Probabilistic Machine Learning
Lecture 14
Logistic Regression

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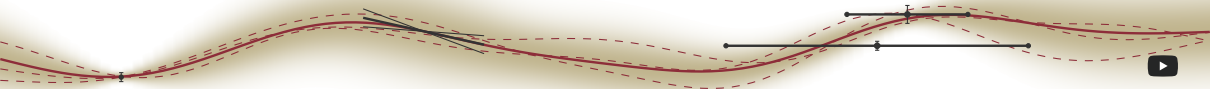


Algorithm 1 Iterative GP regression (Numerics Layer)

Input: sufficient statistics $K = k_{XX} + \sigma^2 I, \bar{y} = y - \mu_X$, initial guesses α_0, C_0
Output: defragmented statistics S, C_i, α_i

```
procedure TRAIN(K, y, C_0 = 0, α_0 = 0)
    for i ∈ {1, ..., n} do
        s_i ⇐ POLICY(S = [s_{j<i}], Z = [z_{j<i}])        // Action – load, s_i ∈ ℝ^{N×k_i}
        z_i ⇐ K s_i                                       // Observation – compute, z_i ∈ ℝ^{N×k_i}
        d_i ⇐ (I − C_{i−1} K) s_i = s_i − C_{i−1} z_i     // low-rank update, d_i ∈ ℝ^{N×k_i}
        H_i ⇐ s_i^T K d_i = z_i^T d_i                     // Schur complement, H_i ∈ ℝ^{k_i×k_i}
        C_i ⇐ C_{i−1} + d_i H_i^{−1} d_i^T                // Inverse estimate
        α_i ⇐ C_i y = α_{i−1} + d_i H_i^{−1} d_i^T ȳ      // Solution Estimate
    end for
    return S = [s_j]_{j≤i}, α_i, C_i
end procedure
procedure PREDICT(x, S, α, C)
    k_xS ⇐ k[x, S]                                        // Covariance to Observations
    μ_x ⇐ μ_x + k_xS α                                    // Point estimate
    v_xx ⇐ k_xx − k_xS C k_Sx                             // Uncertainty
end procedure
```


Computation and Inference

There is really no difference

- In least-squares regression, "training" the algorithm reduces to a *linear algebra* computation
- We have now seen that the corresponding *numerical methods* essentially reduce to smartly loading *projections* of the data in the right order
  - $s_i = e_{j(i)}$ yields the **pivoted** Cholesky decomposition, where $j(i)$ is the pivoting policy
  - the Lanczos process, initialized with $s_0 = \boldsymbol{K}\alpha_0 - \boldsymbol{C}_0\boldsymbol{y}$, yields the **preconditioned** conjugate gradient method, where $\boldsymbol{C}_0$ is the preconditioner.
  - We can think of $\alpha_0, \boldsymbol{C}_0$ as a **prior guess** for $\alpha, \boldsymbol{K}^{-1}$. Then our algorithm computes updated estimates of $\boldsymbol{K}^{-1}$.
- Side note: It turns out there are Bayesian interpretations of these point estimates with associated uncertainty for α and $\boldsymbol{K}^{-1}$ [Hennig, 2015, Wenger & Hennig, 2021, Hennig, Osborne, Kersting, 2022]

Relationship to Gradient Descent

connection to previous lecture

Lecture 12: Jacobian/Sensitivity of minimizer

$$\boldsymbol{\alpha}^\star = \arg\min_{\alpha \in \mathbb{R}^N} f(\boldsymbol{\alpha}) = \arg\min_{\alpha \in \mathbb{R}^N} \frac{1}{2}\boldsymbol{\alpha}^\intercal (k_{XX} + \sigma^2 I_N)\boldsymbol{\alpha} - \underbrace{(\boldsymbol{y} - \mu_X)}_{=\tilde{\boldsymbol{y}}}{}^\intercal \boldsymbol{\alpha}$$

$$= (k_{XX} + \sigma^2 I_N)^{-1}(\boldsymbol{y} - \mu_X)$$

$$\Rightarrow \qquad \frac{\mathrm{d}\boldsymbol{\alpha}^\star}{\mathrm{d}\boldsymbol{y}} = (k_{XX} + \sigma^2 I_N)^{-1}$$

