

# Advanced Bayesian Learning

## Gaussian Process Regression and Classification - Lecture 2

Mattias Villani

**Department of Statistics  
Stockholm University**

Department of Computer and Information Science  
Linköping University



# Stationary processes and smoothness

- A stochastic process (field)  $\{f(\mathbf{x}), \mathbf{x} \in \mathbb{R}^D\}$  is **weakly stationary** if  $E(f(\mathbf{x})) = \mu$  and its covariance function  $k(\mathbf{x}, \mathbf{x}')$  is a function of  $\mathbf{t} = \mathbf{x} - \mathbf{x}'$

$$k(\mathbf{x}, \mathbf{x}') = \text{Cov} [f(\mathbf{x}), f(\mathbf{x}')] = k(\mathbf{t}).$$

- The covariance function is **isotropic** if it only depends on the distance  $t = \|\mathbf{x} - \mathbf{x}'\|$  (invariant to directions)

$$k(\mathbf{x}, \mathbf{x}') = \text{Cov} [f(\mathbf{x}), f(\mathbf{x}')] = k(t).$$

- A stationary process is **continuous in quadratic mean**

$$E \left( |f(\mathbf{x} + t) - f(\mathbf{x})|^2 \right) \rightarrow 0 \text{ as } t \rightarrow 0$$

iff  $k(t)$  is continuous at  $t = 0$ .

- A stationary process is **differentiable in quadratic mean**

$$\frac{f(\mathbf{x} + t) - f(\mathbf{x})}{t} \xrightarrow{q.m.} f'(\mathbf{x}) \text{ as } t \rightarrow 0$$

iff  $k(t)$  is twice continuously differentiable at  $t = 0$ .

# Fourier analysis and orthogonal functions

- **Fourier series** for functions:

$$f(x) = \sum_k a_k \cos(2\pi s_k x) + \sum_k b_k \sin(2\pi s_k x)$$

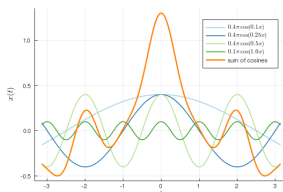
$$a_k = \int f(x) \cos(2\pi s_k x) dx \text{ and } b_k = \int f(x) \sin(2\pi s_k x) dx.$$

- cos and sin are **orthogonal** at Fourier frequencies  $s_k$  and  $s_l$ :

$$\int \sin(2\pi s_k x) \cos(2\pi s_l x) dx = \delta_{kl}$$

- **Complex exponential**:  $e^{it} \equiv \cos t + i \cdot \sin(t)$ .

- Fourier:  $f(x) = \sum_k c_k e^{i2\pi s_k x}$  where  $c_k = \int f(x) e^{i2\pi s_k x} dx$ .



# Spectral density

- **Bochner's theorem:** A function  $k(\cdot)$  is the covariance function of a stationary continuous process iff

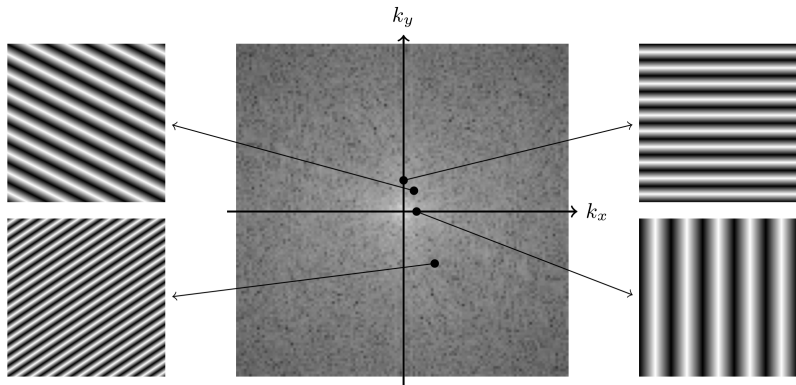
$$k(t) = \int_{\mathbb{R}^D} e^{2\pi i s^T t} S(s) ds$$

- $S(s)$  is the **spectral density**.  $S(s)$  is the energy allocated to the basis function  $e^{2\pi i s^T t}$  at frequency  $s$ .
- $S(s) \iff k(t) \iff$  Smoothness of  $f(x)$ .
- **Multivariate Bochner's:** A function  $k(\cdot)$  on  $\mathbb{R}^D$  is the covariance function of a stationary continuous process iff

$$k(\mathbf{t}) = \int_{\mathbb{R}^D} e^{2\pi i \mathbf{s}^T \mathbf{t}} S(\mathbf{s}) d\mathbf{s}$$

- $e^{2\pi i \mathbf{s}^T \mathbf{t}}$  is a  $D$ -dimensional sine wave with frequency  $\mathbf{s}$  (with direction).

# Fourier in 2D



# Spectral density determines smoothness

- A stationary process  $f(x)$  is continuous in q.m. if

$$\int S(s) ds < \infty$$

- The  $k$ th q.m. derivative process  $f^{(k)}(x)$  has spectral density

$$S_{f^{(k)}}(s) = s^{2k} S_f(s)$$

- $f(x)$  is q.m. differentiable of order  $k$  iff  $S(s)$  has moments order  $2k$ .

# Spectral densities of common kernels

- Let  $r = \|x - x'\|$ . All kernels can be scaled by  $\sigma_f > 0$ .
- **Squared exponential (SE)** ( $\ell > 0$ )

$$K_{SE}(r) = \exp\left(-\frac{r^2}{2\ell^2}\right)$$

- ▶ Spectral density  $S(s) = (2\pi\ell^2)^{D/2} \exp(-2\pi^2\ell^2s^2)$ .
- ▶ Higher freq tail of like a Gaussian with variance  $1/(4\pi^2\ell^2)$ .
- ▶ Infinitely mean square differentiable. Very smooth.

