Non parametric regression

Course of Machine Learning
Master Degree in Computer Science

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a.a. 2020-2021

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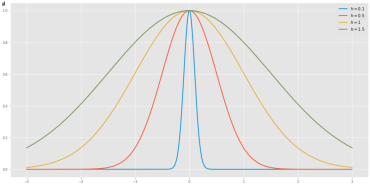
Kernel regression

- 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

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

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

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

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 $\mathbf{x} = (x_1, \dots, x_n)^T$ 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:

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

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 $\chi = (\mathbf{x}_1, \dots, \mathbf{x}_m)$ 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 $(f(\mathbf{x}_1), \dots, f(\mathbf{x}_m))$
    - Any vector $(y_1, \dots, y_m)$ 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 $\mathbb{R}$

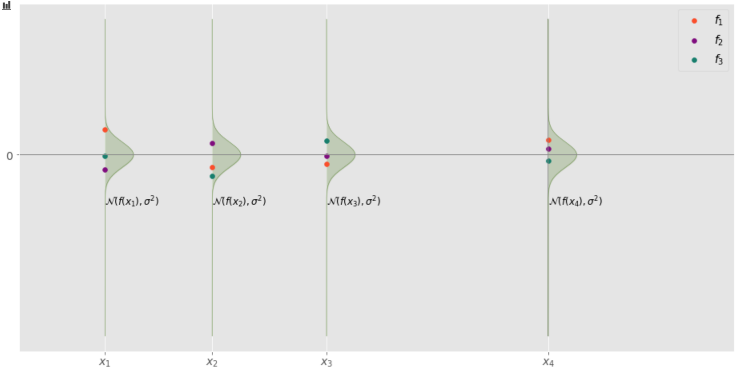
Gaussian distributions over functions with finite domains

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 σ^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

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

Gaussian distributions over functions with infinite domains

- In the case of infinite χ, 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 χ, known as the index set.
- A Gaussian process is a stochastic process such that for any finite subset $\mathbf{x}_1, \dots, \mathbf{x}_n$ of χ, the function values $f(\mathbf{x}_1), \dots, f(\mathbf{x}_n)$ 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 κ 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 κ.

Sampling functions from gaussian processes

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

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

RBF kernel

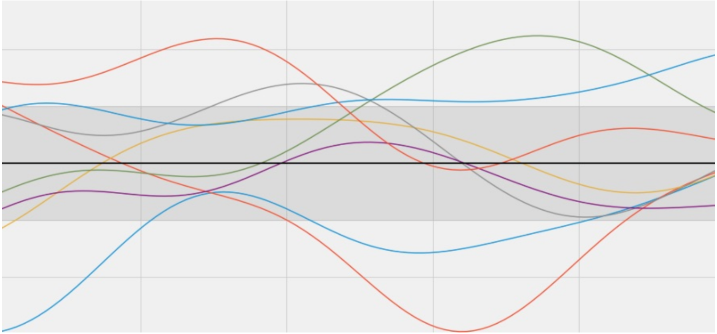
- One of the most applied kernel is the RBF kernel

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

  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 τ.