Compare to gradient descent:

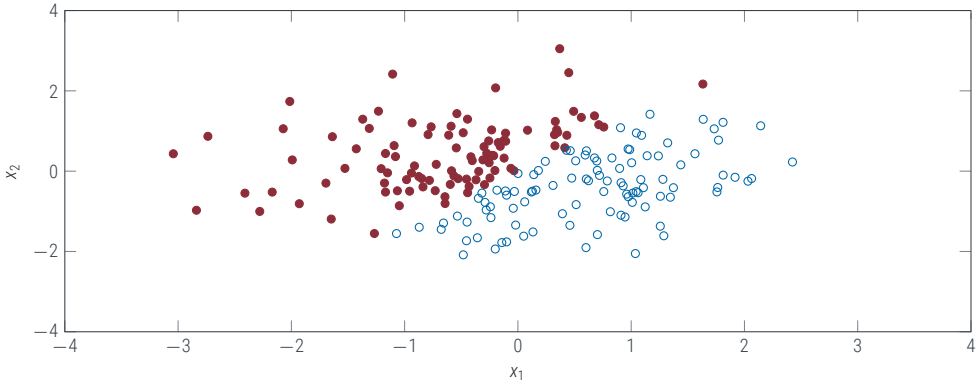
$$\frac{\partial \boldsymbol{\alpha}^*}{\partial \boldsymbol{y}} = \frac{\partial \nabla_\alpha f(\alpha)}{\partial \boldsymbol{y}} = \eta I$$

Cholesky iteratively computes a *total* derivative (a matrix inverse), while GD computes a *partial* derivative. This is why gradient descent does not converge in finite time. We pay for reducing complexity to $\mathcal{O}(N)$ and below, by losing convergence, and uncertainty.

Classification

Classification Problems

a typography of supervised learning problems



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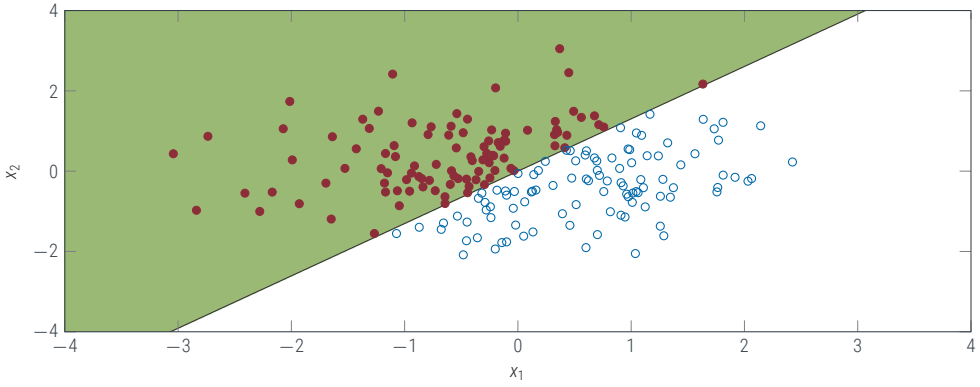

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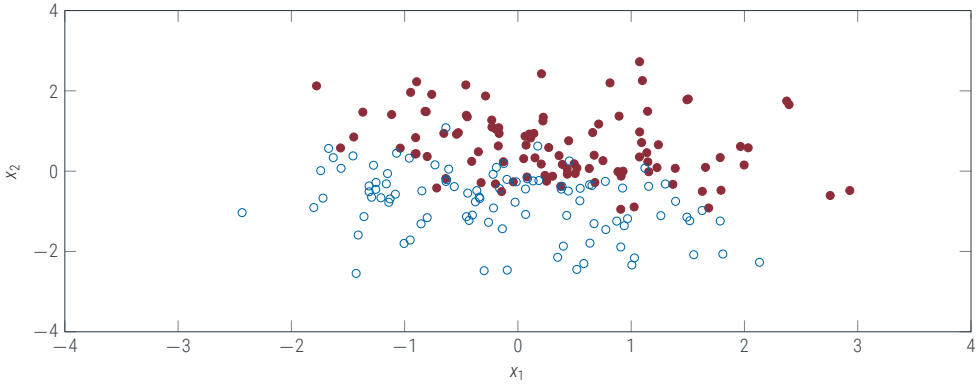

