Advanced Bayesian Learning
Gaussian Processes
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Topic overview

- Gaussian process regression
  - Recall: Bayesian inference for Gaussian linear/nonlinear regression.
  - Gaussian processes for nonparametric regression
  - Covariance kernels
  - Properties of GPs
  - Selecting the kernel and hyperparameters
- Gaussian process classification
  - Flexible classification
  - Laplace approximation of the posterior
- Main literature: Rasmussen and Williams (2006). *Gaussian Processes for Machine Learning*.

Flexible nonlinear regression

- **Linear regression**

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

$$f(\mathbf{x}) = \mathbf{x}^T \cdot \mathbf{w}$$

  and $\varepsilon \sim N(0, \sigma_n^2)$ and iid over observations.
- The weights $\mathbf{w}$ are called regression coefficients (β) in statistics.
- **Polynomial regression**: $\mathbf{x} = (1, x, x^2, x^3, ..., x^k)^T$.
- **Spline regression**:

$$f(\mathbf{x}) = \phi(\mathbf{x})^T \cdot \mathbf{w}$$

  where $\phi(\mathbf{x}) = (\phi_1(\mathbf{x}), \phi_2(\mathbf{x}), ..., \phi_N(\mathbf{x}))^T$ for N basis functions
- Example: **thin plate splines** with N knots $\kappa_1, ..., \kappa_N$ in $\mathbf{x}$-space

$$\phi_k(\mathbf{x}) = \ln\left(\|\mathbf{x} - \kappa_k\|\right) \|\mathbf{x} - \kappa_k\|^2$$

- Note: these models are still linear in the weights.

Bayesian linear regression - inference

- $\mathbf{w}$ is unknown. σ_n is assumed known.
- **Prior** [note: RW do *not* use $\Sigma_p = \sigma_n^2 \Omega$]

$$\mathbf{w} \sim N(0, \Sigma_p)$$

- **Posterior**

$$\begin{aligned}
\mathbf{w}|\mathbf{X},\mathbf{y} &\sim N\left(\bar{\mathbf{w}}, \mathbf{A}^{-1}\right) \\
\mathbf{A} &= \sigma_n^{-2}\mathbf{X}\mathbf{X}^T + \Sigma_p^{-1} \\
\bar{\mathbf{w}} &= \sigma_n^{-2}\mathbf{A}^{-1}\mathbf{X}\mathbf{y} = \left(\mathbf{X}\mathbf{X}^T + \sigma_n^2\Sigma_p^{-1}\right)^{-1}\mathbf{X}\mathbf{y}
\end{aligned}$$

- Recall: **Posterior precision = Data Precision + Prior Precision** and all of that.
- Posterior of $\mathbf{w}$ is multivariate student-t when σ_n^2 is unknown with Inv-χ^2 prior (and $\Sigma_p = \sigma_n^2\Omega$).

Bayesian linear regression - prediction

- **Predictive density for mean** $f(\mathbf{x}_*)$ at new location $\mathbf{x}_*$

$$f(\mathbf{x}_*)|\mathbf{x}_*, \mathbf{X}, \mathbf{y} \sim N\left(\mathbf{x}_*^T \bar{\mathbf{w}}, \mathbf{x}_*^T \mathbf{A}^{-1} \mathbf{x}_*\right)$$

- Proof: $f(\mathbf{x}_*) = \mathbf{x}_*^T \mathbf{w}$ and $\mathbf{w}$ has a normal posterior. Use that linear combs of normals is normal.

- **Predictive density for new response** y_*

$$\mathbf{y}_*|\mathbf{x}_*, \mathbf{X}, \mathbf{y} \sim N\left(\mathbf{x}_*^T \bar{\mathbf{w}}, \mathbf{x}_*^T \mathbf{A}^{-1} \mathbf{x}_* + \sigma_n^2\right)$$

- Replace $\mathbf{X}$ with $\Phi(\mathbf{X})$ in the above for the case with basis expansion (e.g. splines).

Non-parametric regression

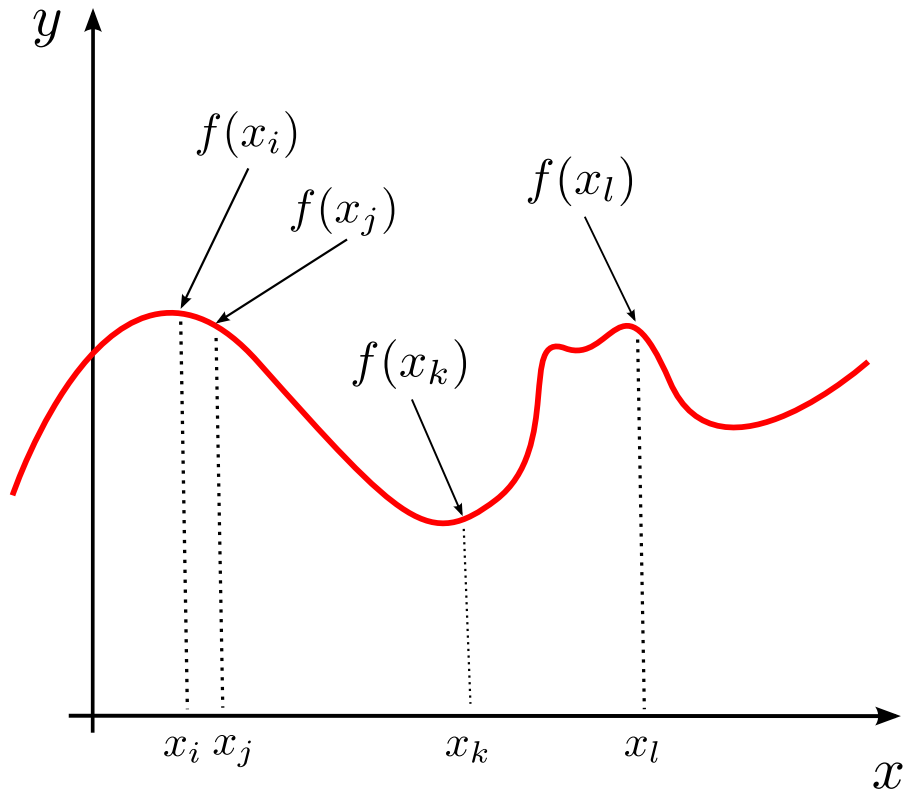
- **Non-parametric regression**: avoiding a parametric form for $f(\cdot)$. Treat $f(\mathbf{x})$ as an unknown parameter for every $\mathbf{x}$.

- **Weight space view**
  - Restrict attention to a grid of (ordered) x-values: $x_1, x_2, .., x_k$.
  - Put a joint prior on the k function values: $f(x_1), f(x_2), ..., f(x_k)$.

- **Function space view**
  - Treat f as an **unknown function**.
  - Put a **prior over a set of functions**.

- Kolmogorov's existence theorem for stochastic processes equates the two views.

NONPARAMETRIC = ONE PARAMETER FOR EVERY X!



The multivariate normal distribution

- The **density function** of a p-variate normal vector $\mathbf{x} \sim N(\mu, \Sigma)$ is

$$f(\mathbf{x}) = \left(\frac{1}{2\pi}\right)^{p/2} \frac{1}{\sqrt{\det \Sigma}} \exp\left\{-\frac{1}{2}(\mathbf{x}-\mu)'\Sigma^{-1}(\mathbf{x}-\mu)\right\}$$

- Example: **Bivariate normal** $(p = 2)$

$$\Sigma = \begin{pmatrix} \sigma_1^2 & \rho\sigma_1\sigma_2 \\ \rho\sigma_1\sigma_2 & \sigma_2^2 \end{pmatrix}$$

- **Linear combinations**. Let $\mathbf{y} = \mathbf{B}\mathbf{x} + \mathbf{b}$, where $\mathbf{x}$ is $n \times 1$ and $\mathbf{B}$ is a $m \times n$ constant matrix. Then

$$\mathbf{y} \sim N(\mathbf{B}\mu + \mathbf{b}, \mathbf{B}\Sigma\mathbf{B}')$$

The multivariate normal distribution, cont.

