

Introduction to Probabilistic Machine Learning

Gaussian Processes

Ralf Herbrich

Overview

1. Basic Concepts
2. Gaussian Processes for Regression
 - Weight-Space View
3. Gaussian Processes for Classification
4. Evidence Maximization for Gaussian Processes

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Unit 10 – Gaussian Processes

1. **Basic Concepts**
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Gaussian Processes

- So far, we assumed that we have a set of **parameterized** functions $f(x; \mathbf{w})$ and parameterized a distribution over f via the vector space $\mathbb{R}^M \ni \mathbf{w}$

- Required *explicit* definition of M basis functions $\phi: \mathcal{X} \rightarrow \mathbb{R}$
- The most expensive operation was $O(M^3)$ (matrix inversion)

- **Gaussian Process.** A Gaussian process is a probability distribution over functions $f: \mathcal{X} \rightarrow \mathbb{R}$ that has the property that for any $x_1, \dots, x_n \in \mathcal{X}$

$$p\left(\begin{bmatrix} f(x_1) \\ \vdots \\ f(x_n) \end{bmatrix}\right) = \mathcal{N}\left(\mathbf{f}; \begin{bmatrix} m(x_1) \\ \vdots \\ m(x_n) \end{bmatrix}, \begin{bmatrix} C(x_1, x_1) & \dots & C(x_1, x_n) \\ \vdots & \ddots & \vdots \\ C(x_n, x_1) & \dots & C(x_n, x_n) \end{bmatrix}\right)$$

- Fully parameterized by a mean *function* $m: \mathcal{X} \rightarrow \mathbb{R}$ and covariance *function* $C: \mathcal{X} \times \mathcal{X} \rightarrow \mathbb{R}$
- Mean function is arbitrary, but the covariance function must be positive definite!

- **Gaussian processes** have a long history in engineering (“Kriging”)

- In 1950, Danie G. Krige was studying gold locations predicted from a few boreholes
- In 1960, Georges Matheron rediscovered Krige’s work and formalized it for statistics
- In 1999, Prof. David MacKay rediscovered Gaussian Processes for machine learning



Danie G. Krige
(1919 – 2013)



Georges Matheron
(1930 – 2000)



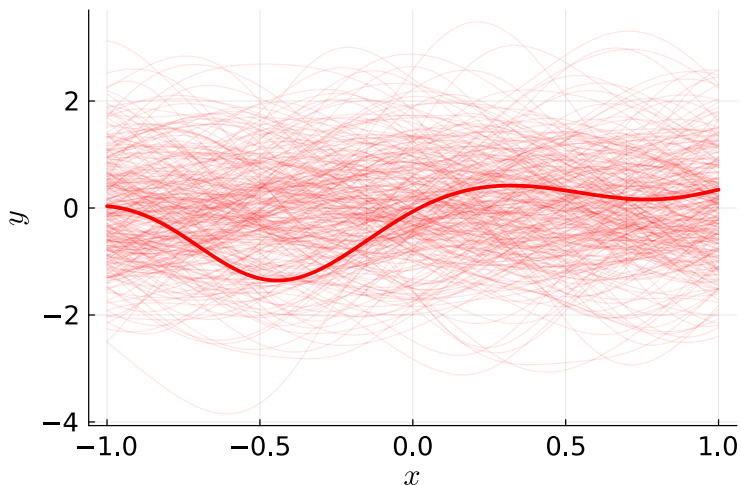
Sir David JC MacKay
(1967 – 2016)

Gaussian Process: Example

$$m(x) = 0$$

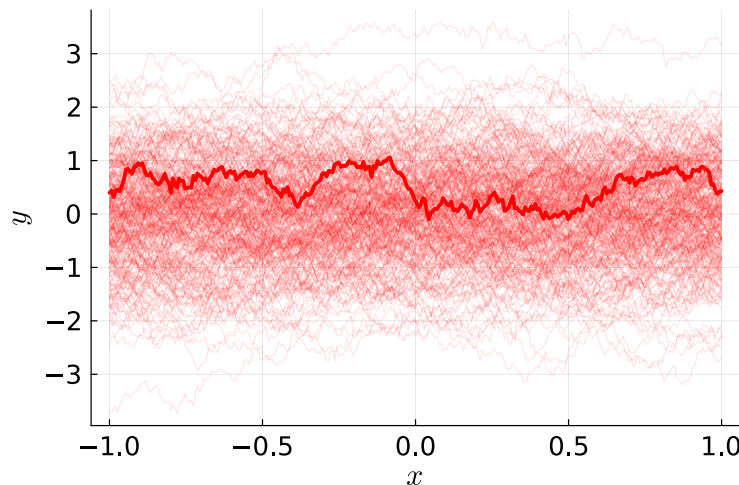
RBF Kernel

$$C(x, x') = \exp\left(-\frac{(x - x')^2}{\lambda^2}\right)$$



Ornstein-Uhlenbeck Kernel

$$C(x, x') = \exp\left(-\frac{|x - x'|}{\lambda}\right)$$



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Partitioned Multivariate Normal Distribution

