Machine Learning 2

2. Gaussian Process Models (GPs)

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Syllabus

		A. Advanced Supervised Learning
Tue. 5.4.	(1)	A.1 Generalized Linear Models
Tue. 12.4.	(2)	A.2 Gaussian Processes
Tue. 19.4.	(3)	A.3 Advanced Support Vector Machines
Tue. 26.4.	(4)	A.4 Neural Networks
Tue. 3.5.	(5)	A.5 Ensembles
Tue. 10.5.	(6)	A.5b Ensembles (ctd.)
Tue. 17.5.	(7)	A.6 Sparse Linear Models — L1 regularization
Tue. 24.5.	—	— Pentecoste Break —
Tue. 31.5.	(8)	A.6b Sparse Linear Models — L1 regularization (ctd.)
Tue. 7.6.	(9)	A.7. Sparse Linear Models — Further Methods
		B. Complex Predictors
Tue. 14.6.	(10)	B.1 Latent Dirichlet Allocation (LDA)
Tue. 21.6.	(11)	B.1b Latent Dirichlet Allocation (LDA; ctd.)
Tue. 28.6.	(12)	B.2 Deep Learning
Tue. 5.7.	(13)	Questions and Answers

Outline

1. GPs for Regression

2. GPs for Classification

Outline

Gaussian Process Model

Gaussian Processes describe

- the **vector** $y := (y_1, \ldots, y_N)^T$ **of all targets**
- as a sample from a **normal distribution**
- where targets of different instances are **correlated by a kernel** Σ:
- and thus depend on the **matrix** X **of all predictors**:

$$y \mid X \sim \mathcal{N}(y \mid \mu(X), \Sigma(X))$$

with

$$\begin{aligned} \mu(X)_n &:= m(x_n) \\ \Sigma(X)_{n,m} &:= k(x_n, x_m), \quad n, m \in \{1, \ldots, N\} \end{aligned}$$

with a **kernel function** k and **mean function** m (often $m = 0$).

Kernels

The kernel k measures how much targets y, y' correlate given their predictors x, x'.

Example: **squared exponential kernel**

$$k(x, x') := \sigma_f^2 e^{-\frac{1}{2\ell^2}||x-x'||^2}$$

with **kernel (hyper)parameters**

ℓ horizontal length scale (x)

σ_f^2 vertical variation (y)

Conditional Distributions of Multivariate Normals

Let y_A, y_B be jointly Gaussian

$$y := \begin{pmatrix} y_A \\ y_B \end{pmatrix} \sim \mathcal{N}(\begin{pmatrix} y_A \\ y_B \end{pmatrix} \mid \begin{pmatrix} \mu_A \\ \mu_B \end{pmatrix}, \begin{pmatrix} \Sigma_{AA} & \Sigma_{AB} \\ \Sigma_{BA} & \Sigma_{BB} \end{pmatrix})$$

then the **conditional distribution** is

$$p(y_B \mid y_A) = \mathcal{N}(y_B \mid \mu_{B|A}, \Sigma_{B|A})$$

with

$$\mu_{B|A} := \mu_B + \Sigma_{BA}\Sigma_{AA}^{-1}(y_A - \mu_A)$$
$$\Sigma_{B|A} := \Sigma_{BB} - \Sigma_{BA}\Sigma_{AA}^{-1}\Sigma_{AB}$$

Predictions w/o Noise

Let y, X be the training data,
X_* be the test data and
y_* be the test targets to predict.

$$\begin{pmatrix} y \\ y_* \end{pmatrix} \mid X, X_* \sim \mathcal{N}(\begin{pmatrix} y \\ y_* \end{pmatrix} \mid \begin{pmatrix} \mu \\ \mu_* \end{pmatrix}, \begin{pmatrix} \Sigma & \Sigma_* \\ \Sigma_*^T & \Sigma_{**} \end{pmatrix})$$

with

$$\mu := m(X), \quad \mu_* := m(X_*)$$
$$\Sigma := k(X, X), \quad \Sigma_* := k(X, X_*), \quad \Sigma_{**} := k(X_*, X_*)$$

