Kernel Methods

Machine Learning

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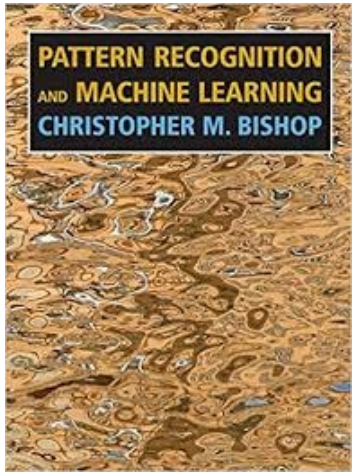
Outline and References

- Outline
  - Introduction [PRML 6]
  - Kernel Ridge Regression [PRML 6.1]
  - Kernel Design [PRML 6.2]
  - Kernel Regression [PRML 6.3, 2.5.1]
  - Gaussian Processes [PRML 6.4]

- References
  - This slides are based on material of prof. Marcello Restelli
  - Pattern Recognition and Machine Learning, Bishop [PRML]

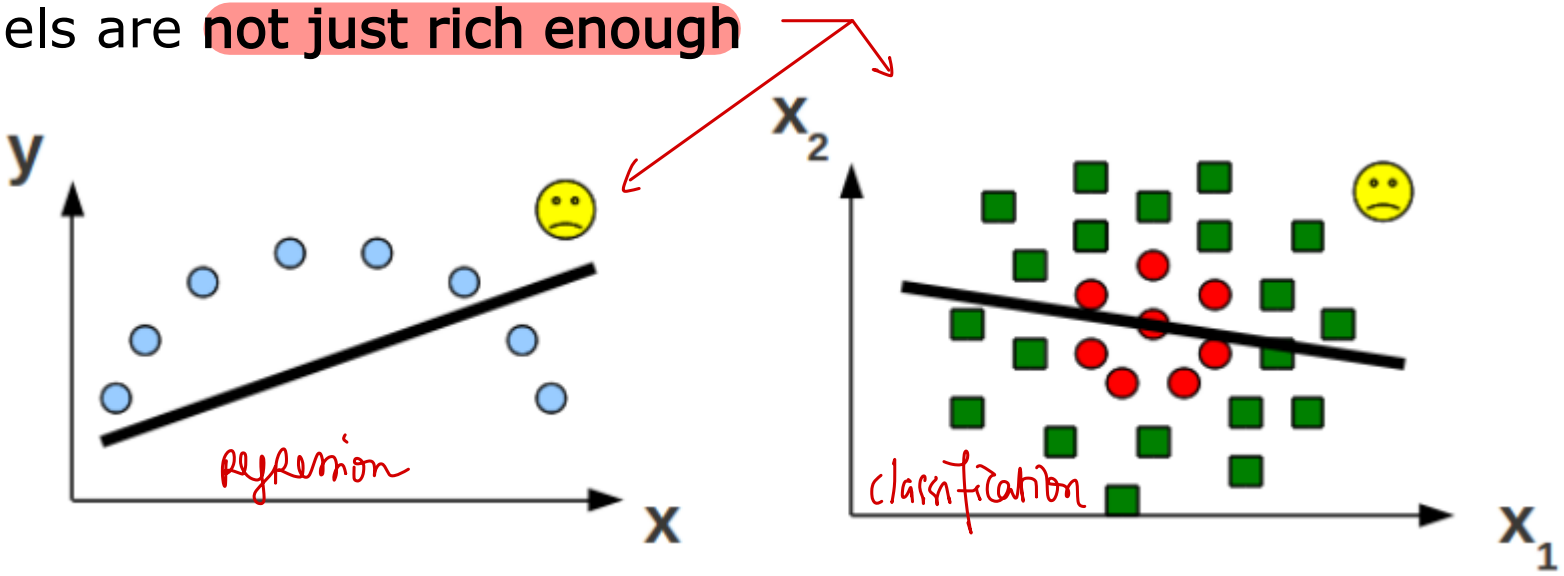


Introduction to Kernel Methods

"extension of what we saw in linear regression, & linear classification"

