Machine Learning 2

2. Gaussian Process Models (GPs)

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Syllabus

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Tue. 19.4.	(3)	A.3 Advanced Support Vector Machines
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Outline

1. GPs for Regression

2. GPs for Classification

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2. GPs for Classification

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

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

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

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

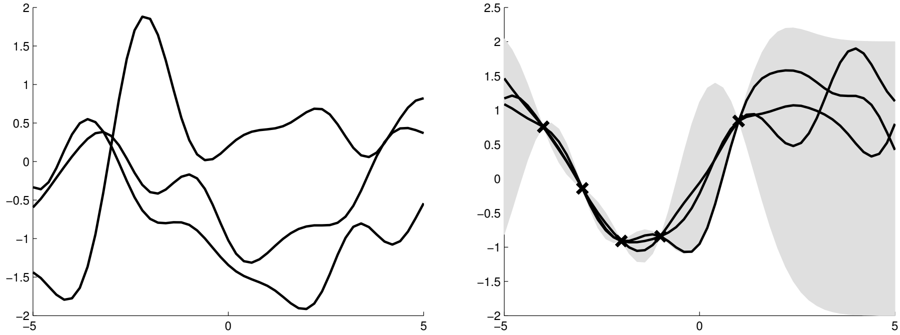
Then

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

with

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

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

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

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

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

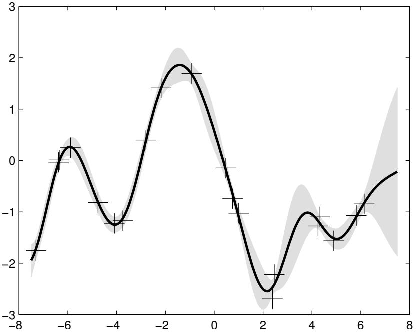
Prediction $\hat{y}$ for a single instance x:

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

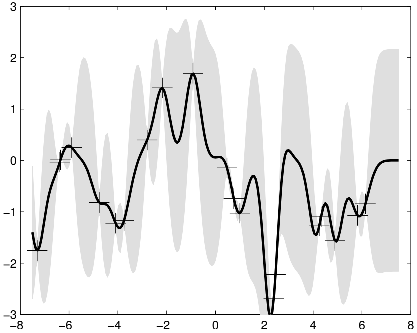
with

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

Example with Noise



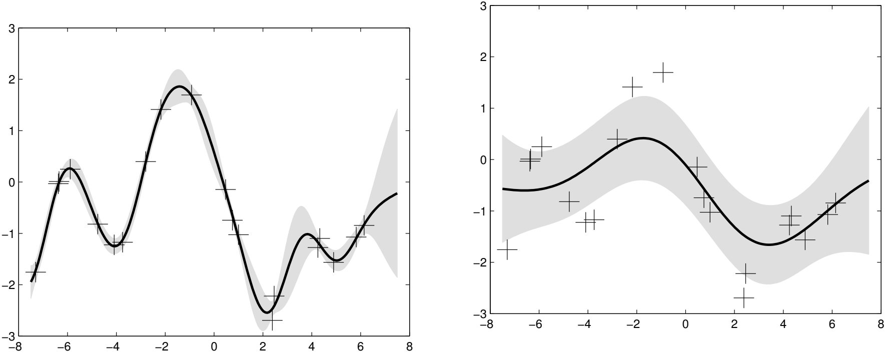
$$(\ell, \sigma_f, \sigma_y) = (1, 1, 0.1)$$



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

[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; grad. desc.).

Model:

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

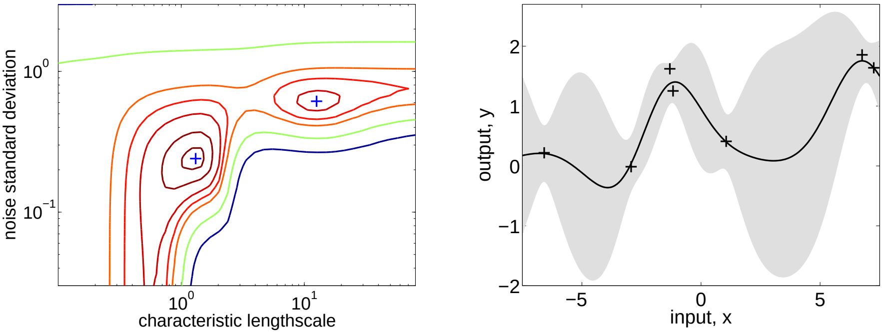
negative log likelihood:

