Machine Learning

Kernel Methods

Marcello Restelli

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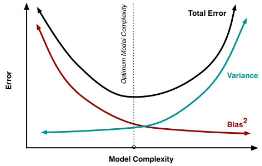
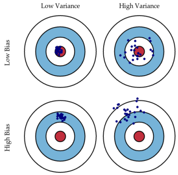
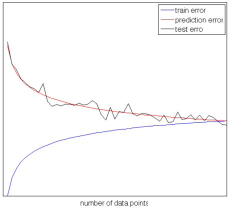






Outline

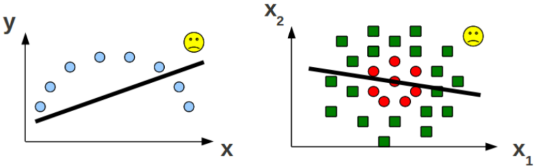
1. Kernel Methods
   - Dual Representation
   - Constructing Kernels
2. Radial Basis Functions Networks
3. Gaussiann Processes

Kernel Methods

- Kernel methods are memory**-based** (like nearest neighbor)
  - **Training data** are used in **prediction phase**
  - **Fast** to train, **slow** to predict
  - Require a **metric** to be defined

Motivations

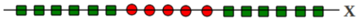
- Often we want to **capture nonlinear patterns** in the data
  - Nonlinear Regression: input-output relationship may not be linear
  - Nonlinear Classification: Classes may not be separable by a linear boundary
- Linear models are **not just rich enough**



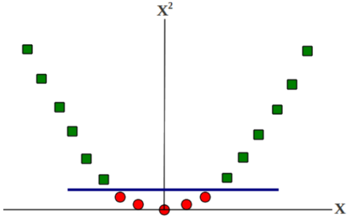
- **Kernels**: make linear models work in nonlinear settings
  - By **mapping data to higher dimensions** where it exhibits linear patterns
  - Apply the **linear model** in the **new input space**
  - Mapping $\equiv$ changing the **feature representation**
- Mappings can be **expensive** to compute
- Kernels give such mappings **for (almost) free**: **Kernel trick!**

Example: 1D

- Consider this binary classification problem

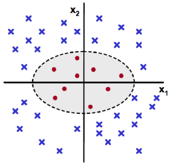


  - Each example represented by a **single feature** x
  - **No linear separator** exists for this data
- Now map each example as $x \rightarrow \{x, x^2\}$
  - Each example now has **two features** (derived from the old representation)
- Data now becomes **linear separable** in the **new representation**

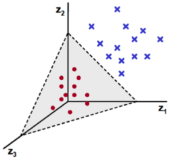


Example: 2D

- Let's look at another example:



  - Each example defined by a two features $\mathbf{x} = \{x_1, x_2\}$
  - **No linear separator** exists for this data
- Now map each example as $\mathbf{x} = \{x_1, x_2\} \rightarrow \mathbf{z} = \{x_1^2, \sqrt{2}x_1x_2, x_2^2\}$
  - Each example now has **three features**
- Data now becomes **linearly separable** in the **new representation**



Feature Mapping

- Consider the following mapping ϕ for an example $\mathbf{x} = \{x_1, \dots, x_M\}$

$$\phi : \mathbf{x} \to \{x_1^2, x_2^2, \dots, x_M^2, x_1 x_2, x_2 x_3, \dots, x_1 x_M, \dots, x_{M-1} x_M\}$$

- It's an example of a **quadratic** mapping
  - Each new feature uses a **pair** of the original features
- **Problem**: Mapping usually leads to the number of features **blow up**!
  - Computing the mapping itself can be **inefficient**
  - Moreover, **using** the mapped representation could be inefficient too
- Thankfully, **kernels** help avoid both these issues!
  - The mapping doesn't have to be **explicitly** computed
  - Computations with the mapped features remain **efficient**

Kernel Functions

- Many linear **parametric** models can be re-cast into equivalent **dual representations** where predictions are based on a **kernel function** evaluated at **training points**
- Kernel function is given by

