Machine learning for graphs and with graphs

Graph kernels

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ENS DE LYON

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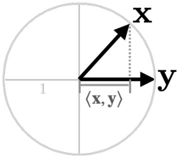
Acknowledgments

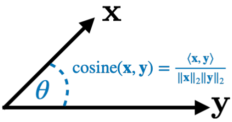
Some slides adapted from those of Jean-Philippe Vert and Rémi Flamary.

What is a kernel ?

Measuring similarities between objects

- Two "objects" $\mathbf{x}, \mathbf{y}$ in **an abstract space** $\mathcal{X}$.
- A kernel aims at measuring "how similar" is $\mathbf{x}$ from $\mathbf{y}$.
- e.g. $\mathcal{X} = \mathbb{R}^d$, $\text{kernel}(\mathbf{x}, \mathbf{y}) = \langle \mathbf{x}, \mathbf{y} \rangle$ or cosine similarity.





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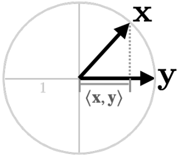

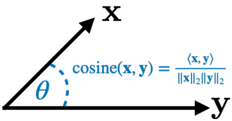

ML with kernels

- ML methods based on **pairwise comparisons**.
- By imposing constraints on the kernel (positive definite), we obtain a **general framework for learning from data** (RKHS).
- $+$ **without making any assumptions regarding the type of data** (vectors, strings, graphs, images, ...)

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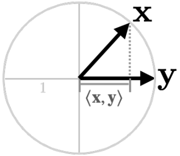

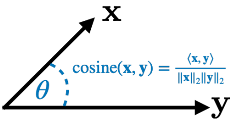

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A principle method for ERM

$\min_{f \in ?} \frac{1}{n} \sum_{i=1}^{n} \ell(\mathbf{y}_i, f(\mathbf{x}_i)) \rightarrow$ look for f in specific space (RKHS)

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The definition

Positive definite (PD) kernel

Let $\mathcal{X}$ be some space. A function $\kappa : \mathcal{X} \times \mathcal{X} \mapsto \mathbb{R}$ is a PD kernel if

- It is symmetric $\kappa(\mathbf{x}, \mathbf{y}) = \kappa(\mathbf{y}, \mathbf{x})$.
- For any $\mathbf{x}_1, \cdots, \mathbf{x}_n \in \mathcal{X}$ and $c_1, \cdots, c_n \in \mathbb{R}$

$$\sum_{i,j=1}^{n} c_i c_j \kappa(\mathbf{x}_i, \mathbf{x}_j) \geq 0 \, . \tag{1}$$

The definition

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Remarks

- (1) equiv. $\mathbf{K} := (\kappa(\mathbf{x}_i, \mathbf{x}_j))_{ij} \in \mathbb{R}^{n \times n}$ is a PSD matrix $\forall \mathbf{x}_1, \cdots, \mathbf{x}_n \in \mathcal{X}$.
- For $\kappa(\mathbf{x}, \mathbf{y}) = \langle \mathbf{x}, \mathbf{y} \rangle$ if $\mathbf{X} = (\mathbf{x}_1, \cdots, \mathbf{x}_n)^\top$ then $\mathbf{c}^\top \mathbf{K} \mathbf{c} = \|\mathbf{X}^\top \mathbf{c}\|_2^2 \geq 0$.
- Works also for $\kappa(\mathbf{x}, \mathbf{y}) = \langle \Phi(\mathbf{x}), \Phi(\mathbf{y}) \rangle$ for any Φ.
- Not entirely obvious $\kappa(\mathbf{x}, \mathbf{y}) = \exp(-\|\mathbf{x} - \mathbf{y}\|_2^2 / 2\sigma^2)$. (see TD)

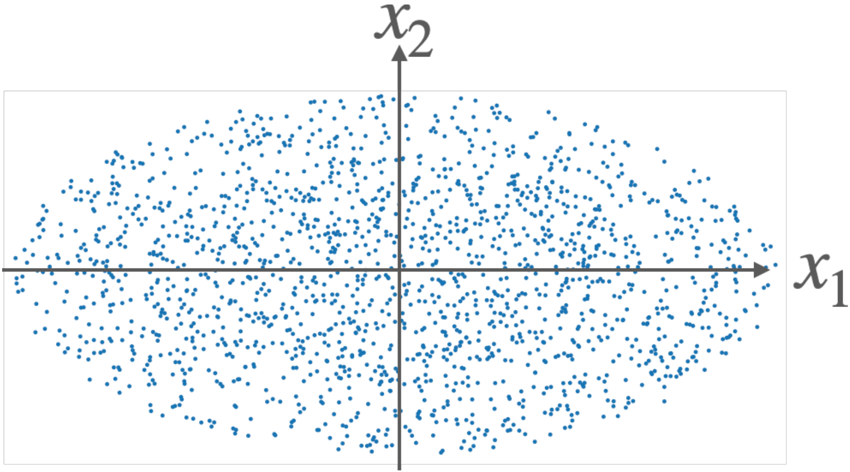
Properties of PD kernel

Basic properties (see TD)

Let $\kappa_1, \kappa_2, \cdots$ be fixed PD kernels.

- $\gamma\kappa_1$ for any $\gamma > 0$ is a PD kernel.
- $\kappa_1 + \kappa_2$ is a PD kernel.
- $\kappa(\mathbf{x}, \mathbf{y}) := \lim_{n \to +\infty} \kappa_n(\mathbf{x}, \mathbf{y})$ is a PD kernel (provided it exists).
- $\kappa(\mathbf{x}, \mathbf{y}) := \kappa_1(\mathbf{x}, \mathbf{y})\kappa_2(\mathbf{x}, \mathbf{y})$ is a PD kernel.
- If $f : \mathcal{X} \to \mathbb{R}$ then $\kappa(\mathbf{x}, \mathbf{y}) := f(\mathbf{x})\kappa_1(\mathbf{x}, \mathbf{y})f(\mathbf{y})$ is a PD kernel.

Changing the features



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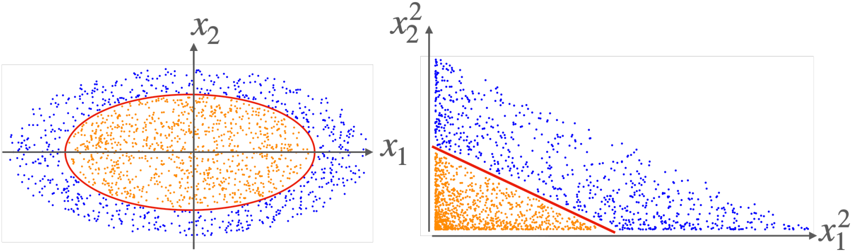

Polynomial kernel

Consider $\Phi : \mathbb{R}^2 \to \mathbb{R}^3$ defined by $\Phi(\mathbf{x} = (x_1, x_2)) = (x_1^2, \sqrt{2}x_1x_2, x_2^2)$. Then:

$$\kappa(\mathbf{x}, \mathbf{y}) := \langle \Phi(\mathbf{x}), \Phi(\mathbf{y}) \rangle_{\mathbb{R}^3} = \cdots = (\langle \mathbf{x}, \mathbf{y} \rangle_{\mathbb{R}^2})^2 .$$

Basic properties show that it defines a PD kernel.

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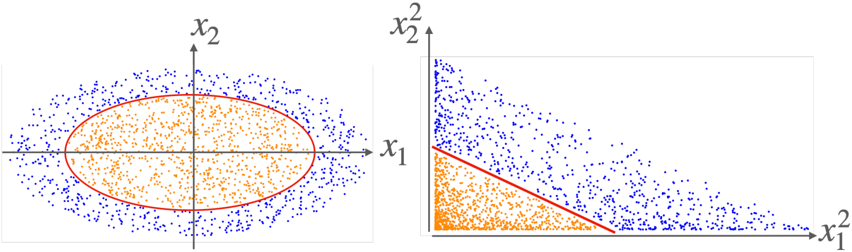

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Basic properties show that it defines a PD kernel.

- More generally $\kappa(\mathbf{x}, \mathbf{y}) = \langle \mathbf{x}, \mathbf{y} \rangle^m$.

Translation invariant kernels

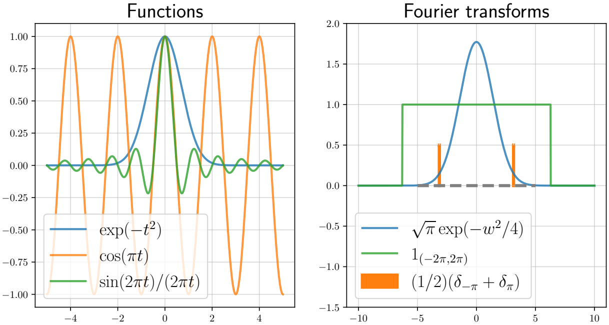
A generic form of kernel on $\mathcal{X} = \mathbb{R}^d$

- For $\kappa_0 : \mathbb{R}^d \to \mathbb{R}$, kernel defined by

$$\kappa(\mathbf{x}, \mathbf{y}) = \kappa_0(\mathbf{x} - \mathbf{y})$$

- e.g. Gaussian kernel $\kappa(\mathbf{x}, \mathbf{y}) = \exp(-\|\mathbf{x} - \mathbf{y}\|_2^2 / (2\sigma^2))$.
- Recall Fourier transform: $\widehat{f}(\boldsymbol{\omega}) = \int_{\mathbb{R}^d} f(\mathbf{x}) e^{-i\langle \boldsymbol{\omega}, \mathbf{x}\rangle} \mathrm{d}\mathbf{x}$.
- Based on Bochner's theorem (see Wendland 2004, Theorem 6.11):

$$\kappa \text{ is a PD kernel } \iff \forall \boldsymbol{\omega} \in \mathbb{R}^d, \widehat{\kappa_0}(\boldsymbol{\omega}) \geq 0$$



