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Statistical Learning Theory and Applications

Class 03: Regularized Least Squares

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Learning problem and algorithms

Solve

$$\min_{f\in\mathcal{F}} L(f), \qquad L(f) = \mathbb{E}_{(x,y)\sim P}[\ell(y, f(x))],$$

given only

$$S_n = (x_1, y_1), \ldots, (x_n, y_n) \sim P^n.$$

Learning algorithm

$$S_n \to \widehat{f} = \widehat{f}_{S_n},$$

$\widehat{f}$ estimates f_P given the observed examples S_n.

Learning problem and algorithms

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$\widehat{f}$ estimates f_P given the observed examples S_n.

How can we design a learning algorithm?

Algorithm design: complexity and regularization

The design of most algorithms proceed as follows:

- Pick a (possibly large) class of function $\mathcal{H}$, ideally

$$\min_{f \in \mathcal{H}} L(f) = \min_{f \in \mathcal{F}} L(f).$$

- Define a procedure $A_\gamma(S_n) = \hat{f}_\gamma \in \mathcal{H}$ to *explore* the space $\mathcal{H}$.

Empirical risk minimization

A classical example (called M-estimation in statistics).

Consider $(\mathcal{H}_\gamma)_\gamma$ such that

$$\mathcal{H}_1 \subset \mathcal{H}_2, \dots \mathcal{H}_\gamma \subset \dots \mathcal{H}.$$

Then, let

$$\hat{f}_\gamma = \min_{f \in \mathcal{H}_\gamma} \widehat{L}(f), \qquad \widehat{L}(f) = \frac{1}{n} \sum_{i=1}^{n} \ell(y_i, f(x_i)).$$

This is the idea we discuss next.

Linear functions

Let $\mathcal{H}$ be the space of linear functions

$$f(x) = w^\top x.$$

Then,

- $f \leftrightarrow w$ is one to one,
- inner product $\left\langle f, \bar{f} \right\rangle_{\mathcal{H}} := w^\top \bar{w}$,
- norm/metric $\left\| f - \bar{f} \right\|_{\mathcal{H}} := \| w - \bar{w} \|$.

Linear functions are the conceptual building block of most functions.

Linear least squares

ERM with least squares also called ordinary least squares (OLS)

$$\min_{w \in \mathbb{R}^d} \underbrace{\frac{1}{n} \sum_{i=1}^{n} (y_i - w^\top x_i)^2}_{\widehat{L}(w)}.$$

- Statistics later...
- ...now **computations**.

Matrices and linear systems

Let $\widehat{X} \in \mathbb{R}^{nd}$ and $\widehat{Y} \in \mathbb{R}^{n}$. Then

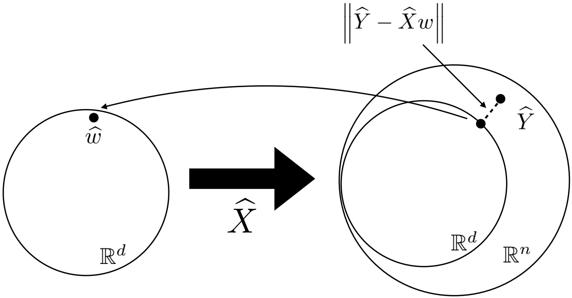
$$\frac{1}{n}\sum_{i=1}^{n}(y_i - w^\top x_i)^2 = \frac{1}{n}\left\|\widehat{Y} - \widehat{X}w\right\|^2.$$

This is the least squares problem associated to the linear system

$$\widehat{X}w = \widehat{Y}.$$

Overdetermined lin. syst.

$n > d$



$$\nexists\, \widehat{w} \quad \text{s.t.} \quad \widehat{X}w = \widehat{Y}$$

Least squares solutions

From the optimality conditions

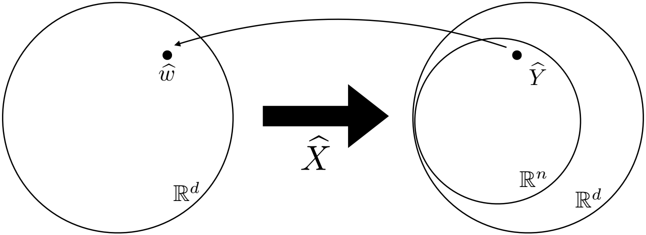
$$\nabla_w \frac{1}{n} \left\| \widehat{Y} - \widehat{X} w \right\|^2 = 0$$

we can derive the normal equation

$$\widehat{X}^\top \widehat{X} w = \widehat{X}^\top \widehat{Y} \qquad \Leftrightarrow \qquad \widehat{w} = (\widehat{X}^\top \widehat{X})^{-1} \widehat{X}^\top \widehat{Y}.$$

Underdetermined lin. syst.

