Statistical Learning II

Lecture 12 - Kernel methods

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Feature maps

Idea: Introduce a feature map:

$$\boldsymbol{\varphi} : \mathbb{R}^d \to \mathbb{R}^p$$
$$\boldsymbol{x} \mapsto \boldsymbol{\varphi}(\boldsymbol{x})$$

And consider a linear predictor in feature space:

$$f_\theta(\boldsymbol{x}) = \langle \boldsymbol{\theta}, \boldsymbol{\varphi}(\boldsymbol{x}) \rangle$$

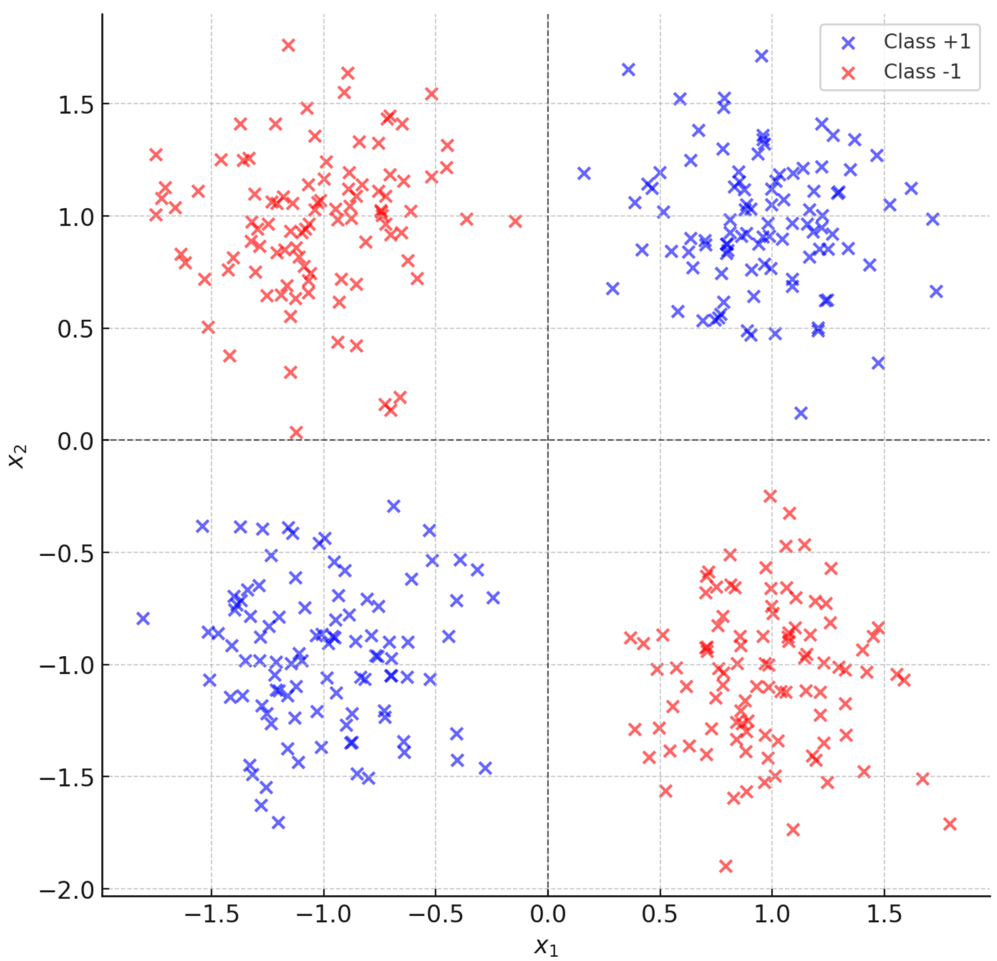
- Now we have $\boldsymbol{\theta} \in \mathbb{R}^p$.
- f_θ still a linear function of $\boldsymbol{\theta}$.
- Typically $p > d$.
- More generally, we can consider $\boldsymbol{\varphi} : \mathscr{X} \to \mathbb{R}^p$

