# Non parametric regression

Course of Machine Learning
Master Degree in Computer Science

University of Rome "Tor Vergata"

a.a. 2020-2021

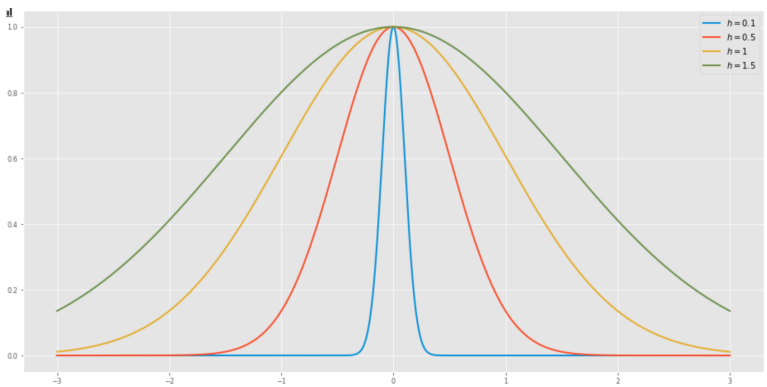
Giorgio Gambosi

# Kernel regression

- In kernel regression methods, the target value corresponding to any item $\mathbf{x}$ is predicted by referring to items in the training set, and in particular to the items which are closer to $\mathbf{x}$.
- This is controlled by referring to a kernel function $\kappa_h(\mathbf{x})$, which is non zero only in an interval around $0$
- $h$ is the bandwidth of the kernel, which controls the width of $\kappa_h(\mathbf{x})$

A possible, common kernel, is the gaussian (or RBF) kernel

$$g(\mathbf{x}) = e^{-\frac{\|\mathbf{x}\|^2}{2h^2}}$$



# Kernel regression

In regression, we are interested in estimating the conditional expectation

$$f(\mathbf{x}) = E[t|\mathbf{x}] = \int tp(t|\mathbf{x})dt = \int t\frac{p(\mathbf{x},t)}{p(\mathbf{x})}dt = \frac{\int t\ p(\mathbf{x},t)dt}{p(\mathbf{x})} = \frac{\int t\ p(\mathbf{x},t)dt}{\int p(\mathbf{x},t)dt}$$

The joint distribution $p(\mathbf{x},t)$ is approximated by means of a kernel function as

$$p(\mathbf{x},t) \approx \frac{1}{n}\sum_{i=1}^{n}\kappa_h(\mathbf{x}-\mathbf{x}_i)\kappa_h(t-t_i)$$

# Kernel regression

This results into

$$f(\mathbf{x}) = \frac{\int t \frac{1}{n} \sum_{i=1}^{n} \kappa_t(\mathbf{x} - \mathbf{x}_i) \kappa_h(t - t_i) dt}{\int \frac{1}{n} \sum_{i=1}^{n} \kappa_h(\mathbf{x} - \mathbf{x}_i) \kappa_h(t - t_i) dt} = \frac{\sum_{i=1}^{n} \kappa_h(\mathbf{x} - \mathbf{x}_i) \int t \kappa_h(t - t_i) dy}{\sum_{i=1}^{n} \kappa_h(\mathbf{x} - \mathbf{x}_i) \int \kappa_h(t - t_i) dt}$$

and, since $\int \kappa_h(t - t_i) dt = 1$ and $\int t \kappa_h(t - t_i) dt = t_i$, we get

$$f(\mathbf{x}) = \frac{\sum_{i=1}^{n} \kappa_h(\mathbf{x} - \mathbf{x}_i) t_i}{\sum_{i=1}^{n} \kappa_h(\mathbf{x} - \mathbf{x}_i)}$$

# Kernel regression

By setting

$$w_i(\mathbf{x}) = \frac{\kappa_h(\mathbf{x} - \mathbf{x}_i)}{\sum_{j=1}^{n} \kappa_h(\mathbf{x} - \mathbf{x}_j)}$$

we can write

$$f(\mathbf{x}) = \sum_{i=1}^{n} w_i(\mathbf{x}) t_i$$

that is, the predicted value is computed as a normalized linear combination of all target values, weighted by kernels (Nadaraya-Watson)

# Locally weighted regression

In Nadaraya-Watson model, the prediction is performed by means of a normalized weighted combination of constant values (target values in the training set).

Locally weighted regression (LOESS) improves that approach by referring to a weighted version of the sum of squared differences loss function used in regression.

If a value $t$ has to be predicted for an item $\mathbf{x}$, a "local" version of the loss function is considered, with weight $\mathbf{w}_i$ dependent from the "distance" between $\mathbf{x}$ and $\mathbf{x}_i$.

$$L(\mathbf{x}) = \sum_{i=1}^{n} \kappa_h(\mathbf{x} - \mathbf{x}_i)(\mathbf{w}^T \overline{\mathbf{x}}_i - t_i)^2$$

# Locally weighted regression

The minimization of this loss function

$$\hat{\mathbf{w}}(\mathbf{x}) = \underset{\mathbf{w}}{\operatorname{argmin}} \sum_{i=1}^{n} \kappa_h(\mathbf{x} - \mathbf{x}_i)(\mathbf{w}^T \overline{\mathbf{x}}_i - t_i)^2$$

has solution

$$\hat{\mathbf{w}}(\mathbf{x}) = (\overline{\mathbf{X}}^T \Psi(\mathbf{x}) \overline{\mathbf{X}})^{-1} \overline{\mathbf{X}}^T \Psi(\mathbf{x}) \mathbf{t}$$

where $\Psi(\mathbf{x})$ is a diagonal $n \times n$ matrix with $\Psi(\mathbf{x})_{ii} = \kappa_h(\mathbf{x} - \mathbf{x}_i)$.