Main property of PD kernel

Main property: Moore–Aronszajn theorem Aronszajn 1950

A function $\kappa : \mathcal{X} \times \mathcal{X} \to \mathbb{R}$ is a PD kernel if and only if **there exists a Hilbert space** $\mathcal{H}$ and **a mapping** $\Phi : \mathcal{X} \to \mathcal{H}$ such that

$$\forall \mathbf{x}, \mathbf{y} \in \mathcal{X}, \;\; \kappa(\mathbf{x}, \mathbf{y}) = \langle \Phi(\mathbf{x}), \Phi(\mathbf{y}) \rangle_{\mathcal{H}} \, .$$

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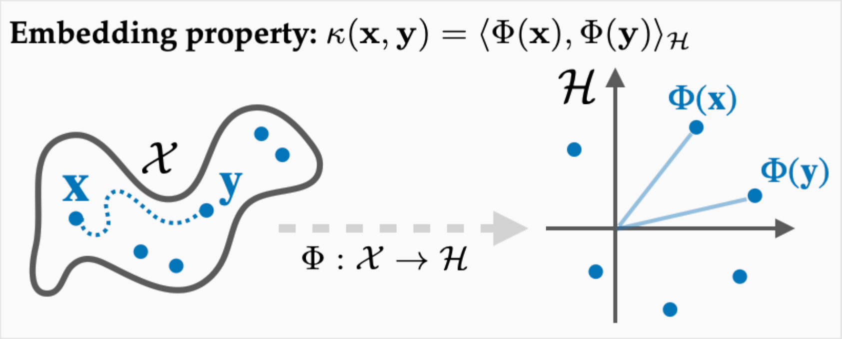


Main property of PD kernel

Some reminders

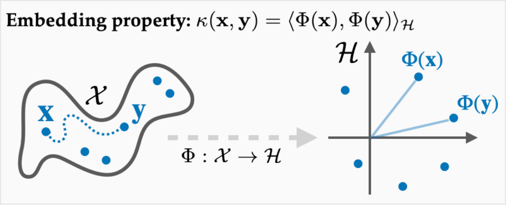
- $\langle \cdot, \cdot \rangle_{\mathcal{H}} : \mathcal{H} \times \mathcal{H} \to \mathbb{R}$ is a bilinear, symmetric and such that $\langle \mathbf{x}, \mathbf{x} \rangle_{\mathcal{H}} > 0$ for any $\mathbf{x} \neq 0$.
- A vector space endowed with an inner product is called pre-Hilbert. It is endowed with $\|\mathbf{x}\|_{\mathcal{H}} := \sqrt{\langle \mathbf{x}, \mathbf{x} \rangle_{\mathcal{H}}}$.
- A Hilbert space is a pre-Hilbert space complete for the norm defined by the inner product.

Proof of the theorem in the discrete case

On the board

Complete proof Steinwart and Christmann 2008, Theorem 4.16.

About the feature space



The feature map Φ and feature space $\mathcal{H}$

- The feature space may have **infinite dimension** and is **not unique**.
- Polynomial kernel in $2D$ $\kappa(\mathbf{x}, \mathbf{y}) = (\langle \mathbf{x}, \mathbf{y} \rangle)^2$:

$$\Phi(\mathbf{x} = (x_1, x_2)) = (x_1^2, x_2^2, x_1 x_2, x_1 x_2), \; \mathcal{H} = \mathbb{R}^4$$

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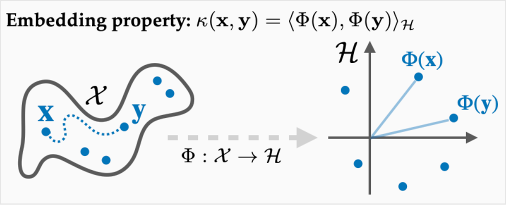

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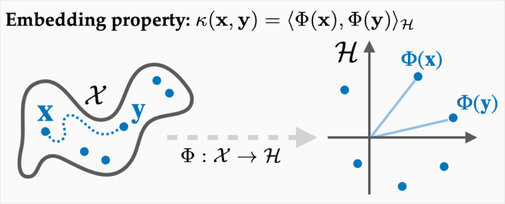
- Another possibility:

$$\Phi(\mathbf{x} = (x_1, x_2)) = (x_1^2, x_2^2, \sqrt{2} x_1 x_2),\ \mathcal{H} = \mathbb{R}^3$$

About the feature space



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$$\Phi(x) = e^{-\frac{x^2}{2\sigma^2}} \left(1, \sqrt{\frac{1}{1!\sigma^2}}x, \sqrt{\frac{1}{2!\sigma^4}}x^2, \sqrt{\frac{1}{3!\sigma^6}}x^3, \cdots\right)^\top \text{ (Taylor series)}$$

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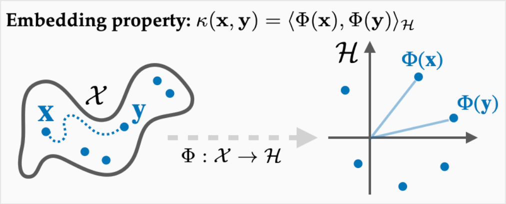

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- Or $\mathcal{H} = L_2(\mathbb{R})$ using $\kappa(x,y) = \frac{1}{\sigma}\sqrt{\frac{2}{\pi}} \int_{-\infty}^{+\infty} \exp(-\frac{(x-t)^2}{\sigma^2}) \exp(-\frac{(y-t)^2}{\sigma^2}) \mathrm{d}t$:

$$\Phi(x) = t \to \frac{2^{\frac{1}{4}}}{\sqrt{\sigma}\pi^{\frac{1}{4}}} \exp(-\frac{(x-t)^2}{\sigma^2})$$

Reproducing Kernel Hilbert Space (RKHS)

From kernels to functions: motivating example

- Kernels can be used to define functions from $\mathcal{X}$ to $\mathbb{R}$.

$$\Phi : \mathbb{R}^2 \to \mathbb{R}^3 = \mathcal{H}$$

$$\mathbf{x} = \begin{bmatrix} x_1 \\ x_2 \end{bmatrix} \mapsto \Phi(\mathbf{x}) = \begin{bmatrix} x_1 \\ x_2 \\ x_1 x_2 \end{bmatrix} \text{ and } f(\mathbf{x}) = a \cdot x_1 + b \cdot x_2 + c \cdot x_1 x_2 \; (\mathbb{R}^2 \to \mathbb{R})$$

- Consider $\boldsymbol{\theta} = (a, b, c)^\top \in \mathcal{H}$ then $f(\mathbf{x}) = \langle \boldsymbol{\theta}, \Phi(\mathbf{x}) \rangle_{\mathcal{H}}$.
- **Evaluation of** f **at** $\mathbf{x}$ **is an inner product in feature space**.

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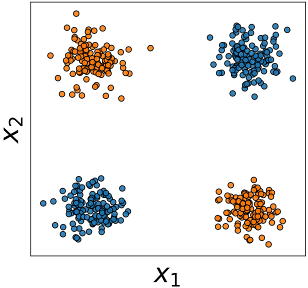
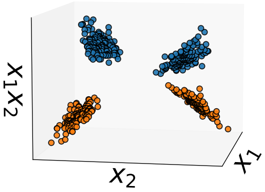
Go into higher dimensions to **linearly** separate the classes !





Reproducing Kernel Hilbert Space (RKHS)

From kernels to functions: first idea

- **Given** $\mathcal{H}$ **and** $\Phi : \mathcal{X} \to \mathcal{H}_0$: defines a kernel $\kappa(\mathbf{x}, \mathbf{y}) = \langle \Phi(\mathbf{x}), \Phi(\mathbf{y}) \rangle_{\mathcal{H}_0}$
- And a space of functions from $\mathcal{X}$ to $\mathbb{R}$.

$$\mathcal{H} := \{ f : \exists \boldsymbol{\theta} \in \mathcal{H}_0, \forall \mathbf{x} \in \mathcal{X}, f(\mathbf{x}) = \langle \boldsymbol{\theta}, \Phi(\mathbf{x}) \rangle_{\mathcal{H}_0} \} .$$

- Endowed with the norm

$$\|f\|_{\mathcal{H}} := \inf\{ \|\boldsymbol{\theta}\|_{\mathcal{H}_0} : \boldsymbol{\theta} \in \mathcal{H}_0 \text{ with } f = \langle \boldsymbol{\theta}, \Phi(\cdot) \rangle_{\mathcal{H}_0} \} \tag{2}$$

- It is a Hilbert space of functions called the RKHS of κ.
- We can stop here... but...

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From kernels to functions: second idea

- **Given a PSD kernel** $\kappa : \mathcal{X} \times \mathcal{X} \to \mathbb{R}$.
- 1°) Find a "suitable" $(\Phi, \mathcal{H})$ such that $\kappa(\mathbf{x}, \mathbf{y}) = \langle \Phi(\mathbf{x}), \Phi(\mathbf{y}) \rangle_{\mathcal{H}}$ (recall: many possible)
- 2°) Build upon it to define a suitable space of functions.

Reproducing Kernel Hilbert Space (RKHS)

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Reproducing Kernel Hilbert Space (RKHS)

Let κ be fixed

- Among all $(\Phi, \mathcal{H})$ mentioned in Aronszjan's theorem one $\mathcal{H}$, called **RKHS**, is of interest to us.
- This is a **space of functions from $\mathcal{X}$ to** $\mathbb{R}$.
- Each data point $\mathbf{x} \in \mathcal{X}$ will be represented **by a function** given by the **canonical feature map**

$$\Phi(\mathbf{x}) = \kappa(\cdot, \mathbf{x}) : \mathcal{X} \to \mathbb{R}$$

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Example

- Consider $\mathcal{X} = \mathbb{R}$ we could decide to represent $x \in \mathbb{R}$ as a Gaussian function centered at x:

$$\Phi(x) = y \to \exp(-(x-y)^2/(2\sigma^2))$$

- What is the corresponding space $\mathcal{H}$ (if it exists)? What would be the inner-product?