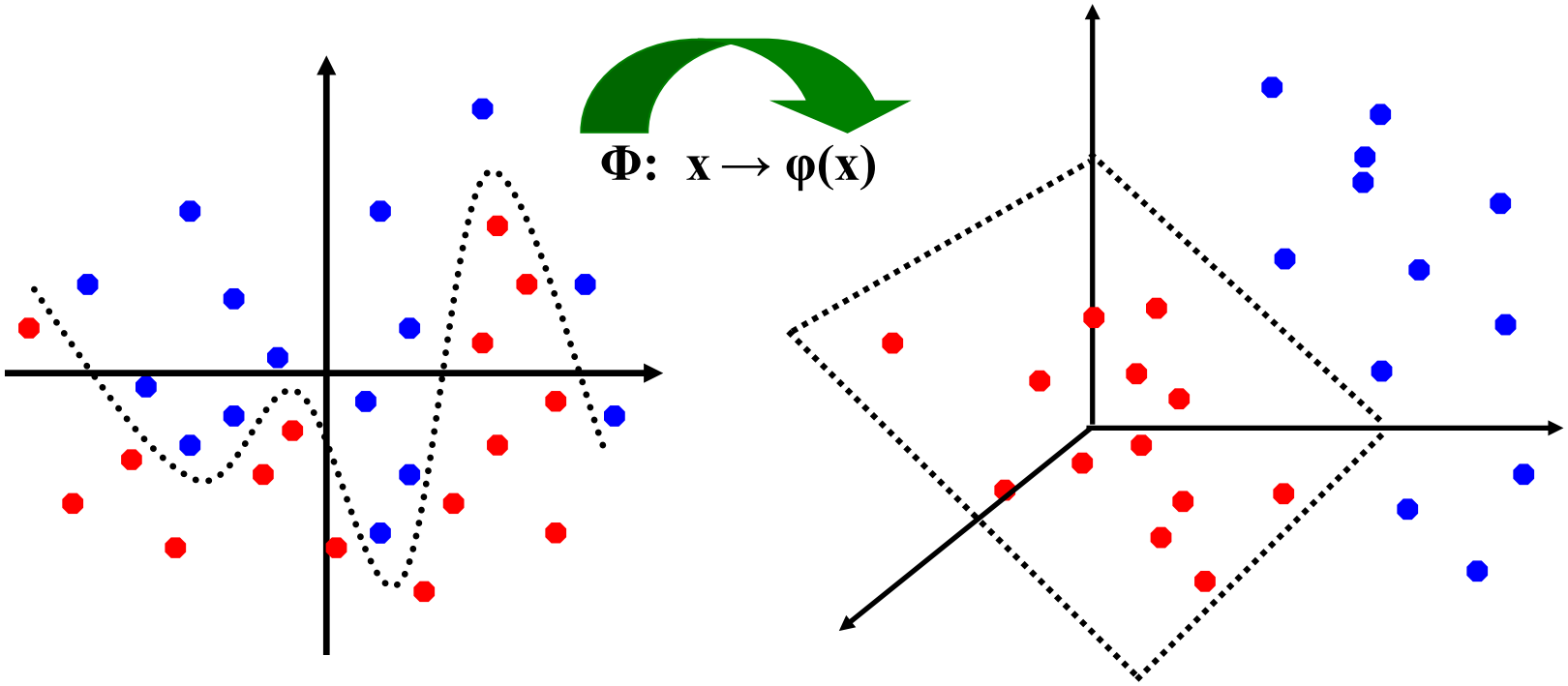
Feature Mapping

- Often we want to **capture nonlinear patterns** in the data
  - Nonlinear Regression: input-output relationship may not be linear
  - Nonlinear Classification: Classes may not be separable by a linear boundary
- Linear models are **not just rich enough**



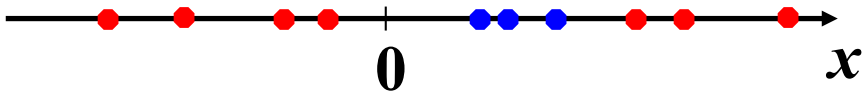
- **Kernel methods** allow to make linear models work in nonlinear settings by **mapping data to higher dimensions** where it exhibits linear patterns

Feature Mapping (2)

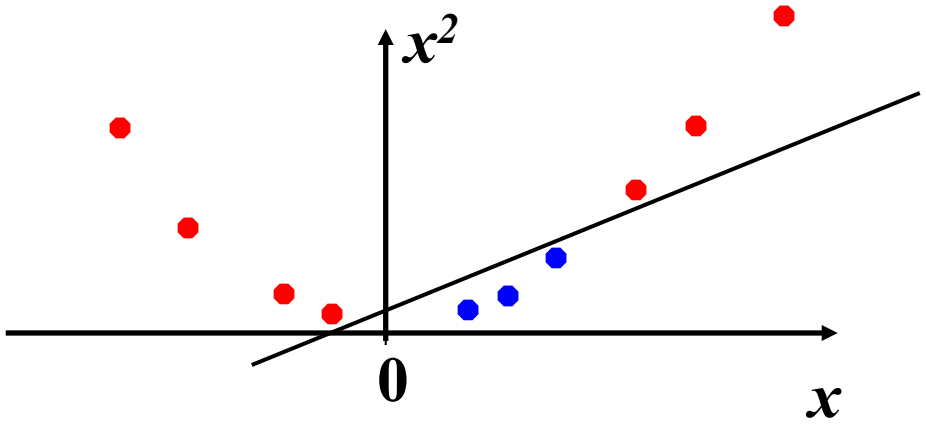


Example: 1D Binary Classification

- Let consider this binary classification problem for which **no linear separator** exists:

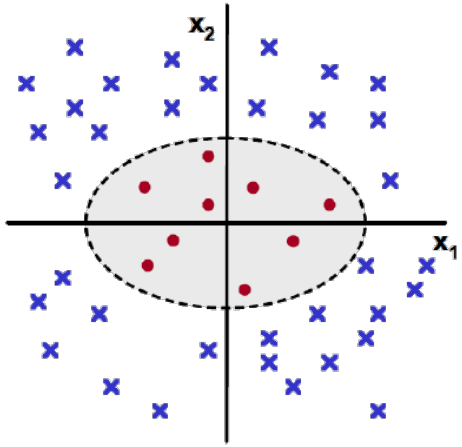


- Now let map the input space (single variable x) to a feature space with **two features**: $x \rightarrow \{x, x^2\}$
- Data is now linear separable:

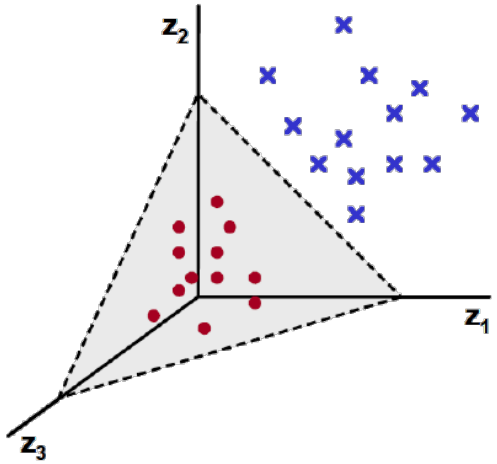


Example: 2D Binary Classification

- Let consider the following binary classification problem for which **no linear separator** exists in the input space $\mathbf{x} = \{x_1, x_2\}$



- We can make data linearly separable by mapping the input space to a suitable feature space: $\mathbf{x} = \{x_1, x_2\} \rightarrow \boldsymbol{z} = \{x_1^2, \sqrt{2}x_1x_2, x_2^2\}$



Why kernel methods?

- Let consider a **quadratic mapping** for a problem with M input variables:

$$\mathbf{x} = \{x_1, \ldots, x_M\} \rightarrow \phi(\mathbf{x}) = \{x_1^2, x_2^2, \ldots, x_M^2, x_1x_2, x_2x_3, \ldots, x_1x_M, \ldots, x_{M-1}x_M\}$$

→ the dimension of my space will explode very quickly !

- **Curse of dimensionality!** The number of features grows significantly with the number of input variable and the mapping become quickly **computationally unfeasible**
- **Kernels methods** deal with this issue:
  - they **don't require to explicitly compute** the feature mapping
  - they are **expensive** but computationally **feasible**

different mathematical technique ...

Kernel Functions

- The **kernel function** is defined as the **scalar product** between the feature vectors of two data samples:

$$k(x, x') = \phi(\mathbf{x})^T \phi(\mathbf{x}')$$

} Scalar product in our high dimensional feature space.

By def:

- Kernel function is **symmetric:** $k(\mathbf{x}, \mathbf{x}') = k(\mathbf{x}', \mathbf{x})$
- Kernel function can be interpreted as a **similarity measure** between $\mathbf{x}$ and $\mathbf{x}'$ → in our feature space.
- Very large feature vectors (even non finite ones) might result in an easy to compute kernel function → In fact we don't need to compute $\phi(x)$ & $\phi(x')$ to compute $k(x,x')$.

we'll prove this later.