- **Matérn** ( $\ell > 0, \nu > 0$ )

$$K_{Matern}(r) = \frac{2^{1-\nu}}{\Gamma(\nu)} \left(\frac{\sqrt{2\nu}r}{\ell}\right)^\nu K_\nu\left(\frac{\sqrt{2\nu}r}{\ell}\right)$$

- ▶ Spectral density: student- $t$  density with  $2\nu$  degrees of freedom.
- ▶  $\nu = 1/2$ ,  $S(s)$  is Cauchy. Continuous in q.m., no derivatives.
- ▶ As  $\nu \rightarrow \infty$ , Matérn approaches SE.

# Spectral mixture kernels

- Bochner's theorem for stationary processes:

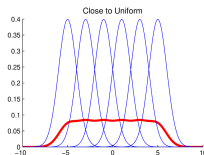
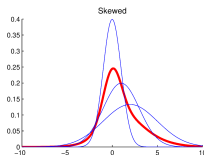
$$k(t) = \int e^{2\pi i s t} S(s) ds.$$

- Mixture of normals in frequency domain

$$S(s) = \sigma^2 \sum_{k=1}^K \pi_k \mathcal{N}(s | \mu_k, \psi_k^2)$$

- Bochner's theorem gives kernel in time domain

$$k(t) = \sigma^2 \sum_{k=1}^K \pi_k \cos(2\pi \mu_k t) \exp(-2\pi^2 \psi_k^2 t^2)$$





# SE as infinite basis expansion

- Regression with basis functions  $\phi_1(x), \dots, \phi_N(x)$

$$y = \sum_{c=1}^N w_c \phi_c(x) + \varepsilon$$

$$\phi_c(x) = \exp\left(-\frac{(x-c)^2}{2\ell^2}\right).$$

- Prior  $\mathbf{w} \sim N\left(0, \frac{\sigma_p^2}{N} I\right)$ .
- This is a GP with kernel

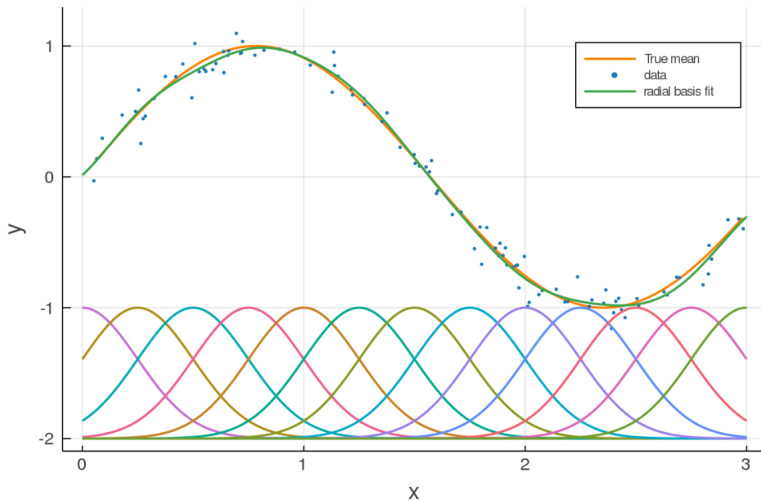
$$k(x_p, x_q) = \text{cov}\left(\sum_{c=1}^N w_c \phi_c(x_p), \sum_{c=1}^N w_c \phi_c(x_q)\right) = \frac{\sigma_p^2}{N} \sum_{c=1}^N \phi_c(x_p) \phi_c(x_q) \rightarrow \sigma_p^2 \int_{c_{\min}}^{c_{\max}} \phi_c(x_p) \phi_c(x_q) dc$$

as the number of bases  $N \rightarrow \infty$  over  $[c_{\min}, c_{\max}]$ .

- Letting  $c_{\min} \rightarrow -\infty$  and  $c_{\max} \rightarrow \infty$  we get

$$k(x_p, x_q) = \sigma_p^2 \int_{-\infty}^{\infty} \exp\left(-\frac{(x_p - c)^2}{2\ell^2}\right) \exp\left(-\frac{(x_q - c)^2}{2\ell^2}\right) dc = \sqrt{\pi}\ell\sigma_p^2 \exp\left(-\frac{(x_p - x_q)^2}{2(\sqrt{2}\ell)^2}\right)$$

# Fitting basis expansion



# Kernel composition

- **Periodic kernels.** When  $f(x)$  is believed to be periodic with period  $d$ . Example:

$$k(x, x') = \sigma_f^2 \exp \left( -\frac{2 \sin^2 (\pi |x - x'| / d)}{\ell^2} \right).$$

- **Product** of kernels is a kernel.
- Example: Locally periodic. Two nearby peaks are more dependent than two distant peaks.

$$k(x, x') = \sigma_f^2 \exp \left( -\frac{2 \sin^2 (\pi |x - x'|^2 / d)}{\ell^2} \right) \times \exp \left( -\frac{1}{2} \frac{|x - x'|^2}{\ell^2} \right)$$

- **Sum** of kernels is a kernel.
- Let  $f_a \sim GP [m_a(\mathbf{x}), k_a(\mathbf{x}, \mathbf{x}')] ]$  independently of  $f_b \sim GP [m_b(\mathbf{x}), k_b(\mathbf{x}, \mathbf{x}')] ]$  then

$$f_a + f_b \sim GP [m_a(\mathbf{x}) + m_b(\mathbf{x}), k_a(\mathbf{x}, \mathbf{x}') + k_b(\mathbf{x}, \mathbf{x}')] ]$$

# Anisotropic kernels - ARD

- Anisotropic version of isotropic kernels by setting  $r^2(\mathbf{x}, \mathbf{x}') = (\mathbf{x} - \mathbf{x}')^T \mathbf{M} (\mathbf{x} - \mathbf{x}')$  where  $\mathbf{M}$  is positive definite.
- **Automatic Relevance Determination (ARD)**:  $\mathbf{M} = \text{Diag}(\ell_1^{-2}, \dots, \ell_D^{-2})$  is diagonal with different length scales.
- ARD does 'variable selection' since large  $\ell_j$  means that the  $j$ th input essentially drops out of  $f(\mathbf{x})$ .
- ARD is a product of  $D$  one-dimensional kernels, one for each input variable

$$k_{ARD}(\mathbf{x}, \mathbf{x}') = \prod_{d=1}^D k_{SE, \ell_d}(x_d, x'_d)$$

- **Factor kernels**:  $\mathbf{M} = \Lambda \Lambda^T + \Psi$ , where  $\Lambda$  is  $D \times k$  for low rank  $k$ .

