5. Kernel methods

5.1. Positive semi-definite kernels

Representation of the data

- **What we have seen so far:** linear classification / linear regression
- works well if the data is linearly separable
- **Problem:** that is not always the case!
- what if we could transport the data to another space where it is well-behaved?
- for instance a very high-dimensional space
- first we define a (positive-definite) *kernel*
- **many** definitions in maths, introduced in machine learning by Aizerman, Braverman, and Rozonoer in the 60s[7]

[7] Aizerman, Braverman, Rozonoer, *Theoretical foundations of the potential function method in pattern recognition learning*, Automation and Remote Control, 1964

Positive semi-definite kernels

Definition: a function $k : \mathcal{X} \times \mathcal{X} \to \mathbb{R}$ is called a *positive semi-definite kernel* if $k(x, x') = k(x', x)$ for any $x, x' \in \mathcal{X}$, and

$$\forall x_1, \ldots, x_n \in \mathcal{X}, \forall c_1, \ldots, c_n \in \mathbb{R}, \quad \sum_{i=1}^{n} \sum_{j=1}^{n} c_i c_j k(x_i, x_j) \geq 0\,.$$

- in other words, the Gram matrix $K = (k(x_i, x_j))_{i,j=1}^{n}$ is positive definite for any input data $x_1, \ldots, x_n$
- *kernel methods* take this K as input
- **Remark:** this is *costly*, $\mathcal{O}\left(n^2\right)$ whatever we do, with possible dependency in the dimensionality of the data
- Beware: unlike the name suggests, k has no reason to be *positive*

Fundamental example

- suppose that $\mathcal{X} = \mathbb{R}$
- then $k(x, y) := xy$ is a positive definite kernel
- **Why?** first, we check that $k(x, y) = k(y, x)$
- second, let $n \geq 1$, $x_1, \ldots, x_n \in \mathbb{R}^d$, and $c_1, \ldots, c_n \in \mathbb{R}$, then

$$\begin{aligned}\sum_{i=1}^{n} \sum_{j=1}^{n} c_i c_j k(x_i, x_j) &= \sum_{i=1}^{n} \sum_{j=1}^{n} c_i c_j x_i x_j \\ &= \left(\sum_{i=1}^{n} c_i x_i \right)^2 \\ &\geq 0 \,.\end{aligned}$$

Fundamental example, ctd.

- we can extend this example: set $k(x, y) := x^\top y$ on $\mathcal{X} = \mathbb{R}^d$
- let $n \geq 1$, $x_1, \ldots, x_n \in \mathbb{R}^d$, and $c_1, \ldots, c_n \in \mathbb{R}$, then

$$\begin{aligned}\sum_{i=1}^{n}\sum_{j=1}^{n} c_i c_j k(x_i, x_j) &= \sum_{i=1}^{n}\sum_{j=1}^{n} c_i c_j x_i^\top x_j \\ &= \left\| \sum_{i=1}^{n} c_i x_i \right\|^2 \\ &\geq 0\,.\end{aligned}$$

- $k(x, y) := x^\top y$ is usually called the **linear kernel**
- **Intuition:** kernels are a generalization of inner product

Other examples

- **Polynomial kernel:**
$$\mathcal{X} = \mathbb{R}^d, \qquad k(x, y) = (x^\top y + c)^k \,.$$
- **min kernel:**
$$\mathcal{X} = \mathbb{R}, \qquad k(x, y) = \min(x, y) \,.$$
- **Gaussian kernel:**
$$\mathcal{X} = \mathbb{R}^d, \qquad k(x, y) = \exp\left(\frac{-\|x - y\|^2}{2\nu^2}\right) \,.$$
- **Exponential kernel:**
$$\mathcal{X} = \mathbb{R}^d, \qquad k(x, y) = \exp\left(\frac{-\|x - y\|}{2\nu}\right) \,.$$
- ...

Choosing the bandwidth

- Gaussian and Laplace kernel: one has to choose the bandwidth parameter ν
- indeed, if ν is *too large* with respect to the typical value of $\|x_i - x_j\|$, then $K \approx I_n$
- in the other direction, if ν is *too small*, then $K \approx \mathbf{1}\mathbf{1}^\top$
- both cases are degenerate: whatever we do with K is not going to work very well
- one possible solution: **median heuristic**[8]

$$\nu = \mathrm{Med}\{\|x_i - x_j\|\,, \quad 1 \leq i, j \leq n\}\,.$$

- preferable to the mean (too sensitive to extreme values)
- we can pick other quantiles

[8] Garreau, Jitkrittum, Kanagawa, *Large sample analysis of the median heuristic*, 2017

Hilbert spaces

Definition: A *Hilbert space* is a real or complex vector space which is also a complete metric space with respect to the distance function induced by the inner product.

