02477 – Bayesian Machine Learning: Lecture 5

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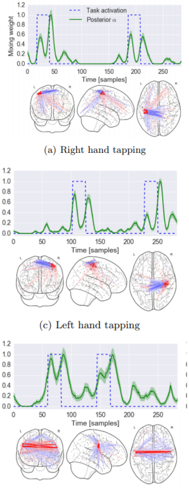
Outline

Multitude of Gaussian processes applications

- Regression (supervised learning)
  - Time series analysis
  - EEG brain imaging
  - Survival analysis for cancer data
  - Predicting rainfall
  - Robot dynamics
  - ...
- Classification (supervised learning)
  - Recognizings human movements
  - Brain decoding
  - ...
- Used as building block in more complex models
- Dimensionality reduction (unsupervised learning)
- Optimization of black functions (Bayesian optimization)
- Numerical integration (Bayesian quadrature)
- Solving differential equations (probabilistic numerics)



(a) Right hand tapping
(c) Left hand tapping
(b) Tongue wagging

Towards prior distributions for function spaces

Parametric models

- In week 3, we studied linear models of the form

$$y_n = f_n + e_n = \phi(\boldsymbol{x}_n)^T \boldsymbol{w} + e_n$$

- In week 4, we studied Bayesian logistic regression

$$y_n | f_n \sim Ber(\sigma(f_n))$$
$$f_n = \phi(\boldsymbol{x}_n)^T \boldsymbol{w}$$

- Typical workflow
  1. Specify prior $p(\boldsymbol{w})$ and likelihood $p(\boldsymbol{y}|\boldsymbol{w})$
  2. Calculate posterior distribution $p(\boldsymbol{w}|\boldsymbol{y})$
  3. Make predictions based on the predictive distribution $p(y^*|\boldsymbol{y}, \boldsymbol{x}^*)$

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- Linear and logistic regression are both *parametric models*: probability distributions indexed by finite dimensional parameters

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$$p(\boldsymbol{y}, \boldsymbol{f}, \boldsymbol{w}) = p(\boldsymbol{y}|\boldsymbol{f})p(\boldsymbol{f}|\boldsymbol{w})p(\boldsymbol{w})$$

- The model is the same - we can recover the old model formulation via the sum rule

$$p(\boldsymbol{y}, \boldsymbol{w}) = \int p(\boldsymbol{y}|\boldsymbol{f})p(\boldsymbol{f}|\boldsymbol{w})p(\boldsymbol{w})\mathrm{d}\boldsymbol{f}$$

From parameters to functions II

- The augmented model

$$p(\boldsymbol{y}, \boldsymbol{f}, \boldsymbol{w}) = p(\boldsymbol{y}|\boldsymbol{f})p(\boldsymbol{f}|\boldsymbol{w})p(\boldsymbol{w})$$

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- We could do the integral directly, let's use this result instead

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Changing perspective from weight space to function space

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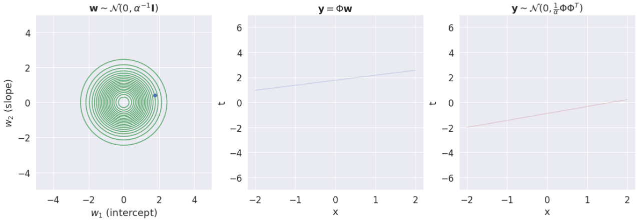

- Two ways to generate samples of $\boldsymbol{f} \sim p(\boldsymbol{f})$

- Weight space-perspective

  Step 1: Generate a sample $\boldsymbol{w}^{(i)} \sim p(\boldsymbol{w})$
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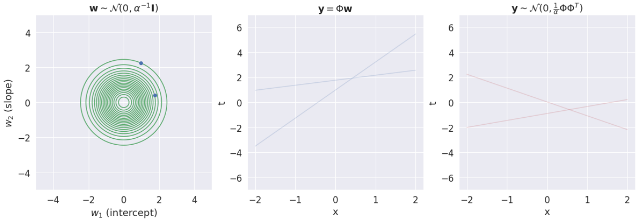

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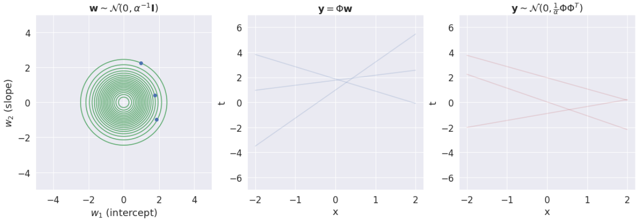

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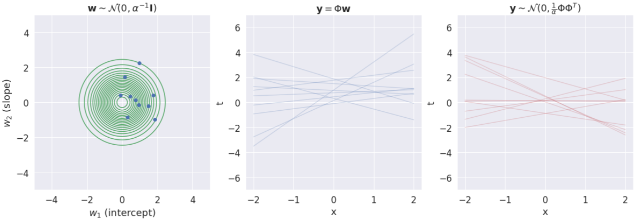

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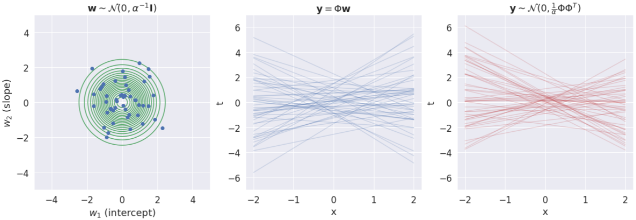

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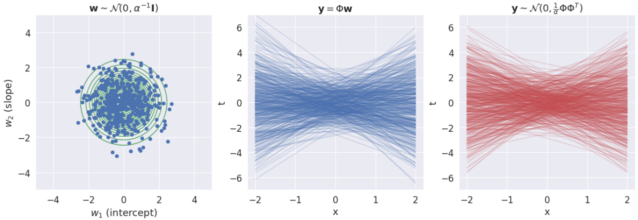

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A closer look at the covariance

- A prior on linear functions: $p(\boldsymbol{f}) = \mathcal{N}\left(\boldsymbol{f}|\mathbf{0}, \boldsymbol{K}\right)$, where $\boldsymbol{K} = \frac{1}{\alpha}\boldsymbol{\Phi}\boldsymbol{\Phi}^T$

- A closer look on the covariance between f_i and f_j

$$\boldsymbol{K}_{ij} = \text{cov}\left(y_i, y_j\right) = \text{cov}\left(f(\boldsymbol{x}_i), f(\boldsymbol{x}_j)\right)$$

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&= \frac{1}{\alpha} \phi(\boldsymbol{x}_i)^T \phi(\boldsymbol{x}_j) \\
&\equiv k(\boldsymbol{x}_i, \boldsymbol{x}_j)
\end{aligned}$$

A closer look at the covariance

- A prior on linear functions: $p(\boldsymbol{f}) = \mathcal{N}(\boldsymbol{f}|\boldsymbol{0}, \boldsymbol{K})$, where $\boldsymbol{K} = \frac{1}{\alpha}\boldsymbol{\Phi}\boldsymbol{\Phi}^T$

