Lecture 10

Gaussian Processes

Luigi Freda

ALCOR Lab DIAG University of Rome "La Sapienza"

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Distribution over functions

- in supervised learning, we observe some input vector \mathbf{x}_i and some scalar outputs y_i
- we assume that $y_i = f(\mathbf{x}_i)$, for some **unknown function** f, possibly corrupted by **noise** ϵ
- the optimal approach is to infer a **distribution over functions** given the data, $p(f|\mathbf{X}, \mathbf{y})$, and then to use this to make predictions given new inputs, i.e., to compute

$$\rho(y^*|\mathbf{x}^*,\mathbf{X},\mathbf{y}) = \int \rho(\mathbf{y}^*,f|\mathbf{x}^*,\mathbf{X},\mathbf{y})df = \int \rho(\mathbf{y}^*|f,\mathbf{x}^*)\rho(f|\mathbf{X},\mathbf{y})df$$

- question: how can we characterize a **distribution over functions** p(f)?
- in order to answer, we first need to introduce the concept of stochastic process

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Stochastic Process

 a stochastic process is a statistical model where each observation correspond to a function

more formally

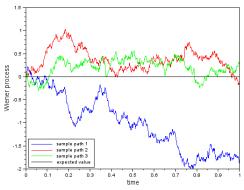
- let \mathcal{T} be a subset of $[0,\infty)$
- a family of random variables $\{X_t\}_{t\in\mathcal{T}}$, indexed by \mathcal{T} , is called a **stochastic process**
- when $\mathcal{T} = \mathbb{N}$, $\{X_t\}_{t \in \mathcal{T}}$ is said to be a **discrete-time process**
- when $T = [0, \infty)$, it is called a continuous-time process

note that

- when $\mathcal T$ is a singleton (say $\mathcal T=\{1\}$), the process $\{X_t\}_{t\in\mathcal T}\equiv X_1$ is really just a single random variable
- when \mathcal{T} is finite (e.g., $\mathcal{T} = \{1, 2, ..., n\}$), we get a random vector

Stochastic Process

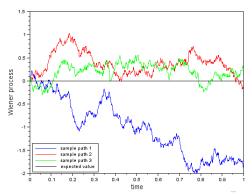
- ullet every stochastic process can be viewed as a **function** of **two variables** t and $\omega \in \Omega$
- ullet for each fixed $(t,\omega) o X_t(\omega)$ is a random variable
- if we change our point of view and keep ω fixed, the stochastic process is a function mapping ω to the real-valued function $t \to X_t(\omega)$ (these functions are called the **trajectories** of the stochastic process X)



Stochastic Process

how can we study/characterize a stochastic process $\{X_t\}_{t\in\mathcal{T}}$?

- ullet we can start by fixing $t=t_1$ and characterizing the PDF $p_{X_1}(x_1)$ of the RV X_1
- then we can consider two values $t_1, t_2 \in \mathcal{T}$ and characterize the joint PDF $p_{X_1, X_2}(x_1, x_2)$ of the RVs X_1 and X_2
- in general we can consider any arbitrary finite set of values $t_1, ..., t_n$ and its corresponding joint PDF $p_{X_1,...,X_n}(x_1,...,x_n)$



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Gaussian processes

in a Gaussian process representing an unknown function f

• every point $y_i = f(\mathbf{x}_i)$ is associated with a normally distributed random variable, i.e.

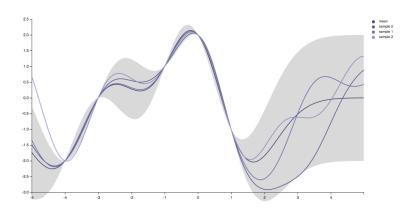
$$f(\mathbf{x}_i) \sim \mathcal{N}(\mu(\mathbf{x}_i), \sigma(\mathbf{x}_i))$$

• every finite collection of random variables $f(\mathbf{x}_1),...,f(\mathbf{x}_n)$ has a multivariate normal distribution

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

the covariance $\Sigma(\mathbf{x}_1,...,\mathbf{x}_n)$ has elements $\Sigma_{ij} = \kappa(\mathbf{x}_i,\mathbf{x}_j)$ where κ is a positive definite kernel function

An Example



different observations (trajectories) of a Gaussian process with

- $\bullet \ \ \mathsf{mean} \ \mathsf{function} \ \mu \ \mathsf{(black)}$
- $\mu \pm 2\sigma$ functions (95% confidence)

Why Gaussian Processes?

why should we use a Gaussian processes?