- **Partitioned Gaussians.** Given a joint distribution $\mathcal{N}(\mathbf{x}; \boldsymbol{\mu}, \boldsymbol{\Sigma})$ and a partitioning

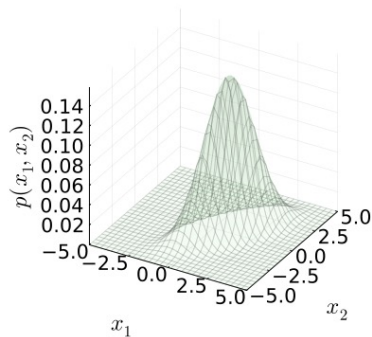
$$\mathbf{x} = \begin{bmatrix} \mathbf{x}_a \\ \mathbf{x}_b \end{bmatrix}, \quad \boldsymbol{\mu} = \begin{bmatrix} \boldsymbol{\mu}_a \\ \boldsymbol{\mu}_b \end{bmatrix}, \quad \boldsymbol{\Sigma} = \begin{bmatrix} \boldsymbol{\Sigma}_{aa} & \boldsymbol{\Sigma}_{ab} \\ \boldsymbol{\Sigma}_{ba} & \boldsymbol{\Sigma}_{bb} \end{bmatrix}$$

we have the following for the marginal $p(\mathbf{x}_a)$ and the conditional $p(\mathbf{x}_a | \mathbf{x}_b)$

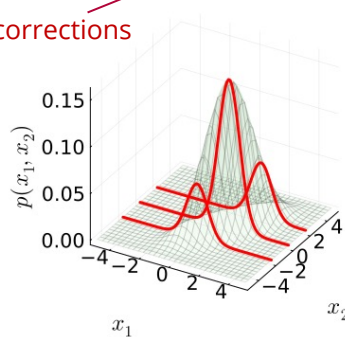
$$p(\mathbf{x}_a) = \mathcal{N}(\mathbf{x}_a; \boldsymbol{\mu}_a, \boldsymbol{\Sigma}_{aa})$$

$$p(\mathbf{x}_b | \mathbf{x}_a) = \mathcal{N}(\mathbf{x}_b; \boldsymbol{\mu}_b + \boldsymbol{\Sigma}_{ba} \boldsymbol{\Sigma}_{aa}^{-1} (\mathbf{x}_a - \boldsymbol{\mu}_a), \boldsymbol{\Sigma}_{bb} - \boldsymbol{\Sigma}_{ba} \boldsymbol{\Sigma}_{aa}^{-1} \boldsymbol{\Sigma}_{ab})$$

additive corrections



$$p(x_1) = \mathcal{N}(x_1; 1, 1)$$



$$p(x_1 | x_2) = \mathcal{N}\left(x_1; 1 + \frac{1}{2}x_2, \frac{1}{2}\right)$$

$$\boldsymbol{\mu} = \begin{bmatrix} 1 \\ 0 \end{bmatrix}$$

$$\boldsymbol{\Sigma} = \begin{bmatrix} 1 & 1 \\ 1 & 2 \end{bmatrix}$$

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Bayes' Theorem for Normal Distributions

- **Conjugate Gaussians.** Given a normally distributed variable

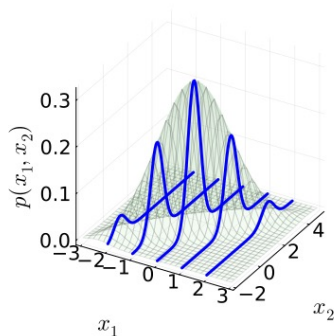
$$\mathbf{x} \sim \mathcal{N}(\mathbf{x}; \boldsymbol{\mu}, \boldsymbol{\Sigma})$$

and a conditional distribution for \mathbf{y} given \mathbf{x} such that $\mathbf{y}|\mathbf{x} \sim \mathcal{N}(\mathbf{y}; \mathbf{A}\mathbf{x} + \mathbf{b}, \mathbf{S})$ we have the following for the marginal $p(\mathbf{y})$ and the "inverse" conditional $p(\mathbf{x}|\mathbf{y})$