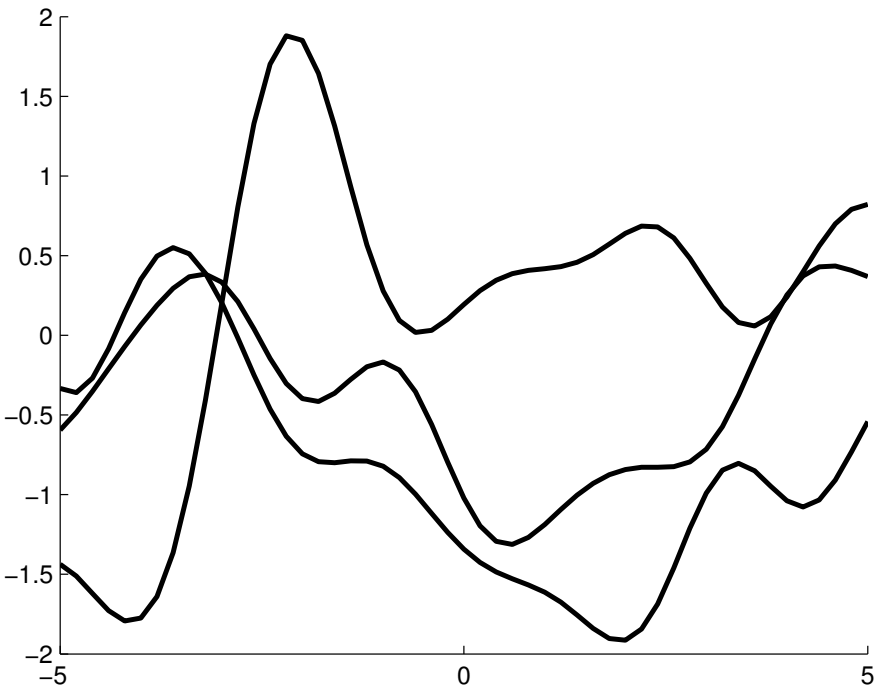
Then

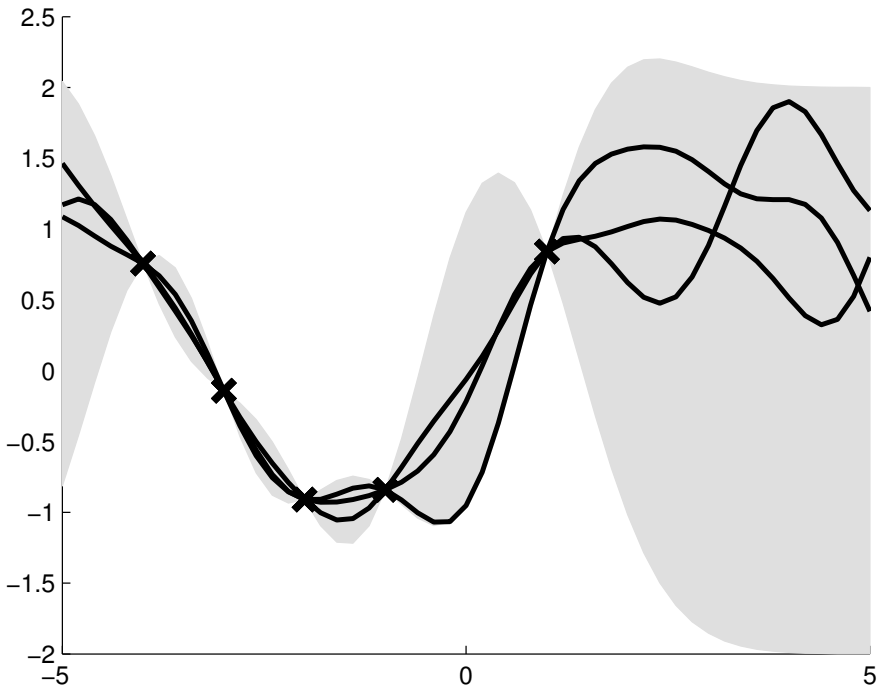
$$p(y_* \mid y) = \mathcal{N}(y_* \mid \tilde{\mu}_*, \tilde{\Sigma}_*)$$

with

$$\tilde{\mu}_* := \mu_* + \Sigma_*^T \Sigma^{-1}(y - \mu)$$
$$\tilde{\Sigma}_* := \Sigma_{**} - \Sigma_*^T \Sigma^{-1} \Sigma_*$$

Example w/o Noise





Without noise the data is interpolated.

[Mur12, fig. 15.2]

Predictions with Noise

No noise:

$$\Sigma := K$$

With noise:

$$\Sigma := K + \sigma_y^2 I$$

Then as before

$$p(y_* \mid y) = \mathcal{N}(y_* \mid \tilde{\mu}_*, \tilde{\Sigma}_*)$$

now with

$$\tilde{\mu}_* := \mu_* + K_*^T (K + \sigma_y^2 I)^{-1} (y - \mu)$$
$$\tilde{\Sigma}_* := K_{**} + \sigma_y^2 I - K_*^T (K + \sigma_y^2)^{-1} K_*$$

where

$$K := k(X, X), \quad K_* := k(X, X_*), \quad K_{**} := k(X_*, X_*)$$

Predictions with Noise, Zero Means

$$p(y_* \mid y) = \mathcal{N}(y_* \mid \tilde{\mu}_*, \tilde{\Sigma}_*)$$

with

$$\begin{aligned}\tilde{\mu}_* :=& \mu_* + K_*^T (K + \sigma_y^2 I)^{-1} (y - \mu) \\ \tilde{\Sigma}_* :=& K_{**} + \sigma_y^2 I - K_*^T (K + \sigma_y^2)^{-1} K_*\end{aligned}$$

