Regression

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From classification to regression

Classification:

- there is a joint distribution of $(X, Y) \sim \rho$ where typically $X \in \mathbb{R}^d$ and $Y \in \{1, \dots, K\}$ is discrete
- Goal: given input x, find the label y with the highest posterior probability

$$\arg\max_{y \in \{1,\dots,K\}} \mathbb{P}\big(Y = y | X = x\big)$$

Regression:

- there is a joint distribution of $(X, Y) \sim \rho$ where $X \in \mathbb{R}^d$ and $Y \in \mathbb{R}$
- Goal: given input x, find a prediction $f(x)$ for Y conditional on $X = x$, that minimizes MSE

$$\mathbb{E}\big[(Y - f(x))^2 | X = x\big]$$

Target of regression problem

Theorem 4.1

For any random variable Z, we have

$$\arg\min_{c\in\mathbb{R}} \mathbb{E}[(Z-c)^2] = \mathbb{E}[Z].$$

Implications for regression problem:

- Conditional on $X = x$, the optimal prediction for Y that minimizes MSE is

$$f^\star(x) = \mathbb{E}[Y|X = x]$$

- Rewrite the model

$$Y = \underbrace{\mathbb{E}[Y|X]}_{\text{regression function}} + \underbrace{Y - \mathbb{E}[Y|X]}_{\text{mean-zero noise}}$$

Regression problem

We will consider the regression problem in a more straightforward way:

$$y = f^\star(\boldsymbol{x}) + \varepsilon$$

- $\boldsymbol{x} \in \mathbb{R}^d$ is the input, $y \in \mathbb{R}$ is the output
- ε is some mean-zero random noise, e.g., $\varepsilon \sim \mathcal{N}(0, \sigma^2)$
- $f^\star : \mathbb{R}^d \to \mathbb{R}$ is the *unknown* regression function
- Training data: $(\boldsymbol{x}_1, y_1), \ldots, (\boldsymbol{x}_n, y_n)$ satisfying

  $$y_i = f^\star(\boldsymbol{x}_i) + \varepsilon_i$$

  where $\varepsilon_1, \ldots, \varepsilon_n$ are i.i.d. noise with $\mathbb{E}[\varepsilon_i] = 0$, and
  - in some cases, we assume $\boldsymbol{x}_1, \ldots, \boldsymbol{x}_n$ are deterministic (fixed design)
  - sometimes we may assume that $\boldsymbol{x}_1, \ldots, \boldsymbol{x}_n \overset{\text{i.i.d.}}{\sim} \rho_X$ (random design)
- Learn the regression function $f^\star$ based on training data

Overview

- **Linear regression:** model the regression function $f^\star$ as a linear function

$$f^\star(\boldsymbol{x}) = \boldsymbol{x}^\top \boldsymbol{\beta}^\star$$

  where we assume $\boldsymbol{x}$ includes a constant variable 1. Here $\boldsymbol{\beta}^\star \in \mathbb{R}^d$ is the unknown parameter.

- **Nonparametric regression:** assume that

$$f^\star \in \mathcal{F}$$

  where $\mathcal{F}$ is certain function class, e.g.,

  - class of quadratic function
  - class of convex function
  - Reproducing Kernel Hilbert Space (RKHS)

Linear regression: classical setting

Linear regression

- Linear regression:

$$y_i = \boldsymbol{x}_i^\top \boldsymbol{\beta}^\star + \varepsilon_i \quad (i = 1, \ldots, n)$$

where $\boldsymbol{x}_1, \ldots, \boldsymbol{x}_n$ are fixed design, and $\varepsilon_1, \ldots, \varepsilon_n$ are i.i.d. noise satisfying $\mathbb{E}[\varepsilon_i] = 0$ and $\mathsf{var}(\varepsilon_i) = \sigma^2$

- Consider matrix notation

$$\boldsymbol{Y} = \boldsymbol{X}\boldsymbol{\beta}^\star + \boldsymbol{\varepsilon}$$

where

$$\boldsymbol{Y} = \begin{bmatrix} y_1 \\ \vdots \\ y_n \end{bmatrix} \in \mathbb{R}^n, \quad \boldsymbol{X} = \begin{bmatrix} \boldsymbol{x}_1^\top \\ \vdots \\ \boldsymbol{x}_n^\top \end{bmatrix} \in \mathbb{R}^{n \times d}, \quad \boldsymbol{\varepsilon} = \begin{bmatrix} \varepsilon_1 \\ \vdots \\ \varepsilon_n \end{bmatrix} \in \mathbb{R}^n$$

Least square estimator

- The most popular estimation method is *least squares*, which estimates $\boldsymbol{\beta}^\star$ by minimizing the residual sum of squares

$$\sum_{i=1}^{n}(y_i - \boldsymbol{x}_i^\top \boldsymbol{\beta})^2 = \|\boldsymbol{Y} - \boldsymbol{X}\boldsymbol{\beta}\|_2^2.$$

- Ordinary least squares (OLS) estimator:

$$\widehat{\boldsymbol{\beta}} := \arg\min_{\boldsymbol{\beta}\in\mathbb{R}^d} \|\boldsymbol{Y} - \boldsymbol{X}\boldsymbol{\beta}\|_2^2$$

  It has minimizer

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

- Suppose the noise are i.i.d. Gaussian, then OLS is the MLE

Theoretical properties

- Linear estimator: estimator of the form $\boldsymbol{AY}$ for some matrix $\boldsymbol{A} \in \mathbb{R}^{d\times n}$
- OLS achieves the minimum variance among all linear unbiased estimators
- Furthermore, when the noise is i.i.d. Gaussian, OLS achieves the minimum variance among all unbiased estimators

Theorem 4.2

- **Gauss-Markov:** *The OLS estimator $\widehat{\boldsymbol{\beta}}$ is the best linear unbiased estimator of $\boldsymbol{\beta}^\star$, i.e. for any linear and unbiased estimator $\widetilde{\boldsymbol{\beta}}$ of $\boldsymbol{\beta}^\star$,*

$$\mathrm{cov}(\widehat{\boldsymbol{\beta}}) \preceq \mathrm{cov}(\widetilde{\boldsymbol{\beta}}).$$

- **Cramér-Rao lower bound:** *when $\varepsilon_1, \dots, \varepsilon_n$ are i.i.d. $\mathcal{N}(0, \sigma^2)$, the variance of OLS matches the Cramér-Rao lower bound, i.e. for any unbiased estimator $\widetilde{\boldsymbol{\beta}}$ of $\boldsymbol{\beta}^\star$,*

$$\mathrm{cov}(\widehat{\boldsymbol{\beta}}) \preceq \mathrm{cov}(\widetilde{\boldsymbol{\beta}}).$$

Cramér-Rao lower bound

- Consider $X_1, \ldots, X_n$ be i.i.d. samples from a density f_θ
- The unknown parameter $\theta \in \Theta$
- Let $T(X_1, \ldots, X_n)$ be any unbiased estimator for θ
- Under some regularity condition,

$$\mathsf{cov}(T(X_1, \ldots, X_n)) \succeq [I(\theta)]^{-1}$$

where $I(\theta)$ is the **Fisher information matrix**

$$\begin{aligned} I(\theta) &= n\mathbb{E}_{X \sim f_\theta}\left[\nabla_\theta \log f_\theta(X) \left[\nabla_\theta \log f_\theta(X)\right]^\top\right] \\ &= -n\mathbb{E}_{X \sim f_\theta}\left[\nabla_\theta^2 \log f_\theta(X)\right] \end{aligned}$$

Implications

- The OLS estimator is the best one among all unbiased estimator for $\boldsymbol{\beta}^\star$ in terms of minimizing MSE (why?)
- Is it also the best estimator among any estimator for $\boldsymbol{\beta}^\star$, including those biased ones?

