Probabilistic Machine Learning
Lecture 22
Summary and Cleanup

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The course so far

Intermediate summary, more to come in the final lectures

Probabilities: the language of reasoning under uncertainty

Lectures 1–3

- We can describe all inference tasks by assigning **probabilities**, (or, for continuous variables probability density functions) jointly to all variables in the problem.
- Probabilities and pdfs satisfy "the rules of probability":

$$\int_{\mathbb{R}^d} p(x)\,dx = 1$$

$$p_{X_1}(x_1) = \int_{\mathbb{R}} p_X(x_1, x_2)\,dx_2 \qquad \textbf{sum rule}$$

$$p(x_1 \mid x_2) = \frac{p(x_1, x_2)}{p(x_2)} \qquad \textbf{product rule}$$

$$p(x_1 \mid x_2) = \frac{p(x_1) \cdot p(x_2 \mid x_1)}{\int p(x_1) \cdot p(x_2 \mid x_1)\,dx_1} \qquad \textbf{Bayes' Theorem.}$$

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Definition (Exponential Family, simplified form)

Consider a random variable X taking values $x \in \mathbb{X} \subset \mathbb{R}^n$. A probability distribution for X with pdf of the functional form

$$p_w(x) = h(x) \exp\left[\phi(x)^\intercal w - \log Z(w)\right] = \frac{h(x)}{Z(w)} e^{\phi(x)^\intercal w} = p(x \mid w)$$

is called an **exponential family** of probability measures. The function $\phi : \mathbb{X} \rightharpoonup \mathbb{R}^d$ is called the **sufficient statistics**. The parameters $w \in \mathbb{R}^d$ are the **natural parameters** of p_w. The normalization constant $Z(w) : \mathbb{R}^d \rightharpoonup \mathbb{R}$ is the **partition function**. The function $h(x) : \mathbb{X} \rightharpoonup \mathbb{R}_+$ is the **base measure**. For notational convenience, it can be useful to re-parametrize the natural parameters w as $w := \eta(\theta)$ in terms of *canonical parameters* θ.

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Exponential Families have Conjugate Priors

- Consider the exponential family $p_w(x \mid w) = h(x) \exp\left[\phi(x)^\intercal w - \log Z(w)\right]$
- its conjugate prior is the exponential family $F(\alpha, \nu) = \int \exp(\alpha^\intercal w - \nu \log Z(w))\, dw$

$$p_\alpha(w \mid \alpha, \nu) = \exp\left[\begin{pmatrix} w \\ -\log Z(w) \end{pmatrix}^\intercal \begin{pmatrix} \alpha \\ \nu \end{pmatrix} - \log F(\alpha, \nu)\right]$$

$$\text{because } p_\alpha(w \mid \alpha, \nu) \prod_{i=1}^{n} p_w(x_i \mid w) \propto p_\alpha\left(w \,\middle|\, \alpha + \sum_i \phi(x_i), \nu + n\right)$$

- and the predictive is

$$p(x) = \int p_w(x \mid w) p_\alpha(w \mid \alpha, \nu)\, dw = h(x) \int e^{(\phi(x)+\alpha)^\intercal w + (\nu+1) \log Z(w) - \log F(\alpha,\nu)}\, dw$$

$$= h(x) \frac{F(\phi(x) + \alpha, \nu + 1)}{F(\alpha, \nu)}$$

Computing $F(\alpha, \nu)$ can be tricky. In general, this is **the** challenge when constructing an EF.

Gaussians: Inference as Linear Algebra

Lectures 5–6

- products of Gaussians are Gaussians

$$\begin{aligned}&\mathcal{N}(x; a, A)\mathcal{N}(x; b, B)\\ &= \mathcal{N}(x; c, C)\mathcal{N}(a; b, A+B)\end{aligned}$$

$$C := (A^{-1} + B^{-1})^{-1} \qquad c := C(A^{-1}a + B^{-1}b)$$

- linear projections of Gaussians are Gaussians

$$\begin{aligned}&p(z) = \mathcal{N}(z; \mu, \Sigma)\\ \Rightarrow \quad &p(Az) = \mathcal{N}(Az, A\mu, A\Sigma A^\intercal)\end{aligned}$$