With $m = 0$:

$$p(y_* \mid y) = \mathcal{N}(y_* \mid \tilde{\mu}_*, \tilde{\Sigma}_*)$$

with

$$\begin{aligned}\tilde{\mu}_* :=& K_*^T (K + \sigma_y^2 I)^{-1} y \\ \tilde{\Sigma}_* :=& K_{**} + \sigma_y^2 I - K_*^T (K + \sigma_y^2)^{-1} K_*\end{aligned}$$

Prediction for a single instance

$$p(y_* \mid y) = \mathcal{N}(y_* \mid \tilde{\mu}_*, \tilde{\Sigma}_*)$$

with

$$\begin{aligned}\tilde{\mu}_* :=& K_*^T (K + \sigma_y^2 I)^{-1} y \\ \tilde{\Sigma}_* :=& K_{**} + \sigma_y^2 I - K_*^T (K + \sigma_y^2)^{-1} K_*\end{aligned}$$

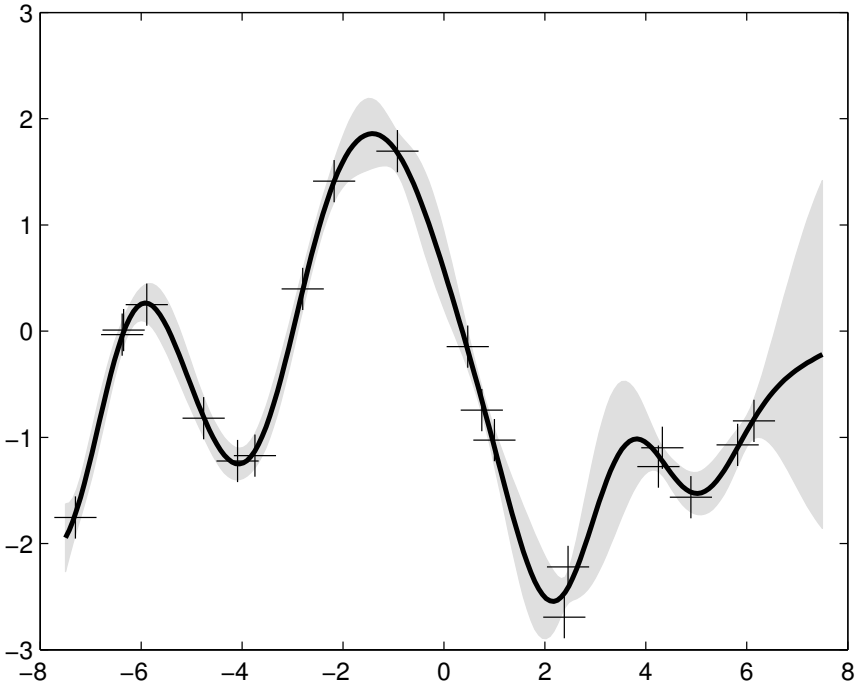
Prediction $\hat{y}$ for a single instance x:

$$\hat{y}(x) := k_*^T (K + \sigma_y^2 I)^{-1} y = \sum_{n=1}^{N} \alpha_n k(x_n, x), \quad \alpha := (K + \sigma_y^2 I)^{-1} y$$

