Kernel regression and gaussian processes

Course of Machine Learning
Master Degree in Computer Science

University of Rome “Tor Vergata”

a.a. 2019-2020

Giorgio Gambosi

Kernel regression

Kernel smoothers methods can be applied also to regression: in this case, the 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 $\mathbf{x}$).

In regression, we are interested in estimating the conditional expectation

$$f(\mathbf{x}) = E[y|\mathbf{x}] = \int yp(y|\mathbf{x})dy = \int y\frac{p(\mathbf{x},y)}{p(\mathbf{x})}dy = \frac{\int yp(\mathbf{x},y)dy}{p(\mathbf{x})} = \frac{\int yp(\mathbf{x},y)dy}{\int p(\mathbf{x},y)dy}$$

Applying kernels, we have

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

Kernels regression

This results into

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

and, since $\displaystyle\int \kappa_h(y-t_i)dy = 1$ and $\displaystyle\int y\kappa_h(y-t_i)dy = t_i$, we get

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

Kernels 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 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 weighted combination of constant values (target values in the training set).

Locally weighted regression improves that approach by referring to a weighted version of the sum of squared differences loss function used in regression.
If a value y has to be predicted for a provided 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

An instance of the weighted regression problem must be solved,

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

which 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.
A suitable modification of the IRLS algorithm for logistic regression can be applied here to compute

$$\hat{\mathbf{w}}(\mathbf{x}) = \underset{\mathbf{w}}{\operatorname{argmax}} \sum_{i=1}^{n} \kappa_h(\mathbf{x} - \mathbf{x}_i)(t_i \log p_i - (1 - t_i) \log(1 - p_i))$$

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.

Consider a random vector $\mathbf{x} = (x_1, \ldots, x_n)^T$ with $p(\mathbf{x}) = \mathcal{N}(\boldsymbol{\mu}, \boldsymbol{\Sigma})$ 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, both $\boldsymbol{\mu}$ and $\boldsymbol{\Sigma}$ can be partitioned as

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

Clearly, $\boldsymbol{\mu}_A \in \mathbb{R}^r$, $\boldsymbol{\mu}_B \in \mathbb{R}^{n-r}$, $\boldsymbol{\Sigma}_{AA} \in \mathbb{R}^r \times \mathbb{R}^r$, $\boldsymbol{\Sigma}_{BB} \in \mathbb{R}^{n-r} \times \mathbb{R}^{n-r}$, $\boldsymbol{\Sigma}_{AB} \in \mathbb{R}^r \times \mathbb{R}^{n-r}$

Some properties of Gaussian distribution

Properties of $\mathbf{x}_A, \mathbf{x}_B$.

- Marginal densities are gaussian with

$$p(\mathbf{x}_A) = \mathcal{N}(\boldsymbol{\mu}_A, \boldsymbol{\Sigma}_{AA}) \qquad p(\mathbf{x}_B) = \mathcal{N}(\boldsymbol{\mu}_B, \boldsymbol{\Sigma}_{BB})$$

- Conditional densities are gaussian with

$$p(\mathbf{x}_A|\mathbf{x}_B) = \mathcal{N}(\boldsymbol{\mu}_A + \boldsymbol{\Sigma}_{AB}\boldsymbol{\Sigma}_{BB}^{-1}(\mathbf{x}_B - \boldsymbol{\mu}_B), \boldsymbol{\Sigma}_{AA} - \boldsymbol{\Sigma}_{AB}\boldsymbol{\Sigma}_{BB}^{-1}\boldsymbol{\Sigma}_{BA})$$
$$p(\mathbf{x}_B|\mathbf{x}_A) = \mathcal{N}(\boldsymbol{\mu}_B + \boldsymbol{\Sigma}_{BA}\boldsymbol{\Sigma}_{AA}^{-1}(\mathbf{x}_A - \boldsymbol{\mu}_A), \boldsymbol{\Sigma}_{BB} - \boldsymbol{\Sigma}_{BA}\boldsymbol{\Sigma}_{AA}^{-1}\boldsymbol{\Sigma}_{AB})$$

Gaussian processes

Multivariate Gaussian distributions: useful for modeling finite collections of real-valued variables. Nice analytical properties.

