Kernel Methods: Theory

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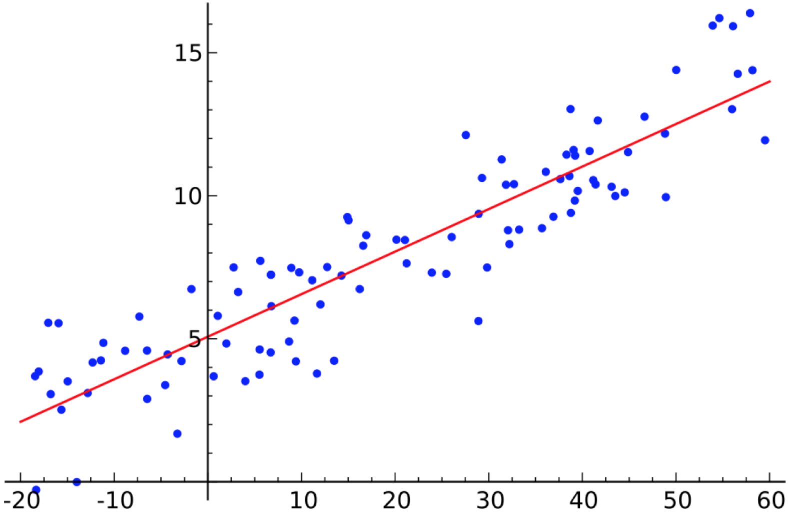
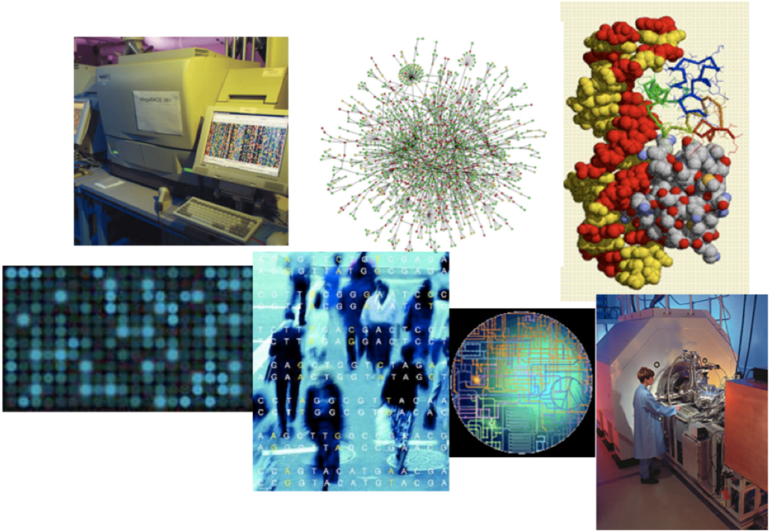
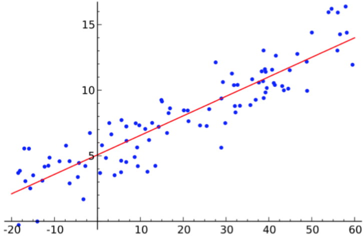
Outline

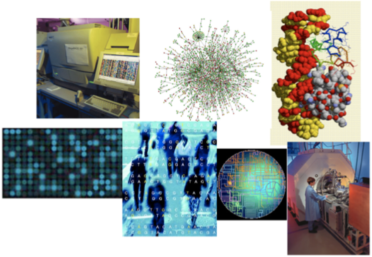
What we know how to solve



But real data are often more complicated ...





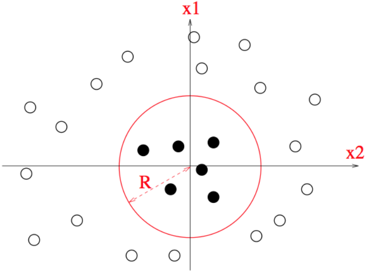


Show some classical examples how to extend well-understood, linear statistical learning techniques to real-world, complicated, structured, high-dimensional data (texts, time series, graphs, distributions, permutations, ...)