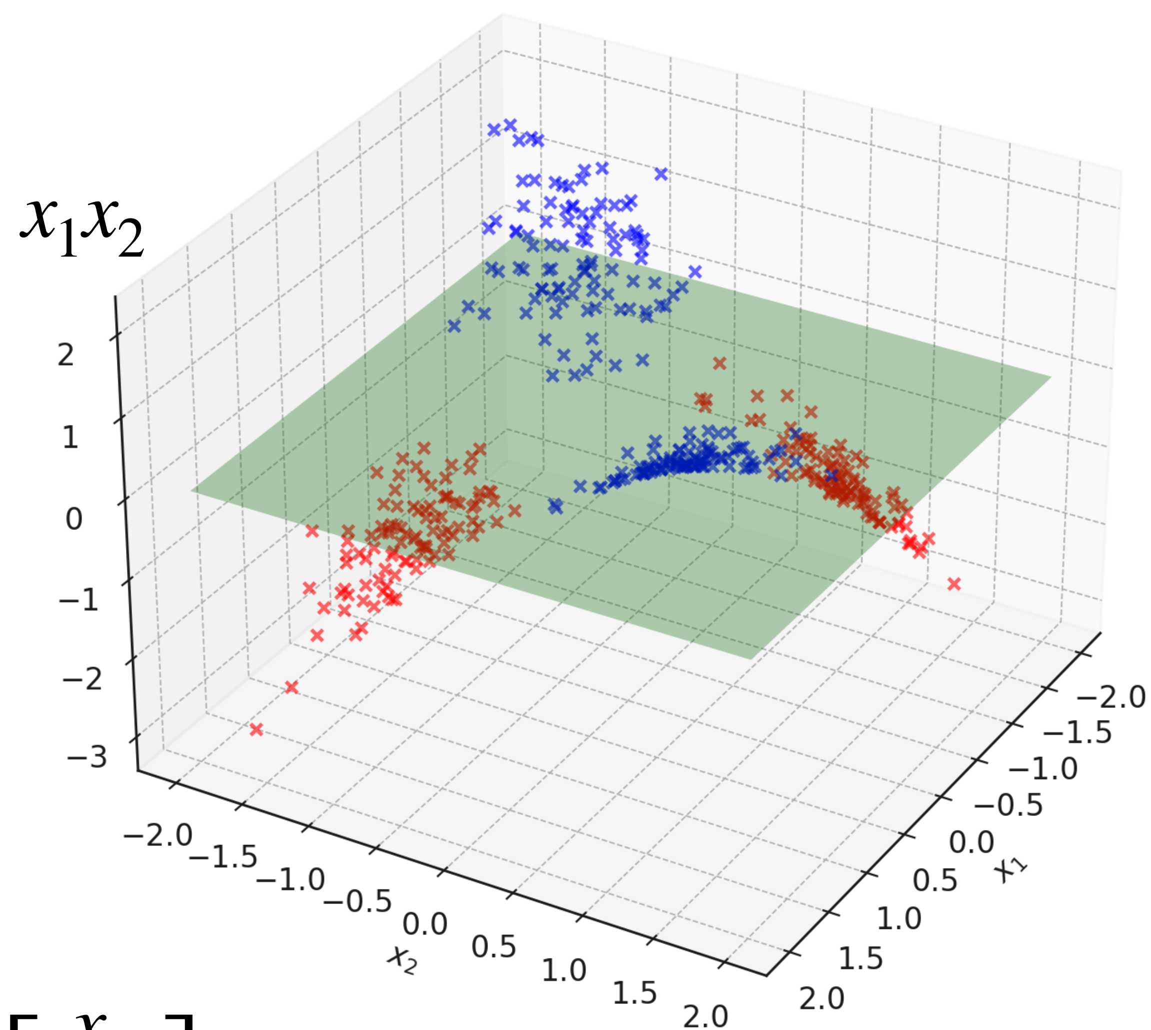
Example: $\mathscr{X}$ a collection of books.

Examples: XOR Gaussian mixture

$x \in \mathbb{R}^2 \quad (d = 2)$

$$p(\boldsymbol{x}) = \frac{1}{4} \sum_{k=1}^{4} \mathcal{N}(\boldsymbol{\mu}_k, \boldsymbol{I}_2)$$





$$\boldsymbol{\varphi}(\boldsymbol{x}) = \begin{bmatrix} x_1 \\ x_2 \\ x_1 x_2 \end{bmatrix}$$

Ridge regression on feature space

Let $\mathscr{D} = \{(x_i, y_i) \in \mathscr{X} \times \mathbb{R} : i \in [n]\}$ denote training data and $\varphi : \mathscr{X} \to \mathbb{R}^p$ a feature map.

$$\min_{\boldsymbol{\theta} \in \mathbb{R}^p} \frac{1}{2n} \sum_{i=1}^{n} (y_i - \langle \boldsymbol{\theta}, \boldsymbol{\varphi}(x_i) \rangle)^2 + \frac{\lambda}{2} ||\boldsymbol{\theta}||_2^2$$