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- The OLS estimator is the best one among all unbiased estimator for $\boldsymbol{\beta}^\star$ in terms of minimizing MSE (why?)
- Is it also the best estimator among any estimator for $\boldsymbol{\beta}^\star$, including those biased ones?

  — *No! There are biased estimator which can achieve smaller MSE.*
- Examples of biased estimator with smaller MSE:
  - James-Stein estimator
  - Ridge regression

  — *shrinkage estimators*

Shrinkage estimator

Bias-variance tradeoff

- Suppose that the unknown parameter is $\boldsymbol{\beta}^\star \in \mathbb{R}^d$
- For any estimator $\widehat{\boldsymbol{\beta}}$ (more generally, any random vector), the mean squared error (MSE) can be decomposed into

$$\underbrace{\mathbb{E}[\|\widehat{\boldsymbol{\beta}} - \boldsymbol{\beta}^\star\|_2^2]}_{=:\text{MSE}} = \underbrace{\|\mathbb{E}[\widehat{\boldsymbol{\beta}}\,] - \boldsymbol{\beta}^\star\|_2^2}_{\text{bias}} + \underbrace{\mathsf{tr}(\mathsf{cov}(\widehat{\boldsymbol{\beta}}))}_{\text{variance}}$$

- For unbiased estimator (e.g., OLS), the bias is zero
- By tolerating a small amount of bias we may be able to achieve a larger reduction in variance, thus achieving smaller MSE

James-Stein estimator

- Consider a Gaussian sequence model,

$$\boldsymbol{Y} = \boldsymbol{\beta}^\star + \boldsymbol{\varepsilon}, \qquad \boldsymbol{\varepsilon} \sim \mathcal{N}(\boldsymbol{0}, \boldsymbol{I}_n)$$

  which is a special linear regression by taking $d = n$ and $\boldsymbol{X} = \boldsymbol{I}_n$

- OLS / MLE: $\widehat{\boldsymbol{\beta}}_{\text{OLS}} = \boldsymbol{Y}$
- James-Stein estimator:

$$\widehat{\boldsymbol{\beta}}_{\text{JS}} = \left(1 - \frac{n-2}{\|\boldsymbol{Y}\|_2^2}\right)\boldsymbol{Y}$$

Theorem 4.3

James-Stein estimator has smaller MSE than OLS when $n \geq 3$, i.e.,

$$\text{MSE}(\widehat{\boldsymbol{\beta}}_{\text{JS}}) < \text{MSE}(\widehat{\boldsymbol{\beta}}_{\text{OLS}}) \quad \textit{for any} \quad \boldsymbol{\beta}^\star$$

Implications

- By shrinking the OLS towards zero, we achieve smaller MSE

  — *inadmissability of OLS (or MLE)*

- It is not even necessary to shrink towards zero: for any fixed $\boldsymbol{c} \in \mathbb{R}^n$,

$$\widehat{\boldsymbol{\beta}}_{\boldsymbol{c}} \coloneqq \boldsymbol{Y} - \frac{p-2}{\|\boldsymbol{Y} - \boldsymbol{c}\|_2^2}(\boldsymbol{Y} - \boldsymbol{c})$$

  also satisfy the same property as Theorem 4.3

- Can be extended to linear regression:

$$\widehat{\boldsymbol{\beta}}_{\mathsf{JS}} = \widehat{\boldsymbol{\beta}}_{\mathsf{OLS}} - \frac{(d-2)\widehat{\sigma}^2}{\|\boldsymbol{X}^\top \boldsymbol{X} \widehat{\boldsymbol{\beta}}_{\mathsf{OLS}}\|_2^2} \boldsymbol{X}^\top \boldsymbol{X} \widehat{\boldsymbol{\beta}}_{\mathsf{OLS}}.$$

Ridge regression

- Ridge regression: ℓ_2-penalized least squares estimator

$$\widehat{\boldsymbol{\beta}}_\lambda = \underset{\boldsymbol{\beta} \in \mathbb{R}^d}{\arg\min} \, \|\boldsymbol{Y} - \boldsymbol{X}\boldsymbol{\beta}\|_2^2 + \lambda \|\boldsymbol{\beta}\|_2^2,$$

  where λ is the tuning parameter.

- The ridge regression estimator admits closed-form solution:

$$\widehat{\boldsymbol{\beta}}_\lambda = (\boldsymbol{X}^\top \boldsymbol{X} + \lambda \boldsymbol{I}_d)^{-1} \boldsymbol{X}^\top \boldsymbol{Y}.$$

  It is well defined even when $\boldsymbol{X}^\top \boldsymbol{X}$ is not invertible

- As $\lambda \to 0$, ridge regression recovers the OLS
- Interpretation as MAP estimator with a Gaussian prior on $\boldsymbol{\beta}^\star$

MAP estimate

Consider observing X from a density $f_{\theta^\star}$, where $\theta^\star \in \Theta$ is unknown

Frequentist's viewpoint: $\theta^\star$ is fixed (though unknown)

- Likelihood function: $f_\theta(X)$ (a function of $\theta \in \Theta$)
- Estimate $\theta^\star$ by the maximizer of the likelihood function

— *maximum likelihood estimation (MLE)*

Bayesian's viewpoint: θ is also random

- We have a prior distribution $g(\theta)$ over Θ, and conditional on θ, $X \sim f_\theta$
- Posterior probability of θ after observing X:

$$\mathbb{P}(\theta|X) = \frac{g(\theta) f_\theta(X)}{\int_\Theta g(\theta') f_{\theta'}(X) \mathrm{d}\theta'} \propto g(\theta) f_\theta(X)$$

- Estimate θ by the maximizer of the posterior probability

— *maximum a posteriori estimation (MAP)*

Properties of ridge regression

Ridge regression:

$$\widehat{\boldsymbol{\beta}}_\lambda = \arg\min_{\boldsymbol{\beta}\in\mathbb{R}^d} \|\boldsymbol{Y} - \boldsymbol{X}\boldsymbol{\beta}\|_2^2 + \lambda\|\boldsymbol{\beta}\|_2^2 = (\boldsymbol{X}^\top\boldsymbol{X} + \lambda\boldsymbol{I}_d)^{-1}\boldsymbol{X}^\top\boldsymbol{Y}.$$

Theorem 4.4

There exists $\lambda_0 > 0$ such that ridge regression $\widehat{\boldsymbol{\beta}}_\lambda$ achieves smaller MSE than OLS estimate

$$\mathsf{MSE}(\widehat{\boldsymbol{\beta}}_\lambda) < \mathsf{MSE}(\widehat{\boldsymbol{\beta}}_{\mathsf{OLS}})$$

for any $\lambda \in (0, \lambda_0]$.

