

# Lecture 10

## Gaussian Processes

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## 1 Intro

- Distribution over functions
- Stochastic Processes
- Gaussian Processes

## 2 GPs for Regression

- GP Prior
- Predictions Using Noisy-free Observations
- Predictions Using Noisy Observations
- Effect of Kernel Parameters
- Estimating the Kernel Parameters

## 3 Linear Smoothers

- Linear Smoothers

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# Introduction

## 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**  $\epsilon$
- 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

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

- 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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- 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  $\mathcal{T} = [0, \infty)$ , it is called a **continuous-time process**

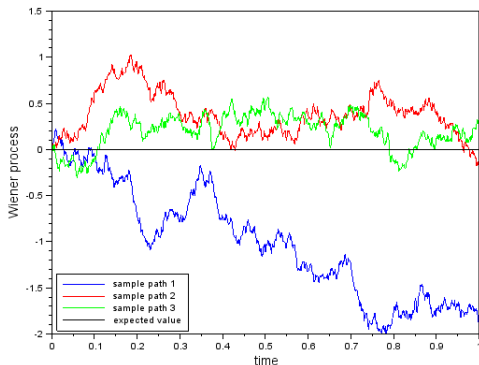
note that

- 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.,  $\mathcal{T} = \{1, 2, \dots, n\}$ ), we get a **random vector**

# Introduction

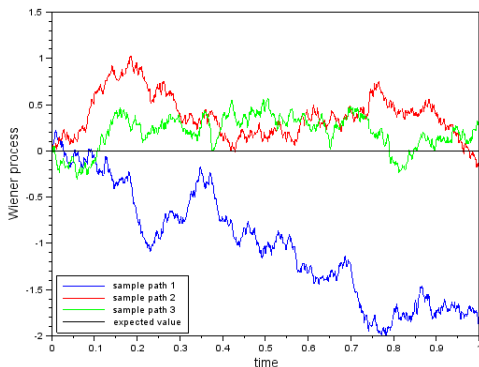
## Stochastic Process

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



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

- 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  $t_1, \dots, t_n$  and its corresponding joint PDF  $p_{X_1, \dots, X_n}(x_1, \dots, x_n)$





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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.

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

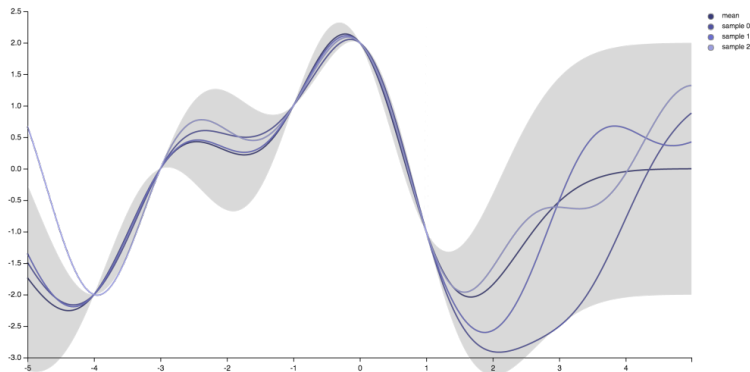
- every finite collection of random variables  $f(\mathbf{x}_1), \dots, f(\mathbf{x}_n)$  has a multivariate normal distribution

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

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

# Introduction

## An Example



different observations (trajectories) of a Gaussian process with

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

# Introduction

## 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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- 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**

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

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

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**

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

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

- note that it is common to use a mean function of  $\mathbf{m}(\mathbf{x}) = 0$ , 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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# Predictions Using Noisy-free Observations

- 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  $\mathbf{X}_*$  of size  $N_* \times D$ , we want to predict the function outputs  $\mathbf{f}_*$

what do we expect?