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

  - where $\phi(\mathbf{x})$ is a fixed nonlinear feature space mapping (**basis function**)
- Kernel is a **symmetric** function of its arguments

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

- Kernel function can be interpreted as **similarity** of $\mathbf{x}$ and $\mathbf{x}'$
- Simplest is **identity mapping** in feature space: $\phi(\mathbf{x}) = \mathbf{x}$
  - In which case $k(\mathbf{x}, \mathbf{x}') = \mathbf{x}^T \mathbf{x}'$
  - Called **linear kernel**

Kernel Trick

- Formulated as **inner product** allows extending well-known algorithms
  - by using the **kernel trick**
- **Basic idea** of kernel trick
  - If an input vector $\mathbf{x}$ appears only in the form of **scalar products** then we can replace scalar products with some other choice of kernel
- **Used widely**
  - Ridge Regression
  - Perceptron
  - Nonlinear variant of PCA
  - Support Vector Machines
  - Lots more...

Other Forms of Kernel Functions

- Function of difference between arguments

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

  - Called **stationary kernel** since invariant to translation in space
- **Homogeneous kernels**, also known as **radial basis functions**

$$k(\mathbf{x}, \mathbf{x}') = k(\left\|\mathbf{x} - \mathbf{x}'\right\|)$$

  - Depend only on the magnitude of the **distance** between arguments
- Note that the kernel function is a **scalar** value while **x** is an M-dimensional **vector**
- The kernel functions are valid if can be expressed as $k(\mathbf{x}, \mathbf{x}') = \phi(\mathbf{x})^T\phi(\mathbf{x})$

Dual Representation

- Many linear models for regression and classification can be reformulated in terms of dual representation in which the **kernel function arises naturally**
- Plays important role in SVMs (we see this later)
- Consider linear regression model
  - The parameters are obtained by minimizing **regularized sum-of-squares** error function

$$L_{\mathbf{w}} = \frac{1}{2}\sum_{n=1}^{N}\left(\mathbf{w}^T\phi(\mathbf{x}_n) - t_n\right)^2 + \frac{\lambda}{2}\mathbf{w}^T\mathbf{w}$$

  - Setting the gradient of $L_{\mathbf{w}}$ with respect to $\mathbf{w}$ equal to zero:

$$\mathbf{w} = -\frac{1}{\lambda}\sum_{n=1}^{N}\left(\mathbf{w}^T\phi(\mathbf{x}_n) - t_n\right)\phi(\mathbf{x}_n) = \sum_{n=1}^{N} a_n\phi(\mathbf{x}_n) = \mathbf{\Phi}^T\mathbf{a}$$

    - $\mathbf{\Phi}$ is the design matrix whose n^{th} row is $\phi(\mathbf{x}_n)^T$
    - The coefficients a_n are functions of $\mathbf{w}$: $a_n = -\frac{1}{\lambda}\left(\mathbf{w}^T\phi(\mathbf{x}_n) - t_n\right)$

Gram Matrix and Kernel Function

- Define the **Gram matrix** $K = \mathbf{\Phi} \times \mathbf{\Phi}^T$ an $N \times N$ matrix, with elements

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

- Given N vectors, the Gram Matrix is the matrix of all **inner products**

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

- Notes:
  - $\mathbf{\Phi}$ is $N \times M$ and K is $N \times N$
  - K is a matrix of **similarities** of pairs of samples (is **symmetric**)

Error Function in Terms of Gram Matrix of Kernel

- Substituting $\mathbf{w} = \mathbf{\Phi}^T\mathbf{a}$ into $L_\mathbf{w}$ gives

$$L_\mathbf{w} = \frac{1}{2}\mathbf{a}^T\mathbf{\Phi}\mathbf{\Phi}^T\mathbf{\Phi}\mathbf{\Phi}^T\mathbf{a} - \mathbf{a}^T\mathbf{\Phi}\mathbf{\Phi}^T\mathbf{t} + \frac{1}{2}\mathbf{t}^T\mathbf{t} + \frac{\lambda}{2}\mathbf{a}^T\mathbf{\Phi}\mathbf{\Phi}^T\mathbf{a}$$

  where $\mathbf{t} = (t_1, \ldots, t_N)^T$
- Sum of squares error function is written in terms of Gram matrix as

$$L_\mathbf{a} = \frac{1}{2}\mathbf{a}^T K K\mathbf{a} - \mathbf{a}^T K\mathbf{t} + \frac{1}{2}\mathbf{t}^T\mathbf{t} + \frac{\lambda}{2}\mathbf{a}^T K\mathbf{a}$$