- GP based methods can be thought of as a Bayesian alternative to the presented kernel methods (including SVM)
- although those kernel methods are sparser and therefore faster, they do not give well-calibrated probabilistic outputs (i.e. estimates plus confidences)

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GP Prior

- a GP defines a **prior** over functions, which can be converted into a **posterior** over functions once we have seen some data $\mathcal{D} = \{\mathbf{x}_i, y_i\}_{i=1}^N$
- the GP prior on the regression function is denoted by

$$f(\mathbf{x}) \sim GP(m(\mathbf{x}), \kappa(\mathbf{x}, \mathbf{x}'))$$

where $m(\mathbf{x}) \in \mathbb{R}$ is the mean function and $\kappa(\mathbf{x}, \mathbf{x}') \in \mathbb{R}$ is the kernel or covariance function

$$m(\mathbf{x}) = \mathbb{E}[f(\mathbf{x})]$$

$$\kappa(\mathbf{x}, \mathbf{x}') = \mathbb{E}[(f(\mathbf{x}) - \mathbf{m}(\mathbf{x}))(f(\mathbf{x}') - \mathbf{m}(\mathbf{x}'))^T]$$

N.B.: $\kappa(\mathbf{x}, \mathbf{x}')$ is required to be a **positive definite kernel**

• for any finite set of points, the process defines a joint Gaussian

$$ho(\mathbf{f},\mathbf{X}) = \mathcal{N}(\mathbf{f}|\boldsymbol{\mu},\mathbf{K})$$

where $\mathbf{f} \triangleq [f(\mathbf{x}_1),...,f(\mathbf{x}_N)]^T \in \mathbb{R}^N$, $K_{ij} = \kappa(\mathbf{x}_i,\mathbf{x}_j)$, $\boldsymbol{\mu} = [m(\mathbf{x}_1),...,m(\mathbf{x}_N)]^T \in \mathbb{R}^N$,

- note that it is common to use a mean function of m(x) = 0, since the GP is flexible enough to model the mean arbitrarily well
- it is also possible to consider parametric models for the mean function

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- suppose we observe a training set $\mathcal{D} = \{(\mathbf{x}_i, f_i), i = 1 : N\}$, where $f_i = f(\mathbf{x}_i)$ is the **noise-free** observation of the function evaluated at \mathbf{x}_i
- given a test set X_* of size $N_* \times D$, we want to predict the function outputs f_*

what do we expect?

- we have assumed the observations are noiseless
- if we ask the GP to predict f(x) for a value of x that it has already seen, we want the GP to return the answer f(x) with no uncertainty
- in other words, it should act as an interpolator of the training data

• by definition of the GP, the joint distribution has the following form

$$\begin{bmatrix} \mathbf{f} \\ \mathbf{f}_* \end{bmatrix} \sim \mathcal{N} \bigg(\begin{bmatrix} \boldsymbol{\mu} \\ \boldsymbol{\mu}_* \end{bmatrix}, \begin{bmatrix} \mathbf{K} & \mathbf{K}_* \\ \mathbf{K}_*^\mathsf{T} & \mathbf{K}_{**} \end{bmatrix} \bigg)$$

$$\begin{split} \boldsymbol{\mu} &= \boldsymbol{\mu}(\mathbf{X}), \ \boldsymbol{\mu}_* = \boldsymbol{\mu}(\mathbf{X}_*), \\ \mathbf{K} &= \kappa(\mathbf{X}, \mathbf{X}) \in \mathbb{R}^{N \times N} \ , \ \mathbf{K}_* = \kappa(\mathbf{X}, \mathbf{X}_*) \in \mathbb{R}^{N \times N_*}, \ \mathbf{K}_{**} = \kappa(\mathbf{X}_*, \mathbf{X}_*) \in \mathbb{R}^{N_* \times N_*} \end{split}$$