# Discrete covariates

- Suppose:  $x_1$  is continuous (mg/week) and  $x_2$  is binary (sex).
- Linear regression: just use  $x_2$  coded as  $x_2 = 0$  if male,  $x_2 = 1$  if female.
- Implicit model:

$$y = \begin{cases} \beta_0 + \beta_1 x_1 & \text{if } x_2 = 0 \\ \beta_0 + \tilde{\beta}_0 + (\beta_1 + \tilde{\beta}_1) x_1 & \text{if } x_2 = 1 \end{cases}$$

- GP: add the 0-1 coded covariate and use ARD kernel:

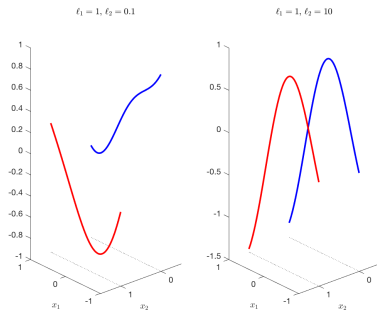
$$\exp\left(-\frac{1}{2}\left(\frac{x_1 - x'_1}{\ell_1}\right)^2\right) \exp\left(-\frac{1}{2}\left(\frac{x_2 - x'_2}{\ell_2}\right)^2\right)$$

So the covariance between  $f(x_1, 0)$  and  $f(x_1, 1)$  is

$$\exp\left(-\frac{1}{2}\left(\frac{1}{\ell_2}\right)^2\right)$$

# Discrete covariates

- Large  $\ell_2$ : men and female are believed to have similar profiles with respect to  $x_1$ .
- Small  $\ell_2$ : men and female are believed to have potentially very different profiles with respect to  $x_1$ .



- Categorical covariates with  $K$  levels: create  $K$  *one-hot* variables.

# Eigenfunction decomposition

- **Eigenvalue decomposition** of a  $n \times n$  **covariance matrix**:

$$K = V\Lambda V^T, \text{ or}$$

$$K = \sum_{j=1}^n \lambda_j \mathbf{v}_j \mathbf{v}_j^T,$$

where  $\Lambda = \text{Diag}(\lambda_1, \dots, \lambda_n)$ ,  $K\mathbf{v}_j = \lambda_j \mathbf{v}_j$ ,  $\mathbf{v}_j^T \mathbf{v}_j = \delta_{ij}$ .

- Simulation from  $y \sim N(\mu, K)$ :  $y = \mu + V\Lambda^{1/2}\mathbf{z}$ , and  $\mathbf{z} \sim N(0, I)$ . Principal components.
- **Mercer's theorem** for covariance kernels

$$k(\mathbf{x}, \mathbf{x}') = \sum_{i=1}^{\infty} \lambda_i \phi_i(\mathbf{x}) \phi_i^*(\mathbf{x}')$$

$$\int k(\mathbf{x}, \mathbf{x}') \phi(\mathbf{x}) p(\mathbf{x}) d\mathbf{x} = \lambda \phi(\mathbf{x}')$$

the **eigenfunctions**  $\phi(\mathbf{x})$  are orthogonal with respect  $p(\mathbf{x})$ .

- The **eigenvalues** determine the **smoothness** of the kernel.
- Bochner:  $e^{2\pi i \mathbf{s} \cdot \mathbf{x}}$  are the eigenfunctions of stationary kernels.

# Karhunen-Loève decomposition

- **Karhunen-Loève theorem**: a stochastic process  $X_t$  can be represented as

$$X_t = \sum_{k=1}^{\infty} Z_k e_k(t),$$

where  $Z_k$  are uncorrelated variables and  $e_k(t)$  orthogonal basis.

- $e_k(t)$  are determined by the covariance function of  $X_t$ .
- Karhunen-Loève adapts to  $X_t$  optimally.
- If  $X_t$  is a GP: the  $Z_k$  are Gaussian and independent.
- Can be use for simulation
- Truncate an infinite-dimensional process to finite dimension.



# Large scale GPs

- GPs are **computationally challenging**.
- Need to invert  $n \times n$  matrices such as  $[K(\mathbf{x}, \mathbf{x}) + \sigma^2 I]^{-1}$ .
- **Scales as  $O(n^3)$** . Also with Cholesky.
- **Banded covariance functions**.
  - ▶ Special covariance functions that makes  $K(\mathbf{x}, \mathbf{x})$  sparse.
  - ▶ Observations at a certain distance apart are uncorrelated.
  - ▶ Sparse matrix algebra.

# Large scale GPs

- Introduce  $m$  latent **inducing variables**  $\mathbf{u} = \{u_1, \dots, u_m\}$  with inputs  $\mathbf{X}_u = \{\mathbf{x}_{u_1}, \mathbf{x}_{u_2}, \dots, \mathbf{x}_{u_m}\}$ . Pseudo inputs.
- The **Fully Independent Conditional (FIC)** method *assumes* elements in  $\mathbf{f}$  are independent given  $\mathbf{u}$

$$p(\mathbf{f}|\mathbf{X}, \mathbf{X}_u, \mathbf{u}, \theta) = \prod_{i=1}^n p_i(f_i|\mathbf{X}, \mathbf{X}_u, \mathbf{u}, \theta)$$

- Computations are now  $O(m^2 n)$ , and often  $m \ll n$ . Fast!
- **Partially Independent Conditional (PIC)**. Partition into blocks  $\mathbf{f} = (\mathbf{f}_1, \dots, \mathbf{f}_k)$ , where each  $\mathbf{f}_i$  has  $b$  elements. Assume indep. blocks given  $\mathbf{u}$ , but full dependence with blocks.
- $b = 1$  gives FIC.  $b = n$  gives the original GP.
- The locations of  $\mathbf{X}_u$  are learned by optimization.