The prediction is then performed as usual, as

$$y = \hat{\mathbf{w}}(\mathbf{x})^T \overline{\mathbf{x}}$$

# Local logistic regression

The same approach applied in the case of local regression can be applied for classification, by defining a weighted loss function to be minimized, with weights dependent from the item whose target must be predicted.

In this case, a weighted version of the cross entropy function is considered, which has to be maximized

$$L(\mathbf{x}) = \sum_{i=1}^{n} \kappa_h(\mathbf{x} - \mathbf{x}_i)(t_i \log p_i - (1 - t_i) \log(1 - p_i))$$

with $p_i = \sigma(\mathbf{w}^T \overline{\mathbf{x}}_i)$, as usual.

The loss function minimization can be performed, for example, by applying a suitable modification of the IRLS algorithm for logistic regression

# Recap: some properties of Gaussian distribution

In order to introduce Gaussian processes and how they can be exploited for regression, let us first provide a short reminder on some properties of multivariate gaussian distributions.

Let $\mathbf{x} = (x_1, \ldots, x_n)^T$ be a random vector with gaussian distribution $p(\mathbf{x}) = \mathcal{N}(\boldsymbol{\mu}, \boldsymbol{\Sigma})$ and let $\mathbf{x} = (\mathbf{x}_A, \mathbf{x}_B)$ be a partition of the components $\mathbf{x}$ such that:

- $\mathbf{x}_A = (x_1, \ldots, x_r)^T$
- $\mathbf{x}_B = (x_{r+1}, \ldots, x_n)^T$

Then, the marginal densities $p(\mathbf{x}_A)$ and $p(\mathbf{x}_B)$ are both gaussian with means $\boldsymbol{\mu}_A, \boldsymbol{\mu}_B$ and covariance matrices $\boldsymbol{\Sigma}_A, \boldsymbol{\Sigma}_B$ which can be derived from $\boldsymbol{\mu}, \boldsymbol{\Sigma}$ by observing that

$$\boldsymbol{\mu} = (\boldsymbol{\mu}_A, \boldsymbol{\mu}_B)^T \qquad \boldsymbol{\Sigma} = \begin{pmatrix} \boldsymbol{\Sigma}_A & \boldsymbol{\Sigma}_{AB} \\ \boldsymbol{\Sigma}_{AB}^T & \boldsymbol{\Sigma}_B \end{pmatrix}$$

# Recap: some properties of the Gaussian distribution

In the same situation, the conditional densities $p(\mathbf{x}_A|\mathbf{x}_B)$ and $p(\mathbf{x}_B|\mathbf{x}_A)$ are also gaussian with means

$$\boldsymbol{\mu}_{A|B} = \boldsymbol{\mu}_A + \boldsymbol{\Sigma}_{AB}\boldsymbol{\Sigma}_B^{-1}(\mathbf{x}_B - \boldsymbol{\mu}_B)$$
$$\boldsymbol{\mu}_{B|A} = \boldsymbol{\mu}_B + \boldsymbol{\Sigma}_{BA}\boldsymbol{\Sigma}_A^{-1}(\mathbf{x}_A - \boldsymbol{\mu}_A)$$

and covariance matrices

$$\boldsymbol{\Sigma}_{A|B} = \boldsymbol{\Sigma}_A - \boldsymbol{\Sigma}_{AB}\boldsymbol{\Sigma}_B^{-1}\boldsymbol{\Sigma}_{BA}$$
$$\boldsymbol{\Sigma}_{B|A} = \boldsymbol{\Sigma}_B - \boldsymbol{\Sigma}_{BA}\boldsymbol{\Sigma}_A^{-1}\boldsymbol{\Sigma}_{AB}$$

# Gaussian processes

- Multivariate gaussians on random vectors are useful for modeling finite collections of real-valued variables. They have nice analytical properties (see previous slides).
- Gaussian processes: extension of multivariate gaussians to infinite-sized collections of real-valued variables.
- We may think of gaussian processes as distributions not just over random vectors but over random real functions.

# Probability distributions over functions with finite domains

Let us first consider the case of functions defined over finite vectors.