- Special class of kernels
  - **Stationary kernels:** $k(\mathbf{x}, \mathbf{x}') = k(\mathbf{x} - \mathbf{x}')$
  - **Homogeneous kernels** (or **radial basis functions**): $k(\mathbf{x}, \mathbf{x}') = k(||\mathbf{x} - \mathbf{x}'||)$

Kernel Trick

- What kernel function is used for?
  - It is possible to rework the representation of linear models to replace all the terms that involve $\phi(\mathbf{x})$ with other terms that involve only $k(\mathbf{x},\cdot)$
  - In other words, the output of linear model can be computed only on the basis of the similarities between data samples (computed with the kernel function)
- This approach, called **kernel trick**, is used in several learning algorithm
  - Ridge Regression
  - K-NN Regression
  - Perceptron
  - (Nonlinear) PCA
  - Support Vector Machines
  - ...

Kernel Trick

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  - K-NN Regression
  - Perceptron
  - (Nonlinear) PCA
  - Gaussian Processes (Bayesian Linear Regression)
  - Support Vector Machines
  - ...

Kernel Ridge Regression

Dual Representation

- Let's go back to the loss function used for the **ridge regression:**

$$L(\mathbf{w}) = \underbrace{\frac{1}{2}\sum_{n=1}^{N}\left(\mathbf{w}^T\boldsymbol{\phi}(\mathbf{x}_n) - t_n\right)^2}_{\text{RSS}} + \underbrace{\frac{\lambda}{2}\mathbf{w}^T\mathbf{w}}_{\text{Regularization } \|.\|_2} = \overbrace{\frac{1}{2}(\mathbf{t}-\boldsymbol{\Phi}\mathbf{w})^T(\mathbf{t}-\boldsymbol{\Phi}\mathbf{w}) + \frac{\lambda}{2}\mathbf{w}^T\mathbf{w}}^{\text{Matrix form.}}$$

- To solve it, we set to zero the gradient of L with respect to $\mathbf{w}$:

$$\frac{\partial L(\mathbf{w})}{\partial \mathbf{w}} = \lambda\mathbf{w} - \boldsymbol{\Phi}^T(\mathbf{t}-\boldsymbol{\Phi}\mathbf{w}) = 0$$

- Now, instead of solving it for $\mathbf{w}$, let do a variable change:

$$\mathbf{a} = \lambda^{-1}(\mathbf{t}-\boldsymbol{\Phi}\mathbf{w})$$

Instead we do a variable change:

$$\mathbf{w} = \boldsymbol{\Phi}^T\lambda^{-1}(\mathbf{t}-\boldsymbol{\Phi}\mathbf{w}) = \boldsymbol{\Phi}^T\mathbf{a}$$

We don't want to follow this path today! Indeed we don't want to compute Φ matrix because it would mean computing $\phi(x)$, $\forall x \in$ DATASET. → Too expensive.

Dual Representation (2)

- Now we can replace **w** in the gradient:

By:

$$\mathbf{w} = \boldsymbol{\Phi}^T \mathbf{a}$$

$$\frac{\partial L(\mathbf{w})}{\partial \mathbf{w}} = \lambda \mathbf{w} - \boldsymbol{\Phi}^T (\mathbf{t} - \boldsymbol{\Phi}\mathbf{w}) = 0$$

$$\boldsymbol{\Phi}^T \left(\lambda \mathbf{a} - \left(\mathbf{t} - \boldsymbol{\Phi}\boldsymbol{\Phi}^T \mathbf{a} \right) \right) = 0$$

$$\boldsymbol{\Phi}\boldsymbol{\Phi}^T \mathbf{a} + \lambda \mathbf{a} = \mathbf{t} \longrightarrow (\Phi\Phi^T + \lambda I)a = t$$

$$\mathbf{a} = (\mathbf{K} + \lambda \mathbf{I})^{-1} \mathbf{t}$$

$$\mathbf{K} = \boldsymbol{\Phi}\boldsymbol{\Phi}^T$$

Gram Matrix

Φ = [N×M] $\begin{pmatrix} \vec{\phi}^T(x_1) \\ \vec{\phi}^T(x_2) \\ \vdots \\ \vec{\phi}^T(x_N) \end{pmatrix}$ Φ^T = [M×N] $\left(\vec{\phi}(x_1) \dots \vec{\phi}(x_N)\right)$

So $\Phi\Phi^T$ looks like cf the next slide...

Gram Matrix and Kernel Function

- The **Gram matrix** is a NxN matrix, where each element is the inner product between the feature vectors:

we didn't have to compute the $\phi(x)$... we use only $k(x_n, x_m)$!

$$K = \begin{bmatrix} k(\mathbf{x}_1, \mathbf{x}_1) & \dots & k(\mathbf{x}_1, \mathbf{x}_N) \\ \vdots & \ddots & \vdots \\ k(\mathbf{x}_N, \mathbf{x}_1) & \dots & k(\mathbf{x}_N, \mathbf{x}_N) \end{bmatrix}$$

Recall :

$$k(\mathbf{x}_n, \mathbf{x}_m) = \boldsymbol{\phi}(\mathbf{x}_n)^T \boldsymbol{\phi}(\mathbf{x}_m)$$

  - K matrix represents the **similarities** between each pair of samples in the training data

Prediction Function

- How can we compute the prediction using the dual representation?

$$\mathbf{w} = \mathbf{\Phi}^T \mathbf{a} \longrightarrow w^T = a^T \phi^{TT} = a^T \phi$$

$$y(\mathbf{x}) = \mathbf{w}^T \phi(\mathbf{x}) = \mathbf{a}^T \mathbf{\Phi}\phi(\mathbf{x}) = \mathbf{k}(\mathbf{x})^T (K + \lambda \mathbf{I}_N)^{-1} \mathbf{t}$$

$$\mathbf{a} = (\mathbf{K} + \lambda \mathbf{I})^{-1} \mathbf{t}$$

LR model formula for prediction.

(*)

we transposed everything since the result is a $\mathbb{R}$: $a^T k(x) = k(x)^T a$.

(*) $\begin{bmatrix} \vec{\phi}^T(x_1) \\ \vdots \\ \vec{\phi}^T(x_N) \end{bmatrix}$ $N \times M$

$\phi(X)$ $M \times 1$ = $\begin{bmatrix} \vec{\phi}^T(x_1)\,\phi(X) \\ \vdots \\ \vec{\phi}^T(x_N)\,\phi(X) \end{bmatrix} = \begin{bmatrix} k(x_1, X) \\ \vdots \\ k(x_N, X) \end{bmatrix} = k(x)$

The actual input I'm considering.