- Solving for $\mathbf{a}$ by combining $\mathbf{w} = \mathbf{\Phi}^T\mathbf{a}$ and $a_n = -1/\lambda(\mathbf{w}^T\phi(\mathbf{x}_n) - t_n)$

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

- Solution for $\mathbf{a}$ can be expressed as a linear combination of elements of $\phi(\mathbf{x})$ whose coefficients are **entirely in terms of kernel** $k(\mathbf{x}, \mathbf{x}')$ from which we can recover original formulation in terms of parameters $\mathbf{w}$

Prediction Function

- Prediction for new input $\mathbf{x}$
  - We can write $\mathbf{a} = (K + \lambda \mathbf{I}_N)^{-1}\mathbf{t}$
  - Substituting back into linear regression model

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

  where $\mathbf{k}(\mathbf{x})$ has elements $k_n(\mathbf{x}) = k(\mathbf{x}_n, \mathbf{x})$
- Prediction is a linear combination of the **target values** from the **training set**

Advantage of Dual Representation

- Solution for $\mathbf{a}$ is expressed entirely in terms of kernel function $k(\mathbf{x}, \mathbf{x}')$
- Once we get $\mathbf{a}$ we can recover $\mathbf{w}$ as linear combination of elements of $\phi(\mathbf{x})$ using $\mathbf{w} = \mathbf{\Phi}^T\mathbf{a}$
- In parametric formulation, solution is $\mathbf{w}_{ML} = (\mathbf{\Phi}^T\mathbf{\Phi})^{-1}\mathbf{\Phi}^T\mathbf{t}$
  - Instead of inverting an $M \times M$ matrix we are inverting an $N \times N$ matrix (an **apparent disadvantage**)
- But, advantage of dual formulation is that we can work with kernel function $k(\mathbf{x}, \mathbf{x}')$ and therefore
  - **avoid** working with a feature vector $\phi(\mathbf{x})$ and
  - problems associated with **very high or infinite dimensionality** of $\mathbf{x}$
  - kernel functions can be defined not only over simply vectors of real numbers, but also **over objects** as diverse as graphs, sets, string, and text documents

Constructing Kernels

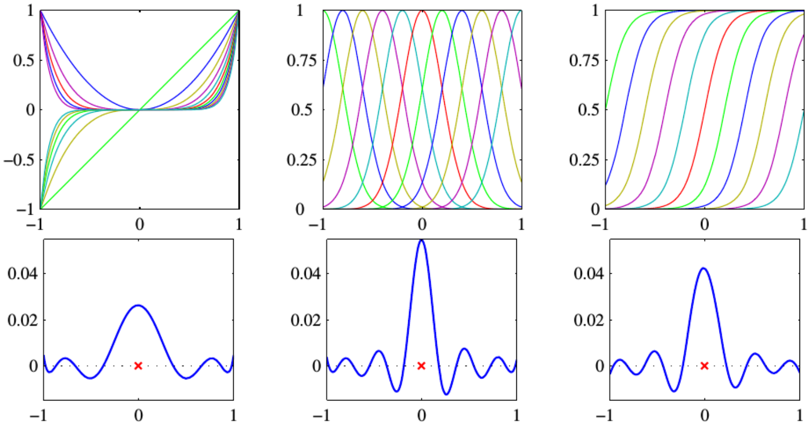
- To exploit kernel substitution need **valid** kernel functions
- First method
  - **Choose a feature space** mapping $\boldsymbol{\phi}(\mathbf{x})$ and use it to find corresponding kernel
  - One-dimensional input space