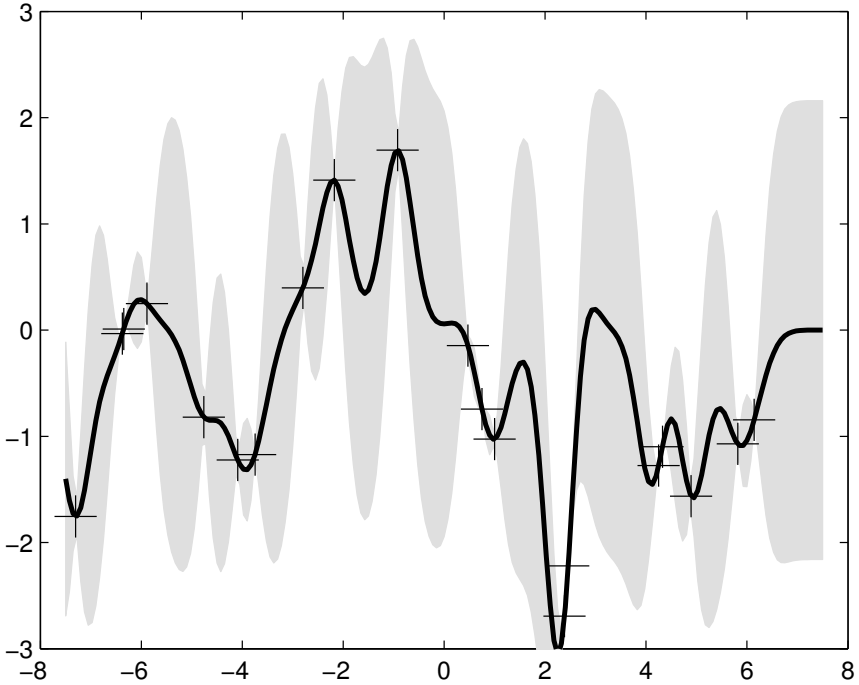
with

$$k_* := k(X, x)$$

Example with Noise



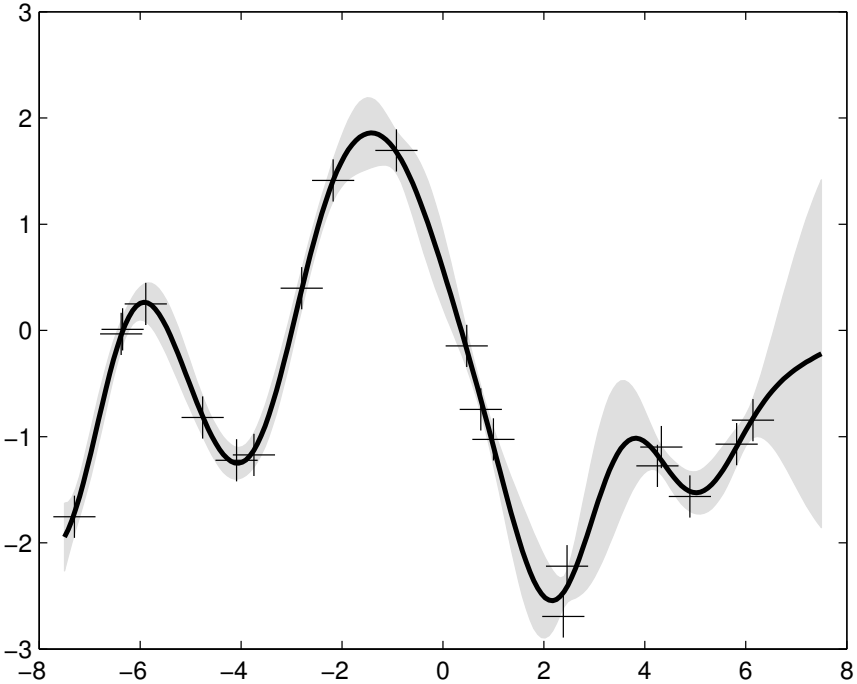
$$(\ell, \sigma_f, \sigma_y) = (1, 1, 0.1)$$



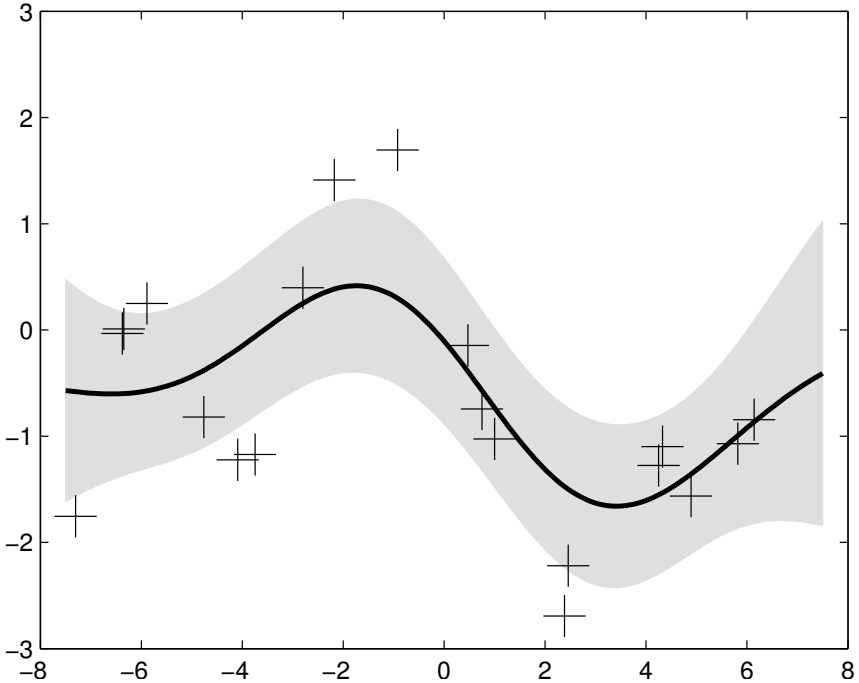
$$(\ell, \sigma_f, \sigma_y) = (0.3, 0.1?, 0.00005)$$