Motivation

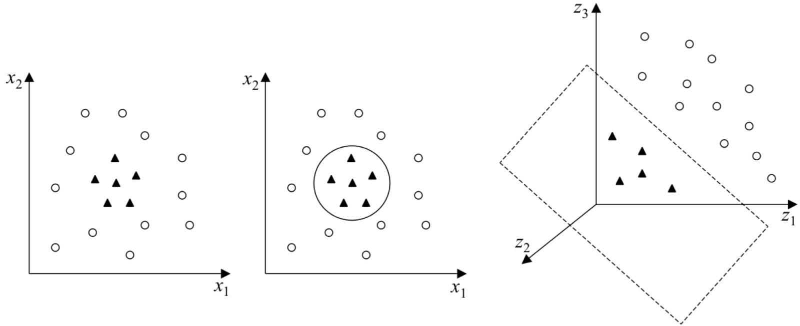
- Efficient computation of inner products in high dimension
- Non-linear decision boundary
- Learning with non-vectorial inputs
- More informative features
- Kernels allow to perform pairwise comparisons

Recall: Non-linear separation



- Linear separation impossible in most problems
- Non-linear mapping $\Phi : X \to \mathbb{H}$ from input space to high-dimensional feature space
- Generalization ability: independent of $\dim(\mathbb{H})$, depends only on d and m

Example: polynomial kernel



For $\mathbf{x} = (x_1, x_2) \in \mathbb{R}^2$, let $\Phi(\mathbf{x}) = (x_1^2, \sqrt{2}x_1x_2, x_2^2) \in \mathbb{R}^3$. Then

$$\begin{aligned} K(\mathbf{x}', \mathbf{x}) &= \Phi(\mathbf{x}') \cdot \Phi(\mathbf{x})^\top \quad \text{[dot product of features]} \\ &= x_1^2(x_1')^2 + 2x_1x_2x_1'x_2' + x_2^2(x_2')^2 \\ &= (x_1x_1' + x_2x_2')^2 = (\mathbf{x}' \cdot \mathbf{x}^\top)^2 \end{aligned}$$

- **Idea**:
  - Define $K : X \times X \to \mathbb{R}$ called kernel, such that

$$\Phi(\mathbf{x}) \cdot \Phi(\mathbf{x}')^\top = K(\mathbf{x}, \mathbf{x}')$$

  - K is often interpreted as a similarity measure

- **Benefits**:
  - Efficiency: K is often more efficient to compute than Φ and the dot product
  - Flexibility: K can be chosen arbitrarily so long as the existence of Φ is guaranteed (PDS condition or Mercer's condition)

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- **Definition**:

$$\forall \mathbf{x}, \mathbf{x}' \in \mathbb{R}^d,\ K(\mathbf{x}, \mathbf{x}') = (\mathbf{x}' \cdot \mathbf{x}^\top + c)^p,\ c > 0$$

- **Example**: for $p = 2$ and $d = 2$,

$$K(\mathbf{x}, \mathbf{x}') = (x_1 x_1' + x_2 x_2' + c)^2$$

$$= \left[x_1^2, x_2^2, \sqrt{2} x_1 x_2, \sqrt{2c} x_1, \sqrt{2c} x_2, c\right] \cdot \begin{bmatrix} {x_1'}^2 \\ {x_2'}^2 \\ \sqrt{2} x_1' x_2' \\ \sqrt{2c} x_1' \\ \sqrt{2c} x_2' \\ c \end{bmatrix}$$

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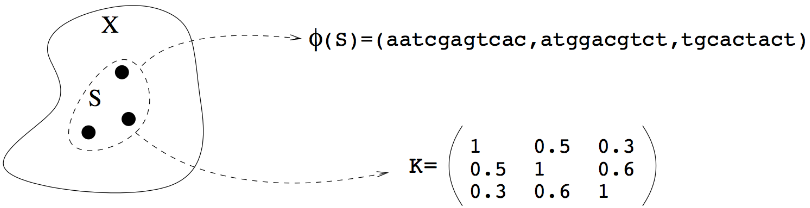
- **Gaussian kernel**:

$$K(\mathbf{x}, \mathbf{x}') = \exp\left(-\frac{\|\mathbf{x} - \mathbf{x}'\|^2}{2\sigma^2}\right), \ \sigma \neq 0$$

- **Sigmoid kernels**:

$$K(\mathbf{x}, \mathbf{x}') = \tanh(a(\mathbf{x} \cdot \mathbf{x}') + b), \ \ a, b >$$



Idea:

- Define a "comparison function": $K : X \times X \to \mathbb{R}$
- Represent a set of m data points $S = \{\mathbf{x}_1, \ldots, \mathbf{x}_m\}$ by the $m \times m$ matrix
$$[K]_{i,j} := K(\mathbf{x}_i, \mathbf{x}_j)$$

- **Definition**: a kernel $K : X \times X \to \mathbb{R}$ is *positive definite symmetric* (PDS) is for any $\{\mathbf{x}_1, \ldots, \mathbf{x}_m\} \subseteq X$ the matrix $\mathrm{K} = [K(\mathbf{x}_i, \mathbf{x}_j)]_{ij} \in \mathbb{R}^{m \times m}$ is symmetric positive semi-definite (SPSD)