- Let $\chi = (\mathbf{x}_1, \ldots, \mathbf{x}_m)$ be any finite vector, and let $\mathcal{H}$ be the set of functions $f : \chi \mapsto \mathbb{R}$: $f$ assigns a value $f(\mathbf{x}_i)$ to each $\mathbf{x}_i \in \chi$
  - A function $f \in \mathcal{H}$ can be described by the vector $(f(\mathbf{x}_1), \ldots, f(\mathbf{x}_m))$
  - Any vector $(y_1, \ldots, y_m)$ can be seen as the description of a function $f \in \mathcal{H}$ such that $f(\mathbf{x}_i) = y_i$
  - The set $\mathcal{H}$ is then in 1-to-1 correspondence with the set of vectors in $\mathbb{R}^m$
- A probability distribution $p(\mathbf{x}), \mathbf{x} \in \mathbb{R}^m$ over $m$-dimensional real vectors is also a distribution $p(f), f \in \mathcal{H}$ over functions from $\mathbb{R}^m$ to $\mathbb{R}$

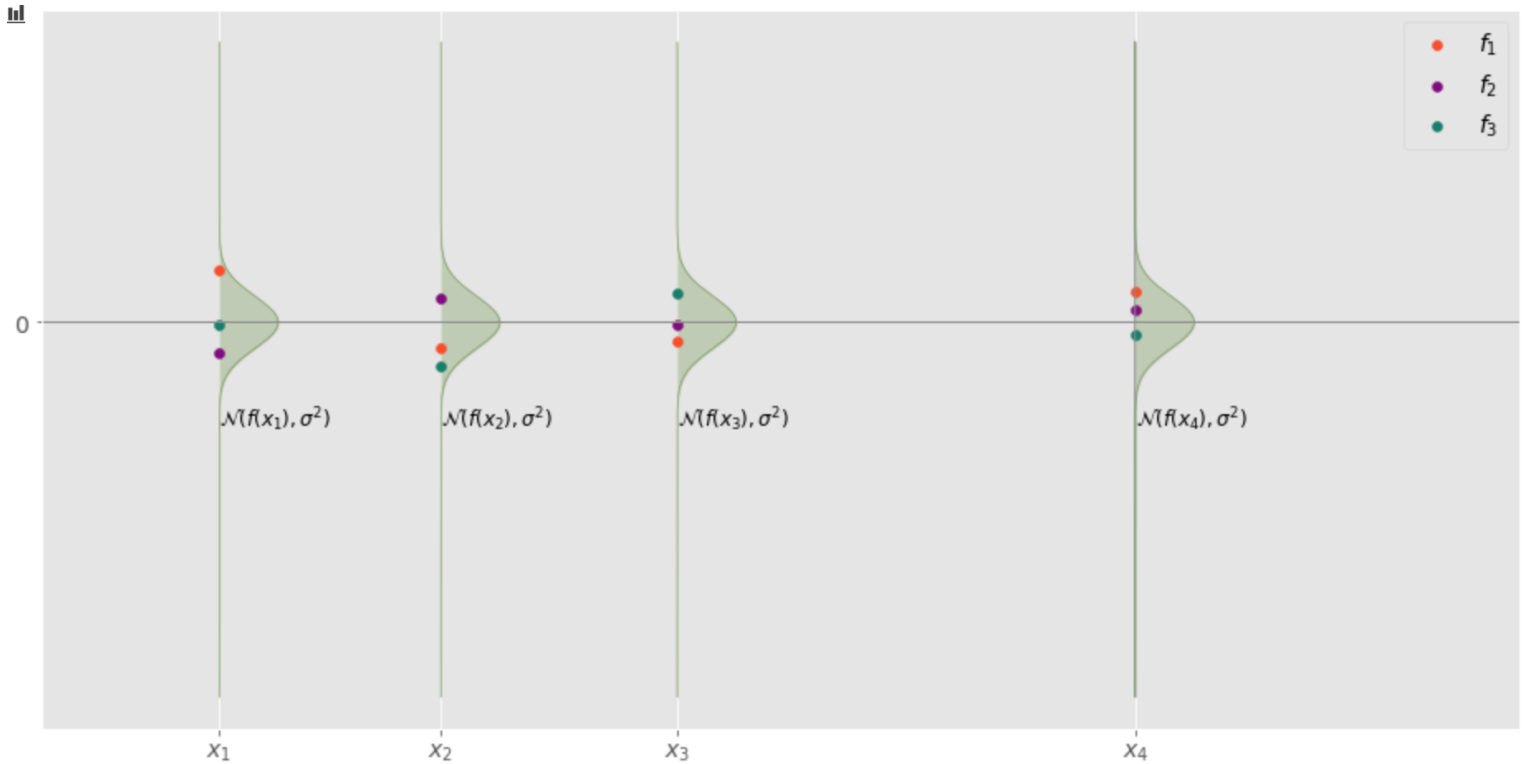
# Gaussian distributions over functions with finite domains

Assume that $p(\mathbf{x})$ (or, equivalently, $p(f)$) is a (multivariate, $m$-dimensional) Gaussian distribution centered on $\mathbf{0}$ and with diagonal covariance $\sigma^2\mathbf{I}$, that is

$$p(f|\sigma^2) = \mathcal{N}(f|\mathbf{0}, \sigma^2\mathbf{I}) = \prod_{i=1}^{m} \frac{1}{\sqrt{2\pi}\sigma} e^{-\frac{f(\mathbf{x}_i)^2}{2\sigma^2}}$$

- This is equivalent to assuming that each function value $f(\mathbf{x}_i)$ has normal distribution with mean $0$ and variance $\sigma^2$, and that items are independent
- A dependence between function values at different points could be modeled through a non-diagonal covariance matrix

# Gaussian distributions over functions with finite domains




We may consider $p(f|\sigma^2)$ as a prior distribution of functions, with respect to the observation of the value $t_j$ actually taken by any variable $\mathbf{x}_j$, $1 \leq j \leq m$.