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Defining the feature matrix and label vector:

$$\boldsymbol{\Phi} = \begin{bmatrix} \boldsymbol{\varphi}(x_1) \\ \vdots \\ \boldsymbol{\varphi}(x_n) \end{bmatrix} \in \mathbb{R}^{n \times p} \qquad \boldsymbol{y} = \begin{bmatrix} y_1 \\ \vdots \\ y_n \end{bmatrix} \in \mathbb{R}^n$$

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The above admits an explicit solution:

$$\hat{\boldsymbol{\theta}}_\lambda(\boldsymbol{\Phi}, \boldsymbol{y}) = (\boldsymbol{\Phi}^\top \boldsymbol{\Phi} + n\lambda \boldsymbol{I}_p)^{-1} \boldsymbol{\Phi}^\top \boldsymbol{y}$$

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Note we can equivalently write:

$$\hat{\boldsymbol{\theta}}_\lambda(\boldsymbol{\Phi}, \boldsymbol{y}) = \begin{cases} (\boldsymbol{\Phi}^\top \boldsymbol{\Phi} + n\lambda \boldsymbol{I}_p)^{-1} \boldsymbol{\Phi}^\top \boldsymbol{y} \\ \boldsymbol{\Phi}^\top (\boldsymbol{\Phi} \boldsymbol{\Phi}^\top + n\lambda \boldsymbol{I}_n)^{-1} \boldsymbol{y} \end{cases}$$

Same result, but one might be cheaper than the other.

Kernels

Note that the solution:

$$\hat{\boldsymbol{\theta}}_\lambda(\boldsymbol{\Phi}, \boldsymbol{y}) = \boldsymbol{\Phi}^\top(\boldsymbol{\Phi}\boldsymbol{\Phi}^\top + n\lambda \boldsymbol{I}_n)^{-1}\boldsymbol{y}$$

Actually lives in the $\mathrm{span}(\boldsymbol{\varphi}(x_1), \ldots, \boldsymbol{\varphi}(x_n))$.

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And the predictor:

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This is also known as a *kernel*.

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This is true for any linear predictor, and goes under the name of "representer theorem"

Kernel methods

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A Hilbert space $\mathscr{H}$ is a vector space (over $\mathbb{R}$ or $\mathbb{C}$) with an inner product $\langle \cdot , \cdot \rangle_{\mathscr{H}} : \mathscr{H} \times \mathscr{H} \to \mathbb{R}$ which is complete.

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Informally, an inner product is the minimum we need to do linear algebra in infinite dimensions

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  - $||f||^2_{\mathscr{H}} = \langle f, f \rangle_{\mathscr{H}} \geq 0$ with equality iff $f = 0$
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Inner product induces norm, but converse not always true.

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- Complete: Cauchy sequences $f_n \in \mathscr{H}$ converge $f_\infty \in \mathscr{H}$

Examples of Hilbert spaces

- $\mathscr{H} = \mathbb{R}^d$ with the usual Euclidean inner product:

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- $L^2(\mathbb{R})$: functions $f : \mathbb{R} \to \mathbb{R}$ with $$\langle f, g \rangle_{L^2(\mathbb{R})} = \int_{-\infty}^{\infty} f(x) g(x) \mathrm{dx}$$

Such that: $$||f||_{L^2(\mathbb{R})}^2 = \langle f, f \rangle_{L^2(\mathbb{R})} = \int_{-\infty}^{\infty} |f(x)|^2 \mathrm{dx} < \infty$$

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Let $\mathscr{H}$ denote a Hilbert space with inner product $\langle \cdot\,, \cdot \rangle_{\mathscr{H}}$.

<u>Idea</u>: Given data $x \in \mathscr{X}$, define features:

$$\begin{aligned} \varphi : \mathscr{X} &\to \mathscr{H} \\ x &\mapsto \varphi(x) \end{aligned}$$

and predictors: $\quad f_\theta(x) = \langle \theta, \varphi(x) \rangle_{\mathscr{H}} \quad$ with $\theta \in \mathscr{H}$.

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Problems:

- In general $f \notin \mathscr{H}$.
- Class of functions $f : \mathscr{X} \to \mathbb{R}$ defined this way can be small.

Example

Let $\mathscr{H} \subset \mathbb{R}^2$ with standard Euclidean inner product.

