Probabilistic Machine Learning
Lecture 15
Gaussian Process Classification

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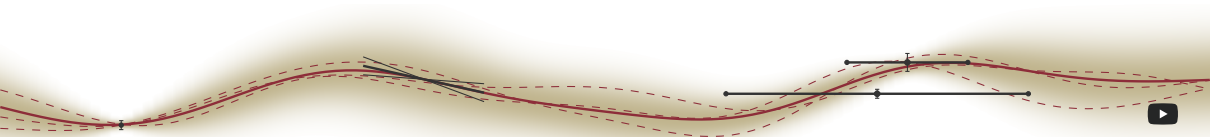

A Gaussian Process model for Classification

Logistic Regression

$$p(f) = \mathcal{GP}(f; m, k)$$

$$p(y \mid f_x) = \sigma(y f_x) = \begin{cases} \sigma(f) & \text{if } y = 1 \\ 1 - \sigma(f) & \text{if } y = -1 \end{cases} \qquad \text{using } \sigma(x) = 1 - \sigma(-x).$$

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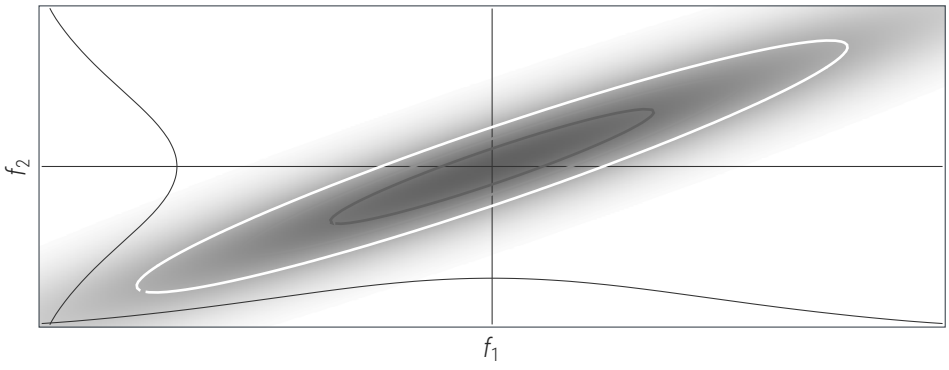
The problem: The posterior is not Gaussian!

$$p(f_X \mid Y) = \frac{p(Y \mid f_X) p(f_X)}{p(Y)} = \frac{\mathcal{N}(f_X; m, k) \prod_{i=1}^n \sigma(y_i f_{x_i})}{\int \mathcal{N}(f_X; m, k) \prod_{i=1}^n \sigma(y_i f_{x_i}) \, df_X}$$

$$\log p(f_X \mid Y) = -\frac{1}{2} f_X^\intercal k_{XX}^{-1} f_X + \sum_{i=1}^n \log \sigma(y_i f_{x_i}) + \text{const.}$$

Logistic Regression is not analytic

We'll have to break out the toolbox



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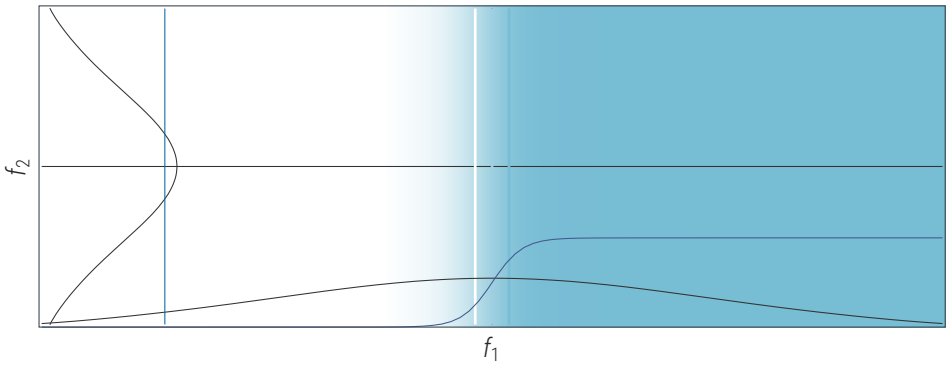

