Advanced Statistical Inference
Gaussian Processes

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Suggested readings

Gaussian Processes for Machine Learning
Carl E. Rasmussen and Christopher K. I. Williams

Pattern Recognition and Machine Learning
C. Bishop

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Weight Space View
Function Space View
Example
Optimizing Kernel Parameters

Gaussian Processes

- Linear models requires specifying a set of basis functions
  - Polynomials, Trigonometric, ...??
- Can we use Bayesian inference to let data tell us this?
- Gaussian Processes work implicitly with an infinite set of basis functions and learn a probabilistic combination of these

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Gaussian Processes

Gaussian Processes can be explained in two ways
- Weight Space View
  - Bayesian linear regression with infinite basis functions
- Function Space View
  - Defined as priors over functions

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Gaussian Processes

Gaussian Processes can be explained in two ways

- **Weight Space View**
  - **Bayesian linear regression with infinite basis functions**
- Function Space View
  - Defined as priors over functions

Bayesian Linear Regression - recap

- Modeling observations as noisy realizations of a linear combination of the features:

$$p(\mathbf{t}|\mathbf{w}, \mathbf{X}, \sigma^2) = \mathcal{N}(\mathbf{X}\mathbf{w}, \sigma^2 \mathbf{I})$$

- Gaussian prior over model parameters:

$$p(\mathbf{w}) = \mathcal{N}(\mathbf{0}, \mathbf{S})$$

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Bayesian Linear Regression - recap

- Posterior **must be** Gaussian

$$p(\mathbf{w}|\mathbf{X}, \mathbf{t}, \sigma^2) = \mathcal{N}(\boldsymbol{\mu}, \boldsymbol{\Sigma})$$

- Covariance:

$$\boldsymbol{\Sigma} = \left(\frac{1}{\sigma^2} \mathbf{X}^{\mathsf{T}} \mathbf{X} + \mathbf{S}^{-1} \right)^{-1}$$

- Mean:

$$\boldsymbol{\mu} = \frac{1}{\sigma^2} \boldsymbol{\Sigma} \mathbf{X}^{\mathsf{T}} \mathbf{t}$$

- Predictions

$$p(t_* | \mathbf{X}, \mathbf{t}, \mathbf{x}_*, \sigma^2) = \mathcal{N}(\mathbf{x}_*^{\mathsf{T}} \boldsymbol{\mu}, \sigma^2 + \mathbf{x}_*^{\mathsf{T}} \boldsymbol{\Sigma} \mathbf{x}_*)$$

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Introducing basis functions

- Imagine transforming the inputs using a set of D functions

$$\mathbf{x} \rightarrow \boldsymbol{\phi}(\mathbf{x}) = (\phi_1(\mathbf{x}), \ldots, \phi_D(\mathbf{x}))^{\top}$$

- The functions $\phi_1(\mathbf{x})$ are also known as basis functions
- Define:

$$\boldsymbol{\Phi} = \begin{bmatrix} \phi_1(\mathbf{x}_1) & \ldots & \phi_D(\mathbf{x}_1) \\ \vdots & \ddots & \vdots \\ \phi_1(\mathbf{x}_N) & \ldots & \phi_D(\mathbf{x}_N) \end{bmatrix}$$

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Introducing basis functions

- Applying Bayesian Linear Regression on the transformed features gives

$$p(\mathbf{w}|\mathbf{X}, \mathbf{t}, \sigma^2) = \mathcal{N}(\boldsymbol{\mu}, \boldsymbol{\Sigma})$$

- Covariance:

$$\boldsymbol{\Sigma} = \left(\frac{1}{\sigma^2} \boldsymbol{\Phi}^{\mathrm{T}} \boldsymbol{\Phi} + \mathbf{S}^{-1} \right)^{-1}$$

- Mean:

$$\boldsymbol{\mu} = \frac{1}{\sigma^2} \boldsymbol{\Sigma} \boldsymbol{\Phi}^{\mathrm{T}} \mathbf{t}$$

- Predictions:

$$p(t_*|\mathbf{X}, \mathbf{t}, \mathbf{x}_*, \sigma^2) = \mathcal{N}(\phi_*^{\mathrm{T}} \boldsymbol{\mu}, \sigma^2 + \phi_*^{\mathrm{T}} \boldsymbol{\Sigma} \phi_*)$$

Bayesian Linear Regression as a Kernel Machine

- We are going to show that predictions can be expressed exclusively in terms of scalar products as follows

$$k(\mathbf{x}, \mathbf{x}') = \psi(\mathbf{x})^{\top} \psi(\mathbf{x}')$$

- This allows us to work with either $k(\cdot, \cdot)$ or $\psi(\cdot)$
- Why is this useful??