- Let $\mathbf{x} = \begin{pmatrix} \mathbf{x}_1 \\ \mathbf{x}_2 \end{pmatrix}$ where $\mathbf{x}_1$ is $p_1 \times 1$ and $\mathbf{x}_2$ is $p_2 \times 1$ ($p_1 + p_2 = p$).
- Partition μ and Σ accordingly as

$$\mu = \begin{pmatrix} \mu_1 \\ \mu_2 \end{pmatrix} \text{ and } \Sigma = \begin{pmatrix} \Sigma_{11} & \Sigma_{12} \\ \Sigma_{21} & \Sigma_{22} \end{pmatrix}$$

- **Marginals are normal**. Let $\mathbf{x} \sim N(\mu, \Sigma)$, then

$$\mathbf{x}_1 \sim N(\mu_1, \Sigma_1)$$

- **Conditionals are normal**. Let $\mathbf{x} \sim N(\mu, \Sigma)$, then

$$\mathbf{x}_1 | \mathbf{x}_2 = \mathbf{x}_2^* \sim N\left[\mu_1 + \Sigma_{12}\Sigma_{22}^{-1}(x_2^* - \mu_2),\ \Sigma_{11} - \Sigma_{12}\Sigma_{22}^{-1}\Sigma_{21}\right]$$

- Life is beautiful ...

Gaussian process regression

- Natural choice. Multivariate normal (Gaussian):

$$\begin{pmatrix} f(x_1) \\ \vdots \\ f(x_k) \end{pmatrix} \sim N(\mathbf{m}, \mathbf{K})$$

- But how do we specify the $k \times k$ **covariance matrix** $\mathbf{K}$?

$$Cov(f(x_p), f(x_q))$$

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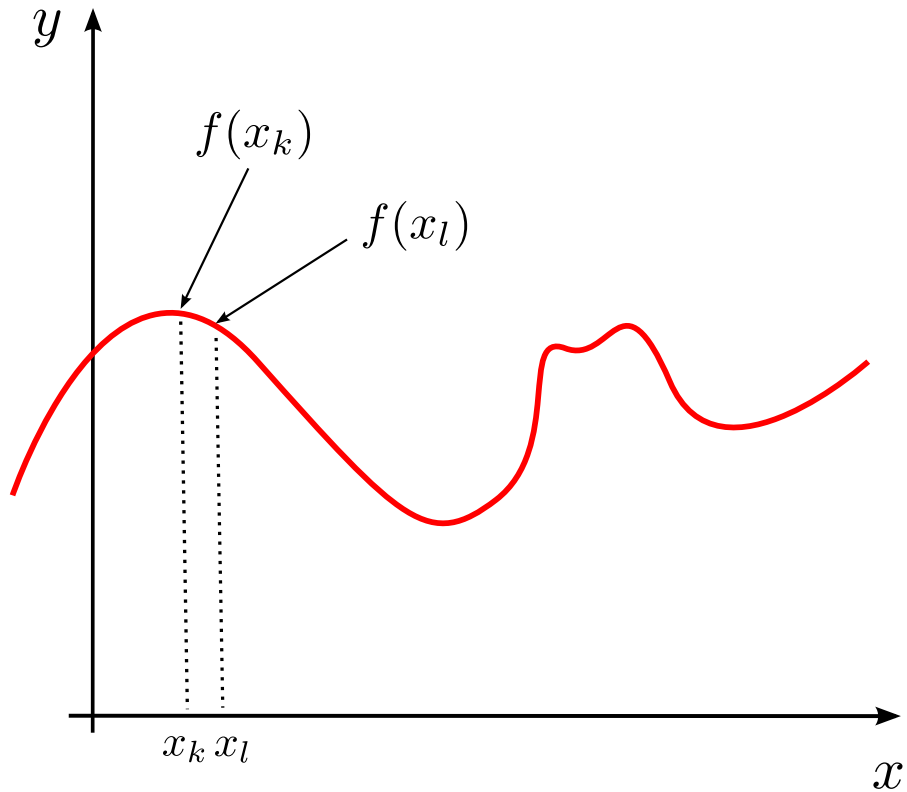
$$Cov\left(f(x_p), f(x_q)\right)$$

- **Squared exponential covariance function**

$$Cov\left(f(x_p), f(x_q)\right) = K(x_p, x_q) = \sigma_f^2 \exp\left(-\frac{1}{2}(x_p - x_q)^2\right)$$

- The covariance between $f(x_p)$ and $f(x_q)$ is a function of x_p and x_q.
- Nearby x's have highly correlated function ordinates $f(x)$.
- We can compute $Cov\left(f(x_p), f(x_q)\right)$ for *any* x_p and x_q (no need for a pre-determined grid)

Smooth f(x) - points nearby



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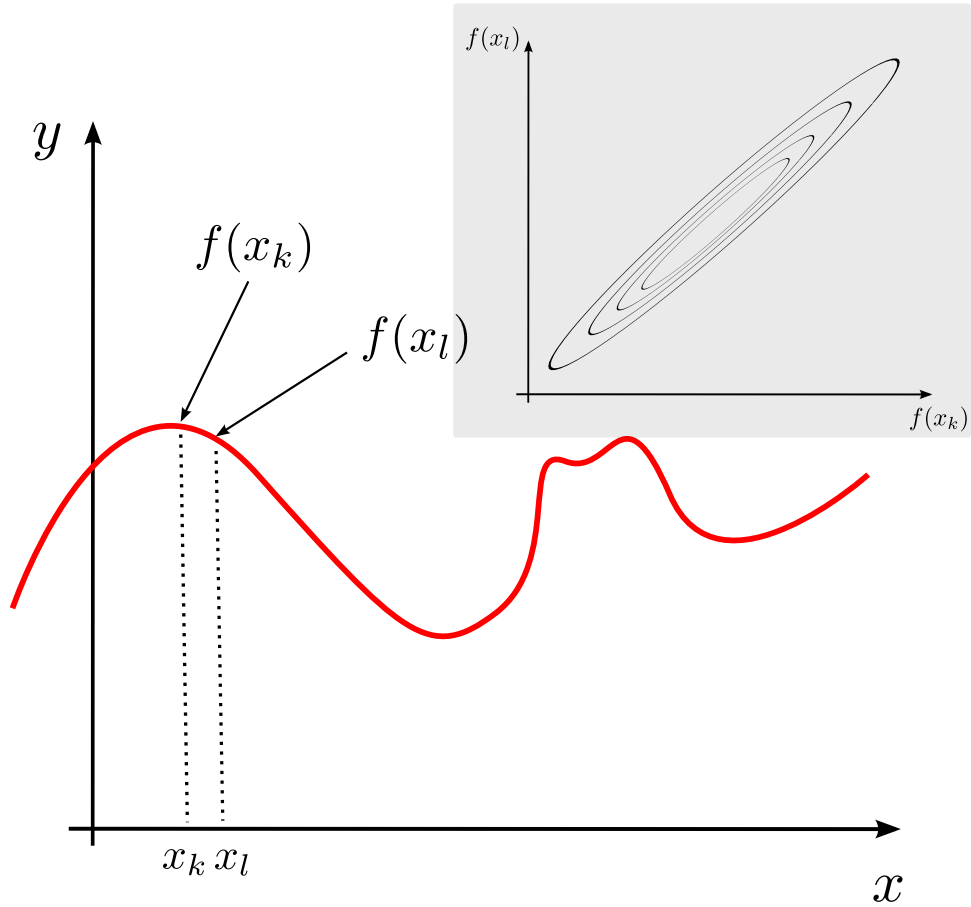
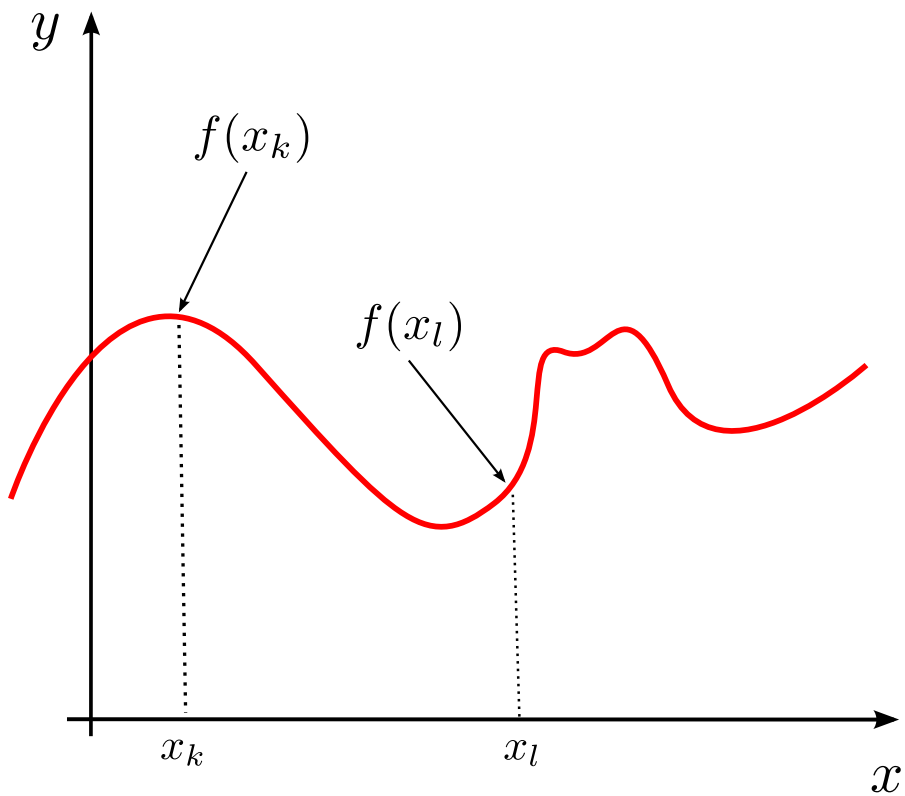