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$$\widehat{\boldsymbol{\beta}}_\lambda = \arg\min_{\boldsymbol{\beta} \in \mathbb{R}^d} \|\boldsymbol{Y} - \boldsymbol{X}\boldsymbol{\beta}\|_2^2 + \lambda\|\boldsymbol{\beta}\|_2^2 = (\boldsymbol{X}^\top \boldsymbol{X} + \lambda \boldsymbol{I}_d)^{-1} \boldsymbol{X}^\top \boldsymbol{Y}.$$

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- To prove this theorem, we need some tool from linear algebra

Singular Value Decomposition (SVD)

For any rank-r matrix $\boldsymbol{X} \in \mathbb{R}^{n \times d}$, it can be expressed as

$$\boldsymbol{X} = \boldsymbol{U}\boldsymbol{\Sigma}\boldsymbol{V}^\top$$

- $\boldsymbol{U} \in \mathbb{R}^{n \times r}$ and $\boldsymbol{V} \in \mathbb{R}^{d \times r}$ are orthogonal matrices:

$$\boldsymbol{U} = [\boldsymbol{u}_1, \dots, \boldsymbol{u}_r], \qquad \boldsymbol{V} = [\boldsymbol{v}_1, \dots, \boldsymbol{v}_r],$$

  where $\{\boldsymbol{u}_i\}_{i=1}^r$ (resp. $\{\boldsymbol{v}_i\}_{i=1}^r$) are orthonormal vectors in $\mathbb{R}^m$ (resp. $\mathbb{R}^n$)

- $\boldsymbol{\Sigma} \in \mathbb{R}^{r \times r}$ is a diagonal matrix

$$\boldsymbol{\Sigma} = \mathsf{diag}\{\sigma_1, \dots, \sigma_r\}$$

  where $\sigma_1 \geq \sigma_2 \geq \cdots \geq \sigma_r > 0$ are the singular values of $\boldsymbol{X}$

More about SVD

For any rank-r matrix $\boldsymbol{X} \in \mathbb{R}^{n\times d}$ with SVD $\boldsymbol{X} = \boldsymbol{U}\boldsymbol{\Sigma}\boldsymbol{V}^\top$

- Connection to eigen-decomposition

$$\boldsymbol{X}\boldsymbol{X}^\top = \boldsymbol{U}\boldsymbol{\Sigma}^2\boldsymbol{U}^\top = \begin{bmatrix}\boldsymbol{U} & \boldsymbol{U}_\perp\end{bmatrix}\begin{bmatrix}\boldsymbol{\Sigma}^2 & \boldsymbol{0} \\ \boldsymbol{0} & \boldsymbol{0}_{n-r}\end{bmatrix}\begin{bmatrix}\boldsymbol{U}^\top \\ \boldsymbol{U}_\perp^\top\end{bmatrix}$$

$$\boldsymbol{X}^\top\boldsymbol{X} = \boldsymbol{V}\boldsymbol{\Sigma}^2\boldsymbol{V}^\top = \begin{bmatrix}\boldsymbol{V} & \boldsymbol{V}_\perp\end{bmatrix}\begin{bmatrix}\boldsymbol{\Sigma}^2 & \boldsymbol{0} \\ \boldsymbol{0} & \boldsymbol{0}_{d-r}\end{bmatrix}\begin{bmatrix}\boldsymbol{V}^\top \\ \boldsymbol{V}_\perp^\top\end{bmatrix}$$

  where $\boldsymbol{U}_\perp$ (resp. $\boldsymbol{V}_\perp$) is the orthogonal complement of $\boldsymbol{U}$ (resp. $\boldsymbol{V}$)

- The operator (spectral) norm of $\boldsymbol{X}$

$$\|\boldsymbol{X}\| = \sup_{\|\boldsymbol{a}\|_2=1} \|\boldsymbol{X}\boldsymbol{a}\|_2 = \sigma_1$$

- The Frobenius norm of $\boldsymbol{X}$

$$\|\boldsymbol{X}\|_{\mathrm{F}}^2 = \sum_{i=1}^{r} \sigma_i^2$$

Implications to ridge regression

Suppose that the design matrix $\boldsymbol{X}$ has SVD $\boldsymbol{U\Sigma V}^\top$

- Bias-variance decomposition

$$\mathbb{E}[\|\widehat{\boldsymbol{\beta}}_\lambda - \boldsymbol{\beta}^\star\|_2^2] = \|\mathbb{E}[\widehat{\boldsymbol{\beta}}_\lambda] - \boldsymbol{\beta}^\star\|_2^2 + \mathsf{tr}(\mathsf{cov}(\widehat{\boldsymbol{\beta}}_\lambda))$$

- Bias term

$$\|\mathbb{E}[\widehat{\boldsymbol{\beta}}_\lambda] - \boldsymbol{\beta}^\star\|_2^2 = \sum_{i=1}^{d} \Big(\frac{\lambda \widetilde{\beta}_i}{\lambda + \sigma_i^2}\Big)^2 \quad \text{where} \quad \widetilde{\boldsymbol{\beta}} = [\boldsymbol{V}, \boldsymbol{V}_\perp]^\top \boldsymbol{\beta}^\star$$

- Variance term

$$\mathsf{cov}(\widehat{\boldsymbol{\beta}}_\lambda) = \sigma^2 \sum_{i=1}^{d} \Big(\frac{\sigma_i}{\lambda + \sigma_i^2}\Big)^2$$

- This allows us to prove Theorem 4.4

Linear regression: high-dimensional setting

What happens in high-dimension?

High-dimensional linear regression:

$$\boldsymbol{Y} = \boldsymbol{X}\boldsymbol{\beta}^\star + \boldsymbol{\varepsilon}$$

where the dimension d is much larger than the sample size n

- OLS fails because $\boldsymbol{X}^\top \boldsymbol{X}$ is not invertible
- In general, it is not possible to say something meaningful about $\boldsymbol{\beta}^\star \in \mathbb{R}^d$ from n samples $\boldsymbol{Y} \in \mathbb{R}^n$ (identifiability issue)

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- In general, it is not possible to say something meaningful about $\boldsymbol{\beta}^\star \in \mathbb{R}^d$ from n samples $\boldsymbol{Y} \in \mathbb{R}^n$ (identifibility issue)
- A meaningful and workable setup: assume $\boldsymbol{\beta}^\star$ is sparse, i.e.,

$$s := \|\boldsymbol{\beta}^\star\|_0 \equiv |\{j : \beta_j^\star \neq 0\}| \ll d$$

Sparse linear regression

High-dimensional linear regression:

$$\boldsymbol{Y} = \boldsymbol{X}\boldsymbol{\beta}^\star + \boldsymbol{\varepsilon}$$

where $d \geq n$, but $s = \|\boldsymbol{\beta}^\star\|_0 \ll d$

- **Genomics:** only a small subset of genes is expected to be associated with a particular trait or disease
- **Finance and Economics:** only a small subset of macroeconomic variables or market signals may be relevant to stock returns or economic growth
- $\cdots\cdots$

Insights

- Motivated by ridge regression, we may consider

$$\arg\min_{\boldsymbol{\beta}\in\mathbb{R}^d} \|\boldsymbol{Y} - \boldsymbol{X}\boldsymbol{\beta}\|_2^2 + \lambda\|\boldsymbol{\beta}\|_0$$

- Issue: computationally hard ($\|\cdot\|_0$ is discontinuous, non-convex...)
- Idea: use $\|\cdot\|_1$ instead
- Insights from compressed sensing (noiseless): under certain conditions (known as restricted isometry property), ℓ_1 minimization problem

$$\arg\min_{\boldsymbol{\beta}\in\mathbb{R}^d} \|\boldsymbol{\beta}\|_1 \quad \text{s.t.} \quad \boldsymbol{X}\boldsymbol{\beta} = \boldsymbol{Y}$$

has unique minimizer that coincides with the minimizer to

$$\arg\min_{\boldsymbol{\beta}\in\mathbb{R}^d} \|\boldsymbol{\beta}\|_0 \quad \text{s.t.} \quad \boldsymbol{X}\boldsymbol{\beta} = \boldsymbol{Y}\,.$$

LASSO

LASSO (Least Absolute Shrinkage and Selection Operator) estimates $\boldsymbol{\beta}^\star$ by solving the following convex optimization problem:

$$\widehat{\boldsymbol{\beta}} = \arg\min_{\boldsymbol{\beta}\in\mathbb{R}^d} \|\boldsymbol{Y} - \boldsymbol{X}\boldsymbol{\beta}\|_2^2 + \lambda\|\boldsymbol{\beta}\|_1,$$

where:

- $\|\boldsymbol{Y} - \boldsymbol{X}\boldsymbol{\beta}\|_2^2$: residual sum of squares (RSS).
- $\|\boldsymbol{\beta}\|_1 = \sum_{j=1}^p |\beta_j|$: ℓ_1-norm penalty.
- $\lambda > 0$: tuning parameter that controls the trade-off between goodness of fit and sparsity.
- Interpretation as MAP estimator with a Laplace prior on $\boldsymbol{\beta}^\star$
- Questions:
  - How to compute LASSO estimate?
  - What is the statistical properties of LASSO?