# Classification with logistic regression

- **Classification: binary response**  $y \in \{-1, 1\}$ .
- Example: linear logistic regression

$$Pr(y = 1|\mathbf{x}) = \lambda(\mathbf{x}^T \mathbf{w})$$

where  $\lambda(z)$  is the logistic **link function**

$$\lambda(z) = \frac{1}{1 + \exp(-z)}$$

- $\lambda(z)$  'squashes' the linear prediction  $\mathbf{x}^T \mathbf{w} \in \mathbb{R}$  into  $\in [0, 1]$ .
- Logistic regression has **linear decision boundaries**.

# GP classification

- Obvious **GP extension** of logistic regression: replace  $\mathbf{x}^T \mathbf{w}$  by

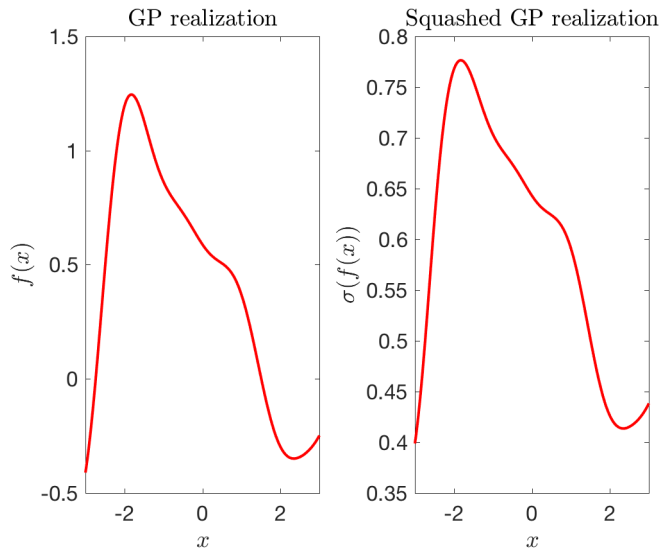
$$f(\mathbf{x}) \sim GP(0, k(\mathbf{x}, \mathbf{x}'))$$

and squash

$$Pr(y = 1|\mathbf{x}) = \lambda(f(\mathbf{x}))$$

- **Flexible decision boundaries (non-parametric, GP-style).**

# Squashing a GP function



# GP classification - inference

- **Prediction** for a test case  $\mathbf{x}_*$ :

$$Pr(y_* = +1 | \mathbf{X}, \mathbf{y}, \mathbf{x}_*) = \int \sigma(f_*) p(f_* | \mathbf{x}_*, \mathbf{X}, \mathbf{y}) df_*$$

- ▶  $\sigma(f_*)$  is some sigmoidal function (logistic, normal CDF...)
- ▶  $f_*$  is the latent  $f$  at the test input  $\mathbf{x}_*$ .

- The posterior distribution of  $f_*$  is

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

where  $p(\mathbf{f} | \mathbf{X}, \mathbf{y})$  is the posterior of  $\mathbf{f}$  from the training data

$$p(\mathbf{f} | \mathbf{X}, \mathbf{y}) \propto p(\mathbf{y} | \mathbf{f}) p(\mathbf{f} | \mathbf{X})$$

- $p(\mathbf{y} | \mathbf{f})$  is no longer Gaussian. Posterior  $p(\mathbf{f} | \mathbf{X}, \mathbf{y})$  intractable.

# The Laplace approximation

- Approximates  $p(\mathbf{f}|\mathbf{X}, \mathbf{y})$  with  $N(\hat{\mathbf{f}}, \mathbf{A}^{-1})$ , where
  - ▶  $\hat{\mathbf{f}}$  is the posterior mode
  - ▶  $\mathbf{A} = -\nabla\nabla \log p(\mathbf{f}|\mathbf{y})$  is negative Hessian at  $\mathbf{f} = \hat{\mathbf{f}}$ .
- Log posterior

$$\begin{aligned}\Psi(\mathbf{f}) &= \log p(\mathbf{y}|\mathbf{f}) + \log p(\mathbf{f}|\mathbf{X}) \\ &= \log p(\mathbf{y}|\mathbf{f}) - \frac{1}{2}\mathbf{f}^T K^{-1}\mathbf{f} - \frac{1}{2}\log |K| - \frac{n}{2}\log 2\pi\end{aligned}$$

- Differentiating wrt  $\mathbf{f}$

$$\begin{aligned}\nabla\Psi(\mathbf{f}) &= \nabla \log p(\mathbf{y}|\mathbf{f}) - K^{-1}\mathbf{f} \\ \nabla\nabla\Psi(\mathbf{f}) &= \nabla\nabla \log p(\mathbf{y}|\mathbf{f}) - K^{-1} = -W - K^{-1}\end{aligned}$$

where  $W$  is a diagonal matrix since  $y_i$  only depends on  $f_i$ .

- Use **Newton's method** to iterate to the mode.
- Approximate inference for  $f_*$  is possible.
- **Predictions** of  $y_*$  by one-dim numerical integration.

# Saddlepoint approximation of marginal likelihood

## ■ Saddlepoint approximation of marginal likelihood

$$p(\mathbf{y}|\theta) = \int p(\mathbf{y}, \mathbf{f}|\theta) d\mathbf{f} \approx \sqrt{2\pi} p(\mathbf{y}, \hat{\mathbf{f}}_\theta|\theta) \left( \frac{\partial^2 p(\mathbf{y}, \mathbf{f}|\theta)}{\partial \mathbf{f} \partial \mathbf{f}^T} \Big|_{\mathbf{f}=\hat{\mathbf{f}}_\theta} \right)^{-1/2},$$

where  $\hat{\mathbf{f}}_\theta$  and  $\frac{\partial^2 \log p(\mathbf{f}, \theta|\mathbf{y})}{\partial \mathbf{f} \partial \mathbf{f}^T}$  are the mode and Hessian for given  $\theta$ .