Smooth f(x) - points far apart



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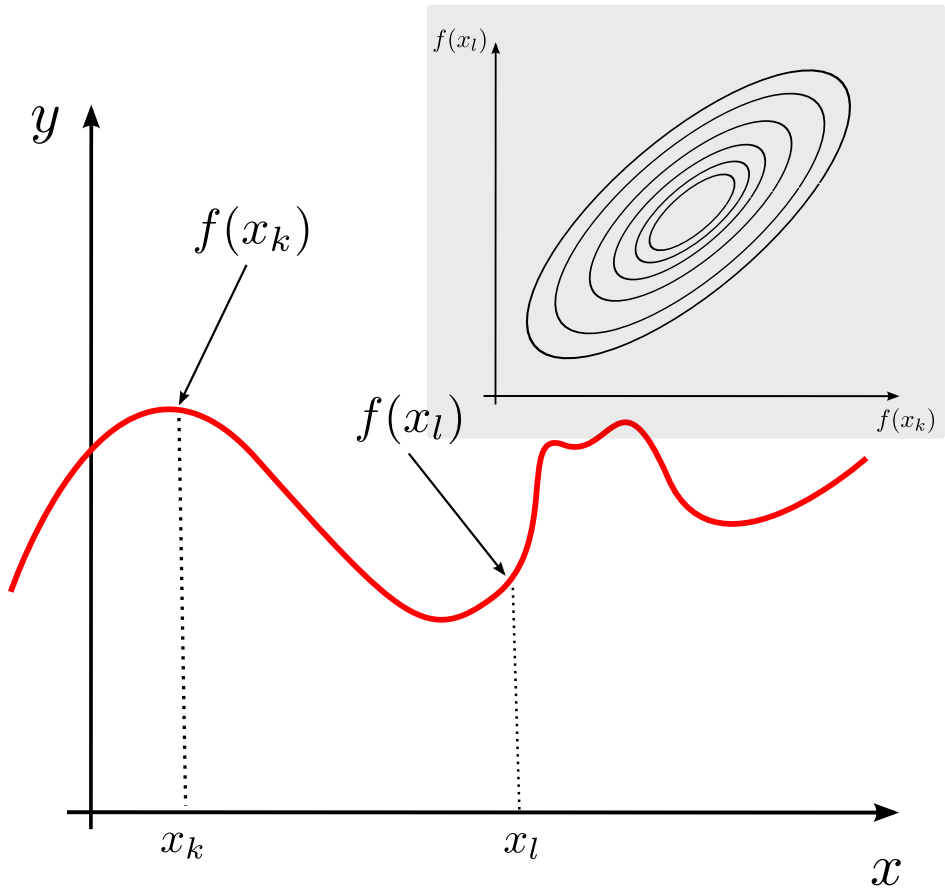
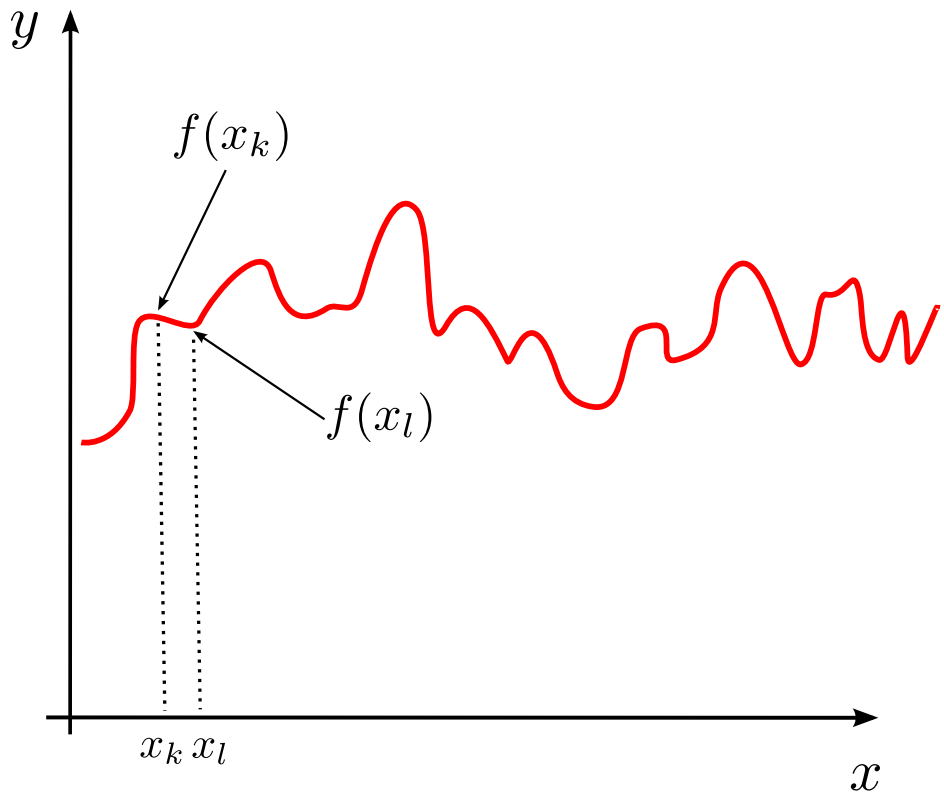


Jagged f(x) - points nearby



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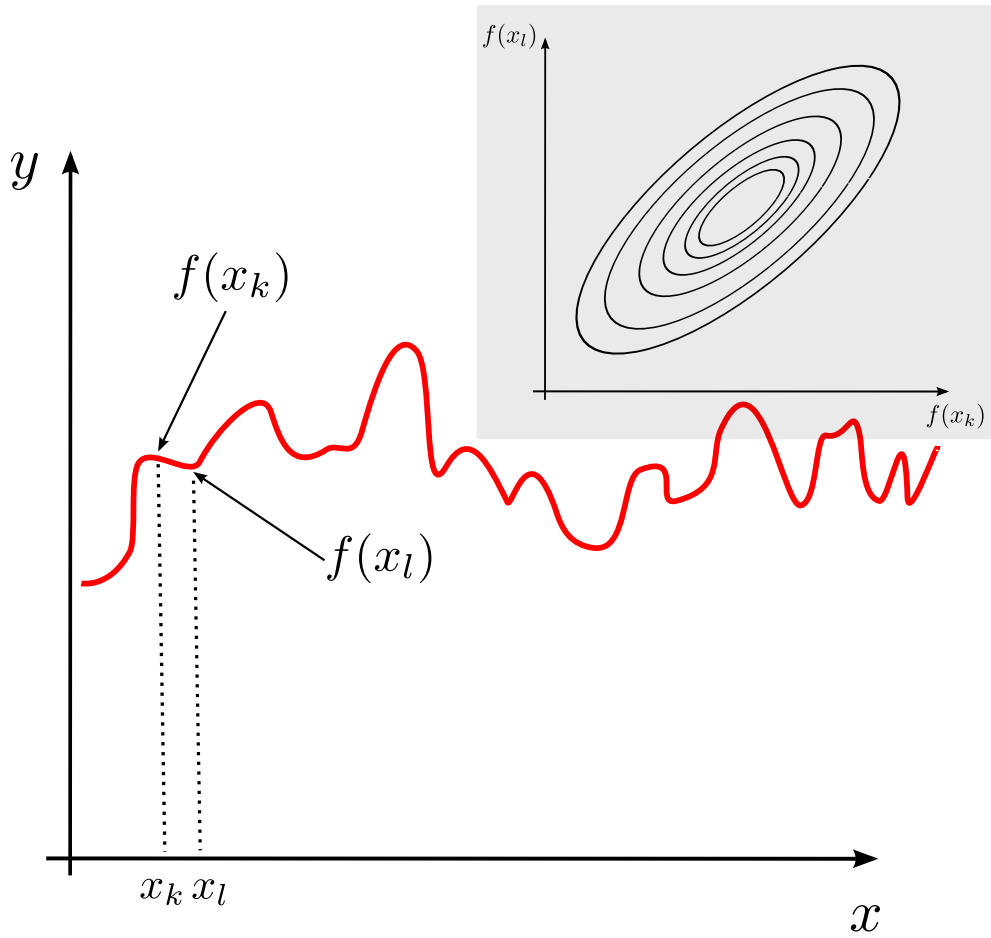