- **Remark:** recall the linear kernel, all we used were properties of inner product
- let $\Phi : \mathcal{X} \to \mathcal{H}$ be some mapping, $\mathcal{H}$ a Hilbert space with scalar product $\langle \cdot, \cdot \rangle$
- then $k(x, y) = \langle \Phi(x), \Phi(y) \rangle$ is positive definite:

$$\sum_{i=1}^{n} \sum_{j=1}^{n} c_i c_j \langle \Phi(x), \Phi(y) \rangle = \left\| \sum_{i=1}^{n} c_i \Phi(x_i) \right\|^2 \geq 0 \, ,$$

by linearity of the inner product.

Kernel as inner products

- **Remarkable fact:** the converse statement is true!

Theorem:[9] For any kernel k on $\mathcal{X}$, there exists a Hilbert space $(\mathcal{H}, \langle \cdot, \cdot \rangle)$ and a mapping $\Phi : \mathcal{X} \to \mathcal{H}$ such that

$$\forall x, y \in \mathcal{X}, \qquad k(x, y) = \langle \Phi(x), \Phi(y) \rangle \, .$$

- **Reminder:** Hilbert space = inner product + *complete* for the associated norm (Cauchy sequences converge in $\mathcal{H}$)
- **Consequence:** we can think of any kernel as a dot product in the *feature space*
- **Main idea:** forget about Φ and work only with kernel evaluations (more on that later)

[9] Aronszajn, *Theory of reproducing kernels*, Transactions of the American Mathematical Society, 1950

Proof in the finite case

- assume that $\mathcal{X} = \{x_1, \ldots, x_N\}$ is finite of size N
- any kernel k is entirely defined by the $N \times N$ positive semi-definite matrix $K := (k(x_i, x_j))_{i,j=1}^N$
- we can diagonalize K in an orthonormal basis $(u_1, \ldots, u_N)$ with associated (non-negative) eigenvalues $\lambda_1, \ldots, \lambda_N$: $K = U \Lambda U^\top$, with $U_{:,i} = u_i$, $\Lambda = \mathrm{diag}(\lambda)$, $UU^\top = U^\top U = \mathrm{I}$
- then we write

$$
\begin{aligned}
k(x_i, x_j) &= \left(\sum_{\ell=1}^N \lambda_\ell u_\ell u_\ell^\top \right)_{i,j} \\
&= \sum_{\ell=1}^N \lambda_\ell (u_\ell)_i (u_\ell)_j = \langle \Phi(x_i), \Phi(x_j) \rangle ,
\end{aligned}
$$

with

$$
\Phi(x_i) := \left(\sqrt{\lambda_1} (u_1)_i, \cdots, \sqrt{\lambda_n} (u_N)_i \right)^\top .
$$

$\square$

5.2. Reproducing kernel Hilbert spaces

Function spaces

- among all spaces in the previous statement, one of them has interesting properties
- in particular, it is a **space of functions**
- *i.e.*, we can map each point $x \in \mathcal{X}$ to a *function* $\Phi(x) = k_x \in \mathcal{H}$
- **Example:** $\mathcal{X} = \mathbb{R}$, we map each x to the function $t \mapsto xt$
- $\rightarrow$ space of linear functions
- more complicated in general...

Reproducing Kernel Hilbert Space (RKHS)

Definition: let $\mathcal{X}$ be a set and $\mathcal{H}$ be a function space forming a Hilbert space with inner product $\langle \cdot, \cdot \rangle$. The function $k : \mathcal{X} \times \mathcal{X} \to \mathbb{R}$ is called a *reproducing kernel* of $\mathcal{H}$ if

- $\mathcal{H}$ contains all functions of the form $k_x : t \mapsto k(x, t)$
- for every $x \in \mathcal{X}$ and $f \in \mathcal{H}$, the *reproducing property* holds:

$$f(x) = \langle f, k_x \rangle \, .$$

- if a reproducing kernel exists, then $\mathcal{H}$ is called a *reproducing kernel Hilbert space* (RKHS)

Equivalent definition

Theorem: the Hilbert space $\mathcal{H} \subseteq \mathbb{R}^{\mathcal{X}}$ is a RKHS if, and only if, for any $x \in \mathcal{X}$, the mapping $f \mapsto f(x)$ is continuous.