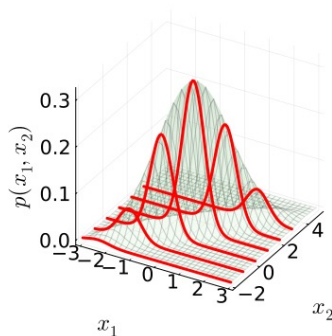
$$p(\mathbf{y}) = \mathcal{N}(\mathbf{y}; \mathbf{A}\boldsymbol{\mu} + \mathbf{b}, \mathbf{S} + \mathbf{A}\boldsymbol{\Sigma}\mathbf{A}^T)$$

$$p(\mathbf{x}|\mathbf{y}) = \mathcal{G}(\mathbf{x}; \boldsymbol{\Sigma}^{-1}\boldsymbol{\mu} + \mathbf{A}^T\mathbf{S}^{-1}(\mathbf{y} - \mathbf{b}), \boldsymbol{\Sigma}^{-1} + \mathbf{A}^T\mathbf{S}^{-1}\mathbf{A}),$$

$$p(x_1) = \mathcal{N}(x_1; 0, 1)$$



$$p(x_2|x_1) = \mathcal{N}\left(x_2; x_1 + 1, \frac{1}{2}\right)$$



$$p(x_1|x_2) = \mathcal{N}\left(x_1; \frac{2}{3}(x_2 - 1), \frac{1}{3}\right)$$

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Inference in a Gaussian Processes (GP)

- Observation:** *The only part of our data that is predicted is the targets \mathbf{y} and everything is conditioned on the locations $\{x_1, \dots, x_n\} =: X$.*

$$p(\mathbf{y}|X) = \int p(\mathbf{y}|\mathbf{f}, X) \cdot \overbrace{p(\mathbf{f}|X)}^{\text{GP}(\mathbf{f}; \mathbf{0}, \mathbf{C})} d\mathbf{f}$$

$$p(\mathbf{y}|X) = \int \mathcal{N}(\mathbf{y}; \mathbf{f}, \sigma^2 \mathbf{I}) \cdot \mathcal{N}(\mathbf{f}; \mathbf{0}, \mathbf{C}_X) d\mathbf{f}$$

$$p(\mathbf{y}|X) = \mathcal{N}(\mathbf{y}; \mathbf{0}, \sigma^2 \mathbf{I} + \mathbf{C}_X)$$

- Observation:** *The marginal distribution of data over all functions is also a GP with the covariance/kernel function modified by an identity function!*

$$\mathcal{N}(\mathbf{y}; \mathbf{0}, \sigma^2 \mathbf{I} + \mathbf{C}_X) = \text{GP}(\mathbf{y}; \mathbf{0}, \mathbf{C} + \sigma^2 \mathbb{I}(x = x')) \leftarrow \tilde{\mathbf{C}}$$

- Inference** of the predictive distribution at a new point $x^* \in \mathcal{X}$ in a Gaussian Process can be done by conditioning!

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

$$p(y^*|x^*, X, \mathbf{y}) = \mathcal{N}(y^*; \mathbf{k}^T \tilde{\mathbf{C}}^{-1} \mathbf{y}, C(x^*, x^*) + \sigma^2 - \mathbf{k}^T \tilde{\mathbf{C}}^{-1} \mathbf{k})$$

where $\mathbf{k} := (\tilde{C}(x_1, x^*), \dots, \tilde{C}(x_n, x^*))^T$ and $\tilde{C}_{ij} := \tilde{C}(x_i, x_j)$

Properties of Gaussians

$$p(\mathbf{f}) = \mathcal{N}(\mathbf{w}; \boldsymbol{\mu}, \boldsymbol{\Sigma})$$

$$p(\mathbf{y}|\mathbf{f}) = \mathcal{N}(\mathbf{y}; \mathbf{A}\mathbf{f}, \boldsymbol{\Sigma})$$

$$p(\mathbf{y}) = \mathcal{N}(\mathbf{y}; \mathbf{A}\boldsymbol{\mu}, \mathbf{S} + \mathbf{A}\boldsymbol{\Sigma}\mathbf{A}^T)$$

Partitioned Gaussians

$$\mathbf{x} = \begin{bmatrix} \mathbf{x}_a \\ \mathbf{x}_b \end{bmatrix}, \boldsymbol{\mu} = \begin{bmatrix} \boldsymbol{\mu}_a \\ \boldsymbol{\mu}_b \end{bmatrix}, \boldsymbol{\Sigma} = \begin{bmatrix} \boldsymbol{\Sigma}_{aa} & \boldsymbol{\Sigma}_{ab} \\ \boldsymbol{\Sigma}_{ba} & \boldsymbol{\Sigma}_{bb} \end{bmatrix}$$

$$p(\mathbf{x}_b|\mathbf{x}_a) = \mathcal{N}(\mathbf{x}_b; \mathbf{m}, \mathbf{S})$$

$$\mathbf{m} = \boldsymbol{\mu}_b + \boldsymbol{\Sigma}_{ba} \boldsymbol{\Sigma}_{aa}^{-1} (\mathbf{x}_a - \boldsymbol{\mu}_a)$$

$$\mathbf{S} = \boldsymbol{\Sigma}_{bb} - \boldsymbol{\Sigma}_{ba} \boldsymbol{\Sigma}_{aa}^{-1} \boldsymbol{\Sigma}_{ab}$$