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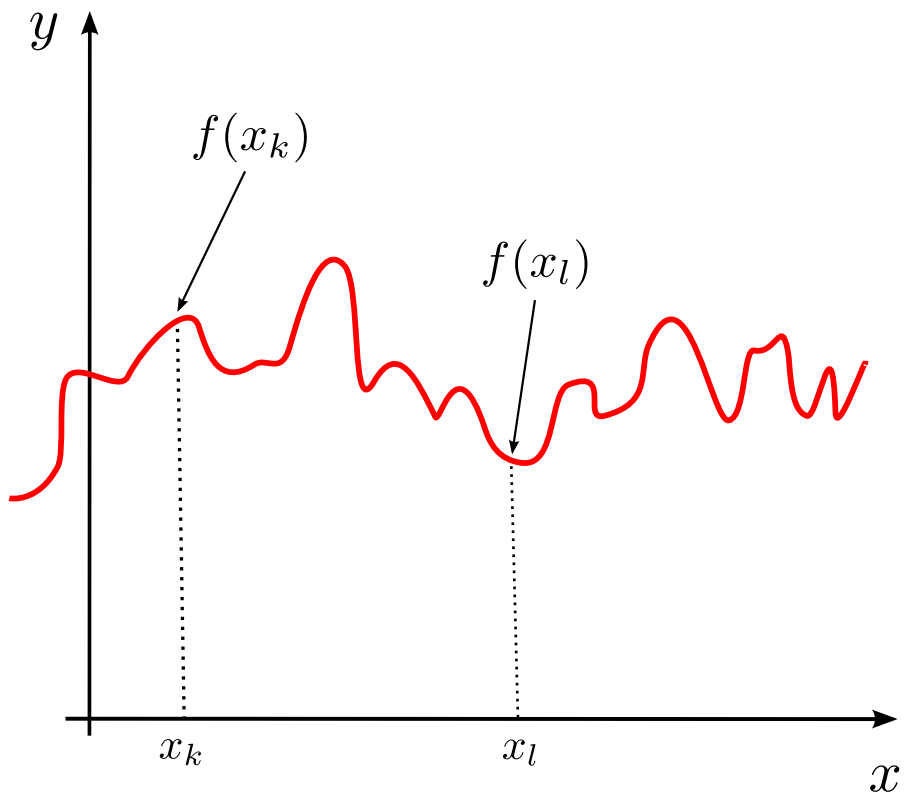

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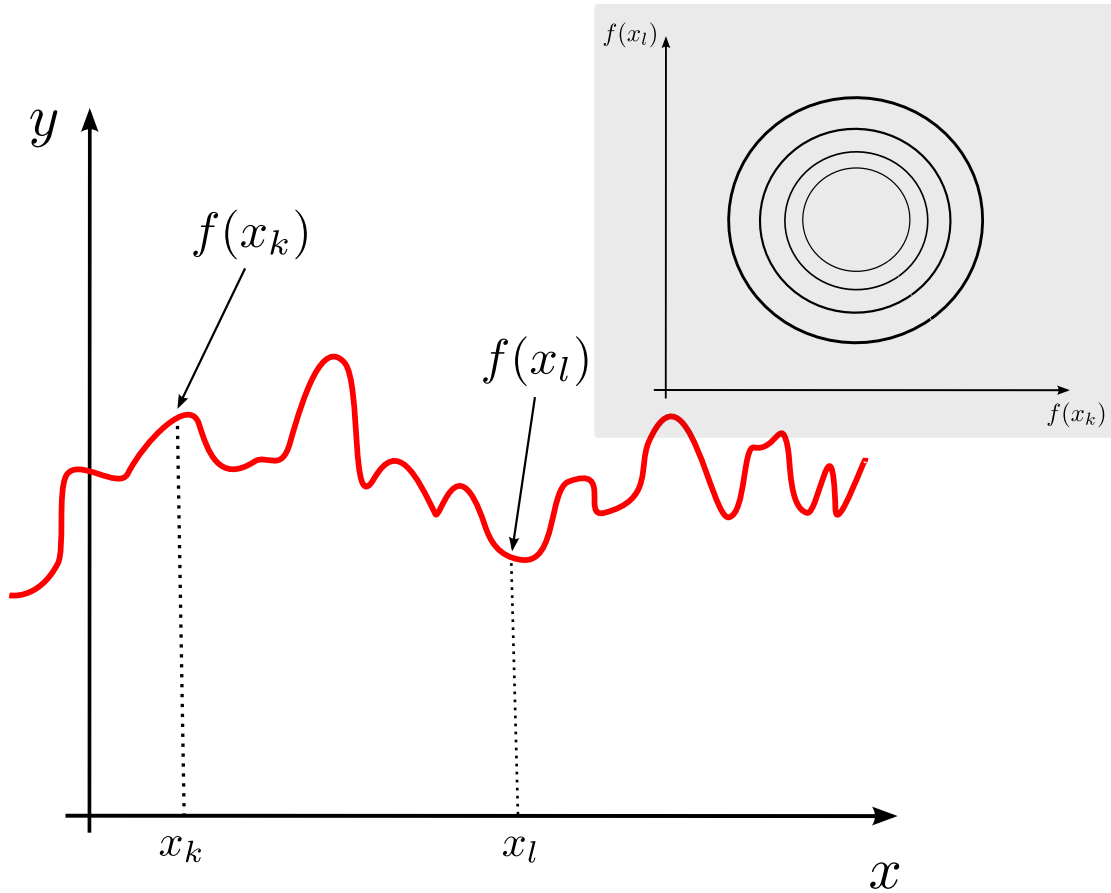


Gaussian process regression, cont.

Definition

A **Gaussian process** (**GP**) is a collection of random variables, any finite number of which have a multivariate Gaussian distribution.

- A Gaussian process is really a **probability distribution over functions** (curves). No need for a grid!
- A GP is completely specified by a mean and a covariance function

$$m(x) = \mathrm{E}\left[f(x)\right]$$

$$K(x, x') = E\left[\left(f(x) - m(x)\right)\left(f(x') - m(x')\right)\right]$$

  for any two inputs x and x' (note: this is *not* the transpose here).
- A Gaussian process (prior) is denoted by

$$f(x) \sim GP\left(m(x), K(x, x')\right)$$

Gaussian process regression, cont.

- Example:

$$m(x) = \sin(x)$$

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

  where $\ell > 0$ is the length scale.
- Larger l gives more smoothness in $f(x)$.
- Simulate draw from $f(x) \sim GP\left(m(x), K(x, x')\right)$ over a grid $x_* = (x_1, ..., x_n)$ by using that