Let $\mathscr{X} = \{x_1, x_2, x_3\}$ be a discrete data space. Define $\varphi : \mathscr{X} \to \mathscr{H}$

$$\varphi(x_1) = \begin{bmatrix} 1 \\ 0 \end{bmatrix} \qquad \varphi(x_2) = \begin{bmatrix} 0 \\ 1 \end{bmatrix} \qquad \varphi(x_3) = \begin{bmatrix} 1 \\ 1 \end{bmatrix}$$

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For any $\theta = \begin{bmatrix} \theta_1 \\ \theta_2 \end{bmatrix} \in \mathscr{H}$, define the function: $\quad f(x) = \langle \theta, \varphi(x) \rangle$

We have: $\quad f(x_1) = \theta_1 \quad f(x_2) = \theta_2 \quad f(x_3) = \theta_1 + \theta_2$

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Only few functions on $\mathscr{X}$ can be expressed this way.

e.g. can't express $\quad f(x_1) = 1 \quad f(x_2) = 0 \quad f(x_3) = 2$

Reproducing property

To make the Hilbert space compatible with $\mathscr{X}$, we need the following reproducing property:

Definition (RKHS)

A Hilbert space $\mathscr{H}$ of functions over $\mathscr{X}$ is said to be a "Reproducing Kernel Hilbert Space" (RKHS) if there exists $\varphi \in \mathscr{H}$ such that:

$$\forall x \in \mathscr{X} \quad \forall f \in \mathscr{H} \qquad f(x) = \langle f, \varphi(x) \rangle_{\mathscr{H}}$$

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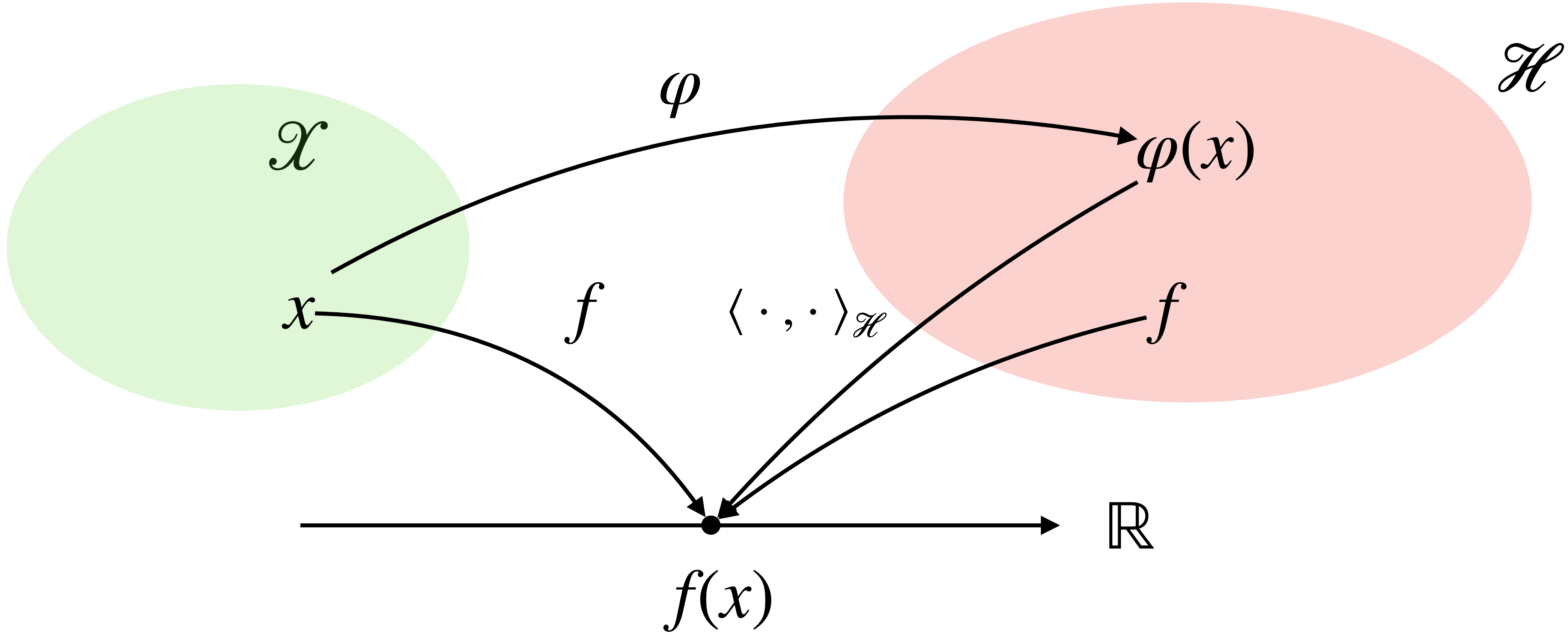

Kernel ridge regression

Let $\mathscr{D} = \{(x_i, y_i) \in \mathscr{X} \times \mathbb{R} : i \in [n]\}$ denote training data. We now have everything we need to define ERM on a RKHS.

$$\min_{f \in \mathscr{H}} \frac{1}{2n} \sum_{i=1}^{n} (y_i - f(x_i))^2 + \frac{\lambda}{2} ||f||_{\mathscr{H}}^2$$

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Closed-form in terms of "infinite dimensional" matrices "$\Phi \in \mathbb{R}^{n \times \infty}$"?