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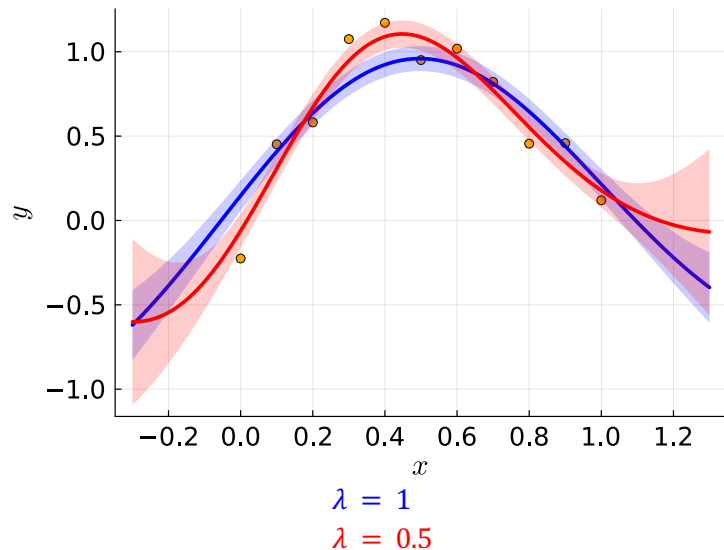
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Gaussian Process: Example

$$m(x) = 0$$

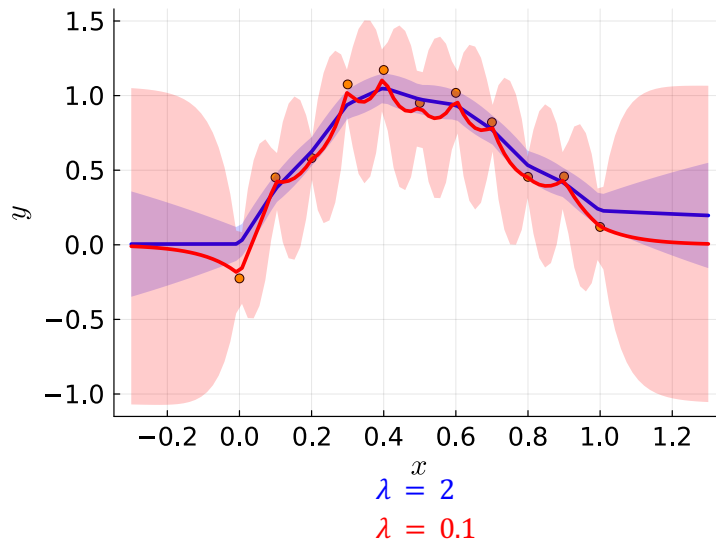
RBF Kernel

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Ornstein-Uhlenbeck Kernel

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Bayesian Linear Regression Revisited

- **Bayesian Linear Regression:** Linear basis function model $f(x; \mathbf{w}) := \mathbf{w}^T \boldsymbol{\phi}(x)$

- Likelihood: $p(\mathbf{y}|\mathbf{w}, X) = \mathcal{N}(\mathbf{y}; \boldsymbol{\Phi}\mathbf{w}, \sigma^2 \mathbf{I})$
- Prior: $p(\mathbf{w}) = \mathcal{N}(\mathbf{w}; \mathbf{0}, \mathbf{I})$
- Marginal Likelihood: $p(\mathbf{y}|X) = \int p(\mathbf{y}|\mathbf{w}, X) \cdot p(\mathbf{w}) d\mathbf{w}$

$$p(\mathbf{y}|X) = \mathcal{N}(\mathbf{y}; \mathbf{0}, \sigma^2 \mathbf{I} + \boldsymbol{\Phi}\boldsymbol{\Phi}^T) = \text{GP}(\mathbf{y}; \mathbf{0}, \boldsymbol{\phi}(x)^T \boldsymbol{\phi}(x') + \sigma^2 \mathbb{I}(x = x'))$$

- **Equivalence:** A Gaussian Process is equivalent to the marginal likelihood of a linear basis function model with the prior $p(\mathbf{w}) = \mathcal{N}(\mathbf{w}; \mathbf{0}, \mathbf{I})$ and the covariance function $C(x, x') = \boldsymbol{\phi}(x)^T \boldsymbol{\phi}(x')$.