- A closer look on the covariance between f_i and f_j

$$
\begin{aligned}
\boldsymbol{K}_{ij} = \text{cov}\left(y_i, y_j\right) &= \text{cov}\left(f(\boldsymbol{x}_i), f(\boldsymbol{x}_j)\right) \\
&= \text{cov}\left(\phi(\boldsymbol{x}_i)^T\boldsymbol{w}, \phi(\boldsymbol{x}_j)^T\boldsymbol{w}\right) \\
&= \phi(\boldsymbol{x}_i)^T\text{cov}\left(\boldsymbol{w}, \boldsymbol{w}\right)\phi(\boldsymbol{x}_j) \\
&= \phi(\boldsymbol{x}_i)^T\mathbb{V}\left(\boldsymbol{w}\right)\phi(\boldsymbol{x}_j) \\
&= \phi(\boldsymbol{x}_i)^T\frac{1}{\alpha}\boldsymbol{I}\phi(\boldsymbol{x}_j) \\
&= \frac{1}{\alpha}\phi(\boldsymbol{x}_i)^T\phi(\boldsymbol{x}_j) \\
&\equiv k(\boldsymbol{x}_i, \boldsymbol{x}_j)
\end{aligned}
$$

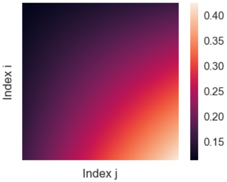
- What happens if we change the *covariance function* k?

Covariance functions

Linear

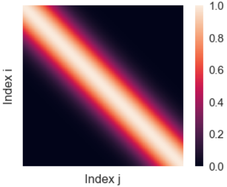
$$k\left(\boldsymbol{x}_i, \boldsymbol{x}_j\right) = \frac{1}{\alpha}\phi(\boldsymbol{x}_i)^T\phi(\boldsymbol{x}_j)$$

$\boldsymbol{K}$



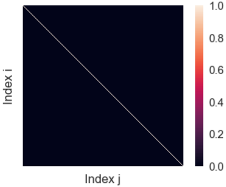
Squared exponential

$$k\left(\boldsymbol{x}_i, \boldsymbol{x}_j\right) = \exp\left(-\frac{\|\boldsymbol{x}_i - \boldsymbol{x}_j\|^2}{2\ell^2}\right)$$



White noise

$$k\left(\boldsymbol{x}_i, \boldsymbol{x}_j\right) = \delta\left(\boldsymbol{x}_i - \boldsymbol{x}_j\right)$$



Covariance functions

Linear | **Squared exponential** | **White noise**

$$k\left(\boldsymbol{x}_i, \boldsymbol{x}_j\right) = \frac{1}{\alpha}\phi(\boldsymbol{x}_i)^T\phi(\boldsymbol{x}_j)$$

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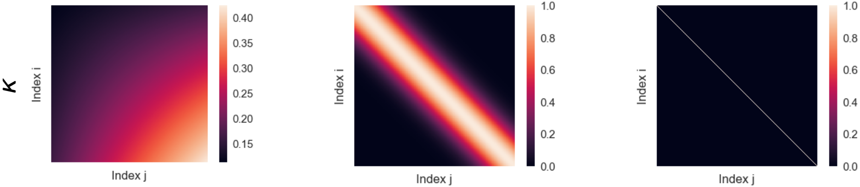

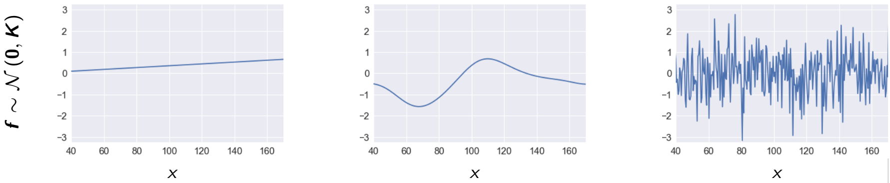

Covariance functions

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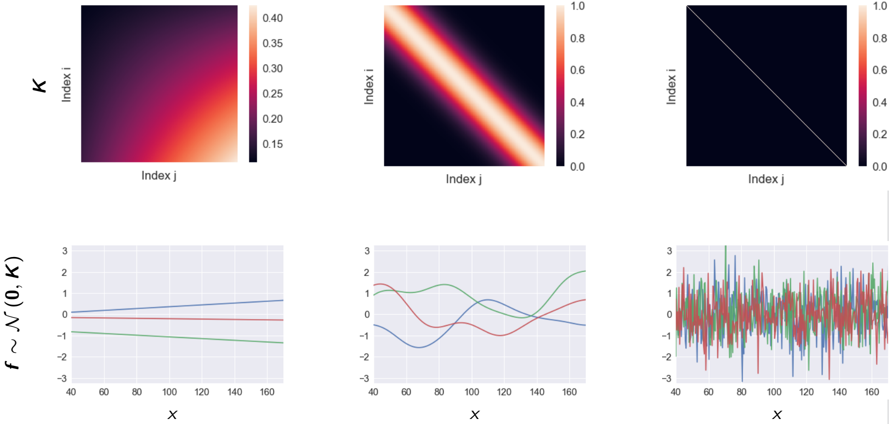

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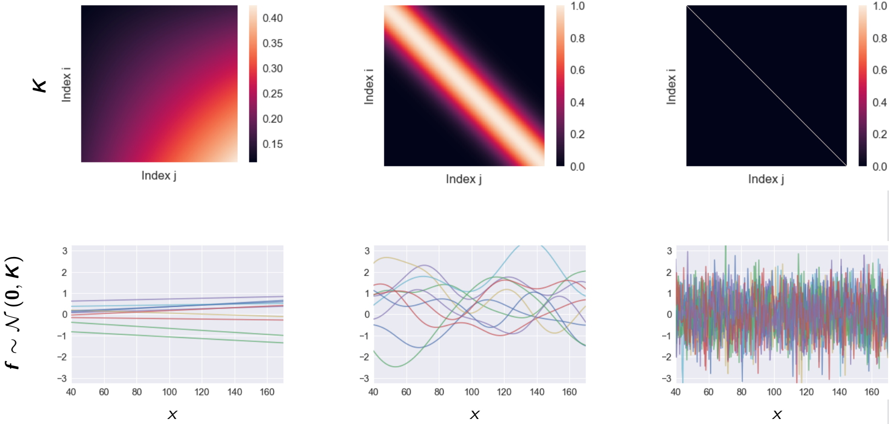
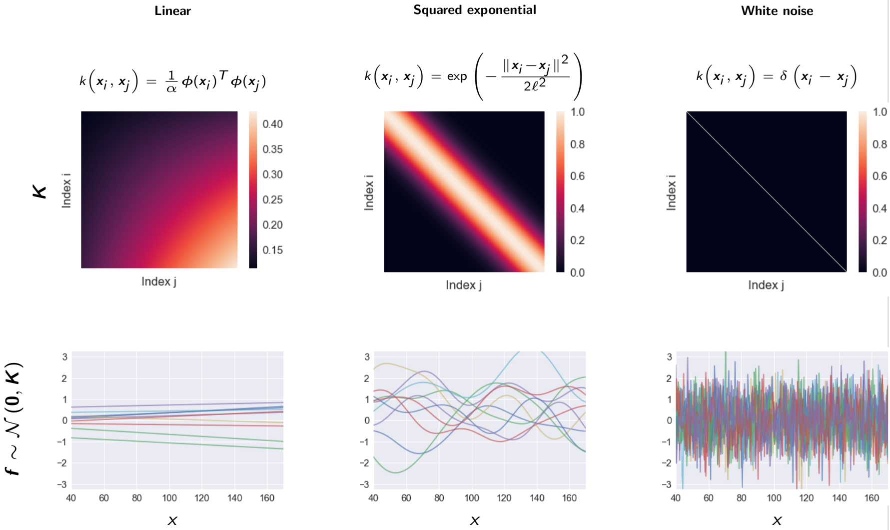