## ■ Joint posterior

$$\log p(\mathbf{y}, \mathbf{f}|\theta) = \log p(\mathbf{y}|\mathbf{f}, \theta) + \log p(\mathbf{f}|\theta)$$

## ■ Saddlepoint approx = local Laplace approximation for given $\theta$ .



# Hamiltonian Monte Carlo

- HMC/MCMC to **sample from training posterior**

$$\mathbf{f}|\mathbf{x}, \mathbf{y}, \theta$$

Produces  $\mathbf{f}^{(1)}, \dots, \mathbf{f}^{(N)}$  draws.

- For each  $\mathbf{f}^{(i)}$ , **sample the test posterior**  $\mathbf{f}_*$  from

$$\mathbf{f}_*|\mathbf{f}^{(i)}, \mathbf{x}, \mathbf{x}_* \sim N\left(K(\mathbf{x}_*, \mathbf{x})K(\mathbf{x}, \mathbf{x})^{-1}\mathbf{f}^{(i)}, K(\mathbf{x}_*, \mathbf{x}_*) - K(\mathbf{x}_*, \mathbf{x})K(\mathbf{x}, \mathbf{x})^{-1}K(\mathbf{x}, \mathbf{x}_*)\right)$$

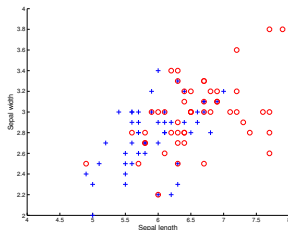
Note that this does not depend on  $\mathbf{y}$  since we condition on  $\mathbf{f}$ .

Noise-free GP fit. Produces  $\mathbf{f}_*^{(1)}, \dots, \mathbf{f}_*^{(N)}$  draws.

- For each  $\mathbf{f}_*^{(i)}$ , **sample a prediction** from

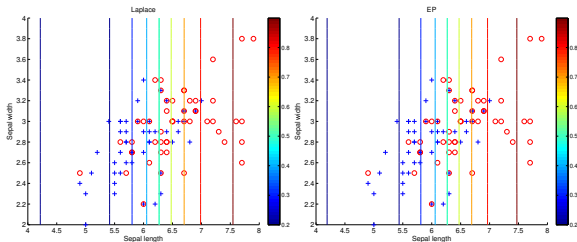
$$p(\mathbf{y}_*|\mathbf{f}_*^{(i)}, \theta).$$

# Iris data - sepal - SE kernel with ARD

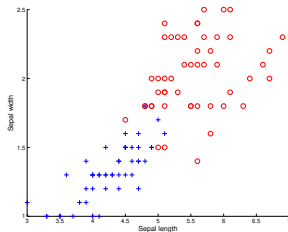


Laplace:  $\hat{\ell}_1 = 1.7214, \hat{\ell}_2 = 185.5040, \sigma_f = 1.4361$

EP:  $\hat{\ell}_1 = 1.7189, \hat{\ell}_2 = 55.5003, \sigma_f = 1.4343$

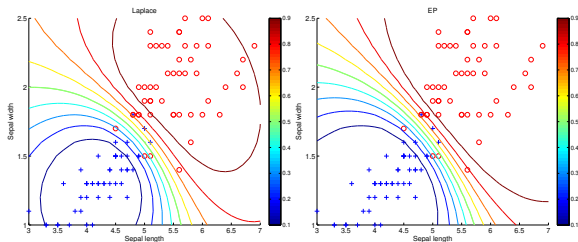


# Iris data - petal - SE kernel with ARD

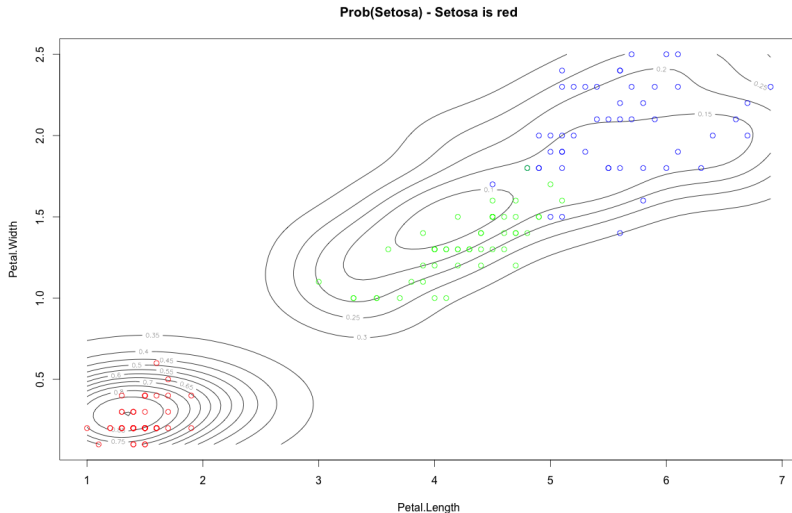


Laplace:  $\hat{\ell}_1 = 1.7606, \hat{\ell}_2 = 0.8804, \sigma_f = 4.9129$

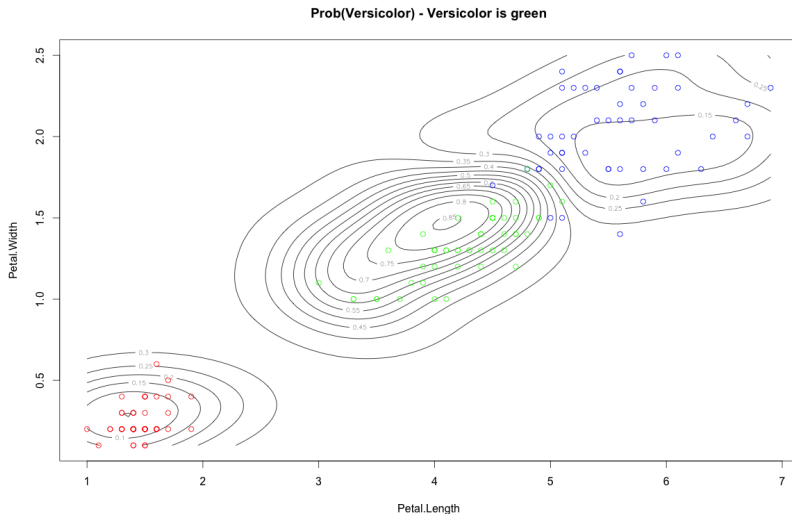
EP:  $\hat{\ell}_1 = 2.1139, \hat{\ell}_2 = 1.0720, \sigma_f = 5.3369$