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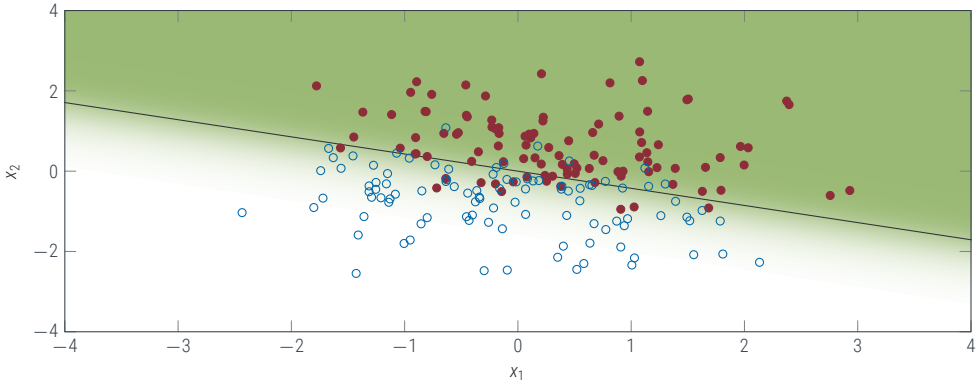

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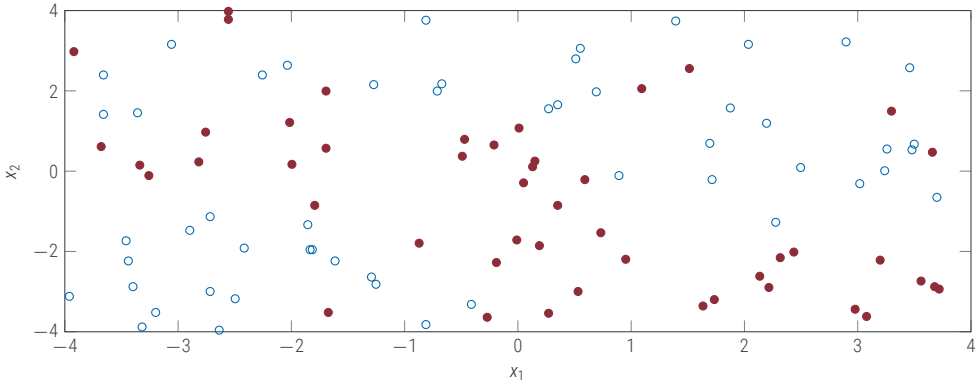

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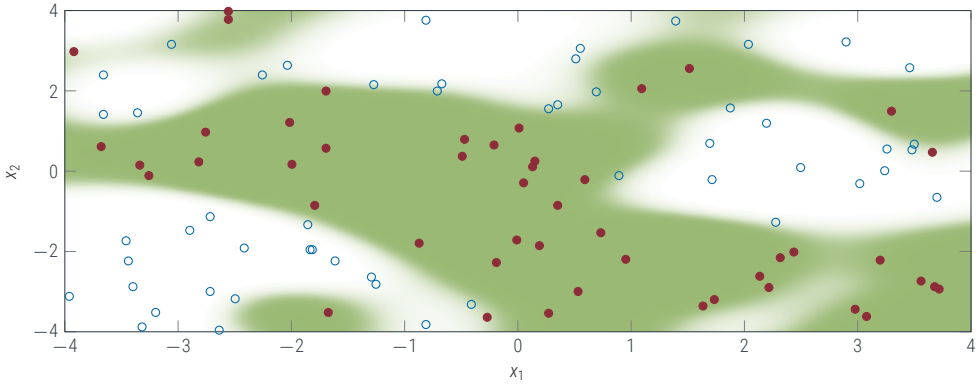