	Number of Basis Functions	Computational Cost
Linear Basis Function Model	M	$O(M^3)$
Gaussian Process	∞	$O(n^3)$

Properties of Gaussians

$$p(\mathbf{w}) = \mathcal{N}(\mathbf{w}; \boldsymbol{\mu}, \boldsymbol{\Sigma})$$

$$p(\mathbf{y}|\mathbf{w}) = \mathcal{N}(\mathbf{y}; \boldsymbol{\Phi}\mathbf{w}, \mathbf{S})$$

$$p(\mathbf{y}) = \mathcal{N}(\mathbf{y}; \boldsymbol{\Phi}\boldsymbol{\mu}, \mathbf{S} + \mathbf{A}\boldsymbol{\Sigma}\mathbf{A}^T)$$

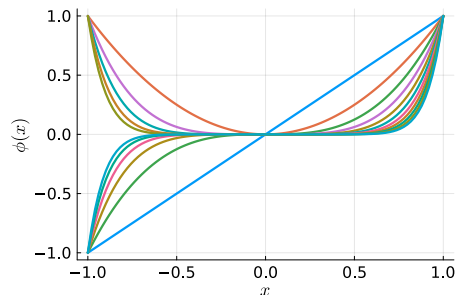
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Constructing Covariance Functions

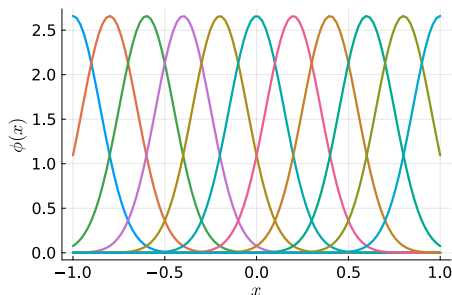
Polynomial Basis

$$\phi_j(x) = x^j$$



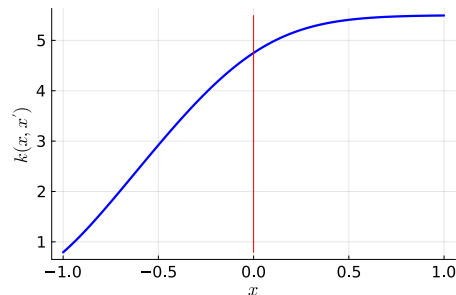
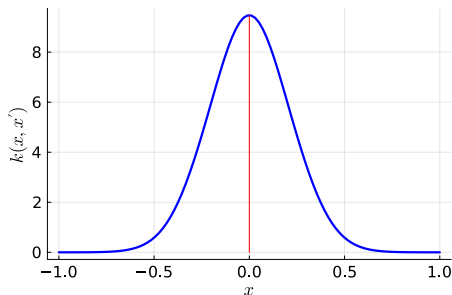
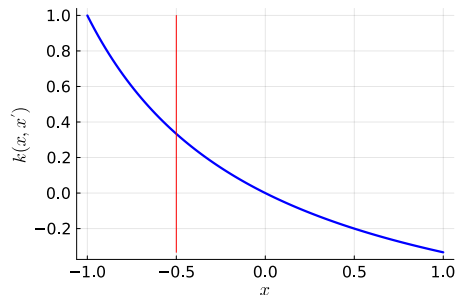
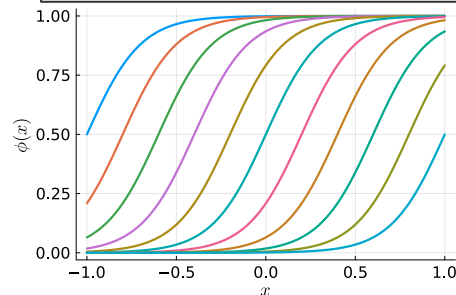
Gaussian Basis

$$\phi_j(x) = \mathcal{N}\left(x; \frac{j}{5} - 1, 0.15^2\right)$$



Sigmoid Basis

$$\phi_j(x) = \frac{\exp(x - 0.2j + 1)}{1 + \exp(x - 0.2j + 1)}$$



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Gaussian Processes with Logit for Classification

- A **Gaussian Process (GP) prior** is a prior $p(f)$ over functions f such that for any $x_1, \dots, x_n \in \mathcal{X}$

$$p(\mathbf{f}|X) = p\left(\begin{bmatrix} f(x_1) \\ \vdots \\ f(x_n) \end{bmatrix}\right) = \mathcal{N}\left(\mathbf{f}; \mathbf{0}, \begin{bmatrix} C(x_1, x_1) & \dots & C(x_1, x_n) \\ \vdots & \ddots & \vdots \\ C(x_n, x_1) & \dots & C(x_n, x_n) \end{bmatrix}\right) = \mathcal{N}(\mathbf{f}; \mathbf{0}, \mathbf{C}_X)$$

