IFT6390
Fondements de l’apprentissage machine

Kernel Trick

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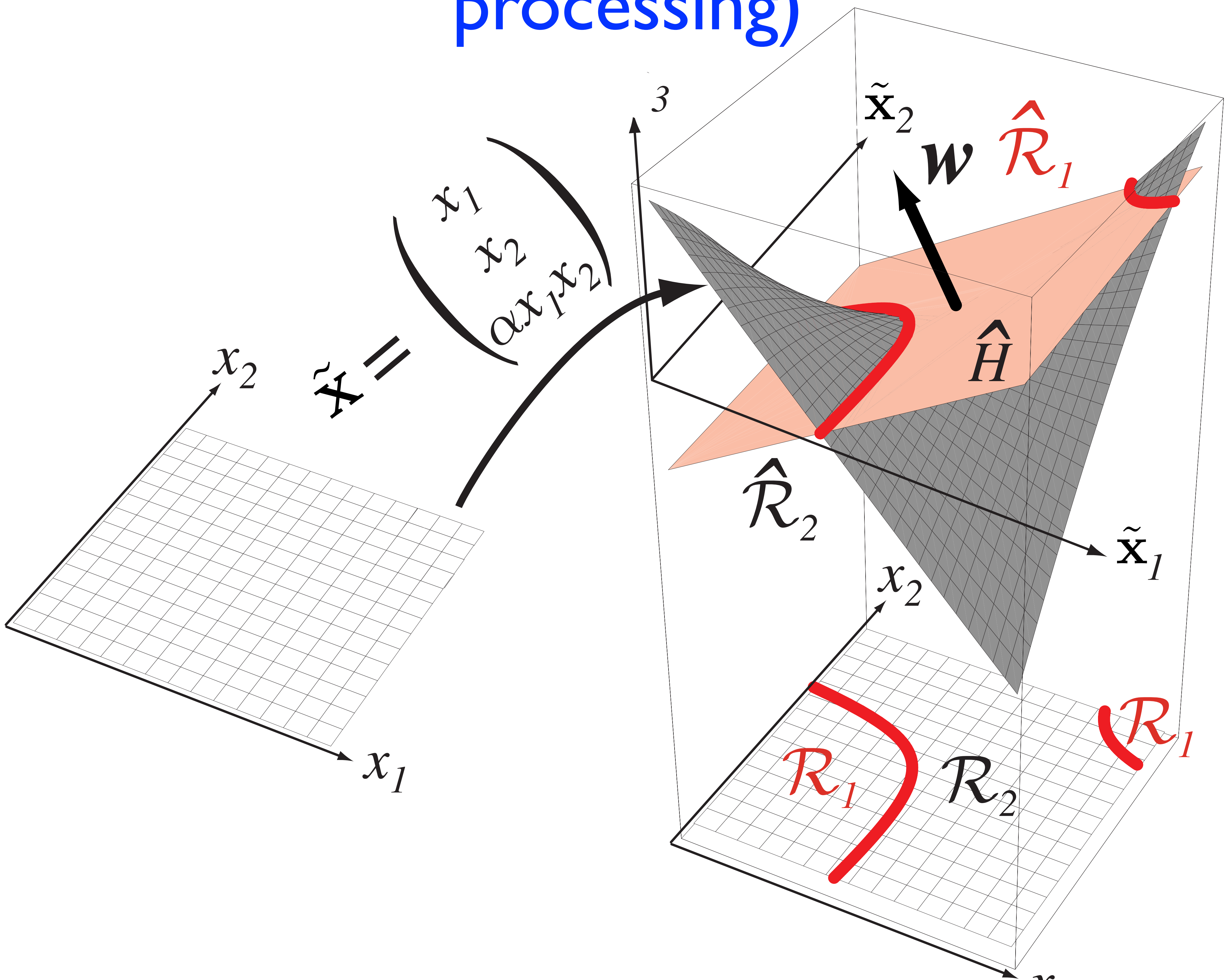
Reminder