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 functions.

Probability distributions over functions with finite domains

Let $\chi = (\mathbf{x}_1, \ldots, \mathbf{x}_m)$ be any finite array of elements, and let $\mathcal{H}$ be the set of functions from χ to $\mathbb{R}$

A function $f \in \mathcal{H}$ can be described by the array $(f(\mathbf{x}_1), \ldots, f(\mathbf{x}_m))$ and any array $(y_1, \ldots, y_m)$ 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 density distribution $p(f), f \in \mathcal{H}$ over functions $f \in \mathcal{H}$, corresponds then to a density distribution $p(\mathbf{x}), \mathbf{x} \in \mathbb{R}^m$

Gaussian distributions over functions with finite domains

If we assume that $p(f)$ is a multivariate Gaussian distribution centered on $\mathbf{0}$ and with diagonal covariance $\sigma^2\mathbf{I}$, it results

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

This can be seen as a *prior* distribution of functions, with respect to the observation of any pair $(\mathbf{x}_j, t_j)$, $1 \leq j \leq m$.

Gaussian distributions over functions with finite domains

Given a set $I \subset \{1, \ldots, m\}$ of indices, let $\mathbf{X} = \{(\mathbf{x}_j, t_j), j \in I\}$ be a set of observed pairs.

The posterior distribution $p(f|\mathbf{X})$ of functions (wrt to $\mathbf{X}$) can be defined and derived according to Bayes' rule, provided a likelihood model is defined such as the usual $t_i = y_i + \varepsilon$, $p(\varepsilon) = \mathcal{N}(\varepsilon|0, \beta)$.

The predictive distribution $p(y_k|\mathbf{x}_k, \mathbf{X}) = \displaystyle\int p(y_k|f, \mathbf{x}_k)p(f|\mathbf{X})df$ for any $k \notin I$ can be also derived.

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 any finite subset of random variables has a 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 $m(\mathbf{x})$ onto $\mathbb{R}$ for each $\mathbf{x} \in \chi$
- a kernel function $\kappa(\mathbf{x}_1, \mathbf{x}_2)$ onto $\mathbb{R}$ for each pair from $(\mathbf{x}_i, \mathbf{x}_j) \in \chi^2$

Given a finite subset $\mathbf{X} = (\mathbf{x}_1, \ldots, \mathbf{x}_m)$ of χ, the distribution of the corresponding set of random variables $(f(\mathbf{x}_1), \ldots, f(\mathbf{x}_m))$ is given by

$$p(f(\mathbf{x}_1), \ldots, f(\mathbf{x}_m) = \mathcal{N}(f | \boldsymbol{\mu}(\mathbf{X}), \boldsymbol{\Sigma}(\mathbf{X}))$$

where $\boldsymbol{\mu}(\mathbf{X}) = (m(\mathbf{x}_1), \ldots, m(\mathbf{x}_m))^T$ and $\boldsymbol{\Sigma}(\mathbf{X})_{ij} = \kappa(\mathbf{x}_i, \mathbf{x}_j)$.

Gaussian processes

That is, in a Gaussian process:

- the expectation of $f(\mathbf{x})$ is provided by function $m(\mathbf{x})$
- the covariance $E_f[(f(\mathbf{x}_1) - m(\mathbf{x}_1))^2 (f(\mathbf{x}_2) - m(\mathbf{x}_2))^2]$ between $f(\mathbf{x}_1)$ and $f(\mathbf{x}_2)$ is provided by the kernel function $\kappa(\mathbf{x}_1, \mathbf{x}_2)$.

It can be shown that κ must be such that for any subset $\mathbf{X}$ of χ, the corresponding covariance matrix $\mathbf{\Sigma}(\mathbf{X})$ is positive semidefinite (that is, for any $\mathbf{x}$ it must be $\mathbf{x}^T \mathbf{\Sigma}(\mathbf{X})\mathbf{x} \geq 0$)

Gaussian processes

Given a Gaussian process $\mathcal{GP}(m, \kappa)$, a function$f$ drawn from it can be intuitively seen as an extremely high-dimensional vector drawn from an extremely high-dimensional multivariate Gaussian.