Covariance functions



The form of the covariance function determines the characteristics of the functions

The big picture: Summary so far

1. We started with a Bayesian linear model

$$p(\boldsymbol{y}, \boldsymbol{w}) = p(\boldsymbol{y}|\boldsymbol{w})p(\boldsymbol{w})$$

2. We introduced $\boldsymbol{f}$ into the model and marginalized over the weights $\boldsymbol{w}$

$$p(\boldsymbol{y}, \boldsymbol{f}) = \int p(\boldsymbol{y}|\boldsymbol{f})p(\boldsymbol{f}|\boldsymbol{w})p(\boldsymbol{w})\mathrm{d}\boldsymbol{w} = p(\boldsymbol{y}|\boldsymbol{f})p(\boldsymbol{f})$$

3. This gave us a prior for linear functions in function space $p(\boldsymbol{f})$, where the covariance function for $\boldsymbol{f}$ was given by

$$k(\boldsymbol{x}_i, \boldsymbol{x}_j) = \frac{1}{\alpha}\phi(\boldsymbol{x}_i)^T\phi(\boldsymbol{x}_j)$$

4. By changing the form of the covariance function $k(\boldsymbol{x}_i, \boldsymbol{x}_j)$, we can model much more interesting functions

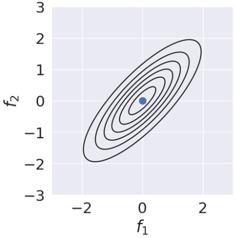
A visual approach towards Gaussian process regression

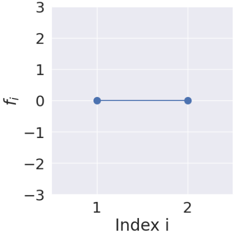
Visualizing samples in higher dimensions

- How can a multivariate normal distribution represent functions?

- Visualizations in 2D

$$\boldsymbol{K} = \begin{bmatrix} 1 & 0.8 \\ 0.8 & 1 \end{bmatrix}$$





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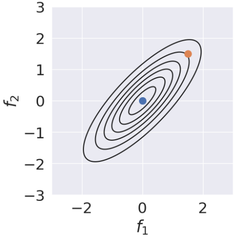

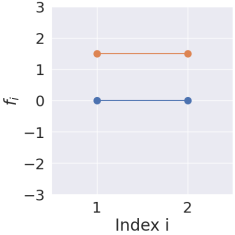

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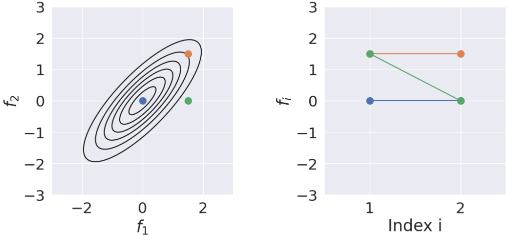

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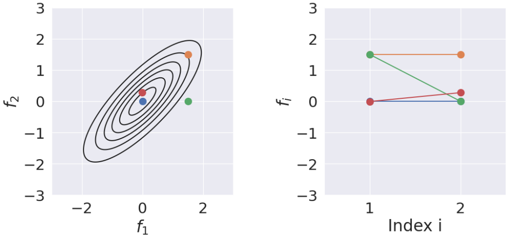

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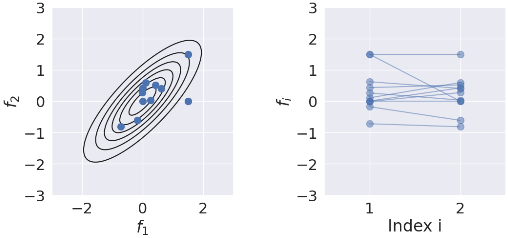
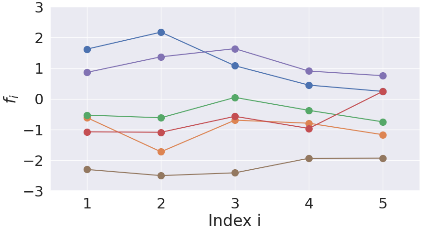


Visualizing samples in higher dimensions

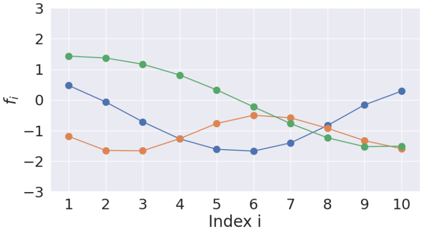
- Visualizations in 5D



$$\boldsymbol{K} = \begin{bmatrix} 1 & 0.8^1 & 0.8^2 & 0.8^3 & 0.8^4 \\ 0.8^1 & 1 & 0.8^1 & 0.8^2 & 0.8^3 \\ 0.8^2 & 0.8^1 & 1 & 0.8^1 & 0.8^2 \\ 0.8^3 & 0.8^2 & 0.8^1 & 1 & 0.8^1 \\ 0.8^4 & 0.8^3 & 0.8^2 & 0.8^1 & 1 \end{bmatrix}$$

Visualizing samples in higher dimensions

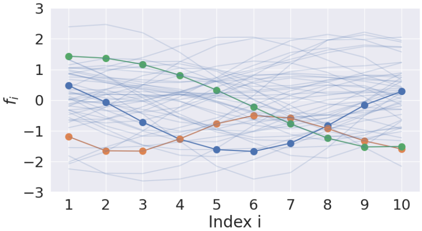
- Visualizations in 10D



$$\boldsymbol{K} = \begin{bmatrix} 1 & 0.8^1 & 0.8^2 & \dots & 0.8^9 \\ 0.8^1 & 1 & 0.8^1 & & \vdots \\ 0.8^2 & 0.8^1 & 1 & & \vdots \\ \vdots & & & \ddots & \vdots \\ 0.8^9 & \dots & \dots & \dots & 1 \end{bmatrix}$$

Visualizing samples in higher dimensions

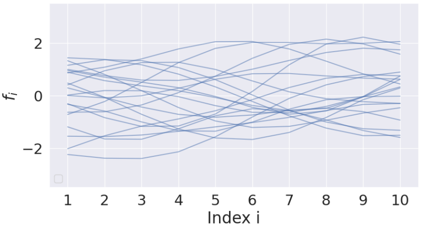
- Visualizations in 10D



$$\boldsymbol{K} = \begin{bmatrix} 1 & 0.8^1 & 0.8^2 & \dots & 0.8^9 \\ 0.8^1 & 1 & 0.8^1 & & \vdots \\ 0.8^2 & 0.8^1 & 1 & & \vdots \\ \vdots & & & \ddots & \vdots \\ 0.8^9 & \dots & \dots & \dots & 1 \end{bmatrix}$$