$$f(x_*) \sim N\left(m(x_*), K(x_*, x_*)\right)$$

Simulating a GP

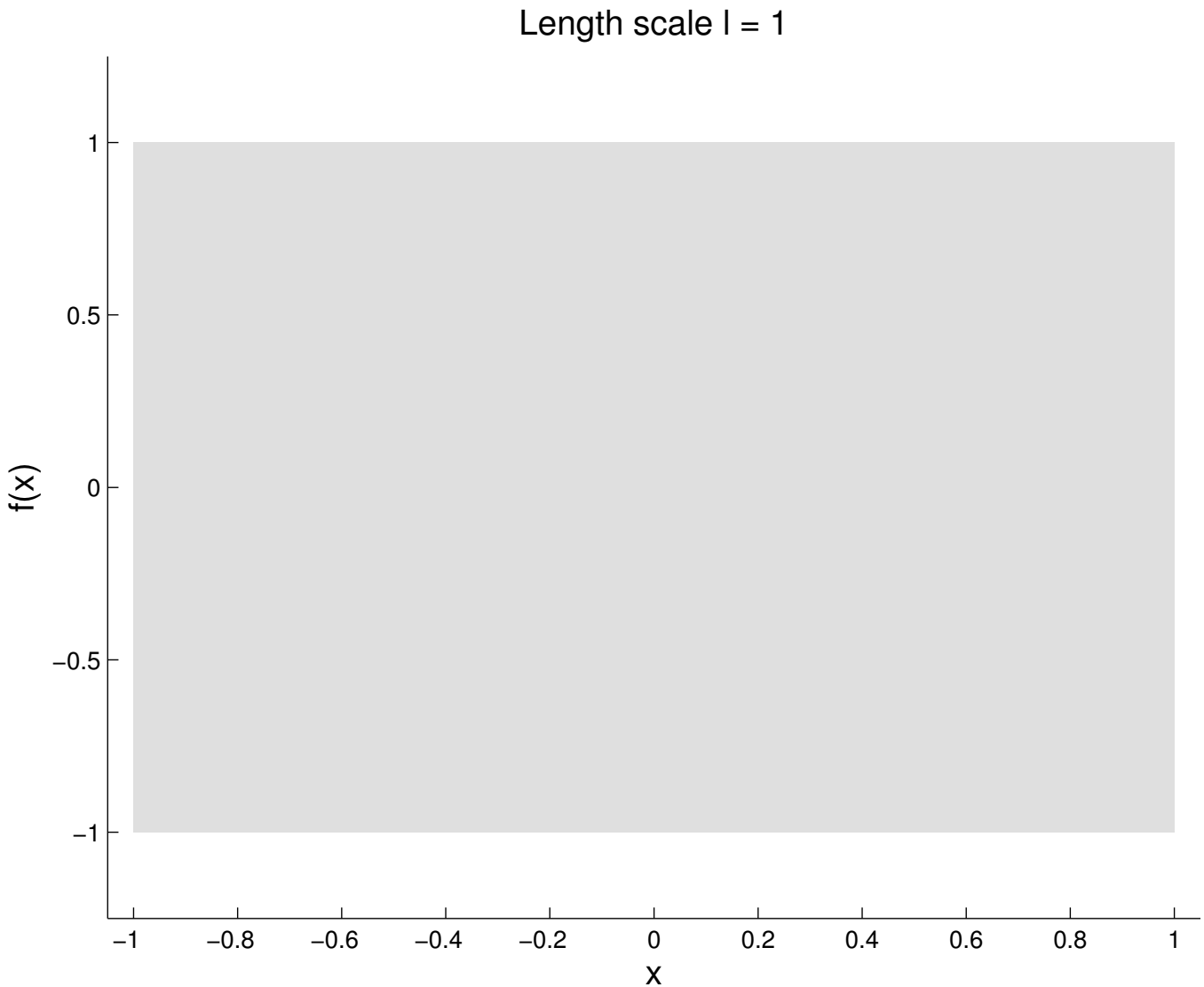
- The joint way: Choose a grid $x_1, ..., x_k$. Simulate the k-vector

$$\begin{pmatrix} f(x_1) \\ \vdots \\ f(x_k) \end{pmatrix} \sim N(\mathbf{m}, \mathbf{K})$$

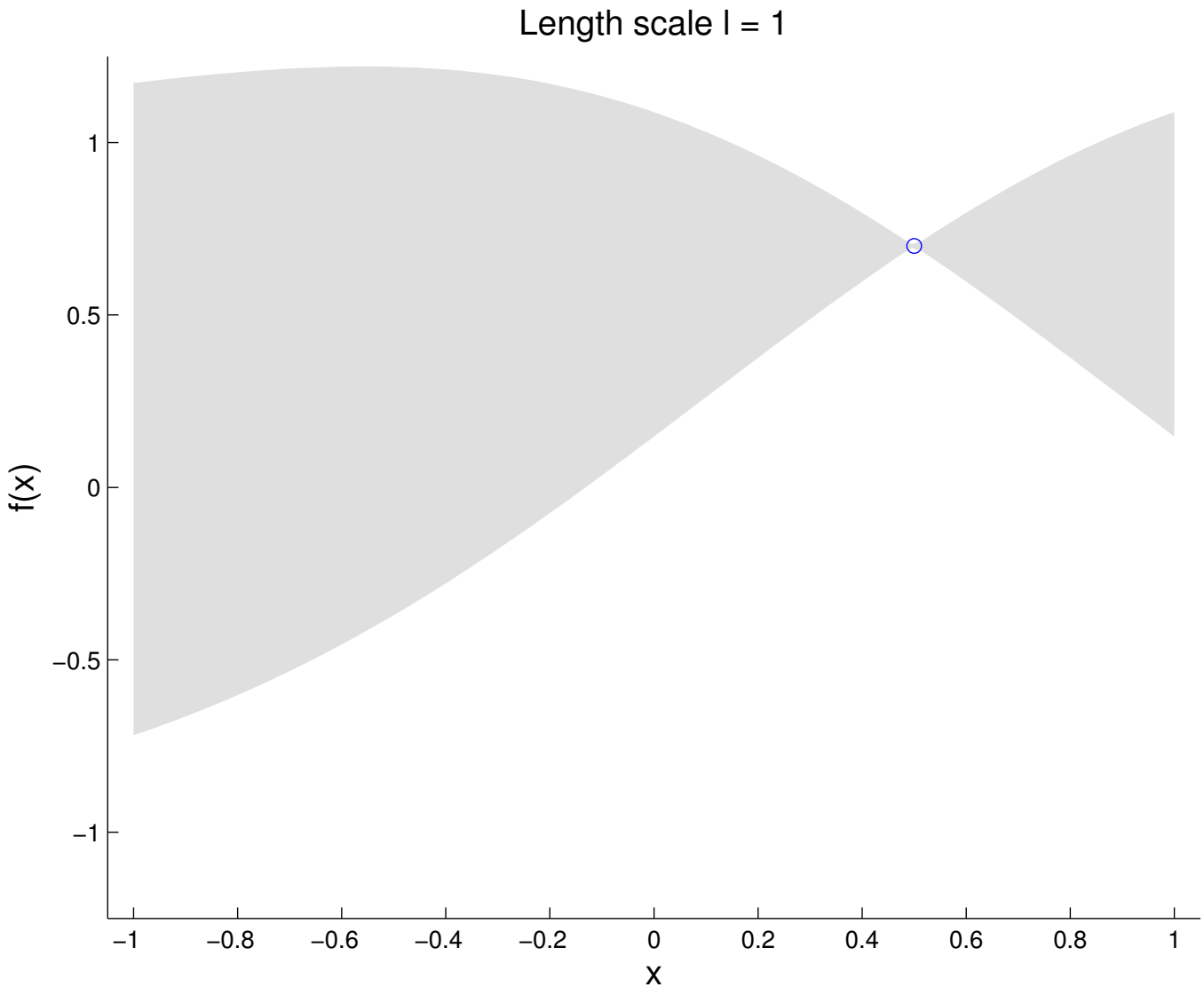
- More intuition from the conditional decomposition

$$p(f(x_1), f(x_2), ..., f(x_k)) = p(f(x_1))\, p(f(x_2)|f(x_1)) \cdots \\ \times p(f(x_k)|f(x_1), ..., f(x_{k-1}))$$

