

1 Kernel Machines

Consider a linear model

$$Y_i = x_i^T \beta^0 + \varepsilon_i, \quad i = 1, \dots, n, \quad x_i \in \mathbb{R}^p \text{ fixed}$$

where $\mathbb{E}\varepsilon = 0$, $\text{Var}(\varepsilon) = \sigma^2 I_n$. We have

$$\begin{aligned} \hat{\beta}^{\text{ols}} &= \underset{\beta \in \mathbb{R}^p}{\text{argmin}} \sum_{i=1}^n (Y_i - x_i^T \beta)^2 \\ &= \underset{\beta \in \mathbb{R}^p}{\text{argmin}} \|Y - X\beta\|^2 \\ &= (X^T X)^{-1} X^T Y. \end{aligned}$$

Classical theory:

- $\hat{\beta}^{\text{ols}}$ unbiased,

$$\text{Var}(\hat{\beta}^{\text{ols}}) = \sigma^2 (X^T X)^{-1} = i^{-1}(\beta^0)$$

Where i is the Fisher information.

- Cramér-Rao lower bound: if an estimator $\tilde{\beta}$ is unbiased then

$$\text{Var}(\tilde{\beta}) - i^{-1}(\beta^0) \underset{\text{positive semi-definite}}{\geq} 0.$$

- If $\varepsilon \sim \mathcal{N}(0, \sigma^2 I_n)$, then $\hat{\beta}^{\text{ols}}$ is the MLE of β^0 . Furthermore $\sqrt{n}(\hat{\beta}^{\text{ols}} - \beta^0) \sim \mathcal{N}(0, n\sigma^2(X^T X)^{-1})$. From this we can derive confidence intervals, hypothesis test, etc.

In a general model with parameter $\theta \in \mathbb{R}^p$, n independent observations, under regularity, we have asymptotic normality, i.e. $\sqrt{n}(\hat{\theta}^{\text{MLE}} - \theta^0) \xrightarrow{d} \mathcal{N}(0, I^{-1}(\theta^0))$ (with p fixed).

Question: what happens when p is large relative to n ?

- If $p > n$, $\hat{\beta}^{\text{ols}}$ is not even defined.
- If $p \approx n$, $\text{Var}(\hat{\beta}^{\text{ols}})$ explodes since $X^T X$ is near singular.
- More generally, if $p, n \rightarrow \infty$ then asymptotic normality can break down.

Recall the bias-variance decomposition:

$$\begin{aligned} \text{mse}(\tilde{\beta}) &= \mathbb{E}_{\beta^0, \sigma^2} [(\tilde{\beta} - \beta^0)(\tilde{\beta} - \beta^0)] \\ &= \mathbb{E}_{\beta^0, \sigma^2} \left\| \tilde{\beta} - \mathbb{E}\tilde{\beta} + \mathbb{E}\tilde{\beta} - \beta^0 \right\|^2 \\ &= \text{Var}(\tilde{\beta}) + \left\| \mathbb{E}(\tilde{\beta}) - \beta^0 \right\|^2. \end{aligned}$$

We introduce bias to reduce the variance.

1.1 Ridge regression

Define

$$(\hat{\mu}_\lambda^R, \hat{\beta}_\lambda^R) = \operatorname{argmin}_{(\mu, \beta) \in \mathbb{R} \times \mathbb{R}^p} \left[\|Y - \mu \mathbf{1} - X\beta\|^2 + \underbrace{\lambda \|\beta\|^2}_{\text{penalty for large } \beta} \right].$$

λ is called a *regularisation* or *tuning* parameter. We shall assume the columns of X have been standardised (mean 0, variance 1).

After standardisation, we can show that

$$\hat{\mu}_\lambda^R = \frac{1}{n} \sum_{i=1}^n Y_i = \bar{Y}.$$

Hence, if we replace Y with $Y - \mathbf{1}\bar{Y}$ we can write

$$\begin{aligned} \hat{\beta}_\lambda^R &= \operatorname{argmin}_{\beta \in \mathbb{R}^p} [\|Y - X\beta\|^2 + \lambda \|\beta\|^2] \\ &= \underbrace{(X^T X + \lambda I_p)^{-1}}_{\text{always invertible}} X^T Y. \end{aligned}$$

Theorem 1.1. For $\lambda > 0$ sufficiently small,

$$\operatorname{mse}(\hat{\beta}^{\text{ols}}) - \operatorname{mse}(\hat{\beta}_\lambda^R) = \mathbb{E}\|\hat{\beta}^{\text{ols}} - \beta^0\|^2 - \mathbb{E}\|\hat{\beta}_\lambda^R - \beta^0\|^2 > 0. \quad (*)$$

Proof. We have

$$Y = X\beta^0 + \varepsilon.$$

The bias of $\hat{\beta}_\lambda^R$ is

$$\begin{aligned} \mathbb{E}(\hat{\beta}_\lambda^R - \beta^0) &= (X^T X + \lambda I)^{-1} X^T X \beta^0 - \beta^0 \\ &= (X^T X + \lambda I)^{-1} (X^T X + \lambda I - \lambda I) \beta^0 - \beta^0 \\ &= -\lambda (X^T X + \lambda I)^{-1} \beta^0. \end{aligned}$$

While we have variance

$$\begin{aligned} \operatorname{Var}(\hat{\beta}_\lambda^R) &= \mathbb{E} \|(X^T X + \lambda I)^{-1} X^T \varepsilon\|^2 \\ &= \sigma^2 [(X^T X + \lambda I)^{-1} X^T X (X^T X + \lambda I)^{-1}]. \end{aligned}$$

Then (*) becomes

$$\begin{aligned} &\mathbb{E}\|\hat{\beta}^{\text{ols}} - \beta^0\|^2 - \mathbb{E}\|\hat{\beta}_\lambda^R - \beta^0\|^2 \\ &= \sigma^2 (X^T X)^{-1} - \sigma^2 (X^T X + \lambda I) X^T X (X^T X + \lambda I)^{-1} \\ &\quad - \lambda^2 (X^T X + \lambda I)^{-1} \beta^0 (\beta^0)^T (X^T X + \lambda I)^{-1} \\ &= \vdots \quad \quad \quad (\text{use SVD } X = UDV^T) \\ &= \lambda (X^T X + \lambda I)^{-1} [\sigma^2 \{2I_p + \lambda (X^T X)^{-1}\} - \lambda \beta^0 (\beta^0)^T] (X^T X + \lambda I)^{-1}. \end{aligned}$$

We want to show this is positive definite. This is equivalent to

$$\begin{aligned}\sigma^2 [2I + \lambda(X^T X)^{-1}] - \lambda\beta^0(\beta^0)^T &> 0 \\ \iff 2\sigma^2 I - \lambda\beta^0(\beta^0)^T &> 0 \\ \iff 2\sigma^2 \|z\|^2 - \lambda(z^T \beta^0)^2 &> 0 \quad \forall z \in \mathbb{R}^p.\end{aligned}\tag{†}$$

We also have $(z^T \beta^0)^2 \leq \|z\|^2 \|\beta^0\|^2$ by Cauchy-Schwarz. Hence (†) holds for all $\lambda < \frac{2\sigma^2}{\|\beta^0\|^2}$. \square

Singular value decomposition

Suppose $n \geq p$, so we can always write $X \in \mathbb{R}^{n \times p}$ as

$$X = UDV^T \quad (\text{“thin SVD”})$$

where $U \in \mathbb{R}^{n \times p}$, $V \in \mathbb{R}^{p \times p}$, with orthonormal columns, $D \in \mathbb{R}^{p \times p}$ diagonal with $D_{11} \geq D_{22} \geq \dots \geq D_{pp} \geq 0$.

The fitted values in ridge regression are

$$\begin{aligned} \hat{Y}_\lambda^R &= X\hat{\beta}_\lambda^R = X(X^T X + \lambda I)^{-1} X^T Y \\ &= UDV^T (VD^2 V^T + \lambda I)^{-1} V D U^T Y \quad (\text{using } VV^T = V^T V = I) \\ &= UD(D^2 + \lambda I)^{-1} D U^T Y \\ &= \sum_{j=1}^p U_j \frac{D_{jj}^2}{D_{jj}^2 + \lambda} U_j^T Y \end{aligned}$$

where U_j denotes the j th column of U . For reference, in OLS regression

$$\hat{Y}^{ols} = X\hat{\beta}^{ols} = X(X^T X)^{-1} X^T Y = \sum_{j=1}^p U_j U_j^T Y.$$

So ridge “projects” onto columns of U , but it shrinks j th component by a factor

$$\frac{D_{jj}^2}{D_{jj}^2 + \lambda}.$$

Hence it shrinks small singular values to 0 rapidly.

Note. The matrix $X(X^T X)^{-1} X^T Y$ is known as the “hat matrix” and it represents an orthogonal projection onto the column space of X .

The SVD of X is related to principal component analysis.

Definition. The k th *principal component* $U^{(k)}$ of X and *principal direction* $v^{(k)}$ of X are defined recursively by

$$v^{(k)} = \operatorname{argmax}_{v \in \mathbb{R}^p} \|Xv\|^2 \text{ subject to } \|v\| = 1, (v^{(j)})^T X^T X v = 0 \quad \forall j < k$$

and

$$u^{(k)} = Xv^{(k)}.$$

Lemma 1.2. If $D_{jj} > 0$ for all $j \in \{1, \dots, p\}$ then $v^{(k)} = V_k$, $u^{(k)} = D_{kk} U_k$.

Message: ridge is good when the signal (β^0) is large for the top principal components of X .

Computation: we can compute \hat{Y}_λ^R for any value of λ quickly after doing an SVD, which has cost $\mathcal{O}(np^2)$.