# Gaussian distributions over functions with finite domains

- Assume now that for some subset $\mathbf{X} = \{\mathbf{x}_{i_1}, \ldots, \mathbf{x}_{i_k}\}$ of component indices, the corresponding targets $\mathbf{t} = \{t_{i_1}, \ldots, t_{i_k}\}$ are available.
- the posterior distribution $p(f|\mathbf{X}, \mathbf{t})$ of functions (wrt to $\mathbf{X}, \mathbf{t}$) can be defined and derived according to Bayes' rule, provided a likelihood model is defined

$$p(\mathbf{X}, \mathbf{t}|f) = \prod_{\mathbf{x}_i \in \mathbf{X}} p(\mathbf{x}_i, t_i|f) = \prod_{\mathbf{x}_i \in \mathbf{X}} p(t_i|\mathbf{x}_i, f) p(\mathbf{x}_i|f) \propto \prod_{\mathbf{x}_i \in \mathbf{X}} p(t_i|\mathbf{x}_i, f)$$

- for example, we could assume the usual likelihood $p(t|\mathbf{x}, f, \beta) = \mathcal{N}(t|f(\mathbf{x}), \beta)$, which implies

$$p(\mathbf{X}, \mathbf{t}|f, \beta) \propto \prod_{\mathbf{x}_i \in \mathbf{X}} \mathcal{N}(t_i|f(\mathbf{x}_i), \beta)$$

- the posterior distribution then would be

$$p(f|\mathbf{X}, \mathbf{t}, \beta, \sigma^2) \propto \prod_{\mathbf{x}_i \in \mathbf{X}} \mathcal{N}(t_i|f(\mathbf{x}_i), \beta) p(f|\sigma^2)$$

# Gaussian distributions over functions with finite domains

Since both the prior and the posterior distributions of $f$ are gaussian, the predictive distribution

$$p(t|\mathbf{x}, \mathbf{X}, \mathbf{t}, \beta, \sigma^2) = \int p(t|\mathbf{x}, f, \beta) p(f|\mathbf{X}, \mathbf{t}, \beta, \sigma^2) df$$

is itself a gaussian.

That would the case also in the more general case when some dependancy between function points is assumed. In this case, a general covariance matrix is defined for the prior distribution

$$p(f|\mathbf{\Sigma}) = \mathcal{N}(f|\mathbf{0}, \mathbf{\Sigma})$$

# Gaussian distributions over functions with infinite domains

- In the case of infinite $\chi$, we have to deal with an infinite collection of random variables.
- In this case, the role of multidimensional distributions is covered by stochastic processes.
  - A *stochastic process* is a collection of random variables, $\{f(\mathbf{x}) : \mathbf{x} \in \chi\}$, indexed by elements from some set $\chi$, known as the index set.
- A Gaussian process is a stochastic process such that for any finite subset $\mathbf{x}_1, \ldots, \mathbf{x}_n$ of $\chi$, the function values $f(\mathbf{x}_1), \ldots, f(\mathbf{x}_n)$ have joint multivariate Gaussian distribution

# Gaussian processes

- In order to define a Gaussian process, both a mean and a covariance function must be defined.
  - a mean function $m : \mathbb{R}^d \mapsto \mathbb{R}$ mapping each point $\mathbf{x}_i \in \chi$ to the expectation
    $$m(\mathbf{x}_i) = E_f[f(\mathbf{x}_i)]$$
    of $f(x)$ over all functions $f$
  - a covariance function $\kappa : \mathbb{R}^d \times \mathbb{R}^d \mapsto \mathbb{R}$ mapping each pair of variables $(\mathbf{x}_i, \mathbf{x}_j) \in \chi^2$ to the covariance
    $$\kappa(\mathbf{x}_i, \mathbf{x}_j) = E_f[(f(\mathbf{x}_i) - m(\mathbf{x}_i))^2 (f(\mathbf{x}_j) - m(\mathbf{x}_j))^2]$$
    of $f(x_j)$ and $f(x_j)$ over all functions $f$.

# Kernels in gaussian processes

- The covariance function $\kappa$ is assumed to be a positive definite (Mercer) kernel.
- This means that for any set of distinct points $\mathbf{x}_1, \ldots, \mathbf{x}_n$ it must be

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

  for any choice of the constants $c_1, \ldots, c_n$ such that not all $c_i$ are equal to $0$.
- Equivalently, the square Gram matrix $G$ defined as

$$G = \begin{pmatrix} \kappa(\mathbf{x}_1, \mathbf{x}_1) & \kappa(\mathbf{x}_1, \mathbf{x}_2) & \cdots & \kappa(\mathbf{x}_1, \mathbf{x}_n) \\ \kappa(\mathbf{x}_2, \mathbf{x}_1) & \kappa(\mathbf{x}_2, \mathbf{x}_2) & \cdots & \kappa(\mathbf{x}_2, \mathbf{x}_n) \\ \cdots & \cdots & \cdots & \cdots \\ \kappa(\mathbf{x}_n, \mathbf{x}_1) & \kappa(\mathbf{x}_n, \mathbf{x}_2) & \cdots & \kappa(\mathbf{x}_n, \mathbf{x}_n) \end{pmatrix}$$

  must have positive eigenvalues.
- A collection of positive definite kernels is known in the literature and can be constructed by applying suitable rules.

