - \Phi_1$$

3. Hence, we have

$$\begin{aligned} -\|u\|_2^2 &\leq \sum_{t=1}^{T} (\Phi_{t+1} - \Phi_t) \\ &\leq \sum_{t=1}^{T} \left(-\eta l_t^2 + \left(\frac{\eta}{1-\eta} \right) g_t^2 \right) = -\eta L_{WH} + \left(\frac{\eta}{1-\eta} \right) L_{\mathbf{u}}. \end{aligned}$$

4. By simplifying this inequality, we obtain $L_{WH} \leq \left(\frac{\eta}{1-\eta} \right) L_{\mathbf{u}} + \frac{\|u\|_2^2}{\eta}$.
5. Since $\mathbf{u}$ was arbitrary, the above inequality must hold for **the best vector**.

□

1. We can look at the average loss per time step

$$\frac{L_{WH}}{T} \leq \min_{\mathbf{u}} \left[\left(\frac{\eta}{1-\eta} \right) \frac{L_{\mathbf{u}}}{T} + \frac{\|u\|_2^2}{\eta T} \right].$$

2. As T gets large, we have

$$\left(\frac{\|u\|_2^2}{\eta T} \right) \to 0.$$

3. If step-size (η) is very small,

$$\left(\frac{\eta}{1-\eta} \right) \frac{L_{\mathbf{u}}}{T} \to \min_{\mathbf{u}} \left(\frac{L_{\mathbf{u}}}{T} \right), \qquad \text{Show it.}$$

   which is **the average loss of the best regressor**.

4. This means that the Widrow-Hoff algorithm is performing almost as well as the best regressor vector as the number of rounds gets large.

Summary

- We study the bounded regression problem.
- For unbounded regression, there is the main issue for deriving uniform convergence bounds.
- We defined pseudo-dimension for real-valued function classes.
- We study the generalization bounds based on Rademacher complexity.
- We study several regression algorithms and analysis their bounds.
- We study an online regression algorithms and analysis its bound.

Readings

1. Chapter 11 of Mehryar Mohri, Afshin Rostamizadeh, and Ameet Talwalkar (2018). *Foundations of Machine Learning*. Second Edition. MIT Press.
2. Chapter 11 of Martin Anthony and Peter L. Bartlett (1999). *Learning in Neural Networks : Theoretical Foundations*. Cambridge University Press.

References

Anthony, Martin and Peter L. Bartlett (1999). *Learning in Neural Networks : Theoretical Foundations*. Cambridge University Press.

Mohri, Mehryar, Afshin Rostamizadeh, and Ameet Talwalkar (2018). *Foundations of Machine Learning*. Second Edition. MIT Press.

Questions?