- K SPSD if symmetric and one of the 2 equiv. cond.'s:
  - its eigenvalues are non-negative
  - for any $\mathbf{c} \in \mathbb{R}^{m \times 1}$, $\mathbf{c}^\top \mathrm{K} \mathbf{c} = \sum_{i,j=1}^{m} c_i c_j K(\mathbf{x}_i, \mathbf{x}_j) \geq 0$

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$$\forall \mathbf{x}, \mathbf{x}' \in X,\ \widetilde{K}(\mathbf{x}, \mathbf{x}') = \begin{cases} 0, \text{ if } \ K(\mathbf{x}, \mathbf{x}) = 0 \text{ or } K(\mathbf{x}', \mathbf{x}') = 0 \\ \frac{K(\mathbf{x},\mathbf{x}')}{\sqrt{K(\mathbf{x},\mathbf{x})K(\mathbf{x}',\mathbf{x}')}} \end{cases}$$

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$$\sum_{i,j=1}^{m} \frac{c_i c_j K(\mathbf{x}_i, \mathbf{x}_j)}{\sqrt{K(\mathbf{x}_i, \mathbf{x}_i) K(\mathbf{x}_j, \mathbf{x}_j)}} = \sum_{i,j=1}^{m} \frac{c_i c_j \langle \Phi(\mathbf{x}_i), \Phi(\mathbf{x}_j) \rangle}{\|\Phi(\mathbf{x}_i)\|_{\mathbb{H}} \|\Phi(\mathbf{x}_j)\|_{\mathbb{H}}}$$

$$= \left\| \sum_{i=1}^{m} \frac{c_i \Phi(\mathbf{x}_i)}{\|\Phi(\mathbf{x}_i)\|_{\mathbb{H}}} \right\|_{\mathbb{H}}^2 \geq 0$$

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Gaussian kernel is a normalized kernel of

$$(\mathbf{x}, \mathbf{x}') \to \exp\left(\frac{\mathbf{x} \cdot \mathbf{x}'}{\sigma^2}\right) = \sum_{n=0}^{\infty} \frac{(\mathbf{x} \cdot \mathbf{x}')^n}{\sigma^n n!}$$

- Let $\mathbf{x}, \mathbf{z} \in \mathbb{R}^d$. We consider the space of functions $\mathbb{H}$ generated by the linear span of $\{K(\cdot, \mathbf{z}), \mathbf{z} \in \mathbb{R}^d\}$; i.e. arbitrary linear combinations of the form

$$f(\mathbf{x}) = \sum_m a_m K(\mathbf{x}, \mathbf{z}_m),$$

  where each kernel term is viewed as a function of the first argument, and indexed by the second
- Suppose K has an eigen-expansion

$$K(\mathbf{x}, \mathbf{z}) = \sum_{i=1}^{\infty} a_i \phi_i(\mathbf{x}) \phi_i(\mathbf{z})$$

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$$\langle K(\cdot, \mathbf{x}_i), f\rangle = f(\mathbf{x}_i),\ \langle K(\cdot, \mathbf{x}_i), K(\cdot, \mathbf{x}_j)\rangle = K(\mathbf{x}_i, \mathbf{x}_j)$$

- Thus for $f(\mathbf{x}) = \sum_{i=1}^{m} \alpha_i K(\mathbf{x}, \mathbf{x}_i)$ we get that

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- **Theorem**: Let $X \subset \mathbb{R}^d$ be a compact set and $K : X \times X \to \mathbb{R}$ be a continuous and symmetric. Then, K admits a uniformly convergent expansion
$$K(\mathbf{x}, \mathbf{x}') = \sum_{n=0}^{\infty} a_n \phi_n(\mathbf{x}) \phi_n(\mathbf{x}'),$$
with $a_n > 0$ iff for any square integrable function c ($c \in L_2(X)$), the following condition holds
$$\int \int_{X \times X} c(\mathbf{x}) c(\mathbf{x}') K(\mathbf{x}, \mathbf{x}') d\mathbf{x} d\mathbf{x}' \geq 0$$
- This condition is important to guarantee the convexity of the optimization problem for algorithms such as SVMs
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$$\forall \mathbf{x}, \mathbf{x}' \in X,\ K(\mathbf{x}, \mathbf{x}') = \Phi(\mathbf{x}) \cdot \Phi(\mathbf{x}')^\top$$

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  does not depend on representations of f and g
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for any $f_1, \ldots, f_m$ and $c_1, \ldots, c_m$

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  does not depend on representations of f and g
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Reproducing Kernel Hilbert Space IV