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

    - where $\boldsymbol{\phi}(\mathbf{x})$ are basis functions such as polynomial
    - for each i we choose $\phi_i(\mathbf{x}) = \mathbf{x}^i$

Construction of Kernel Functions from Basis Functions

One-dimensional input space



Second Method: Direct Construction of Kernels

- Function we choose has to correspond to a **scalar product** in some (perhaps infinite dimensional) space
- Consider kernel function $k(x, z) = (x^T z)^2$
  - In **two dimensional space**

$$\begin{aligned} k(x, z) &= (\mathbf{x}^T\mathbf{z})^2 = (x_1 z_1 + x_2 z_2)^2 = x_1^2 z_1^2 + 2x_1 z_1 x_2 z_2 + x_2^2 z_2^2 \\ &= (x_1^2, \sqrt{2}x_1x_2, x_2^2)(z_1^2, \sqrt{2}z_1z_2, z_2^2)^T = \phi(\mathbf{x})^T\phi(\mathbf{z}) \end{aligned}$$

  - Feature mapping takes the form $\phi(\mathbf{x}) = (x_1^2, \sqrt{2}x_1x_2, x_2^2)$
  - Comprises of **all second order terms** with a specific weighting
    - Inner product needs computing six feature values and $3 \times 3 = 9$ multiplications
    - Kernel function $k(\mathbf{x}, \mathbf{z})$ has 2 multiplications and a squaring
  - By considering $(\mathbf{x}^T\mathbf{z} + c)^2$ we get constant, linear, second order terms
  - By considering $(\mathbf{x}^T\mathbf{z} + c)^p$ we get all terms up to degree p

Testing whether a function is a valid kernel

- Without having to construct the function $\phi(\mathbf{x})$ explicitly
- **Necessary and sufficient** condition for a function $k(\mathbf{x}, \mathbf{x}')$ to be a kernel is
  - Gram matrix K, whose elements are given by $k(\mathbf{x}_n, \mathbf{x}_m)$ is positive semi-definite for all possible choices of the set $\{\mathbf{x}_n\}$
    - Positive semi-definite is **not** the same thing as a matrix whose elements are non-negative
    - It means $\mathbf{x}^T K\mathbf{x} \geq 0$ for non-zero vectors $\mathbf{x}$ with real entries, i.e., $\sum_n \sum_m K_{n,m}\mathbf{x}_n\mathbf{x}_m \geq 0$ for any real numbers $\mathbf{x}_n$, $\mathbf{x}_m$

Theorem

*Mercer's theorem **Any** continuous, symmetric, positive semi-definite kernel function $k(x, y)$ can be expressed as a **dot product** in a high-dimensional space*

- **New kernels** can be constructed from simpler kernels as **building blocks**

Techniques for Constructing Kernels

Given valid kernels $k_1(\mathbf{x}, \mathbf{x}')$ and $k_2(\mathbf{x}, \mathbf{x}')$ the following new kernels will be valid

1. $k(\mathbf{x}, \mathbf{x}') = ck_1(\mathbf{x}, \mathbf{x}')$
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 $q(\cdot)$ 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 $\phi(\mathbf{x})$ is a function from $\mathbf{x}$ to $\mathbb{R}^M$
8. $k(\mathbf{x}, \mathbf{x}') = \mathbf{x}^T A\mathbf{x}'$, where A is a symmetric positive semidefinite matrix
9. $k(\mathbf{x}, \mathbf{x}') = k_a(\mathbf{x}_a, \mathbf{x}'_a) + k_b(\mathbf{x}_b, \mathbf{x}'_b)$, where x_a and x_b are variables with $\mathbf{x} = (x_a, x_b)$
10. $k(\mathbf{x}, \mathbf{x}') = k_a(\mathbf{x}_a, \mathbf{x}'_a)k_b(\mathbf{x}_b, \mathbf{x}'_b)$