- marginals of Gaussians are Gaussians

$$\int \mathcal{N}\left[\begin{pmatrix} x \\ y \end{pmatrix}; \begin{pmatrix} \mu_x \\ \mu_y \end{pmatrix}, \begin{pmatrix} \Sigma_{xx} & \Sigma_{xy} \\ \Sigma_{yx} & \Sigma_{yy} \end{pmatrix}\right] dy = \mathcal{N}(x; \mu_x, \Sigma_{xx})$$

- (linear) conditionals of Gaussians are Gaussians

$$\begin{aligned}p(x \mid y) &= \frac{p(x, y)}{p(y)}\\ &= \mathcal{N}\left(x; \mu_x + \Sigma_{xy}\Sigma_{yy}^{-1}(y - \mu_y), \Sigma_{xx} - \Sigma_{xy}\Sigma_{yy}^{-1}\Sigma_{yx}\right)\end{aligned}$$

Bayesian inference becomes linear algebra

If $p(x) = \mathcal{N}(x; \mu, \Sigma)$ and $p(y \mid x) = \mathcal{N}(y; A^\intercal x + b, \Lambda)$, then

$$p(B^\intercal x + c \mid y) = \mathcal{N}[B^\intercal x + c; B^\intercal \mu + c + B^\intercal \Sigma A(A^\intercal \Sigma A + \Lambda)^{-1}(y - A^\intercal \mu - b), B^\intercal \Sigma B - B^\intercal \Sigma A(A^\intercal \Sigma A + \Lambda)^{-1} A^\intercal \Sigma B]$$

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$$\text{prior} \quad p(w) = \mathcal{N}(w; \mu, \Sigma) \quad \Rightarrow \quad p(f) = \mathcal{N}(f_x; \phi_x^\intercal \mu, \phi_x \Sigma \phi_x)$$

$$\text{likelihood} \quad p(y \mid w, \phi_X) = \mathcal{N}(y; \phi_X^\intercal w, \sigma^2 I) = \mathcal{N}(y; f_X, \sigma^2 I)$$

$$\begin{aligned}
\text{posterior on } \boldsymbol{w} \quad p(w \mid \boldsymbol{y}, \phi_X) &= \mathcal{N}(w; \mu + \Sigma\phi_X(\phi_X^\intercal \Sigma \phi_X + \sigma^2 I)^{-1}(\boldsymbol{y} - \phi_X^\intercal \mu), \\
&\qquad \Sigma - \Sigma\phi_X(\phi_X^\intercal \Sigma \phi_X + \sigma^2 I)^{-1}\phi_X^\intercal \Sigma) \\
&= \mathcal{N}\left(w; (\Sigma^{-1} + \sigma^{-2}\phi_X\phi_X^\intercal)^{-1}\left(\Sigma^{-1}\mu + \sigma^{-2}\phi_X \boldsymbol{y}\right),\right. \\
&\qquad \left.(\Sigma^{-1} + \sigma^{-2}\phi_X\phi_X^\intercal)^{-1}\right)
\end{aligned}$$

$$\begin{aligned}
\text{posterior on } f \quad p(f_x \mid y, \phi_X) &= \mathcal{N}(f_x; \phi_x^\intercal \mu + \phi_x^\intercal \Sigma\phi_X(\phi_X^\intercal \Sigma \phi_X + \sigma^2 I)^{-1}(y - \phi_X^\intercal \mu), \\
&\qquad \phi_x^\intercal \Sigma \phi_x - \phi_x^\intercal \Sigma\phi_X(\phi_X^\intercal \Sigma \phi_X + \sigma^2 I)^{-1}\phi_X^\intercal \Sigma \phi_x) \\
&\qquad \mathcal{N}\left(f_x; \phi_x(\Sigma^{-1} + \sigma^{-2}\phi_X\phi_X^\intercal)^{-1}\left(\Sigma^{-1}\mu + \sigma^{-2}\phi_X \boldsymbol{y}\right),\right. \\
&\qquad \left.\phi_x(\Sigma^{-1} + \sigma^{-2}\phi_X\phi_X^\intercal)^{-1}\phi_x^\intercal\right)
\end{aligned}$$