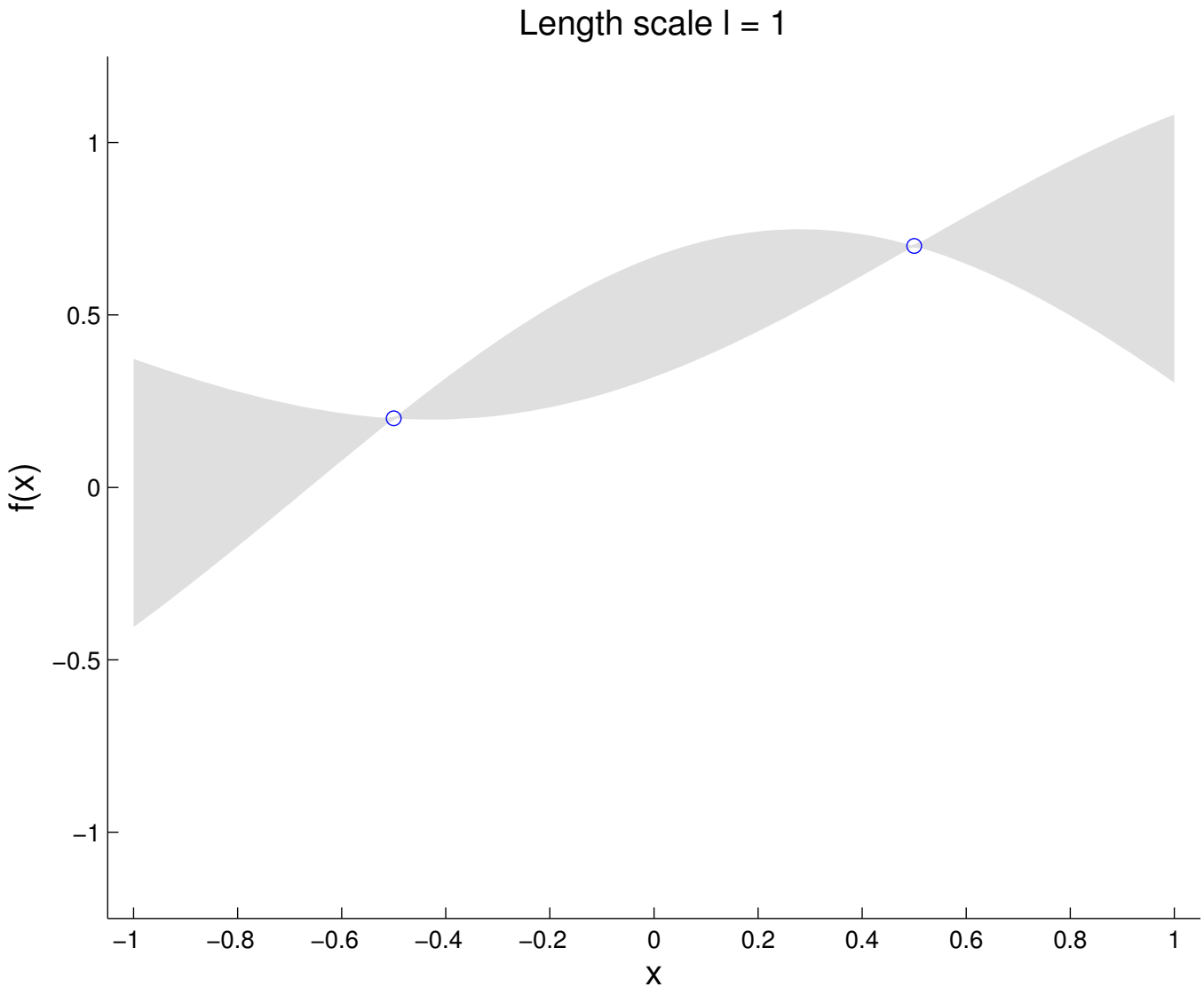
Density before first draw



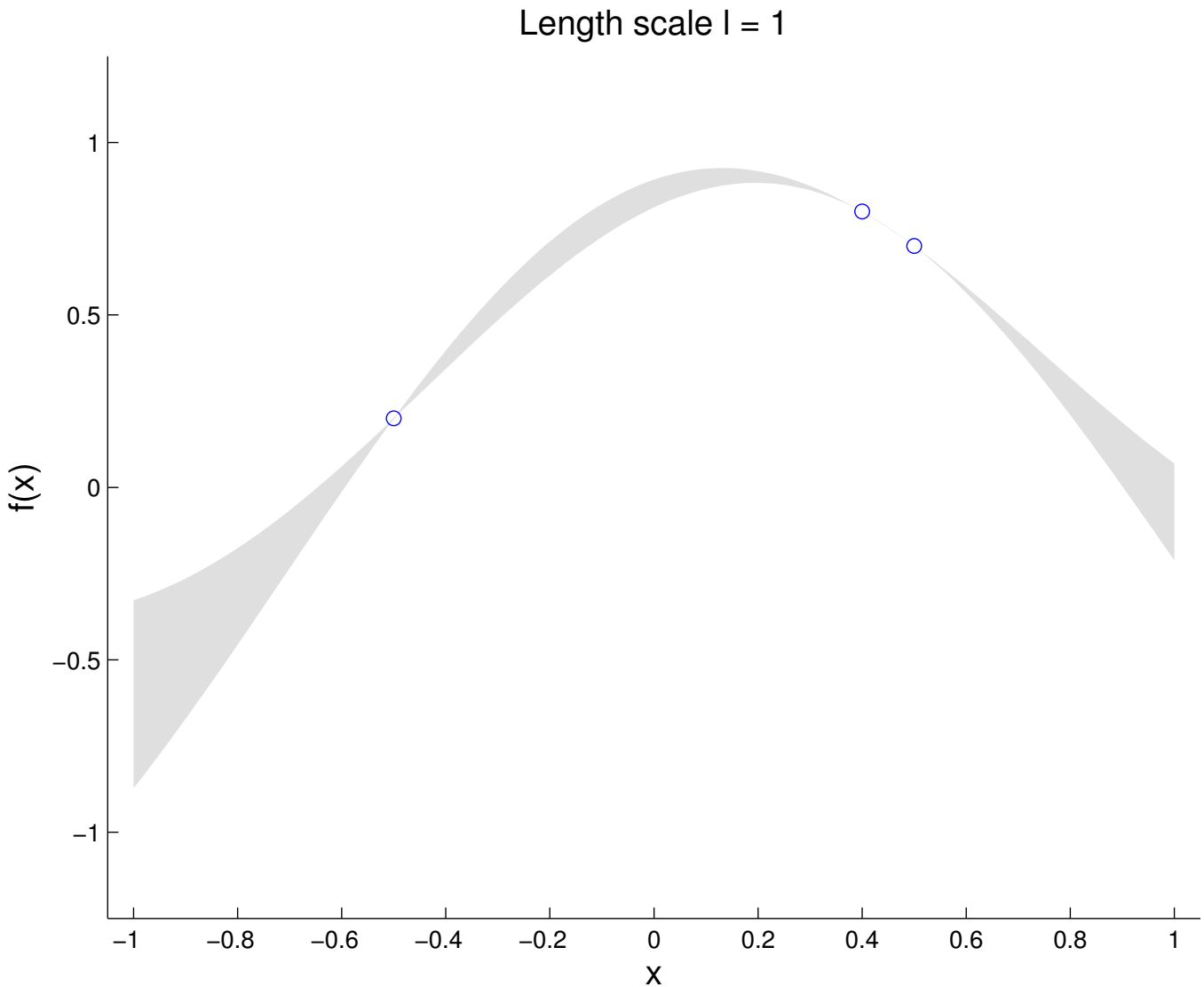
Density before second draw



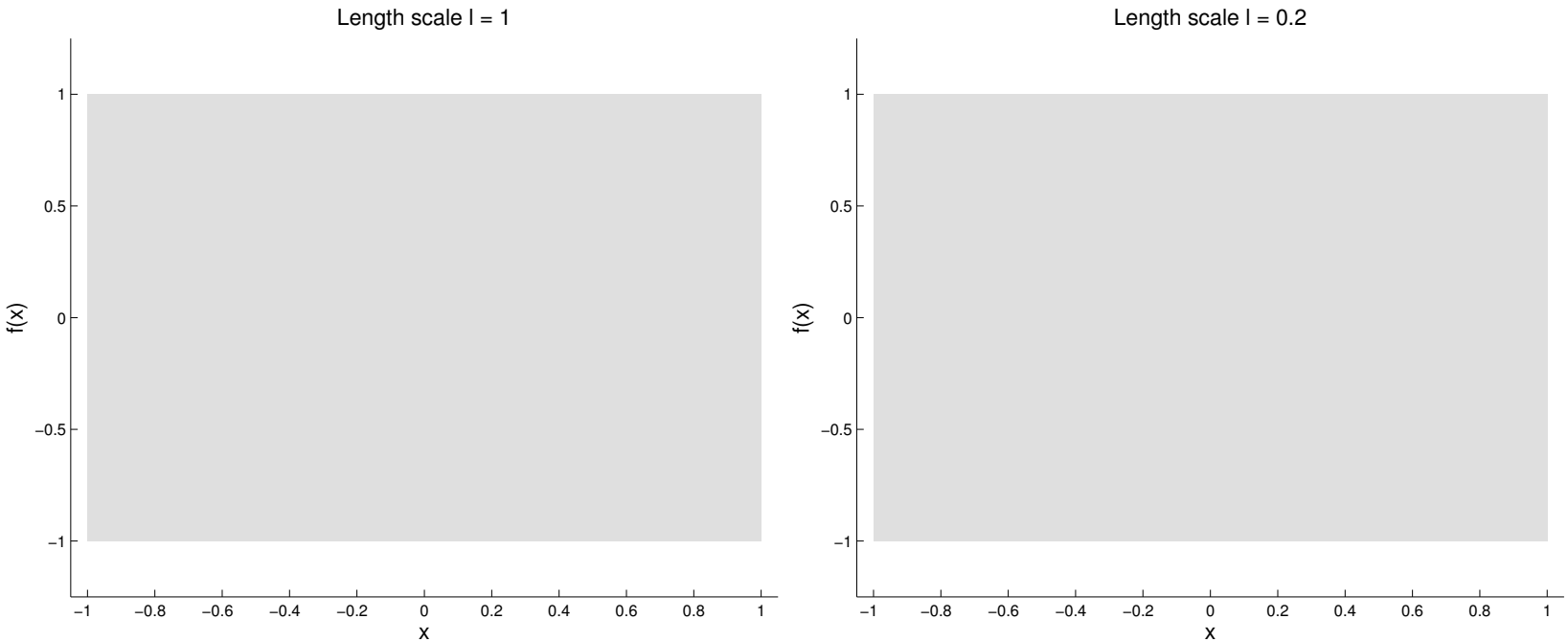
Density before third draw



Density before fourth draw



Simulation from l=1 vs l=0.2. Before first draw.