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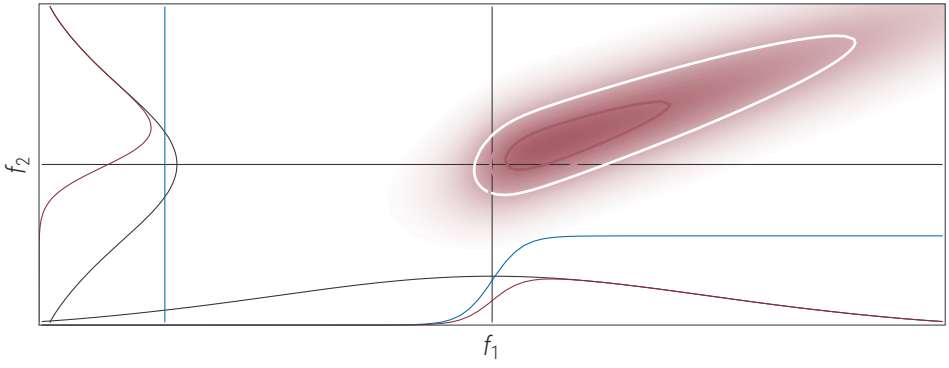
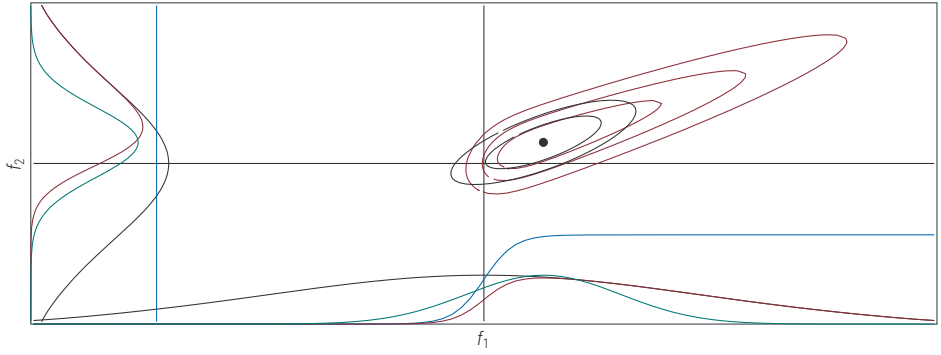


The Laplace Approximation

A local Gaussian approximation

Pierre Simon M. de Laplace, 1814



The Laplace Approximation

recap

- Consider a probability distribution $p(\theta)$ (may be a posterior $p(\theta \mid D)$ or something else)
- find a (local) **maximum** of $p(\theta)$ or (equivalently) $\log p(\theta)$

$$\hat{\theta} = \arg\max \log p(\theta) \qquad \Rightarrow \qquad \nabla \log p(\hat{\theta}) = 0$$

- perform **second order Taylor expansion** around $\theta = \hat{\theta} + \delta$ in log space

$$\log p(\delta) = \log p(\hat{\theta}) + \frac{1}{2}\delta^\intercal \left(\underbrace{\nabla\nabla^\intercal \log p(\hat{\theta})}_{=:\Psi} \right) \delta + \mathcal{O}(\delta^3)$$

- define **the Laplace approximation** q **to** p

$$q(\theta) = \mathcal{N}(\theta; \hat{\theta}, -\Psi^{-1})$$

The Laplace Approximation for GP Classification

conceptual step (implementation details coming up) [based on Rasmussen & Williams, 2006, §3.4]

- Find maximum posterior probability for **latent** f at **training points**

$$\hat{f} = \arg\max \log p(f_X \mid y)$$

- Assign approximate Gaussian posterior at training points

$$q(f_X) = \mathcal{N}(f_X; \hat{f}, -(\nabla\nabla^\intercal \log p(f_X \mid y)|_{f_X=\hat{f}})^{-1}) =: \mathcal{N}(f_X; \hat{f}, \hat{\Sigma})$$