Reproducing Kernel Hilbert Space (RKHS)

Reproducing kernel and RKHS

Let $\mathcal{H}$ be a **Hilbert space** of functions from $\mathcal{X}$ to $\mathbb{R}$ with inner product $\langle \cdot, \cdot \rangle_{\mathcal{H}}$. $\kappa : \mathcal{X} \times \mathcal{X} \to \mathbb{R}$ is called a **reproducing kernel** of $\mathcal{H}$ if

- $\forall \mathbf{x} \in \mathcal{X}, \kappa(\cdot, \mathbf{x}) \in \mathcal{H}$
- κ satisfies the reproducing property: for any $f \in \mathcal{H}$,

$$\forall \mathbf{x} \in \mathcal{X},\ f(\mathbf{x}) = \langle f, \kappa(\cdot, \mathbf{x}) \rangle_{\mathcal{H}}\,.$$

If a reproducing kernel of $\mathcal{H}$ exists, then $\mathcal{H}$ is called a **RKHS**.

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Important properties

- If $\mathcal{H}$ is a RKHS, then it has a unique reproducing kernel κ.
- (the feature map is not unique only the kernel is)
- A function κ can be the reproducing kernel of at most one RKHS.

Reproducing Kernel Hilbert Space (RKHS)

Reproducing kernel and RKHS

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If a reproducing kernel of $\mathcal{H}$ exists, then $\mathcal{H}$ is called a **RKHS**.

RKHS and feature spaces

Let $\mathcal{H}$ be a RKHS with reproducing kernel κ. Then $\mathcal{H}$ is **one** feature space associated to κ, where the feature map is $\forall \mathbf{x} \in \mathcal{X}, \Phi(\mathbf{x}) = \kappa(\cdot, \mathbf{x})$.

Examples of RKHS

So far these functions are a little bit abstract:

Two questions

- Given a PD kernel κ what is the RKHS associated to κ ?
- Given a function space, is it a RKHS and what is the reproducing kernel ?

Examples of RKHS

So far these functions are a little bit abstract:

Two questions

- Given a PD kernel κ what is the RKHS associated to κ ?
- Given a function space, is it a RKHS and what is the reproducing kernel ?

Battery of examples

- (on the board) The RKHS associated to $\kappa(\mathbf{x}, \mathbf{y}) = \langle \mathbf{x}, \mathbf{y} \rangle$ is

$$\mathcal{H} = \{ f_{\boldsymbol{\theta}} = \mathbf{x} \rightarrow \langle \boldsymbol{\theta}, \mathbf{x} \rangle ; \boldsymbol{\theta} \in \mathbb{R}^d \}$$

  endowed with the dot product $\langle f_{\boldsymbol{\theta}_1}, f_{\boldsymbol{\theta}_2} \rangle_{\mathcal{H}} := \langle \boldsymbol{\theta}_1, \boldsymbol{\theta}_2 \rangle$.
- (homework) What is the RKHS associated to $\kappa(\mathbf{x}, \mathbf{y}) = \langle \mathbf{x}, \mathbf{y} \rangle^2$?
- The space $L_2(\mathbb{R}^d)$ **is not** a RKHS.

Examples of RKHS

Battery of examples

- The Paley-Wiener space (bandwidth limited Fourier transform):

  $$\mathcal{F}_\pi := \{f \in L_2(\mathbb{R}) : \operatorname{supp} \hat{f} \in [-\pi, \pi]\}$$

  where $\hat{f}$ is the Fourier transform of f.

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  - Inverse Fourier transform

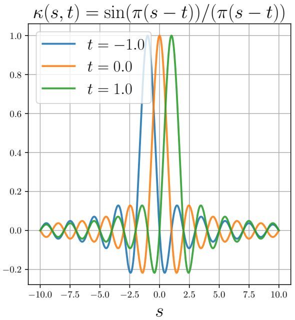
$$f(t) = \frac{1}{\sqrt{2\pi}} \int_{-\pi}^{\pi} \hat{f}(\omega) e^{i\omega t} \mathrm{d}\omega = \langle \hat{f}, \omega \to \frac{e^{-i\omega t}}{\sqrt{2\pi}} \rangle_{L_2([-\pi,\pi])}$$

  - Plancherel-Parseval theorem

$$\forall t \in \mathbb{R},\ f(t) = \langle \hat{f}, \omega \to \frac{e^{-i\omega t}}{\sqrt{2\pi}} \rangle_{L_2([-\pi,\pi])} = \langle f, \frac{\sin(\pi(\cdot - t))}{\pi(\cdot - t)} \rangle_{L_2(\mathbb{R})}$$

  - The kernel $\kappa(s, t) = \frac{\sin(\pi(s-t))}{\pi(s-t)}$

Examples of RKHS



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Examples of RKHS

Battery of examples

- Translation invariant PD kernels on $\mathbb{R}^d$ $\kappa(\mathbf{x}, \mathbf{y}) = \kappa_0(\mathbf{x} - \mathbf{y})$ with $\kappa_0 \in L_1(\mathbb{R}^d) \cap C(\mathbb{R}^d)$ and $\forall \boldsymbol{\omega} \in \mathbb{R}^d, \widehat{\kappa_0}(\boldsymbol{\omega}) \geq 0$.

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- The corresponding RKHS is

$$\mathcal{H} = \{f \in L_2(\mathbb{R}^d) \cap C(\mathbb{R}^d) : \hat{f}/\sqrt{\widehat{\kappa_0}} \in L_2(\mathbb{R}^d)\}$$

- The inner product is given by:

$$\langle f, g\rangle_{\mathcal{H}} := (2\pi)^{-d/2} \int_{\mathbb{R}^d} \frac{\hat{f}(\boldsymbol{\omega})\overline{\widehat{g}(\boldsymbol{\omega})}}{\widehat{\kappa_0}(\boldsymbol{\omega})} \mathrm{d}\boldsymbol{\omega}\,.$$

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- Special case: Matèrn kernel $\widehat{\kappa_0}(\boldsymbol{\omega}) \propto (\alpha^2 + \|\boldsymbol{\omega}\|_2^2)^{-s}, s > d/2$
- Sobolev spaces of order s: $\|f\|_{\mathcal{H}}^2 =$ smoothness of the functions as its derivatives in $L_2(\mathbb{R}^d)$.

Reproducing Kernel Hilbert Space (RKHS)

Reproducing kernels are PD kernels

A function $\kappa : \mathcal{X} \times \mathcal{X} \to \mathbb{R}$ is a reproducing kernel if and only if it is a PD kernel.

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Remarks

- One direction easy: a reproducing kernel is a PD kernel (on the board).
- The other more work: use Moore–Aronszajn theorem + $\mathcal{F}$ + Steinwart and Christmann 2008, Theorem 4.21.

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Important consequence

- Any PSD kernel defines a Hilbert space of functions from $\mathcal{X}$ to $\mathbb{R}$.
- These functions satisfy

$$\forall \mathbf{x} \in \mathcal{X},\ f(\mathbf{x}) = \langle f, \kappa(\cdot, \mathbf{x}) \rangle_{\mathcal{H}} .$$

- Abstract view of $\mathcal{H}$:

$$\mathcal{H} = \overline{\mathrm{Span}\{\kappa(\cdot, \mathbf{x}); \mathbf{x} \in \mathcal{X}\}} .$$

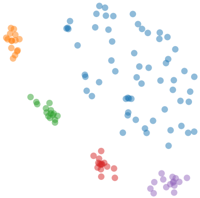
Table of contents

Recap on supervised ML

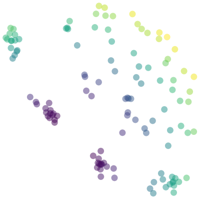
Samples + labels:

$$\mathbf{X} = \begin{bmatrix} \mathbf{x}_1^\top \\ \mathbf{x}_2^\top \\ \vdots \\ \mathbf{x}_n^\top \end{bmatrix} \quad \mathbf{y} = \begin{bmatrix} y_1 \\ y_2 \\ \vdots \\ y_n \end{bmatrix}$$

Classification



Regression



Supervised learning

- The dataset contains the samples $(\mathbf{x}_i, y_i)_{i=1}^n$ where $\mathbf{x}_i$ is the feature sample and $y_i \in \mathcal{Y}$ its label.
- Prediction space $\mathcal{Y}$ can be:
  - $\mathcal{Y} = \{-1, 1\}$ or $\mathcal{Y} = \{1, \dots, K\}$ for classification problems.
  - $\mathcal{Y} = \mathbb{R}$ for regression problems ($\mathbb{R}^p$ for multi-output regression).

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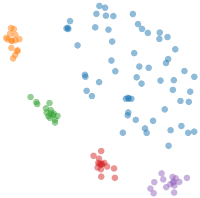

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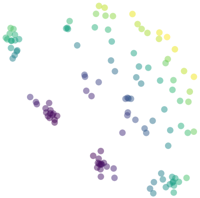

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Minimizing the averaged error on the training data

To find $f : \mathcal{X} \to \mathcal{Y}$ the idea is to minimize:

$$\min_f \frac{1}{n} \sum_{i=1}^{n} \ell(y_i, f(\mathbf{x}_i)) + \lambda \operatorname{Reg}(f) \tag{ERM}$$

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- How to properly regularize ?
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One solution

- When $\mathcal{Y} \subset \mathbb{R}$ we can consider $f \in \mathcal{H}$ where $\mathcal{H}$ is a RKHS.
- A natural candidate $\text{Reg}(f) = \|f\|_{\mathcal{H}}^2$: the higher the smoother f is.
- How to ensure that this is not so difficult ?