$n < d$



$$\exists\ \widehat{w} \quad \text{s.t.} \quad \widehat{X}w = \widehat{Y}$$

possibly not unique...

Minimal norm solution

There can be many solutions

$$\widehat{X}\widehat{w} = \widehat{Y}, \quad \text{and} \quad \widehat{X}w_0 = 0 \quad \Rightarrow \widehat{X}(\widehat{w} + w_0) = \widehat{Y}.$$

Consider

$$\min_{w \in \mathbb{R}^d} \|w\|^2, \qquad \text{subj. to} \qquad \widehat{X}w = \widehat{Y}.$$

Using the method of Lagrange multipliers, the solution is

$$\widehat{w} = \widehat{X}^\top (\widehat{X}\widehat{X}^\top)^{-1}\widehat{Y}.$$

Pseudoinverse

$$\widehat{w} = \widehat{X}^{\dagger}\widehat{Y}$$

For $n > d$, (independent columns)

$$\widehat{X}^{\dagger} = (\widehat{X}^{\top}\widehat{X})^{-1}\widehat{X}^{\top}.$$

For $n < d$, (independent rows)

$$\widehat{X}^{\dagger} = \widehat{X}^{\top}(\widehat{X}\widehat{X}^{\top})^{-1}.$$

Spectral view

Consider the SVD of $\widehat{X}$

$$\widehat{X} = USV^\top \quad \Leftrightarrow \quad \widehat{X}w = \sum_{j=1}^{r} s_j (v_j^\top w) u_j,$$

here $r \leq n \wedge d$ is the rank of $\widehat{X}$.

Then,

$$\widehat{w}^\dagger = \widehat{X}^\dagger \widehat{Y} = \sum_{j=1}^{r} \frac{1}{s_j} (u_j^\top \widehat{Y}) v_j.$$

Pseudoinverse and bias

$$\widehat{w}^\dagger = \widehat{X}^\dagger \widehat{Y} = \sum_{j=1}^{r} \frac{1}{s_j} (u_j^\top \widehat{Y}) v_j.$$

$(v_j)_j$ are principal components of $\widehat{X}$: OLS "likes" principal components.

Not all linear functions are the same for OLS!

The pseudoinverse introduces a bias towards certain solutions.

From OLS to ridge regression

Recall, it also holds,

$$\widehat{X}^{\dagger} = \lim_{\lambda \to 0_+} (\widehat{X}^\top \widehat{X} + \lambda I)^{-1} \widehat{X}^\top = \lim_{\lambda \to 0_+} \widehat{X}^\top (\widehat{X}\widehat{X}^\top + \lambda I)^{-1}.$$

Consider for $\lambda > 0$,

$$\widehat{w}^{\lambda} = (\widehat{X}^\top \widehat{X} + \lambda I)^{-1} \widehat{X}^\top \widehat{Y}.$$

This is called ridge regression.

Spectral view on ridge regression

$$\widehat{w}^{\lambda} = (\widehat{X}^{\top}\widehat{X} + \lambda I)^{-1}\widehat{X}^{\top}\widehat{Y}$$

Considering the SVD of $\widehat{X}$,

$$\widehat{w}^{\lambda} = \sum_{j=1}^{r} \frac{s_j}{s_j^2 + \lambda}(u_j^{\top}\widehat{Y})v_j.$$

Ridge regression as filtering

$$\widehat{w}^{\lambda} = \sum_{j=1}^{r} \frac{s_j}{s_j^2 + \lambda} (u_j^\top \widehat{Y}) v_j$$

The function

$$F(s) = \frac{s}{s^2 + \lambda},$$

acts as a low pass filter (low frequencies= principal components).

- For s small, $F(s) \approx 1/\lambda$.
- For s big, $F(s) \approx 1/s$.