Conditioning

- So far, we have seen samples from the distribution $p(\boldsymbol{f}) = \mathcal{N}\left(\boldsymbol{f} \middle| \boldsymbol{0}, \boldsymbol{K}\right)$



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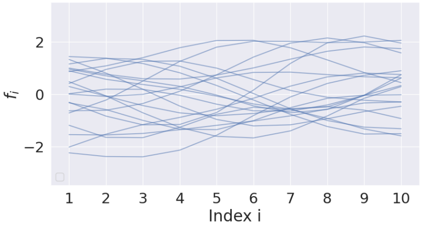

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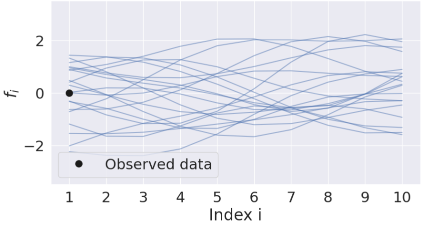
- We now observe $f_1 = 0$



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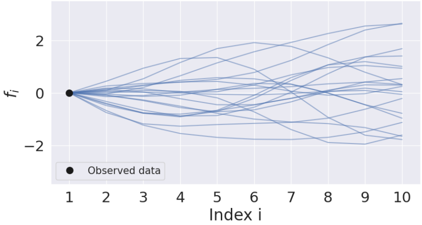

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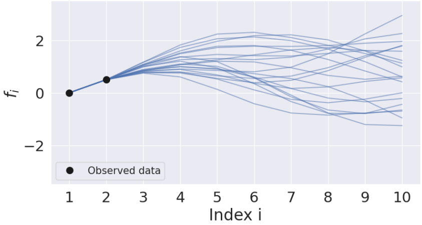

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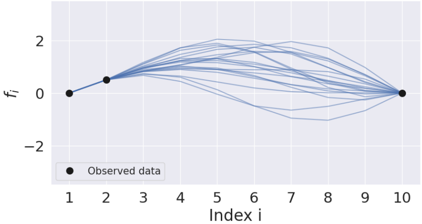

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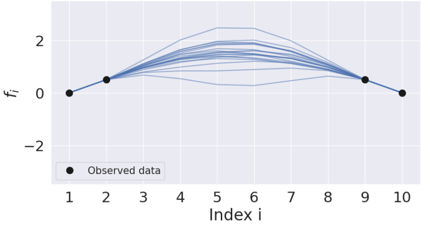

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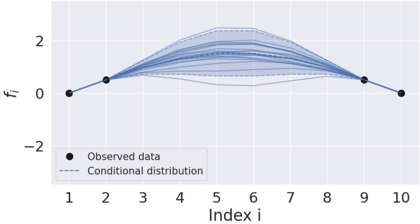
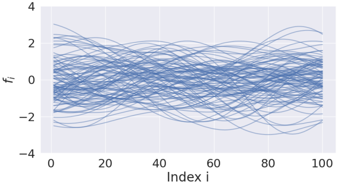


Conditioning II

- Let's now consider a case with $\boldsymbol{f} \in \mathbb{R}^{100}$ dimensions with 5 observations



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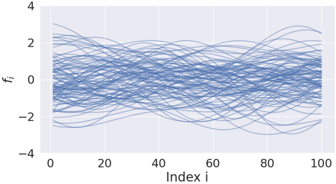

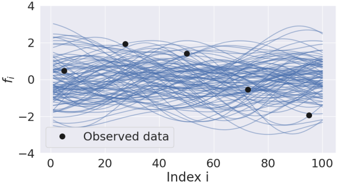

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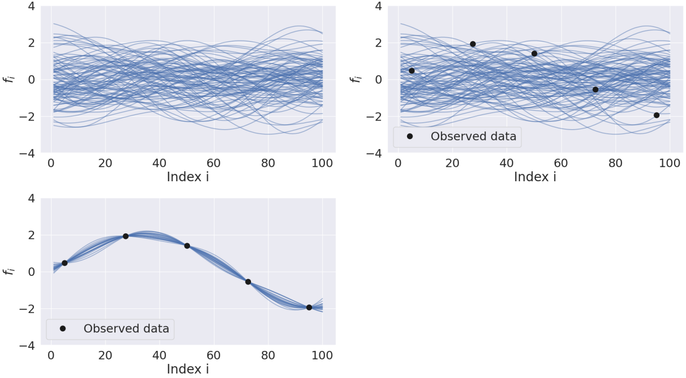

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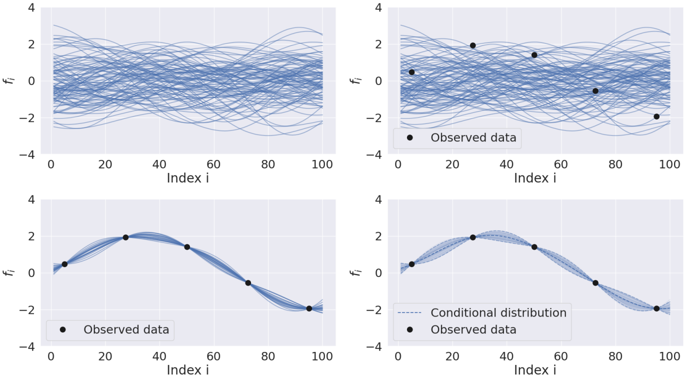

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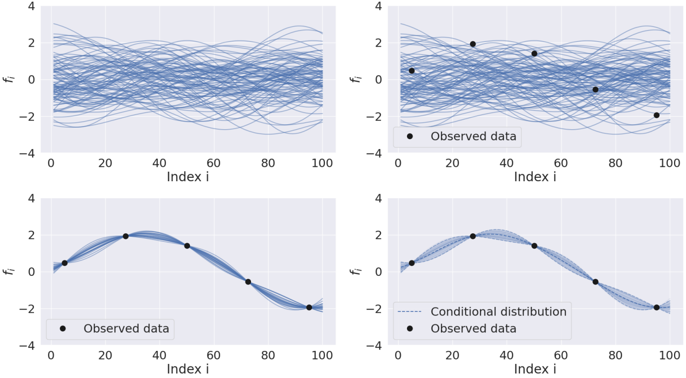

- Informally: We can think functions as vectors with infinite dimensions
- Using conditining in multivariate Gaussian distributions, we can do non-linear regression!