# Gaussian processes

Given a gaussian process $p(f) = \mathcal{GP}(m, \kappa)$, then for any set of items $\mathbf{X} = (\mathbf{x}_1, \ldots, \mathbf{x}_n)$, the distribution of $f(\mathbf{x}_1), \ldots, f(\mathbf{x}_n)$ is a gaussian

$$(f(\mathbf{x}_1), \ldots, f(\mathbf{x}_n)) \sim \mathcal{N}(\boldsymbol{\mu}(\mathbf{X})|\boldsymbol{\Sigma}(\mathbf{X}))$$

where

- $\boldsymbol{\mu}(\mathbf{X}) = (m(\mathbf{x}_1), \ldots, m(\mathbf{x}_n))^T$
- $\boldsymbol{\Sigma}(\mathbf{X})$ is the Gram matrix wrt $\mathbf{x}_1, \ldots, \mathbf{x}_n$ of a kernel function $\kappa(\mathbf{x}, \mathbf{x}')$

The mean vector - at least initially, with no information from data - is usually assumed to be $\mathbf{0}$: different processes are then characterized only by their covariance kernel $\kappa$.

# Sampling functions from gaussian processes

- For any finite subset $\mathbf{X} = (\mathbf{x}_1, \ldots, \mathbf{x}_n)$ of $\chi$ it is possible to sample from $p(f)$ the values of $f(\mathbf{x}_1), \ldots, f(\mathbf{x}_m)$ by sampling from $\mathcal{N}(f|\mathbf{0}, \boldsymbol{\Sigma}(\mathbf{X}))$, where, as stated before

$$\boldsymbol{\mu}(\mathbf{X})_i = m(\mathbf{x}_i)$$
$$\boldsymbol{\Sigma}(\mathbf{X})_{ij} = \kappa(\mathbf{x}_i, \mathbf{x}_j)$$

# RBF kernel

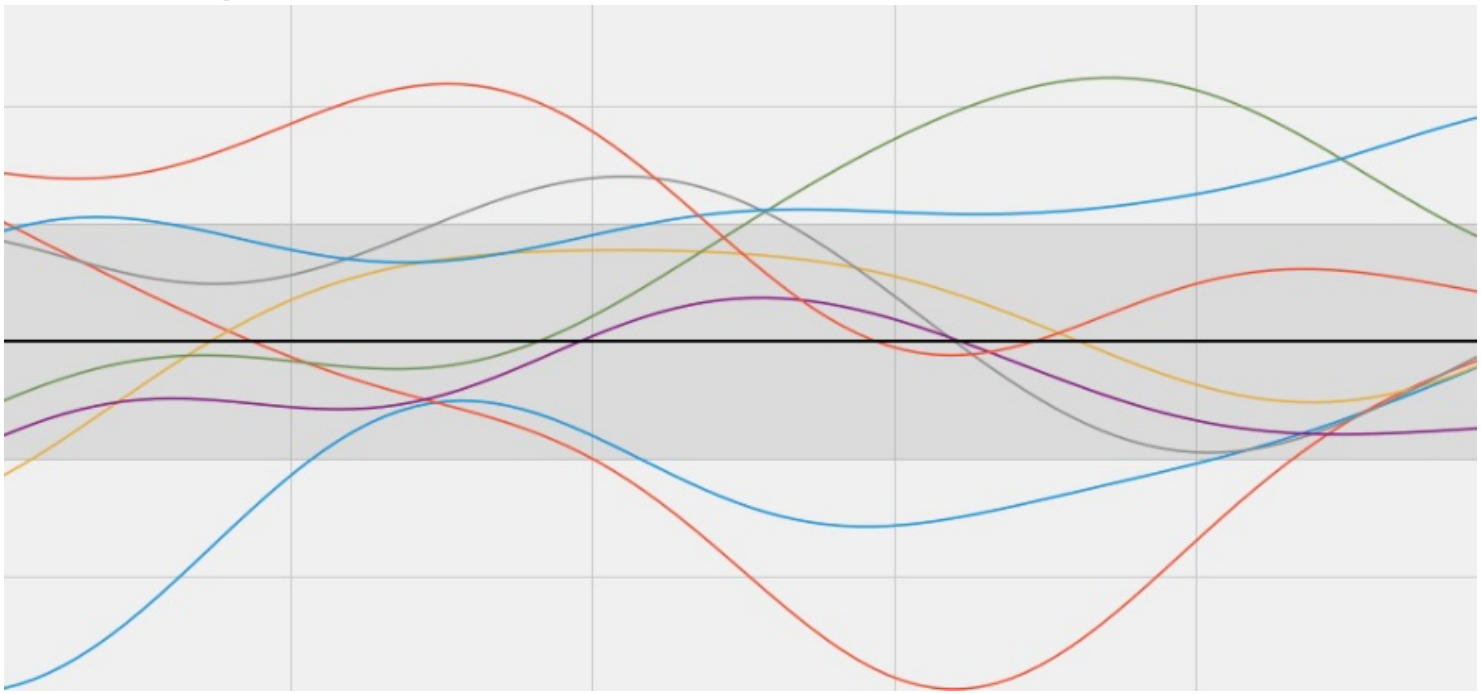
- One of the most applied kernel is the RBF kernel