How to compute LASSO: proximal gradient method

A more general class of convex optimization

Consider unconstrained convex optimization problem of the form

$$\min_{\boldsymbol{x} \in \mathbb{R}^d} F(\boldsymbol{x}) := f(\boldsymbol{x}) + h(\boldsymbol{x})$$

where

- $f(\boldsymbol{x})$: a differentiable, convex function
- $h(\boldsymbol{x})$: a convex, potentially non-differentiable function (e.g., ℓ_1-norm).
- Example: LASSO can be viewed as taking

$$f(\boldsymbol{x}) = \|\boldsymbol{Y} - \boldsymbol{X}\boldsymbol{\beta}\|_2^2, \qquad h(\boldsymbol{x}) = \lambda \|\boldsymbol{\beta}\|_1.$$

Issue: gradient descent (GD) does not work (due to non-smoothness)

A Proximal View of Gradient Descent

- To motivate proximal gradient methods, we first revisit gradient descent for $\min_{\boldsymbol{x}} f(\boldsymbol{x})$, where $f(\cdot)$ is convex and smooth
- Gradient descent update: $\boldsymbol{x}_{t+1} = \boldsymbol{x}_t - \eta \nabla f(\boldsymbol{x}_t)$
- This is equivalent to

$$\boldsymbol{x}_{t+1} = \arg\min_{\boldsymbol{x}} \Big\{ \underbrace{f(\boldsymbol{x}_t) + \langle \nabla f(\boldsymbol{x}_t), \boldsymbol{x} - \boldsymbol{x}_t \rangle}_{\text{first-order approximation at } \boldsymbol{x}_t} + \underbrace{\frac{1}{2\eta} \|\boldsymbol{x} - \boldsymbol{x}_t\|_2^2}_{\text{proximal term}} \Big\}$$

- Heuristics: search for $\boldsymbol{x}_{t+1}$ that
  - aim to minimize $f(\cdot)$ (through minimizing first-order approximation)
  - remains close to $\boldsymbol{x}_t$ such that first-order approximation at $\boldsymbol{x}_t$ is valid (enforced by proximal term)
- Benefit: minimizing a quadratic function, admits simple solution (i.e., GD)

Proximal gradient method: algorithm

Consider an iterative algorithm: starting from $\boldsymbol{x}_t$, update

$$\boldsymbol{x}_{t+1} = \arg\min_{\boldsymbol{x}} \Big\{ \underbrace{f(\boldsymbol{x}_t) + \langle \nabla f(\boldsymbol{x}_t), \boldsymbol{x} - \boldsymbol{x}_t \rangle}_{\text{first-order approximation at } \boldsymbol{x}_t} + h(\boldsymbol{x}) + \underbrace{\frac{1}{2\eta} \|\boldsymbol{x} - \boldsymbol{x}_t\|_2^2}_{\text{proximal term}} \Big\}$$

- Define proximal operator

$$\mathsf{prox}_h(\boldsymbol{v}) = \arg\min_{\boldsymbol{x} \in \mathbb{R}^d} \left\{ h(\boldsymbol{x}) + \frac{1}{2} \|\boldsymbol{x} - \boldsymbol{v}\|_2^2 \right\}$$

- If this proximal operator is easy to compute, then we can express

$$\boldsymbol{x}_{t+1} = \mathsf{prox}_{\eta h}(\boldsymbol{x}_t - \eta \nabla f(\boldsymbol{x}_t))$$

- alternates between gradient updates on f and proximal minimization on h

Proximal gradient method: properties

Proximal gradient algorithm: for $t = 1, 2, \ldots$

$$\boldsymbol{x}_{t+1} = \mathsf{prox}_{\eta h}(\boldsymbol{x}_t - \eta \nabla f(\boldsymbol{x}_t))$$

- fast convergence when f is convex and L-smooth: take $\eta = 1/L$,

$$F(\boldsymbol{x}_t) - F^\star \leq \frac{L}{2t}\|\boldsymbol{x}_0 - \boldsymbol{x}^\star\|_2^2$$

- exponential convergence when f is μ-strongly convex

$$\|\boldsymbol{x}_t - \boldsymbol{x}^\star\|_2^2 \leq (1 - \mu/L)^t \|\boldsymbol{x}_0 - \boldsymbol{x}^\star\|_2^2$$

- when $h(\boldsymbol{x}) = 0$ when $\boldsymbol{x} \in \mathcal{A}$ and $h(\boldsymbol{x}) = \infty$ otherwise, this gives the projected gradient descent for $\min_{\boldsymbol{x} \in \mathcal{A}} f(\boldsymbol{x})$:

$$\boldsymbol{x}_{t+1} = \mathcal{P}_{\mathcal{A}}(\boldsymbol{x}_t - \eta \nabla f(\boldsymbol{x}_t))$$

- Recommended reading material: Lecture 5 of the course Large-Scale Optimization for Data Science

Application to LASSO

- LASSO:

$$f(\boldsymbol{\beta}) = \|\boldsymbol{Y} - \boldsymbol{X}\boldsymbol{\beta}\|_2^2 \qquad \text{and} \qquad h(\boldsymbol{\beta}) = \lambda\|\boldsymbol{\beta}\|_1$$

- The proximal operator admits closed-form expression

$$\mathsf{prox}_h(\boldsymbol{v}) = \arg\min_{\boldsymbol{\beta}\in\mathbb{R}^d} \left\{ \frac{1}{2}\|\boldsymbol{\beta} - \boldsymbol{v}\|_2^2 + \lambda\|\boldsymbol{\beta}\|_1 \right\} = \mathsf{shrink}_\lambda(\boldsymbol{v})$$

where $\mathsf{shrink}_\lambda(\cdot)$ applies entrywise shrinkage to $\boldsymbol{v}$ towards zero:

$$[\mathsf{shrink}_\lambda(\boldsymbol{v})]_j = \begin{cases} v_j - \lambda, & \text{if } v_j \geq \lambda, \\ v_j + \lambda, & \text{if } v_j \leq -\lambda, \\ 0, & \text{otherwise.} \end{cases}$$

- Proximal gradient algorithm for LASSO:

$$\boldsymbol{\beta}_{t+1} = \mathsf{shrink}_{\eta\lambda}\big(\boldsymbol{\beta}_t - 2\eta\boldsymbol{X}^\top\boldsymbol{X}\boldsymbol{\beta}_t + 2\eta\boldsymbol{X}^\top\boldsymbol{Y}\big)$$

Statistical properties of LASSO

Setup

LASSO:

$$\widehat{\boldsymbol{\beta}} = \arg\min_{\boldsymbol{\beta}\in\mathbb{R}^d} \Big\{ \frac{1}{2}\|\boldsymbol{Y} - \boldsymbol{X}\boldsymbol{\beta}\|_2^2 + \lambda\|\boldsymbol{\beta}\|_1 \Big\},$$

- Independent, sub-Gaussian noise $\|\varepsilon_i\|_{\psi_2} \le \sigma$
- Sparsity: $n \gg s \log d$
- Theory-informed tuning parameter selection:

$$\lambda \asymp \sigma\sqrt{n \log d}$$

- Question:
  - Does LASSO recover the support of $\boldsymbol{\beta}^\star$?
  - Does LASSO provide reliable estimate for $\boldsymbol{\beta}^\star$?