Formal definitions

Definition of the multivariate Gaussian distribution

A random vector $\boldsymbol{x} = [x_1, x_2, \cdots, x_D]$ is said to have the **multivariate Gaussian distribution** if all linear combinations of $\boldsymbol{x}$ are (univariate) Gaussian distributed:

$$f = a_1 x_1 + a_2 x_2 + \cdots + a_D x_D \sim \mathcal{N}(m, v)$$

for all $\boldsymbol{a} \in \mathbb{R}^D$

Definition of Gaussian process

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

Notation and characterization

- We'll use the notation

$$f(\boldsymbol{x}) \sim \mathcal{GP}\left(m(\boldsymbol{x}), k\left(\boldsymbol{x}, \boldsymbol{x}'\right)\right)$$

- A Gaussian process can be considered as a prior distribution over functions $f : \mathcal{X} \rightarrow \mathbb{R}$ (the domain $\mathcal{X}$ is typically $\mathbb{R}^D$)

- A Gaussian process is completely characterized by its mean function $m(\boldsymbol{x})$ and its covariance function $k\left(\boldsymbol{x}, \boldsymbol{x}'\right)$.

$$\begin{aligned} m(\boldsymbol{x}) &= \mathbb{E}\left[f(\boldsymbol{x})\right] \\ k\left(\boldsymbol{x}, \boldsymbol{x}'\right) &= \mathbb{E}\left[\left(f(\boldsymbol{x}) - m(\boldsymbol{x})\right)\left(f(\boldsymbol{x}') - m\left(\boldsymbol{x}'\right)\right)\right] \end{aligned}$$

- This means that $f(\boldsymbol{x})$ and $f(\boldsymbol{x}')$ are jointly Gaussian distributed with covariance $k\left(\boldsymbol{x}, \boldsymbol{x}'\right)$

- Not all functions are valid covariance functions - more on that later

Gaussian process regression

DTU

Recall: Linear Gaussian-systems in general (see Section 3.3 in Murphy1)

- For *linear* systems: the Gaussian distribution is *conjugate* to itself
- The *posterior* for a *linear* Gaussian model with Gaussian prior is also *Gaussian*

$$p(\boldsymbol{y}|\boldsymbol{z}) = \mathcal{N}(\boldsymbol{y}|\boldsymbol{W}\boldsymbol{z} + \boldsymbol{b}, \boldsymbol{\Sigma}_y) \qquad\qquad p(\boldsymbol{z}) = \mathcal{N}(\boldsymbol{z}|\boldsymbol{\mu}_z, \boldsymbol{\Sigma}_z)$$

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- The *joint* distribution $p(\boldsymbol{z}, \boldsymbol{y}) = \mathcal{N}\left(\begin{bmatrix}\boldsymbol{z}\\ \boldsymbol{y}\end{bmatrix} |\boldsymbol{\mu}, \boldsymbol{\Sigma}\right)$

$$\boldsymbol{\mu} = \begin{bmatrix}\boldsymbol{\mu}_z \\ \boldsymbol{W}\boldsymbol{\mu}_z + \boldsymbol{b}\end{bmatrix} \qquad \boldsymbol{\Sigma} = \begin{bmatrix}\boldsymbol{\Sigma}_z & \boldsymbol{\Sigma}_z\boldsymbol{W}^T \\ \boldsymbol{W}\boldsymbol{\Sigma}_Z & \boldsymbol{\Sigma}_y + \boldsymbol{W}\boldsymbol{\Sigma}_z\boldsymbol{W}^T\end{bmatrix}$$

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- The *posterior* distribution of $\boldsymbol{z}$ given $\boldsymbol{y}$

$$p(\boldsymbol{z}|\boldsymbol{y}) = \mathcal{N}\left(\boldsymbol{z}|\boldsymbol{\mu}_{z|y}, \boldsymbol{\Sigma}_{z|y}\right)$$
$$\boldsymbol{\Sigma}_{z|y}^{-1} = \boldsymbol{\Sigma}_z^{-1} + \boldsymbol{W}^T\boldsymbol{\Sigma}_y\boldsymbol{W}$$
$$\boldsymbol{\mu}_{z|y} = \boldsymbol{\Sigma}_{z|y}\left[\boldsymbol{W}^T\boldsymbol{\Sigma}_y^{-1}(\boldsymbol{y} - \boldsymbol{b}) + \boldsymbol{\Sigma}_z^{-1}\boldsymbol{\mu}_z\right]$$

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$$\boldsymbol{\Sigma}_{z|y}^{-1} = \boldsymbol{\Sigma}_z^{-1} + \boldsymbol{W}^T\boldsymbol{\Sigma}_y\boldsymbol{W}$$
$$\boldsymbol{\mu}_{z|y} = \boldsymbol{\Sigma}_{z|y}\left[\boldsymbol{W}^T\boldsymbol{\Sigma}_y^{-1}(\boldsymbol{y} - \boldsymbol{b}) + \boldsymbol{\Sigma}_z^{-1}\boldsymbol{\mu}_z\right]$$

- The *marginal* distribution $\boldsymbol{y}$

$$p(\boldsymbol{y}) = \mathcal{N}(\boldsymbol{y}|\boldsymbol{W}\boldsymbol{\mu}_z + \boldsymbol{b}, \boldsymbol{\Sigma}_y + \boldsymbol{W}\boldsymbol{\Sigma}_z\boldsymbol{W}^T)$$

Conditioning for multivariate Gaussians (Murphy1 Section 3.2.3)

- Suppose $\boldsymbol{y} = (\boldsymbol{y}_1, \boldsymbol{y}_2)$ is jointly Gaussian $\mathcal{N}(\boldsymbol{y}|\boldsymbol{\mu}, \boldsymbol{\Sigma})$ with mean and covariance

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

- The precision matrix $\boldsymbol{\Lambda}$

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

- The marginals are given by

$$\begin{aligned} p(\boldsymbol{y}_1) &= \mathcal{N}(\boldsymbol{y}_1|\boldsymbol{\mu}_1, \boldsymbol{\Sigma}_{11}) \\ p(\boldsymbol{y}_2) &= \mathcal{N}(\boldsymbol{y}_1|\boldsymbol{\mu}_2, \boldsymbol{\Sigma}_{22}) \end{aligned}$$

- The conditional

$$\begin{aligned} p(\boldsymbol{y}_1|\boldsymbol{y}_2) &= \mathcal{N}(\boldsymbol{y}_1|\boldsymbol{\mu}_{1|2}, \boldsymbol{\Sigma}_{1|2}) \\ \boldsymbol{\mu}_{1|2} &= \boldsymbol{\mu}_1 + \boldsymbol{\Sigma}_{12}\boldsymbol{\Sigma}_{22}^{-1}(\boldsymbol{y}_2 - \boldsymbol{\mu}_2) \\ \boldsymbol{\Sigma}_{1|2} &= \boldsymbol{\Sigma}_{11} - \boldsymbol{\Sigma}_{12}\boldsymbol{\Sigma}_{22}^{-1}\boldsymbol{\Sigma}_{21} = \boldsymbol{\Lambda}_{11}^{-1} \end{aligned}$$

Gaussian process regression I

- Our model

$$y_n = f(\boldsymbol{x}_n) + e_n$$

Gaussian process regression I

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- Likelihood for all datapoints (assuming homoscedastic noise)

$$p(\boldsymbol{y}|\boldsymbol{f}) = \prod_{n=1}^{N} \mathcal{N}(y_n|f_n, \beta^{-1}) = \mathcal{N}(\boldsymbol{y}|\boldsymbol{f}, \beta^{-1}\boldsymbol{I})$$

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- We impose a prior directly on the *function values* $\boldsymbol{f} = \begin{bmatrix} f(\boldsymbol{x}_1) & f(\boldsymbol{x}_2) & \dots & f(\boldsymbol{x}_N) \end{bmatrix}$

$$p(\boldsymbol{f}) = \mathcal{N}(\boldsymbol{f}|\boldsymbol{0}, \boldsymbol{K}) \qquad \text{for} \qquad (\boldsymbol{K})_{ij} = k(\boldsymbol{x}_i, \boldsymbol{x}_j)$$