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As before, defining the kernel function and matrix

$$K(x, x') = \langle \varphi(x), \varphi(x') \rangle_{\mathscr{H}} \qquad \boldsymbol{K}_{ij} = \langle \varphi(x_i), \varphi(x_j) \rangle_{\mathscr{H}}$$

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The solution can be written as:

$$\hat{f}(x) = \sum_{i=1}^{n} \hat{\alpha}_{\lambda,i} K(x, x_i) \qquad \hat{\boldsymbol{\alpha}}_{\lambda}(\boldsymbol{\Phi}, \boldsymbol{y}) = (\boldsymbol{K} + n\lambda \boldsymbol{I}_n)^{-1} \boldsymbol{y}$$

Kernels

Note that in practice, to do ridge regression on $\mathscr{H}$ we don't even need to know what φ is. It suffices to have K.

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Theorem (Aronszajn, 1950)

A function $K : \mathscr{X} \times \mathscr{X} \to \mathbb{R}$ defines a positive definite Kernel if and only if there exists a Hilbert space $\mathscr{H}$ and a map $\varphi : \mathscr{X} \to \mathscr{H}$ such that:

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A kernel can correspond to several feature maps. e.g. $\mathscr{X} = \mathbb{R}$

$$\varphi(x) = x \qquad \varphi(x) = \frac{1}{\sqrt{2}} \begin{bmatrix} x \\ x \end{bmatrix} \qquad K(x, x') = xx'$$

Examples of Kernels

- Gaussian kernel: $K(\boldsymbol{x}, \boldsymbol{x}') = e^{-\frac{1}{2\sigma^2}||\boldsymbol{x}-\boldsymbol{x}'||_2^2}$ (a.k.a. RBF)
- Laplace kernel: $K(\boldsymbol{x}, \boldsymbol{x}') = e^{-\lambda||\boldsymbol{x}-\boldsymbol{x}'||_2}$
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- Translational invariant kernels $K(\boldsymbol{x}, \boldsymbol{x}') = \kappa(\boldsymbol{x} - \boldsymbol{x}')$
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- Polynomial kernel: $K(\boldsymbol{x}, \boldsymbol{x}') = (\langle \boldsymbol{x}, \boldsymbol{x}' \rangle + b)^k$
- Translational invariant kernels $K(\boldsymbol{x}, \boldsymbol{x}') = \kappa(\boldsymbol{x} - \boldsymbol{x}')$
- Rotationally invariant kernels $K(\boldsymbol{x}, \boldsymbol{x}') = \kappa(\langle \boldsymbol{x}, \boldsymbol{x}' \rangle)$

Or any other positive-definite function…

Examples of Kernels

- Gaussian kernel: $K(\boldsymbol{x}, \boldsymbol{x}') = e^{-\frac{1}{2\sigma^2}||\boldsymbol{x}-\boldsymbol{x}'||_2^2}$ (a.k.a. RBF)

- Laplace kernel: $K(\boldsymbol{x}, \boldsymbol{x}') = e^{-\lambda||\boldsymbol{x}-\boldsymbol{x}'||_2}$

- Polynomial kernel: $K(\boldsymbol{x}, \boldsymbol{x}') = (\langle \boldsymbol{x}, \boldsymbol{x}' \rangle + b)^k$

- Translational invariant kernels $K(\boldsymbol{x}, \boldsymbol{x}') = \kappa(\boldsymbol{x} - \boldsymbol{x}')$

- Rotationally invariant kernels $K(\boldsymbol{x}, \boldsymbol{x}') = \kappa(\langle \boldsymbol{x}, \boldsymbol{x}' \rangle)$

Or any other positive-definite function…

In general, finding φ associated to these is not obvious.

Examples of Kernels

$$y_i = \sin(x) + \varepsilon \qquad n = 100$$

$$\varepsilon \sim \mathcal{N}(0, 0.2^2) \qquad \lambda = 0.1$$