Bayesian Linear Regression as a Kernel Machine

- Working with $\psi(\cdot)$ costs $O(D^2)$ storage, $O(D^3)$ time
- Working with $k(\cdot, \cdot)$ costs $O(N^2)$ storage, $O(N^3)$ time
- Pick the one that makes computations faster ... or
- What if we could pick $k(\cdot, \cdot)$ so that $\psi(\cdot)$ is infinite dimensional?

Kernels

- It is possible to show that for

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

there exists a corresponding $\psi(\cdot)$ that is infinite dimensional!!!
- There are other kernels satisfying this property

Kernels

Proof that the Gaussian kernel induces an infinite dimensional $\psi(\cdot)$

- For simplicity consider one dimensional inputs x, y
- Expand the Gaussian kernel $k(x, y)$ as

$$\exp\left(-\frac{(x-y)^2}{2}\right) = \exp\left(-\frac{x^2}{2}\right)\exp\left(-\frac{y^2}{2}\right)\exp(xy)$$

- Focusing on the last term and applying the Taylor expansion of the $\exp(\cdot)$ function

$$\exp(xy) = 1 + (xy) + \frac{(xy)^2}{2!} + \frac{(xy)^3}{3!} + \frac{(xy)^4}{4!} + \dots$$

Kernels

Proof that the Gaussian kernel induces an infinite dimensional $\psi(\cdot)$

- Define the infinite dimensional mapping

$$\psi(x) = \exp\left(-\frac{x^2}{2}\right)\left(1, x, \frac{x^2}{\sqrt{2!}}, \frac{x^3}{\sqrt{3!}}, \frac{x^4}{\sqrt{4!}}, \dots\right)^{\top}$$

- It is easy to verify that

$$k(x, y) = \exp\left(-\frac{(x-y)^2}{2}\right) = \psi(x)^{\top}\psi(y)$$

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Bayesian Linear Regression as a Kernel Machine

Proof

- To show that Bayesian Linear Regression can be formulated through scalar products only, we need Woodbury identity:

$$(A + UCV)^{-1} = A^{-1} - A^{-1}U(C^{-1} + VA^{-1}U)^{-1}VA^{-1}$$

- Do not memorize this!

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Bayesian Linear Regression as a Kernel Machine

Proof

- Woodbury identity:

$$(A + UCV)^{-1} = A^{-1} - A^{-1}U(C^{-1} + VA^{-1}U)^{-1}VA^{-1}$$

- We can rewrite:

$$\begin{aligned}\mathbf{\Sigma} &= \left(\frac{1}{\sigma^2}\mathbf{\Phi}^{\mathrm{T}}\mathbf{\Phi} + \mathbf{S}^{-1}\right)^{-1} \\ &= \mathbf{S} - \mathbf{S}\mathbf{\Phi}^{\mathrm{T}}\left(\sigma^2\mathbf{I} + \mathbf{\Phi}\mathbf{S}\mathbf{\Phi}^{\mathrm{T}}\right)^{-1}\mathbf{\Phi}\mathbf{S}\end{aligned}$$

- We set $A = \mathbf{S}$, $U = V^{\top} = \mathbf{\Phi}^{\mathrm{T}}$, and $C = \frac{1}{\sigma^2}\mathbf{I}$

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Bayesian Linear Regression as a Kernel Machine

Proof

- Mean and variance of the predictions:

$$p(t_* | \mathbf{X}, \mathbf{t}, \mathbf{x}_*, \sigma^2) = \mathcal{N}(\phi_*^{\mathrm{T}} \boldsymbol{\mu}, \sigma^2 + \phi_*^{\mathrm{T}} \boldsymbol{\Sigma} \phi_*)$$