[Mur12, fig. 15.3]

Example with Noise



$$(\ell, \sigma_f, \sigma_y) = (1, 1, 0.1)$$



$$(\ell, \sigma_f, \sigma_y) = (3, 1.16, 0.89)$$

[Mur12, fig. 15.3]

Estimating Kernel Parameters

Either treating them as hyperparameters (grid search, random search) or maximize the marginal likelihood (empirical Bayes approach).

Model:

$$p(y \mid X) = \mathcal{N}(y \mid 0, K + \sigma_y^2 I)$$

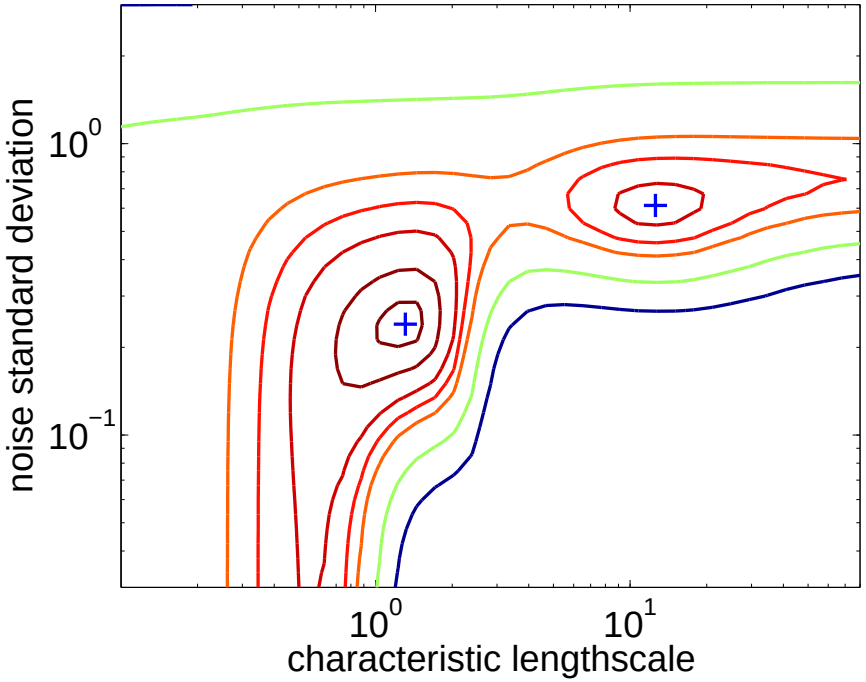
negative log likelihood:

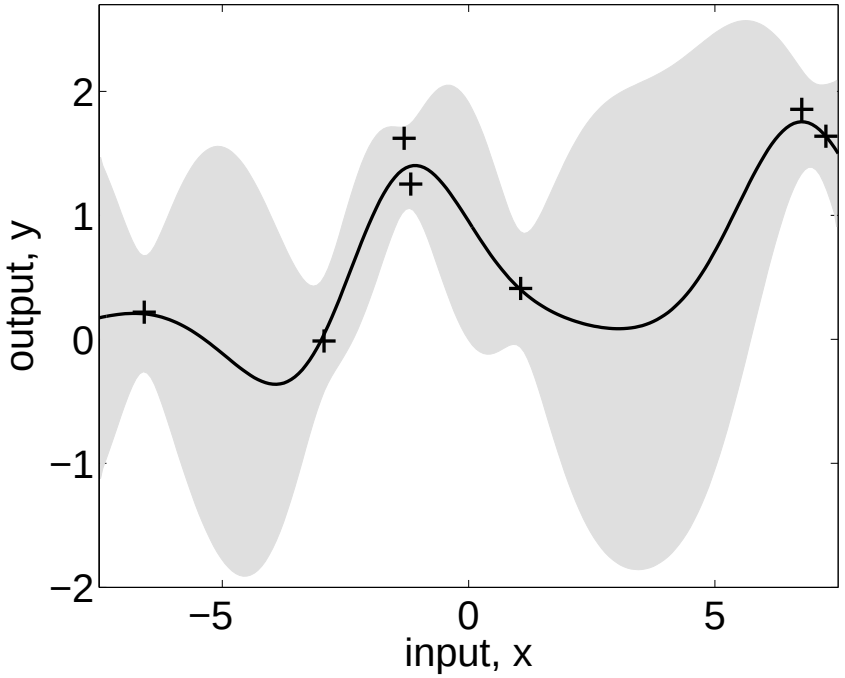
$$\begin{aligned}
L(\ell, \sigma_f) &:= -\log p(y \mid X) \\
&= \frac{1}{2} y^T (K + \sigma_y^2)^{-1} y + \frac{1}{2} \log |K + \sigma_y^2 I| + \frac{N}{2} \log(2\pi) \\
\frac{\partial L}{\partial \theta} &= -\frac{1}{2} y^T (K + \sigma_y^2)^{-1} \frac{\partial K}{\partial \theta} (K + \sigma_y^2)^{-1} y + \frac{1}{2} \mathrm{tr}((K + \sigma_y^2 I)^{-1} \frac{\partial K}{\partial \theta}) \\
&= -\frac{1}{2} \mathrm{tr}((\alpha \alpha^T - (K + \sigma_y^2 I)^{-1}) \frac{\partial K}{\partial \theta})
\end{aligned}$$