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



# Predictions Using Noisy-free Observations

- by definition of the GP, the **joint distribution** has the following form

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

$$\boldsymbol{\mu} = \boldsymbol{\mu}(\mathbf{X}), \boldsymbol{\mu}_* = \boldsymbol{\mu}(\mathbf{X}_*),$$

$$\mathbf{K} = \kappa(\mathbf{X}, \mathbf{X}) \in \mathbb{R}^{N \times N}, \mathbf{K}_* = \kappa(\mathbf{X}, \mathbf{X}_*) \in \mathbb{R}^{N \times N_*}, \mathbf{K}_{**} = \kappa(\mathbf{X}_*, \mathbf{X}_*) \in \mathbb{R}^{N_* \times N_*}$$

## 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

$$p(\mathbf{x}_1) = \mathcal{N}(\mathbf{x}_1|\boldsymbol{\mu}_1, \boldsymbol{\Sigma}_{11})$$

$$p(\mathbf{x}_2) = \mathcal{N}(\mathbf{x}_2|\boldsymbol{\mu}_2, \boldsymbol{\Sigma}_{22})$$

and the **posterior conditional** is given by

$$p(\mathbf{x}_1|\mathbf{x}_2) = \mathcal{N}(\mathbf{x}_1|\boldsymbol{\mu}_{1|2}, \boldsymbol{\Sigma}_{1|2})$$

$$\begin{aligned} \boldsymbol{\mu}_{1|2} &= \boldsymbol{\mu}_1 + \boldsymbol{\Sigma}_{12}\boldsymbol{\Sigma}_{22}^{-1}(\mathbf{x}_2 - \boldsymbol{\mu}_2) \\ &= \boldsymbol{\mu}_1 - \boldsymbol{\Lambda}_{11}^{-1}\boldsymbol{\Lambda}_{12}(\mathbf{x}_2 - \boldsymbol{\mu}_2) \end{aligned}$$

$$\boldsymbol{\Sigma}_{1|2} = \boldsymbol{\Sigma}_{11} - \boldsymbol{\Sigma}_{12}\boldsymbol{\Sigma}_{22}^{-1}\boldsymbol{\Sigma}_{21} = \boldsymbol{\Lambda}_{11}^{-1}$$

# Predictions Using Noisy-free Observations

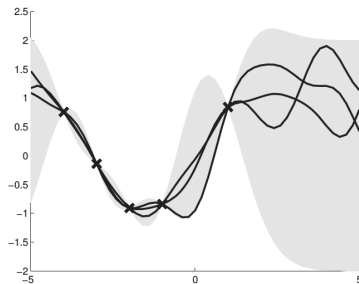
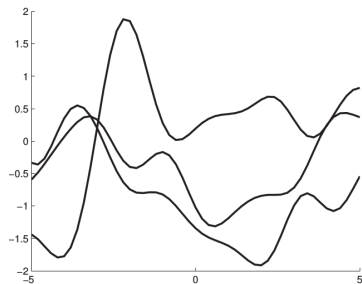
- by definition of the GP, the **joint distribution** has the following form

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

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

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

# Predictions Using Noisy-free Observations



- *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**
- the shaded area represents  $\mathbb{E}[f(\mathbf{x})] \pm 2\text{std}(f(\mathbf{x}))$
- 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**

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

- $l$  controls the **horizontal length scale** over which the function varies
- $\sigma_f^2$  controls the **vertical scale** (variation) of the function

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# Predictions Using Noisy Observations

- 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  $\epsilon \sim \mathcal{N}(0, \sigma_y^2)$

- 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

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

which, given the noise terms  $\epsilon_i$  are iid, entails

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

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

# Predictions Using Noisy Observations

- we have  $\mathbf{y} = \mathbf{f} + \boldsymbol{\epsilon}$  where  $\mathbf{y} \triangleq [y_1, \dots, y_N] \in \mathbb{R}^N$ ,  $\mathbf{f} \triangleq [f(\mathbf{x}_1), \dots, f(\mathbf{x}_N)]^T \in \mathbb{R}^N$ ,  $\boldsymbol{\epsilon} \triangleq [\epsilon_1, \dots, \epsilon_N] \in \mathbb{R}^N$
- 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