Interpretation of minimization on a RKHS

- Suppose $\mathcal{X} = \mathbb{R}^d$ and $\mathcal{H}$ a RKHS. Consider ERM

$$\min_{f \in \mathcal{H}} \frac{1}{n} \sum_{i=1}^{n} \ell(y_i, f(\mathbf{x}_i)) + \lambda \|f\|_{\mathcal{H}}^2$$

- Since $f \in \mathcal{H}$, then $f(\mathbf{x}) = \langle f, \kappa(\cdot, \mathbf{x}) \rangle_{\mathcal{H}} = \langle f, \Phi(\mathbf{x}) \rangle_{\mathcal{H}}$.
- Rewriting ERM in RKHS as

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Important interpretation

- $\Phi : \mathcal{X} \to \mathcal{H}$ pushes the points to a potentially very high-dimensional space (even ∞): more powerful representation.
- Then linear classification/regression is made on this high-dim space $\mathcal{H}$
- We can deduce the function in low-dim from the high-dim.

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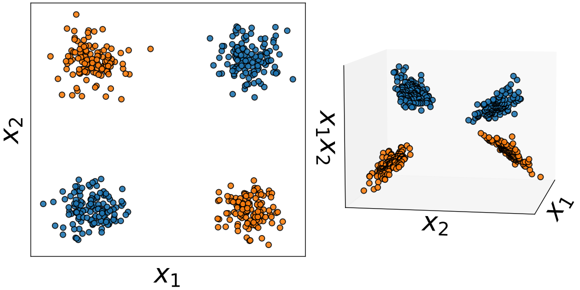
Go into higher dimensions to **linearly** separate the classes !



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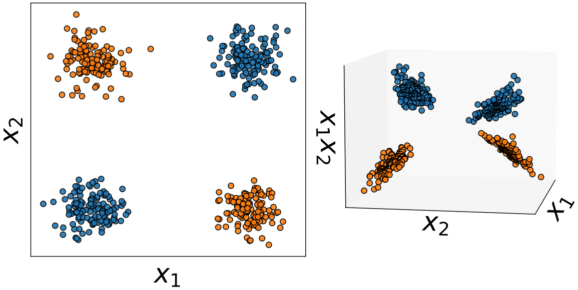
Go into higher dimensions to **linearly** separate the classes !

- But how to implement $\Phi(\mathbf{x}) \in \mathcal{H}$ on a computer if $\dim \mathcal{H} = \infty$?????
- How to solve ERM in $\mathcal{H}$????



The representer theorem

Main result

- Let $\mathcal{X}$ be any space, $\mathcal{D} = \{\mathbf{x}_1, \cdots, \mathbf{x}_n\} \subset \mathcal{X}$ a finite set of points.
- $\mathcal{H}$ a RKHS with reproducing kernel $\kappa : \mathcal{X} \times \mathcal{X} \to \mathbb{R}$.
- Let $\Psi : \mathbb{R}^{n+1} \to \mathbb{R}$ any function that is strictly increasing with respect to the last variable.
- Then any solution $f^\star$ of the minimization problem

$$\min_{f \in \mathcal{H}} \Psi(f(\mathbf{x}_1), \cdots, f(\mathbf{x}_n), \|f\|_{\mathcal{H}}^2)$$

can be written as

$$\forall \mathbf{x} \in \mathcal{X}, \;\; f^\star(\mathbf{x}) = \sum_{i=1}^{n} \theta_i \kappa(\mathbf{x}, \mathbf{x}_i) \text{ for some } \boldsymbol{\theta} \in \mathbb{R}^n .$$

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Important remarks

- Although the RKHS can be of infinite dimension any solution lives in $\mathrm{Span}\{\kappa(\cdot, \mathbf{x}_1), \cdots, \kappa(\cdot, \mathbf{x}_n)\}$ which is a subspace of dimension n.
- Works for any $\mathcal{X}$ and $\Psi = \Psi_0 + g$ with $g \nearrow$!!!

Practical use of the representer theorem (1/2)

- When the representer theorem holds we can simply look for f as

$$\forall \mathbf{x} \in \mathcal{X},\ f(\mathbf{x}) = \sum_{i=1}^{n} \theta_i \kappa(\mathbf{x}, \mathbf{x}_i) \text{ for some } \boldsymbol{\theta} \in \mathbb{R}^n .$$

- Define $\mathbf{K} := \left(\kappa(\mathbf{x}_i, \mathbf{x}_j)\right)_{ij}$.
- Then , for any $j \in [\![n]\!]$

$$f(\mathbf{x}_j) = \sum_{i=1}^{n} \theta_i \kappa(\mathbf{x}_i, \mathbf{x}_j) = [\mathbf{K}\boldsymbol{\theta}]_j .$$

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- Also

$$\begin{aligned}\|f\|_{\mathcal{H}}^2 &= \|\sum_{i=1}^{n} \theta_i \kappa(\cdot, \mathbf{x}_i)\|_{\mathcal{H}}^2 = \langle \sum_{i=1}^{n} \theta_i \kappa(\cdot, \mathbf{x}_i), \sum_{j=1}^{n} \theta_j \kappa(\cdot, \mathbf{x}_j) \rangle_{\mathcal{H}} \\ &= \sum_{ij} \theta_i \theta_j \langle \kappa(\cdot, \mathbf{x}_i), \kappa(\cdot, \mathbf{x}_j) \rangle_{\mathcal{H}} = \sum_{ij} \theta_i \theta_j \kappa(\mathbf{x}_i, \mathbf{x}_j) \\ &= \boldsymbol{\theta}^\top \mathbf{K} \boldsymbol{\theta} .\end{aligned}$$

Practical use of the representer theorem (2/2)

- Therefore the problem

$$\min_{f \in \mathcal{H}} \Psi(f(\mathbf{x}_1), \cdots, f(\mathbf{x}_n), \|f\|_{\mathcal{H}}^2)$$

- is equivalent to

$$\min_{\boldsymbol{\theta} \in \mathbb{R}^n} \Psi([\mathbf{K}\boldsymbol{\theta}]_1, \cdots, [\mathbf{K}\boldsymbol{\theta}]_n, \boldsymbol{\theta}^\top \mathbf{K}\boldsymbol{\theta})$$

- 1°) To tackle it we only need the Gram matrix $\mathbf{K}$: **kernel trick** !
- 2°) Can be used whatever $\mathcal{X}, \kappa$!
- 3°) We can solve it on a computer since finite dimensional !
- 4°) It can usually be solved analytically or by numerical methods.

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Application to ERM

If we look for f in a RKHS then we need to solve

$$\min_{\boldsymbol{\theta}\in\mathbb{R}^n} \frac{1}{n}\sum_{i=1}^{n} \ell(\mathbf{y}_i, [\mathbf{K}\boldsymbol{\theta}]_i) + \lambda\boldsymbol{\theta}^\top \mathbf{K}\boldsymbol{\theta}$$

Application to regression

Setting

- $\mathbf{x}_i \in \mathcal{X}$ (not necessarily $\mathbb{R}^d$!) and $y_i \in \mathbb{R}, \mathbf{y} = (y_1, \cdots, y_n)^\top \in \mathbb{R}^n$
- We consider the square loss $\ell(y, y') = (y - y')^2$
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Kernel Ridge Regression

The ERM in the RKHS is equivalent to the minimization problem:

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How can we solve it ? What is the time/memory complexity ?

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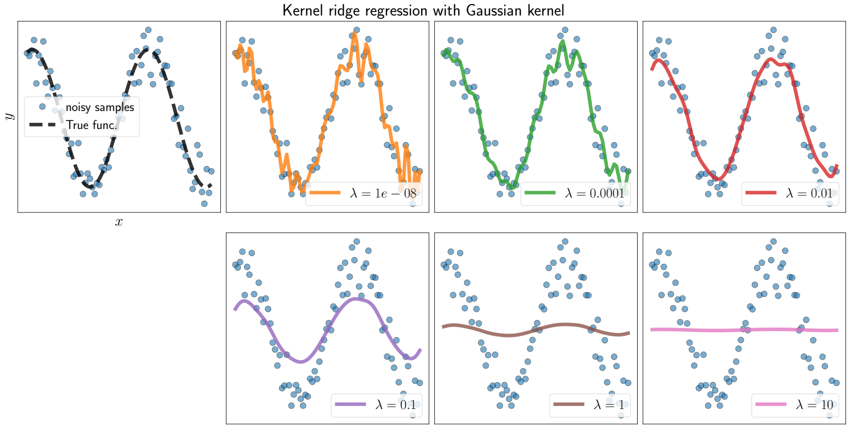
Solution

Given by $\boldsymbol{\theta}^\star = (\mathbf{K} + \lambda n \mathbf{I})^{-1}\mathbf{y}, \ \forall \mathbf{x} \in \mathcal{X}, f^\star(\mathbf{x}) = \sum_{i=1}^n \theta_i^\star \kappa(\mathbf{x}, \mathbf{x}_i)$.

Application to regression

- Gaussian kernel $\kappa(x, x') = \exp(-|x - x'|^2/(2\sigma^2))$
- Regularization parameter λ



Kernel ridge regression vs linear regression

- Take $\mathcal{X} = \mathbb{R}^d$ and the linear kernel $\kappa(\mathbf{x}, \mathbf{y}) = \langle \mathbf{x}, \mathbf{y} \rangle$.
- Let $\mathbf{X} = (\mathbf{x}_1, \cdot, \mathbf{x}_n)^\top \in \mathbb{R}^{n \times d}$ the data. The Gram matrix is $\mathbf{K} = \mathbf{X}\mathbf{X}^\top$.
- Then corresponding function is

$$f^\star(\mathbf{x}) = \sum_{i=1}^{n} \theta_i^\star \kappa(\mathbf{x}, \mathbf{x}_i) = \langle \mathbf{x}, \sum_{i=1}^{n} \theta_i^\star \mathbf{x}_i \rangle = \langle \mathbf{x}, \mathbf{w}^\star \rangle.$$

- We have $\mathbf{w}^\star = \mathbf{X}^\top (\mathbf{X}\mathbf{X}^\top + \lambda n \mathbf{I}_n)^{-1} \mathbf{y}$.