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- $\langle\cdot,\cdot\rangle$ is well-defined:
  - Let us consider **Cauchy-Schwarz** inequality for PDS kernels. If K is PDS, then
  $$\mathbf{M} = \begin{pmatrix} K(\mathbf{x},\mathbf{x}) & K(\mathbf{x},\mathbf{z}) \\ K(\mathbf{z},\mathbf{x}) & K(\mathbf{z},\mathbf{z}) \end{pmatrix}$$
  is SPSD for all $\mathbf{x},\mathbf{z} \in X$.
  - In particular, the product of its eigenvalues, $\det(\mathbf{M})$ is non-negative:
  $$\det(\mathbf{M}) = K(\mathbf{x},\mathbf{x})K(\mathbf{z},\mathbf{z}) - K(\mathbf{x},\mathbf{z})^2 \geq 0$$
  - Since $\langle\cdot,\cdot\rangle$ is a PDS kernel, for any $f \in \mathbb{H}_0$ and $\mathbf{x} \in X$
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$$\max_{\alpha} \sum_{i=1}^{m} \alpha_i - \frac{1}{2} \sum_{i,j}^{m} \alpha_i \alpha_j y_i y_j \underbrace{K(\mathbf{x}_i, \mathbf{x}_j)}_{\Phi(\mathbf{x}_i)\cdot\Phi(\mathbf{x}_j)^\top}$$

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$$\min_{f \in \mathbb{H}} \left[\sum_{i=1}^{m} L(y_i, f(\mathbf{x}_i)) + \lambda J(f) \right]$$

where $L(y, f(\mathbf{x}))$ is a loss function, $J(f)$ is a penalty functional, $\mathbb{H}$ is a space of functions

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General regularization problem statement I

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- PDS kernels are used to extend a variety of algorithms in classification and other areas
  - regression
  - ranking
  - dimensionality reduction
  - clustering
- How to define PDS kernels?

- **Theorem**: Positive definite symmetric (PDS) kernels are closed under:
  - sum
  - product
  - tensor product
  - pointwise limit
  - composition with a power series

- **Proof**:
  - closure under *sum*

$$\mathbf{c}^\top \mathrm{K}\mathbf{c} \geq 0 \text{ and } \mathbf{c}^\top \mathrm{K}'\mathbf{c} \geq 0 \Rightarrow \mathbf{c}^\top (\mathrm{K} + \mathrm{K}')\mathbf{c} \geq 0$$

  - closure under *product*: $\mathrm{K} = \mathbf{M}\mathbf{M}^\top$

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- Closure under *composition with power series*
  - assumption: K is a PDS kernel with $|K(\mathbf{x}, \mathbf{z})| < \rho$ for all $\mathbf{x}, \mathbf{z} \in X$ and $f(\mathbf{x}) = \sum_{n=0}^{\infty} a_n x^n$, $a_n \geq 0$ is a power series with radius of convergence ρ
  - $f \circ K$ is a PDS kernel since K^n is a PDS by closure under product, $\sum_{n=0}^{N} a_n K^n$ is PDS by closure under sum, and closure under pointwise limit
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- The squared distance $\|\mathbf{x}-\mathbf{z}\|^2$ in a Hilbert space $\mathbb{H}$ defines an NDS kernel. If $\sum_{i=1}^m c_i = 0$

$$\begin{aligned}\sum_{i,j=1}^m c_i c_j \|\mathbf{x}_i - \mathbf{x}_j\|^2 &= \sum_{i,j=1}^m c_i c_j (\mathbf{x}_i - \mathbf{x}_j)\cdot(\mathbf{x}_i - \mathbf{x}_j)\\ &= \sum_{i,j=1}^m c_i c_j (\|\mathbf{x}_i\|^2 + \|\mathbf{x}_j\|^2 - 2\mathbf{x}_i\cdot\mathbf{x}_j)\\ &= \sum_{i,j=1}^m c_i c_j (\|\mathbf{x}_i\|^2 + \|\mathbf{x}_j\|^2) - 2\sum_{i=1}^m c_i \mathbf{x}_i \cdot \sum_{j=1}^m c_j \mathbf{x}_j\end{aligned}$$

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Examples — cont.'d

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- The kernel defined by $K(\mathbf{x},\mathbf{z}) = \exp(-t\|\mathbf{x}-\mathbf{z}\|^2)$ is PDS for all $t > 0$ since $\|\mathbf{x}-\mathbf{z}\|^2$ is NDS
- The kernel $\exp(-|x-z|^p)$ is not PDS for $p > 2$. Otherwise, for any $t > 0$, $\{x_1,\ldots,x_m\} \subseteq X$ and $\mathbf{c} \in \mathbb{R}^{m\times 1}$

$$\sum_{i,j=1}^{m} c_i c_j e^{-t|x_i - x_j|^p} = \sum_{i,j=1}^{m} c_i c_j e^{-|t^{1/p}x_i - t^{1/p}x_j|^p} \geq 0$$

- This would imply that $|x-z|^p$ is NDS for $p > 2$, but that is not true (prove!!!)