Ridge regression as ERM

$$\widehat{w}^{\lambda} = (\widehat{X}^{\top}\widehat{X} + \lambda I)^{-1}\widehat{X}^{\top}\widehat{Y}$$

is the solution of

$$\min_{w \in \mathbb{R}^d} \underbrace{\left\|\widehat{Y} - \widehat{X}w\right\|^2 + \lambda\|w\|^2}_{\widehat{L_{\lambda}}(w)}.$$

It follows from,

$$\Delta\widehat{L_{\lambda}}(w) = -\frac{2}{n}\widehat{X}^{\top}(\widehat{Y} - \widehat{X}w) + 2\lambda w = 2(\frac{1}{n}\widehat{X}^{\top}\widehat{X} + \lambda I)w - \frac{2}{n}\widehat{X}^{\top}\widehat{Y}.$$

Ridge regression as ERM

ERM interpretation suggests the rescaling

$$\widehat{w}^{\lambda} = (\widehat{X}^{\top}\widehat{X} + n\lambda I)^{-1}\widehat{X}^{\top}\widehat{Y}$$

since

$$\min_{w\in\mathbb{R}^d} \underbrace{\frac{1}{n}\left\|\widehat{Y} - \widehat{X}w\right\|^2 + \lambda\|w\|^2}_{\widehat{L_\lambda}(w)}.$$

Related ideas

Tikhonov

$$\min_{w \in \mathbb{R}^d} \frac{1}{n} \left\| \widehat{Y} - \widehat{X} w \right\|^2 + \lambda \|w\|^2$$

Morozov

$$\min_{w \in \mathbb{R}^d} \|w\|^2 \qquad \text{subj. to} \qquad \frac{1}{n} \left\| \widehat{Y} - \widehat{X} w \right\|^2 \leq \delta$$

Ivanov

$$\min_{w \in \mathbb{R}^d} \frac{1}{n} \left\| \widehat{Y} - \widehat{X} w \right\|^2, \qquad \text{subj. to} \qquad \|w\|^2 \leq R$$

Ridge regression and SRM

The constraint

$$\|w\|^2 \leq R$$

- restricts the search of solution,
- shrinks the solution coefficients.

Different views on regularization

$$\widehat{w} = \widehat{X}^{\dagger}\widehat{Y} \qquad \widehat{w}_\lambda = (\widehat{X}^\top \widehat{X} + \lambda I)^{-1}\widehat{X}^\top \widehat{Y}$$

$$\min_{w \in \mathbb{R}^d \text{ s.t. } \widehat{X}w = \widehat{Y}} \|w\|^2 \qquad \min_{w \in \mathbb{R}^d} \frac{1}{n}\sum_{i=1}^{n}(y_i - w^\top x_i)^2 + \lambda \|w\|^2$$

- Introduces a *bias* towards certain solutions: small norm/principal components,
- controls the *stability* of the solution .

Complexity of ridge regression

Back to computations.

Solving

$$\widehat{w}^{\lambda} = (\widehat{X}^\top \widehat{X} + \lambda I)^{-1} \widehat{X}^\top \widehat{Y}$$

requires essentially (using a direct solver)

- time $O(nD^2 + D^3)$,
- memory $O(nd \vee D^2)$.

What if $n \ll D$?

Representer theorem in disguise

A simple observation

Using SVD we can see that

$$(\widehat{X}^\top \widehat{X} + \lambda I)^{-1} \widehat{X}^\top = \widehat{X}^\top (\widehat{X}\widehat{X}^\top + \lambda I)^{-1}$$

More on complexity

Then

$$\widehat{w}^{\lambda} = \widehat{X}^{\top}(\widehat{X}\widehat{X}^{\top} + \lambda I)^{-1}\widehat{Y}.$$

requires essentially (using a direct solver)

- time $O(n^2 D + n^3)$,
- memory $O(nd \vee n^2)$.

Representer theorem

Note that

$$\widehat{w}^{\lambda} = \widehat{X}^{\top} \underbrace{(\widehat{X}\widehat{X}^{\top} + \lambda I)^{-1} \widehat{Y}}_{c \in \mathbb{R}^n} = \sum_{i=1}^{n} x_i c_i.$$

The coefficients vector is a linear combination of the input points.

Then

$$\hat{f}^{\lambda}(x) = x^{\top} \widehat{w}^{\lambda} = x^{\top} \widehat{X}^{\top} c = \sum_{i=1}^{n} x^{\top} x_i c_i$$

The function we obtain is a linear combination of *inner products*.

This will be the key to nonparametric learning.

Summing up

- From OLS to ridge regression
- Different views: (spectral) filtering and ERM
- Regularization and bias.

TBD

- Beyond linear models.
- Optimization.
- Model selection.