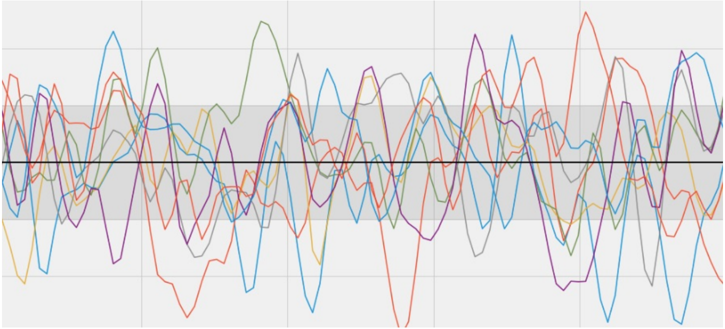
RBF kernel

Larger smoothing



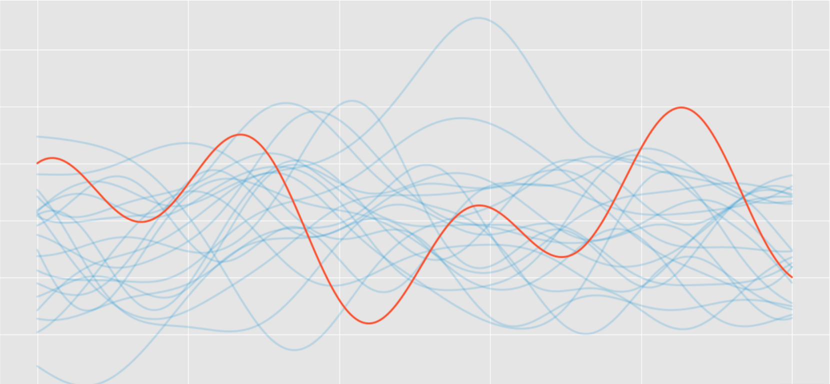
RBF kernel

Smaller smoothing



Gaussian process regression: no noise

- By the gaussian process definition, $\mathbf{f}$ is distributed as a multivariate gaussian such that the mean of any value $\mathbf{x}$ is $m(\mathbf{x})$ and the covariance of any pair $\mathbf{x}, \mathbf{x}'$ is $\kappa(\mathbf{x}, \mathbf{x}')$
- as a consequence, for any finite set of points $\mathbf{X}$, we have that $\mathbf{f}(\mathbf{X})$ is distributed as a multivariate gaussian with mean $\boldsymbol{\mu}(\mathbf{X})$ defined as $\boldsymbol{\mu}(\mathbf{X})_i = m(\mathbf{x}_i)$ and covariance matrix $\boldsymbol{\Sigma}(\mathbf{X})$, defined as $\boldsymbol{\Sigma}(\mathbf{X})_{i,j} = \kappa(\mathbf{x}_i, \mathbf{x}_j)$



Gaussian process regression: no noise

- Let us now assume that for a set of points $\mathbf{X} = (\mathbf{x}_1, \ldots, \mathbf{x}_n)^T$ the corresponding values $\mathbf{f} = (f(\mathbf{x}_1), \ldots, f(\mathbf{x}_n))^T$ are known
- that is, we assume that a training set $\mathbf{X}, \mathbf{t}$ is available such 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

In this case, for any new set of points $\mathbf{X}^*$, the joint distribution of $(\mathbf{f}(\mathbf{X}), \mathbf{f}(\mathbf{X}^*))$ is a multivariate gaussian distribution with mean $\boldsymbol{\mu}(\mathbf{X}, \mathbf{X}^*)$ and covariance $\boldsymbol{\Sigma}(\mathbf{X}, \mathbf{X}^*)$

- $\boldsymbol{\mu}(\mathbf{X}, \mathbf{X}^*) = (\boldsymbol{\mu}(\mathbf{X}), \boldsymbol{\mu}(\mathbf{X}^*))^T$
- $$\boldsymbol{\Sigma}(\mathbf{X}, \mathbf{X}^*) = \begin{pmatrix} \boldsymbol{\Sigma}(\mathbf{X}) & \boldsymbol{\Sigma}(\mathbf{x}, \mathbf{X}) \\ \boldsymbol{\Sigma}(\mathbf{x}, \mathbf{X})^T & \boldsymbol{\Sigma}(\mathbf{X}^*) \end{pmatrix}$$

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

The posterior distribution of $\mathbf{f}(\mathbf{X}^*)$, given $\mathbf{X}, \mathbf{X}^*, \mathbf{t}$ can be derived by gaussian distribution properties, and turns out to be a gaussian distribution with mean and covariance defined as

- $\boldsymbol{\mu}^* = \boldsymbol{\mu}(\mathbf{X}^*) + \boldsymbol{\Sigma}(\mathbf{x}, \mathbf{X})\boldsymbol{\Sigma}(\mathbf{X})^{-1}(\mathbf{t} - \boldsymbol{\mu}(\mathbf{X}))$
- $\boldsymbol{\Sigma}^* = \boldsymbol{\Sigma}(\mathbf{X}^*) - \boldsymbol{\Sigma}(\mathbf{x}, \mathbf{X})\boldsymbol{\Sigma}(\mathbf{X})^{-1}\boldsymbol{\Sigma}(\mathbf{x}, \mathbf{X})^T$

Gaussian process regression: no noise

In particular, for a single test point $\mathbf{x}$, we have that the corresponding predictive distribution is