Each dimension of the Gaussian corresponds to an element x from χ, and the corresponding component of the random vector represents the value of $f(x)$

Using the marginalization property for multivariate Gaussians, we can obtain the multivariate Gaussian density corresponding to any finite subset of variables.

RBF kernel

One of the most applied kernel is the RBF kernel

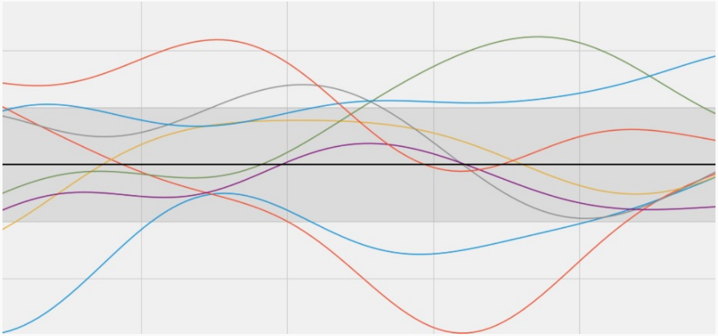
$$\kappa(\mathbf{x}_1, \mathbf{x}_2) = \sigma^2 e^{-\frac{||\mathbf{x}_1 - \mathbf{x}_2||^2}{2\tau^2}}$$

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.

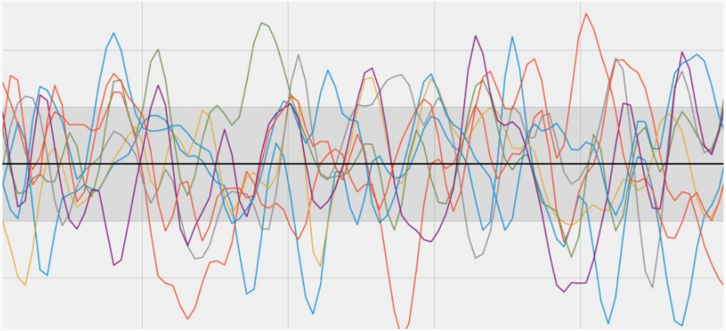
RBF kernel

Larger smoothing



RBF kernel

Smaller smoothing



Gaussian process regression

- Assume, as usual, that observed data derive from function f with an additional gaussian and independent noise.

$$y = f(\mathbf{x}) + \varepsilon \qquad\qquad p(\varepsilon) = \mathcal{N}(\varepsilon|\mathbf{0}, \sigma^2\mathbf{I})$$

  that is, $p(y|f, \mathbf{x}) = \mathcal{N}(y|f(\mathbf{x}), \sigma^2\mathbf{I})$
- A Gaussian process $p(f) = \mathcal{GP}(m, \kappa)$ provides a prior distribution on functions in $\mathcal{H}$.

Gaussian process regression

Given a set of observations $\{\mathbf{X} = \{\mathbf{x}_i\}, \mathbf{y} = \{y_i\}\}, i = 1, \ldots, m\}$ we could now derive a posterior distribution of functions.

It is possible to show that

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

with

$$\begin{aligned} m_p(\mathbf{x}) &= k(\mathbf{x}, \mathbf{X})(\mathbf{\Sigma}(\mathbf{X}) + \sigma^2\mathbf{I})^{-1}\mathbf{y} \\ \kappa_p(\mathbf{x}, \mathbf{x}') &= \kappa(\mathbf{x}, \mathbf{x}') - k(\mathbf{x}, \mathbf{X})(\mathbf{\Sigma}(\mathbf{X}) + \sigma^2\mathbf{I})^{-1}k(\mathbf{X}, \mathbf{x}') \end{aligned}$$

where

$$\begin{aligned} k(\mathbf{x}, \mathbf{X}) &= \begin{bmatrix} \kappa(\mathbf{x}, \mathbf{x}_1) & \cdots & \kappa(\mathbf{x}, \mathbf{x}_m) \end{bmatrix} \\ k(\mathbf{X}, \mathbf{x}') &= \begin{bmatrix} \kappa(\mathbf{x}_1, \mathbf{x}') & \cdots & \kappa(\mathbf{x}_m, \mathbf{x}') \end{bmatrix}^T = k(\mathbf{x}', \mathbf{X})^T \end{aligned}$$