NB: we never computed explicitely the feature mapping ϕ !

Prediction Function

It's way less expensive to compute K, $k(x_i, x_j)$, etc. than to compute ϕ...

- How can we compute the prediction using the dual representation?

$$y(\mathbf{x}) = \mathbf{w}^T \boldsymbol{\phi}(\mathbf{x}) = \mathbf{a}^T \boldsymbol{\Phi} \boldsymbol{\phi}(\mathbf{x}) = \mathbf{k}(\mathbf{x})^T (K + \lambda \mathbf{I}_N)^{-1} \mathbf{t}$$

$y(\mathbf{x}) \in \mathbb{R}$.

$1 \times N$ vec.

$N \times 1$ vector

"$\phi'(x)$"

"Let's call it w'"

"$y(x) = \phi'(x)\, w'$"

  - Where $\mathbf{k}(\mathbf{x})$ is such that $k_n(\mathbf{x}) = k(\mathbf{x}_n, \mathbf{x}) \; \forall \mathbf{x}_n \in \mathcal{D}$

- Accordingly the prediction is computed as the linear combination of the **target values** of the samples in the **training set**

Here: non-parametric type of model since I don't choose the amount of parameters that I have, it's the data that determine it.

Original vs Dual Representation?

- Original representation
  - Requires to compute the inverse of $(\boldsymbol{\Phi}^T\boldsymbol{\Phi} + \lambda \boldsymbol{I_M})$ which is a MxM matrix
  - Is computationally convenient when M is rather small
- Dual representation
  - Requires to compute the inverse of $(\mathbf{K} + \lambda \boldsymbol{I_N})$ which is a NxN matrix
  - Is computationally convenient when M **is very large or even infinite**
  - Does not require to explicitly compute $\boldsymbol{\Phi}$, making it possible to apply this approach also to complex type of data (e.g., graphs, sets, strings, text, etc.)
  - The **similarity between data samples** (i.e., the **kernel function**) is generally both less expensive to compute and easy to design than computing $\boldsymbol{\Phi}$

Kernel Function Design

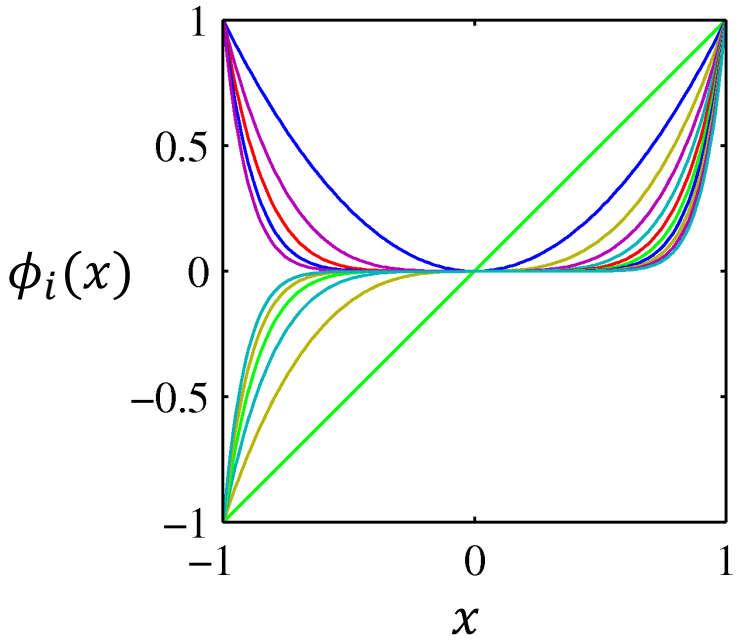
Design of Kernels

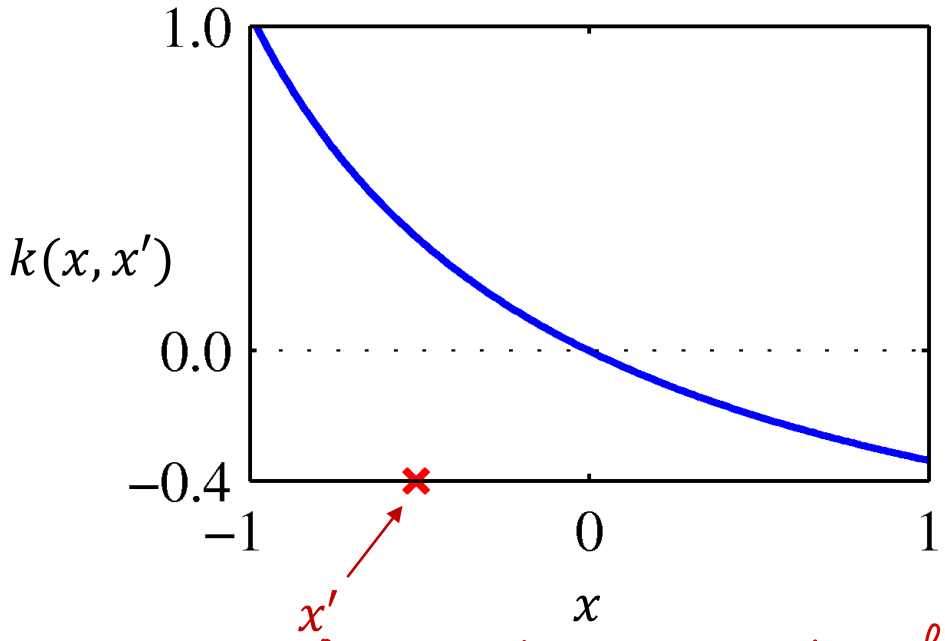
- We defined the kernel function as the dot product in the feature space:

DEF:

$$k(x, x') = \boldsymbol{\phi}(\mathbf{x})^T \boldsymbol{\phi}(\mathbf{x}') = \sum_{i=1}^{M} \phi_i(\mathbf{x}) \phi_i(\mathbf{x}')$$

- Examples (1D input space)





one of the point, x', is fixed. And x moves.