- approximate posterior **predictions** at f_x for **latent function**

$$\begin{aligned} q(f_x \mid y) &= \int p(f_x \mid f_X) q(f_X)\, df_X = \int \mathcal{N}(f_x; m_x + k_{xX}K_{XX}^{-1}(f_X - m_X), k_{xx} - k_{xX}K_{XX}^{-1}k_{Xx}) q(f_X)\, df_X \\ &= \mathcal{N}(f_x;\ m_x + k_{xX}K_{XX}^{-1}(\hat{f} - m_X),\ k_{xx} - k_{xX}K_{XX}^{-1}k_{Xx} + k_{xX}K_{XX}^{-1}\hat{\Sigma}K_{XX}^{-1}k_{Xx}) \end{aligned}$$

Compare with *exact* predictions

$$\mathbb{E}_{p(f_x, f_X \mid y)}(f_x) = \int (\mathbb{E}_{p(f_x \mid f_X)}(f_x)) p(f_X \mid y)\, df_X = m_x + k_{xX}K_{XX}^{-1}(\mathbb{E}_{p(f_X \mid y)}(f_X) - m_X) =: \bar{f}_x$$

Recall: $p(x) = \mathcal{N}(x; m, V), p(z \mid x) = \mathcal{N}(z; Ax, B) \ \Rightarrow\ p(z) = \int p(z \mid x) p(x)\, dx = \mathcal{N}(z; Am, AVA^\intercal + B)$.

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Compare with *exact* predictions

$$\mathrm{var}_{p(f_x, f_X \mid y)}(f_x) = \int (f_x - \bar{f}_x)^2\, dp(f_x \mid f_X)\, dp(f_X) = k_{xx} - k_{xX}K_{XX}^{-1}k_{Xx} + k_{xX}K_{XX}^{-1}\mathrm{var}_{p(f_X \mid y)}(f_X)K_{XX}^{-1}k_{Xx})$$

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- compute predictions for **label probabilities**:

$$\mathbb{E}_{p(f|y)}[\pi_x] \approx \mathbb{E}_q[\pi_x] = \int \sigma(f_x) q(f_x \mid y)\, df_x \quad \text{or (not the same!)} \quad \hat{\pi}_x = \sigma(\mathbb{E}_q(f_x))$$

- the Laplace approximation is only very roughly motivated (see above)
- it can be **arbitrarily wrong**, since it is a **local** approximation
- but it is still better than a point estimate!
- and it is typically the most computationally efficient thing to try, because it uses only auto-diff and linear algebra
- for logistic regression, it tends to work relatively well, because
  - the log posterior is concave (see below)
  - the algebraic structure of the link function yields "almost" a Gaussian posterior (cf. picture above)

Today, we will focus on the Hessian/uncertainty

Loss, Gradient, Hessian for Logistic Regression

Derivation

[based on Rasmussen & Williams, 2006, §3.4]

$$p(f) = \mathcal{GP}(f, m, k) \qquad p(\boldsymbol{y} \mid \boldsymbol{f}_X) = \prod_{i=1}^{n} \sigma(y_i f_{x_i}) \qquad \sigma(z) = \frac{1}{1+e^{-x}}$$

$$\begin{aligned}
\log p(\boldsymbol{f}_X \mid \boldsymbol{y}) &= \log p(\boldsymbol{y} \mid \boldsymbol{f}_X) + \log p(\boldsymbol{f}_X) - \log p(\boldsymbol{y}) \quad \text{with} \quad \log \sigma(y_i f_{x_i}) = -\log(1 + e^{-y_i f_{x_i}}) \\
&= \sum_{i=1}^{n} \log \sigma(y_i f_{x_i}) - \frac{1}{2}(\boldsymbol{f}_X - \boldsymbol{m}_X)^\intercal K_{XX}^{-1}(\boldsymbol{f}_X - \boldsymbol{m}_X) + \text{const.} \\
\nabla \log p(\boldsymbol{f}_X \mid \boldsymbol{y}) &= \sum_{i=1}^{n} \nabla \log \sigma(y_i f_{x_i}) - K_{XX}^{-1}(\boldsymbol{f}_X - \boldsymbol{m}_X) \quad \text{with} \quad \frac{\partial \log \sigma(y_i f_{x_i})}{\partial f_{x_j}} = \delta_{ij}\left(\frac{y_i + 1}{2} - \sigma(f_{x_i})\right) \\
\nabla\nabla^\intercal \log p(\boldsymbol{f}_X \mid \boldsymbol{y}) &= \sum_{i=1}^{n} \nabla\nabla^\intercal \log \sigma(y_i f_{x_i}) - K_{XX}^{-1} \quad \text{with} \quad \frac{\partial^2 \log \sigma(y_i f_{x_i})}{\partial f_{x_a} \partial f_{x_b}} = -\delta_{ia}\delta_{ib} \underbrace{\sigma(f_{x_i})(1 - \sigma(f_{x_i}))}_{=: w_i \text{ with } 0 < w_i < 1} \\
&=: -\operatorname{diag} \boldsymbol{w} - K^{-1} = -(W + K^{-1}) \quad \leftarrow \text{convex minimization / concave maximization!}
\end{aligned}$$