- There is a lot of ways to learn a linear classifier (e.g. Perceptron, logistic regression, SVM.)
- We saw that we can obtain a non-linear classifier using a linear classifier by simply pre-processing the input data.
- We just need to apply a non φ to data points x to project them into a feature space of higher dimension:

$$\tilde{\mathbf{x}} = \varphi(\mathbf{x})$$

Ex. *a priori* linear transform (pre-processing)



To obtain a non-linear classifier

We can:

- Use a mapping φ **that we explicitly choose *a priori*** and explicitly compute each $\tilde{\mathbf{x}} = \varphi(\mathbf{x})$

Ex: $\varphi : \underbrace{(x_{[1]}, x_{[2]})}_{\mathbf{x}} \mapsto \underbrace{(1, x_{[1]}, x_{[2]}, x_{[1]}x_{[2]}, x_{[1]}^2, x_{[2]}^2, \sin x_{[1]}, \cos x_{[2]})}_{\tilde{\mathbf{x}}}$

- **Learn a non-linear mapping** φ within some parametrized class of functions. Neural networks can be seen from this perspective (e.g. first layer computes φ)

Ex: $\tilde{\mathbf{x}} = \varphi(\mathbf{x}) = \mathrm{sigmoid}(\mathbf{W}\mathbf{x} + \mathbf{b})$

- Use the **kernel trick**

What's bad with *explicitly choosing the mapping?*

- If *x* is already of high dimension, a polynomial mapping will lead to computing $\tilde{\mathrm{x}}$ in a space of very high dimension.
- Ex: $\mathbf{x} \in \mathbb{R}^d$ and *polynomial mapping* of degree *k* (all products within *k* components of *x*), we need to compute $\tilde{\mathrm{x}}$ in space of dimension ~ d^k .

Ex: d=100, k=5 $\longrightarrow$ 10 000 000 000

The kernel trick

- Can be applied to any learning algorithm that can be expressed in terms of *dot products between input points.*
- The trick consists in supposing that we can compute the dot product $\langle \varphi(\mathbf{x}_i), \varphi(\mathbf{x}_j) \rangle$ directly without having to explicitly compute $\varphi(\mathbf{x})$.
- We choose a kernel K satisfying

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

Example

$$\varphi : \underbrace{(x_{[1]},\, x_{[2]})}_{\mathbf{x}} \quad \mapsto \quad (x_{[1]}^2,\, \sqrt{2}\, x_{[1]} x_{[2]},\, x_{[2]}^2)$$

$$\begin{aligned}
K(\mathbf{x}, \mathbf{y}) &= \langle \varphi(\mathbf{x}),\, \varphi(\mathbf{y}) \rangle \\
&= \left\langle (x_{[1]}^2,\, \sqrt{2}\, x_{[1]} x_{[2]},\, x_{[2]}^2), (y_{[1]}^2,\, \sqrt{2}\, y_{[1]} y_{[2]},\, y_{[2]}^2) \right\rangle \\
&= x_{[1]}^2 y_{[1]}^2 + \sqrt{2} x_{[1]} x_{[2]} \sqrt{2} y_{[1]} y_{[2]} + x_{[2]}^2 y_{[2]}^2 \\
&= x_{[1]}^2 y_{[1]}^2 + 2 x_{[1]} x_{[2]} y_{[1]} y_{[2]} + x_{[2]}^2 y_{[2]}^2 \\
&= (x_{[1]} y_{[1]} + x_{[2]} y_{[2]})^2 \\
&= (\langle \mathbf{x}, \mathbf{y} \rangle)^2
\end{aligned}$$

We can compute dot products in the new feature space without having to explicitly use the feature map!

Terminology

- We call the input space where the original inputs *x* belong the *starting/original/raw input space.*
- The space where φ *maps* the data is *feature space*)
- The kernel *K* corresponds to a *dot product in the feature space.*

Kernel trick: details

- A linear model takes the form

$$g(\mathbf{x}) = \underbrace{\mathbf{w}^T\mathbf{x}}_{\text{dot product}} + b \qquad \mathbf{x} \in \mathbb{R}^d$$

$$g(\mathbf{x}) = b + \underbrace{\langle \mathbf{w}, \mathbf{x} \rangle}_{\text{dot product}} \qquad \mathbf{w} \in \mathbb{R}^d, b \in \mathbb{R}$$

- For many learning algorithms **w** will always be a linear combination of input points:

$$\mathbf{w} = \sum_{i=1}^{n} \alpha_i \mathbf{x}_i$$

Hence **w** can be implicitly represented by using the scalars α_i (sometimes, most of them will be 0, e.g. in SVM)

- Ex: Perceptron find **w** starting from 0 and adding/subtracting vectors that are collinear to input points from the training set (the $\mathbf{x}_i$'s).