Design of Kernels

- We defined the kernel function as the dot product in the feature space:

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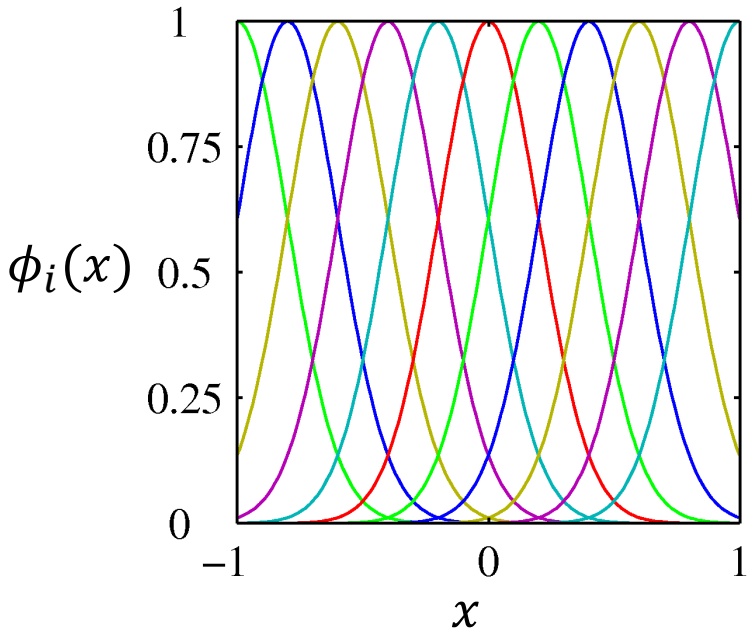

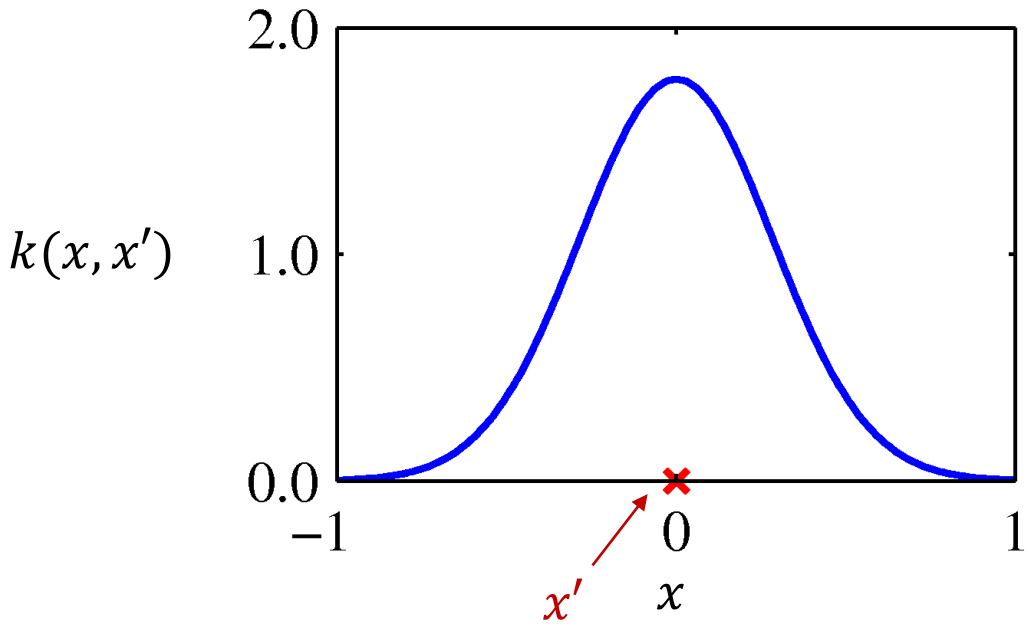

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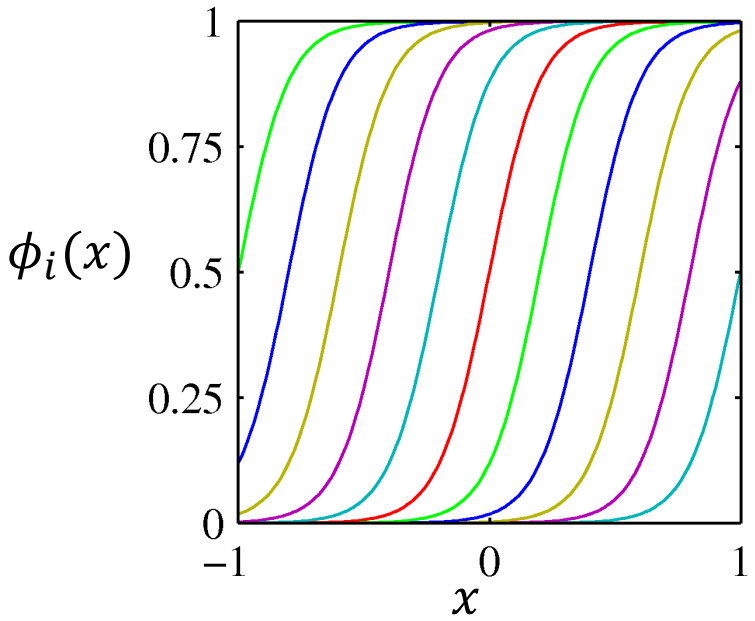
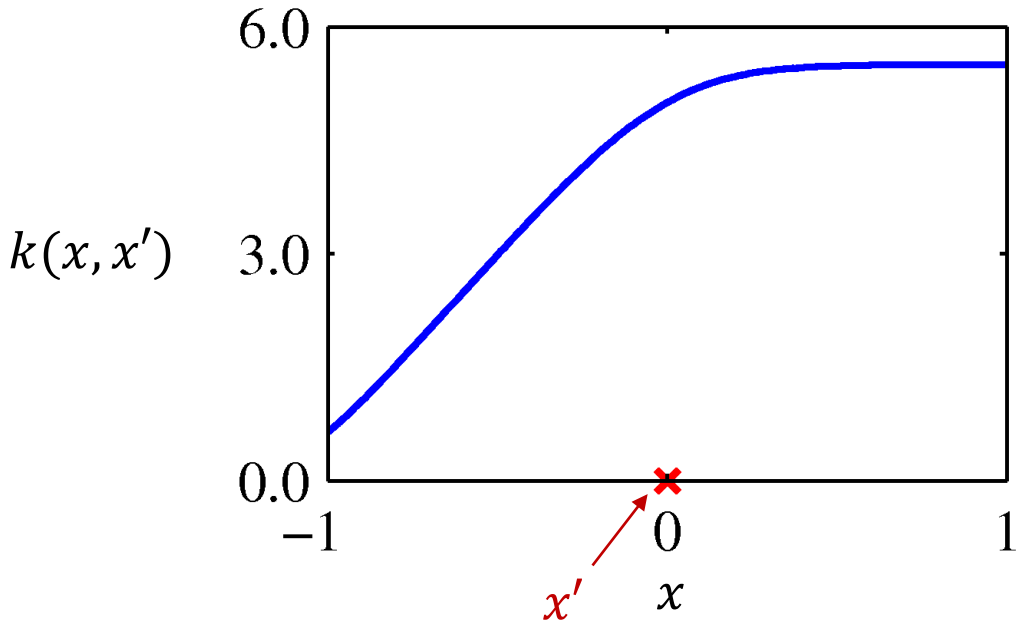