- **Problem:** The data model $p(y_i|f_i) = \text{Ber}(y_i; g(f_i))$ is not conjugate to the Gaussian resulting a non-Gaussian $p(\mathbf{f}|X, \mathbf{y}) \propto p(\mathbf{y}|\mathbf{f}) \cdot p(\mathbf{f}|X)$!
- **Predictions.** By marginalization over $p(f^*|x^*, X, \mathbf{y})$ we can get the predictive distribution over $y^* \in \{0,1\}$ at a new point $x^* \in \mathcal{X}$

$$p(y^*|x^*, X, \mathbf{y}) = \int_{-\infty}^{+\infty} p(y^*|f^*) \cdot p(f^*|x^*, X, \mathbf{y}) df^*$$

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

$$p(f^*|x^*, X, \mathbf{f}) = \frac{p(f^*, \mathbf{f}|x^*, X)}{p(\mathbf{f}|X)} = \mathcal{N}(f^*; \mathbf{k}^T \mathbf{C}_X^{-1} \mathbf{f}, C(x^*, x^*) - \mathbf{k}^T \mathbf{C}_X^{-1} \mathbf{k})$$

Partitioned Gaussians

$$\mathbf{x} = \begin{bmatrix} x_a \\ x_b \end{bmatrix}, \boldsymbol{\mu} = \begin{bmatrix} \mu_a \\ \mu_b \end{bmatrix}, \boldsymbol{\Sigma} = \begin{bmatrix} \Sigma_{aa} & \Sigma_{ab} \\ \Sigma_{ba} & \Sigma_{bb} \end{bmatrix}$$

$$p(x_b|x_a) = \mathcal{N}(x_b; \mathbf{m}, S)$$

$$\mathbf{m} = \mu_b + \Sigma_{ba} \Sigma_{aa}^{-1} (x_a - \mu_a)$$

$$S = \Sigma_{bb} - \Sigma_{ba} \Sigma_{aa}^{-1} \Sigma_{ab}$$

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Approximate Gaussian Processes for Classification

- **Idea:** We approximate $p(\mathbf{f}|X, \mathbf{y}) \propto p(\mathbf{y}|\mathbf{f}) \cdot p(\mathbf{f}|X)$ with a Gaussian $\mathcal{N}(\mathbf{f}; \mathbf{m}, \mathbf{A})$.

$$p(y^*|x^*, X, \mathbf{y}) = \int_{-\infty}^{+\infty} p(y^*|f^*) \cdot \mathcal{N}(f^*; \mathbf{k}^T \mathbf{C}_X^{-1} \mathbf{m}, C(x^*, x^*) - \mathbf{k}^T (\mathbf{C}_X^{-1} - \mathbf{C}_X^{-1} \mathbf{A} \mathbf{C}_X^{-1}) \mathbf{k}) df^*$$

- **Laplace Approximation:** Similar to Bayesian Linear Logit Regression, we use the Laplace approximation on the distribution $p(\mathbf{f}|X, \mathbf{y}) \propto p(\mathbf{y}|\mathbf{f}) \cdot p(\mathbf{f}|X)$!

Properties of Gaussians

$$p(\mathbf{w}) = \mathcal{N}(\mathbf{w}; \boldsymbol{\mu}, \boldsymbol{\Sigma})$$

$$p(\mathbf{v}|\mathbf{w}) = \mathcal{N}(\mathbf{v}; \mathbf{A}\mathbf{w}, \boldsymbol{\Xi})$$

$$p(\mathbf{v}) = \mathcal{N}(\mathbf{v}; \mathbf{A}\boldsymbol{\mu}, \boldsymbol{\Xi} + \mathbf{A}\boldsymbol{\Sigma}\mathbf{A}^T)$$

1. **Initialize:** A the latent function values vector $\mathbf{m} = \mathbf{0}$ and compute the covariance matrix $\mathbf{C} \in \mathbb{R}^{n \times n}$ once

2. **Iterate** until convergence

$$\square \text{ Compute } g_i = \frac{\exp(m_i)}{1 + \exp(m_i)} \text{ and } \mathbf{R} = \text{diag} \left(\begin{bmatrix} -g_1(1 - g_1) \\ \vdots \\ -g_n(1 - g_n) \end{bmatrix} \right)$$

$$\square \text{ Update } \mathbf{m} \leftarrow \mathbf{m} - (\mathbf{R} - \mathbf{C}^{-1})^{-1}((\mathbf{y} - \mathbf{g}) - \mathbf{C}^{-1}\mathbf{m})$$

3. **Set** the covariance \mathbf{A} of Gaussian approximation to $\mathbf{A} = (\mathbf{C}^{-1} - \mathbf{R})^{-1}$