Gaussian Processes: Models with "infinite freedom"

Lectures 8-11

$$
\begin{aligned}
p(f(\bullet) \mid \boldsymbol{w}) &= \mathcal{N}(f(\bullet); \phi(\bullet)^\intercal \boldsymbol{w}, \sigma I) \\
p(f(\bullet)) &= \int p(f(\bullet) \mid \boldsymbol{w}) p(\boldsymbol{w}) \, \mathrm{d}\boldsymbol{w} \\
&= \mathcal{N}(f(\bullet); \phi(\bullet)^\intercal \mu, \phi(\bullet)^\intercal \Sigma \phi(\circ) + \sigma I)
\end{aligned}
$$

using the abstraction / encapsulation

$m(\bullet) := \phi(\bullet)^\intercal \mu$	$m : \mathbb{X} \to \mathbb{R}$	mean function
$k(\bullet, \circ) := \phi(\bullet)^\intercal \Sigma \phi(\circ)$	$k : \mathbb{X} \times \mathbb{X} \to \mathbb{R}$	covariance function, aka. **kernel**

Algorithm 1 Linear Algebra for/as Gaussian (process) inference – efficient data-loading and book-keeping

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($K, y, C_0 = 0, \alpha_0 = 0$)
    for $i \in \{1, \dots, n\}$ **do**
        $s_i \leftarrow \text{POLICY}(S = [s_{j<i}], Z = [z_{j<i}])$ // Action – `load`, $s_i \in \mathbb{R}^{N \times k_i}$
        $z_i \leftarrow K s_i$ // Observation – `compute`, $z_i \in \mathbb{R}^{N \times k_i}$
        $d_i \leftarrow (I - C_{i-1} K) s_i = s_i - C_{i-1} z_i$ // low-rank update, $d_i \in \mathbb{R}^{N \times k_i}$
        $H_i \leftarrow s_i^\top K d_i = z_i^\intercal d_i$ // Schur complement, $H_i \in \mathbb{R}^{k_i \times k_i}$
        $C_i \leftarrow C_{i-1} + d_i H_i^{-1} d_i^\top$ // Inverse estimate
        $\alpha_i \leftarrow C_i y = \alpha_{i-1} + d_i H_i^{-1} d_i^\intercal \bar{y}$ // Solution Estimate
    end for
    return $S = [s_j]_{j \leq i}, \alpha_i, C_i$
end procedure
procedure PREDICT(x, S, α, C)
    $k_{xS} \leftarrow k[x, S]$ // Covariance to Observations
    $\mu_x \leftarrow \mu_x + k_{xS} \alpha$ // Point estimate
    $v_{xx} \leftarrow k_{xx} - k_{xS} C k_{Sx}$ // Uncertainty
end procedure

Classification: approximate inference with non-Gaussian likelihoods

$$p(f) = \mathcal{GP}(f; m, k) \quad p(y \mid f_x) = \sigma(yf_x) = \begin{cases} \sigma(f) & \text{if } y = 1 \\ 1 - \sigma(f) & \text{if } y = -1 \end{cases} \qquad \text{using } \sigma(x) = 1 - \sigma(-x).$$

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

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

- Assign approximate Gaussian posterior at training points

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

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

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

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

- compute predictions for **label probabilities**:

$$\mathbb{E}_{p(f \mid y)}[\pi_x] \approx \mathbb{E}_q[\pi_x] = \int \sigma(f_x) q(f_x \mid y)\, df_x$$

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1. Realise that the loss is a **negative log-posterior**

$$\mathcal{L}(\boldsymbol{\theta}) = \left(\frac{1}{N} \sum_{i=1}^{N} \underbrace{\ell(y_i; \overbrace{f(x_i, \boldsymbol{\theta})}^{\text{deep net}})}_{\text{empirical risk}} + \underbrace{r(\boldsymbol{\theta})}_{\text{regularizer}} \right) = -\sum_{i=1}^{N} \log p(\boldsymbol{y} \mid \boldsymbol{\theta}) - \log p(\boldsymbol{\theta}) = -\log p(\boldsymbol{\theta} \mid \boldsymbol{y}) + \text{const.}$$