Optimality condition

The optimality condition for unconstrained convex optimization

$$\min_{\boldsymbol{x}\in\mathbb{R}^d} f(\boldsymbol{x})$$

- if f is smooth: $\nabla f(\widehat{\boldsymbol{x}}) = \boldsymbol{0}$
- in general (when f might not be smooth): $\boldsymbol{0} \in \partial f(\widehat{\boldsymbol{x}})$

Here $\partial f(\boldsymbol{x}) \subseteq \mathbb{R}^d$ is the **subgradient** of the confex function f at $\boldsymbol{x}$:

$$\boldsymbol{g} \in \partial f(\boldsymbol{x}) \quad \Longleftrightarrow \quad f(\boldsymbol{y}) \geq f(\boldsymbol{x}) + \boldsymbol{g}^\top(\boldsymbol{y}-\boldsymbol{x}) \quad \text{for all} \quad \boldsymbol{y}\in\mathbb{R}^d$$

Check (in homework):

- if f is smooth at $\boldsymbol{x}$: $\partial f(\boldsymbol{x}) = \{\nabla f(\boldsymbol{x})\}$
- the optimality condition for LASSO is: for each $1 \leq j \leq d$

$$\left[\boldsymbol{X}^\top(\boldsymbol{Y} - \boldsymbol{X}^\top\widehat{\boldsymbol{\beta}})\right]_j \quad \begin{cases} = \lambda\cdot\mathsf{sign}(\widehat{\beta}_j) & \text{if} \quad \widehat{\beta}_j \neq 0 \\ \in [-\lambda,\lambda] & \text{if} \quad \widehat{\beta}_j = 0 \end{cases}$$

Model selection consistency

- Let $S = \{j : \beta_j^\star \neq 0\}$ be the support set (nonzero coefficients) and S^{c} be its complement.
- **Irrepresentable condition:**

$$\|\boldsymbol{X}_{S^c}^\top \boldsymbol{X}_S (\boldsymbol{X}_S^\top \boldsymbol{X}_S)^{-1} \boldsymbol{\beta}_S^\star\|_\infty < 1,$$

  where $\boldsymbol{X}_S$ and $\boldsymbol{X}_{S^c}$ as submatrices of $\boldsymbol{X}$ with columns corresponding to S and S^{c}, and $\boldsymbol{\beta}_S^\star$ is the sub-vector of $\boldsymbol{\beta}^\star$ corresponding to S
- **Model Selection Consistency:** If the irrepresentable condition holds, under certain assumptions, the Lasso estimator satisfies:

$$\mathbb{P}(\widehat{S} = S) \to 1 \quad \text{as } n \to \infty,$$

  where $\widehat{S} = \{j : \widehat{\beta}_j \neq 0\}$.

Estimation guarantees

- **Restricted eigenvalue condition:** For any $\boldsymbol{v} \in \mathbb{R}^p$ such that $\|\boldsymbol{v}_{S^c}\|_1 \le 3\|\boldsymbol{v}_S\|_1$, the restricted eigenvalue condition is:

$$\min_{\|\boldsymbol{v}\|_2=1, \|\boldsymbol{v}_{S^c}\|_1 \le 3\|\boldsymbol{v}_S\|_1} \boldsymbol{v}^\top \Big(\frac{1}{n}\boldsymbol{X}^\top \boldsymbol{X}\Big)\boldsymbol{v} > 0.$$

  This is satisfied by e.g., i.i.d. Gaussian matrix $\boldsymbol{X}$.

- **Estimation error:** If the restricted eigenvalue condition holds, under certain assumptions, the LASSO estimator satisfies:

$$\frac{1}{n}\|\boldsymbol{X}(\widehat{\boldsymbol{\beta}} - \boldsymbol{\beta}^\star)\|_2^2 \lesssim \sigma^2 s \frac{\log d}{n},$$

  and

$$\|\widehat{\boldsymbol{\beta}} - \boldsymbol{\beta}^\star\|_1 \lesssim \sigma s \sqrt{\frac{\log d}{n}}.$$

Reference

Model selection:

- *Peng Zhao, and Bin Yu. "On model selection consistency of Lasso." The Journal of Machine Learning Research 7 (2006): 2541-2563.*
- *Martin J. Wainwright. "Sharp thresholds for High-Dimensional and noisy sparsity recovery using ℓ_1-Constrained Quadratic Programming (Lasso)." IEEE transactions on information theory 55.5 (2009): 2183-2202.*

Estimation error bounds:

- *Peter J. Bickel, Ya'acov Ritov, and Alexandre B. Tsybakov. "Simultaneous analysis of Lasso and Dantzig selector." Annals of Statistics 37.4 (2009): 1705-1732.*

Nonparametric regression

Setup: we have data $(\boldsymbol{x}_1, y_1), \ldots, (\boldsymbol{x}_n, y_n)$ satisfying

$$y_i = f^\star(\boldsymbol{x}_i) + \varepsilon_i$$

- unknown $f^\star \in \mathcal{F}$ where $\mathcal{F}$ is certain function class
- i.i.d. Gaussian noise $\varepsilon_1, \ldots, \varepsilon_n \sim \mathcal{N}(0, \sigma^2)$
- fixed design ($\boldsymbol{x}_1, \ldots, \boldsymbol{x}_n$ are fixed) or random design ($\boldsymbol{x}_1, \ldots, \boldsymbol{x}_n \overset{\text{i.i.d.}}{\sim} \rho$)

Goal: estimate $f^\star$ using the data

Error metric: for any estimator f, consider squared L_2 norm

$$\|f - f^\star\|_n^2 := \frac{1}{n}\sum_{i=1}^n \big(f(\boldsymbol{x}_i) - f^\star(\boldsymbol{x}_i)\big)^2 \qquad \text{(for fixed design)}$$

$$\|f - f^\star\|_\rho^2 := \mathbb{E}_{\boldsymbol{x}\sim\rho}\big[(f(\boldsymbol{x}) - f^\star(\boldsymbol{x}))^2\big] \qquad \text{(for random design)}$$

Nonparametric least squares

Least squares estimate:

$$\widehat{f} := \arg\min_{f \in \mathcal{F}} \sum_{i=1}^{n} \big(f(\boldsymbol{x}_i) - y_i \big)^2$$

- this estimator depends on $\mathcal{F}$
- computational: how to compute this least squares estimate?
- statistical: what is the convergence rate of $\widehat{f}$?