Design of Kernels: alternative methods

- We do not necessarily have to compute the kernel function starting from the feature space, as we do not want to explicitly compute the feature vectors
- There are two major alternatives to design a kernel function:
  1. **Directly** design the kernel functions from scratch
  2. Design **from existing** kernel functions by applying a **set of rules**
- In general, we must make sure that the designed kernel functions is **valid**, that is it correspond to a scalar product into any feature space
- **Mercer Theorem:** Any **continuous, symmetric, positive semi-definite** kernel function $k(x, x')$ can be expressed as a dot product in a high-dimensional space
  - **Necessary and sufficient** condition for a function $k(\mathbf{x}, \mathbf{x}')$ to be a valid kernel is that Gram matrix K is positive semi-definite for all possible choice of $\mathcal{D} = \{\mathbf{x}_i\}$
  - It means $\mathbf{x}^T K \mathbf{x} > 0$ for any non zero real vector $\mathbf{x}$, i.e., $\sum_i \sum_j K_{ij} x_i x_j$ for any real numbers x_i and x_j

Kernel direct design: an example

- Let consider the following kernel function: $k(\mathbf{x}, \mathbf{x}') = (\mathbf{x}^T\mathbf{x}')^2$
- Is it a valid kernel function?
- Let check it in a **two dimensional space:**

$$k(\mathbf{x}, \mathbf{x}') = (\mathbf{x}^T\mathbf{x}')^2 = (x_1x_1' + x_2x_2')^2 = x_1^2{x_1'}^2 + 2x_1x_1'x_2x_2' + x_2^2{x_2'}^2$$
$$= (x_1^2, \sqrt{2}x_1x_2, x_2^2)({x_1'}^2, \sqrt{2}x_1'x_2', {x_2'}^2)^T = \boldsymbol{\phi}(\mathbf{x})^T\boldsymbol{\phi}(\mathbf{x}')$$

  - It does correspond to the scalar product in a feature space with only second order terms (also notice that is **less computationally expensive to compute**)
- To get also constant and linear terms, we can define $k(\mathbf{x}, \mathbf{x}') = (\mathbf{x}^T\mathbf{x}' + c)^2$
- To get all the terms up to degree z, we can define $k(\mathbf{x}, \mathbf{x}') = (\mathbf{x}^T\mathbf{x}' + c)^z$

Rules to design valid kernels

From valid kernels, how to generate other valid kernels ?

- Given valid kernels $k_1(\mathbf{x},\mathbf{x}')$ and $k_2(\mathbf{x},\mathbf{x}')$ the following rules can be applied to design a new valid kernel:

1. $k(\mathbf{x},\mathbf{x}') = ck_1(\mathbf{x},\mathbf{x}')$, where $c > 0$ is a constant
2. $k(\mathbf{x},\mathbf{x}') = f(\mathbf{x})k_1(\mathbf{x},\mathbf{x}')f(\mathbf{x}')$, where $f(\cdot)$ is any function
3. $k(\mathbf{x},\mathbf{x}') = q(k_1(\mathbf{x},\mathbf{x}'))$, where $\mathrm{q}(\cdot)$ is a polynomial with non-negative coefficients
4. $k(\mathbf{x},\mathbf{x}') = exp(k_1(\mathbf{x},\mathbf{x}'))$
5. $k(\mathbf{x},\mathbf{x}') = k_1(\mathbf{x},\mathbf{x}') + k_2(\mathbf{x},\mathbf{x}')$
6. $k(\mathbf{x},\mathbf{x}') = k_1(\mathbf{x},\mathbf{x}')k_2(\mathbf{x},\mathbf{x}')$
7. $k(\mathbf{x},\mathbf{x}') = k_3(\phi(\mathbf{x}),\phi(\mathbf{x}'))$, where $\phi(\mathbf{x})$ maps $\mathbf{x}$ to $\mathbb{R}^M$ and $k_3(\cdot,\cdot)$ is a valid kernel in $\mathbb{R}^M$
8. $k(\mathbf{x},\mathbf{x}') = \mathbf{x}^T\mathbf{A}\,\mathbf{x}'$, where $\mathbf{A}$ is a symmetric semidefinite matrix
9. $k(\mathbf{x},\mathbf{x}') = k_a(\mathbf{x}_a,\mathbf{x}'_a) + k_b(\mathbf{x}_b,\mathbf{x}'_b)$
10. $k(\mathbf{x},\mathbf{x}') = k_a(\mathbf{x}_a,\mathbf{x}'_a)k_b(\mathbf{x}_b,\mathbf{x}'_b)$

} Where $\mathbf{x} = \{\mathbf{x}_a\} \cup \{\mathbf{x}_b\}$ are two subsets no necessarily disjoints of variables and k_a, k_b are valid kernels

Gaussian Kernel

The most used type of kernels.

↳ The corresponding feature space is of ∞-dimension.

- This is a commonly used kernel:

$$k(\mathbf{x}, \mathbf{x}') = \exp(-\|\mathbf{x} - \mathbf{x}'\|^2 / 2\sigma^2)$$

  - We can check it is a valid kernel, expanding the square:

$$\|\mathbf{x} - \mathbf{x}'\|^2 = \mathbf{x}^T\mathbf{x} + \mathbf{x}'^T\mathbf{x}' - 2\mathbf{x}^T\mathbf{x}'$$

$$\Rightarrow \quad k(\mathbf{x}, \mathbf{x}') = \underbrace{\exp(-\mathbf{x}^T\mathbf{x}/2\sigma^2)}_{f(\mathbf{x})} \exp(\mathbf{x}^T\mathbf{x}'/\sigma^2) \underbrace{\exp(-\mathbf{x}'^T\mathbf{x}'/2\sigma^2)}_{f(\mathbf{x}')}$$

If previous slide → valid kernel.

Rule 2 and 4

- The feature space corresponding to Gaussian kernel has infinite dimension
- We can extend Gaussian Kernel by replacing $\mathbf{x}^T\mathbf{x}'$ with a nonlinear kernel $\kappa(\mathbf{x}, \mathbf{x}')$:

$$k(\mathbf{x}, \mathbf{x}') = \exp\left(-\frac{1}{2\sigma^2}(\kappa(\mathbf{x}, \mathbf{x}) + \kappa(\mathbf{x}', \mathbf{x}') - 2\kappa(\mathbf{x}, \mathbf{x}'))\right)$$

Kernels for Symbolic Data

Non-numerical data.