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$$f^\star(\mathbf{x}) = \sum_{i=1}^{n} \theta_i^\star \kappa(\mathbf{x}, \mathbf{x}_i) = \langle \mathbf{x}, \sum_{i=1}^{n} \theta_i^\star \mathbf{x}_i \rangle = \langle \mathbf{x}, \mathbf{w}^\star \rangle.$$

- We have $\mathbf{w}^\star = \mathbf{X}^\top (\mathbf{X}\mathbf{X}^\top + \lambda n \mathbf{I}_n)^{-1} \mathbf{y}$.

ℓ_2 penalized linear regression: ridge regression

The problem

$$\min_{\mathbf{w} \in \mathbb{R}^d} \frac{1}{n} \sum_{i=1}^{n} (y_i - \mathbf{w}^\top \mathbf{x}_i)^2 + \lambda \|\mathbf{w}\|_2^2 \text{ has solution } \mathbf{w}^\star = (\mathbf{X}^\top \mathbf{X} + \lambda n \mathbf{I}_d)^{-1} \mathbf{X}^\top \mathbf{y}.$$

Kernel ridge regression vs linear regression

- Take $\mathcal{X} = \mathbb{R}^d$ and the linear kernel $\kappa(\mathbf{x}, \mathbf{y}) = \langle \mathbf{x}, \mathbf{y} \rangle$.
- Let $\mathbf{X} = (\mathbf{x}_1, \cdot, \mathbf{x}_n)^\top \in \mathbb{R}^{n \times d}$ the data. The Gram matrix is $\mathbf{K} = \mathbf{X}\mathbf{X}^\top$.
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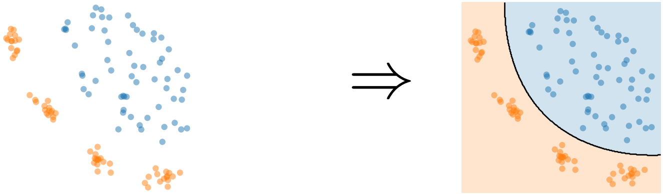
Matrix inversion lemma

$$(\mathbf{X}^\top \mathbf{X} + \lambda n \mathbf{I}_d)^{-1} \mathbf{X}^\top = \mathbf{X}^\top (\mathbf{X}\mathbf{X}^\top + \lambda n \mathbf{I}_n)^{-1}$$

- Both agree !
- Complexity roughly: KRR $O(n^3)$, RR $O(\min\{d^3, n^3\})$.

Binary classification



Objective

$$(\mathbf{x}_i, y_i)_{i=1}^n \quad \Rightarrow \quad f : \mathbb{R}^d \to \{-1, 1\}$$

- Train a function $f(\mathbf{x}) = y \in \mathcal{Y}$ predicting a binary value ($\mathcal{Y} = \{-1, 1\}$).
- $f(\mathbf{x}) = 0$ defines the boundary on the partition of the feature space.

ERM in RKHS

$$\min_{f \in \mathcal{H}} \frac{1}{n} \sum_{i=1}^{n} \ell(y_i, f(\mathbf{x}_i)) + \lambda \|f\|_{\mathcal{H}}^2 .$$

Loss functions

A focus on classification problems $\mathcal{Y} = \{-1, 1\}$

$$\ell(y_i, f(\mathbf{x}_i)) = \Phi(y_i f(\mathbf{x}_i)) \text{ with } \Phi \text{ non-increasing.}$$

Loss functions

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$$\ell(y_i, f(\mathbf{x}_i)) = \Phi(y_i f(\mathbf{x}_i)) \text{ with } \Phi \text{ non-increasing.}$$

- $y_i f(\mathbf{x}_i)$ is **the margin** (on the board).
- $\ell(y_i, f(\mathbf{x}_i)) = \mathbf{1}_{y_i f(\mathbf{x}_i) \leq 0}$ (0/1 loss)
- $\ell(y_i, f(\mathbf{x}_i)) = \max\{0, 1 - y_i f(\mathbf{x}_i)\}$ (hinge loss: **SVM**)
- $\ell(y_i, f(\mathbf{x}_i)) = \log(1 + e^{-y_i f(\mathbf{x}_i)})$ (logistic loss)

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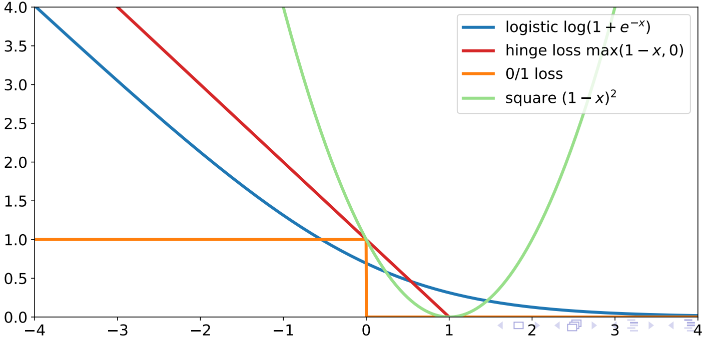


Support Vector Machines (SVM)

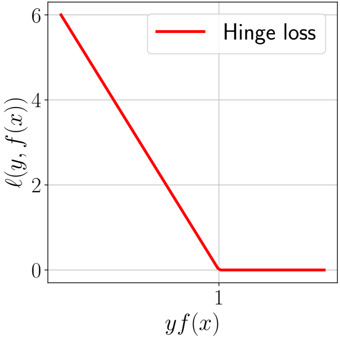
Definition

- The hinge-loss is the function $\mathbb{R} \to \mathbb{R}_+$:

$$\begin{aligned}\Phi_{\text{hinge}}(x) &= \max(1-x, 0) \\ &= \begin{cases} 0 & \text{if } x \geq 1 \\ 1-x & \text{otherwise}\end{cases}\end{aligned}$$

- SVM is the corresponding large-margin classifier, which solves:

$$\min_{f \in \mathcal{H}} \frac{1}{n} \sum_{i=1}^{n} \Phi_{\text{hinge}}(y_i f(\mathbf{x}_i)) + \lambda \|f\|_{\mathcal{H}}^2 \,.$$



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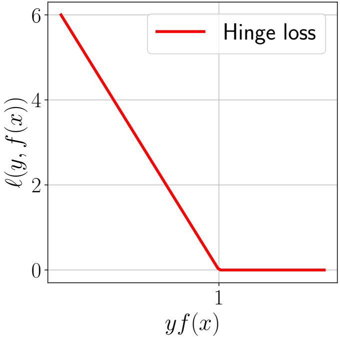
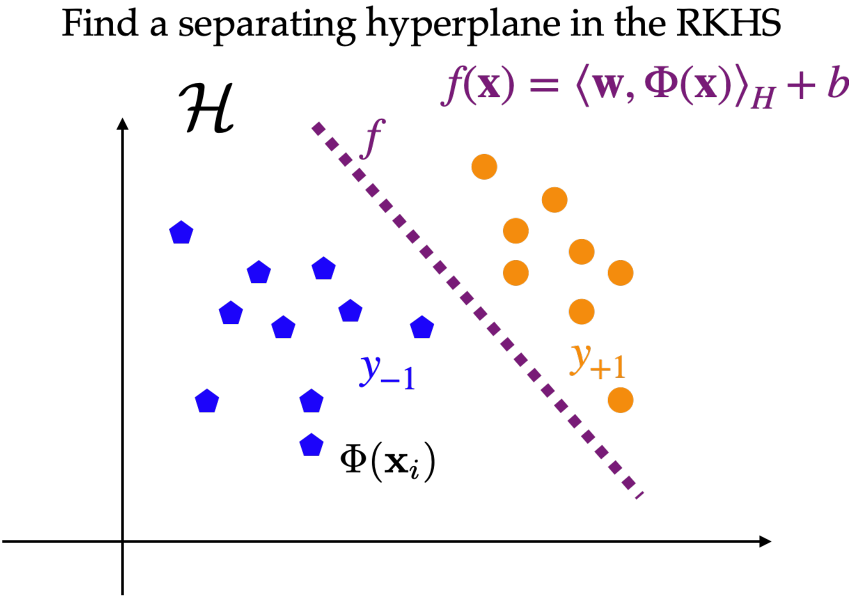


Solving for the SVM (details in Steinwart and Christmann 2008)

- Representer theorem: sol. of the form $f^\star(\mathbf{x}) = \sum_{i=1}^{n} \theta_i^\star \kappa(\mathbf{x}, \mathbf{x}_i)$.
- $\boldsymbol{\theta}^\star$ can be found by solving a quadratic program (QP).
- Again: we only need to know the Gram matrix $\mathbf{K} = (\kappa(\mathbf{x}_i, \mathbf{x}_j))_{ij}$.

What is SVM doing ?