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- Two-step strategy

  1. Calculate the joint Gaussian distribution $p(\boldsymbol{y}, y^*|\boldsymbol{x}^*)$
  2. Use rule for conditioning in Gaussian distributions to compute $p(y^*|\boldsymbol{y}, \boldsymbol{x}^*)$

Gaussian process regression II

- Recall: General Linear Gaussian systems (Murphy1 page 86-77).
  If

$$p(\mathbf{z}) = \mathcal{N}(\boldsymbol{z}|\boldsymbol{\mu}_z, \Sigma_z)$$
$$p(\boldsymbol{y}|\boldsymbol{z}) = \mathcal{N}(\boldsymbol{y}|\boldsymbol{W}\boldsymbol{z} + \boldsymbol{b}, \boldsymbol{\Sigma}_y)$$

  then

$$p(\boldsymbol{y}) = \int p(\boldsymbol{y}|\boldsymbol{z})p(\boldsymbol{z})\mathbf{d}\boldsymbol{z} = \mathcal{N}(\boldsymbol{y}|\boldsymbol{W}\boldsymbol{\mu}_z + \boldsymbol{b}, \boldsymbol{\Sigma}_y + \boldsymbol{W}\boldsymbol{\Sigma}_z\boldsymbol{W}^T)$$

- We can compute the marginal distribution of $\boldsymbol{y}$ using the *sum rule*

$$\begin{aligned} p(\boldsymbol{y}) &= \int p(\boldsymbol{y}|\boldsymbol{f})p(\boldsymbol{f})\mathrm{d}\boldsymbol{f} \\ &= \int \mathcal{N}(\boldsymbol{y}|\boldsymbol{f}, \beta^{-1}\boldsymbol{I})\mathcal{N}(\boldsymbol{f}|\mathbf{0}, \boldsymbol{K})\mathrm{d}\boldsymbol{f} \\ &= \mathcal{N}(\boldsymbol{y}|\ ?\ ,\ ?\ ) \end{aligned}$$

- Spend 5 minutes calculating the mean and variance of $p(\boldsymbol{y})$

$$p(\boldsymbol{y}) = \mathcal{N}(\boldsymbol{y}|\ ?\ ,\ ?\ )$$

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Gauasian process regression III

- The distribution of $\boldsymbol{y} \in \mathbf{R}^N$

$$p(\boldsymbol{y}) = \mathcal{N}(\boldsymbol{y}|\mathbf{0}, \boldsymbol{C}) \qquad \text{for} \qquad \boldsymbol{C} = \boldsymbol{K} + \beta^{-1}\boldsymbol{I}$$

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Example

Key equations for Gaussian process regression

$$p(y^*|\boldsymbol{y}) = \mathcal{N}\left(y^*\middle|\mu_{y^*|\boldsymbol{y}}, \sigma^2_{y^*|\boldsymbol{y}}\right)$$

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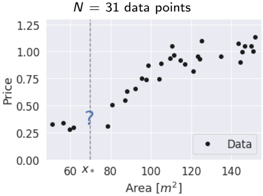

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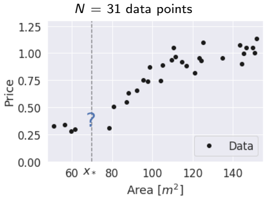
- Predict $y^* = f(x_*) + e^*$ for test input $x_* = 70$



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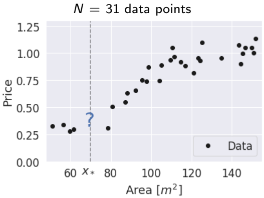

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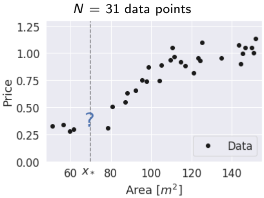

Example

Key equations for Gaussian process regression

$$p(y^*|\boldsymbol{y}) = \mathcal{N}\left(y^*|\mu_{y^*|\boldsymbol{y}}, \sigma^2_{y^*|\boldsymbol{y}}\right)$$

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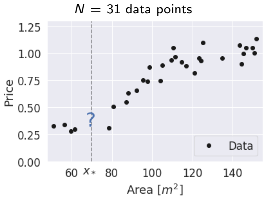

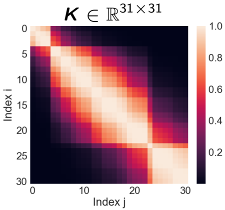

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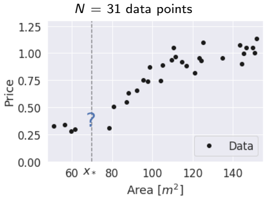

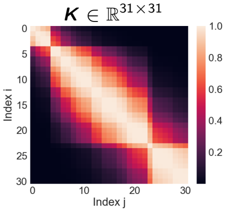

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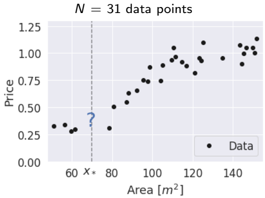

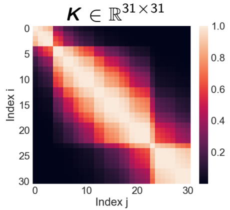

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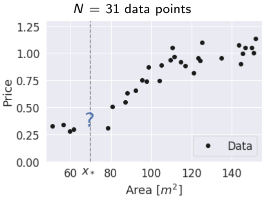

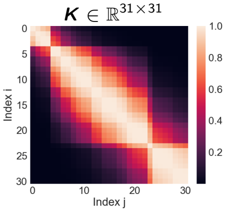

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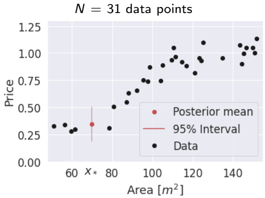

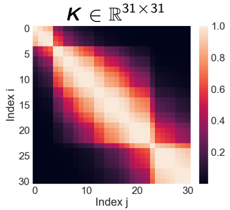

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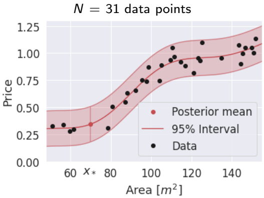

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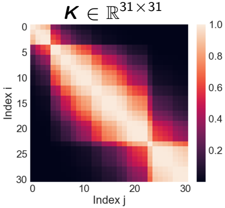

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Gaussian process intuition

- Gaussian process implements the assumption

$$\boldsymbol{x} \approx \boldsymbol{x}' \quad \Rightarrow \quad f(\boldsymbol{x}) \approx f(\boldsymbol{x}')$$

- In words: If the inputs are similar, the outputs should be similar as well.

- Using the squared exponential covariance function as example

$$k(\boldsymbol{x}, \boldsymbol{x}') = \exp\left(-\frac{\|\boldsymbol{x} - \boldsymbol{x}'\|^2}{2}\right)$$

- Then covariance between $f(\boldsymbol{x})$ and $f(\boldsymbol{x})'$ is given by

$$\mathrm{cov}\left[f(\boldsymbol{x}), f(\boldsymbol{x}')\right] = k(\boldsymbol{x}, \boldsymbol{x}') = \exp\left(-\frac{\|\boldsymbol{x} - \boldsymbol{x}'\|^2}{2}\right)$$

- Note: the covariance between outputs are given in terms of the inputs

True or false?