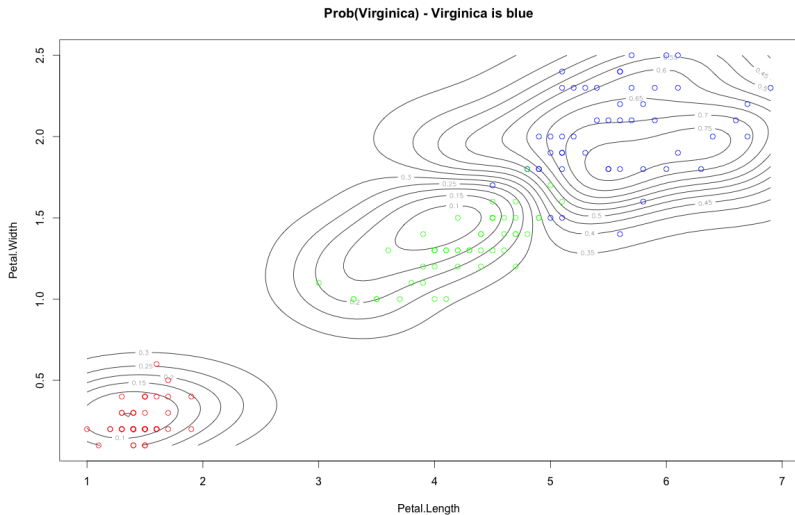
# Iris data - petal - all three classes



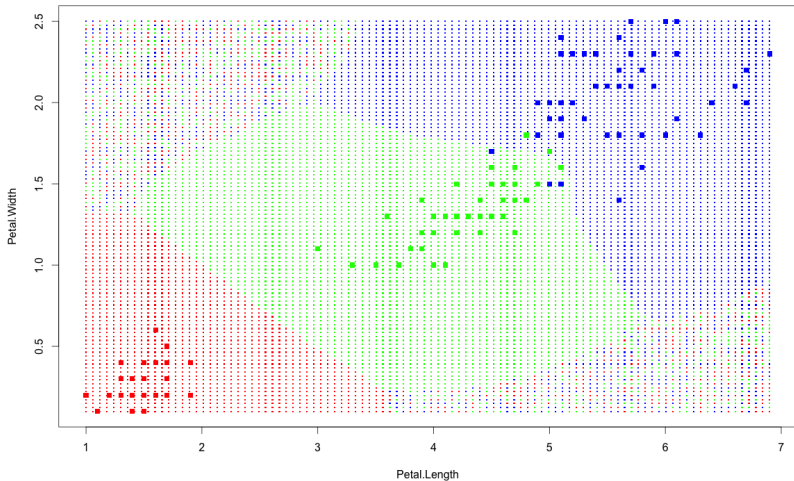
# Iris data - petal - all three classes



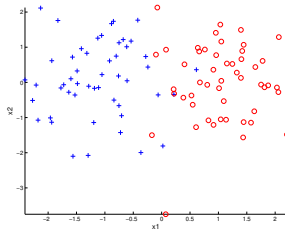
# Iris data - petal - all three classes



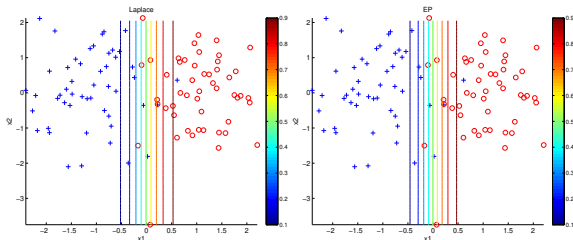
# Iris data - petal - decision boundaries



# Toy data 1 - SE kernel with ARD

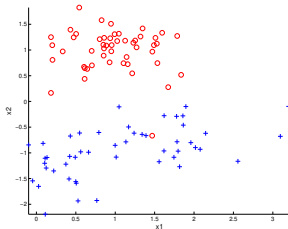


EP:  $\hat{\ell}_1 = 2.4503, \hat{\ell}_2 = 721.7405, \sigma_f = 4.7540$

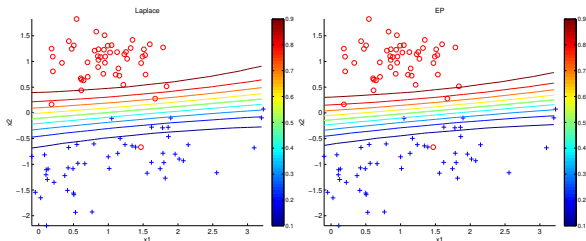




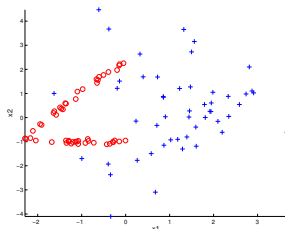
# Toy data 2 - SE kernel with ARD



EP:  $\hat{\ell}_1 = 8.3831, \hat{\ell}_2 = 1.9587, \sigma_f = 4.5483$

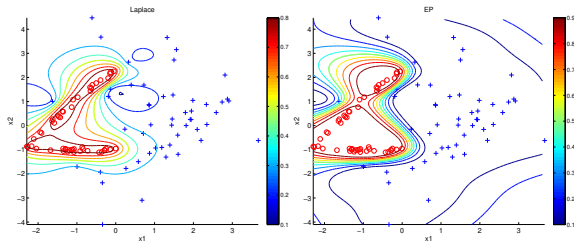


## Toy data 3 - SE kernel with ARD



Laplace:  $\hat{\ell}_1 = 0.7726, \hat{\ell}_2 = 0.6974, \sigma_f = 11.7854$

EP:  $\hat{\ell}_1 = 1.2685, \hat{\ell}_2 = 1.0941, \sigma_f = 17.2774$



# Bayesian Optimization (BO)

- Minimization of **expensive** function

$$\operatorname{argmin}_{\mathbf{x} \in \mathcal{X}} f(\mathbf{x})$$

- **Hyperparameter estimation** from marginal likelihood.