- Kernel methods can be extended also to inputs different from real vectors, such as graphs, sets, strings, texts, etc.
- In fact, the kernel function represents a measure of the similarity between two samples
- A common kernel used for set is:

$$k(A_1, A_2) = 2^{|A_1 \cap A_2|}$$

Cardinal of $A_1 \cap A_2$.

This is a possible "similarity" measure between two sets A_1 & A_2.

Kernels Based on Generative Models

- It is also possible to define a kernel function based on probability distribution
- Given a generative model $p(\mathbf{x})$ we can define a kernel as:

$$k(\mathbf{x}, \mathbf{x}') = p(\mathbf{x})p(\mathbf{x}')$$

- It is a valid kernel, since it corresponds to the inner product in the one dimensional feature space defined mapping $\mathbf{x}$ to $p(\mathbf{x})$

Kernel Regression

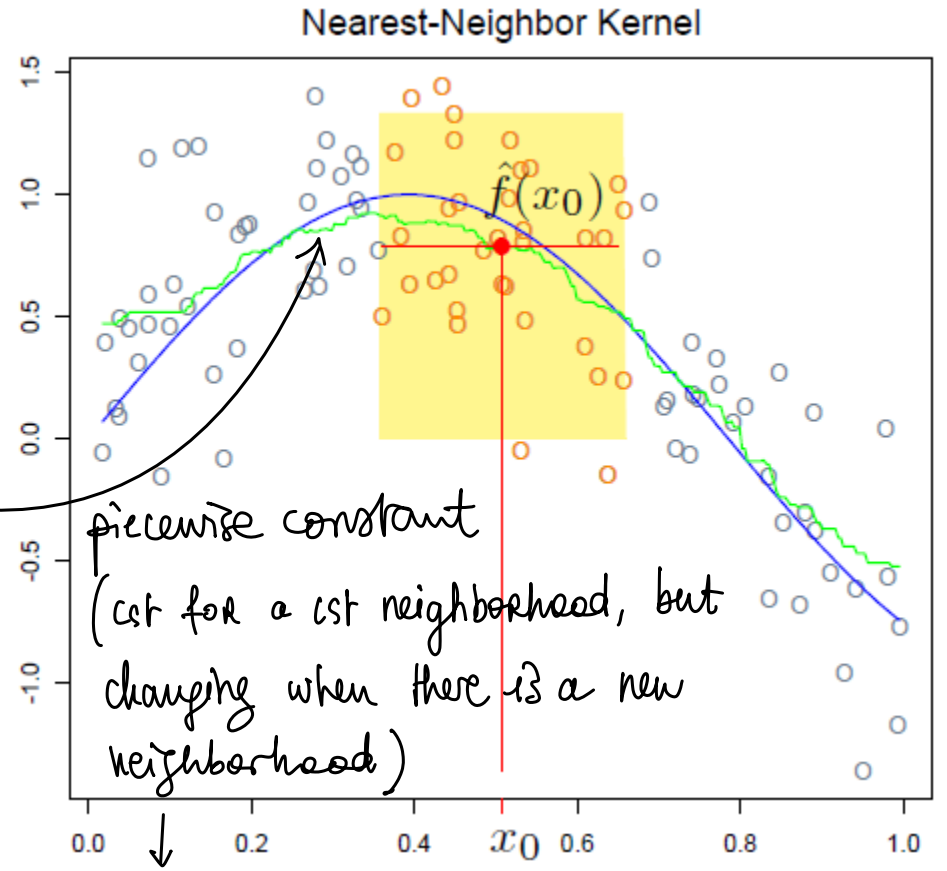
k-NN Regression

- The k Nearest Neighbour (k-NN) can be applied to solve a regression problem by averaging the K nearest samples in the training data:

AVG of the target data in $N_k(x)$.

$$\hat{f}(\mathbf{x}) = \frac{1}{k} \sum_{\mathbf{x}_i \in N_k(\mathbf{x})} t_i$$

The set of k-closest points of the training data to X.



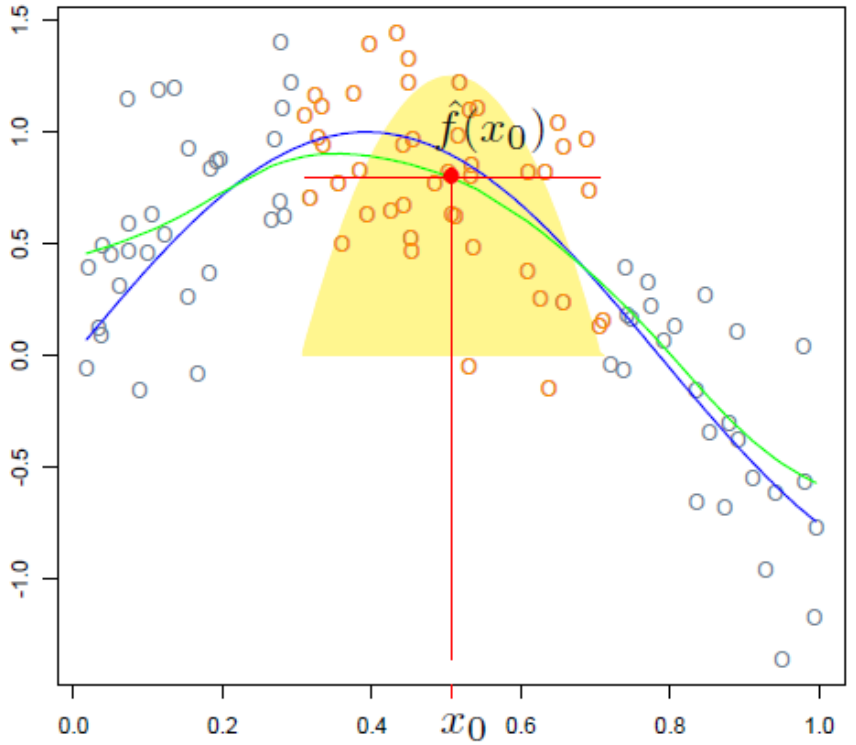
Not amazing : we want a smoother prediction fct.