- Rewrite the variance:

$$\begin{aligned} \sigma^2 &+ \phi_*^{\mathrm{T}} \boldsymbol{\Sigma} \phi_* = \\ \sigma^2 &+ \phi_*^{\mathrm{T}} \mathbf{S} \phi_* - \phi_*^{\mathrm{T}} \mathbf{S} \boldsymbol{\Phi}^{\mathrm{T}} \left(\sigma^2 \mathbf{I} + \boldsymbol{\Phi} \mathbf{S} \boldsymbol{\Phi}^{\mathrm{T}} \right)^{-1} \boldsymbol{\Phi} \mathbf{S} \phi_* \end{aligned}$$

... continued

Bayesian Linear Regression as a Kernel Machine

Proof

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- Mean and variance of the predictions:

$$p(t_* | \mathbf{X}, \mathbf{t}, \mathbf{x}_*, \sigma^2) = \mathcal{N}(\phi_*^{\mathrm{T}} \boldsymbol{\mu}, \sigma^2 + \phi_*^{\mathrm{T}} \boldsymbol{\Sigma} \phi_*)$$

- Rewrite the variance:

$$\begin{aligned} \sigma^2 &+ \phi_*^{\mathrm{T}} \mathbf{S} \phi_* - \phi_*^{\mathrm{T}} \mathbf{S} \boldsymbol{\Phi}^{\mathrm{T}} \left(\sigma^2 \mathbf{I} + \boldsymbol{\Phi} \mathbf{S} \boldsymbol{\Phi}^{\mathrm{T}} \right)^{-1} \boldsymbol{\Phi} \mathbf{S} \phi_* = \\ \sigma^2 &+ k_{**} - \mathbf{k}_*^{\mathrm{T}} \left(\sigma^2 \mathbf{I} + \mathbf{K} \right)^{-1} \mathbf{k}_* \end{aligned}$$

- Where the mapping defining the kernel is

$$\psi(\mathbf{x}) = \mathbf{S}^{1/2} \phi(\mathbf{x})$$

and

$$\begin{aligned} k_{**} &= k(\mathbf{x}_*, \mathbf{x}_*) = \psi(\mathbf{x}_*)^{\mathrm{T}} \psi(\mathbf{x}_*) \\ (\mathbf{k}_*)_i &= k(\mathbf{x}_*, \mathbf{x}_i) = \psi(\mathbf{x}_*)^{\mathrm{T}} \psi(\mathbf{x}_i) \\ (\mathbf{K})_{ij} &= k(\mathbf{x}_i, \mathbf{x}_j) = \psi(\mathbf{x}_i)^{\mathrm{T}} \psi(\mathbf{x}_j) \end{aligned}$$

Bayesian Linear Regression as a Kernel Machine

Proof

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- Mean and variance of the predictions:

$$p(t_* | \mathbf{X}, \mathbf{t}, \mathbf{x}_*, \sigma^2) = \mathcal{N}(\phi_*^{\mathrm{T}} \boldsymbol{\mu}, \sigma^2 + \phi_*^{\mathrm{T}} \boldsymbol{\Sigma} \phi_*)$$

- Rewrite the mean:

$$\begin{aligned} \phi_*^{\mathrm{T}} \boldsymbol{\mu} &= \frac{1}{\sigma^2} \phi_*^{\mathrm{T}} \boldsymbol{\Sigma} \boldsymbol{\Phi}^{\mathrm{T}} \mathbf{t} \\ &= \frac{1}{\sigma^2} \phi_*^{\mathrm{T}} \left(\mathbf{S} - \mathbf{S} \boldsymbol{\Phi}^{\mathrm{T}} \left(\sigma^2 \mathbf{I} + \boldsymbol{\Phi} \mathbf{S} \boldsymbol{\Phi}^{\mathrm{T}} \right)^{-1} \boldsymbol{\Phi} \mathbf{S} \right) \boldsymbol{\Phi}^{\mathrm{T}} \mathbf{t} \\ &= \frac{1}{\sigma^2} \phi_*^{\mathrm{T}} \mathbf{S} \boldsymbol{\Phi}^{\mathrm{T}} \left(\mathbf{I} - \left(\sigma^2 \mathbf{I} + \boldsymbol{\Phi} \mathbf{S} \boldsymbol{\Phi}^{\mathrm{T}} \right)^{-1} \boldsymbol{\Phi} \mathbf{S} \boldsymbol{\Phi}^{\mathrm{T}} \right) \mathbf{t} \\ &= \frac{1}{\sigma^2} \phi_*^{\mathrm{T}} \mathbf{S} \boldsymbol{\Phi}^{\mathrm{T}} \left(\mathbf{I} - \left(\mathbf{I} + \frac{\boldsymbol{\Phi} \mathbf{S} \boldsymbol{\Phi}^{\mathrm{T}}}{\sigma^2} \right)^{-1} \frac{\boldsymbol{\Phi} \mathbf{S} \boldsymbol{\Phi}^{\mathrm{T}}}{\sigma^2} \right) \mathbf{t} \end{aligned}$$