Marginals and Conditionals

Theorem 1

(Marginals and conditionals for an MVN) Suppose $\mathbf{x} = (\mathbf{x}_1, \mathbf{x}_2) \sim \mathcal{N}(\mathbf{x} | \boldsymbol{\mu}, \boldsymbol{\Sigma})$, i.e. \mathbf{x} is jointly Gaussian with parameters

$$\boldsymbol{\mu} = \begin{bmatrix} \boldsymbol{\mu}_1 \\ \boldsymbol{\mu}_2 \end{bmatrix}, \quad \boldsymbol{\Sigma} = \begin{bmatrix} \boldsymbol{\Sigma}_{11} & \boldsymbol{\Sigma}_{12} \\ \boldsymbol{\Sigma}_{21} & \boldsymbol{\Sigma}_{22} \end{bmatrix}, \quad \boldsymbol{\Lambda} = \boldsymbol{\Sigma}^{-1} = \begin{bmatrix} \boldsymbol{\Lambda}_{11} & \boldsymbol{\Lambda}_{12} \\ \boldsymbol{\Lambda}_{21} & \boldsymbol{\Lambda}_{22} \end{bmatrix}$$

then the marginals are given by

$$egin{aligned}
ho(\mathbf{x}_1) &= \mathcal{N}(\mathbf{x}_1|oldsymbol{\mu}_1, oldsymbol{\Sigma}_{11}) \
ho(\mathbf{x}_2) &= \mathcal{N}(\mathbf{x}_2|oldsymbol{\mu}_2, oldsymbol{\Sigma}_{22}) \end{aligned}$$

and the posterior conditional is given by

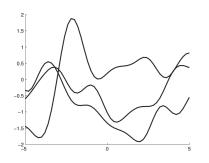
$$egin{aligned}
ho(\mathbf{x}_1|\mathbf{x}_2) &= \mathcal{N}(\mathbf{x}_1|oldsymbol{\mu}_{1|2}, oldsymbol{\Sigma}_{1|2}) \ oldsymbol{\mu}_{1|2} &= oldsymbol{\mu}_1 + oldsymbol{\Sigma}_{12}oldsymbol{\Sigma}_{22}^{-1}(\mathbf{x}_2 - oldsymbol{\mu}_2) \ &= oldsymbol{\mu}_1 - oldsymbol{\Lambda}_{11}^{-1}oldsymbol{\Lambda}_{12}(\mathbf{x}_2 - oldsymbol{\mu}_2) \ oldsymbol{\Sigma}_{1|2} &= oldsymbol{\Sigma}_{11} - oldsymbol{\Sigma}_{12}oldsymbol{\Sigma}_{21}^{-1}oldsymbol{\Sigma}_{21} &= oldsymbol{\Lambda}_{11}^{-1} \end{aligned}$$

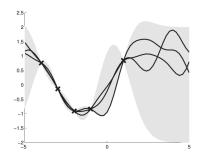
• by definition of the GP, the joint distribution has the following form

$$\begin{bmatrix} \mathbf{f} \\ \mathbf{f}_* \end{bmatrix} \sim \mathcal{N} \bigg(\begin{bmatrix} \boldsymbol{\mu} \\ \boldsymbol{\mu}_* \end{bmatrix}, \begin{bmatrix} \mathbf{K} & \mathbf{K}_* \\ \mathbf{K}_*^\mathsf{T} & \mathbf{K}_{**} \end{bmatrix} \bigg)$$

 by the standard rules for conditioning Gaussians (see lec. 5), the posterior has the following form

$$\begin{split} \rho(\mathbf{f}_*|\mathbf{X}_*,\mathbf{X},\mathbf{f}) &= \mathcal{N}(\mathbf{f}_*|\boldsymbol{\mu}_*,\boldsymbol{\Sigma}_*) \\ \boldsymbol{\mu}_* &= \boldsymbol{\mu}(\mathbf{X}_*) + \mathbf{K}_*^{\mathsf{T}}\mathbf{K}^{-1}(\mathbf{f} - \boldsymbol{\mu}(\mathbf{X})) \\ \boldsymbol{\Sigma}_* &= \mathbf{K}_{**} - \mathbf{K}_*^{\mathsf{T}}\mathbf{K}^{-1}\mathbf{K}_* \end{split}$$





- *left*: some functions sampled from a GP prior with SE (Squared Exponential) kernel
- right: some samples from a GP posterior, after conditioning on 5 noise-free observations
- ullet the shaded area represents $\mathbb{E}[f(\mathbf{x})] \pm 2\mathsf{std}(f(x))$
- the model perfectly interpolates the training data
- the predictive uncertainty increases as we move further away from the observed data