1.2 v -fold cross-validation

We assume that (x_i, Y_i) , $i = 1, \dots, n$ is iid from some distribution (random design matrix). Let (x^*, Y^*) be another independent observation from this distribution. We may wish to pick λ minimising the mean-squared prediction error (MSPE) conditional on (X, Y) :

$$\mathbb{E}\{(Y^* - (x^*)^T \hat{\beta}_\lambda^R(X, Y))^2 | (X, Y)\}.$$

A less ambitious goal is to minimise the MSPE

$$\mathbb{E}\{(Y^* - (x^*)^T \hat{\beta}_\lambda^R(X, Y))^2\} = \mathbb{E}\left[\mathbb{E}\{(Y^* - (x^*)^T \hat{\beta}_\lambda^R(X, Y))^2 | (X, Y)\}\right]. \quad (\ddagger)$$

We can try to estimate this quantity for different values of λ , using data splitting.

- Let $(X^{(1)}, Y^{(1)}), \dots, (X^{(v)}, Y^{(v)})$ be groups of data points of roughly equal size. These are called *folds*.
- Let $(X^{(-k)}, Y^{(-k)})$ denote all the folds except the k th.
- Let $\kappa(i)$ be the fold to which sample i (i.e. (X_i, Y_i)) belongs.

Our estimator of (\ddagger) is

$$\text{CV}(\lambda) = \frac{1}{n} \sum_{i=1}^n \left\{ Y_i - x_i^T \underbrace{\hat{\beta}_\lambda^R(X^{(-\kappa(i))}, Y^{(-\kappa(i))})}_{\text{using all folds except the ones containing } (x_i, Y_i)} \right\}^2.$$

Then define

$$\lambda_{\text{CV}} = \operatorname{argmin}_{\lambda \in \{\lambda_1, \dots, \lambda_m\}} \text{CV}(\lambda).$$

We use the estimator

$$\hat{\beta}_{\lambda_{\text{CV}}}^R(X, Y).$$

How to choose v ?

Note.

- The expectation of each summand in $\text{CV}(\lambda)$ is almost the same as \ddagger , which is what we want to estimate. The only difference is the size of the training set. Hence the bias of $\text{CV}(\lambda)$ is small when v is large [the extreme of this is $v = n$, called “leave one out” cross-validation].
- When v is large, the estimator $\hat{\beta}_\lambda^R(X^{(-k)}, Y^{(-k)})$ is similar for different values of k , which leads to positively correlated summands in $\text{CV}(\lambda)$, leading to high variance.
- A common choice is $v = 5$ or $v = 10$.

1.3 Kernel trick

We have

$$\hat{Y}_\lambda^R = X(X^T X + \lambda I)^{-1} X^T Y.$$

Note that

$$\begin{aligned} X^T (X X^T + \lambda I) &= (X^T X + \lambda I) X^T \\ \implies (X^T X + \lambda I)^{-1} X^T &= X^T (X X^T + \lambda I)^{-1} \\ \implies X \underbrace{(X^T X + \lambda I)^{-1}}_{p \times p} X^T Y &= X X^T \underbrace{(X X^T + \lambda I)^{-1}}_{n \times n} Y. \end{aligned}$$

The computation cost of the LHS is $\mathcal{O}(np^2 + p^3)$ while the RHS is $\mathcal{O}(pn^2 + n^3)$.

- When $p \gg n$, the 2nd expression is cheaper to compute;
- The fitted values in ridge regression only depend on X through the “Gram matrix” $K = X X^T$, with entries $K_{ij} = \langle x_i, x_j \rangle$.

Suppose we wish to fit a quadratic model:

$$Y_i = x_i^T \beta + \sum_{k,l} x_{ik} x_{il} \theta_{kl} + \varepsilon_i.$$

This can be done with a linear model where we replace the predictors $x_i \in \mathbb{R}^p$ with a new “feature” vector:

$$\phi(x_i) = (x_{i1}, x_{i2}, \dots, x_{ip}, x_{i1}x_{i1}, x_{i1}x_{i2}, \dots, x_{ip}x_{ip}) \in \mathbb{R}^{p+p^2}.$$

We call ϕ a “feature map”. Now we have $\mathcal{O}(p^2)$ predictors. If $p^2 \gg n$, to compute ridge fitted values, we want to use the 2nd expression, with cost $\mathcal{O}(p^2 n^2 + n^3)$.

However, the part that scales as $\mathcal{O}(p^2 n^2)$ is just the computation of the Gram matrix with entries $K_{ij} = \langle \phi(x_i), \phi(x_j) \rangle$.

The *kernel trick* offers a shortcut for computing K .

Idea:

$$\begin{aligned} \left(\frac{1}{2} + x_i^T x_j \right)^2 - \frac{1}{4} &= \left(\frac{1}{2} + \sum_k x_{ik} x_{jk} \right)^2 - \frac{1}{4} \\ &= \sum_k x_{ik} x_{jk} + \sum_{k,l} x_{ik} x_{il} x_{jk} x_{jl} \\ &= \langle \phi(x_i), \phi(x_j) \rangle = K_{ij}. \end{aligned}$$

The LHS can be computed in $\mathcal{O}(p)$ iterations, so we can obtain K in $\mathcal{O}(n^2 p)$ iterations, and we can compute the fitted values in ridge regression in $\mathcal{O}(n^2 p + n^3)$, which is not worse than the linear model!

Notes.

- For many feature maps ϕ , there are similar shortcuts.
- Instead of focusing on ϕ , we can directly think of the function $k(x_i, x_j) = \langle \phi(x_i), \phi(x_j) \rangle$ as a measure of “similarity” between inputs x_i, x_j .

Question: for which similarities k is there a feature map ϕ such that

$$k(x_i, x_j) = \langle \phi(x_i), \phi(x_j) \rangle?$$

1.4 Kernels

Definition. An *inner product space* is a real vector space \mathcal{H} endowed with a map $\langle \cdot, \cdot \rangle : \mathcal{H} \times \mathcal{H} \rightarrow \mathbb{R}$ satisfying:

- (i) Symmetry: for all $u, v \in \mathcal{H}$ we have $\langle u, v \rangle = \langle v, u \rangle$;
- (ii) Bilinearity: for all $a, b \in \mathbb{R}$ and all $u, v, w \in \mathcal{H}$ we have

$$\langle au + bv, w \rangle = a\langle u, w \rangle + b\langle v, w \rangle.$$

- (iii) Positive-definiteness: we have $\langle u, u \rangle \geq 0$ for all $u \in \mathcal{H}$, with equality if and only if $u = 0$.

Suppose that regression inputs x_1, \dots, x_n take values in an abstract set \mathcal{X} (so far we’ve had $\mathcal{X} = \mathbb{R}^p$, but the x_i ’s could be functions; images; graphs; etc.).

Goal: characterise similarity functions $k : \mathcal{X} \times \mathcal{X} \rightarrow \mathbb{R}$ for which there is an inner product space \mathcal{H} and a feature map $\phi : \mathcal{X} \rightarrow \mathcal{H}$ such that

$$k(x, x') = \langle \phi(x), \phi(x') \rangle \quad \forall x, x' \in \mathcal{X}.$$

Definition. A (*positive-definite*) *kernel* k is a symmetric map $k : \mathcal{X} \times \mathcal{X} \rightarrow \mathbb{R}$ such that for all $n \in \mathbb{N}$ and all $x_1, \dots, x_n \in \mathcal{X}$, the matrix K with entries $K_{ij} = k(x_i, x_j)$ is positive semi-definite.

Remark. A kernel is not an inner product on \mathcal{X} in general. Indeed, \mathcal{X} does not even need to be a vector space, and k need not be bilinear. However, we do have a version of the Cauchy-Schwarz inequality for kernels.

Proposition 1.3. *Let k be a kernel on \mathcal{X} . Then*

$$k(x, x')^2 \leq k(x, x)k(x', x') \quad \forall x, x' \in \mathcal{X}.$$

Proof. Since k is a kernel,

$$\begin{pmatrix} k(x, x) & k(x, x') \\ k(x', x) & k(x', x') \end{pmatrix} \geq 0.$$

Hence this has non-negative determinant and $k(x, x)k(x', x') - k(x, x')^2 \geq 0$. \square

Proposition 1.4. *Any similarity k defined by*

$$k(x, x') = \langle \phi(x), \phi(x') \rangle \quad \forall x, x' \in \mathcal{X}$$

is a kernel.

Proof. Symmetry of k is clear. Let $x_1, \dots, x_n \in \mathcal{X}$ be arbitrary and take any vector $\alpha \in \mathbb{R}^n$. We need to show $\alpha^T K \alpha \geq 0$. Indeed

$$\begin{aligned} \alpha^T K \alpha &= \sum_{i,j} \alpha_i K_{ij} \alpha_j \\ &= \sum_{i,j} \alpha_i \langle \phi(x_i), \phi(x_j) \rangle \alpha_j \\ &= \left\langle \sum_{i=1}^n \alpha_i \phi(x_i), \sum_{j=1}^n \alpha_j \phi(x_j) \right\rangle && \text{(linearity of } \langle \cdot, \cdot \rangle \text{)} \\ &\geq 0. && \text{(positive-definiteness of } \langle \cdot, \cdot \rangle \text{)} \end{aligned}$$

□

Examples of kernels

Proposition 1.5 (Closure property). *Suppose k_1, k_2, \dots are kernels on \mathcal{X} . Then*

- (i) *If $\alpha_1, \alpha_2 \geq 0$, then $\alpha_1 k_1 + \alpha_2 k_2$ is a kernel. If $k(x, x') := \lim_{m \rightarrow \infty} k_m(x, x')$ exists for all $x, x' \in \mathcal{X}$, then k is a kernel.*
- (ii) *The pointwise product $k(x, x') = k_1(x, x')k_2(x, x')$ is a kernel.*

Proof. Example Sheet 1. □

Some examples of kernels are:

- Linear kernel: $k(x, x') = x^T x'$ (for $\mathcal{X} = \mathbb{R}^p$);
- Polynomial kernel: $k(x, x') = (1 + x^T x')^d$, $d \in \mathbb{N}$ ($\mathcal{X} = \mathbb{R}^p$). Note $(x, x') \mapsto 1$ is a kernel so this is a kernel by the previous proposition;
- Gaussian kernel: $k(x, x') = \exp\left(-\frac{\|x - x'\|^2}{2\sigma^2}\right)$, $\sigma^2 > 0$ the *bandwidth* of the kernel. Indeed note

$$\exp\left(-\frac{\|x - x'\|^2}{2\sigma^2}\right) = \underbrace{\exp\left(-\frac{\|x\|^2}{2\sigma^2}\right)}_{:=k_1(x, x')} \underbrace{\exp\left(-\frac{\|x'\|^2}{2\sigma^2}\right)}_{:=k_2(x, x')} \exp\left(\frac{x^T x'}{\sigma^2}\right).$$

It suffices to show k_1, k_2 are kernels. For k_1 we have $k_1(x, x') = \langle \phi(x), \phi(x') \rangle$ where $\phi : \mathbb{R}^p \rightarrow \mathbb{R}$ is defined by

$$\phi(x) = \exp\left(-\frac{\|x\|^2}{2\sigma^2}\right).$$

For k_2 we have that $(x, x') \mapsto x^T x'$ is a kernel and k_2 can be Taylor expanded so is the limit of kernels;

- Sobolev kernel: let $\mathcal{X} = [0, 1]$ and set $k(x, x') = \min(x, x') = \text{Cov}(Wx, Wx')$ where $(W_t)_{t \geq 0}$ a Brownian motion (positive definite as a covariance);
- Jaccard similarity kernel: let $\mathcal{X} = \mathcal{P}(\{1, \dots, p\})$ and set

$$k(x, x') = \begin{cases} \frac{|x \cap x'|}{|x \cup x'|} & \text{if } x \cup x' \neq \emptyset \\ 0 & \text{otherwise} \end{cases}.$$

(For proof this is a kernel see Example Sheet 1.)

Remark. There is no finite-dimensional feature map $\phi : \mathbb{R}^p \rightarrow \mathbb{R}^m$ representing the Gaussian kernel.

Theorem 1.6 (Moore-Aronzajn Theorem). *For every kernel $k : \mathcal{X} \times \mathcal{X} \rightarrow \mathbb{R}$, there exists a feature map ϕ taking values in some inner product space \mathcal{H} such that $k(x, x') = \langle \phi(x), \phi(x') \rangle$ for all $x, x' \in \mathcal{X}$.*

Proof. Take \mathcal{H} to be the vector space of functions from \mathcal{X} to \mathbb{R} of the form

$$f(\cdot) = \sum_{i=1}^n \alpha_i k(\cdot, x_i) \quad n \in \mathbb{N}, \alpha_i \in \mathbb{R}, x_i \in \mathcal{X}.$$

In other words, \mathcal{H} is the linear span of functions of the form $f(\cdot, x)$ for $x \in \mathcal{X}$. Our feature map $\phi : \mathcal{X} \rightarrow \mathcal{H}$ will be $\phi(x) = k(\cdot, x)$. We now define the inner product $\langle \cdot, \cdot \rangle$ on \mathcal{H} . Let

$$f(\cdot) = \sum_{i=1}^n \alpha_i k(\cdot, x_i) \quad n \in \mathbb{N}, \alpha_i \in \mathbb{R}, x_i \in \mathcal{X}$$

and

$$g(\cdot) = \sum_{j=1}^m \beta_j k(\cdot, x'_j).$$

Then define

$$\langle f, g \rangle := \sum_{i=1}^n \sum_{j=1}^m \alpha_i \beta_j k(x_i, x'_j) = \sum_{i=1}^n \alpha_i g(x_i) = \sum_{j=1}^m \beta_j f(x'_j).$$

In particular, the final two expressions show $\langle \cdot, \cdot \rangle$ is well-defined (it doesn't matter how we represent f, g as these linear combinations).

We observe directly from the definition that $\langle \phi(x), \phi(x') \rangle = \langle k(\cdot, x), k(\cdot, x') \rangle = k(x, x')$ as required. We must show $\langle \cdot, \cdot \rangle$ is indeed an inner product. It is certainly bilinear and symmetric. So we show it is positive-definite. Note that

$$\langle f, f \rangle = \sum_{i=1}^n \sum_{j=1}^n \alpha_i k(x_i, x_j) \alpha_j \geq 0 \quad (\ddagger)$$

since k is a kernel. It remains to show $\langle f, f \rangle$ implies $f(x) = 0$ for all $x \in \mathcal{X}$.

Note that $\langle \cdot, \cdot \rangle : \mathcal{H} \times \mathcal{H} \rightarrow \mathbb{R}$ is a kernel. Indeed, given functions f_1, \dots, f_m and $\gamma_1, \dots, \gamma_n \in \mathbb{R}$ we have

$$\sum_{i=1}^n \sum_{j=1}^n \gamma_i \langle f_i, f_j \rangle \gamma_j = \left\langle \sum_{i=1}^n \gamma_i f_i, \sum_{j=1}^n \gamma_j f_j \right\rangle \geq 0$$

by (\ddagger) .

Now note that

$$f(x)^2 = \langle f, k(\cdot, x) \rangle^2 \leq \langle f, f \rangle \langle k(\cdot, x), k(\cdot, x) \rangle$$

by the Cauchy-Schwarz property for kernels. Hence $\langle f, f \rangle = 0$ implies $f(x) = 0$ for all $x \in \mathcal{X}$. \square

Remark. The space $(\mathcal{H}, \langle \cdot, \cdot \rangle)$ constructed in the proof has the property that

$$f(x) = \langle f, \underbrace{k(\cdot, x)}_{\phi(x)} \rangle.$$

As a consequence

$$|f(x) - g(x)| = |\langle f - g, k(\cdot, x) \rangle| \leq \|f - g\|_{\mathcal{H}} k(x, x)^{1/2}.$$

Hence convergence in $(\mathcal{H}, \|\cdot\|)$ implies pointwise convergence.

Lemma 1.7. Let \mathcal{H} be a Hilbert space and $\mathcal{V} \subseteq \mathcal{H}$ a closed subspace. Then $\mathcal{H} = \mathcal{V} \oplus \mathcal{V}^\perp$, i.e for any $f \in \mathcal{H}$ we have $f = u + v$ where $u \in \mathcal{V}$ and $v \in \mathcal{V}^\perp$ and u, v are unique.

Proof. See Part II Linear Analysis. \square

Definition. A Hilbert space of functions $f : \mathcal{X} \rightarrow \mathbb{R}$ is a *reproducing kernel Hilbert space* (RKHS) if for all $x \in \mathcal{X}$, there exists $k_x \in \mathcal{H}$ such that $f(x) = \langle k_x, f \rangle$ for all $f \in \mathcal{H}$.

The function $k : \mathcal{X} \times \mathcal{X} \rightarrow \mathbb{R}$ defined by $(x, x') \mapsto \langle k_x, k_{x'} \rangle = k_x(x')$ is known as the reproducing kernel of \mathcal{H} .

Remark. By the Riesz Representation Theorem, it is equivalent to define an RKHS as a Hilbert space where the evaluation operator $E_x : f \mapsto f(x)$ is a continuous linear operator.

The Moore-Aronzajn Theorem says that whenever k is a kernel, there is an inner product space \mathcal{H} of functions $f : \mathcal{X} \rightarrow \mathbb{R}$ where $f(x) = \langle f, k(\cdot, x) \rangle$ and thus $k(x, x') = \langle k(\cdot, x), k(\cdot, x') \rangle$.

This implies that if $(f_n)_{n \geq 1}$ is Cauchy in \mathcal{H} ,

$$|f_n(x) - f_m(x)| \leq \sqrt{k(x, x)} \|f_n - f_m\|_{\mathcal{H}} \rightarrow 0.$$

Hence $(f_n)_{n \geq 1}$ has a pointwise limit $f^* : \mathcal{X} \rightarrow \mathbb{R}$ by completeness of \mathbb{R} . So we can complete \mathcal{H} by including all limits of Cauchy sequences (Hausdorff completion) to obtain a Hilbert space $\overline{\mathcal{H}}$. By construction, $\overline{\mathcal{H}}$ is a RKHS with reproducing kernel k .

Proposition 1.8. If \mathcal{G} is a RKHS of functions $f : \mathcal{X} \rightarrow \mathbb{R}$ such that $\mathcal{G} \supseteq \mathcal{H}$, then $\overline{\mathcal{H}} = \mathcal{G}$.

Proof. Example Sheet 1. \square

Notation: from now on the RKHS is \mathcal{H} (i.e $\mathcal{H} = \overline{\mathcal{H}}$).

Examples.

- Linear kernel: $k(x, x') = x^T x'$. Then $\mathcal{H} = \{f : f(x) = x^T \beta, \beta \in \mathbb{R}^p\}$. If $f(x) = x^T \beta$ then $\|f\|_{\mathcal{H}}^2 = \|\beta\|^2$.
- Sobolev kernel: $k(x, x') = \min(x, x')$ with $\mathcal{X} = [0, 1]$. Then \mathcal{H} is the space of continuous functions $f : [0, 1] \rightarrow \mathbb{R}$ with $f(0) = 0$, for which

$$\int_0^1 |f'(x)|^2 dx < \infty$$

where f' is the weak derivative.