... continued

Bayesian Linear Regression as a Kernel Machine

Proof

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- Define $\mathbf{H} = \frac{\boldsymbol{\Phi} \mathbf{S} \boldsymbol{\Phi}^{\mathrm{T}}}{\sigma^2}$
- The term in the parenthesis

$$\left(\mathbf{I} - \left(\mathbf{I} + \frac{\boldsymbol{\Phi} \mathbf{S} \boldsymbol{\Phi}^{\mathrm{T}}}{\sigma^2} \right)^{-1} \frac{\boldsymbol{\Phi} \mathbf{S} \boldsymbol{\Phi}^{\mathrm{T}}}{\sigma^2} \right)$$

becomes

$$\left(\mathbf{I} - (\mathbf{I} + \mathbf{H})^{-1} \mathbf{H} \right) = \mathbf{I} - (\mathbf{H}^{-1} + \mathbf{I})^{-1}$$

- Using Woodbury ($A, U, V = \mathbf{I}$ and $C = \mathbf{H}^{-1}$)

$$\mathbf{I} - (\mathbf{H}^{-1} + \mathbf{I})^{-1} = (\mathbf{I} + \mathbf{H})^{-1}$$

Bayesian Linear Regression as a Kernel Machine

Proof

- Substituting into the expression of the predictive mean

$$
\begin{aligned}
\phi_*^{\mathsf{T}}\boldsymbol{\mu} &= \frac{1}{\sigma^2}\phi_*^{\mathsf{T}}\mathbf{S}\boldsymbol{\Phi}^{\mathsf{T}}\left(\mathbf{I}-\left(\mathbf{I}+\frac{\boldsymbol{\Phi}\mathbf{S}\boldsymbol{\Phi}^{\mathsf{T}}}{\sigma^2}\right)^{-1}\frac{\boldsymbol{\Phi}\mathbf{S}\boldsymbol{\Phi}^{\mathsf{T}}}{\sigma^2}\right)\mathbf{t} \\
&= \frac{1}{\sigma^2}\phi_*^{\mathsf{T}}\mathbf{S}\boldsymbol{\Phi}^{\mathsf{T}}\left(\mathbf{I}+\frac{\boldsymbol{\Phi}\mathbf{S}\boldsymbol{\Phi}^{\mathsf{T}}}{\sigma^2}\right)^{-1}\mathbf{t} \\
&= \phi_*^{\mathsf{T}}\mathbf{S}\boldsymbol{\Phi}^{\mathsf{T}}\left(\sigma^2\mathbf{I}+\boldsymbol{\Phi}\mathbf{S}\boldsymbol{\Phi}^{\mathsf{T}}\right)^{-1}\mathbf{t} \\
&= \mathbf{k}_*^{\mathsf{T}}\left(\sigma^2\mathbf{I}+\mathbf{K}\right)^{-1}\mathbf{t}
\end{aligned}
$$

- All definitions as in the case of the variance

$$
\begin{aligned}
\psi(\mathbf{x}) &= \mathbf{S}^{1/2}\phi(\mathbf{x}) \\
(\mathbf{k}_*)_i &= k(\mathbf{x}_*,\mathbf{x}_i) = \psi(\mathbf{x}_*)^{\mathsf{T}}\psi(\mathbf{x}_i) \\
(\mathbf{K})_{ij} &= k(\mathbf{x}_i,\mathbf{x}_j) = \psi(\mathbf{x}_i)^{\mathsf{T}}\psi(\mathbf{x}_j)
\end{aligned}
$$