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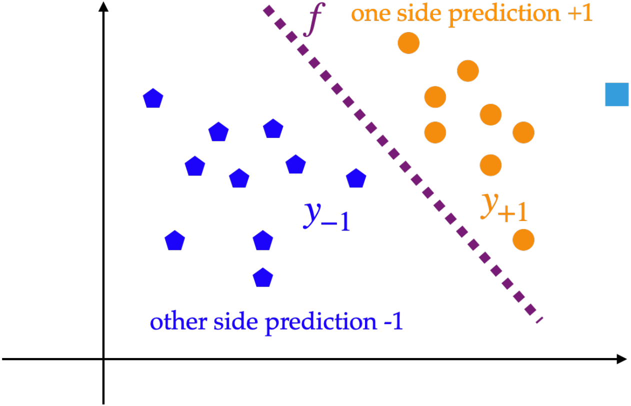


- Classification:

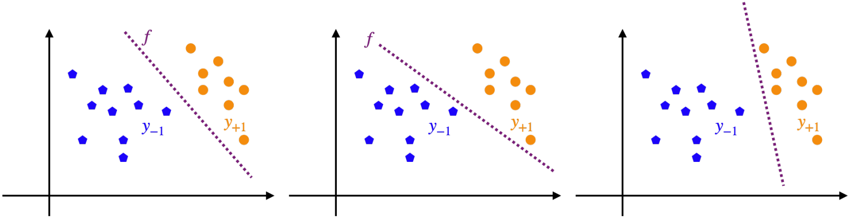
  $\text{sign}(f)$

  $if\ f(\mathbf{x}) > 0 \rightarrow +1$

  $if\ f(\mathbf{x}) < 0 \rightarrow -1$

What is SVM doing ?

But there could be an infinity of separating hyperplanes or zero !



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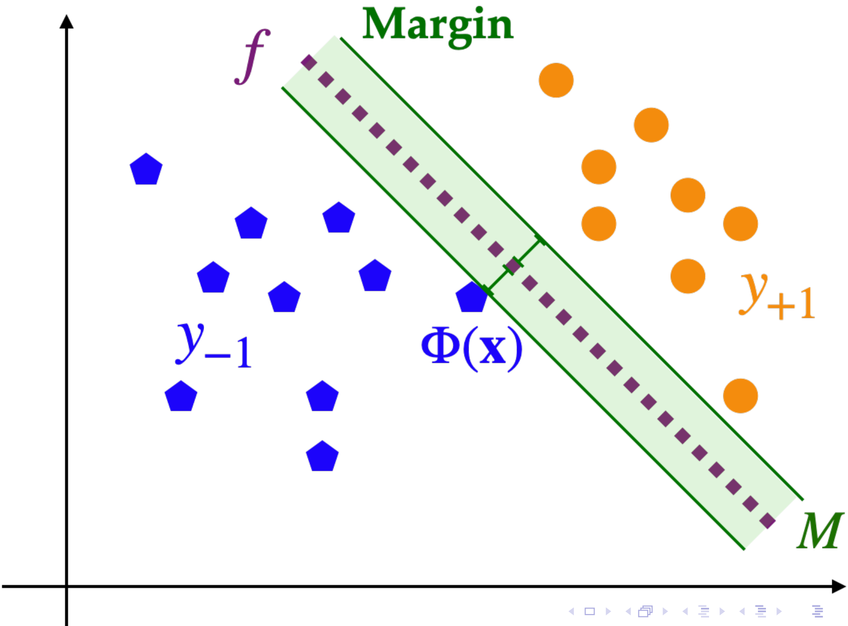
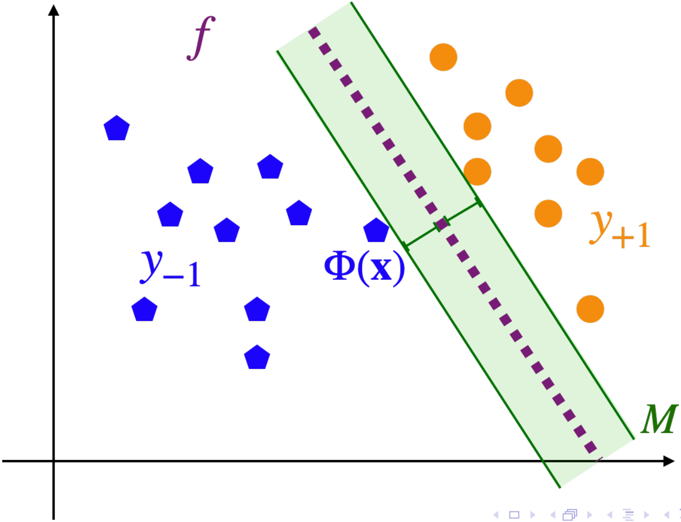


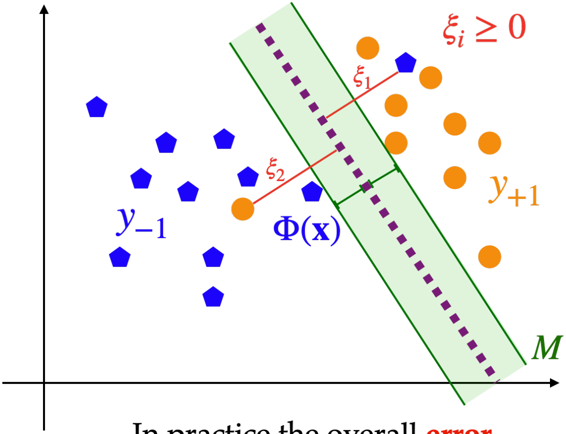
What is SVM doing ?

SVM finds the hyperplane
that maximizes the **margin**



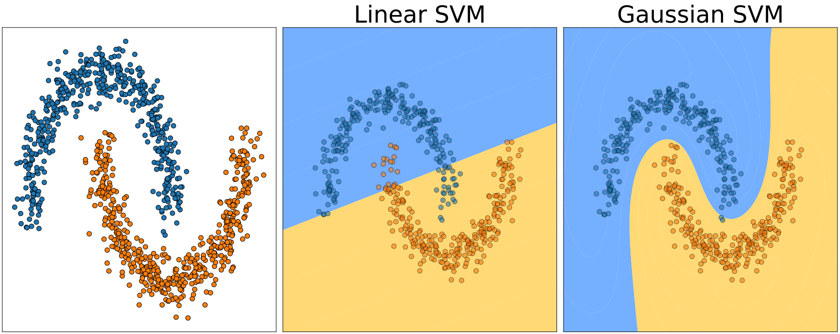
What is SVM doing ?

+ We allow **some errors** to be made



In practice the overall **error**
is controlled by a regularization param. C

Example



Conclusion

- Kernel theory is very rich, kernels are quite simple but also versatile.
- Defines a very general way of learning classifiers/regressors on any kind of space.
- Based on the representer theorem: we only need the Gram matrix !
- Difficulties: the choice of the kernel (see TD), also can be expensive.

Table of contents

Kernels for structured data

Objective

Given a dataset of graphs $(G_1, \cdots, G_n)$ can we build machine learning models to do:

- Supervised learning: each graph associated to $y_i \in \mathcal{Y}$.
- Unsupervised learning: PCA, Kernel PCA, graph embedding...

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Application of RKHS for graphs

Let $\mathcal{X} = \{$ set of all graphs $\}$ can we build interesting kernels $\kappa : \mathcal{X} \times \mathcal{X} \to \mathbb{R}$?

- For $G, G' \in \mathcal{X}, \kappa(G, G')$ is a notion of "similarity" between graphs.
- Gram matrix $\mathbf{K} = (\kappa(G_i, G_j))_{(i,j) \in [\![n]\!]^2}$.
- Then do stuff...

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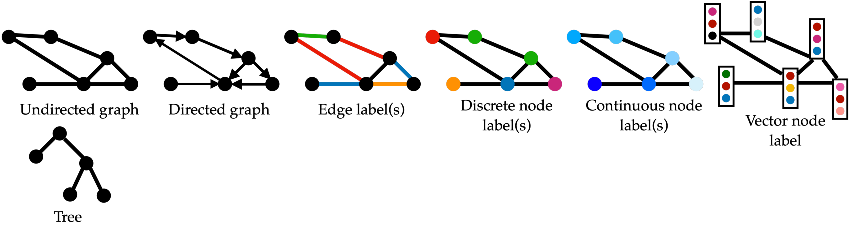
Some notations

A graph $G = (V, E)$. Labeling function if attributes/labels $\ell_G : V \cup E \to S$ (S discrete or continuous $\subset \mathbb{R}^N$)

What is a good graph kernel ?

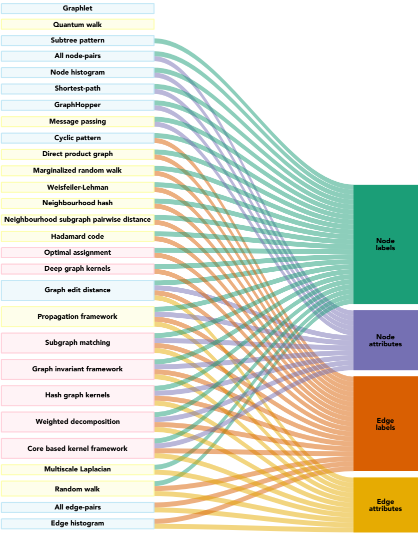
Properties of the graph kernel

- Handle graphs that are directed (or undirected) ?
- Handle node or edge labels or attributes that are present in the graphs?
- Efficient to compute ? Complexity *w.r.t.* $|V|, |E|, \dim$?
- Is there a particular relevant substructure (*e.g.* tree patterns) that would preclude the choice of a particular kernel?