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

with

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

Local Minima for Kernel Parameters

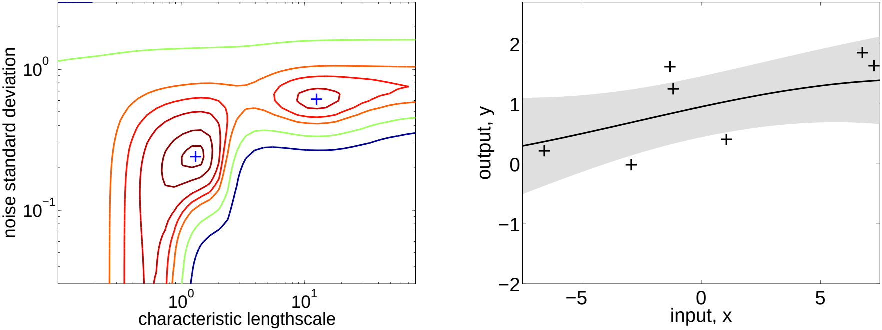


lower left minimum:

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

[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

1. GPs for Regression

2. GPs for Classification

Model

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

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:

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

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:

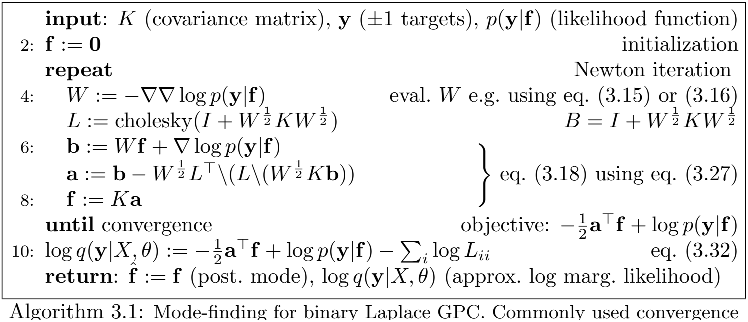
$$\mathrm{Var}_q(f_* \mid X, y, x_*) = k(x_*, x_*) - k_*^T (K + W)^{-1} k_*$$

predictions:

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

solve integral via MCMC or
probit approximation (Murphy 8.4.4.2)

Algorithm (Step 1)



```
input: $K$ (covariance matrix), $\mathbf{y}$ ($\pm 1$ 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), $\mathbf{y}$ ($\pm 1$ targets), $k$ (covariance function),
                 $p(\mathbf{y}|\mathbf{f})$ (likelihood function), $\mathbf{x}_*$ test input
2:  $W := -\nabla\nabla \log p(\mathbf{y}|\hat{\mathbf{f}})$
    $L := \text{cholesky}(I + W^{\frac{1}{2}} K W^{\frac{1}{2}})$                $B = I + W^{\frac{1}{2}} K W^{\frac{1}{2}}$
4:  $\bar{f}_* := \mathbf{k}(\mathbf{x}_*)^\top \nabla \log p(\mathbf{y}|\hat{\mathbf{f}})$                eq. (3.21)
    $\mathbf{v} := L \backslash (W^{\frac{1}{2}} \mathbf{k}(\mathbf{x}_*))$                  $\Big\}$ eq. (3.24) using eq. (3.29)
6:  $\mathbb{V}[f_*] := k(\mathbf{x}_*, \mathbf{x}_*) - \mathbf{v}^\top \mathbf{v}$
    $\bar{\pi}_* := \int \sigma(z) \mathcal{N}(z|\bar{f}_*, \mathbb{V}[f_*]) dz$                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

Approximation Methods for Large Datasets

See recent literature:

- Filippone, M. and Engler, R. 2015.
  Enabling scalable stochastic gradient-based inference for Gaussian processes by employing the Unbiased LInear System SolvEr (ULISSE), arXiv preprint arXiv:1501.05427. (2015).
- Dai, B., Xie, B., He, N., Liang, Y., Raj, A., Balcan, M.-F. and Song, L. 2014.
  Scalable Kernel Methods via Doubly Stochastic Gradients. arXiv:1407.5599 [cs, stat]. (Jul. 2014).
- Hensman, J., Fusi, N. and Lawrence, N.D. 2013.
  Gaussian processes for big data. arXiv preprint arXiv:1309.6835. (2013).

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

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

References

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