Squared Exponential Kernel

• in the previous 1D example, we used the squared exponential kernel

$$\kappa(x, x') = \sigma_f^2 \exp\left(-\frac{1}{2l^2}(x - x')^2\right)$$

- I controls the horizontal length scale over which the function varies
- σ_f^2 controls the **vertical scale** (variation) of the function

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 now let's consider the case where what we observe is a noisy version of the underlying function, i.e.

$$y = f(\mathbf{x}) + \epsilon$$

where $\epsilon \sim \mathcal{N}(0, \sigma_v^2)$

- in this case, the model is not required to interpolate the data (since they are noisy), but it must come "close" to the observed data
- one has that $y|\mathbf{x} \sim \mathcal{N}(m(\mathbf{x}), \sigma_y^2)$ since $\mathbb{E}[y|\mathbf{x}] = E[f(\mathbf{x}) + \epsilon] = E[f(\mathbf{x})] = m(\mathbf{x})$
- the covariance of the observed noisy responses is

$$cov[y_p, y_q] = cov[f(\mathbf{x}_p) + \epsilon_p, f(\mathbf{x}_q) + \epsilon_q]$$

which, given the noise terms ϵ_i are iid, entails

$$cov[y_p, y_q] = \kappa(\mathbf{x}_p, \mathbf{x}_q) + \sigma_y^2 \delta_{pq}$$

where $\delta_{pq} \triangleq \mathbb{I}(p=q)$



- we have $\mathbf{y} = \mathbf{f} + \boldsymbol{\epsilon}$ where $\mathbf{y} \triangleq [y_1, ..., y_N] \in \mathbb{R}^N$, $\mathbf{f} \triangleq [f(\mathbf{x}_1), ..., f(\mathbf{x}_N)]^T \in \mathbb{R}^N$, $\boldsymbol{\epsilon} \triangleq [\epsilon_1, ..., \epsilon_N] \in \mathbb{R}^N$
- this is a Gaussian linear system (see lec. 5) with $p(\mathbf{f}|\mathbf{X}) = \mathcal{N}(\mathbf{f}|\boldsymbol{\mu}, \mathbf{K})$ and $p(\mathbf{y}|\mathbf{f}) = \prod_i \mathcal{N}(y_i|f_i, \sigma_y^2)$
- considering that $\mathbb{E}[y|\mathbf{x}] = m(\mathbf{x})$ and $\text{cov}[y_p,y_q] = \kappa(\mathbf{x}_p,\mathbf{x}_q) + \sigma_y^2 \delta_{pq}$ we obtain

$$p(\mathbf{y}|\mathbf{X}) = \mathcal{N}(\mathbf{y}|\boldsymbol{\mu}, \mathbf{K}_y)$$
 with $\mathbf{K}_y \triangleq \text{cov}[\mathbf{y}|\mathbf{X}] = \mathbf{K} + \sigma_y^2 \mathbf{I}_N$

- for notational simplicity let's assume that the mean function is zero, i.e. m(x) = 0
- the joint density of the observed data y and the latent noise-free function on the test points f** is given by

$$\begin{bmatrix} \mathbf{y} \\ \mathbf{f}_* \end{bmatrix} \sim \mathcal{N} \bigg(\mathbf{0}, \begin{bmatrix} \mathbf{K}_{y} & \mathbf{K}_* \\ \mathbf{K}_*^T & \mathbf{K}_{**} \end{bmatrix} \bigg)$$

 again, by the standard rules for conditioning Gaussians, we have that the posterior predictive density is

$$\begin{split} \rho(\mathbf{f}_*|\mathbf{X}_*,\mathbf{X},\mathbf{y}) &= \mathcal{N}(\mathbf{f}_*|\boldsymbol{\mu}_*,\boldsymbol{\Sigma}_*) \\ \boldsymbol{\mu}_* &= \mathbf{K}_y^{\mathsf{T}} \mathbf{K}_y^{-1} \mathbf{y} \\ \boldsymbol{\Sigma}_* &= \mathbf{K}_{**} - \mathbf{K}_y^{\mathsf{T}} \mathbf{K}_y^{-1} \mathbf{K}_* \end{split}$$