Our plan: focus on $\mathcal{F}$ that leads to *computationally feasible* estimate

- **isotonic regression:** $\mathcal{F} = \{$monotone function in $\mathbb{R}\}$
- **convex regression:** $\mathcal{F} = \{$convex function in $\mathbb{R}^d\}$
- **kernel ridge regression:** $\mathcal{F} =$ reproducing kernel hilbert space (RKHS)

Isotonic regression

Isotonic regression: setup

- **Setup:** $\mathcal{F}$ is the set of increasing (or decreasing) function in $\mathbb{R}$
- Suppose without loss of generality that $x_1 < x_2 < \cdots < x_n$
- **Key observation:** $f^\star(x)$ is only identifiable for $x \in \{x_1, \ldots, x_n\}$
- **Equivalent formulation:**
  - Unknown parameters: $f_1^\star \le f_2^\star \le \cdots \le f_n^\star$ (corresponds to $f^\star(x_1), \ldots, f^\star(x_n)$)
  - Observations: one sample per parameter

$$y_i = f_i^\star + \varepsilon_i \quad (i = 1, \ldots, n)$$

  - Goal: estimate $f_1^\star \le f_2^\star \le \cdots \le f_n^\star$

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$$y_i = f_i^\star + \varepsilon_i \quad (i = 1, \ldots, n)$$

  - Goal: estimate $f_1^\star \le f_2^\star \le \cdots \le f_n^\star$
- **Questions:** (1) How to estimate $f_1^\star, \ldots, f_n^\star$; (2) How to reconstruct $f^\star$?

Isotonic regression: estimation

- **Estimation:** solve the following convex optimization problem

$$(\widehat{f}_1, \ldots, \widehat{f}_n) := \mathop{\arg\min}_{f_1 \le \cdots \le f_n} \sum_{i=1}^{n} (y_i - f_i)^2$$

  to estimate $f^\star(x_1), \ldots, f^\star(x_n)$

- **Reconstruction:** the least squares solution

$$\mathop{\arg\min}_{f \nearrow} \sum_{i=1}^{n} \big(f(x_i) - y_i\big)^2$$

  is any increasing function $\widehat{f}(x)$ that interploates $(x_i, \widehat{f}_i)$ for $1 \le i \le n$:

$$\widehat{f}(x_i) = \widehat{f}_i \qquad (i = 1, \ldots, n).$$

Isotonic regression: convergence rate

Theorem 4.5

Consider the class of increasing function with bounded variation

$$\mathcal{F} = \{f : [0,1] \to [0,1] \mid f \text{ is monotonically increasing}\}.$$

Then the isotonic regression estimate $\widehat{f}$ *satisfies*

$$\frac{1}{n}\sum_{i=1}^{n}\mathbb{E}\Big[\big(\widehat{f}(x_i) - f^{\star}(x_i)\big)^2\Big] \lesssim \left(\frac{\sigma^2}{n}\right)^{2/3}$$

- **Remark:** in comparison, without using the monotonic structure, the squared error of MLE does not decrease as n grows:

$$\frac{1}{n}\sum_{i=1}^{n}\mathbb{E}\Big[\big(y_i - f^{\star}(x_i)\big)^2\Big] = \sigma^2.$$

- **Reference:** Cun-Hui Zhang. "Risk bounds in isotonic regression." The Annals of Statistics (2002)

Convex regression

Convex regression: setup

- **Setup:** $\mathcal{F}$ is the set of convex function in $\mathbb{R}^d$
- **Key observation:** $f^\star(\boldsymbol{x})$ is only identifiable for $\boldsymbol{x} \in \{\boldsymbol{x}_1, \ldots, \boldsymbol{x}_n\}$
- **Equivalent formulation:**
  - Unknown parameters:
    - $f_1^\star, \ldots, f_n^\star \in \mathbb{R}$ (correspond to $f^\star(x_1), \ldots, f^\star(x_n)$)

Convex regression: setup

- **Setup:** $\mathcal{F}$ is the set of convex function in $\mathbb{R}^d$
- **Key observation:** $f^\star(\boldsymbol{x})$ is only identifible for $\boldsymbol{x} \in \{\boldsymbol{x}_1, \ldots, \boldsymbol{x}_n\}$
- **Equivalent formulation:**
  - Unknown parameters:
    - $f_1^\star, \ldots, f_n^\star \in \mathbb{R}$ (correspond to $f^\star(x_1), \ldots, f^\star(x_n)$)
    - $\boldsymbol{g}_1^\star, \ldots, \boldsymbol{g}_n^\star \in \mathbb{R}^d$ (correspond to $\partial f^\star(x_1), \ldots, \partial f^\star(x_n)$)
  - Constraint: for each i,
$$f_j^\star \geq f_i^\star + \boldsymbol{g}_i^{\star\top}(\boldsymbol{x}_j - \boldsymbol{x}_i) \quad \text{holds for all } j \neq i$$
  - Observations: one sample per parameter
$$y_i = f_i^\star + \varepsilon_i \quad (i = 1, \ldots, n)$$
  - Goal: estimate $f_1^\star, \ldots, f_n^\star \in \mathbb{R}$

Convex regression: setup

- **Setup:** $\mathcal{F}$ is the set of convex function in $\mathbb{R}^d$
- **Key observation:** $f^\star(\boldsymbol{x})$ is only identifible for $\boldsymbol{x} \in \{\boldsymbol{x}_1, \ldots, \boldsymbol{x}_n\}$
- **Equivalent formulation:**
  - Unknown parameters:
    - $f_1^\star, \ldots, f_n^\star \in \mathbb{R}$ (correspond to $f^\star(x_1), \ldots, f^\star(x_n)$)
    - $\boldsymbol{g}_1^\star, \ldots, \boldsymbol{g}_n^\star \in \mathbb{R}^d$ (correspond to $\partial f^\star(x_1), \ldots, \partial f^\star(x_n)$)
  - Constraint: for each i,
    $$f_j^\star \geq f_i^\star + \boldsymbol{g}_i^{\star\top}(\boldsymbol{x}_j - \boldsymbol{x}_i) \quad \text{holds for all } j \neq i$$
  - Observations: one sample per parameter
    $$y_i = f_i^\star + \varepsilon_i \quad (i = 1, \ldots, n)$$
  - Goal: estimate $f_1^\star, \ldots, f_n^\star \in \mathbb{R}$
- **Questions:** (1) How to estimate $f_1^\star, \ldots, f_n^\star$; (2) How to reconstruct $f^\star$?

Convex regression: estimation

- **Estimation:** solve the following convex optimization problem

$$\begin{array}{ll} \underset{f_1,\ldots,f_n\in\mathbb{R},\boldsymbol{g}_1,\ldots,\boldsymbol{g}_n\in\mathbb{R}^d}{\text{minimize}} & \sum_{i=1}^n (y_i - f_i)^2 \\ \text{subject to} & f_j \geq f_i + \boldsymbol{g}_i^\top(\boldsymbol{x}_j - \boldsymbol{x}_i) \quad \text{for all } 1 \leq i,j \leq n \end{array}$$

- **Reconstruction:** the least squares solution

$$\arg\min_{f \text{ convex}} \sum_{i=1}^n \big(f(x_i) - y_i\big)^2$$

is any convex function $\widehat{f}(\boldsymbol{x})$ such that

$$\widehat{f}(\boldsymbol{x}_i) = \widehat{f}_i, \quad \widehat{\boldsymbol{g}}_i \in \partial \widehat{f}(\boldsymbol{x}_i) \qquad (i = 1, \ldots, n).$$

Convex regression: convergence rate

Theorem 4.6

Consider the class of convex function in $\mathbb{R}$

$$\mathcal{F} = \{f : [0,1] \to [0,1] \mid f \text{ is convex}\}.$$

Then the convex regression estimate $\widehat{f}$ *satisfies*

$$\frac{1}{n}\sum_{i=1}^{n} \mathbb{E}\left[\left(\widehat{f}(x_i) - f^\star(x_i)\right)^2\right] \lesssim \left(\frac{\sigma^2}{n}\right)^{4/5}$$

- **Remark:** for convex regression in $\mathbb{R}^d$, the error is of order $n^{-4/(d+4)}$
- **Reference:** Adityanand Guntuboyina and Bodhisattva Sen. "Global risk bounds and adaptation in univariate convex regression." Probability Theory and Related Fields (2015)