$$\kappa(\mathbf{x}_1, \mathbf{x}_2) = \sigma^2 e^{-\frac{||\mathbf{x}_1 - \mathbf{x}_2||^2}{2\tau^2}}$$

  which tends to assign higher covariance between $f(\mathbf{x}_1)$ and $f(\mathbf{x}_2)$ if $\mathbf{x}_1$ and $\mathbf{x}_2$ are nearby points.
- Functions drawn from a Gaussian process with RBF kernel tend to be smooth (values computed for nearby points tend to have similar values). Smoothing is larger for larger $\tau$.

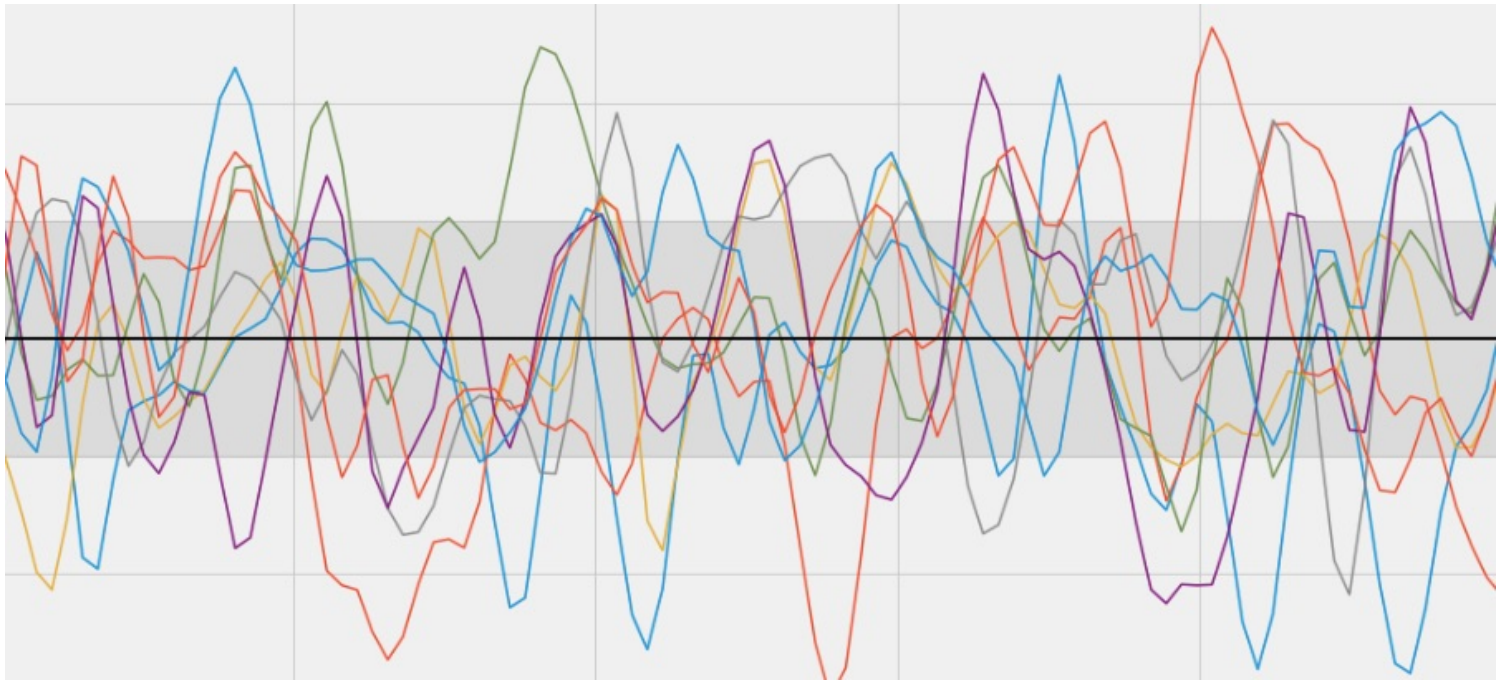
# RBF kernel

Larger smoothing



# RBF kernel

Smaller smoothing



# Gaussian process regression: no noise

Based on gaussian marginalization properties

- Given a gaussian process $\mathcal{GP}(m, \kappa)$, assume $\mathbf{X} = (\mathbf{x}_1, \ldots, \mathbf{x}_n)^T$ is a set of points such that $\mathbf{f} = (f(\mathbf{x}_1), \ldots, f(\mathbf{x}_n))^T$ are known
- that is, we assume that the target values in the training set correspond exactly to the function value $t_i = f(\mathbf{x}_i)$. Note that in the probabilistic model of regression this is not true, since a (gaussian) error is assumed