This makes it possible to sample functions from the posterior distribution

Gaussian process regression

In order to derive the predictive distribution of a new item $\mathbf{x}$, let us observe that for any function f drawn from $\mathcal{GP}(\mathbf{0}, \kappa)$, the marginal distribution over any set of input points $\mathbf{X} = (\mathbf{x}_1, \ldots, \mathbf{x}_m)$ is a multivariate Gaussian distribution.

$$p(f(\mathbf{x}_1), \ldots, f(\mathbf{x}_m)) = \mathcal{N}(\mathbf{x}|\mathbf{0}, \mathbf{\Sigma}(\mathbf{X}))$$

Let $\mathbf{X}_t$ be the set of points in the training set, and let $\mathbf{x}$ be a new item. Then,

$$(f(\mathbf{x}_1), \ldots, f(\mathbf{x}_m), f(\mathbf{x})) \sim \mathcal{N}(\mathbf{0}, \mathbf{\Sigma}(\mathbf{X} \cup \{\mathbf{x}\}))$$

where

$$\mathbf{\Sigma}(\mathbf{X} \cup \{\mathbf{x}\}) = \left[\begin{array}{cc} \mathbf{\Sigma}(\mathbf{X}) & k(\mathbf{X}, \mathbf{x}) \\ k(\mathbf{x}, \mathbf{X}) & \kappa(\mathbf{x}, \mathbf{x}) \end{array} \right]$$

Gaussian process regression

By the assumption of gaussian noise

$$\begin{aligned} y_i &= f(\mathbf{x}_i) + \varepsilon \qquad\qquad i = 1, \ldots, m \\ y &= f(\mathbf{x}) + \varepsilon \end{aligned}$$

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

$$(y_1, \ldots, y_m, y) \sim (f(\mathbf{x}_1) + \varepsilon, \ldots, f(\mathbf{x}_m) + \varepsilon, f(\mathbf{x}) + \varepsilon) \sim \mathcal{N}(\mathbf{0}, \mathbf{\Sigma}(\mathbf{X} \cup \{\mathbf{x}\} + \sigma^2\mathbf{I})$$

From the properties of multivariate gaussian distributions, namely

$$p(\mathbf{x}_B|\mathbf{x}_A) = \mathcal{N}(\boldsymbol{\mu}_B + \mathbf{\Sigma}_{BA}\mathbf{\Sigma}_{AA}^{-1}(\mathbf{x}_A - \boldsymbol{\mu}_A), \mathbf{\Sigma}_{BB} - \mathbf{\Sigma}_{BA}\mathbf{\Sigma}_{AA}^{-1}\mathbf{\Sigma}_{AB})$$

it results

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

with

$$\begin{aligned} \overline{\mu}(\mathbf{x}) &= k(\mathbf{x}, \mathbf{X})(\mathbf{\Sigma}(\mathbf{X}) + \sigma^2\mathbf{I})^{-1}\mathbf{y} = \sum_{i=1}^{m} \alpha(\mathbf{x}_i, \mathbf{x}) y_i \\ \overline{\sigma}^2(\mathbf{x}) &= \kappa(\mathbf{x}, \mathbf{x}) + \sigma^2 - k(\mathbf{x}, \mathbf{X})(\mathbf{\Sigma}(\mathbf{X}) + \sigma^2\mathbf{I})^{-1} k(\mathbf{x}, \mathbf{X})^T \end{aligned}$$

Estimating kernel parameters

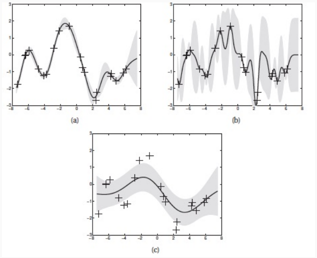
The predictive performance of gaussian processes depends exclusively on the suitability of the chosen kernel.

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

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

It can be shown that

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

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