Nadaraya-Watson Model

- In k-NN regression the model output is generally very noisy due to the discontinuity of neighborhood averages
- **Nadaraya-Watson** model (or **kernel regression**) deal with this issue by using kernel function to compute a weighted average of samples:

$$\hat{f}(\mathbf{x}) = \frac{\sum_{i=1}^{N} k(\mathbf{x}, \mathbf{x}_i) t_i}{\sum_{i=1}^{N} k(\mathbf{x}, \mathbf{x}_i)}$$

- Typical choices for kernels are:
  - Epanechnikov Kernel (bounded support)
  - Gaussian Kernel (infinite support)



Gaussian Processes

Kernel version of the Bayesian Linear Regression.

Linear Regression Revisited

- Let's start from the same assumptions used in Bayesian Linear Regression

$$y(\mathbf{x}, \mathbf{w}) = \mathbf{w}^T \boldsymbol{\phi}(\mathbf{x})$$

$$p(\mathbf{w}) = \mathcal{N}\left(\mathbf{w}|0, \tau^2\mathbf{I}\right)$$ } typical choice of PRIOR.

- Now compute the prior distribution of the outputs of the regression function:

$$\mathbf{y} = \boldsymbol{\Phi}\mathbf{w} \quad \Rightarrow \quad p(\mathbf{y}) = \mathcal{N}\left(\mathbf{y}|\boldsymbol{\mu}, \mathbf{S}\right)$$ } PRIOR of the output y.

$$\boldsymbol{\mu} = \mathbb{E}[\mathbf{y}] = \boldsymbol{\Phi}\mathbb{E}[\mathbf{w}] = \mathbf{0}$$

$$\mathbf{S} = \text{cov}[\mathbf{y}] = \mathbb{E}[\mathbf{y}\mathbf{y}^T] = \boldsymbol{\Phi}\mathbb{E}[\mathbf{w}\mathbf{w}^T]\boldsymbol{\Phi}^T = \tau^2\boldsymbol{\Phi}\boldsymbol{\Phi}^T = \mathbf{K}$$

$\mathbb{E}[\mathbf{w}\mathbf{w}^T] = \text{VAR}(\mathbf{w})$

Gram matrix

Gaussian Processes and Gram Matrix

- In general, a **Gaussian Process** is defined as a distribution probability over a function y(x) such that **the set of values $y(x_i)$** – for an arbitrary $\{x_i\}$ – **jointly have a Gaussian Distribution.**
- In our specific case,

$$p(\mathbf{y}) = \mathcal{N}(\mathbf{y}|\mathbf{0}, \mathbf{K})$$

  - where **K** is the Gram matrix defined as:

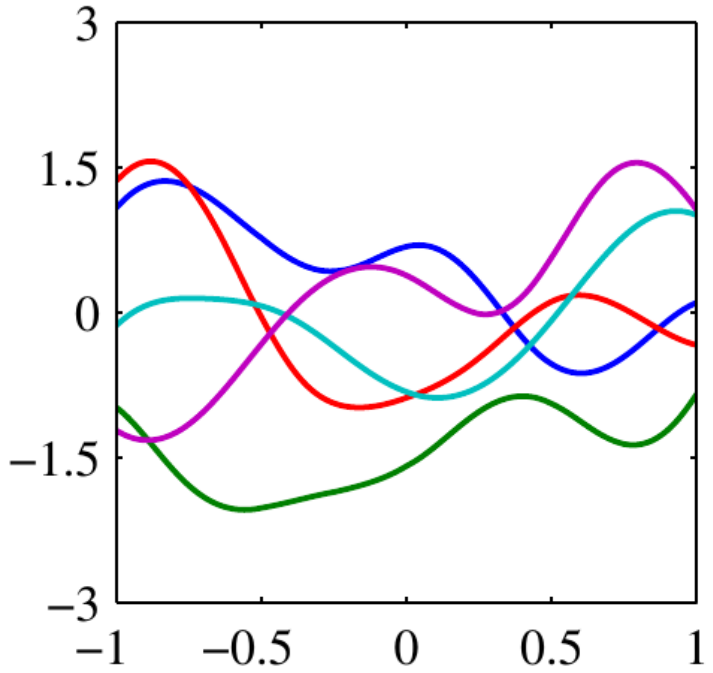
$$K_{nm} = k(\mathbf{x}_n, \mathbf{x}_m) = \tau^2 \boldsymbol{\phi}(\mathbf{x}_n)^T \boldsymbol{\phi}(\mathbf{x}_m)$$

- This gives a probabilistic interpretation of the Kernel function as:

$$k(\mathbf{x}_n, \mathbf{x}_m) = \mathbb{E}[y(\mathbf{x}_n) y(\mathbf{x}_m)]$$

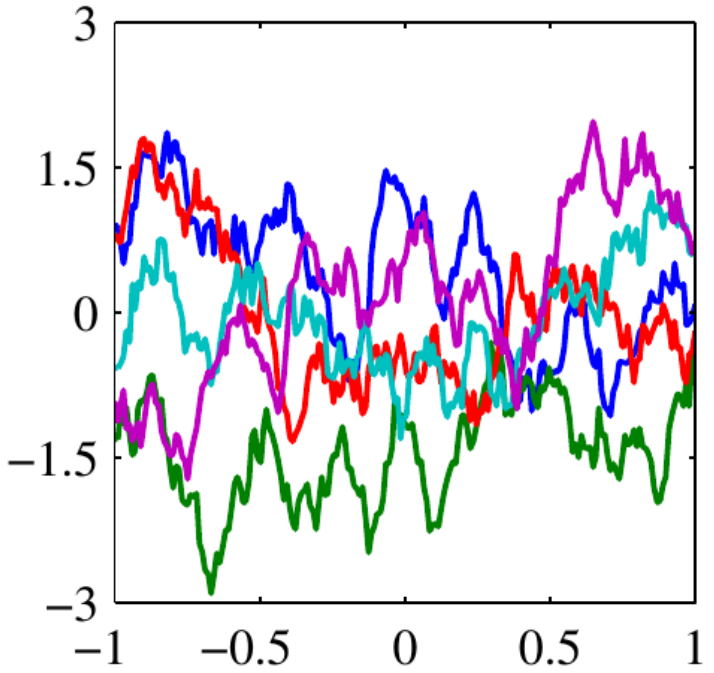
Kernel Design

- We can apply the usual approaches to design the kernels
- Two families of kernels typically used with GP are:



Gaussian Kernel

$$k(\mathbf{x}, \mathbf{x}') = \exp(-\|\mathbf{x} - \mathbf{x}'\|_2^2 / 2\sigma^2)$$



Exponential Kernel

$$k(\mathbf{x}, \mathbf{x}') = \exp(-\theta|\mathbf{x} - \mathbf{x}'|))$$