with

$$\alpha := (K + \sigma_y^2)^{-1} y, \quad \theta = \ell, \sigma_f$$

Local Minima for Kernel Parameters



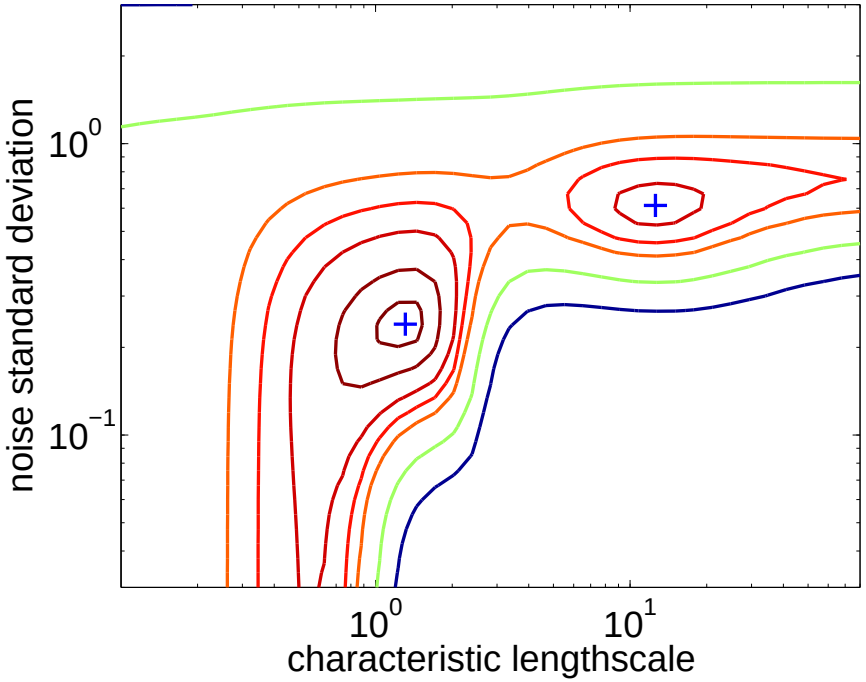


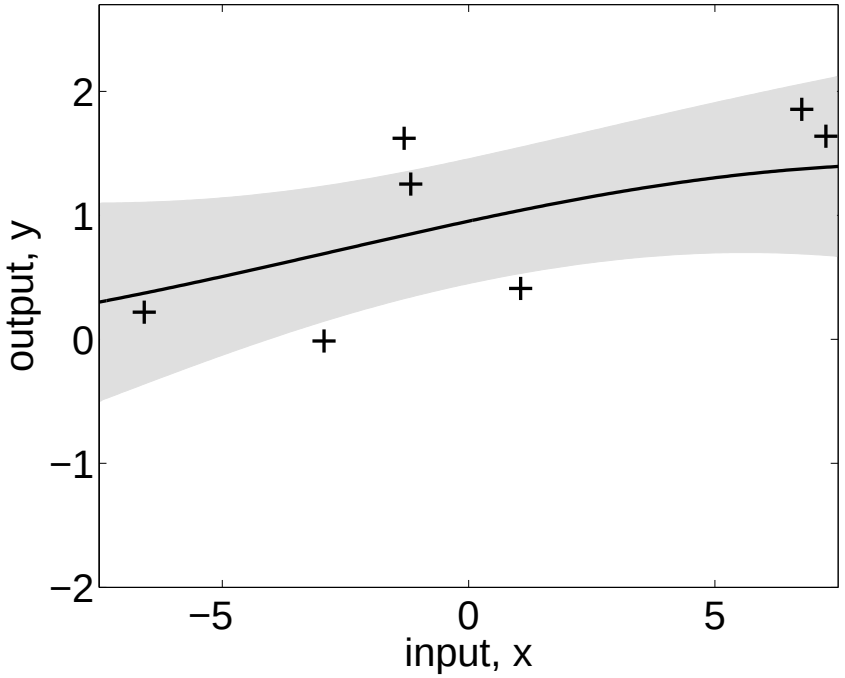
lower left minimum:

$$(\ell, \sigma_f) = (1, 0.2)$$

[Mur12, fig. 15.5]