The Representer Theorem

If \mathcal{H} is the RKHS of the linear kernel, we can express ridge regression as

$$\hat{f} = \operatorname{argmin}_{f \in \mathcal{H}} \left\{ \sum_{i=1}^n \underbrace{(Y_i - f(x_i))^2}_{x_i^T \beta} + \lambda \underbrace{\|f\|_{\mathcal{H}}^2}_{\|\beta\|^2} \right\}.$$

In *kernel ridge regression*, we solve this problem in a more general RKHS with kernel k , e.g the Gaussian kernel.

Theorem 1.9 (Representer Theorem). *Let:*

- $c : \mathbb{R}^n \times \mathcal{X}^n \times \mathbb{R}^n \rightarrow \mathbb{R}$ be an arbitrary loss;
- $J : [0, \infty) \rightarrow \mathbb{R}$ be strictly increasing;
- $x_1, \dots, x_n \in \mathcal{X}$, $Y \in \mathbb{R}^n$;
- \mathcal{H} an RKHS with representing kernel k ;
- $K_{ij} = k(x_i, x_j)$, $i, j \in [n]$.

Then \hat{f} minimises

$$Q_1(f) = c(Y, x_1, \dots, x_n, f(x_1), \dots, f(x_n)) + J(\|f\|_{\mathcal{H}}^2)$$

over $f \in \mathcal{H}$ if and only if $\hat{f}(\cdot) = \sum_{i=1}^n \hat{\alpha}_i k(\cdot, x_i)$ and $\hat{\alpha}$ minimises Q_2 over $\alpha \in \mathbb{R}^n$ where

$$Q_2(\alpha) = c(Y, x_1, \dots, x_n, K\alpha) + J(\alpha^T K \alpha).$$

Example. In kernel ridge regression we just need to solve the quadratic program

$$\hat{\alpha} = \operatorname{argmin}_{\alpha \in \mathbb{R}^n} \|Y - K\alpha\|^2 + \lambda \alpha^T K \alpha = (K + I\lambda)^{-1}.$$

Then the fitted values are given by $\hat{f}(\cdot) = \sum_{i=1}^n \hat{\alpha}_i k(\cdot, x_i)$.

Intuition: to make a prediction at “test” point x^* the terms in $\hat{f}(x^*)$ that contribute the most are those for training points x_i with similarity $k(x^*, x_i)$ large.

Proof of the Representer Theorem. Note $V = \operatorname{span}\{k(\cdot, x_1), \dots, k(\cdot, x_n)\}$ is a closed (as its finite dimensional) subspace of \mathcal{H} . Hence any $f \in \mathcal{H}$ can be written as $f = u + v$ for $u \in V$ and $v \in V^\perp$.

We have $f(x_i) = \langle k(\cdot, x_i), u + v \rangle = \langle k(\cdot, x_i), u \rangle = u(x_i)$. Then

$$\|f\|_{\mathcal{H}}^2 = \|v\|_{\mathcal{H}}^2 + \|u\|_{\mathcal{H}}^2.$$

In the expression for Q_1 , the first term only depends on u , and the second term is $J(\|f\|_{\mathcal{H}}^2) \geq J(\|u\|_{\mathcal{H}}^2)$ with equality if and only if $v = 0$. Hence any minimiser

of Q_1 is contained in \mathcal{V} .

So write $f(\cdot) = \sum_{i=1}^n \alpha_i k(\cdot, x_i)$ for the minimiser. Now note

$$(f(x_1), \dots, f(x_n)) = K\alpha$$

$$\|f\|_{\mathcal{H}}^2 = \sum_{i,j=1}^n \alpha_i k(x_i, x_j) \alpha_j = \alpha^T K \alpha$$

so therefore for any $f \in \mathcal{V}$, $Q_1(f) = Q_2(\alpha)$. Hence $\hat{f}(\cdot) = \sum_{i=1}^n \hat{\alpha}_i k(\cdot, x_i)$ minimises Q_1 if and only if $\hat{\alpha}$ minimises Q_2 . \square

Now we will assume that

$$Y_i = f^0(x_i) + \varepsilon_i, \quad \mathbb{E}\varepsilon = 0, \quad \text{Var}(\varepsilon) = \sigma^2 I$$

where $\|f^0\|_{\mathcal{H}} \leq 1$.

Note. This is equivalent to $cY_i = cf^0(x_i) + c\varepsilon_i$ so $\|cf^0\|_{\mathcal{H}} = c\|f^0\|_{\mathcal{H}}$, $\text{Var}(c\varepsilon_i) = \sigma^2 c^2$. So the “signal-to-noise ratio” is

$$\frac{\text{Var}(c\varepsilon_i)}{\|cf^0\|_{\mathcal{H}}^2} = \frac{\text{Var}(\varepsilon_i)}{\|f^0\|_{\mathcal{H}}^2} \geq \sigma^2.$$

Theorem 1.10. *Let K have eigenvalues $d_1 \geq d_2 \geq \dots \geq d_n \geq 0$. Then*

$$\begin{aligned} \text{MSPE}(\hat{f}_n) &= \frac{1}{n} \mathbb{E} \left\{ \sum_{i=1}^n (f^0(x_i) - \hat{f}_n(x_i))^2 \right\} \\ &\leq \frac{\sigma^2}{n} \sum_{i=1}^n \frac{d_i^2}{(d_i + \lambda)^2} + \frac{\lambda}{4n} \\ &\leq \frac{\sigma^2}{n} \frac{1}{\lambda} \sum_{i=1}^n \min\left(\frac{d_i}{4}, \lambda\right) + \frac{\lambda}{4n}. \end{aligned}$$

Proof. From the Representer Theorem $(\hat{f}_n(x_1), \dots, \hat{f}_n(x_n))^T = K(K + \lambda I)^{-1}Y$. As $f^0 \in \mathcal{H}$ we have $(f^0(x_1), \dots, f^0(x_n))^T = K\alpha$ for some $\alpha \in \mathbb{R}^n$ (see Example Sheet). Moreover, $\|f^0\|_{\mathcal{H}}^2 \geq \alpha^T K \alpha$. Let the UDU^T be the eigen-decomposition of K , with $D_{ii} = d_i$. Define $\Theta = U^T K \alpha$. Then

$$\begin{aligned} n\text{MSPE}(\hat{f}_n) &= \mathbb{E} \left\| K(K + \lambda I)^{-1} \underbrace{(U\Theta + \varepsilon)}_Y - \underbrace{U\Theta}_{(f^0(x_1), \dots, f^0(x_n))^T} \right\|^2 \\ &= \mathbb{E} \|UDU^T(UDU^T + \lambda I)^{-1}(U\Theta + \varepsilon) - U\Theta\|^2 \\ &= \mathbb{E} \|D(D + \lambda I)^{-1}(\Theta + U^T \varepsilon) - \Theta\|^2 \quad (U^T U = I) \\ &= \underbrace{\mathbb{E} \|\{D(D + \lambda I)^{-1} - I\}\varepsilon\|^2}_{:= (1)} + \underbrace{\mathbb{E} \|D(D + \lambda I)^{-1}U^T \varepsilon\|^2}_{:= (2)}. \quad (\mathbb{E}\varepsilon = 0) \end{aligned}$$

So

$$\begin{aligned} (2) &= \mathbb{E} [\{D(D + \lambda I)^{-1}U^T \varepsilon\}^T \{D(D + \lambda I)^{-1}U^T \varepsilon\}] \\ &= \mathbb{E} [\text{tr}(\{D(D + \lambda I)^{-1}U^T \varepsilon\}^T \{D(D + \lambda I)^{-1}U^T \varepsilon\})] \\ &= \mathbb{E} [\text{tr}(D(D + \lambda I)^{-1} \varepsilon \varepsilon^T D(D + \lambda I)^{-1})] \quad (\text{circular property of tr}) \\ &= \text{tr}(D(D + \lambda I)^{-1} \sigma^2 I D(D + \lambda I)^{-1}) \\ &= \sigma^2 \sum_{i=1}^n \frac{d_i^2}{(d_i + \lambda)^2}. \end{aligned}$$

Also

$$(1) = \sum_{i=1}^n \frac{\lambda^2 \Theta_i^2}{(d_i + \lambda)^2}.$$

Since $\Theta = DU^T \alpha$, so if $d_i = 0$ then $\Theta_i = 0$. So let D^+ be a diagonal matrix with $D_{ii}^+ = \begin{cases} d_i^{-1} & \text{if } d_i \neq 0 \\ 0 & \text{otherwise} \end{cases}$.

Then,

$$\begin{aligned} \sum_{i:d_i > 0} \frac{\Theta_i^2}{d_i} &= \|\sqrt{D^+} \Theta\|^2 = \alpha^T K U D^+ U^T K \alpha \\ &= \alpha^T U D D^+ D U^T \alpha \\ &= \alpha^T U D U^T \alpha \quad (D D^+ D = D) \\ &= \alpha^T K \alpha \leq 1. \end{aligned}$$

Then

$$\begin{aligned} (1) &= \sum_{i:d_i > 0} \frac{\Theta_i^2}{d_i} \frac{d_i \lambda^2}{(d_i + \lambda)^2} \leq \max_{1 \leq i \leq n} \frac{d_i \lambda^2}{(d_i + \lambda)^2} \sum_{i:d_i > 0} \frac{\Theta_i^2}{d_i} \\ &\leq \max_{1 \leq i \leq n} \frac{d_i \lambda^2}{(d_i + \lambda)^2} \\ &\leq \frac{\lambda}{4}. \quad ((a+b)^2 \geq 4ab) \end{aligned}$$

Combining the bounds for (1) and (2) gives the first inequality. Finally, for the final inequality we note that

$$\frac{d_i^2}{(d_i + \lambda)^2} \leq \min \left\{ 1, \frac{d_i^2}{4d_i \lambda} \right\} = \frac{1}{\lambda} \min \left\{ \lambda, \frac{d_i}{4} \right\}.$$

□

Question: when is the upper bound good?