- **BO idea**<sup>1</sup>:

- ▶ Assign GP prior to the unknown function  $f$ .
- ▶ Evaluate the function at some values  $x_1, x_2, \dots, x_n$ .
- ▶ Update posterior  $f|x_1, \dots, x_n \sim GP$ .
- ▶ Use GP posterior of  $f$  to find new eval point  $x_{n+1}$ .
- ▶ Repeat until convergence

- **Explore** vs **Exploit**.

- **Bayesian Numerics**<sup>2</sup>. Posterior of  $\int f(\mathbf{x}) d\mathbf{x}$  from  $\{f(\mathbf{x}_i)\}$ .

---

<sup>1</sup>Snoek et al (2012). Practical Bayesian Optimization of Machine Learning Algorithms.

<sup>2</sup>Hennig et al (2015). Probabilistic numerics and uncertainty in computations.

# Acquisition functions

## ■ Probability of Improvement (PI)

$$a_{PI}(\mathbf{x}; \mathcal{D}_n) \equiv \Pr(f(\mathbf{x}) < f(\mathbf{x}_{\text{best}}) | \mathcal{D}_n) = \Phi(\gamma(\mathbf{x}))$$

where  $\mathcal{D}_n = \{y_i, \mathbf{x}_i\}_{i=1}^n$  are previous function evaluations and

$$\gamma(\mathbf{x}) = \frac{f(\mathbf{x}_{\text{best}}) - \mu(\mathbf{x}; \mathcal{D}_n)}{\sigma(\mathbf{x}; \mathcal{D}_n)}$$

## ■ Expected Improvement (EI)

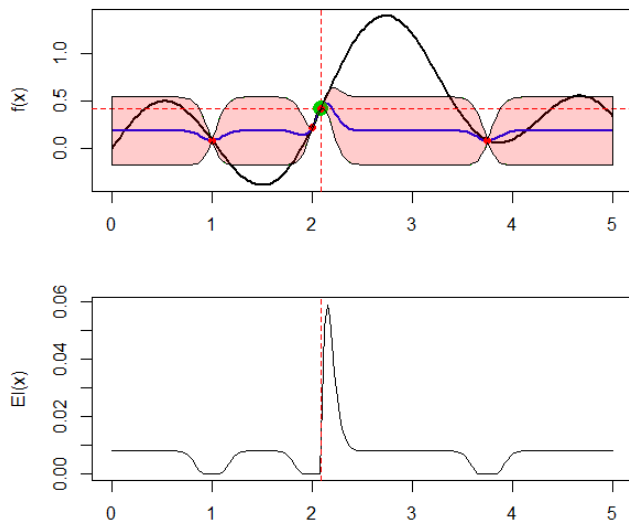
$$a_{EI}(\mathbf{x}; \mathcal{D}_n) = \sigma(\mathbf{x}; \mathcal{D}_n) [\gamma(\mathbf{x})\Phi(\gamma(\mathbf{x})) + \phi(\gamma(\mathbf{x}))]$$

- Maximizing  $a(\mathbf{x})$  to find  $\mathbf{x}_{n+1}$  is simpler than minimizing  $f(\mathbf{x})$ .
- Noisy function evaluations  $\hat{f}(\mathbf{x})$  (e.g. MCMC). Noisy GP.
- When precision of  $\hat{f}(\mathbf{x})$  is controlled by user: BOOP.<sup>3</sup>

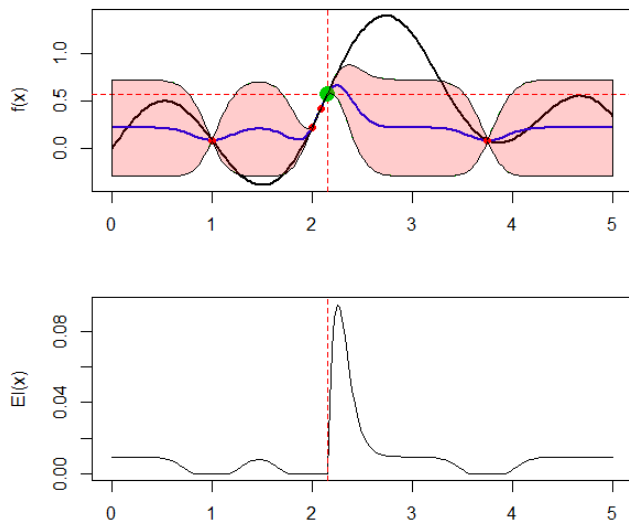
---

<sup>3</sup>Gustafsson et al (2020). Bayesian Optimization of Hyperparameters when the Marginal Likelihood is Estimated by MCMC. On arXiv next week ...