The kernel jungle

Surveys: K. Borgwardt et al. 2020; Nikolentzos, Siglidis, and Vazirgiannis 2021



Graph Kernel	Exp. ϕ	Node Labels	Node Attributes	Type	Complexity
Vertex Histogram	✓	✓	✗	R-convolution	$\mathcal{O}(n)$
Edge Histogram	✓	✓	✗	R-convolution	$\mathcal{O}(m)$
Random Walk	✗†	✓	✓	R-convolution	$\mathcal{O}(n^3)$
Subtree	✗	✓	✓	R-convolution	$\mathcal{O}(n^2 4^{deg^*} h)$
Cyclic Pattern	✓	✓	✗	intersection	$\mathcal{O}((c+2)n+2m)$
Shortest Path	✗†	✓	✓	R-convolution	$\mathcal{O}(n^4)$
Graphlet	✓	✗	✗	R-convolution	$\mathcal{O}(n^k)$
Weisfeiler-Lehman Subtree	✓	✓	✗	R-convolution	$\mathcal{O}(hm)$
Neighborhood Hash	✓	✓	✗	intersection	$\mathcal{O}(hm)$
Neighborhood Subgraph Pairwise Distance	✓	✓	✗	R-convolution	$\mathcal{O}(n^2 m \log(m))$
Lovász ϑ	✓	✗	✗	R-convolution	$\mathcal{O}(n(s+\frac{nm}{\epsilon})+s^2)$
SVM-ϑ	✓	✗	✗	R-convolution	$\mathcal{O}(n(s+n^2)+s^2)$
Ordered Decomposition DAGs	✓	✓	✗	R-convolution	$\mathcal{O}(n \log n)$
Pyramid Match	✗	✓	✗	assignment	$\mathcal{O}(ndL)$
Weisfeiler-Lehman Optimal Assignment	✗	✓	✗	assignment	$\mathcal{O}(hm)$
Subgraph Matching	✗	✓	✓	R-convolution	$\mathcal{O}(kn^{k+1})$
GraphHopper	✗	✓	✓	R-convolution	$\mathcal{O}(n^4)$
Graph Invariant Kernels	✗	✓	✓	R-convolution	$\mathcal{O}(n^6)$
Propagation	✓	✓	✓	R-convolution	$\mathcal{O}(hm)$
Multiscale Laplacian	✗	✓	✓	R-convolution	$\mathcal{O}(n^5 h)$

Bag of structures

A majority of graph kernels are instances of the *convolution kernels* Haussler et al. 1999.

Principle

- Compare graphs by first dividing them into substructures of various granularity.
- E.g. vertices, subgraphs, all shortest paths of a graph.
- Defining *base kernels* at the fine granularity and combine them.
- Of the form $\kappa(G, G') = \sum_{r \in \mathcal{R}, r' \in \mathcal{R}'} \kappa_{\text{substructure}}(r, r')$.

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Advantages & limitations

- Intuitive definitions + relatively good results.
- Sometimes computational limitations.
- Expressiveness limitations.
- "Diagonal dominance problem" Yanardag and Vishwanathan 2015.

All node-pairs kernel

A first idea

- Given $G = (V, E), G' = (V', E')$,
- Suppose the labels of the nodes of both graphs are in S.
- Consider a kernel on the nodes

$$\kappa_{\text{node}} : S \times S \to \mathbb{R}$$

- The all node-pairs kernel is defined by

$$\kappa(G, G') = \sum_{v \in V} \sum_{v' \in V'} \kappa_{\text{node}}(\ell_G(v), \ell_{G'}(v'))$$

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Remarks

- Runtime in $O(|V| \times |V'| \times \dim(S))$.
- Can handle discrete/continuous labels.
- Does not take into account the structures of the graphs.

Node histogram kernel

A baseline kernel (1/2)

- Suppose the labels are discrete over a finite alphabet

$$\Sigma = \{\sigma_1, \cdots, \sigma_{|\Sigma|}\}$$

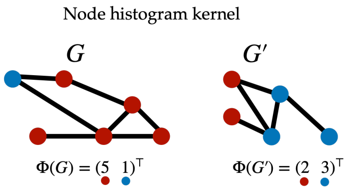
- The node histogram kernel is defined as

$$\kappa_{\mathsf{NH}}(G, G') = \langle \Phi(G), \Phi(G') \rangle \,.$$

where

$$\Phi(G) = \Big(\sum_{v \in V} \mathbf{1}_{\ell_G(v) = \sigma_1}, \cdots, \sum_{v \in V} \mathbf{1}_{\ell_G(v) = \sigma_{|\Sigma|}}\Big) \,.$$

- Simply corresponds to an unnormalised histogram that counts the occurrence of each node label in the graph.



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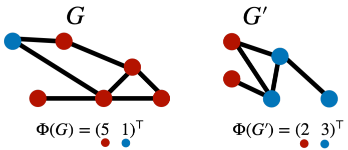

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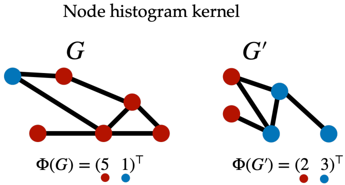

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Edge histogram kernel

A baseline kernel (2/2)

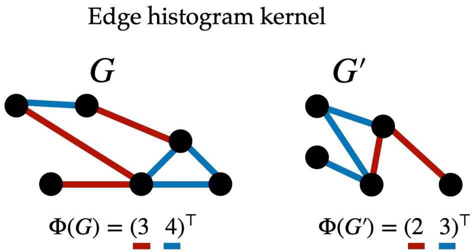
- Suppose the **edges labels** are discrete over a finite alphabet

$$\Sigma = \{\sigma_1, \cdots, \sigma_{|\Sigma|}\}$$

- The edge histogram kernel is defined as

$$\kappa_{\mathsf{EH}}(G, G') = \langle \Phi(G), \Phi(G') \rangle \,.$$

where $\Phi(G) = \left(\sum_{e \in E} \mathbf{1}_{\ell(e)=\sigma_1}, \cdots, \sum_{e \in E} \mathbf{1}_{\ell(e)=\sigma_{|\Sigma|}}\right)$.



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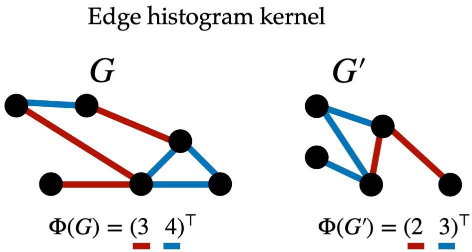


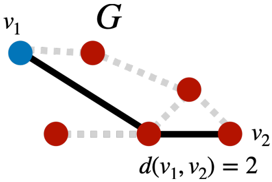
Remarks

- Can be computed in $O(|E| + |E|')$.
- Does not take into account the labels of the nodes.
- Can be combined with the previous one as

$$\kappa(G, G') = \kappa_{\mathsf{EH}}(G, G') \times \kappa_{\mathsf{NH}}(G, G')$$

The shortest-path kernel

K. M. Borgwardt and Kriegel 2005



- Compute all pair-to-pair shortest-paths in G, G' with Floyd-Warshall.
- The kernel is defined as

$$\kappa_{\mathrm{SP}}(G, G') = \sum_{(v_1,v_2)\in V} \sum_{(v_1',v_2')\in V'} \kappa_0(d(v_1, v_2), d(v_1', v_2'))\,.$$

  where $d(v_1, v_2)$ is the shortest-path distance between v_1, v_2.
- κ_0 is a kernel that compares the lengths of the two shortest-paths.
- $\kappa_0(x, y) = x \times y$ (linear kernel) or $\kappa_0(x, y) = \mathbf{1}_{x=y}$ (dirac).

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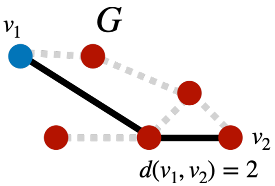

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Remarks

- Complexity Floyd-Warshall on G, $O(|V|^3)$.
- Variants with Bellman–Ford's, Dijkstra's algorithms.
- General complexity for κ_{SP} $O(|V|^2|V'|^2)$.
- Many variants **with attributes**.

GraphHopper kernel

Undirected graphs with edge weights and node attributes.

- Even for real-valued/vector attributes Feragen et al. 2013.

- Kernel is defined as

  $\kappa_{\mathrm{GH}}(G, G') = \sum_{p \in \mathcal{P}_G} \sum_{p' \in \mathcal{P}_{G'}} \kappa_0(p, p')$ where $\mathcal{P}_G$: set of **all shortest-paths**.

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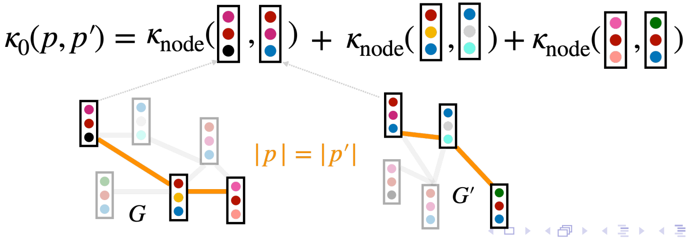
- Base kernel $\kappa_0(p, p') = \begin{cases} \sum_{j=1}^{|p|} \kappa_{\mathrm{node}}(p_j, p'_j) & \text{if equal length} |p| = |p'| \\ 0 & \text{otherwise} \end{cases}$



GraphHopper kernel

Undirected graphs with edge weights and node attributes.