Reproducing kernel hilbert space

Hilbert Space: Definition

A **Hilbert Space** $\mathcal{H}$ is a complete inner product space over $\mathbb{R}$, with:

- Vector space: $\mathcal{H}$ is a vector space over $\mathbb{R}$
  - for any $f, g \in \mathcal{H}$, $f + g \in \mathcal{H}$ (addition)
  - for any $f \in \mathcal{H}$ and $a \in \mathbb{R}$, $af \in \mathcal{H}$ (scalar multiplication)
- Inner product: a function $\langle \cdot, \cdot \rangle : \mathcal{H} \times \mathcal{H} \to \mathbb{R}$ satisfies:
  - Linearity: $\langle af + bg, h \rangle = a\langle f, h \rangle + b\langle g, h \rangle$
  - Symmetry: $\langle f, g \rangle = \langle g, f \rangle$.
  - Positivity: $\langle f, f \rangle \geq 0$, and $\langle f, f \rangle = 0 \iff f = 0$.
- Completeness: every Cauchy sequence in $\mathcal{H}$ converges to a point in $\mathcal{H}$

Hilbert norm: the norm induced by the inner product

$$\|f\|_{\mathcal{H}} = \sqrt{\langle f, f \rangle}.$$

Hilbert Spaces: Examples

- **Finite-dimensional Euclidean space**: for any $\boldsymbol{x}, \boldsymbol{y} \in \mathbb{R}^d$:

$$\langle \boldsymbol{x}, \boldsymbol{y} \rangle = \sum_{i=1}^{n} x_i y_i.$$

- **Sequence space** $\ell_2 = \{(x_1, x_2, \ldots) : \sum_{i=1}^{\infty} x_i^2 < \infty\}$: for any $\boldsymbol{x}, \boldsymbol{y} \in \ell_2$

$$\langle \boldsymbol{x}, \boldsymbol{y} \rangle = \sum_{i=1}^{\infty} x_i y_i.$$

- **Function spaces**: for any given $\Omega \subseteq \mathbb{R}^d$ and measure ρ over Ω,

$$L^2(\Omega, \rho) := \{f : \mathbb{R}^d \to \mathbb{R} \mid \int |f(x)|^2 \mathrm{d}\rho(x) < \infty\}.$$

  For any function $f, g \in L^2(\Omega, \rho)$, their inner product is given by

$$\langle f, g \rangle = \int_{\Omega} f(\boldsymbol{x}) g(\boldsymbol{x}) \mathrm{d}\rho(x).$$

Reproducing Kernel Hilbert Spaces (RKHS)

RKHS is a space of functions from $\mathcal{X}$ to $\mathbb{R}$ (usually $\mathcal{X} = \mathbb{R}^d$)

- **Positive semi-definite kernel:** a symmetric function $\mathcal{K} : \mathcal{X} \times \mathcal{X} \to \mathbb{R}$ is a PSD kernel if, for any integer $n \geq 1$ and $x_1, \ldots, x_n \in \mathcal{X}$, the kernel matrix $\boldsymbol{K}$ defined by $K_{ij} = \mathcal{K}(x_i, x_j)$ is positive semi-definite.
- Examples of PSD kernels: when $\Omega = \mathbb{R}^d$,
  - Linear kernel: $\mathcal{K}(x, x') = \langle x, x' \rangle$.
  - Polynomial kernel: $\mathcal{K}(x, x') = (\langle x, x' \rangle + c)^d$
  - Gaussian kernel: $\mathcal{K}(x, x') = \exp(-\|x - x'\|_2^2 / 2\sigma^2)$.
- **RKHS** is a Hilbert space $\mathcal{H}$ of functions $f : \mathcal{X} \to \mathbb{R}$ satisfying:

$$f(x) = \langle f, \mathcal{K}(\cdot, x) \rangle_{\mathcal{H}} \quad \text{for any } f \in \mathcal{H} \text{ and } x \in \mathcal{X}.$$

  This is known as the **reproducing property**.

Construction of RKHS

Theorem 4.7

Given any PSD kernel $\mathcal{K} : \mathcal{X} \times \mathcal{X} \to \mathbb{R}$, there is a unique Hilbert space of functions on $\mathcal{X}$ that satisfies the reproducing property, known as the reproducing kernel Hilbert space (RKHS) associated with $\mathcal{K}$.

- **Step 1:** define the function space consists via finite linear combinations

$$\widetilde{\mathcal{H}} := \left\{ \sum_{i=1}^{n} \alpha_i \mathcal{K}(\cdot, x_i) : n \geq 1, x_1, \ldots, x_n \in \mathcal{X} \right\}$$

- **Step 2:** for $f = \sum_{i=1}^{n} \alpha_i \mathcal{K}(\cdot, x_i)$ and $g = \sum_{j=1}^{m} \alpha'_j \mathcal{K}(\cdot, x'_j)$, define

$$\langle f, g \rangle_{\widetilde{\mathcal{H}}} = \sum_{i=1}^{n} \sum_{j=1}^{m} \alpha_i \alpha'_j \mathcal{K}(x_i, x'_j)$$

- **Step 3:** take the complement of $\widetilde{\mathcal{H}}$ to obtain a Hilbert space $\mathcal{H}$

Examples

- The space of linear functions $\mathcal{H} := \{f_{\boldsymbol{\beta}} : \boldsymbol{\beta} \in \mathbb{R}^d\}$ where $f_{\boldsymbol{\beta}}(\boldsymbol{x}) = \boldsymbol{\beta}^\top \boldsymbol{x}$ equipped with inner product

$$\langle f_{\boldsymbol{\beta}}, f_{\boldsymbol{\beta}'} \rangle_{\mathcal{H}} = \langle \boldsymbol{\beta}, \boldsymbol{\beta}' \rangle$$

  is an RKHS associated with linear kernel $\mathcal{K}(\boldsymbol{x}, \boldsymbol{x}') = \langle \boldsymbol{x}, \boldsymbol{x}' \rangle$

- The **Sobolev space** consists of absolutely continuous functions over $[0,1]$

$$\mathcal{H} := \{f : [0,1] \to \mathbb{R} : f(0) = 0, f' \in L^2([0,1])\}$$

  equipped with inner product

$$\langle f, g \rangle_{\mathcal{H}} = \int_0^1 f'(z) g'(z) \mathrm{d}z$$

  is an RKHS with kernel $\mathcal{K}(x, y) = \min\{x, y\}$.