Newton Optimization

more efficient optimization for convex problems

[Rasmussen & Williams, 2006, §3.4]

- since we're already computing the Hessian, we can use it to optimize the log posterior, with updates

$$f \leftarrow f - \left(\nabla\nabla^\intercal \log p(\boldsymbol{f}_X \mid \boldsymbol{y})\right)^{-1} \nabla \log p(\boldsymbol{f}_X \mid \boldsymbol{y})$$

- Newton-Raphson optimization converges in *one step* on quadratic functions
- For non-quadratic, convex problems, it asymptotically converges with quadratic convergence rate:

$$\|f_{t+1} - f^*\| \leq C \cdot \|f_t - f^*\|^2$$

- Newton's method has (at least on paper) no learning rate, and no other parameters to tune.
- It requires computing and decomposing the Hessian, though

Implementing Newton Optimization

Concrete Algorithm, preliminary form

[Rasmussen & Williams, 2006, §3.4]

$$\nabla \log p(\boldsymbol{f}_X \mid \boldsymbol{y}) = \sum_{i=1}^{n} \nabla \log \sigma(y_i f_{x_i}) - K_{XX}^{-1}(\boldsymbol{f}_X - \boldsymbol{m}_X) \quad \text{with} \quad \frac{\partial \log \sigma(y_i f_{x_i})}{\partial f_{x_j}} = \delta_{ij}\left(\frac{y_i+1}{2} - \sigma(f_{x_i})\right)$$

$$\nabla\nabla^\intercal \log p(\boldsymbol{f}_X \mid \boldsymbol{y}) = \sum_{i=1}^{n} \nabla\nabla^\intercal \log \sigma(y_i f_{x_i}) - K_{XX}^{-1} \quad \text{with} \quad \frac{\partial^2 \log \sigma(y_i f_{x_i})}{\partial f_{x_a} \partial f_{x_b}} = -\delta_{ia}\delta_{ib} \underbrace{\sigma(f_{x_i})(1-\sigma(f_{x_i}))}_{=:w_i \text{ with } 0<w_i<1}$$

$$=: -\operatorname{diag} \boldsymbol{w} - K^{-1} = -(W + K^{-1})$$

procedure GP-CLASSIFY-TRAIN($K_{XX}, m_X, \boldsymbol{y}$)
  $f \leftarrow m_X, \Delta \leftarrow \infty$ // initialize
  while $\Delta > \epsilon$ **do**
    $W \leftarrow \operatorname{diag}(\sigma(f) \odot (1-\sigma(f)))$ // $= -\nabla\nabla \log p(\boldsymbol{y} \mid f_X)$, Hessian of log likelihood
    $g \leftarrow \frac{y+1}{2} - \sigma(f) - K_{XX}^{-1}(f - m_X)$ // compute gradient
    $\Delta \leftarrow -(W + K^{-1})^{-1} g$ // Newton step
    $f \leftarrow f - \Delta$ // perform step
  end while
  return f
end procedure

Numerical stability

some advanced observations

[Rasmussen & Williams, 2006, §3.4]

- The Newton step can be numerically unstable when $(W + K^{-1})$ has very small eigenvalues. It is helpful to consider the matrix

$$B := I + W^{\frac{1}{2}} K W^{\frac{1}{2}}$$

which is symmetric positive definite, and has eigenvalues ≥ 1.