- Even for real-valued/vector attributes Feragen et al. 2013.
- Interestingly averaged overall worst-case complexity $O(|V||V'|\dim(S))$.
- Kernel is defined as

$$\kappa_{\mathrm{GH}}(G, G') = \sum_{p \in \mathcal{P}_G} \sum_{p' \in \mathcal{P}_{G'}} \kappa_0(p, p') \text{ where } \mathcal{P}_G\text{: set of } \textbf{all shortest-paths}.$$

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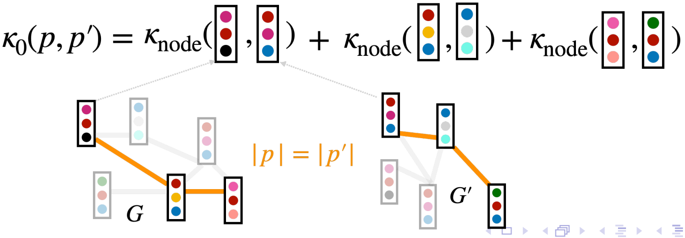


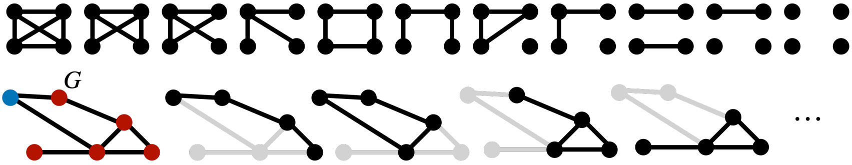
The Graphlet kernel

Principle Shervashidze, Vishwanathan, et al. 2009

- Count substructures in graphs.
- Graphlet = subgraph with k vertices.
- $\mathbb{G} := \{\mathfrak{g}_1, \cdots, \mathfrak{g}_{N_k}\}$ set of k-graphlets (asymptotically $N_k \approx 2^{\binom{k}{2}}/k!$).
- Kernel $\kappa(G, G') = \langle \Phi(G), \Phi(G') \rangle$

$$\Phi(G) \propto (|\{\mathfrak{g}_i \in G\}|, \cdots, |\{\mathfrak{g}_{N_k} \in G\}|)^\top$$

All subgraphs of size 4



Different size 4 graphlets found in G

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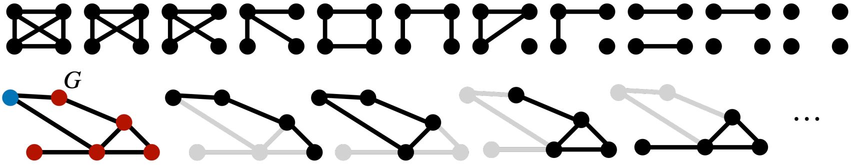
Remarks

- Ignores all labels.
- Computational bottleneck: enumeration of all graphlets.
- Complexity in $O(|V|^k)$ time.
- Typically $k \in \{3, 4, 5\}$.
- Counting all possible subgraphs is NP-hard Gärtner, Flach, and Wrobel 2003.

All subgraphs of size 4



Different size 4 graphlets found in G

The graph isomorphism problem

Checking if two graphs are "identical"

Two graphs $G = (V, E), G' = (V', E')$ are **isomorphic** ($G \cong G'$) if there exists a **bijection** $\Psi : V \to V'$ such that

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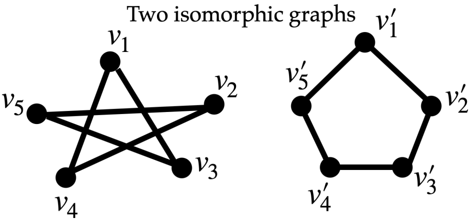

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- Same graphs up to a permutation.
- Currently no known polynomial-time algorithms for solving this problem.
- Not known to be NP-complete.
- Quasi-polynomial algorithm Babai 2016.

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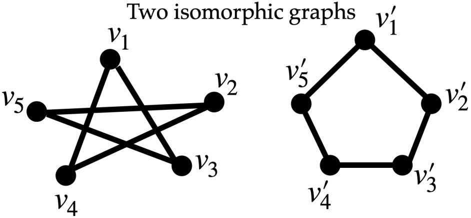

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Weisfeiler-Lehman test of isomorphism Leman and Weisfeiler 1968

On the board

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Multi-set vs set

Key differences

Without being too formal.

- A set $X = \{a, b\}$ is equal to $Y = \{b, a\}$ because $x \in X \iff x \in Y$: **order is irrelevant**.
- A set $Z = \{a, a, b\}$ is also equal to X: **the same element can appear more than once**.
- A **multi-set** denoted with $\{\{\cdots\}\}$ is a “set” where elements can appear more that once.
- The order is still irrelevant.
- For example $\{\{a, a, b\}\}$.
- Formal definition: a multiset is a couple (X, m) where X is a set and a $m : X \to \mathbb{N}$ counts the multiplicity of each element.

Weisfeiler–Lehman kernel

A very popular graph kernel based on Shervashidze, Schweitzer, et al. 2011

- Originally handle graphs with discrete labels.
- Uses **iterative label refinement**.
- Concepts from the Weisfeiler-Lehman test of isomorphism.

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Graphs relabeling/refinement

- Recursively refine the node labels by applying local transformations

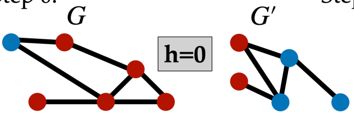
$$a_v = \mathrm{AGGREGATE}\left(\{\{\ell_G^{(\mathrm{old})}(v'); v' \in \mathcal{N}(v)\}\}\right)$$

$$\text{and } \ell_G^{(\mathrm{new})}(v) = \mathrm{COMBINE}\left(\ell_G^{(\mathrm{old})}(v), a_v\right) .$$

- This general idea can give rise to a multitude of distinct graph kernels:
- (i) the specific form of COMBINE, AGGREGATE.
- (ii) which kernels are used to compare the resulting modified graphs.
- (iii) how the graph at multiple scales are aggregated into a single value.

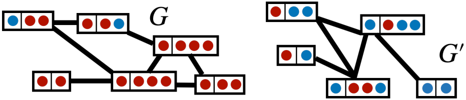
Weisfeiler–Lehman kernel

Step 0:



$\Phi(G) = (5 \quad 1)^\top$ $\Phi(G') = (2 \quad 3)^\top$

Step 1: « Enrich » the labels with neighbors



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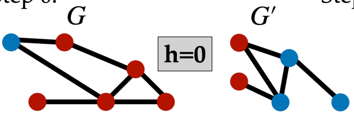

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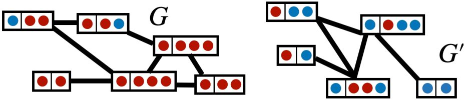

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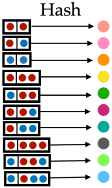
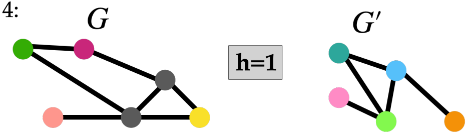


Step 4:



$\Phi(G) = (5 \;\; 1 \;\; 1 \;\; 0 \;\; 0 \;\; 1 \;\; 1 \;\; 1 \;\; 0 \;\; 2 \;\; 0 \;\; 0)^\top$ $\quad$ $\Phi(G') = (2 \;\; 3 \;\; 0 \;\; 1 \;\; 1 \;\; 0 \;\; 0 \;\; 0 \;\; 1 \;\; 0 \;\; 1 \;\; 1)^\top$

-> Step 0 …

-> Terminates after h iterations

Weisfeiler–Lehman kernel

The Weisfeiler–Lehman kernel

- The function AGGREGATE sorts in alphabetic order.
- The function COMBINE hashes to compress the tuple into a single integer-valued label.
- Produces a sequence of graphs $(G_0, \cdots, G_h)$.
- The Weisfeiler–Lehman kernel is

$$\kappa_{\mathrm{WL}}(G, G') = \sum_{i=0}^{h} \kappa_0(G_i, G_i'),$$

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$$\kappa_{\mathrm{WL}}(G, G') = \sum_{i=0}^{h} \kappa_0(G_i, G'_i)\,,$$

  for a base kernel κ_0.
- Most common κ_0 *subtree kernel*: $\Phi(G) =$ number of occurrences of each label in the alphabet of all compressed labels at each step.
- Complexity: for one graph $O(|E| \times h)$.
- Runtime scales only linearly with the number of edges !

Optimal assignment kernel

General setting (Kriege, Giscard, and Wilson 2016)

- Different than "bag of structure" kernels.
- Let $X, Y \subset \Omega$ with $|X| = |Y|$.

$$\kappa_{OA}(X, Y) = \max_{B \in \mathcal{B}(X,Y)} \sum_{x \in X} \kappa_0(x, B(y)) \text{ where } \mathcal{B}(X, Y) = \text{all bijections.}$$

- κ is a valid PSD kernel if $\kappa_0 : \Omega \times \Omega \to \mathbb{R}_+$ is *strong*:

$$\kappa_0(x, y) \geq \min\{\kappa_0(x, z), \kappa_0(z, y)\} \ \forall (x, y, z).$$

- Assign the parts of one objects to the parts of the other *s.t.* the total similarity is maximum possible.

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Weisfeiler-Lehman optimal assignment kernel

- $i \in [\![h]\!], \tau_i(v)$ denotes the color of vertex v at step i of the WL process.
- The base kernel is $\kappa_0(v, v') = \sum_{i=0}^{h} \mathbf{1}_{\tau_i(v) = \tau_i(v')}$ + padding.
- Can also be computed in $O(hm)$.

Continuous alternative to Weisfeiler–Lehman

Hash graph kernel Morris et al. 2016

- Let κ be a graph kernel (such as WL).
- $\mathfrak{H} = \{\mathfrak{h}_1, \mathfrak{h}_2 \cdots\}$ a family of hash functions.
- $\mathfrak{h}_i : \mathbb{R}^d \to \mathbb{N}$ is a hash function.
- $\mathfrak{h}_i(G)$: the discretised graph resulting from applying $\mathfrak{h}_i$ to continuous attributes of the graph.
- The kernel is defined as

$$\kappa_{\mathrm{HGK}}(G, G') = \frac{1}{|\mathfrak{H}|} \sum_{i \in \mathfrak{H}} \kappa(\mathfrak{h}_i(G), \mathfrak{h}_i(G'))\,.$$

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Example of hash functions

- Locality-sensitive hashing schemes Datar et al. 2004.
- Idea: if $\mathbf{x}, \mathbf{y}$ are "close" then $\mathbb{P}[\mathfrak{h}_1(\mathbf{x}) = \mathfrak{h}_2(\mathbf{y})]$ is "high" and conversely.
- More collusion for nearby points.
- e.g. $\mathfrak{h}(\mathbf{x}) = \lfloor \frac{\langle \mathbf{x}, \mathbf{a} \rangle + b}{r} \rfloor, \mathbf{a} \sim \mu, b \sim \mathrm{unif}([0, r])$

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Conclusion

- Graph kernels are very simple but powerful way of using all the ML machinery on graphs.
- The big question is to choose the “right” kernel.
- No straight answer, it depends on the task.
- In practice: always use simple graph kernels as baselines.

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