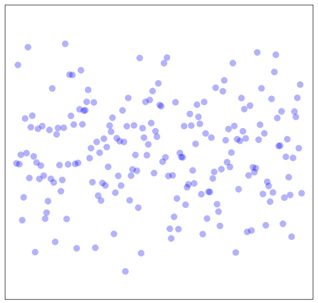
Gaussian Processes

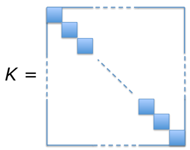
Gaussian Processes can be explained in two ways

- Weight Space View
  - Bayesian linear regression with infinite basis functions
- **Function Space View**
  - **Defined as priors over functions**

Gaussian Processes - Prior over Functions

- Consider an infinite number of Gaussian random variables
- Think of them as indexed by the real line and as independent
- Denote them as $f(x)$





Kernel

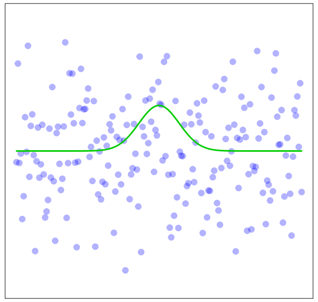
- Consider the Gaussian kernel again

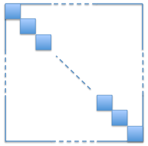
$$k(\mathbf{x},\mathbf{x}') = \alpha\exp(-\beta\|\mathbf{x}-\mathbf{x}'\|^2)$$

- We introduced some parameters for added flexibility

Gaussian Processes - Prior over Functions

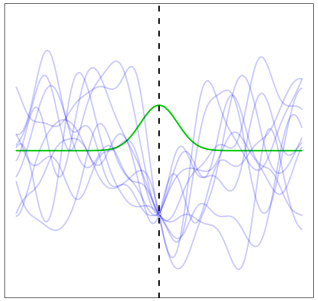
- Impose covariance using the kernel function

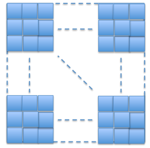


$K =$ 

Gaussian Processes - Prior over Functions

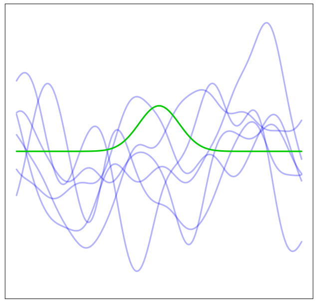
- Draw the infinite random variables again fixing one of them (the one at $x = 0$)

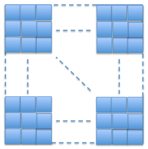


$K =$ 

Gaussian Processes - Prior over Functions

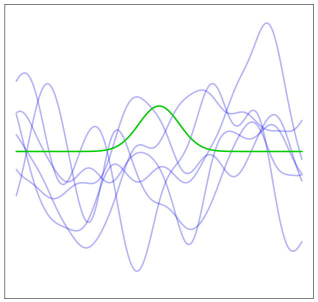
- Draw the infinite random variables again allowing the one at $x = 0$ to be random too

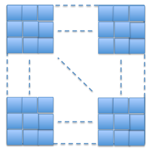


$K =$ 

Gaussian Processes - Prior over Functions

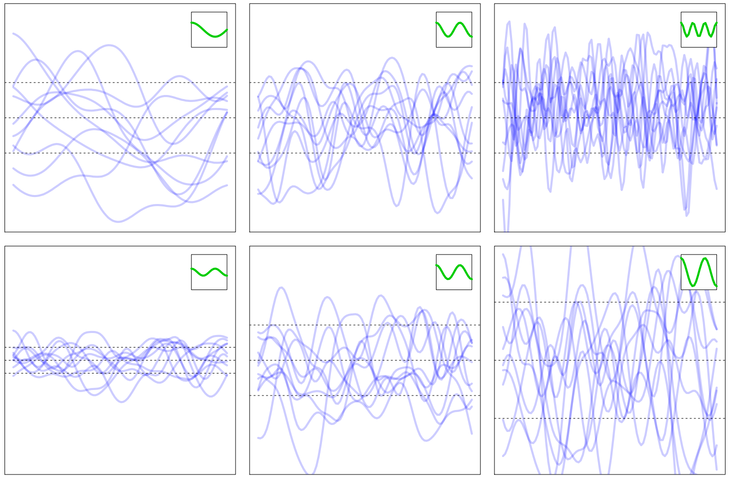
- This can be used as a prior over functions!