Key equations for Gaussian process regression

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True or false?

- Spend 5 minutes on the DTU Learn quiz: "Lecture 5: Key equations for GP Regression."

Covariance functions

Covariance functions

- A covariance function $k : \mathcal{X} \times \mathcal{X} \rightarrow \mathbb{R}$ maps a pair of inputs $\boldsymbol{x}_1, \boldsymbol{x}_2 \in \mathcal{X}$ from some input space $\mathcal{X}$ to the real line $\mathbb{R}$

- Recall: the covariance / kernel matrix is given by

$$\boldsymbol{K}_{ij} = \operatorname{cov}\left(f(\boldsymbol{x}_i), f(\boldsymbol{x})_j\right) = k\left(\boldsymbol{x}_i, \boldsymbol{x}_j\right)$$

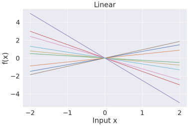
- Covariance functions must be symmetric & Positive Semi-Definite such that

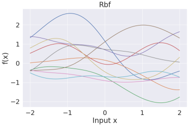
$$\text{(Symmetric)} \quad \boldsymbol{K} = \boldsymbol{K}^T$$

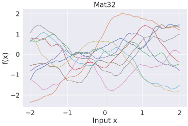
$$\text{(PSD)} \quad \forall \boldsymbol{x} \neq 0 : \quad \boldsymbol{x}^T \boldsymbol{K} \boldsymbol{x} \geq 0$$

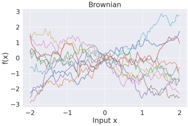
- Must hold for all possible data sets $\{\boldsymbol{x}_n\}_{n=1}^N \subset \mathcal{X}$ in the input space $\mathcal{X}$

- Covariance functions as prior information





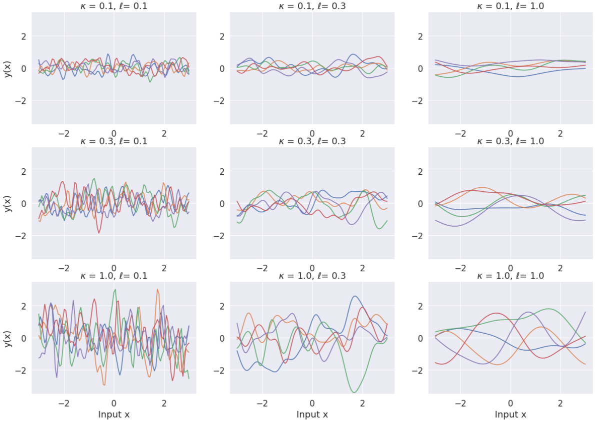




The squared exponential kernel - prior samples

$$k(\boldsymbol{x}, \boldsymbol{x}') = \kappa^2 \exp\left[-\frac{\|\boldsymbol{x} - \boldsymbol{x}'\|_2^2}{2\ell^2}\right]$$

Parameter ℓ is the called the *lengthscale* and parameter κ is the called the *magnitude*



Constructing new kernels from old ones

Techniques for Constructing New Kernels.

Given valid kernels $k_1(\mathbf{x}, \mathbf{x}')$ and $k_2(\mathbf{x}, \mathbf{x}')$, the following new kernels will also be valid:

$$\begin{aligned}
k(\mathbf{x}, \mathbf{x}') &= ck_1(\mathbf{x}, \mathbf{x}') && (6.13)\\
k(\mathbf{x}, \mathbf{x}') &= f(\mathbf{x})k_1(\mathbf{x}, \mathbf{x}')f(\mathbf{x}') && (6.14)\\
k(\mathbf{x}, \mathbf{x}') &= q\left(k_1(\mathbf{x}, \mathbf{x}')\right) && (6.15)\\
k(\mathbf{x}, \mathbf{x}') &= \exp\left(k_1(\mathbf{x}, \mathbf{x}')\right) && (6.16)\\
k(\mathbf{x}, \mathbf{x}') &= k_1(\mathbf{x}, \mathbf{x}') + k_2(\mathbf{x}, \mathbf{x}') && (6.17)\\
k(\mathbf{x}, \mathbf{x}') &= k_1(\mathbf{x}, \mathbf{x}')k_2(\mathbf{x}, \mathbf{x}') && (6.18)\\
k(\mathbf{x}, \mathbf{x}') &= k_3\left(\boldsymbol{\phi}(\mathbf{x}), \boldsymbol{\phi}(\mathbf{x}')\right) && (6.19)\\
k(\mathbf{x}, \mathbf{x}') &= \mathbf{x}^{\mathrm{T}}\mathbf{A}\mathbf{x}' && (6.20)\\
k(\mathbf{x}, \mathbf{x}') &= k_a(\mathbf{x}_a, \mathbf{x}_a') + k_b(\mathbf{x}_b, \mathbf{x}_b') && (6.21)\\
k(\mathbf{x}, \mathbf{x}') &= k_a(\mathbf{x}_a, \mathbf{x}_a')k_b(\mathbf{x}_b, \mathbf{x}_b') && (6.22)
\end{aligned}$$

where $c > 0$ is a constant, $f(\cdot)$ is any function, $q(\cdot)$ is a polynomial with nonnegative coefficients, $\boldsymbol{\phi}(\mathbf{x})$ is a function from $\mathbf{x}$ to $\mathbb{R}^M$, $k_3(\cdot, \cdot)$ is a valid kernel in $\mathbb{R}^M$, $\mathbf{A}$ is a symmetric positive semidefinite matrix, $\mathbf{x}_a$ and $\mathbf{x}_b$ are variables (not necessarily disjoint) with $\mathbf{x} = (\mathbf{x}_a, \mathbf{x}_b)$, and k_a and k_b are valid kernel functions over their respective spaces.

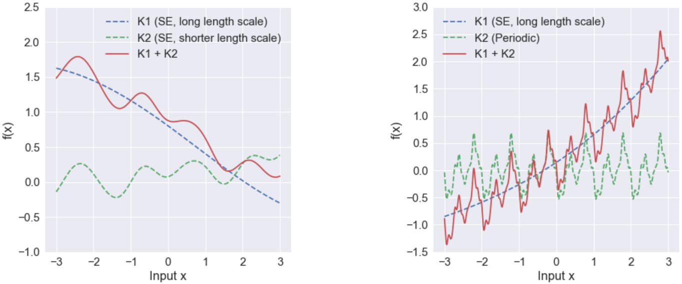
From Chris Bishops book: `https://www.microsoft.com/en-us/research/people/cmbishop`

Additive kernels

- Adding two SEs kernels to model long term trends (long length scale) and short term fluctuations (short length scale)

$$k(\boldsymbol{x}, \boldsymbol{x}') = \kappa_1^2 \exp\left[-\frac{\|\boldsymbol{x} - \boldsymbol{x}'\|_2^2}{2\ell_1^2}\right] + \kappa_2^2 \exp\left[-\frac{\|\boldsymbol{x} - \boldsymbol{x}'\|_2^2}{2\ell_2^2}\right]$$