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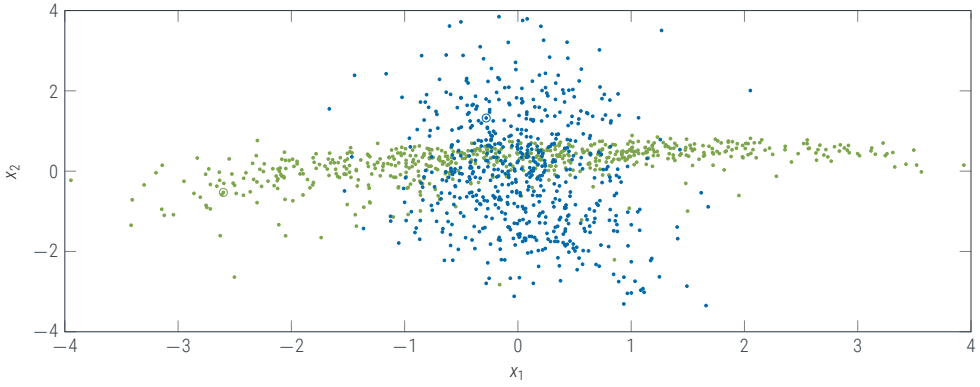

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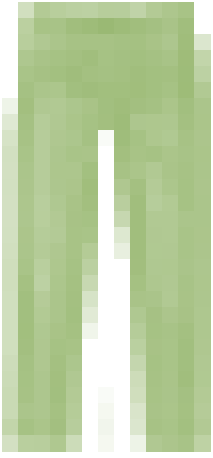

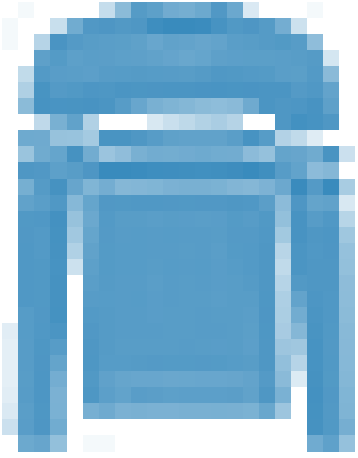

https://github.com/zalandoresearch/fashion-mnist

Classification vs. Regression

Two types of supervised learning problems

Regression:

Given supervised *data* (special case $d = 1$: univariate regression)

$$(X, Y) := (x_i, y_i)_{i=1,\ldots,n} \text{ with } x_i \in \mathbb{X}, y_i \in \mathbb{R}^d$$

find function $f : \mathbb{X} \to \mathbb{R}^d$ such that f "models" $Y \approx f(X)$.

Classification:

Given supervised *data* (special case $d = 2$: binary classification)

$$(X, Y) := (x_i, c_i)_{i=1,\ldots,n} \text{ with } x_i \in \mathbb{X}, c_i \in \{1, \ldots, d\}$$

find probability $\pi : \mathbb{X} \to U^d$ ($U^d = \{p \in [0,1]^d : \sum_{i=1}^d p_i = 1\}$) such that π "models" $y_i \sim \pi_{x_i}$.

Regression predicts a **function**, *classification* predicts a **probability**.

Until further notice, consider only discriminative binary classification:

$$y \in \{-1; +1\} \qquad x \mapsto \pi(x) =: \pi_x \in [0, 1]$$

$$p(y \mid x) = \begin{cases} \pi(x) & \text{if } y = 1 \\ 1 - \pi(x) & \text{if } y = -1 \end{cases}$$