Random design

Let $(\mathcal{X}, \mathcal{B}, \mathbb{P})$ be a probability space, where \mathcal{X} is a metric space, \mathcal{B} is the Borel σ -algebra on \mathcal{X} . Assume that $x_1, \dots, x_n \sim^{\text{iid}} \mathbb{P}$.

Theorem 1.11 (Mercer's Theorem). *Under mild assumptions on k, \mathbb{P} , there is an orthonormal basis (e_i) of $\mathcal{L}^2(\mathbb{P})$, i.e*

$$\int_{\mathcal{X}} e_l(x) e_j(x) d\mathbb{P}(x) = \mathbb{1}\{l = j\}$$

and eigenvalues (μ_i) with $\sum_{i=1}^n \mu_i < \infty$ such that

$$\mu_j e_j(x') = \int_{\mathcal{X}} k(x, x') e_j(x) d\mathbb{P}(x).$$

Furthermore

$$k(x, x') = \sum_{l=1}^{\infty} \mu_l e_l(x) e_l(x')$$

and this series is absolutely convergent.

Proof. Not given. □

Let $\hat{\mu}_1, \dots, \hat{\mu}_n$ be (random) eigenvalues of K/n . As it turns out, when n is large $\hat{\mu}_i \approx \mu_i$. Let $\gamma = \lambda/n$, then a previous theorem gives

$$\text{MSPE}(\hat{f}_{\gamma n}) \leq \frac{\sigma^2}{\gamma} \frac{1}{n} \sum_{i=1}^n \min\left(\frac{\hat{\mu}_i}{4}, \gamma\right) + \frac{\gamma}{4}.$$

Then the MSPE is a random variable depending on x_1, \dots, x_n .

Lemma 1.12.

$$\mathbb{E}\left(\frac{1}{n} \sum_{i=1}^n \min\left(\frac{\hat{\mu}_i}{4}, \gamma\right)\right) \leq \frac{1}{n} \sum_{i=1}^n \min\left(\frac{\mu_i}{4}, \gamma\right).$$

Proof. Not given. □

This lemma means we can bound

$$\underbrace{\mathbb{E}[\text{MSPE}(\hat{f}_{n\gamma})]}_{\text{over } Y \text{ and } x_1, \dots, x_n} \leq \frac{\sigma^2}{\gamma} \frac{1}{n} \sum_{i=1}^n \min\left(\frac{\mu_i}{4}, \gamma\right) + \frac{\gamma}{4}. \quad (*)$$

Theorem 1.13. *Under the assumptions of Mercer's Theorem, there is a sequence $(\gamma_n)_{n \geq 1}$ such that for fixed $\sigma^2 > 0$,*

$$\frac{1}{n} \mathbb{E} \left\{ \sum_{i=1}^n (f^0(x_i) - \hat{f}_{\gamma_n}(x_i))^2 \right\} = o(n^{-1/2}) \text{ as } n \rightarrow \infty.$$

Proof. Let $\phi : [0, \infty) \rightarrow [0, \infty)$ be defined by

$$\phi(\gamma) = \sum_{j=1}^{\infty} \min \left(\frac{\mu_j}{4}, \gamma \right).$$

Note ϕ is increasing, and as $\sum_{j=1}^{\infty} \mu_j < \infty$, $\lim_{\gamma \downarrow 0} \phi(\gamma) = 0$. Define $\gamma_n = n^{-1/2} \sqrt{\phi(n^{-1/2})}$, so $\gamma_n = o(n^{-1/2})$. Thus for n large enough, $\phi(\gamma_n) \leq \phi(n^{-1/2})$ and the upper bound in (*) is

$$\sigma^2 \frac{\phi(\gamma_n)}{n\gamma_n} + \frac{\gamma_n}{4} \leq \frac{\sigma^2 \phi(n^{-1/2})}{n^{1/2} \sqrt{\phi(n^{-1/2})}} + o(n^{-1/2}) = o(n^{-1/2}).$$

□

When we know (μ_j) , in some cases we can get a better bound on the MSPE.

Example. If k is the Sobolev kernel and \mathbb{P} is the Lebesgue measure on $[0, 1]$, one can show that

$$\frac{\mu_i}{4} = \frac{1}{\pi^2 (2i-1)^2}.$$

Then for any integer j ,

$$\sum_{i=1}^{\infty} \min \left(\frac{\mu_i}{4}, \gamma_n \right) \leq \gamma_n j + \sum_{i=j+1}^{\infty} \frac{1}{\pi^2 (2i-1)^2}.$$

So if we take $j = \frac{(\pi^2 \gamma_n)^{-1/2} + 1}{2}$ we get upper bound

$$\begin{aligned} & \frac{\gamma_n}{2} \left(\frac{1}{\sqrt{\pi^2 \gamma_n}} + 1 \right) + \frac{1}{\pi^2} \int_{(\pi^2 \gamma_n)^{-1/2} + 1}^{\infty} \frac{1}{(2x-1)^2} dx \\ &= \mathcal{O}(\gamma_n^{1/2}) + \mathcal{O}(\gamma_n) = \mathcal{O}(\sqrt{\gamma_n}). \end{aligned}$$

By (*) we have

$$\mathbb{E}(\text{MSPE}(\hat{f}_{\gamma_n, n})) \leq \mathcal{O} \left(\frac{\sigma^2}{n\gamma_n} \sqrt{\gamma_n} + \gamma_n \right).$$

Picking $\gamma_n \sim \left(\frac{\sigma^2}{n} \right)^{2/3}$ gives an error of at most $\mathcal{O} \left(\left(\frac{\sigma^2}{n} \right)^{2/3} \right)$.

Support Vector Machines

Suppose we have data $(x_i, Y_i)_{i \in [n]}$ where $x_i \in \mathbb{R}^p$, $Y_i \in \{-1, 1\}$. Suppose the two response classes can be separated by a hyperplane through the origin. Let β be a unit vector which is normal to the hyperplane.

There could be many separating hyperplanes. One way of choosing a single one of these is to maximise an empty margin, i.e

$$\max_{\substack{M > 0 \\ \beta \in \mathbb{S}^{p-1}}} M \text{ subject to } Y_i x_i^T \beta \geq M \text{ for all } i \in [n].$$

Reparameterising by $\beta \rightarrow \beta/M$, this problem becomes

$$\max_{\beta \in \mathbb{R}^p} \frac{1}{\|\beta\|} \text{ subject to } Y_i x_i^T \beta \geq 1 \text{ for all } i \in [n]$$

or equivalently

$$\min_{\beta \in \mathbb{R}^p} \|\beta\|^2 \text{ subject to } Y_i x_i^T \beta \geq 1 \text{ for all } i \in [n].$$

Instead, what if just a few samples fall on the wrong side of the margin? A different estimator, known as a *support vector classifier* replaces the constraint $Y_i x_i^T \beta \geq 1$ with a penalty $[(1 - Y_i)x_i^T \beta]_+$.

Remark. This works even if there is no separating hyperplane.

So our problem is

$$\min_{\beta \in \mathbb{R}^p} \left[\lambda \|\beta\|^2 + \sum_{i=1}^n (1 - Y_i x_i^T \beta)_+ \right].$$

λ is a tuning parameter which balances “maximum margin” objective and penalty.

In general, we may want to estimate a hyperplane which does not pass through the origin; $x^T \beta + \mu = 0$. We can define a similar optimisation:

$$\min_{\substack{\beta \in \mathbb{R}^p \\ \mu \in \mathbb{R}}} \left[\lambda \|\beta\|^2 + \sum_{i=1}^n (1 - Y_i(x_i^T \beta + \mu))_+ \right].$$

If \mathcal{H} is the RKHS for the linear kernel, this problem can be written as

$$(\hat{\mu}, \hat{f}) = \operatorname{argmin}_{(\mu, f) \in \mathbb{R} \times \mathcal{H}} \left[\sum_{i=1}^n (1 - Y_i(f(x_i) + \mu))_+ + \lambda \|f\|_{\mathcal{H}}^2 \right]$$

where $\hat{f}(x) = x^T \hat{\beta}$.

A *support vector machine* is defined by this optimisation with a generic RKHS \mathcal{H} with reproducing kernel k .

Prediction: given $(\hat{\mu}, \hat{f})$ and a new input x^* we predict $\hat{Y}^* = \operatorname{sgn}(\hat{f}(x^*) + \hat{\mu})$.

Note. In \mathcal{X} the separating ‘hyperplane’ is not necessarily linear, but upon mapping (via ϕ) to \mathcal{H} (i.e $x \mapsto \phi(x) = k(\cdot, x)$) it becomes a hyperplane since the class boundary $\{x \in \mathcal{X} : f(x) + \mu = 0\}$ is mapped to $\{k(\cdot, x) : \langle k(\cdot, x), f \rangle_{\mathcal{H}} + \mu = 0\}$.

Using a slight generalisation of the Representer Theorem (see Example Sheet 1), we can show that

$$\hat{f}(\cdot) = \sum_{i=1}^n \hat{\alpha}_i k(x_i, \cdot)$$

where

$$(\hat{\alpha}, \hat{\mu}) = \operatorname{argmin}_{(\alpha, \mu) \in \mathbb{R}^n \times \mathbb{R}} \sum_{i=1}^n (1 - Y_i(K_i^T \alpha + \mu))_+ + \lambda \alpha^T K \alpha$$

where $K_{ij} = k(x_i, x_j)$.

Remark. We can have $\hat{\alpha}_i = 0$ for some i , so we do not use the corresponding x_i at all in the estimator.