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



# Predictions Using Noisy Observations

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

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

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

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

- in the case of a single test input  $\mathbf{x}_*$ , 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  $\mathbf{k}_* = [\kappa(\mathbf{x}_*, \mathbf{x}_1), \dots, \kappa(\mathbf{x}_*, \mathbf{x}_N)]^T$  and  $\mathbf{k}_{**} = \kappa(\mathbf{x}_*, \mathbf{x}_*)$

# Predictions Using Noisy Observations

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

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

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

- another way to write the **posterior mean** is as follows

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

where  $\boldsymbol{\alpha} = \mathbf{K}_y^{-1} \mathbf{y}$

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# Effect of Kernel Parameters

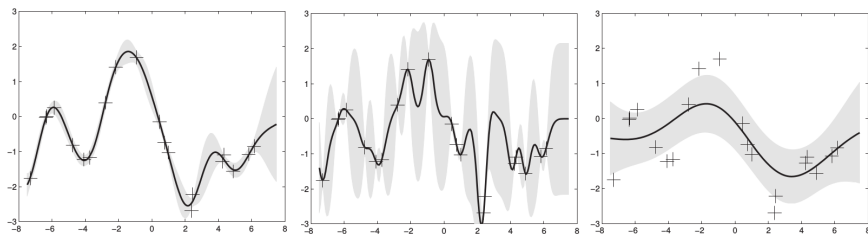
- the predictive performance of GPs depends exclusively on the **suitability** of the **chosen kernel**
- suppose we choose the following squared-exponential (SE) kernel for the 1D noisy observations

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

where  $l$  is the **horizontal scale** over which the function changes,  $\sigma_f^2$  controls the **vertical scale** of the function, and  $\sigma_y^2$  is the **noise variance**

# Effect of Kernel Parameters

effects of changing the parameters  $(l, \sigma_f, \sigma_y)$



- we sampled 20 noisy data points from the SE kernel using  $(l, \sigma_f, \sigma_y) = (1, 1, 0.1)$  and then made predictions changing the parameters, conditional on the data
- *left*:  $(l, \sigma_f, \sigma_y) = (1, 1, 0.1)$ , and the result is a good fit
- *center*:  $(l, \sigma_f, \sigma_y) = (0.3, 1.08, 0.00005)$  (small  $l$ , small noise); now the function looks more “wiggly”; the uncertainty goes up faster when moving far from the training points
- *right*:  $(l, \sigma_f, \sigma_y) = (3, 1.16, 0.89)$  (large  $l$ , 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  $\mathbf{f} \triangleq [f(\mathbf{x}_1), \dots, f(\mathbf{x}_N)]^T \in \mathbb{R}^N$ ,  $\mathbf{y} \triangleq [y_1, \dots, y_N] \in \mathbb{R}^N$ ,  $\boldsymbol{\epsilon} \triangleq [\epsilon_1, \dots, \epsilon_N] \in \mathbb{R}^N$

- 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

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

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

# Estimating the Kernel Parameters

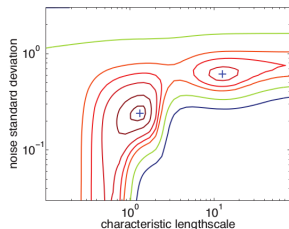
- hence we have to maximize the log-marginal likelihood

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

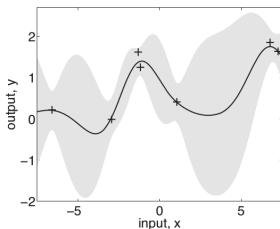
- let  $\theta$  denote the vector of kernel parameters
- once we compute the gradient  $\frac{\partial}{\partial \theta} \log p(\mathbf{y}|\mathbf{X})$  we can estimate the kernel parameters using any standard gradient-based optimizer on the log marginal likelihood
- since the objective is **not convex**,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



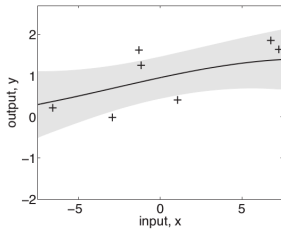
# Estimating the Kernel Parameters



(a)



(b)



(c)

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

- 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

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

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

---

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

- GP regression as a linear smoother

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

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

- Kevin Murphy's book