 \bullet in the case of a single test input x_* , this simplifies as follows

$$p(f_*|\mathbf{x}_*, \mathbf{X}, \mathbf{y}) = \mathcal{N}(f_*|\mathbf{k}_*^T \mathbf{K}_y^{-1} \mathbf{y}, \mathbf{k}_{**} - \mathbf{k}_*^T \mathbf{K}_y^{-1} \mathbf{k}_*)$$

where $\mathbf{k}_* = [\kappa(\mathbf{x}_*, \mathbf{x}_1), ..., \kappa(\mathbf{x}_*, \mathbf{x}_N)]^T$ and $\mathbf{k}_{**} = \kappa(\mathbf{x}_*, \mathbf{x}_*)$



• in the case of a single test input \mathbf{x}_*

$$\rho(f_*|\mathbf{x}_*,\mathbf{X},\mathbf{y}) = \mathcal{N}(f_*|\mathbf{k}_*^T\mathbf{K}_y^{-1}\mathbf{y},\mathbf{k}_{**} - \mathbf{k}_*^T\mathbf{K}_y^{-1}\mathbf{k}_*)$$

where
$$\mathbf{k}_* = [\kappa(\mathbf{x}_*, \mathbf{x}_1), ..., \kappa(\mathbf{x}_*, \mathbf{x}_N)]^T$$
 and $\mathbf{k}_{**} = \kappa(\mathbf{x}_*, \mathbf{x}_*)$

• another way to write the posterior mean is as follows

$$\overline{f}_* = \mathbf{k}_*^T \mathbf{K}_y^{-1} \mathbf{y} = \sum_{i=1}^N \alpha_i \kappa(\mathbf{x}_*, \mathbf{x}_i)$$

where $oldsymbol{lpha} = \mathbf{K}_{y}^{-1}\mathbf{y}$

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Effect of Kernel Parameters

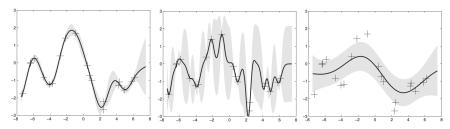
- the predictive performance of GPs depends exclusively on the suitability of the chosen kernel
- suppose we choose the following squared-exponential (SE) kernel for the 1D noisy observations

$$\kappa_y(x_p, x_q) = \sigma_f^2 \exp\left(-\frac{1}{2l^2}(x_p - x_q)^2\right) + \sigma_y^2 \delta_{pq}$$

where I is the **horizontal scale** over which the function changes, σ_f^2 controls the **vertical scale** of the function, and σ_y^2 is the **noise variance**

Effect of Kernel Parameters

effects of changing the parameters (I, σ_f, σ_y)



- we sampled 20 noisy data points from the SE kernel using $(I, \sigma_f, \sigma_y) = (1, 1, 0.1)$ and then made predictions changing the parameters, conditional on the data
- *left*: $(I, \sigma_f, \sigma_y) = (1, 1, 0.1)$, and the result is a good fit
- center: $(I, \sigma_f, \sigma_y) = (0.3, 1.08, 0.00005)$ (small I, small noise); now the function looks more "wiggly"; the uncertainty goes up faster when moving far from the training points
- right: $(I, \sigma_f, \sigma_y) = (3, 1.16, 0.89)$ (large I, large noise); now the function looks smoother

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Estimating the Kernel Parameters

- to estimate the kernel parameters, we could use exhaustive search over a discrete grid of values, with validation loss as an objective, but this can be quite slow (this is the approach used to tune kernels used by SVMs)
- here we consider an empirical Bayes approach, which will allow us to use continuous optimization methods, which are much faster
- in particular, we will maximize the marginal likelihood

$$p(\mathbf{y}|\mathbf{X}) = \int p(\mathbf{y}, \mathbf{f}|\mathbf{X}) d\mathbf{f} = \int p(\mathbf{y}|\mathbf{f}, \mathbf{X}) p(\mathbf{f}|\mathbf{X}) d\mathbf{f}$$

where
$$\mathbf{f} \triangleq [f(\mathbf{x}_1),...,f(\mathbf{x}_N)]^T \in \mathbb{R}^N$$
, $\mathbf{y} \triangleq [y_1,...,y_N] \in \mathbb{R}^N$, $\mathbf{\epsilon} \triangleq [\epsilon_1,...,\epsilon_N] \in \mathbb{R}^N$