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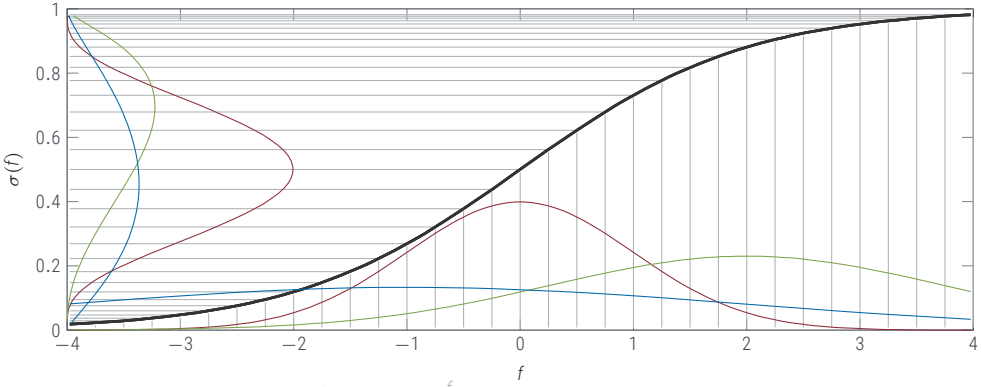
Discriminative learning phrased probabilistically:

- We would like to *learn* $\pi_x(y) = p(y \mid x)$
- This is *almost* like regression: $p(y \mid x) = \mathcal{N}(y; f_x, \sigma^2) = \pi_x(y)$
- only the *domain* is wrong: $y \in \{-1; 1\}$ vs. $y \in \mathbb{R}$.

Link Functions

sigmoids — the **logistic** link function



$$\pi_f = \sigma(f) = \frac{1}{1+\exp(-f)} = \int_{-\infty}^{f} \frac{1}{4}\,\mathrm{sech}^2\left(\frac{x}{2}\right)\,dx$$

$$\sigma(f) = 1 - \sigma(-f) \qquad f(\pi) = \ln \pi - \ln(1-\pi) \qquad \frac{d\pi}{df} = \pi(f)\cdot(1-\pi(f))$$

DEMO

- `git clone https://github.com/philipphennig/ProbML_Apps.git`
- `cd ProbML_Apps/14`
- `pip install -r requirements.txt`
- `streamlit run Lecture_14.py`

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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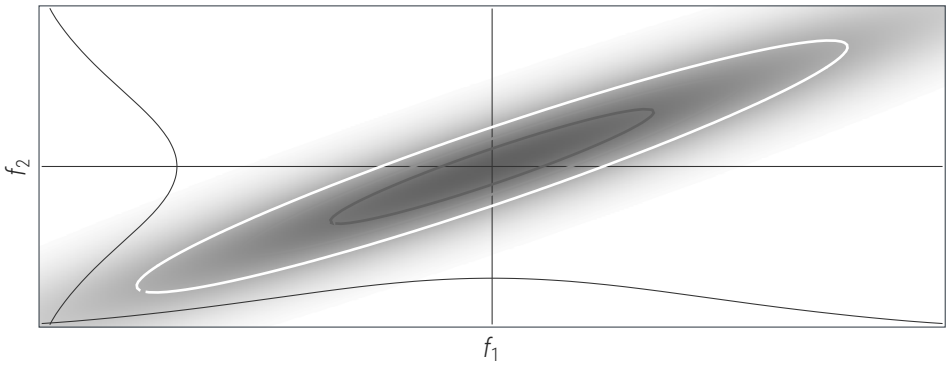
The problem: The posterior is not Gaussian!

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

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

Logistic Regression is not analytic

We'll have to break out the toolbox



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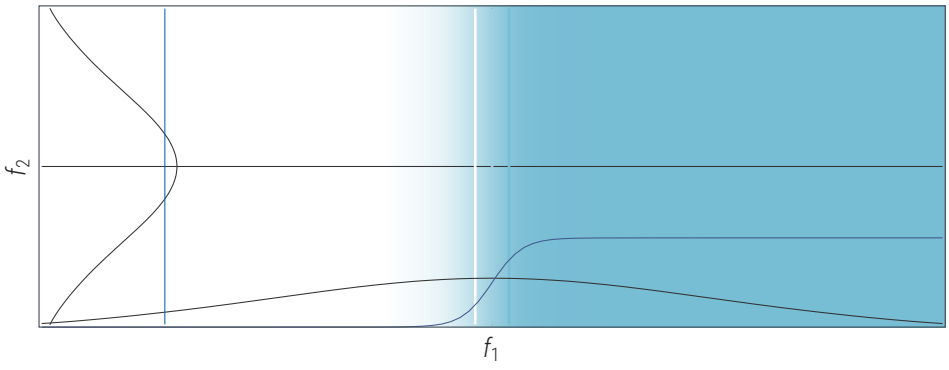