Kernel Logistic Regression

We have standard logistic regression

$$\log \frac{\mathbb{P}(Y_i = 1)}{\mathbb{P}(Y_i = -1)} = x_i^T \beta.$$

Maximising the likelihood with (x_i, Y_i) , $i \in [n]$ is equivalent to solving

$$\min_{\beta \in \mathbb{R}^p} \sum_{i=1}^n \log(1 + \exp(-Y_i x_i^T \beta)).$$

As in ridge regression, we may wish to penalise $\|\beta\|^2$:

$$\min_{\beta \in \mathbb{R}^p} \left[\sum_{i=1}^n \log(1 + \exp(-Y_i x_i^T \beta)) + \lambda \|\beta\|_2^2 \right].$$

This is the same as

$$\min_{f \in \mathcal{H}} \left[\sum_{i=1}^n \log(1 + \exp(-Y_i f(x_i))) + \lambda \|f\|_{\mathcal{H}}^2 \right]$$

where \mathcal{H} is the linear RKHS.

In kernel logistic regression we build the class boundary $\hat{f}(\cdot)$ by solving this problem with an arbitrary RKHS.

Question: how does this compare with the Support Vector Machine?

In each case, the objective is

$$\sum_{i=1}^n l(Y_i f(x_i)) + \lambda \|f\|_{\mathcal{H}}^2$$

with $l(z) = (1 - z)_+$ and $l(z) = \log(1 + e^{-z})$ for the SVM and logistic regression respectively.

1.5 Large-scale Kernel Machines

Suppose for a kernel k , there is a feature map $\phi : \mathcal{X} \rightarrow \mathbb{R}^q$. Let $K_{ij} = k(x_i, x_j)$

and $\Phi = \begin{pmatrix} \phi(x_1) \\ \vdots \\ \phi(x_n) \end{pmatrix} \in \mathbb{R}^{n \times q}$ so that $K = \Phi \Phi^T$.

Consider kernel ridge regression. There are two ways of computing the fitted values:

$$K(\underbrace{K + I\lambda}_{n \times n})^{-1} Y \text{ or;}$$

$$\Phi(\underbrace{\Phi^T \Phi + \lambda I}_{q \times q})^{-1} \Phi^T Y.$$

These have costs $\mathcal{O}(n^3)$ and $\mathcal{O}(q^3 + nq^2)$ respectively. So when n is much larger than q , we want to use the latter expression.

In other kernel machines, it is helpful to have a low rank kernel matrix $K = \Phi \Phi^T$.

Example. Consider the optimisation problem resulting from the representer theorem

$$\min_{\alpha \in \mathbb{R}^n} [c(Y, x_1, \dots, x_n, K\alpha) + \lambda \alpha^T K \alpha].$$

The gradient of the penalty term is $2\lambda K\alpha$. Computing this has cost $\mathcal{O}(n^2)$ (since K is $n \times n$), but if $K = \Phi \Phi^T$ ($q < n$) we can compute $2\lambda \Phi \Phi^T \alpha$ in $\mathcal{O}(nq)$ iterations.

Problem: what if there is no feature map ϕ onto \mathbb{R}^q with $q \ll n$? For example, the Gaussian kernel.

Idea: find an approximation $\hat{\Phi}$ such that $K \approx \hat{\Phi} \hat{\Phi}^T$. Our approach will be to develop a random feature map $\hat{\Psi} : \mathcal{X} \rightarrow \mathbb{R}^b$ satisfying

$$\mathbb{E}[\hat{\Psi}(x)^T \hat{\Psi}(x')] = k(x, x') \text{ for all } x, x' \in \mathcal{X}.$$

Then, we can let $\hat{\Psi}_i, i \in [L]$ be iid copies of $\hat{\Psi}$; define the approximate feature map

$$\hat{\phi} : x \mapsto \frac{1}{\sqrt{L}} (\hat{\Psi}_1(x), \dots, \hat{\Psi}_L(x)) \in \mathbb{R}^{b \times L}.$$

Then $\hat{\phi}(x)^T \hat{\phi}(x') = \frac{1}{L} \sum_{i=1}^L \hat{\Psi}_i(x)^T \hat{\Psi}_i(x')$. In particular $\mathbb{E}[\hat{\phi}(x)^T \hat{\phi}(x)] = k(x, x')$ and $\text{Var}[\hat{\phi}(x)^T \hat{\phi}(x)] = \mathcal{O}(L^{-1})$.

Then approximate $K \approx \hat{\Phi} \hat{\Phi}^T$ where $\hat{\Phi} = \begin{pmatrix} \hat{\phi}(x_1) \\ \vdots \\ \hat{\phi}(x_n) \end{pmatrix}$. In some cases the error

$$\|K - \hat{\Phi}^T \hat{\Phi}\|$$

is small with $Lb \ll n$.

Random Fourier Feature

Theorem 1.14 (Bochner). *Let $k : \mathbb{R}^p \times \mathbb{R}^p \rightarrow \mathbb{R}$ be a continuous kernel. Then k is shift-invariant (there exists h such that $k(x, x') = h(x - x')$) if and only if there exists $c > 0$ and some distribution F in \mathbb{R}^p such that if $W \sim F$, then*

$$k(x, x') = c \mathbb{E}[e^{i(x-x')^T W}] = c \mathbb{E}[\cos((x - x')^T W)].$$

Proof. Not given. □

Example. If $k(x, x') = \exp\left(-\frac{\|x-x'\|^2}{2\sigma^2}\right)$ is the Gaussian kernel, then we have the representation in the theorem with $W \sim \mathcal{N}(0, \sigma^{-2}I)$.

We can use the theorem to construct a random feature map

$$\hat{\Psi}(x) = \sqrt{2c} \cos(W^T x + U) \in \mathbb{R}$$

where $W \sim F$, $U \sim \text{Unif}(-\pi, \pi)$ are independent.

Lemma 1.15.

$$\mathbb{E}(\hat{\Psi}(x)\hat{\Psi}(y)) = k(x, y) \text{ for all } x, y \in \mathbb{R}^p.$$

Proof. The LHS is

$$\begin{aligned} & 2c\mathbb{E}[\cos(W^T x + U) \cos(W^T y + U)] \\ &= 2c\mathbb{E}[\cos(W^T x) \cos U - \sin(W^T x) \sin U] \times [\cos(W^T y) \cos U - \sin(W^T y) \sin U] \\ &= c\mathbb{E}[\cos(W^T x) \cos(W^T y) + \sin(W^T x) \sin(W^T y)] \quad (\text{since } \mathbb{E}[\cos u \sin u] = 0) \\ &= c\mathbb{E}[\cos(W^T(x - y))] \\ &= k(x, y). \end{aligned} \quad (\text{Bochner's Theorem})$$

□

2 The Lasso & Beyond

Consider the standard linear model

$$Y = X\beta^0 + \varepsilon, \quad \mathbb{E}\varepsilon = 0, \text{Var } \varepsilon = \sigma^2 I.$$

Then

$$\begin{aligned} \text{MSPE}(\hat{\beta}^{\text{ols}}) &= \frac{1}{n} \mathbb{E} \|X\beta^0 - X\hat{\beta}^{\text{ols}}\|^2 \\ &= \frac{1}{n} \mathbb{E} [\text{tr}((\beta^0 - \hat{\beta}^{\text{ols}})(\beta^0 - \hat{\beta}^{\text{ols}})^T X^T X)] \\ &= \frac{1}{n} \text{tr} \left(\underbrace{\mathbb{E}[(\beta^0 - \hat{\beta}^{\text{ols}})(\beta^0 - \hat{\beta}^{\text{ols}})^T]}_{\text{Var}(\hat{\beta}^{\text{ols}})} X^T X \right) \\ &= \frac{1}{n} \text{tr}(\sigma^2 (X^T X)^{-1} X^T X) \\ &= \frac{1}{n} \text{tr}(\sigma^2 I_p) = \frac{\sigma^2 p}{n}. \end{aligned}$$

Let $S = \{k : \beta_k^0 \neq 0\}$ be the “relevant” predictors.

Question: what if $s := |S| \ll p$?

The model $Y = X_s \beta_s^0 + \varepsilon$, where X_s is the matrix with columns which are columns of X with index in S , and β_s^0 are the coefficients for predictors in S . So if we fit a model with design matrix X_s instead of X , we get $\text{MSPE} = \frac{\sigma^2 s}{n} \ll \frac{\sigma^2 p}{n}$.

In practice, we don’t know S , but we can try to estimate it (variable selection).

Best subset regression

Fit every model with a subset $M \subseteq \{1, \dots, p\}$ of the predictors. Then choose the best M by cross-validation.

Problem: there are 2^p possibilities, which is too large even for relatively small p .

Forward selection

This is a greedy way of approximating best subset regression.

1. Start by fitting intercept-only model;
2. Add to the model the predictor that decreases the sum-of-squares residuals the most;
3. Repeat step 2 until we have m predictors.

We treat m as a tuning parameter, chosen by cross-validation.

2.1 The Lasso

$$(\hat{\mu}_\lambda^L, \hat{\beta}_\lambda^L) \in \operatorname{argmin}_{(\mu, \beta) \in \mathbb{R} \times \mathbb{R}^p} \left[\frac{1}{2n} \|Y - \mu \mathbf{1} - X\beta\|^2 + \lambda \|\beta\|_1 \right]$$

where $\|\beta\|_1 = \sum_{k=1}^p |\beta_k|$. As we did for ridge regression, we can remove μ by standardising the columns of X and centering the response Y :

$$\hat{\beta}_\lambda^L \in \operatorname{argmin}_{\beta \in \mathbb{R}^p} \left[\frac{1}{2n} \|Y - X\beta\|^2 + \lambda \|\beta\|_1 \right].$$

Note that $\hat{\beta}_\lambda^L$ minimises

$$\|Y - X\beta\|^2 \text{ subject to } \|\beta\|_1 \leq \|\hat{\beta}_\lambda^L\|_1.$$

Similarly, $\hat{\beta}_\lambda^R$ minimises

$$\|Y - X\beta\|^2 \text{ subject to } \|\beta\| \leq \|\hat{\beta}_\lambda^R\|.$$

Fact: in general, $\hat{\beta}_\lambda^R$ has all non-zero entries, whereas $\hat{\beta}_\lambda^L$ can have many entries equal to zero.