- *Proof of* $\Rightarrow$*:* let k be a reproducing kernel, $x \in \mathcal{X}$ and $f_n \to f$ in $\mathcal{H}$
- we write

$$\begin{aligned} |f_n(x) - f(x)| &= |\langle f_n - f, k_x \rangle| \\ &\leq \|f_n - f\| \cdot \|k_x\| \end{aligned}$$

  by Cauchy-Schwarz inequality.
- $\|f_n - f\| \to 0$ and we can conclude
- **Remark:** $\|k_x\|^2 = \langle k_x, k_x \rangle = k(x, x)$, thus $|f(x)| \leq \|f\| \cdot k(x, x)^{1/2}$

Continuity ctd.

- *Proof of* $\Leftarrow$*:* let $x \in \mathcal{X}$
- by the reproducing property, $L : x \mapsto f(x)$ is a *linear functional*
- Riesz theorem: there exists ℓ_x such that $L(x) = \langle f, \ell_x \rangle$
- define $k(x, y) := \ell_y(x)$
- one can check readily the RKHS properties. $\square$

Uniqueness

Theorem: if $\mathcal{H}$ is a RKHS, then it has a unique reproducing kernel. Conversely, a function $k : \mathcal{X} \times \mathcal{X} \to \mathbb{R}$ can be the reproducing kernel of at most one RKHS.

- we talk about *the* RKHS associated to k
- *Proof:* let k and k' be two reproducing kernels
- then for all $x \in \mathcal{X}$,

$$\begin{aligned}\|k_x - k'_x\|^2 &= \langle k_x - k'_x, k_x - k'_x \rangle \\ &= k_x(x) - k'_x(x) - k_x(x) + k'_x(x) \\ &= 0\end{aligned}$$

□

Equivalence psd / RKHS

Theorem: a function $k : \mathcal{X} \times \mathcal{X} \to \mathbb{R}$ is positive definite if, and only if, it is a reproducing kernel.

- **Idea:** build $\mathcal{H}$ as the completion of

$$\mathcal{H}_0 := \left\{ \sum_{i=1}^{n} \alpha_i k(\cdot, x_i), n \in \mathbb{N}, \alpha_i \in \mathbb{R}, x_i \in \mathcal{X} \right\}$$

- **Remark:** showing that a kernel is positive definite is enough to get Φ and $\mathcal{H}$ with the reproducing property "for free"

Example

- **Example:** polynomial kernel of degree 2:

$$k(x, y) = (x^\top y)^2 \,.$$

- **Claim:**

$$k(x, y) = \langle xx^\top, yy^\top \rangle_F \,,$$

  thus k is positive definite
- **Question:** what is the RKHS?
- we know that $\mathcal{H}$ contains all the functions

$$f(x) = \sum_i a_i k(x_i, x) = \sum_i a_i \langle x_i x_i^\top, xx^\top \rangle = \langle \sum_i a_i x_i x_i^\top, xx^\top \rangle$$

Example, ctd.

- spectral theorem: any symmetric matrix can be decomposed as $\sum_i a_i x_i x_i^\top$
- candidate RKHS: set a quadratic functions

$$f_S(x) = \langle S, xx^\top \rangle = x^\top S x\,,$$

  with S symmetric matrix of size $d \times d$
- inner product on $\mathcal{H}$:

$$\langle f_S, f_{S'} \rangle = \langle S, S' \rangle_F\,.$$

- we can check that $\mathcal{H}$ is a Hilbert space (isomorphic to $\mathcal{S}^{d \times d}$)
- finally, we check the reproducing property

5.3. More examples

Elementary properties

Proposition: Let $k_i : \mathcal{X} \times \mathcal{X} \to \mathbb{R}$ be a (potentially infinite) family of p.d. kernels. Then