# Gaussian process regression: no noise

- By the gaussian process definition, $\mathbf{f}$ is distributed as a multivariate gaussian with known mean $\boldsymbol{\mu}(\mathbf{X}) = (m(\mathbf{x}_i), \ldots, m(\mathbf{x}_n))^T$ and covariance matrix $\boldsymbol{\Sigma}(\mathbf{X})$, defined by $\kappa$
- Given a test point $\mathbf{x}$, the set $\mathbf{X} \cup \{\mathbf{x}\} = (\mathbf{x}_1, \ldots, \mathbf{x}_n, \mathbf{x})^T$ is a set of points such that $(f(\mathbf{x}_1), \ldots, f(\mathbf{x}_n), f(\mathbf{x}))^T$ is again a multivariate gaussian with known mean and covariance. This implies that $f(\mathbf{x}|\mathbf{X}, \mathbf{f})$ is gaussian, with

$$m_p(\mathbf{x}|\mathbf{X}, \mathbf{f}) = m(\mathbf{x}) + \boldsymbol{\Sigma}(\mathbf{x}, \mathbf{X})\boldsymbol{\Sigma}(\mathbf{X})^{-1}(\mathbf{f} - \boldsymbol{\mu}(\mathbf{X}))$$
$$\sigma^2 = \kappa_p(\mathbf{x}, \mathbf{x}) = \kappa(\mathbf{x}, \mathbf{x}) - \boldsymbol{\Sigma}(\mathbf{x}, \mathbf{X})\boldsymbol{\Sigma}(\mathbf{X})^{-1}\boldsymbol{\Sigma}(\mathbf{x}, \mathbf{X})^T$$

where $\boldsymbol{\Sigma}(\mathbf{x}, \mathbf{X}) = (\kappa(\mathbf{x}, \mathbf{x}_1), \ldots, \kappa(\mathbf{x}, \mathbf{x}_n))$

# Gaussian process regression: no noise

In this case, an interpolation of the given values is performed: $f(\mathbf{x}_i) = t_i$ for all possible functions, sampled from $f(\mathbf{x}|\mathbf{X}, \mathbf{f})$.
In fact, for all $\mathbf{x}_i \in \mathbf{X}$,

- $\mathbf{\Sigma}(\mathbf{x}_i, \mathbf{X})$ is the $i$-th row of $\mathbf{\Sigma}(\mathbf{X})$: since $\mathbf{\Sigma}(\mathbf{X})\mathbf{\Sigma}(\mathbf{X})^{-1} = \mathbf{I}$ by definition, the product $\mathbf{\Sigma}(\mathbf{x}_i, \mathbf{X})\mathbf{\Sigma}(\mathbf{X})^{-1}$ must be equal to the $i$-th row of $\mathbf{I}$, that is an array $C_i$ such that $C_i[i] = 1$ and $C_i[j] = 0$ otherwise
- as a consequence,

$$m(\mathbf{x}_i|\mathbf{X}, \mathbf{f}) = m(\mathbf{x}_i) + (t_i - m(\mathbf{x}_i)) = t_i$$
$$\sigma^2 = \kappa(\mathbf{x}_i, \mathbf{x}_i) - \kappa(\mathbf{x}_i, \mathbf{x}_i) = 0$$

# Gaussian process regression: noise

In this case, we assume, as usual, that $p(t_i|f, \mathbf{x}_i) = \mathcal{N}(f(\mathbf{x}_i), \sigma_f^2)$

That is, the value $t_i$ observed for variable $\mathbf{x}_i$ differs from the one obtained as $f(\mathbf{x}_i)$ by a gaussian and independent noise

$$t_i = f(\mathbf{x}_i) + \varepsilon \qquad\qquad p(\varepsilon) = \mathcal{N}(\varepsilon|0, \sigma_f^2)$$

# Gaussian process regression

By the assumption of gaussian noise

$$t_i = f(\mathbf{x}_i) + \varepsilon \qquad\qquad i = 1, \ldots, m$$
$$t = f(\mathbf{x}) + \varepsilon$$

with $p(\varepsilon) = \mathcal{N}(\varepsilon|0, \sigma^2)$, it derives that

$$\begin{aligned} p(t_1, \ldots, t_m, t|\mathbf{x}, \mathbf{X}; \sigma^2) &= p(\mathbf{t}, t|\mathbf{x}, \mathbf{X}; \sigma^2) \\ &= p(f(\mathbf{x}_1) + \varepsilon, \ldots, f(\mathbf{x}_m) + \varepsilon, f(\mathbf{x}) + \varepsilon) \\ &= \mathcal{N}(\mathbf{0}, \mathbf{\Sigma}(\mathbf{X} \cup \{\mathbf{x}\} + \sigma^2\mathbf{I}) \end{aligned}$$