Prediction error of the Lasso (slow rate)

Assume the columns of X are standardised, and Y is the centred response

$$Y = X\beta^0 + \varepsilon - \bar{\varepsilon}\mathbf{1}.$$

Further assume $\varepsilon \in \mathcal{N}(0, \sigma^2 I)$.

Theorem 2.1. Let $\hat{\beta}$ be any Lasso solution with $\lambda = A\sigma\sqrt{\log(p)/n}$. Then with probability $\geq 1 - 2p^{-(A^2/2-1)}$,

$$\frac{1}{n} \|X(\beta^0 - \hat{\beta})\|^2 \leq 4A\sigma\sqrt{\frac{\log p}{n}} \|\beta^0\|_1.$$

Remarks.

- Instead of bounding the MSPE (the expectation of the LHS) we bound the SPE with high-probability;
- This is called the “slow rate” with respect to n , since we know the MSPE usually decreases as $\mathcal{O}(n^{-1})$ (e.g MSPE of $\hat{\beta}^{\text{ols}}$).
- However, we trade the factor of p in the numerator with $\sqrt{\log p} \|\beta^0\|_1$, which can be much smaller than in OLS in general.
- We make no assumptions about X !

Lemma 2.2. Let $\|X^T \varepsilon\|_\infty = \max_k |(\varepsilon^T X)_k|$ and let $\Omega = \left\{ \frac{\|X^T \varepsilon\|_\infty}{n} \leq \lambda \right\}$ then

$$\mathbb{P}(\Omega) \geq 1 - 2p^{-(A^2/2-1)}.$$

Proof of slow rate. By the definition of $\hat{\beta}$

$$\frac{1}{2n} \left\| \underbrace{Y - X\hat{\beta}}_{X(\beta^0 - \hat{\beta}) + \varepsilon - \mathbf{1}\bar{\varepsilon}} \right\|^2 + \lambda \|\hat{\beta}\|_1 \leq \frac{1}{2n} \left\| \underbrace{Y - X\beta^0}_{\varepsilon - \mathbf{1}\bar{\varepsilon}} \right\|^2 + \lambda \|\beta^0\|_1.$$

Since $X^T \mathbf{1} = 0$, rearranging terms (and using the previous lemma) gives

$$\begin{aligned} \frac{1}{2n} \|X(\beta^0 - \hat{\beta})\|^2 &\leq \frac{1}{n} \varepsilon^T X(\beta^0 - \hat{\beta}) + \lambda \|\beta^0\|_1 - \lambda \|\hat{\beta}\|_1 \\ &\leq \|\varepsilon^T X\|_\infty \|\beta^0 - \hat{\beta}\|_1 + \lambda \|\beta^0\|_1 - \lambda \|\hat{\beta}\|_1 \\ &\leq \lambda \left[\|\beta^0 - \hat{\beta}\|_1 + \|\beta^0\|_1 - \|\hat{\beta}\|_1 \right]. \quad (\text{On } \Omega) \end{aligned}$$

Thus by the triangle inequality

$$\frac{1}{n} \|X(\beta^0 - \hat{\beta})\|^2 \leq 4\lambda \|\beta^0\|_1.$$

□

Concentration Inequalities

Definition. We say a random variable W is σ -sub-Gaussian for some parameter $\sigma > 0$ if

$$\mathbb{E}[e^{\alpha(W - \mathbb{E}W)}] \leq e^{\frac{\alpha^2 \sigma^2}{2}}.$$

Proposition 2.3. If W is σ -sub-Gaussian, then

$$\mathbb{P}(W - \mathbb{E}W \geq t) \leq e^{-\frac{t^2}{2\sigma^2}}.$$

Proof. Apply Markov's inequality to $\mathbb{P}(W - \mathbb{E}W \geq t) = \mathbb{P}(\exp(\alpha(W - \mathbb{E}W)) \geq \exp(\alpha t))$ and minimise over α (Chernoff bound). \square

All bounded random variables are sub-Gaussian.

Lemma 2.4. If W is a random variable taking values in $[a, b]$, then it is $(\frac{b-a}{2})$ -sub-Gaussian.

Proof. See Part III Topics in Statistical Theory. \square

Proposition 2.5. Let W_1, \dots, W_n be independent random variables where W_i is σ_i -sub-Gaussian. Let $\gamma \in \mathbb{R}^n$. Then $\gamma^T W = \sum_{i=1}^n \gamma_i W_i$ is sub-Gaussian with parameter $\sqrt{\sum_{i=1}^n \gamma_i^2 \sigma_i^2}$.

Proof. Without loss of generality, assume $\mathbb{E}W_i = 0$ for all $i \in [n]$. Then

$$\mathbb{E} \left[\exp \left(\alpha \sum_{i=1}^n \gamma_i W_i \right) \right] = \prod_{i=1}^n \mathbb{E} [\exp(\alpha \gamma_i W_i)] \leq \exp \left(\alpha^2 \sum_{i=1}^n \frac{\gamma_i^2 \sigma_i^2}{2} \right).$$

\square

Recall:

Lemma 2.6. Let $\|X^T \varepsilon\|_\infty = \max_k |(\varepsilon^T X)_k|$ and let $\Omega = \left\{ \frac{\|X^T \varepsilon\|_\infty}{n} \leq \lambda \right\}$ then

$$\mathbb{P}(\Omega) \geq 1 - 2p^{-(A^2/2-1)}.$$

We will prove a stronger result:

Lemma. Suppose $(\varepsilon_i)_{i=1}^n$ are independent mean zero random variables, and are sub-Gaussian with common parameter σ . Let $\lambda = A\sigma \sqrt{\frac{\log p}{n}}$. Then

$$\mathbb{P} \left(\frac{\|X^T \varepsilon\|}{n} \leq \lambda \right) \geq 1 - 2p^{-(A^2/2-1)}.$$

Proof. We have

$$\begin{aligned}\mathbb{P}\left(\frac{\|X^T \varepsilon\|_\infty}{n} > \lambda\right) &\leq \sum_{j=1}^p \mathbb{P}\left(\frac{|X_j^T \varepsilon|}{n} > \lambda\right) \\ &= \sum_{j=1}^p \left[\mathbb{P}\left(\frac{X_j^T}{n} > \lambda\right) + \mathbb{P}\left(-\frac{X_j^T}{n} > \lambda\right) \right].\end{aligned}$$

By the previous proposition, $\pm \frac{X_j^T \varepsilon}{n}$ is mean zero sub-Gaussian with parameter $\left(\frac{\sigma^2 \|X_j\|^2}{n}\right)^{1/2} = \frac{\sigma}{\sqrt{n}}$. Hence, the above expression is bounded above by

$$2p \exp\left(-\frac{\lambda^2}{\left(2\frac{\sigma^2}{n}\right)}\right) = 2p \exp\left(-A^2 \frac{\log p}{2}\right) = 2p^{1-A^2/2}.$$

□

Now we recall some facts from complex analysis.

Proposition 2.7. *Let $C \subseteq \mathbb{R}^d$ be convex.*

- (i) *Let $f_1, \dots, f_m : C \rightarrow \mathbb{R}$ be convex and $c_1, \dots, c_m \geq 0$. Then $c_1 f_1 + \dots + c_m f_m$ is convex.*
- (ii) *Let $A : \mathbb{R}^m \rightarrow \mathbb{R}^d$ be affine ($A(x) = Mx + b$). Let $D = A^{-1}(C) = \{x : A(x) \in C\}$ and let $f : C \rightarrow \mathbb{R}$ be convex. Then D is convex and the composition $f \circ A : D \rightarrow \mathbb{R}$, $x \mapsto f(A(x))$ is a convex function.*
- (iii) *If $f : C \rightarrow \mathbb{R}$ is twice continuously differentiable with C open, then*
 - (a) *f is convex if and only if its Hessian $H(x)$ is positive semi-definite for all $x \in C$;*
 - (b) *f is strictly convex if its Hessian $H(x)$ is positive definite for all $x \in C$.*

Lagrangian method

Consider a problem of the form

$$\text{minimise } f(x) \text{ subject to } g(x) = 0 \text{ } x \in C \subseteq \mathbb{R}^d$$

where $g : C \rightarrow \mathbb{R}^b$. Let c^* be the optimal value. The *Lagrangian* of this problem is defined as

$$L(x, \theta) = f(x) + \theta^T g(x), \quad \theta \in \mathbb{R}^b.$$

Note that for all θ ,

$$\inf_{x \in C} L(x, \theta) \leq \inf_{\substack{x \in C \\ g(x)=0}} L(x, \theta) = c^*.$$

The Lagrangian method involves finding θ^* such that the minimiser x^* of the LHS in the above has $g(x^*) = 0$, in which case this is a minimiser of the original problem.

Subgradient

Definition. Given a convex $C \subseteq \mathbb{R}^d$, convex $f : C \rightarrow \mathbb{R}$, define the *subdifferential* of f at x $\partial f(x) \subseteq \mathbb{R}^d$ defined by

$$\partial f(x) = \{v \in \mathbb{R}^d : f(y) \geq f(x) + v^T(y - x) \quad \forall y \in C\}.$$

An element $v \in \partial f(x)$ is called a *subgradient* of f at x .