- for any $\lambda_1, \ldots, \lambda_p \geq 0$, the sum $\sum_{i=1}^{p} \lambda_i k_i$ is positive definite
- for any $a_1, \ldots, a_p \in \mathbb{N}$, the product $k_1^{a_1} \cdots k_p^{a_p}$ is positive definite
- if it exists, the limit $k = \lim_{p \to +\infty} k_p$ is positive definite

Moreover, let $\mathcal{X}_i$ be a sequence of sets and k_i positive kernels on each $\mathcal{X}_i$. Then

$$k((x_1, \ldots, x_p), (y_1, \ldots, y_p)) := \prod_{i=1}^{p} k_i(x_i, y_i)$$

and

$$k((x_1, \ldots, x_p), (y_1, \ldots, y_p)) := \sum_{i=1}^{p} k_i(x_i, y_i)$$

are positive definite kernels.

Taking the exponential

Theorem: if k is a positive definite kernel, then e^k as well.

- *Proof:* we write

$$\mathrm{e}^{k(x,y)} = \lim_{n \to +\infty} \sum_{p=0}^{n} \frac{k(x,y)^p}{p!} ,$$

  then reason step by step.
- by the product property, $k(x,y)^p$ is a kernel for any $p \geq 0$
- as a positive linear combination of kernels, $\sum_{p=0}^{n} \frac{k(x,y)^p}{p!}$ is a kernel for all $n \geq 1$
- finally, e^k is a kernel as a limit of kernels. □

5.4. The kernel trick and applications

The kernel trick

- input data $x_1, \ldots, x_n \in \mathcal{X}$
- $k : \mathcal{X} \times \mathcal{X}$ kernel with associated RKHS $\mathcal{H}$
- we call $\Phi : \mathcal{X} \to \mathcal{H}$ the feature map
- **Idea:** imagine that our algorithm only depends on scalar products $x_i^\top x_j$
- then we can map the x_i to $\mathcal{H}$ and replace the inner products by kernel evaluations, since

$$\langle \Phi(x_i), \Phi(x_j) \rangle = k(x_i, x_j) \,.$$

- simple “trick” with many, many applications

Example

- **Example:** computing distances
- suppose that our algo relies on distance computation
- that is, $\|x - y\|^2$
- we can write

$$\begin{aligned}\|\Phi(x) - \Phi(y)\|^2 &= \langle \Phi(x) - \Phi(y), \Phi(x) - \Phi(y) \rangle \\ &= \langle \Phi(x), \Phi(x) \rangle - 2\langle \Phi(x), \Phi(y) \rangle + \langle \Phi(y), \Phi(y) \rangle \\ \|\Phi(x) - \Phi(y)\|^2 &= k(x,x) - 2k(x,y) + k(y,y)\,.\end{aligned}$$

- in other words,

$$d_{\mathcal{H}}(x,y) = \sqrt{k(x,x) - 2k(x,y) + k(y,y)}\,.$$

- as promised, **we do not need to know Φ!**

5.5. The representer theorem

Motivation

- let us imagine that we take $\mathcal{H}$ as hypothesis class
- starting from regularized ERM, our optimization problem will look like

$$\operatorname*{arg\,min}_{f\in\mathcal{H}} \left\{ \frac{1}{n}\sum_{i=1}^{n} \ell(y_i, f(x_i)) + \lambda \left\| f \right\|^2 \right\} . \qquad (\star)$$

- we penalize by the norm because it is an indicator of the *smoothness* of f
- **Why?** Cauchy-Schwarz + exercise:

$$|f(x) - f(y)| = |\langle f, k_x - k_y \rangle| \leq \|f\| \cdot \|k_x - k_y\| = \|f\| \cdot d_{\mathcal{H}}(x, y) .$$

- Eq. $(\star)$ is a complicate problem, potentially *infinite-dimensional*
- **Question:** how to solve it in practice?

The representer theorem

Theorem: let $\mathcal{H}$ be the RKHS associated to k defined on $\mathcal{X}$. Let $S = \{x_1, \ldots, x_n\} \subseteq \mathcal{X}$ be a finite set of points. Let $\Psi : \mathbb{R}^{n+1} \to \mathbb{R}$ be a function, increasing in the last variable. Then any solution to the minimization problem

$$\arg\min_{f \in \mathcal{H}} \Psi(f(x_1), \ldots, f(x_n), \|f\|)$$

admits a representation of the form

$$\forall x \in \mathcal{X}, \qquad f(x) = \sum_{i=1}^{n} \alpha_i k(x_i, x)\,.$$

- **Main consequence:** Eq. $(\star)$ is actually a finite-dimensional problem (!)