Gaussian Kernel

- Commonly used kernel is

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

- It is seen as a valid kernel by expanding the square

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

- To give

$$k(\mathbf{x}, \mathbf{x}') = \exp(-\mathbf{x}^T\mathbf{x}/2\sigma^2)\exp(-\mathbf{x}^T\mathbf{x}'/\sigma^2)\exp(-\mathbf{x}'^T\mathbf{x}'/2\sigma^2)$$

- From kernel construction rules 2 and 4, together with validity of linear kernel $k(\mathbf{x}, \mathbf{x}') = \mathbf{x}^T\mathbf{x}'$
- Can be extended to non-Euclidean distances

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

Kernels for Symbolic Data

- Kernels can be extended to inputs that are **symbolic**, rather than simply vectors of real numbers
- Kernel functions can be defined over objects as diverse as graphs, sets, strings, and text documents
- Consider a simple kernel over sets:

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

Kernels based on Generative Models

- Given a generative model $p(\mathbf{x})$ we define a kernel by

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

  - A valid kernel since it is an inner product in the one-dimensional feature space defined by the mapping $p(\mathbf{x})$
- Two inputs $\mathbf{x}$ and $\mathbf{x}'$ are **similar** if they have high probabilities

Radial Basis Function Networks

- **Radial basis functions**: each basis function depends only on the radial distance (typically Euclidean) from a center

$$\phi_j(\mathbf{x}) = h(\|\mathbf{x} - \boldsymbol{\mu}_j\|_2)$$

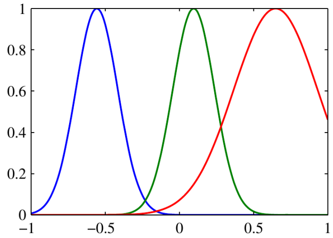
- Used for **exact interpolation**:

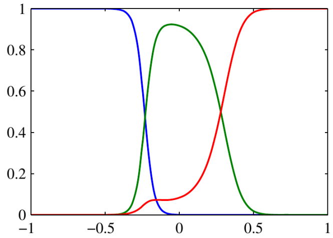
$$f(\mathbf{x}) = \sum_{n=1}^{N} w_n h(\|\mathbf{x} - \mathbf{x}_n\|_2)$$

- Because the data in ML are generally **noisy**, exact interpolation is not very useful

Normalized Basis Functions

- Uses **normalized** radial functions as basis
- Normalization is sometimes used in practice as it avoids having regions of input space where all basis functions take **small values**, which would necessarily lead to **predictions** in such regions that are either **small** or controlled purely by the **bias parameter**





Nadaraya-Watson Model

- Given a training set $\{\mathbf{x}_n, t_n\}$ the **joint distribution** of the two variables can be estimated with **Parzen window**:

$$p(\mathbf{x}, t) = \frac{1}{N}\sum_{n=1}^{N} f(\mathbf{x} - \mathbf{x}_n, t - t_n)$$

- We want to find the regression function $y(\mathbf{x})$

$$\begin{aligned} y(\mathbf{x}) = \mathbb{E}[t|\mathbf{x}] = \int_{-\infty}^{\infty} tp(t|\mathbf{x})\mathrm{d}t = \frac{\int tp(\mathbf{x}, t)\mathrm{d}t}{\int p(\mathbf{x}, t)\mathrm{d}t} \\ = \frac{\sum_{n=1}^{N} g(\mathbf{x} - \mathbf{x}_n)t_n}{\sum_{m=1}^{N} g(\mathbf{x} - \mathbf{x}_m)} = \sum_{n=1}^{N} k(\mathbf{x}, \mathbf{x}_n)t_n \end{aligned}$$