Local Minima for Kernel Parameters





upper right minimum:

$$(\ell, \sigma_f) = (10, 0.8)$$

[Mur12, fig. 15.5]

Semi-parametric GPs

$$
\begin{aligned}
f(x) =& \beta^T \phi(x) + r(x) \\
r(x) \sim& \mathrm{GP}(r \mid 0, k(X, X))
\end{aligned}
$$

Assuming

$$\beta \sim \mathcal{N}(\beta \mid b, B), \quad \text{e.g., } b := 0, B := \sigma_\beta^2 I$$

yields just another GP

$$f(x) \sim \mathrm{GP}(f \mid \phi(X)b, k(X, X) + \phi(X)B\phi(X)^T)$$

where

$$\phi(X) := (\phi(x_1), \ldots, \phi(x_N))^T$$

Outline

Model

$$
\begin{aligned}
p(y \mid x) :=& s(y\, f(x)), \quad y \in \{+1, -1\}, s := \text{logistic} \\
f \sim& \text{GP}(f \mid 0, K(X, X))
\end{aligned}
$$

Inference

Two-step inference:

1. infer latent score variable:

$$p(f_* \mid X, y, x_*) = \int p(f_* \mid X, x_*, f) p(f \mid X, y) df$$

2. infer target:

$$\pi_* := p(y_* = +1 \mid X, y, x_*) = \int s(f_*) p(f_* \mid X, y, x_*) df_*$$

Non Gaussians are analytically intractable.

- $\rightsquigarrow$ Gaussian approximation (**Laplace approximation**)
- $\rightsquigarrow$ **Expectation Propagation (EP)**
- $\rightsquigarrow$ further methods

Posterior

$$
\begin{aligned}
p(f \mid X, y) &= \frac{p(y \mid f)p(f \mid X)}{p(y \mid X)} \propto p(y \mid f)p(f \mid X) \\
\ell(f) &= \log p(y \mid f) + \log p(f \mid X) \\
&= \log p(y \mid f) - \frac{1}{2} f^T K^{-1} f - \frac{1}{2} \log |K| - \frac{N}{2} \log 2\pi \\
\nabla \ell(f) &= \nabla \log p(y \mid f) - K^{-1} f \\
\nabla^2 \ell(f) &= \nabla^2 \log p(y \mid f) - K^{-1}
\end{aligned}
$$

for logistic:

$$
\begin{aligned}
\nabla \log p(y \mid f) &= \frac{1}{2}(y+1) - \pi \\
\nabla^2 \log p(y \mid f) &= \mathrm{diag}(-\pi \circ (1-\pi)) =: W
\end{aligned}
$$

at maximum:

$$
\nabla \ell(f) = 0 \quad \Longrightarrow \quad f = K \nabla \log p(y \mid f)
$$

Posterior

at maximum:

$$\nabla \ell(f) = 0 \quad \Longrightarrow \quad f = K \nabla \log p(y \mid f)$$

Use Newton to find a maximum:

$$\begin{aligned} f^{(t+1)} :=& f^{(t)} - (\nabla^2 \ell)^{-1} \nabla \ell \\ =& f^{(t)} - (K^{-1} + W^{(t)})^{-1} (\nabla \log p(y \mid f) - K^{-1} f^{(t)}) \\ =& (K^{-1} + W^{(t)})^{-1} (W^{(t)} f^{(t)} + \nabla \log p(y \mid f)) \end{aligned}$$

eventually yielding the maximum posterior $\hat{f}$.

Gaussian Approximation

$$p(f \mid X, y) \approx q(f \mid X, y) := \mathcal{N}(f \mid \hat{f}, (K^{-1} + W)^{-1})$$

using the Hessian as covariance matrix.