Practical use

- recall that we defined $K := (k(x_i, x_j))_{i,j=1}^n$
- before turning to concrete examples, we notice that we can simply express the key quantities
- for instance, for any $1 \leq j \leq n$,

$$f(x_j) = \sum_{i=1}^n \alpha_i k(x_i, x_j) = (K\alpha)_j \,.$$

- in the same way,

$$\left\|f\right\|^2 = \left\|\sum_{i=1}^n \alpha_i k(x_i, \cdot)\right\|^2 = \sum_{i=1}^n \sum_{j=1}^n \alpha_i \alpha_j k(x_i, x_j) = \alpha^\top K \alpha \,.$$

5.6. Kernel ridge regression

Kernel Ridge Regression[10] (KRR)

- regression setting: $(x_i, y_i) \in \mathcal{X} \times \mathcal{Y}$
- $\mathcal{Y} \subseteq \mathbb{R}$, but $\mathcal{X}$ could be anything
- we have a kernel k on $\mathcal{X}$
- same idea than with ridge regression:

$$\hat{f} \in \operatorname*{arg\,min}_{f \in \mathcal{H}} \left\{ \frac{1}{n} \sum_{i=1}^{n} (y_i - f(x_i))^2 + \lambda \left\| f \right\|^2 \right\} .$$

- here effect of the regularization is to make $\hat{f}$ smoother

[10] Cristianini and Shawe-Taylor, *An introduction to support vector machines and other kernel-based learning methods*, Cambridge University Press, 2000

Solving KRR

- representer theorem $\Rightarrow$

$$\hat{f}(x) = \sum_{i=1}^{n} \alpha_i k(x_i, x)\,,$$

  for some $\alpha \in \mathbb{R}^n$
- as per the previous remark, we know that

$$(\hat{f}(x_1), \ldots, \hat{f}(x_n))^\top = K\alpha\,,$$

  and

$$\|\hat{f}\|^2 = \alpha^\top K\alpha\,.$$

- thus KRR can be re-written as

$$\hat{\alpha} \in \operatorname*{arg\,min}_{\alpha \in \mathbb{R}^n} \left\{ \frac{1}{n}(K\alpha - y)^\top (K\alpha - y) + \lambda \alpha^\top K\alpha \right\}\,.$$

Solving KRR, ctd.

- convex, smooth objective $\Rightarrow$ set the gradient to zero
- $\hat{\alpha}$ has to be solution of

$$0 = \frac{-2}{n} K(y - K\alpha) + 2\lambda K\alpha = \frac{2}{n} K\left[(K + n\lambda I_n)\alpha - y\right]$$

- since $\lambda > 0$, $K + n\lambda I_n$ is invertible
- a solution is given by

$$\hat{\alpha} = (K + n\lambda I_n)^{-1} y\,.$$

- **Remark:** if $k =$ linear kernel, $K = XX^\top$
- solution we found solving "regular" ridge regression is

$$\hat{\beta} = (X^\top X + n\lambda\, \mathrm{I}_d)^{-1} X^\top y\,.$$

Solving KRR, ctd.

- actually leads to the same solution
- can compare the predictions:
- on one side,

$$K\hat{\alpha} = K(K + n\lambda \, \mathrm{I}_n)^{-1} = XX^\top (XX^\top + n\lambda \, \mathrm{I}_n)^{-1} y \, .$$

- on the other side,

$$X\hat{\beta} = X(X^\top X + n\lambda \, \mathrm{I}_d)^{-1} X^\top y$$

- *Proof:* Woodbury identity:

$$(\mathrm{I} + AA^\top)^{-1} = \mathrm{I} - A(\mathrm{I} + A^\top A)^{-1} A^\top \, .$$

- (Woodbury actually has a more general statement)

Uniqueness

- **Reminder:**
$$\hat{\alpha} = (K + n\lambda \mathrm{I}_n)^{-1} y \, .$$
- **Remark:** not the only solution if K is singular
- **Why?** $K + \lambda n \mathrm{I}$ and $(K + \lambda n \mathrm{I})^{-1}$ both leave $\ker K$ stable, can add ε such that $K\varepsilon = 0$
- but correspond to same element in the RKHS!
- **Why:** compute (squared) norm of the difference:
$$\left\| \sum_i \alpha_i k(\cdot, x_i) - \sum_i (\alpha_i + \varepsilon_i) k(\cdot, x_i) \right\|^2 = (\alpha - \varepsilon)^\top K (\alpha - \varepsilon) = 0 \, .$$