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

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 $\mathbf{x}_i \in \mathbf{X}$,

- $\boldsymbol{\Sigma}(\mathbf{x}_i, \mathbf{X})$ is the i-th row of $\boldsymbol{\Sigma}(\mathbf{X})$: since $\boldsymbol{\Sigma}(\mathbf{X})\boldsymbol{\Sigma}(\mathbf{X})^{-1} = \mathbf{I}$ by definition, the product $\boldsymbol{\Sigma}(\mathbf{x}_i, \mathbf{X})\boldsymbol{\Sigma}(\mathbf{X})^{-1}$ 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,

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

Gaussian process regression: gaussian noise

Let us now 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

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

that is, $p(\mathbf{t}|\mathbf{f}) = \mathcal{N}(\mathbf{t}|\mathbf{f}, \sigma^2\mathbf{I})$

Gaussian process regression: gaussian noise

- $\mathbf{f}$ is now 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 $\hat{\mathbf{\Sigma}}(\mathbf{X}) = \mathbf{\Sigma}(\mathbf{X}) + \sigma_f^2\mathbf{I}$, defined by κ and σ_f^2

Gaussian process regression: gaussian noise

- Let us now assume that a training set $\mathbf{X}, \mathbf{t}$ is available such that the target values in the training set correspond approximately to the function value $t_i = f(\mathbf{x}_i) + \varepsilon$.
- In this case, for any new set of points $\mathbf{X}^*$, the joint distribution of $(\mathbf{t}, \mathbf{f}(\mathbf{X}^*))$ is a multivariate gaussian distribution with mean $\boldsymbol{\mu}(\mathbf{X}, \mathbf{X}^*)$ and covariance $\boldsymbol{\Sigma}(\mathbf{X}, \mathbf{X}^*)$
- $\boldsymbol{\mu}(\mathbf{X}, \mathbf{X}^*) = (\boldsymbol{\mu}(\mathbf{X}), \boldsymbol{\mu}(\mathbf{X}^*))^T$
- $$\boldsymbol{\Sigma}(\mathbf{X}, \mathbf{X}^*) = \begin{pmatrix} \hat{\boldsymbol{\Sigma}}(\mathbf{X}) & \boldsymbol{\Sigma}(\mathbf{x}, \mathbf{X}) \\ \boldsymbol{\Sigma}(\mathbf{x}, \mathbf{X})^T & \boldsymbol{\Sigma}(\mathbf{X}^*) \end{pmatrix}$$

Gaussian process regression: gaussian noise

The posterior distribution of $\mathbf{f}(\mathbf{X}^*)$, given $\mathbf{X}, \mathbf{X}^*, \mathbf{t}$ can be again derived by the gaussian distribution properties, and turns out again to be a gaussian distribution with mean and covariance defined as

- $\boldsymbol{\mu}^* = \boldsymbol{\mu}(\mathbf{X}^*) + \boldsymbol{\Sigma}(\mathbf{x}, \mathbf{X})\hat{\boldsymbol{\Sigma}}(\mathbf{X})^{-1}(\mathbf{t} - \boldsymbol{\mu}(\mathbf{X}))$
- $\boldsymbol{\Sigma}^* = \boldsymbol{\Sigma}(\mathbf{X}^*) - \boldsymbol{\Sigma}(\mathbf{x}, \mathbf{X})\hat{\boldsymbol{\Sigma}}(\mathbf{X})^{-1}\boldsymbol{\Sigma}(\mathbf{x}, \mathbf{X})^T$

Gaussian process regression: gaussian noise

In particular, for a single test point $\mathbf{x}$, we have now that the corresponding predictive distribution is

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

Estimating kernel parameters

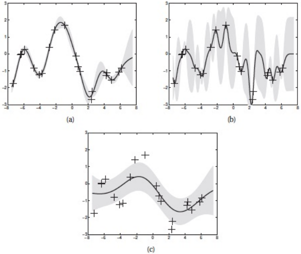
The predictive performance of gaussian processes depends exclusively on the suitability of the chosen kernel.

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 σ_f, σ_y, l returns quite different results.



(figure from K.Murphy “Machine learning: a probabilistic perspective” p. 519, with (l, σ_f, σ_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