$K =$ 

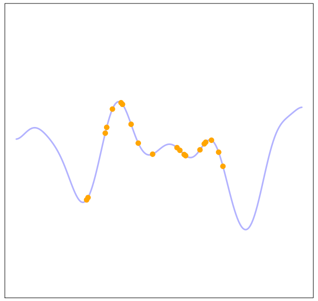
Gaussian Processes - Priors over Functions

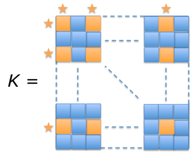
- Infinite Gaussian random variables with parameterized and input-dependent covariance



Gaussian Processes - Prior over Functions

- The distribution of N random variables $f(x_1), \ldots, f(x_N)$ depends exclusively on the corresponding rows and columns of the infinite by infinite kernel matrix K





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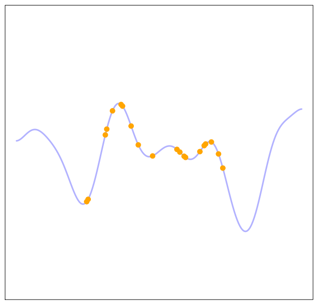
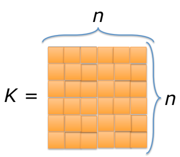
Gaussian Processes - Prior over Functions

- The distribution of N random variables $f(x_1), \ldots, f(x_N)$ depends exclusively on the corresponding rows and columns of the infinite by infinite kernel matrix K





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Gaussian Processes - Prior over Functions

- The marginal distribution of $\mathbf{f} = (f(x_1), \ldots, f(x_N))^\top$ is

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

- The conditional distribution of f_* given $\mathbf{f}$

$$p(f_*|\mathbf{f}, \mathbf{x}_*, \mathbf{X}) = \mathcal{N}(\bar{m}, \bar{s}^2)$$

with

$$\bar{m} = \mathbf{k}_*^\top \mathbf{K}^{-1}$$

$$\bar{s}^2 = k_{**} - \mathbf{k}_*^\top \mathbf{K}^{-1} \mathbf{k}_*$$

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Gaussian Processes - Prior over Functions

- Remember that when we modeled labels $\mathbf{t}$ in the linear model we assumed noise with variance σ around $\mathbf{w}^\top \mathbf{x}$
- We can do the same in Gaussian processes

$$p(\mathbf{t}|\mathbf{f}) = \prod_{i=1}^{N} p(t_i|f_i)$$

with

$$p(t_i|f_i) = \mathcal{N}(t_i|f_i, \sigma^2)$$

- Likelihood and prior are both Gaussian - conjugate!
- We can integrate out Gaussian process prior on $\mathbf{f}$

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

- This gives

$$p(\mathbf{t}|\mathbf{X}) = \mathcal{N}(\mathbf{0}, \mathbf{K} + \sigma^2\mathbf{I})$$

Gaussian Processes - Prior over Functions

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- We can derive the predictive distribution of the function also make predictions as follows:

$$p(f_*|\mathbf{t}, \mathbf{x}_*\mathbf{X}) = \int p(f_*|\mathbf{f}, \mathbf{x}_*, \mathbf{X})p(\mathbf{f}|\mathbf{t}, \mathbf{X})d\mathbf{f}df_* = \mathcal{N}(m, s^2)$$

with

$$m = \mathbf{k}_*^\top \left(\mathbf{K} + \sigma^2\mathbf{I}\right)^{-1}\mathbf{t}$$

$$s^2 = k_{**} - \mathbf{k}_*^\top \left(\mathbf{K} + \sigma^2\mathbf{I}\right)^{-1}\mathbf{k}_*$$