5.7. Kernel logistic regression

Kernel Logistic Regression[11] (KLR)

- classification setting: $(x_i, y_i) \in \mathcal{X} \times \mathcal{Y}$
- $\mathcal{Y} = \{0, 1\}$, but $\mathcal{X}$ could be anything
- we have a kernel k on $\mathcal{X}$
- kernelized version of logistic regression:

$$\hat{f} \in \operatorname*{arg\,min}_{f \in \mathcal{H}} \left\{ \frac{1}{n} \sum_{i=1}^{n} \log\left(1 + \mathrm{e}^{-y_i f(x_i)}\right) + \lambda \left\| f \right\|^2 \right\} .$$

- same regularization effect

[11] Green, Yandell, *Semi-parametric generalized linear models*, Generalized linear models, 1985

Solving KLR

- no explicit solution, but convex and smooth
- again, we can use the representer theorem:

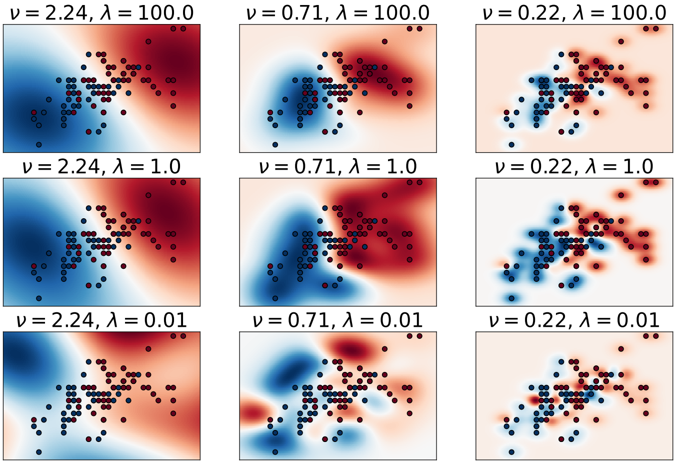
$$\hat{f}(x) = \sum_{i=1}^{n} \alpha_i k(x_i, x)$$

  for some $\alpha \in \mathbb{R}^n$
- again, $(\hat{f}(x_1), \ldots, \hat{f}(x_n))^\top = K\alpha$ and $\|\hat{f}\|^2 = \alpha^\top K \alpha$
- we can rewrite KLR as

$$\hat{\alpha} \in \operatorname*{arg\,min}_{\alpha \in \mathbb{R}^n} \frac{1}{n} \left\{ \sum_{i=1}^{n} \log\left(1 + \mathrm{e}^{-y_i (K\alpha)_i}\right) + \lambda \alpha^\top K \alpha \right\} .$$

- this can be solved (approximately) by gradient descent

Illustration



5.8. Generalization guarantees

Setting

- we consider a minimizer $\hat{f}_D$ of the following problem:

$$\underset{f\in\mathcal{H}}{\text{Minimize}} \frac{1}{n}\sum_{i=1}^{n} \ell(y_i, f(x_i)) \quad \text{such that} \quad \|f\|_{\mathcal{H}} \leq D\,,$$

  with ℓ a L-Lipschitz loss
- **Reminder:** we denote by

$$\mathcal{R}(f) = \mathbb{E}\left[\ell(Y, f(X))\right]$$

  the expected *risk* of f and $f^\star$ one of its minimizers
- in this section, we assume that $\mathcal{X} = \mathbb{R}^d$
- not necessarily the case for kernels, just to make everything simpler
- data has density p over $\mathbb{R}^d$

Consequence of Lipschitzness

- ℓ being Lipschitz allows us to control the excess risk:

Proposition: In our setting,

$$\mathcal{R}(f) - \mathcal{R}^\star \leq L \left\| f - f^\star \right\|_{L^2(p)} .$$

If, furthermore, p is upper bounded (say by C), then

$$\mathcal{R}(f) - \mathcal{R}^\star \leq C^{1/2} L \left\| f - f^\star \right\|_{L^2} .$$