Proposition 2.8. If $f : C \rightarrow \mathbb{R}$ is convex and differentiable at $x \in \text{int}(C)$, then

$$\partial f(x) = \{\nabla f(x)\}.$$

Proposition 2.9. If $f, g : C \rightarrow \mathbb{R}$ are convex with $\text{int}(C) \neq \emptyset$, then

$$\partial(\alpha f)(x) = \alpha \partial f(x) = \{\alpha v : v \in \partial f(x)\}$$

for all $\alpha \in \mathbb{R}$. Also

$$\partial(f + g)(x) = \partial f(x) + \partial g(x) = \{v + w : v \in \partial f(x), w \in \partial g(x)\}.$$

Karush-Kuhn-Tucker (KKT) conditions

Proposition 2.10. *Given $f : C \rightarrow \mathbb{R}$ convex, $x^* \in \operatorname{argmin}_{x \in C} f(x)$ if and only if $0 \in \partial f(x^*)$.*

Proof. Trivial. □

Subdifferential of $\|\cdot\|_1$

By the triangle inequality,

$$\|tx + (1-t)y\|_1 \leq t\|x\|_1 + (1-t)\|y\|_1 \quad \forall t \in (0, 1)$$

so $\|\cdot\|_1$ is convex. Let $A = \{k_1, \dots, k_m\} \subseteq \{1, \dots, d\}$. For $x \in \mathbb{R}^d$ we write x_A for the vector $(x_{k_1}, \dots, x_{k_m}) \in \mathbb{R}^m$. For $X \in \mathbb{R}^{n \times d}$ we write X_A for the matrix with columns $(X_{k_1}, \dots, X_{k_m})$. We also write x_{-j} and x_{-jk} for $x_{\{j\}^c}$ and $x_{\{j,k\}^c}$ respectively. Also X_A^T and X_A^{-1} denote $(X_A)^T$ and $(X_A)^{-1}$ respectively.

We also define the sgn function by

$$\operatorname{sgn}(x_i) = \begin{cases} -1 & \text{if } x_i < 0 \\ 0 & \text{if } x_i = 0 \\ 1 & \text{if } x_i > 0 \end{cases}$$

for $x_i \in \mathbb{R}$. For $x \in \mathbb{R}^d$ we define $\operatorname{sgn}(x) = (\operatorname{sgn}(x_1), \dots, \operatorname{sgn}(x_d))$.

Proposition 2.11. *For $x \in \mathbb{R}^d$, let $A = \{j : x_j \neq 0\}$. Then*

$$\partial\|x\|_1 = \{v \in \mathbb{R}^d : \|v\|_\infty \leq 1, \operatorname{sgn}(v_A) = \operatorname{sgn}(x_A)\}.$$

Proof. Let $g_j : \mathbb{R}^d \rightarrow \mathbb{R}$ be defined by $x \mapsto |x_j|$. Define $g = \sum_{j=1}^d g_j$ so $g(x) = \|x\|_1$ for all $x \in \mathbb{R}^d$. Then by a previous proposition, $\partial g(x) = \sum_{j=1}^d \partial g_j(x)$. When $x_j \neq 0$, g_j is differentiable at x so $\partial g_j(x) = \{\partial g_j(x)\} = \{\operatorname{sgn}(x_j)e_j\}$, where $e_j \in \mathbb{R}^d$ has all entries 0 except j th entry 1.

When $x_j = 0$,

$$\begin{aligned} v \in \partial g(x_j) &\iff g_j(y) \geq g_j(x) + v^T(y - x) \quad \forall y \in \mathbb{R}^d \\ &\iff |y_j| \geq |x_j| + v^T(y - x) \quad \forall y \in \mathbb{R}^d \\ &\iff |y_j| \geq v^T(y - x) \quad \forall y \in \mathbb{R}^d. \end{aligned}$$

We claim this holds if and only if $v_j \in [-1, 1]$ and $v_{-j} = 0$. Indeed if $v_{-j} = 0$ the above becomes $|y_j| \geq v_j y_j$ which holds as long as $v_j \in [-1, 1]$. Conversely, taking $y \in \mathbb{R}^d$ with $y_j = 0$ and $y_{-j} = x_{-j} + v_{-j}$ gives $0 = |y_j| \geq |v_{-j}|^2$, implying $v_{-j} = 0$. Taking $y \in \mathbb{R}^d$ with $y_{-j} = 0$ and $y_j = \operatorname{sgn}(v_j)$ gives $1 \geq |\operatorname{sgn}(v_j)| = |y_j| \geq v_j \operatorname{sgn}(v_j) = |v_j|$.

The proposition now follows from $\partial g(x) = \sum_{j=1}^d \partial g_j(x)$. □

Lasso solutions

We have

$$Q_\lambda(\beta) = \frac{1}{2n} \|Y - X\beta\|_2^2 + \lambda \|\beta\|_1.$$

KKT says that $0 \in \partial Q_\lambda(\hat{\beta}_\lambda^L)$ for any solution $\hat{\beta}_\lambda^L$. This is equivalent to

$$-\frac{1}{n} X^T(Y - X\hat{\beta}_\lambda^L) + \lambda \hat{v} = 0$$

for $\hat{v} \in \partial \|\hat{\beta}_\lambda^L\|_1$, i.e. $\|\hat{v}\|_\infty \leq 1$ and $\text{sgn}(\hat{v}_{\hat{S}_\lambda}) = \text{sgn}(\hat{\beta}_{\lambda, \hat{S}_\lambda}^L)$, where $\hat{S}_\lambda = \{k : \hat{\beta}_{\lambda, k}^L \neq 0\}$.

It turns out the Lasso fitted values are unique!

Proposition 2.12. Fix $\lambda > 0$, suppose $\beta^{(1)}, \beta^{(2)}$ are two lasso solutions. Then $X\beta^{(1)} = X\beta^{(2)}$.

Proof. We have $Q_\lambda(\beta^{(1)}) = Q_\lambda(\beta^{(2)}) = c^*$, the optimal value of Q_λ . By strict convexity of $\|\cdot\|_2^2$,

$$\left\| Y - \frac{X\beta^{(1)}}{2} - \frac{X\beta^{(2)}}{2} \right\|_2^2 \leq \frac{\|Y - X\beta^{(1)}\|_2^2}{2} + \frac{\|Y - X\beta^{(2)}\|_2^2}{2}$$

with equality if and only if $X\beta^{(1)} = X\beta^{(2)}$. We'll show this is an equality. We construct a chain of inequalities

$$\begin{aligned} c^* &\leq Q_\lambda\left(\frac{\beta^{(1)} + \beta^{(2)}}{2}\right) \\ &= \frac{1}{2n} \left\| Y - \frac{X\beta^{(1)}}{2} - \frac{X\beta^{(2)}}{2} \right\|_2^2 + \lambda \left\| \frac{\beta^{(1)}}{2} + \frac{\beta^{(2)}}{2} \right\|_1 \\ &\leq \frac{1}{4n} \|Y - X\beta^{(1)}\|_2^2 + \frac{1}{4n} \|Y - X\beta^{(2)}\|_2^2 + \lambda \left\| \frac{\beta^{(1)} + \beta^{(2)}}{2} \right\|_1 \quad (*) \\ &\leq \frac{1}{4n} \|Y - X\beta^{(1)}\|_2^2 + \frac{1}{4n} \|Y - X\beta^{(2)}\|_2^2 + \lambda \left\| \frac{\beta^{(1)}}{2} \right\|_1 + \left\| \frac{\beta^{(2)}}{2} \right\|_1 \\ &= \frac{Q_\lambda(\beta^{(1)}) + Q_\lambda(\beta^{(2)})}{2} = c^*. \end{aligned}$$

Hence all of these inequalities are in fact equalities. The equality at $(*)$ implies $X\beta^{(1)} = X\beta^{(2)}$. \square

Define the *equicorrelation set*

$$\hat{E}_\lambda = \{k : \frac{1}{n} |X_k^T(Y - X\hat{\beta}_\lambda^L)| = \lambda\}$$

which is well defined, since $X\hat{\beta}_\lambda^L$ does not depend on the choice of $\hat{\beta}_\lambda^L$. The KKT conditions tell us that \hat{E}_λ contains all non-zero entries in $\hat{\beta}_\lambda^L$, i.e. \hat{S}_λ .

Proposition 2.13. *If $\text{rank}(X_{\hat{E}_\lambda}) = |\hat{E}_\lambda|$, then $\hat{\beta}_\lambda^L$ is unique.*

Proof. Say $\beta^{(1)}, \beta^{(2)}$ are lasso solutions. We know $\beta_{-\hat{E}_\lambda}^{(1)} = \beta_{-\hat{E}_\lambda}^{(2)} = 0$ so

$$X(\beta^{(1)} - \beta^{(2)}) = X_{\hat{E}_\lambda}(\beta_{\hat{E}_\lambda}^{(1)} - \beta_{\hat{E}_\lambda}^{(2)}) = 0$$

by uniqueness of the fitted values. If $X_{\hat{E}_\lambda}$ has full column rank, the only solution is $\beta_{\hat{E}_\lambda}^{(1)} - \beta_{\hat{E}_\lambda}^{(2)} = 0$. \square

Variable selection

How good is the lasso at recovering the non-zero entries of β^0 ? When do we have $\text{sgn}(\hat{\beta}_\lambda^L) = \text{sgn}(\beta^0)$?

In the lectures we'll deal with the noiseless case $Y = X\beta^0$ (see Example Sheet for more general case).

Define $S = \{k : \beta_k^0 \neq 0\}$ and $N = S^c$. Assume without loss of generality that $S = \{1, \dots, s\}$. Assume $\text{rank}(X_S) = 1$. Define $\Delta = X_N^T X_S (X_S^T X_S)^{-1} \text{sgn}(\beta^0)$ so $\Delta_k = ((X_S^T X_S)^{-1} X_S^T X_k) \text{sgn}(\beta^0)$, for $k > s$. Note that $(X_S^T X_S)^{-1} X_S^T X_k$ represents the coefficients in regression of non-significant variables X_k onto significant variables X_S .

The irrepresentable condition says $\|\Delta\|_\infty \leq 1$.