Predictions

exact mean

$$
\begin{aligned}
E_p(f_* \mid X, y, x_*) &= \int E(f_* \mid f, X, x_*) p(f \mid X, y) df \\
&= \int k(x_*)^T K^{-1} f p(f \mid X, y) df \\
&= k(x_*)^T K^{-1} E(f \mid X, y)
\end{aligned}
$$

approximated mean:

$$E_q(f_* \mid X, y, x_*) = k(x_*)^T K^{-1} \hat{f}$$

variance:

$$\mathrm{Var}_q(f_* \mid X, y, x_*) = k(x_*, x_*) - k_*^T (K + W)^{-1} k_*$$

predictions:

$$\bar{\pi}_* := E_q(\pi_* \mid X, y, x*) = \int s(f_*) q(f_* \mid X, y, x_*) df_*$$

Algorithm (Step 1)

input: K (covariance matrix), $\mathbf{y}$ (± 1 targets), $p(\mathbf{y}|\mathbf{f})$ (likelihood function)
$\mathbf{f} := \mathbf{0}$ — initialization
repeat — Newton iteration
  $W := -\nabla\nabla \log p(\mathbf{y}|\mathbf{f})$ — eval. W e.g. using eq. (3.15) or (3.16)
  $L := \text{cholesky}(I + W^{\frac{1}{2}} K W^{\frac{1}{2}})$ — $B = I + W^{\frac{1}{2}} K W^{\frac{1}{2}}$
  $\mathbf{b} := W\mathbf{f} + \nabla \log p(\mathbf{y}|\mathbf{f})$
  $\mathbf{a} := \mathbf{b} - W^{\frac{1}{2}} L^\top \backslash (L \backslash (W^{\frac{1}{2}} K \mathbf{b}))$ } eq. (3.18) using eq. (3.27)
  $\mathbf{f} := K\mathbf{a}$
until convergence — objective: $-\frac{1}{2}\mathbf{a}^\top \mathbf{f} + \log p(\mathbf{y}|\mathbf{f})$
$\log q(\mathbf{y}|X, \theta) := -\frac{1}{2}\mathbf{a}^\top \mathbf{f} + \log p(\mathbf{y}|\mathbf{f}) - \sum_i \log L_{ii}$ — eq. (3.32)
return: $\hat{\mathbf{f}} := \mathbf{f}$ (post. mode), $\log q(\mathbf{y}|X, \theta)$ (approx. log marg. likelihood)

Algorithm 3.1: Mode-finding for binary Laplace GPC. Commonly used convergence

[Rasmussen/Williams 200

Algorithm (Step 2)

input: $\hat{\mathbf{f}}$ (mode), X (inputs), $\mathbf{y}$ (± 1 targets), k (covariance function), $p(\mathbf{y}|\mathbf{f})$ (likelihood function), $\mathbf{x}_*$ test input

2: $W := -\nabla\nabla \log p(\mathbf{y}|\hat{\mathbf{f}})$

$L := \text{cholesky}(I + W^{\frac{1}{2}} K W^{\frac{1}{2}})$ $\qquad B = I + W^{\frac{1}{2}} K W^{\frac{1}{2}}$

4: $\bar{f}_* := \mathbf{k}(\mathbf{x}_*)^\top \nabla \log p(\mathbf{y}|\hat{\mathbf{f}})$ $\qquad$ eq. (3.21)

$\mathbf{v} := L \backslash \left(W^{\frac{1}{2}} \mathbf{k}(\mathbf{x}_*)\right)$

6: $\mathbb{V}[f_*] := k(\mathbf{x}_*, \mathbf{x}_*) - \mathbf{v}^\top \mathbf{v}$ $\qquad \Big\}$ eq. (3.24) using eq. (3.29)

$\bar{\pi}_* := \int \sigma(z) \mathcal{N}(z|\bar{f}_*, \mathbb{V}[f_*]) dz$ $\qquad$ eq. (3.25)

8: **return**: $\bar{\pi}_*$ (predictive class probability (for class 1))

Algorithm 3.2: Predictions for binary Laplace GPC. The posterior mode $\hat{\mathbf{f}}$ (which can be computed using Algorithm 3.1) is input. For multiple test inputs lines $4-7$ are applied to each test input. Computational complexity is $n^3/6$ operations once (line 3) plus n^2 operations per test case (line 5). The one-dimensional integral in line 7 can be done analytically for cumulative Gaussian likelihood, otherwise it is computed using an approximation or numerical quadrature.

[Rasmussen/Williams 200

Further Readings

- See also [Mur12, chapter 15].
- Conditioning Gaussians: [Mur12, section 4.3].
- Derivatives of inverse of a matrix etc., see, e.g., *The Matrix Cookbook*, `http://www.mit.edu/~wingated/stuff_i_use/matrix_cookbook.pdf`

Some Matrix Derivatives

$$\partial(X^{-1}) = -X^{-1}(\partial X)X^{-1}$$
$$\partial(\log(|X|)) = \mathrm{tr}(X^{-1}\partial X)$$

References

Kevin P. Murphy.
Machine learning: a probabilistic perspective.
The MIT Press, 2012.