- **Consequence:** controlling the excess risk amounts to controlling the distance in $\mathcal{H}$ between a predictor and $f^\star$

Risk decomposition

- we now make an additional assumption on k: there exists $R < +\infty$ such that

$$\sup_{x \in \mathcal{X}} k(x,x) \leq R^2 \, .$$

- **Remark:** this is reminiscent of the $\left\|\varphi(x)\right\|^2 \leq R^2$ assumption from the linear model chapter
- as announced, the proof technique transfers for kernels and we have

Proposition: Under our assumptions,

$$\mathbb{E}\left[\mathcal{R}(\hat{f}_D)\right] - \mathcal{R}^\star \leq \frac{4LDR}{\sqrt{n}} + L \inf_{\|f\|_{\mathcal{H}} \leq D} \left\|f - f^\star\right\|_{L^2(p)} \, .$$

- *Proof:* first term from Rademacher pipeline, second term previous slide. □

Finding the optimal D

- **From previous slide:**

$$\mathbb{E}\left[\mathcal{R}(\hat{f}_D)\right] - \mathcal{R}^\star \leq \frac{4LDR}{\sqrt{n}} + L \inf_{\|f\|_{\mathcal{H}} \leq D} \|f - f^\star\|_{L^2(p)} .$$

- we can balance the two terms of the upper bound as a function of D:

$$\inf_{D \geq 0} \left\{ \frac{4LDR}{\sqrt{n}} + L \inf_{\|f\|_{\mathcal{H}} \leq D} \|f - f^\star\|_{L^2(p)} \right\} = \inf_{D \geq 0} \left\{ \frac{4LDR}{\sqrt{n}} + L \inf_{\|f\|_{\mathcal{H}} = D} \|f - f^\star\|_{L^2(p)} \right\}$$

(otherwise can choose smaller D)

$$= \frac{4LD^+R}{\sqrt{n}} + L \inf_{\|f\|_{\mathcal{H}} = D^+} \|f - f^\star\|_{L^2(p)}$$

(inf attained at D^+)

$$= \frac{4LR\,\|f^+\|_{\mathcal{H}}}{\sqrt{n}} + L \left\|f^+ - f^\star\right\|_{L^2(p)}$$

(inf attained at f^+)

Finding the optimal D, ctd.

- thus

$$\inf_{D\geq 0}\left\{\frac{4LDR}{\sqrt{n}} + L \inf_{\|f\|_{\mathcal{H}}\leq D} \|f - f^\star\|_{L^2(p)}\right\} = \inf_{f\in\mathcal{H}}\left\{\frac{4LR\,\|f\|_{\mathcal{H}}}{\sqrt{n}} + L\,\|f - f^\star\|_{L^2(p)}\right\}$$

- using $|a| + |b| \leq \sqrt{2(a^2+b^2)}$, we see that the excess risk is bounded by

$$L\sqrt{2\inf_{f\in\mathcal{H}}\left\{\|f - f^\star\|^2_{L^2(p)} + \frac{16R^2}{n}\,\|f\|^2_{\mathcal{H}}\right\}}$$

- define

$$A(\mu, f^\star) = \inf_{f\in\mathcal{H}}\left\{\|f - f^\star\|^2_{L^2(p)} + \mu\,\|f\|^2_{\mathcal{H}}\right\}.$$

- the behavior of $A(\mu, f^\star)$ dictates the convergence of excess risk to zero

Different scenarios

- **Recall:**

$$A(\mu, f^\star) = \inf_{f \in \mathcal{H}} \left\{ \|f - f^\star\|_{L^2(p)}^2 + \mu \|f\|_{\mathcal{H}}^2 \right\} .$$

- different situations are possible:
  - $f^\star \in \mathcal{H}$ **(well-specified problem)**: $A(\mu, f^\star) \leq \mu \|f\|_{\mathcal{H}}^2$, taking $\mu = 16R^2/n$ gives $\mathcal{O}\left(1/\sqrt{n}\right)$ convergence rate
  - $f^\star \notin \mathcal{H}$ **(misspecified problem)**, but can be approached arbitrarily closely in $L^2(p)$-norm by a function in $\mathcal{H}$, then goes to zero but no explicit rate
  - otherwise, incompressible error coming from the choice of the kernel (and thus the associated function space)