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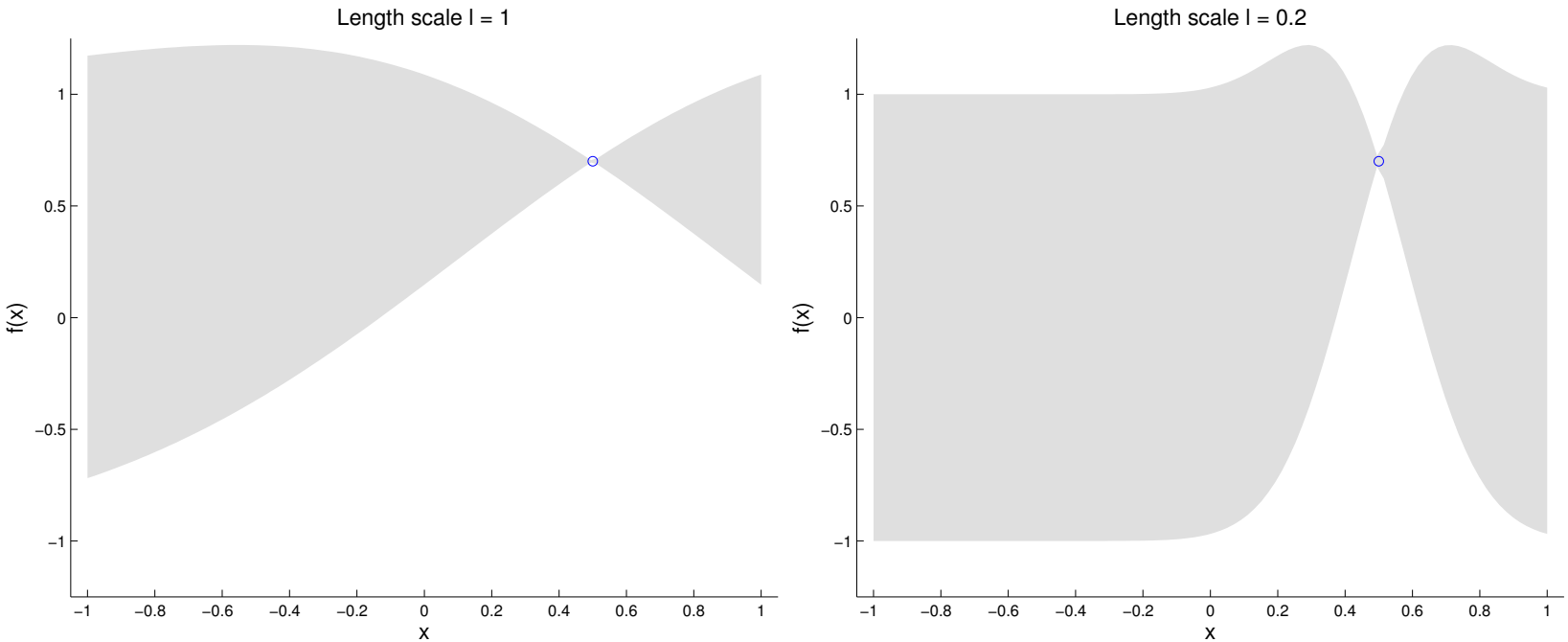

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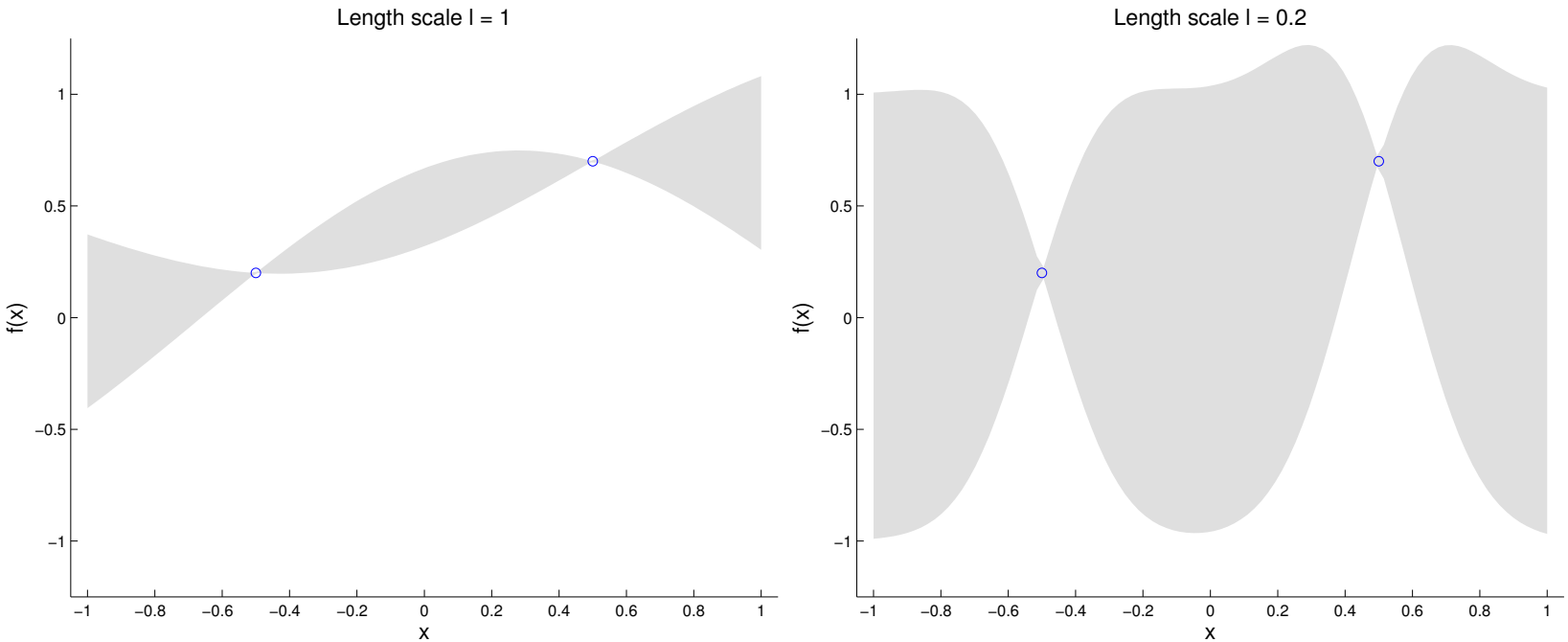

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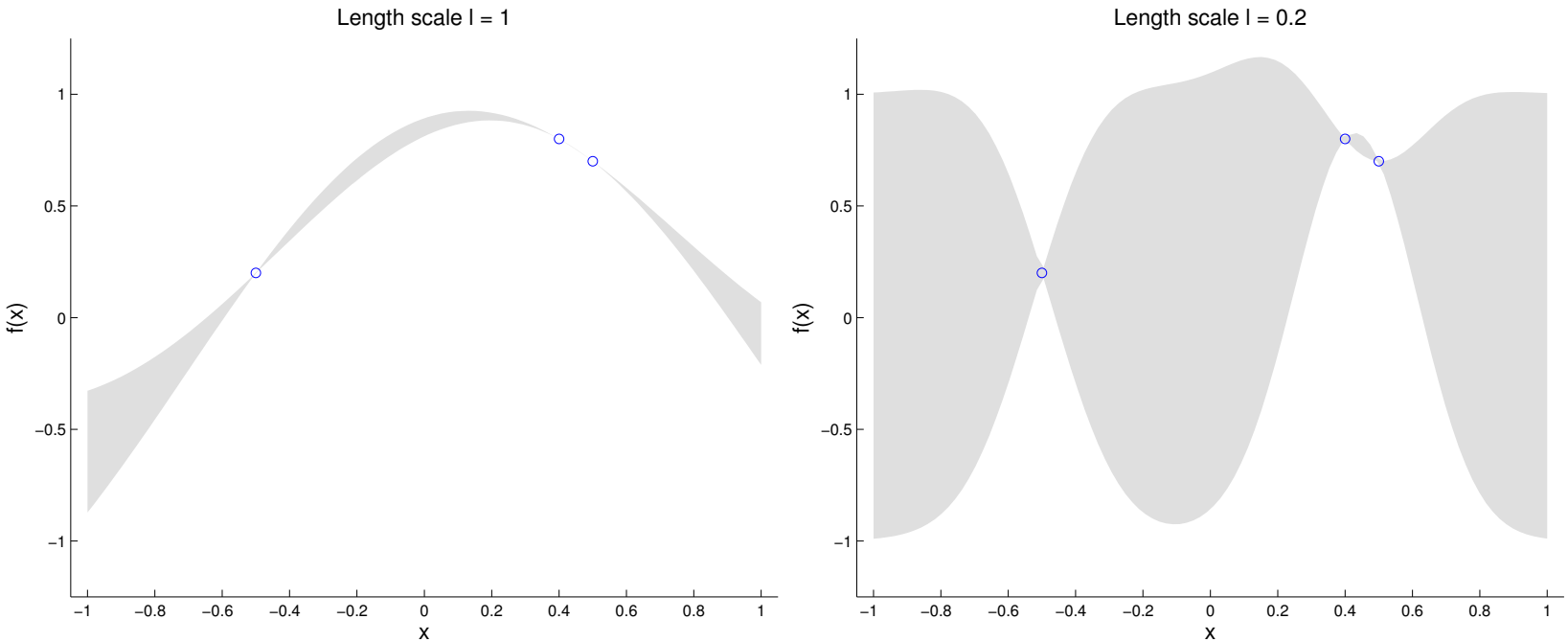

Gaussian process regression, cont.