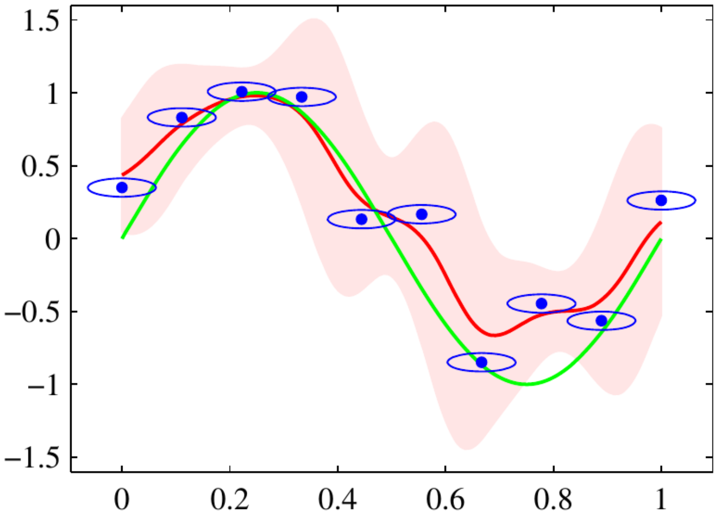
- where $k(\mathbf{x}, \mathbf{x}_n) = \dfrac{g(\mathbf{x} - \mathbf{x}_n)}{\sum_m g(\mathbf{x} - \mathbf{x}_m)}$ and $g(\mathbf{x}) = \int_{-\infty}^{\infty} f(\mathbf{x}, t)\mathrm{d}t$

Nadaraya-Watson Model

- Also called **kernel regression**
- For a localized kernel function, it has the property of giving **more weight** to the data points $\mathbf{x}_n$ that are **close** to $\mathbf{x}$
- The model defines not only a conditional expectation, but also a **full conditional distribution**

Example

Isotropic Gaussian kernels centered around the data points $z_n = (x_n, t_n)$



Gaussian Processes

- We have seen kernels as a **dual model** for a **non-probabilistic** model for regression
- Extend kernels to **probabilistic discriminative models**
- In linear model for regression, we have introduced a prior distribution over $\mathbf{w}$
- Given the training data set, we evaluated the posterior distribution over $\mathbf{w}$ => posterior distribution over the regression functions => predictive distribution $p(t|\mathbf{x})$ for new input $\mathbf{x}$

Gaussian Processes

- Now we define a **prior** probability distribution **over functions directly**
- Might seem difficult to work with a distribution over the uncountable infinite space of functions
- However, for a **finite** training set, we only need to consider the values of the function at the discrete set of input values $\mathbf{x}_n$ of the training set
- So, in practice, we can work in **finite space**

Revisiting Linear Regression

- Let's apply kernels to probabilistic discriminative models

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

- Instead of prior over **w**, let's define a prior over functions directly

$$\begin{aligned} p(\mathbf{w}) &= \mathcal{N}\left(\mathbf{w}|\mathbf{0}, \lambda \mathbf{I}\right) \\ \mathbf{y} &= \mathbf{\Phi w} \\ p(\mathbf{y}) &= ? \end{aligned}$$

- **y** is a **linear combination of Gaussian** distributed variables given by the elements of **w** and hence is itself **Gaussian**

Revisiting Linear Regression

- Thus:

$$\begin{aligned} \mathbb{E}[\mathbf{y}] &= \mathbf{\Phi}\mathbb{E}[\mathbf{w}] = \mathbf{0} \\ \operatorname{cov}[\mathbf{y}] &= \mathbb{E}[\mathbf{y}\mathbf{y}^T] = \mathbf{\Phi}\mathbb{E}[\mathbf{w}\mathbf{w}^T]\mathbf{\Phi}^T = \lambda\mathbf{\Phi}\mathbf{\Phi}^T = \mathbf{K} \end{aligned}$$

- where **K** is the Gram matrix with elements

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

- So the marginal distribution $p(\mathbf{y})$ is defined by a Gram matrix so that $p(\mathbf{y}) = \mathcal{N}(\mathbf{y}|\mathbf{0}, \mathbf{K})$