• we already saw that $\mathbf{y} = \mathbf{f} + \boldsymbol{\epsilon}$ is a Gaussian linear system with $p(\mathbf{f}|\mathbf{X}) = \mathcal{N}(\mathbf{f}|0,\mathbf{K})$ and $p(\mathbf{y}|\mathbf{f}) = \prod_i \mathcal{N}(y_i|f_i,\sigma_y^2)$, and we obtain

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

where $\mathbf{K}_y = \mathbf{K} + \sigma_y^2 \mathbf{I}_N$



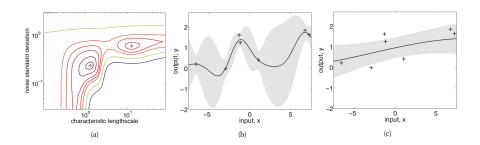
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• hence we have to maximize the log-marginal likelihood

$$\log p(\mathbf{y}|\mathbf{X}) = \log \mathcal{N}(\mathbf{f}|0,\mathbf{K}_y) = -\frac{1}{2}\mathbf{y}^T\mathbf{K}_y^{-1}\mathbf{y} - \frac{1}{2}\log|\mathbf{K}_y| - \frac{N}{2}\log(2\pi)$$

- ullet let eta denote the vector of kernel parameters
- once we compute the gradient $\frac{\partial}{\partial \theta} \log p(\mathbf{y}|\mathbf{X})$ we can we can estimate the kernel parameters using any standard gradient-based optimizer on the log marginal likelihood
- since the objective is not convex, local minima can be a problem

Estimating the Kernel Parameters



- (a) log marginal likelihood vs σ_y^2 and I, for fixed $\sigma_f^2=1$, using the 7 data points; the data was generated using $(I,\sigma_y^2)=(1,0.1)$
- (b) the function corresponding to the lower left local minimum, $(I, \sigma_y^2) \approx (1, 0.2)$; this is quite "wiggly" and has low noise
- (c) the function corresponding to the top right local minimum, $(I, \sigma_y^2) \approx (10, 0.8)$; this is quite smooth and has high noise

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GP as Linear Smoothers

 a linear smoother is a regression function which is a linear function of the training outputs

$$\hat{f}(\mathbf{x}_*) = \sum_i w_i(\mathbf{x}_*) y_i$$

where $w_i(\mathbf{x}_*)$ is the *i*-th weight function ¹

- GP regression is a linear smoother (there are a variety of linear smoothers, such as kernel regression, locally weighted regression, smoothing splines, etc)
- to see that GP regression is a linear smoother, note that the mean of the posterior predictive distribution of a GP is

$$\overline{f}(\mathbf{x}_*) = \mathbf{k}_*^T \mathbf{K}_y^{-1} \mathbf{y} = \mathbf{k}_*^T (\mathbf{K} + \sigma_y \mathbf{I})^{-1} \mathbf{y} = \sum_{i=1}^N w_i(\mathbf{x}_*) y_i$$

with $w_i(\mathbf{x}_*) = [(\mathbf{K} + \sigma_y \mathbf{I})^{-1} \mathbf{k}_*]_i$

¹do not confuse this model with the linear model $\hat{f}(\mathbf{x}_*) \equiv \mathbf{w}^T \mathbf{x} \rightarrow \mathbf{z} \rightarrow \mathbf{z} \rightarrow \mathbf{z}$

GP as Linear Smoothers

GP regression as a linear smoother

$$\overline{f}(\mathbf{x}_*) = \sum_{i=1}^N w_i(\mathbf{x}_*) y_i$$

with
$$w_i(\mathbf{x}_*) = [(\mathbf{K} + \sigma_y \mathbf{I})^{-1} \mathbf{k}_*]_i$$

- for certain GP kernel functions, one can show that $\sum_{i=1}^{N} w_i(\mathbf{x}_*) = 1$, although we may have $w_i(\mathbf{x}_*) < 0$, so we are computing a **linear combination** but not a convex combination of the y_i
- more interestingly, $w_i(\mathbf{x}_*)$ is a **local function**, even if the original kernel used by the GP is not local
- furthermore the effective bandwidth of the equivalent kernel of a GP automatically decreases as the sample size N increases

Credits

Kevin Murphy's book