2. **Train the deep net *as usual*** to find $\boldsymbol{\theta}_* = \arg\max_{\boldsymbol{\theta} \in \mathbb{R}^D} p(\boldsymbol{\theta} \mid \boldsymbol{y})$
3. At $\boldsymbol{\theta}_*$, compute a **Laplace approximation** of the log-posterior, with $\Psi := \nabla\nabla^\intercal \log p(\boldsymbol{\theta}_* \mid \boldsymbol{y})$

$$\log p(\boldsymbol{\theta} \mid \boldsymbol{y}) + \text{const.} = \mathcal{L}(\boldsymbol{\theta}) \approx \mathcal{L}(\boldsymbol{\theta}_*) + {}^1\!/_2(\boldsymbol{\theta} - \boldsymbol{\theta}_*)^\intercal \Psi (\boldsymbol{\theta} - \boldsymbol{\theta}_*) = \log \mathcal{N}(\boldsymbol{\theta}; \boldsymbol{\theta}_*, -\Psi^{-1})$$

4. **Linearize** $f(\boldsymbol{x}, \boldsymbol{\theta})$ around θ_*, with $[J(\boldsymbol{x})]_{ij} = \frac{\partial f_i(\boldsymbol{x}, \boldsymbol{\theta}_*)}{\partial \theta_j}$ as $f(\boldsymbol{x}, \boldsymbol{\theta}) \approx f(\boldsymbol{x}, \boldsymbol{\theta}_*) + J(\boldsymbol{x}, \boldsymbol{\theta}_*)(\boldsymbol{\theta} - \boldsymbol{\theta}_*)$

$$\text{thus } p(f(\bullet) \mid \mathcal{D}) = \int p(f \mid w)\, dp(w) \approx \mathcal{GP}(f(\bullet); f(\bullet, \boldsymbol{\theta}_*), -J(\bullet)\Psi^{-1}J(\circ)) \quad \text{with}$$

$\mathbb{E}(f(\bullet)) = f(\bullet, \boldsymbol{\theta}_*)$ — the **trained net** as the **mean function**

$\operatorname{cov}(f(\bullet), f(\circ)) = -J(\bullet)\Psi^{-1}J(\circ)^\intercal$ — the **Laplace tangent kernel** as the **covariance function**

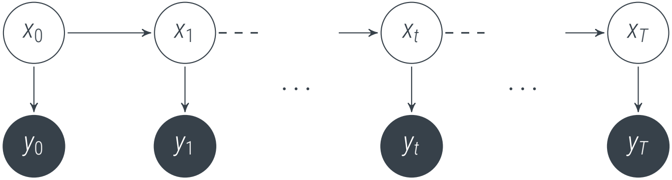
Markov Chains: $\mathcal{O}(T)$ inference in time series

Lectures 20/21

Assume:

$$p(x_t \mid X_{0:t-1}) = p(x_t \mid x_{t-1})$$

and $\quad p(y_t \mid X) = p(y_t \mid x_t)$



$$p(x_t|Y_{1:t-1}) = \int p(x_t|x_{t-1})p(x_{t-1}|Y_{1:t-1})dx_{t-1}$$

$$p(x_t \mid Y_{0:t}) = \frac{p(y_t \mid x_t)p(x_t \mid Y_{0:t-1})}{\int p(y_t \mid x_t)p(x_t \mid Y_{0:t-1})\, dx_t}$$

$$p(x_t \mid Y) = p(x_t \mid Y_{0:t}) \int p(x_{t+1} \mid x_t) \frac{p(x_{t+1} \mid Y)}{p(x_{t+1} \mid Y_{1:t})}\, dx_{t+1}$$

The Toolbox

Framework:

$$\int p(x_1, x_2)\, dx_2 = p(x_1) \qquad p(x_1, x_2) = p(x_1 \mid x_2) p(x_2) \qquad p(x \mid y) = \frac{p(y \mid x) p(x)}{p(y)}$$

Modelling:

- Directed Graphical Models
- Exponential Families (also as likelihoods)
- Gaussian Distributions
- Kernels
- Markov Chains
- Deep Networks

Computation:

- autodiff
- MAP with Laplace approximations
- Linear algebra as a computational primitive
-
-