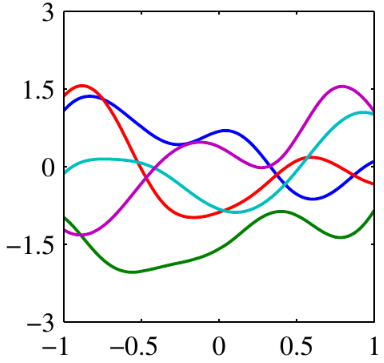
Gaussian Processes: Definition

- A Gaussian process is defined as a **probability distribution over functions** $\mathbf{y}(\mathbf{x})$ such that the set of values of $\mathbf{y}(\mathbf{x})$ evaluated at an arbitrary set of points $\mathbf{x}_1, \ldots \mathbf{x}_N$ **jointly have a Gaussian distribution**
- This distribution is completely specified by the second-order statistics, the mean and the covariance
  - Usually, we do not have any prior information about the **mean** of $y(\mathbf{x})$, so we'll take it to be **zero**
  - The **covariance** is given by the **kernel function**

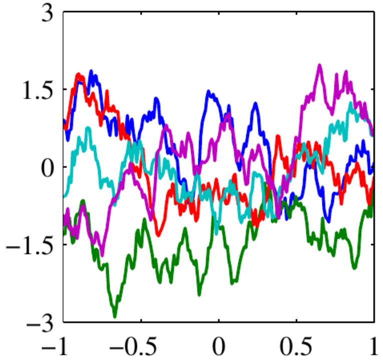
$$\mathbb{E}[y(\mathbf{x}_n)y(\mathbf{x}_m)] = k(\mathbf{x}_n, \mathbf{x}_m)$$

Gaussian Processes: Example

We can also define the kernel function **directly**, rather than indirectly through a choice of basis function



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



Exponential Kernel:
$k(x, x') = \exp(-\theta|x - x'|)$

Gaussian Processes for Regression

- Take into account the noise on the target

$$t_n = y(\mathbf{x}_n) + \epsilon_n$$

- Random noise under a **Gaussian distribution**

$$p(t_n|y(\mathbf{x}_n)) = \mathcal{N}\left(t_n|y(\mathbf{x}_n), \sigma^2\right)$$

- Because the noise is **independent** on each data point, the joint distribution is still **Gaussian**:

$$p(\mathbf{t}|\mathbf{y}) = \mathcal{N}\left(\mathbf{t}|\mathbf{y}, \sigma^2\mathbf{I}_N\right)$$

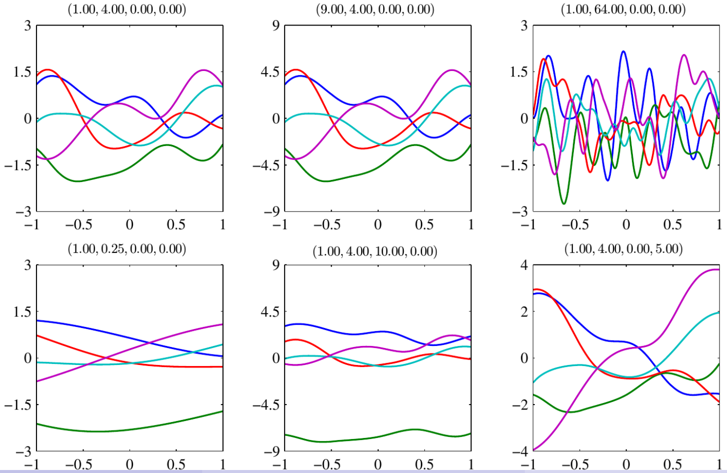
- Since $p(\mathbf{y}) = \mathcal{N}(\mathbf{y}|\mathbf{0}, \mathbf{K})$, we can compute the marginal distribution:

$$p(\mathbf{t}) = \int p(\mathbf{t}|\mathbf{y})p(\mathbf{y})\mathrm{d}\mathbf{y} = \mathcal{N}(\mathbf{t}|\mathbf{0}, \mathbf{C})$$

  where $C(\mathbf{x}_n, \mathbf{x}_m) = k(\mathbf{x}_n, \mathbf{x}_m) + \sigma^2\delta_{nm}$
- Since the two Gaussians are **independent** their covariances simply **add**

Gaussian Processes Examples

$$k(\mathbf{x}_n, \mathbf{x}_m) = \theta_0 \exp\left(-\frac{\theta_1}{2}\left\|\mathbf{x}_n - \mathbf{x}_m\right\|_2^2\right) + \theta_2 + \theta_3 {\mathbf{x}_n}^T \mathbf{x}_m$$