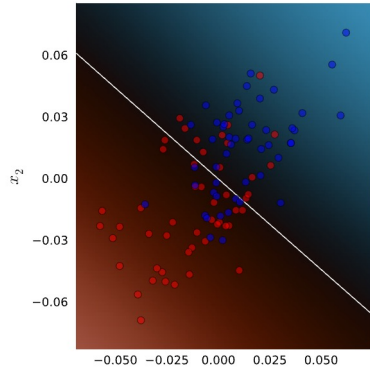
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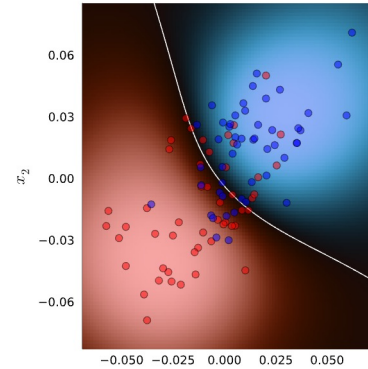
Gaussian Process Logistic Regression in Pictures

$n = 100$

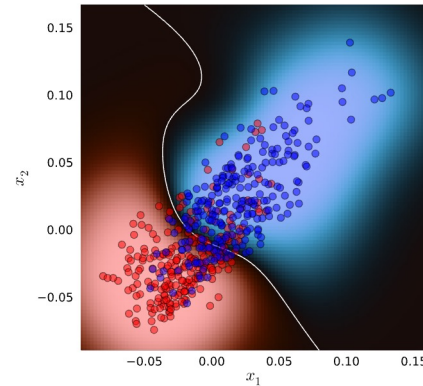
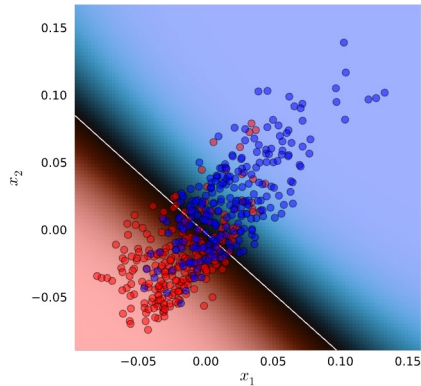
$\lambda = 0.5$



$\lambda = 0.05$



$n = 500$



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Model Averaging and Selection

- All our inference algorithms have **assumed a known and fixed** set of basis functions as well as prior variance τ^2 and data noise variances σ^2 (i.e., **model**)
- **Model.** A model \mathcal{M} is assumed probability distribution over data, $p(D|\mathcal{M})$.
 - Bayesian regression: $p(D|\mathcal{M}) = p(\mathbf{y}|X, \mathcal{M}) = \int p(\mathbf{y}|X, \mathbf{w}, \mathcal{M}) \cdot p(\mathbf{w}|\mathcal{M}) d\mathbf{w}$
 - Gaussian Processes: $p(D|\mathcal{M}) = p(\mathbf{y}|X, \mathcal{M}) = \int p(\mathbf{y}|\mathbf{f}, \mathcal{M}) \cdot p(\mathbf{f}|X, \mathcal{M}) d\mathbf{f}$
- **Model Averaging.** Given a set $\{\mathcal{M}\}$ of models, the predictive distribution for a new example x is obtained via

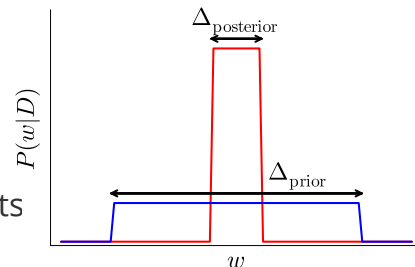
$$p(y|x, D) = \sum_{\mathcal{M}} p(y|x, D, \mathcal{M}) \cdot p(\mathcal{M}|D)$$

- Often too difficult to compute so instead, approximate with a single best model \mathcal{M}
- **Model Selection.** Given a set $\{\mathcal{M}\}$ of models and a dataset D , select the best model

$$\mathcal{M}(D) = \operatorname{argmax}_{\mathcal{M}} p(\mathcal{M}|D) = \operatorname{argmax}_{\mathcal{M}} p(D|\mathcal{M}) \cdot p(\mathcal{M})$$

Model Selection: Intuition

- **Model Evidence.** The probability of the data given a fixed model, $p(D|\mathcal{M})$, is called the model evidence.
 - It's also called **marginal likelihood** because $p(D|\mathcal{M}) = \int p(D|f, \mathcal{M})p(f)df$ and $p(D|f, \mathcal{M})$ is called the likelihood of the function f (actually, really a misnomer!).
 - The **negative logarithm (base 2) of the model evidence** specifies the number of bits that the data can be compressed into without loss given the model \mathcal{M} .
- **Approximation.** Assume that f has one parameter w , that $p(w)$ is uniform and that the posterior for a given dataset is also uniform. Then



$$p(D|\mathcal{M}) = \int p(D|w, \mathcal{M}) \cdot p(w|\mathcal{M})dw = p(D|w_{\text{MAP}}, \mathcal{M}) \cdot \frac{\Delta_{\text{posterior}}}{\Delta_{\text{prior}}}$$