- Same expression as in the “Weight-Space View” section

Gaussian Processes - Prior over Functions

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- We can also make predictions as follows:

$$\begin{aligned} p(t_*|\mathbf{t}, \mathbf{x}_*\mathbf{X}) &= \int p(t_*|f_*)p(f_*|\mathbf{f}, \mathbf{x}_*, \mathbf{X})p(\mathbf{f}|\mathbf{t}, \mathbf{X})d\mathbf{f}df_* \\ &= \mathcal{N}(m_t, s_t^2) \end{aligned}$$

with

$$m_t = \mathbf{k}_*^\top \left(\mathbf{K} + \sigma^2\mathbf{I}\right)^{-1}\mathbf{t}$$

$$s_t^2 = \sigma^2 + k_{**} - \mathbf{k}_*^\top \left(\mathbf{K} + \sigma^2\mathbf{I}\right)^{-1}\mathbf{k}_*$$

- Same expression as in the “Weight-Space View” section

Gaussian Processes - Regression example

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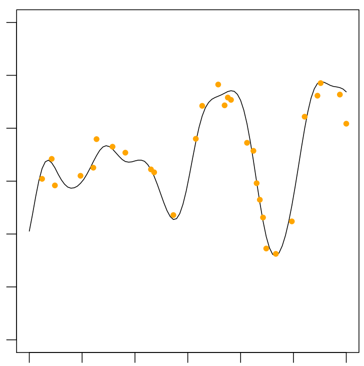
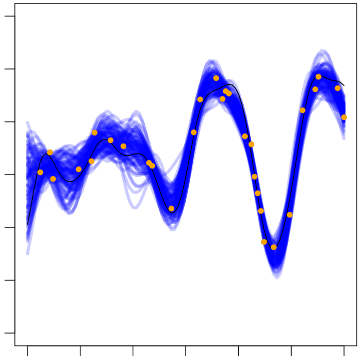
- Some data generated as a noisy version of some function



Gaussian Processes - Regression example

- Draws from the posterior distribution over f_* on the real line



Optimization of Gaussian Process parameters

- The kernel has parameters that have to be tuned

$$k(\mathbf{x}, \mathbf{x}') = \alpha \exp(-\beta \|\mathbf{x} - \mathbf{x}'\|^2)$$

... and there is also the noise parameter σ^2.

- Define $\boldsymbol{\theta} = (\alpha, \beta, \sigma^2)$
- How should we tune them?

Optimization of Gaussian Process parameters

- Define $\mathbf{K}_t = \mathbf{K} + \sigma^2 \mathbf{I}$
- Maximize the logarithm of the likelihood

$$p(\mathbf{t}|\mathbf{X}, \boldsymbol{\theta}) = \mathcal{N}(\mathbf{0}, \mathbf{K}_t)$$

that is

$$-\frac{1}{2} \log |\mathbf{K}_t| - \frac{1}{2} \mathbf{t}^{\mathrm{T}} \mathbf{K}_t^{-1} \mathbf{t} + \mathrm{const.}$$

- Derivatives can be useful for gradient-based optimization

$$\frac{\partial \log[p(\mathbf{t}|\mathbf{X}, \boldsymbol{\theta})]}{\partial \boldsymbol{\theta}_i}$$

Optimization of Gaussian Process parameters

- Log-likelihood

$$-\frac{1}{2} \log |\mathbf{K}_t| - \frac{1}{2} \mathbf{t}^{\mathrm{T}} \mathbf{K}_t^{-1} \mathbf{t} + \mathrm{const.}$$

- Derivatives can be useful for gradient-based optimization:

$$\frac{\partial \log[p(\mathbf{t}|\mathbf{X}, \boldsymbol{\theta})]}{\partial \boldsymbol{\theta}_i} = -\frac{1}{2} \mathrm{Tr} \left(\mathbf{K}_t^{-1} \frac{\partial \mathbf{K}_t}{\partial \boldsymbol{\theta}_i} \right) + \frac{1}{2} \mathbf{t}^{\mathrm{T}} \mathbf{K}_t^{-1} \frac{\partial \mathbf{K}_t}{\partial \boldsymbol{\theta}_i} \mathbf{K}_t^{-1} \mathbf{t}$$

Summary

- Introduced Gaussian Processes
  - Weight space view
  - Function space view
- Gaussian processes for regression
- Optimization of kernel parameters
- To think about:
  - Gaussian processes for classification?
  - Scalability?