RKHS-based estimation procedure

Noiseless case: function interpolation

- **Setup:** an RKHS $\mathcal{H}$ associated with a kernel $\mathcal{K}(\cdot,\cdot)$, unknown $f^\star \in \mathcal{H}$
- **Data:** $(\boldsymbol{x}_1, y_1), \ldots, (\boldsymbol{x}_n, y_n)$ where $y_i = f^\star(\boldsymbol{x}_i)$ — *noiseless observation*
- **Issue:** there might exist multiple $f \in \mathcal{H}$ that fit these data exactly...
- **Remedy:** search for the one with minimal RKHS norm

$$\widehat{f} := \arg\min_{f\in\mathcal{H}} \|f\|_{\mathcal{H}} \quad \text{subject to} \quad f(\boldsymbol{x}_i) = y_i \quad \text{for} \quad i = 1, \ldots, n$$

- Thanks to the reproducing property, this optimization problem can be solved using the kernel matrix $\boldsymbol{K} \in \mathbb{R}^{n\times n}$ where $K_{ij} = \mathcal{K}(\boldsymbol{x}_i, \boldsymbol{x}_j)$

Theorem 4.8

Any optimal solution $\widehat{f}$ can be expressed as

$$\widehat{f} = \sum_{i=1}^{n} \widehat{\alpha}_i \mathcal{K}(\cdot, \boldsymbol{x}_i) \quad \textit{where} \quad \boldsymbol{K}\widehat{\boldsymbol{\alpha}} = \boldsymbol{y}$$

Noisy case: kernel ridge regression

- **Data:** $(\boldsymbol{x}_1, y_1), \ldots, (\boldsymbol{x}_n, y_n)$ where $y_i = f^\star(\boldsymbol{x}_i) + \varepsilon_i$ with $\varepsilon_i \sim \mathcal{N}(0, \sigma^2)$
- **Kernel ridge regression:** solve

$$\widehat{f} := \arg\min_{f \in \mathcal{H}} \sum_{i=1}^{n} (y_i - f(\boldsymbol{x}_i))^2 + \lambda \|f\|_{\mathcal{H}}^2$$

- Recall the kernel matrix $\boldsymbol{K} \in \mathbb{R}^{n \times n}$ where $K_{ij} = \mathcal{K}(\boldsymbol{x}_i, \boldsymbol{x}_j)$

Theorem 4.9

The unique solution $\widehat{f}$ to kernel ridge regression is

$$\widehat{f} = \sum_{i=1}^{n} \widehat{\alpha}_i \mathcal{K}(\cdot, \boldsymbol{x}_i) \quad \textit{where} \quad \widehat{\boldsymbol{\alpha}} = (\boldsymbol{K} + \lambda \boldsymbol{I}_n)^{-1} \boldsymbol{y}$$

Theoretical properties

Eigendecomposition of PSD kernel

- **Setup:** consider $\mathcal{K} : \mathcal{X} \times \mathcal{X} \to \mathbb{R}$ where $\mathcal{X} \subseteq \mathbb{R}^d$ is compact, let ρ be a non-negative measure over $\mathcal{X}$ (e.g., Lebesgue measure)
- Define a linear operator: for any $f : \mathcal{X} \to \mathbb{R}$,

$$\mathcal{T}_{\mathcal{K}}(f) : \boldsymbol{x} \to \int_{\mathcal{X}} \mathcal{K}(\boldsymbol{x}, \boldsymbol{z}) f(\boldsymbol{z}) \rho(\mathrm{d}\boldsymbol{z})$$

- **Mercer's theorem:** under certain regularity conditions,

$$\mathcal{K}(\boldsymbol{x}, \boldsymbol{z}) = \sum_{j=1}^{\infty} \mu_j \phi_j(\boldsymbol{x}) \phi_j(\boldsymbol{z})$$

  where

  - $\{\mu_i\}_{i=1}^{\infty}$ is a sequence of non-negative eigenvalues
  - $\{\phi_i\}_{i=1}^{\infty}$ are the associated **eigenfunctions** from $\mathcal{X}$ to $\mathbb{R}$ satisfying

$$\mathcal{T}_{\mathcal{K}}(\phi_j) = \mu_j \phi_j \quad (j = 1, 2, \ldots)$$

  - $\{\phi_i\}_{i=1}^{\infty}$ forms an orthonormal basis of $L_2(\mathcal{X}, \rho)$

Examples

- **Sobolev space:** $\mathcal{X} = [0,1]$, $\rho =$ Lebesgue,

$$\mu_j = \frac{4}{(2j-1)^2\pi^2}, \quad \phi_j(x) = \sin\frac{(2j-1)\pi t}{2} \quad (j = 1, 2, \ldots)$$

- **Gaussian kernel:** consider $\mathcal{X} = [-1,1]$, $\rho =$ Lebesgue,

$$\mu_j \asymp \exp\left(-cj\log j\right)$$

  for some universal constant $c > 0$; no explicit formula for eigenfunctions

- The decay rate of eigenvalues determines the "expressive power" of RKHS (the slower the larger), and hence the convergence rate of KRR

Compare slow decay $\underbrace{\mu_j \asymp j^{-2}}_{\text{Sololev}}$ vs. fast decay $\underbrace{\mu_j \asymp \exp(-cj\log j)}_{\text{Gaussian}}$

An explicit characterization of RKHS

The RKHS associated with kernel $\mathcal{K} : \mathcal{X} \times \mathcal{X} \to \mathbb{R}$ with eigendecomposition

$$\mathcal{K}(\boldsymbol{x}, \boldsymbol{z}) = \sum_{j=1}^{\infty} \mu_j \phi_j(\boldsymbol{x}) \phi_j(\boldsymbol{z})$$

can be expressed as

$$\mathcal{H} = \Big\{ f = \sum_{j=1}^{\infty} \beta_j \phi_j : (\beta_j)_{j=1}^{\infty} \in \ell^2, \sum_{j=1}^{\infty} \frac{\beta_j^2}{\mu_j} < \infty \Big\}.$$

For $f, g \in \mathcal{H}$, their inner product can be expressed as

$$\langle f, g \rangle_{\mathcal{H}} = \sum_{j=1}^{n} \frac{\langle f, \phi_j \rangle_{L_2(\mathcal{X},\rho)} \langle g, \phi_j \rangle_{L_2(\mathcal{X},\rho)}}{\mu_j} = \sum_{j=1}^{n} \frac{\beta_j \beta_j'}{\mu_j}.$$

where

$$f = \sum_{j=1}^{\infty} \beta_j \phi_j \quad \text{and} \quad g = \sum_{j=1}^{\infty} \beta_j' \phi_j$$

Applications to kernel ridge regression

- **Setup:** $\boldsymbol{x}_1, \ldots, \boldsymbol{x}_n \overset{\text{i.i.d.}}{\sim} \rho$, $y_i = f^\star(\boldsymbol{x}_i) + \varepsilon_i$, $\varepsilon_i \sim \mathcal{N}(0, \sigma^2)$
- Unknown $f^\star \in \mathcal{H}$, suppose access to some $R \geq \|f^\star\|_{\mathcal{H}}$
- Suppose that the eigenvalues of the kernel $\mathcal{K}$ under ρ are $\{\mu_j\}_{j=1}^\infty$
- Let $\delta_n > 0$ be some quantity satisifying

$$\sqrt{\frac{2}{n}\sum_{j=1}^{\infty} \min\{\delta_n^2, \mu_j\}} \leq \frac{R}{\sigma^2}\delta_n^2$$

Theorem 4.10

By taking $\lambda \asymp n\delta_n^2$, then the KRR solution $\widehat{f}$ satisfies

$$\mathbb{E}_{\boldsymbol{x}\sim\rho}\left[\left(\widehat{f}(\boldsymbol{x}) - f^\star(\boldsymbol{x})\right)^2\right] \lesssim R^2\delta_n^2.$$

Examples

- **Gaussian kernel:** $\mu_j \asymp \exp(-cj \log j)$, one can check that

$$\delta_n^2 \asymp \frac{\sigma^2}{nR^2}$$

  This suggests that KRR with Gaussian kernel converges at order $O(n^{-1})$

  — *the RKHS associated with Gaussian kernel is not very large*

- **Sobolev space:** $\mu_j \asymp j^{-2}$, one can check that

$$\delta_n^2 \asymp \left(\frac{\sigma^2}{nR^2}\right)^{2/3}$$

  This suggests that KRR in Sobolev space converges at order $O(n^{-2/3})$

  — *the Sobolev space is much larger*

- In practice, the eigenvalues of $n^{-1}\boldsymbol{K}$ concentrates around corresponding population-level eigenvalues $\{\mu_j\}_{j=1}^{\infty}$