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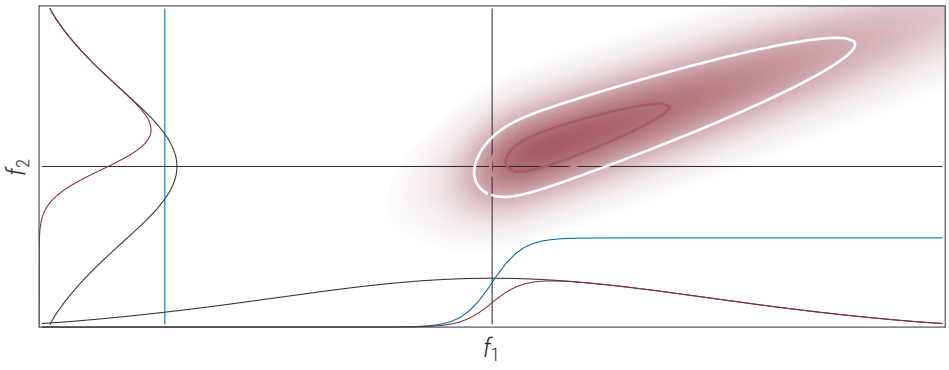
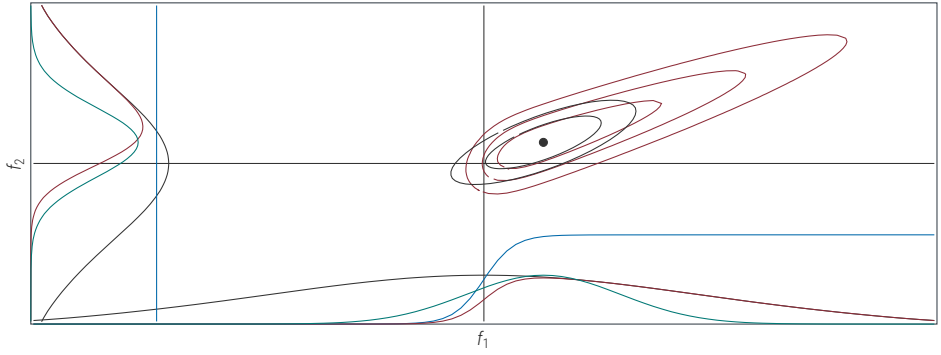


The Laplace Approximation

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**

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

- Assign approximate Gaussian posterior at training points

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

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

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

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

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

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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- 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 only implement the *mode-finding*, and leave the Hessian/uncertainty for next time

Implementing the Laplace Approximation

Derivation

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

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

$$\begin{aligned}\log p(\boldsymbol{f}_X \mid \boldsymbol{y}) &= \log p(\boldsymbol{y} \mid \boldsymbol{f}_X) + \log p(\boldsymbol{f}_X) - \log p(\boldsymbol{y}) \quad \text{with} \quad \log \sigma(y_i f_{x_i}) = -\log(1+e^{-y_i f_{x_i}}) \\ &= \sum_{i=1}^{n} \log \sigma(y_i f_{x_i}) - \frac{1}{2}(\boldsymbol{f}_X - \boldsymbol{m}_X)^\intercal K_{XX}^{-1}(\boldsymbol{f}_X - \boldsymbol{m}_X) + \text{const.}\end{aligned}$$

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

Gaussian Process Classification — (Probabilistic) Logistic Regression:

- 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

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    series = {Lecture Notes
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    institution = {Tübingen AI Center}}
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