Kernel trick: details

In particular, if we work with input points mapped in the feature space $\tilde{\mathbf{x}} = \Phi(\mathbf{x})$, we can implicitly represent $\mathbf{w}$ (potentially of high dimension) with

$$\tilde{\mathbf{w}} = \sum_{i=1}^{n} \alpha_i \tilde{\mathbf{x}}_i = \sum_{i=1}^{n} \alpha_i \varphi(\mathbf{x}_i)$$

In which case we can compute

$$\begin{aligned} g(\tilde{\mathbf{x}}) &= b + \langle \tilde{\mathbf{w}}, \tilde{\mathbf{x}} \rangle \\ &= b + \langle \tilde{\mathbf{w}}, \varphi(\mathbf{x}) \rangle \\ &= b + \left\langle \left(\sum_{i=1}^{n} \alpha_i \varphi(\mathbf{x}_i) \right), \varphi(\mathbf{x}) \right\rangle \\ &= b + \sum_{i=1}^{n} \alpha_i \langle \varphi(\mathbf{x}_i), \varphi(\mathbf{x}) \rangle \\ &= b + \sum_{i=1}^{n} \alpha_i K(\mathbf{x}_i, \mathbf{x}) \end{aligned}$$

Since we only need to compute dot products between points in the feature space, we can use the kernel K without ever having to explicitly use the feature map!

! Warning !

$$\tilde{\mathbf{w}} = \sum_{i=1}^{n} \alpha_i \tilde{\mathbf{x}}_i = \sum_{i=1}^{n} \alpha_i \varphi(\mathbf{x}_i) \neq \varphi\left(\sum_{i=1}^{n} \alpha_i \mathbf{x}_i\right)$$

So you **cannot** simply run the algorithm in the original space, and then apply φ to the weight vector returned by the algorithm!

You need to *implicitly* run the algorithm on the points $\varphi(x)$ (in the feature space).

Kernel trick: summary

- Express an algorithm in the *feature space (corresponding to some feature map φ)* using only dot products between input points.
- In general, this will imply keeping track of some weight vector α used by the algorithm (for a linear combination of input points)
- Replace all dot products with a kernel function *K*.
- This corresponds to running the algorithm in the feature space without ever having to explicitly compute the mappings with the feature map φ.

Common kernel functions

- Usual scalar product: $K(a, b) = \langle a, b \rangle$
- Polynomial kernel of degree *k*: $K_k(a, b) = (1 + \langle a, b \rangle)^k$
- RBF (or Gaussian) kernel: $K_\sigma(a, b) = e^{-\frac{1}{2}\frac{\|a-b\|^2}{\sigma^2}}$

Remarks:

- There are a lot of other useful kernels
- There are also kernels on strings, trees, graphs...
- Kernels can have (hyper)-parameters. ex: $\sigma \text{ ou } k$
- The feature map φ associated with a kernel *K* cannot always be expressed in a nice analytical form: the RBF kernel corresponds to a feature space of infinite dimension!

What it takes to be a kernel...

- Not all functions K(. , .) are kernels: there is not always a mapping φ such that K(a,b) = $< \varphi(a), \varphi(b) >$
- *Mercer Theorem:* This will be the case if, and only if, *K* is continuous, symmetric and positive semi-definite.

Kernel-trick friendly algorithms:

Many learning algorithms that usually return a linear classifier/ regressor can be kernelized. Among others:

classification

- Perceptron => Kernel Perceptron
- Support Vector Machines (SVM)
- Logistic Regression

regression

- Linear Regression
- Ridge Regression
- Support Vector Regression (SVM variant for regression)
- Bayesian Linear Regression => Gaussian Processes (also Kriging in stats).

unsupervised

- Principal Component Analysis (PCA)