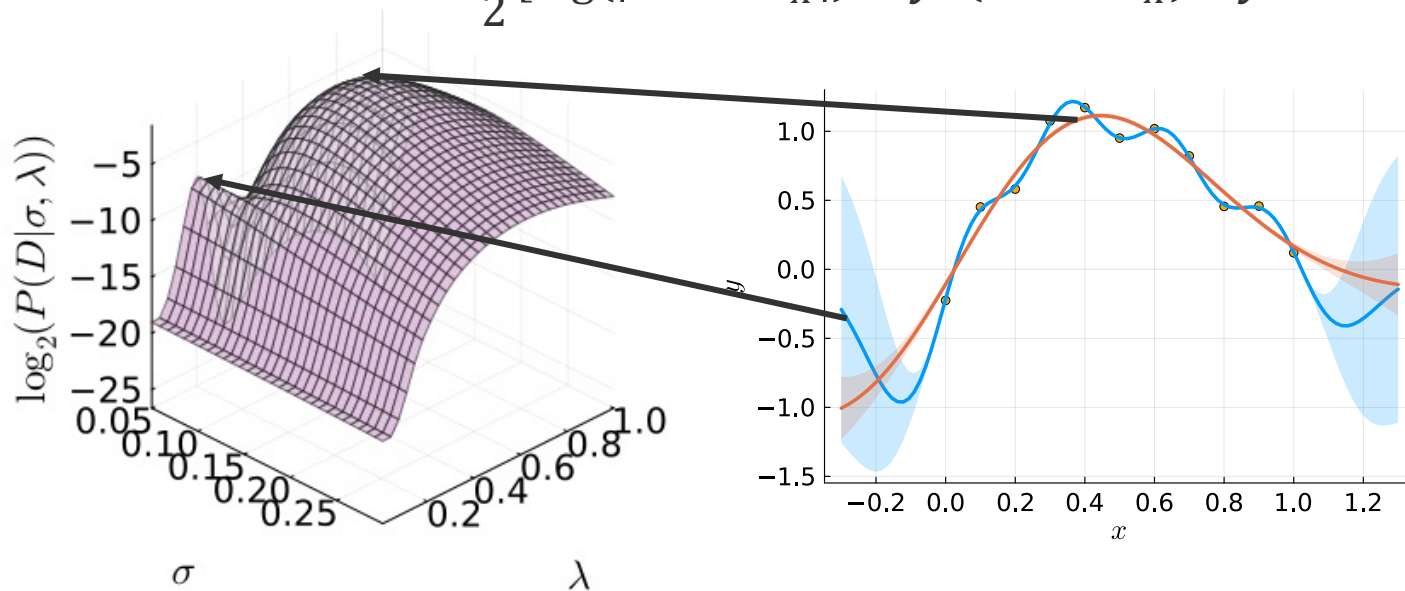
$$\log_2 p(D|\mathcal{M}) = \underbrace{\log_2 p(D|w_{\text{MAP}}, \mathcal{M})}_{\text{fit of the model to data}} - \underbrace{\log_2 \left(\frac{\Delta_{\text{prior}}}{\Delta_{\text{posterior}}} \right)}_{\substack{\text{penalty} \\ \text{for} \\ \text{richness of model}}}$$

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Gaussian Process Evidence Maximization

$$\begin{aligned}\log(p(\mathbf{y}|X)) &= \log(\mathcal{N}(\mathbf{y}; \mathbf{0}, \sigma^2 \mathbf{I} + \mathbf{C}_X)) \\ &= -\frac{1}{2} [\log(|\sigma^2 \mathbf{I} + \mathbf{C}_X|) + \mathbf{y}^T (\sigma^2 \mathbf{I} + \mathbf{C}_X)^{-1} \mathbf{y} + n \cdot \log(2\pi)]\end{aligned}$$



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1. Gaussian Processes

- Distribution over space of functions rather than function parameters
- However, Gaussian Process models are equivalent to linear basis function models with a different parameterization (covariance functions instead of basis functions!)

2. Gaussian Process Classification

- Since the likelihood is no longer Gaussian, we have to approximate the posterior Gaussian process
- Many approximation schemes exist; we introduced the Laplace approximation (Kuss et al., 2005)
- Also possible to use approximate message passing

3. Bayesian Model Comparison and Selection

- Model evidence as the key criterion: The probability of the data given a fixed model, $p(D | \mathcal{M})$.
- Negative log-model evidence equals the compression length of the data (measured in bits): the further we can compress the target values, the better the model (see next lecture!)

See you next week!