# Gaussian process regression

- It is possible to show that the posterior distribution of functions is again a gaussian process, with different mean and covariance functions

$$p(f|\mathbf{X}, \mathbf{t}) = \mathcal{GP}(m_p, \kappa_p)$$

where

$$\begin{aligned} m_p(\mathbf{x}) &= \mathbf{\Sigma}(\mathbf{x}, \mathbf{X})(\mathbf{\Sigma}(\mathbf{X}) + \sigma_f^2 \mathbf{I})^{-1}\mathbf{t} \\ \kappa_p(\mathbf{x}, \mathbf{x}') &= \kappa(\mathbf{x}, \mathbf{x}') - \mathbf{\Sigma}(\mathbf{x}, \mathbf{X})(\mathbf{\Sigma}(\mathbf{X}) + \sigma_f^2 \mathbf{I})^{-1}\mathbf{\Sigma}(\mathbf{x}', \mathbf{X})^T \end{aligned}$$

# Gaussian process regression

By the properties of gaussian distributions wrt to conditioning, it results

$$p(t|\mathbf{x}, \mathbf{X}, \mathbf{t}) = \mathcal{N}(y|\overline{\mu}(\mathbf{x}), \overline{\sigma}^2(\mathbf{x}))$$

with

$$\overline{\mu}(\mathbf{x}) = k(\mathbf{x}, \mathbf{X})(\mathbf{\Sigma}(\mathbf{X}) + \sigma^2\mathbf{I})^{-1}\mathbf{t} = \sum_{i=1}^{m} \alpha(\mathbf{x}_i, \mathbf{x})t_i$$

$$\overline{\sigma}^2(\mathbf{x}) = \kappa(\mathbf{x}, \mathbf{x}) + \sigma^2 - k(\mathbf{x}, \mathbf{X})(\mathbf{\Sigma}(\mathbf{X}) + \sigma^2\mathbf{I})^{-1}k(\mathbf{x}, \mathbf{X})^T$$

# Estimating kernel parameters

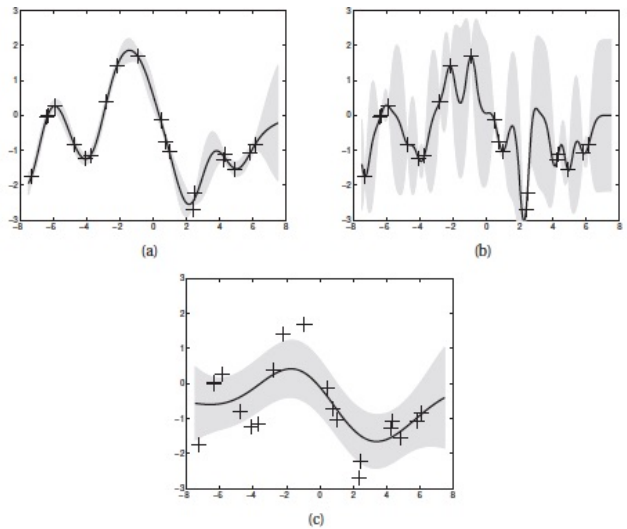
The predictive performance of gaussian processes depends exclusively on the suitability of the chosen kernel.

Let us consider the case of an RBF kernel. Then,

$$\kappa(\mathbf{x}_i, \mathbf{x}_j) = \sigma_f^2 e^{-\frac{1}{2}(\mathbf{x}_i - \mathbf{x}_j)^T \mathbf{M} (\mathbf{x}_i - \mathbf{x}_j)} + \sigma_y^2 \delta_{ij}$$

$\mathbf{M}$ can be defined in several ways: the simplest one is $\mathbf{M} = l^{-2}\mathbf{I}$.

Even in this simple case, varying the values of $\sigma_f, \sigma_y, l$ returns quite different results.




(figure from K.Murphy "Machine learning: a probabilistic perspective" p. 519, with $(l, \sigma_f, \sigma_y)$ equal to $(1, 1, 0.1), (0.3, 1.08, 0.00005), (3.0, 1.16, 0.89)$)

# Estimating kernel parameters

Kernel parameters can be estimated, as usual, through grid search and (cross-)validation.

A different, more efficient approach relies on maximizing the marginal likelihood

$$p(\mathbf{t}|\mathbf{X}) = \int p(\mathbf{t}|\mathbf{f},\mathbf{X})p(\mathbf{f}|\mathbf{X})d\mathbf{f} = \int \mathcal{N}(\mathbf{f}|\mathbf{0},\mathbf{\Sigma}(\mathbf{X})) \prod_{i=1}^{m} \mathcal{N}(t_i|f_i,\sigma_t^2)d\mathbf{f}$$

It can be shown that

$$\begin{aligned}\log p(\mathbf{t}|\mathbf{X}) &= \log \mathcal{N}(\mathbf{t}|\mathbf{0},\mathbf{\Sigma}(\mathbf{X}) + \sigma_t^2\mathbf{I}) \\ &= -\frac{1}{2}\mathbf{y}^T(\mathbf{\Sigma}(\mathbf{X}) + \sigma_t^2\mathbf{I})^{-1}\mathbf{t} - \frac{1}{2}\log|\mathbf{\Sigma}(\mathbf{X})| + \sigma_t^2\mathbf{I} - \frac{n}{2}\log(2\pi)\end{aligned}$$

where the first term measures the fitting of the model to data, the second the complexity of the model, and the third + fourth ones are constants