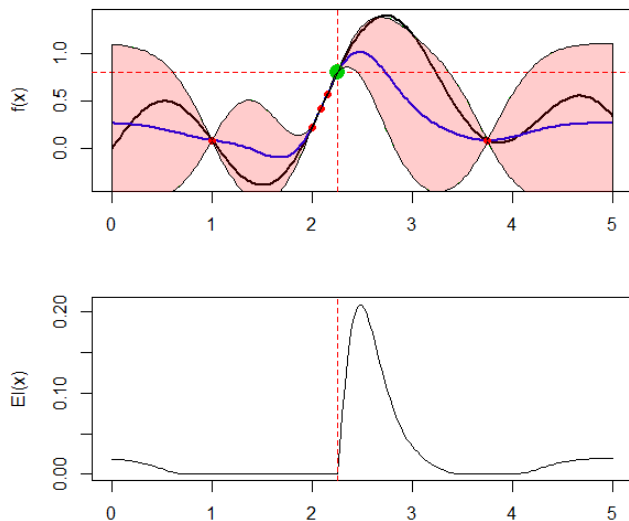
# BO illustration - EI



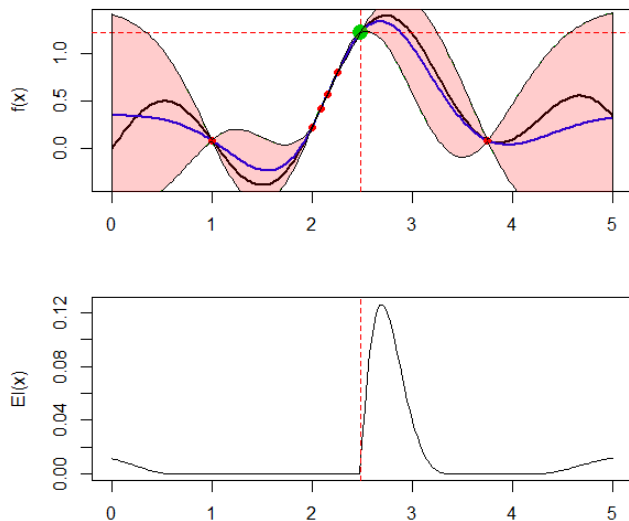
# BO illustration - EI



# BO illustration - EI

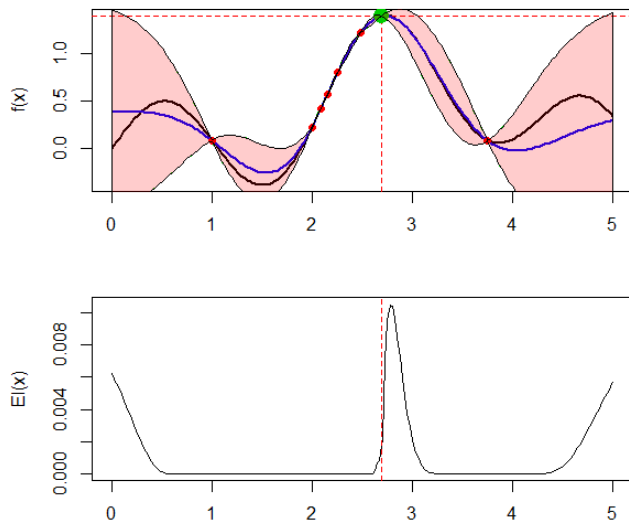


# BO illustration - EI

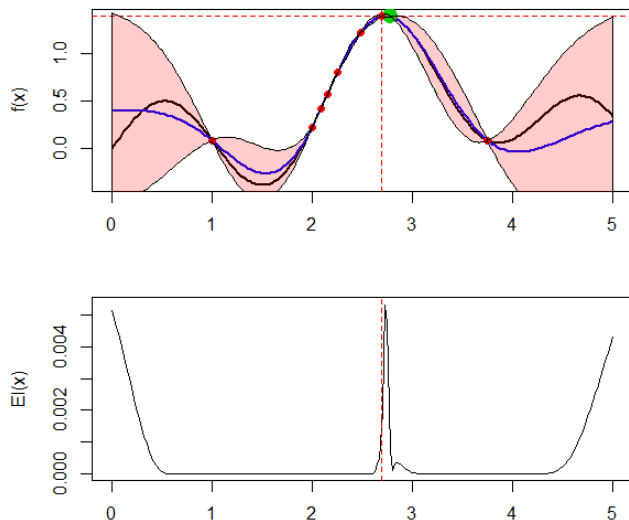




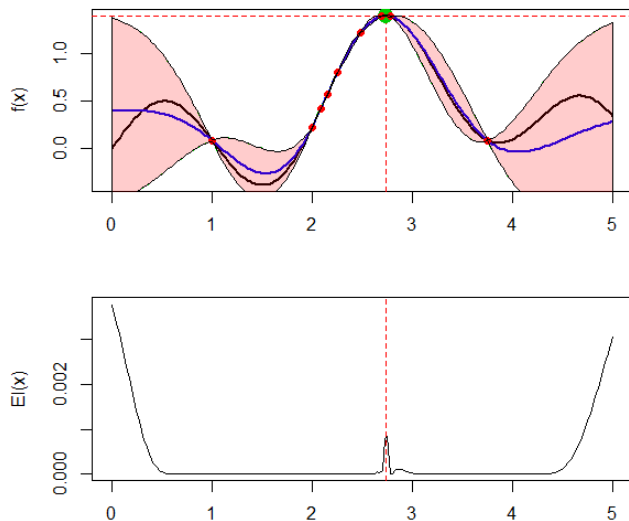
# BO illustration - EI



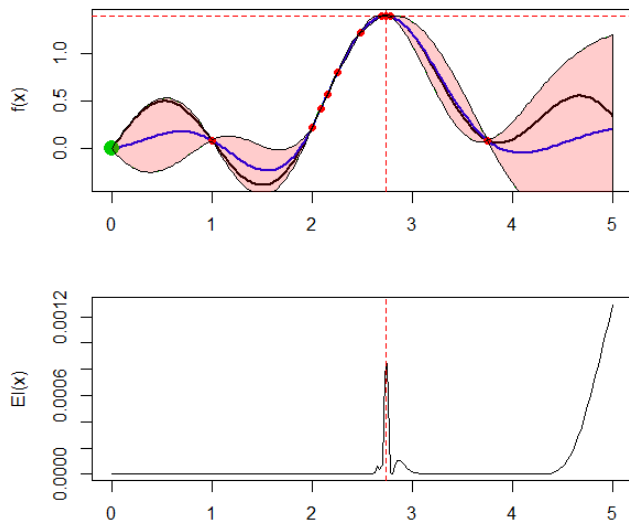
# BO illustration - EI



# BO illustration - EI



# BO illustration - EI



# BO illustration - EI