Making Predictions

- Make prediction for a **new data input**, given the training data
- **Goal**: predict t_{N+1} given $\mathbf{x}_{N+1}$
- Need to evaluate the predictive distribution $p(t_{N+1}|\mathbf{t}_N, \mathbf{x}_1, \ldots, \mathbf{x}_{N+1})$

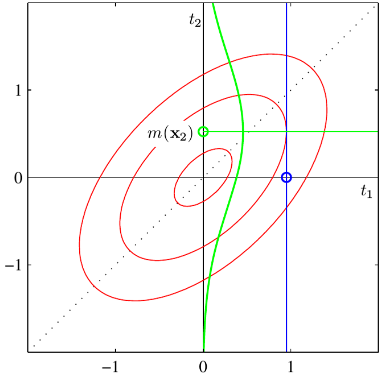
$$p(\mathbf{t}_{N+1}) = \mathcal{N}\left(\mathbf{t}_{N+1}|\mathbf{0}, \mathbf{C}_{N+1}\right)$$

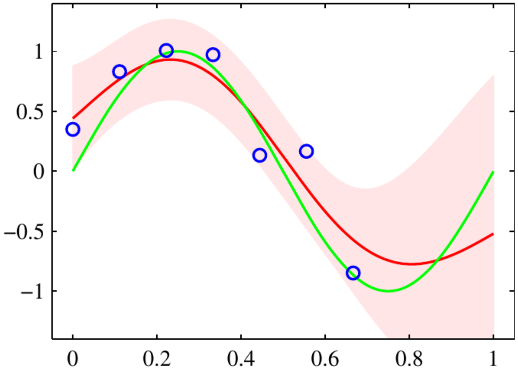
  - where $\mathbf{C}_{N+1} = \begin{pmatrix} \mathbf{C}_N & \mathbf{k} \\ \mathbf{k}^T & c \end{pmatrix}$
  - $\mathbf{k}$ is a vector $k(\mathbf{x}_i, \mathbf{x}_{N+1})$ for $i = 1, \ldots, N$
  - c is a scalar: $c = k(\mathbf{x}_{N+1}, \mathbf{x}_{N+1}) + \sigma^2$
- $p(t_{N+1}|\mathbf{t}_N, \mathbf{x}_1, \ldots, \mathbf{x}_{N+1})$ is a Gaussian:
  - $m(\mathbf{x}_{N+1}) = \mathbf{k}^T\mathbf{C}_N^{-1}\mathbf{t}$
  - $\sigma^2(\mathbf{x}_{N+1}) = c - \mathbf{k}^T\mathbf{C}_N^{-1}\mathbf{k}$
- The mean and variance both depend on $\mathbf{x}_{N+1}$
- $\mathbf{C}$ has to be positive definite $\Leftrightarrow$ the kernel function is positive semi-definite

Computational cost

- The prediction requires to compute the **inversion** of $\mathbf{C}_N$: cost $\mathcal{O}(N^3)$
  - Need to be done **only once** for the given training set
- The computation of the **mean** costs $\mathcal{O}(N)$
- The computation of the **variance** costs $\mathcal{O}(N^2)$
- For **large** training sets **approximated** methods are used
  - random sampling
  - clustering

Prediction Example





Estimating the Kernel Parameters

- The performance of a GP is strongly affected by the choice of **parameters** for the kernels
- The choice of the kernel parameters is a **model selection** problem
  - We can consider a discrete grid of values and use **cross validation**
    - Robust, but **slow**
  - Maximization of the **marginal likelihood** using gradient optimization
    - **Faster**, but multiple local minima
- Other tricks
  - Use **domain knowledge** wherever possible
  - **Standardize input data** and set lengthscales to ~ 1
  - **Standardize targets** and set function variance to ~ 1
  - **Set initial noise level high**, even if you think your data have low noise: The optimization surface for your other parameters will be easier to move in