- Adding SE and period kernels to model long term trends (long length scale) and periodic fluctuations



Hyperparameters and the marginal likelihood

The marginal likelihood I

- Let $\boldsymbol{\theta}$ denote all hyperparameters, then marginal likelihood for Gaussian likelihood

$$
\begin{aligned}
p(\boldsymbol{y}\big|\boldsymbol{\theta}) &= \int p(\boldsymbol{y}|\boldsymbol{f})p(\boldsymbol{f}\big|\boldsymbol{\theta}_K)\mathrm{d}\boldsymbol{f} \\
&= \int \mathcal{N}\left(\boldsymbol{y}\big|\boldsymbol{f}, \beta^{-1}\boldsymbol{I}\right)\mathcal{N}\left(\boldsymbol{f}\big|\boldsymbol{0}, \boldsymbol{K}\right)\mathrm{d}\boldsymbol{f} \\
&= \mathcal{N}\left(\boldsymbol{y}\big|\boldsymbol{0}, \beta^{-1}\boldsymbol{I} + \boldsymbol{K}\right)
\end{aligned}
$$

- We can tune the hyperparameters of the model by optimizing the marginal likelihood as we did for linear regresssion

  1. Hyperparameters of the likelihood (e.g β or σ)
  2. Hyperparameters of the kernel $\boldsymbol{\theta}_K$ (e.g. lengthscales and magnitudes)

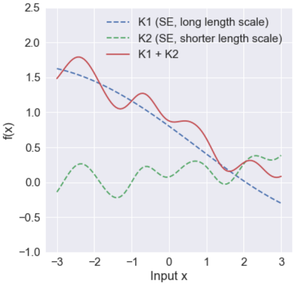
- In practice, we compute the gradient of $p(\boldsymbol{y}\big|\boldsymbol{\theta})$ wrt. $\boldsymbol{\theta}$ and use numerical optimization

The marginal likelihood II

- Suppose we have 5 hyperparameters in total

$$\boldsymbol{\theta} = \{\sigma, \kappa_1, \ell_1, \kappa_2, \ell_2\}$$

- Suppose we want to estimate those using 10-fold cross-validation and test out 10 values for each hyperparameter. How many times do we need to train the model?



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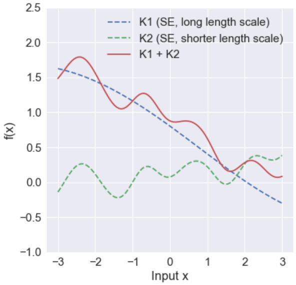
$$10 \cdot 10^5 = 10^6$$



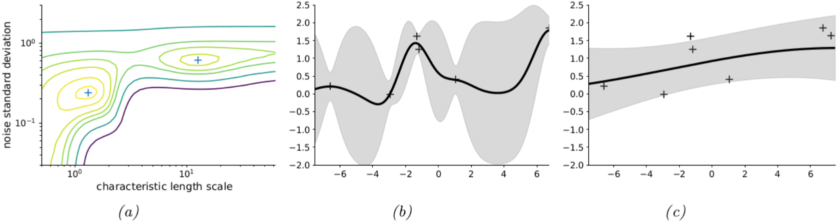
The marginal likelihood III

- The gradients of the marginal likelihood wrt. hyperparameters are given by

$$\frac{\partial}{\partial \theta_j} \log p(\boldsymbol{y}|\boldsymbol{\theta}) = \frac{1}{2}\mathrm{tr}\left((\boldsymbol{\alpha}\boldsymbol{\alpha}^T - \boldsymbol{K}^{-1}) \frac{\partial \boldsymbol{K}}{\partial \theta_j} \right),$$

  where $\boldsymbol{\alpha} = \boldsymbol{K}^{-1}\boldsymbol{y}$ and $\frac{\partial \boldsymbol{K}}{\partial \theta_j}$ depends on the specific choice of kernel.

- $\log p(\boldsymbol{y}|\boldsymbol{\theta})$ is also multimodal wrt. $\boldsymbol{\theta}$



From the Murphy1 book (p. 578)

The marginal likelihood: numerics

- In practice, we should avoid computing determinants and inverses!

$$\ln p(\boldsymbol{y}|\boldsymbol{\theta}) = -\frac{N}{2}\ln(2\pi) - \frac{1}{2}\ln\left|\beta^{-1}\boldsymbol{I} + \boldsymbol{K}\right| - \frac{1}{2}\boldsymbol{y}^T\left(\beta^{-1}\boldsymbol{I} + \boldsymbol{K}\right)^{-1}\boldsymbol{y}$$

- In numpy: $\left|0.1\boldsymbol{I}_{400\times 400}\right| = 0.0$, but $\ln\left|0.1\boldsymbol{I}_{400\times 400}\right| = -2302.58$ and $\exp(-2302.58) > 0$

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$$\ln\left|\boldsymbol{C}\right| =$$

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$$\ln\left|\boldsymbol{C}\right| = \ln\left|\boldsymbol{L}\boldsymbol{L}^T\right| = \ln\left|\boldsymbol{L}\right| \cdot \left|\boldsymbol{L}^T\right|$$

The marginal likelihood: numerics

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- Step 1: Compute Cholesky factorization of $\boldsymbol{C} = \beta^{-1}\boldsymbol{I} + \boldsymbol{K}$ such that $\boldsymbol{C} = \boldsymbol{L}\boldsymbol{L}^T$

- Step 2: Compute the log determinant term as follows

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- Step 4: Sum components

$$\ln p(\boldsymbol{y}|\boldsymbol{\theta}) = -\frac{N}{2}\ln(2\pi) - \frac{1}{2}2\sum_{n=1}^{N}\ln\boldsymbol{L}_{nn} - \frac{1}{2}\boldsymbol{v}^T\boldsymbol{v}$$

- Note that we never compute the determinant or the inverse of $\boldsymbol{C}$ directly!

Computational complexity of Gaussian Processes

Key equations for Gaussian process regression

$$p(y^*|\boldsymbol{y}) = \mathcal{N}\left(y^* \middle| \mu_{y^*|\boldsymbol{y}}, \sigma^2_{y^*|\boldsymbol{y}}\right)$$
$$\mu_{y^*|\boldsymbol{y}} = \boldsymbol{k}\left(\boldsymbol{K} + \beta^{-1}\boldsymbol{I}\right)^{-1}\boldsymbol{y}$$
$$\sigma^2_{y^*|\boldsymbol{y}} = c - \boldsymbol{k}\left(\boldsymbol{K} + \sigma^2\boldsymbol{I}\right)^{-1}\boldsymbol{k}^T$$

- Gaussian processes are *non-parametric models*
- Recall: If $\boldsymbol{A} \in \mathbb{R}^{N\times M}$ and $\boldsymbol{b} \in \mathbb{R}^M$, then the cost of computing $\boldsymbol{Ab}$ is $\mathcal{O}(NM)$
- Recall: If $\boldsymbol{C} \in \mathbb{R}^{N\times N}$, then the cost of computing $\boldsymbol{C}^{-1}$ is $\mathcal{O}\left(N^3\right)$
- What is computational complexity for computing the posterior distribution for 1 test point based on a data set with N observations? $\mathcal{O}(N^3)$
- What about the memory footprint? $\mathcal{O}(N^2)$