- **Model**

$$y_i = f(x_i) + \varepsilon_i, \quad \varepsilon \overset{iid}{\sim} N(0, \sigma^2)$$

- **Prior**

$$f(x) \sim GP\left(0, K(x, x')\right)$$

- You have observed the data: $\mathbf{x} = (x_1, ..., x_n)'$ and $\mathbf{y} = (y_1, ..., y_n)'$.
- Goal: the posterior of $f(\cdot)$ over a grid of x-values: $\mathbf{f}_* = \mathbf{f}(\mathbf{x}_*)$.

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- Intermediate step: joint distribution of $\mathbf{y}$ and $\mathbf{f}_*$

$$\begin{pmatrix} \mathbf{y} \\ \mathbf{f}_* \end{pmatrix} \sim N\left\{ \begin{pmatrix} \mathbf{0} \\ \mathbf{0} \end{pmatrix}, \begin{bmatrix} K(\mathbf{x}, \mathbf{x}) + \sigma^2 I & K(\mathbf{x}, \mathbf{x}_*) \\ K(\mathbf{x}_*, \mathbf{x}) & K(\mathbf{x}_*, \mathbf{x}_*) \end{bmatrix} \right\}$$

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- The **posterior**

$$\mathbf{f}_* | \mathbf{x}, \mathbf{y}, \mathbf{x}_* \sim N\left(\bar{\mathbf{f}}_*, \text{cov}(\mathbf{f}_*)\right)$$

$$\bar{\mathbf{f}}_* = K(\mathbf{x}_*, \mathbf{x}) \left[K(\mathbf{x}, \mathbf{x}) + \sigma^2 I\right]^{-1} \mathbf{y}$$

$$\text{cov}(\mathbf{f}_*) = K(\mathbf{x}_*, \mathbf{x}_*) - K(\mathbf{x}_*, \mathbf{x}) \left[K(\mathbf{x}, \mathbf{x}) + \sigma^2 I\right]^{-1} K(\mathbf{x}, \mathbf{x}_*)$$

Prediction and Decision

- Predicting a new set of y-values $\mathbf{y}_* = f(\mathbf{x}_*) + \epsilon$ is easy

$$\mathbf{y}_* | \mathbf{x}, \mathbf{y}, \mathbf{x}_* \sim N\left(\bar{\mathbf{f}}_*, \text{cov}(\mathbf{f}_*) + \sigma_n^2 I\right)$$

- Choosing a point prediction $\mathbf{y}_{guess}$ can be made by maximizing expected utility

$$\bar{\mathcal{U}}(\mathbf{y}_{guess} | \mathbf{x}_*) = \int \mathcal{U}(\mathbf{y}_*, \mathbf{y}_{guess}) p(\mathbf{y}_* | \mathbf{x}_*, \mathbf{y}, \mathbf{x}) d\mathbf{y}_*$$

- Have to make a decision $a \in \mathcal{A}$ whose consequences (utility) depends on the uncertain $\mathbf{f}_*$ (or $\mathbf{y}_*$)? Just maximize expected utility

$$\bar{\mathcal{U}}(a) = \int \mathcal{U}(a, \mathbf{f}_*) p(\mathbf{f}_* | \mathbf{x}_*, \mathbf{y}, \mathbf{x}) d\mathbf{f}_*$$

where $\mathcal{U}(a, \mathbf{f}_*)$ is the utility of action $a \in \mathcal{A}$ if $\mathbf{f}_*$ turns out to be the "true state of the world".

Stationary processes and smoothness

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

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

- The covariance function is **isotropic** if it only depends on the distance $t = \|\mathbf{x}-\mathbf{x}\|$ (invariant to directions)

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

- The **smoothness** of a stationary process is determined by the smoothness of the covariance function.
- A stationary (isotropic) process is **continuous in quadratic mean**

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

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

- A little more is required to guarantee **continuous sample paths** (continuous $f(\mathbf{x}+t, \omega)$ for any $\mathbf{x} \in \mathbb{R}^D$ and $\omega \in \Omega$).

KERNELS AND SPECTRAL DENSITIES

- $k(\mathbf{x}, \mathbf{x}')$ is a **covariance function** (i.e. positive definite) $\rightarrow$ the $n \times n$ **Gram matrix** $\mathbf{K} = (k(x_i, x_j))_{i,j=1,\ldots,n}$ is a **covariance matrix**.
- **Bochner's theorem**: A complex valued function $k(\cdot)$ on $\mathbb{R}^D$ is the covariance function of a weakly stationary continuous complex-valued stochastic process on $\mathbb{R}^D$ iff

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

- $S(\mathbf{s})$ is the **spectral density**. $S(\mathbf{s})$ is the energy allocated to the complex exponential basis function $e^{2\pi i \mathbf{s}\cdot\mathbf{t}}$ at frequency $\mathbf{s}$.
- For real-valued processes, think of $e^{2\pi i \mathbf{s}\cdot\mathbf{t}}$ as a multi-dimensional sine wave with frequency $\mathbf{s}$ and amplitude $S(\mathbf{s})$.
- Spectral density $\Longleftrightarrow$Covariance function of stationary process $\Longleftrightarrow$Smoothness properties of the process.

Commonly used covariance 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 $S(s) = (2\pi\ell^2)^{D/2} \exp\left(-2\pi^2\ell^2 s^2\right)$. Higher frequencies tail of like a Gaussian (i.e. quickly).
  - 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 behaves like a student-t density with 2ν degrees of freedom. For $\nu = 1/2$, $S(s)$ is Cauchy. Much weight on high frequency. Very rough.
  - $\nu = 3/2$ and $\nu = 5/2$ most useful for ML. As $\nu \to \infty$, Matérn's kernel approaches SE kernel.

Commonly used covariance kernels, cont.

- γ-**exponential** ($\ell > 0$, $0 < \gamma \leq 2$)

$$K_\gamma(r) = \exp\left[-\left(\frac{r}{\ell}\right)^\gamma\right]$$

  - Mean square differentiable only when $\gamma = 2$ (SE).

- **Rational quadratic** ($\ell > 0$, $\alpha > 0$)

$$K_{RQ}(r) = \left(1 + \frac{r^2}{2\alpha\ell^2}\right)^{-\alpha}$$

  - Scale mixture of SE covariance functions with different length-scales.
  - $K_{RQ}(r)$ approaches the SE kernel as $\alpha \to \infty$.

- $k(r) = \int \exp\left(-r^2/2\ell^2\right) p(\ell) d\ell$ is the most general represenation of an isotropic kernel with a valid covariance function in all dimensions D.

More on kernels

- 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): $\mathbf{M} = Diag(\ell_1^{-2}, ..., \ell_D^{-2})$ is diagonal with different length scales.
- **Factor kernels**: $M = \Lambda\Lambda^T + \Psi$, where Λ is $D \times k$ for low rank k.
- Length-scales $\ell(\mathbf{x})$ that vary with $\mathbf{x}$. Non-trivial to make positive definite, but see Gibbs kernel in Eq. 4.32.
- Kernels are often combined into **composite kernels**. Sum of kernels is a kernel. Product of kernels is a kernel.
- Kernels can be used for non-vectorial inputs by defining distance function between objects (e.g. words). String kernels for text analysis. Fisher kernels.

Bayesian inference for hyperparameters

- Kernel depends on hyperparameters θ. Example SE kernel $[\theta = (\sigma_f, \ell)^T]$

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

- If the hyperparameters are unknown, just compute the posterior

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

- We need to compute

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

  where $\mathbf{f} = f(\mathbf{X})$ is a vector with function values in the training data.
- For Gaussian process regression we can actually do this analytically

$$\log p(\mathbf{y}|\mathbf{X}, \theta) = -\frac{1}{2}\mathbf{f}^T K^{-1}\mathbf{f} - \frac{1}{2}\log\left|K + \sigma_n^2 I\right| - \frac{n}{2}\log(2\pi)$$

- RW takes a short-cut and estimates θ by maximizing $\log p(\mathbf{y}|\mathbf{X}, \theta)$.