- From the matrix inversion lemma, we get

$$(W + K^{-1})^{-1} = K - K W^{\frac{1}{2}} B^{-1} W^{\frac{1}{2}} K$$

and thus

$$\begin{aligned}
\boldsymbol{f}_{t+1} &= \boldsymbol{f}_t - (\nabla\nabla^\intercal \log p(\boldsymbol{f}_t \mid \boldsymbol{y}))^{-1} \nabla \log p(\boldsymbol{f}_t \mid \boldsymbol{y}) \\
&= \boldsymbol{f}_t + (W + K^{-1})^{-1} (\nabla \log p(\boldsymbol{y} \mid \boldsymbol{f}_t)) - K^{-1} \boldsymbol{f}_t \\
&= (W + K^{-1})^{-1} (\nabla \log p(\boldsymbol{y} \mid \boldsymbol{f}_t) + W \boldsymbol{f}_t) \\
&= (K - K W^{\frac{1}{2}} B^{-1} W^{\frac{1}{2}} K)(\nabla \log p(\boldsymbol{y} \mid \boldsymbol{f}_t) + W \boldsymbol{f}_t)
\end{aligned}$$

Computing Predictions

from the Laplace approximation

[Rasmussen & Williams, 2006, §3.4]

From above:

$$q(f_x \mid y) = \int p(f_x \mid \boldsymbol{f}_X) q(\boldsymbol{f}_X)\, d\boldsymbol{f}_X = \int \mathcal{N}(f_x; m_x + k_{xX}K_{XX}^{-1}(\boldsymbol{f}_X - m_X), k_{xx} - k_{xX}K_{XX}^{-1}k_{Xx}) q(\boldsymbol{f}_X)\, d\boldsymbol{f}_X$$

$$= \mathcal{N}(f_x;\ m_x + k_{xX}K_{XX}^{-1}(\hat{\boldsymbol{f}} - m_X),\ k_{xx} - k_{xX}K_{XX}^{-1}k_{Xx} + k_{xX}K_{XX}^{-1}\hat{\Sigma}K_{XX}^{-1}k_{Xx})$$

$\log p(\boldsymbol{f}_X \mid \boldsymbol{y})$

with variance

$$= k_{xx} - k_{xX}K_{XX}^{-1}k_{Xx} + k_{xX}K_{XX}^{-1}\hat{\Sigma}K_{XX}^{-1}k_{Xx}$$
$$= k_{xx} - k_{xX}[K_{XX}^{-1} + K_{XX}^{-1}(K^{-1} + W)^{-1}K_{XX}^{-1}]k_{Xx}$$
$$= k_{xx} - k_{xX}(K + W^{-1})^{-1}k_{Xx}$$
$$= k_{xx} - k_{xX}W^{\frac{1}{2}}W^{-\frac{1}{2}}(K + W^{-1})^{-1}W^{-\frac{1}{2}}W^{\frac{1}{2}}k_{Xx}$$
$$= k_{xx} - k_{xX}W^{\frac{1}{2}}B^{-1}W^{\frac{1}{2}}k_{Xx}$$

Computing predictive *probabilities*

DJC MacKay, 1992

- We can compute the pdf of $\sigma(f)$ analytically as

$$p(\sigma(f(x))) = \mathcal{N}(\sigma^{-1}(f(x)); m_x, s_x^2) \left| \frac{\partial \sigma^{-1}(f(x))}{\partial f} \right| = \mathcal{N}(\sigma^{-1}(f); m_x, s_x^2) \frac{1}{(\sigma(1-\sigma))}$$

- but this distribution has no analytic expected value.
- Various approximations have been proposed. A simple (but imperfect) one [MacKay, 1992] is

$$\mathbb{E}_{\mathcal{N}(f;m,s^2)}(\sigma(f)) = \sigma\left(\frac{m}{\sqrt{1+\frac{\pi}{8}s^2}}\right)$$

- a more general, but also more expensive option is to build a regular "Gaussian grid" and compute an approximate integral

Code

Gaussian Process Classification:

- Supervised classification phrased in a **discriminative** model with probabilistic interpretation
- model binary outputs as a **transformation** of a **latent function** with a Gaussian process prior
- due to **non-Gaussian likelihood**, the posterior is non-Gaussian; exact inference **intractable**
- **Laplace approximation:** Find MAP estimator, second order expansion for Gaussian approximation
- tune code for numerical stability, efficient computations
- Laplace approximation provides Gaussian posterior on training points, hence evidence, predictions

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