Bayesian Hierarchical Learning

beyond analytical inference

Bayesian Hierarchical Learning

the formalism for training hyperparameters / fit architectures & models

$$p(f \mid \mathbf{y}, x, \boldsymbol{\theta}) = \frac{p(\mathbf{y} \mid f, x, \boldsymbol{\theta}) p(f \mid, \boldsymbol{\theta})}{\int p(\mathbf{y} \mid f, x, \boldsymbol{\theta}) p(f \mid, \boldsymbol{\theta})\, df} = \frac{p(\mathbf{y} \mid f, x, \boldsymbol{\theta}) p(f \mid, \boldsymbol{\theta})}{p(\mathbf{y} \mid x, \boldsymbol{\theta})}$$

- **Model parameters** like θ are also known as **hyper-parameters**.
- This is largely a computational, practical distinction:

data	are observed	$\rightarrow$ **condition**
variables	are the things we care about	$\rightarrow$ **full probabilistic treatment**
parameters	are the things we have to deal with to get the model right	$\rightarrow$ **integrate out**
hyper-parameters	are the top-level, too expensive to properly infer	$\rightarrow$ **fit**

The **model evidence** in Bayes' Theorem is the (marginal) **likelihood** for the model. So we would like

$$p(\boldsymbol{\theta} \mid \mathbf{y}) = \frac{p(\mathbf{y} \mid \boldsymbol{\theta}) p(\boldsymbol{\theta})}{\int p(\mathbf{y} \mid \boldsymbol{\theta}') p(\boldsymbol{\theta}')\, d\boldsymbol{\theta}'}$$

The Gaussian Base Case

Bayesian Hierarchical Inference for GP regression, from Lecture 10

$$p(f \mid \theta) = \mathcal{GP}(f; m_\theta, k_\theta) \qquad \text{e.g.} \quad m_\theta(\bullet) = \phi(\bullet)^\intercal \boldsymbol{\theta}, \text{ or } k_\theta(\bullet, \circ) = \theta_1 \exp\left(-\frac{(\bullet - \circ)^2}{2\theta_2^2}\right).$$

- The **evidence** in Bayes' theorem is the **marginal likelihood for the model**

$$p(f \mid \boldsymbol{y}, \boldsymbol{x}, \boldsymbol{\theta}) = \frac{p(\boldsymbol{y} \mid f, \boldsymbol{x}, \boldsymbol{\theta}) p(f \mid, \boldsymbol{\theta})}{\int p(\boldsymbol{y} \mid f, \boldsymbol{x}, \boldsymbol{\theta}) p(f \mid, \boldsymbol{\theta})\, df} = \frac{p(\boldsymbol{y} \mid f, \boldsymbol{x}, \boldsymbol{\theta}) p(f \mid, \boldsymbol{\theta})}{p(\boldsymbol{y} \mid \boldsymbol{x}, \boldsymbol{\theta})}$$

- For Gaussians *and Gaussian processes*, die evidence has **analytic form**:

$$\underbrace{\mathcal{N}(\boldsymbol{y}; \phi_X^{\boldsymbol{\theta}\intercal} w + \boldsymbol{b}, \Lambda)}_{p(\boldsymbol{y}|f,\boldsymbol{x},\boldsymbol{\theta})} \cdot \underbrace{\mathcal{N}(w, \mu, \Sigma)}_{p(f)} = \underbrace{\mathcal{N}(w; m_{\text{post}}^{\boldsymbol{\theta}}, V_{\text{post}}^{\boldsymbol{\theta}})}_{p(f|\boldsymbol{y},\boldsymbol{x},\boldsymbol{\theta})} \cdot \underbrace{\mathcal{N}(\boldsymbol{y}; \phi_X^{\boldsymbol{\theta}\intercal} \mu + b, \phi_X^{\boldsymbol{\theta}\intercal} \Sigma \phi_X^{\boldsymbol{\theta}} + \Lambda)}_{p(\boldsymbol{y}|\boldsymbol{\theta},\boldsymbol{x})}$$

$$\mathcal{N}(\boldsymbol{y}; f^{\boldsymbol{\theta}}(X), \Lambda^{\boldsymbol{\theta}}) \cdot \mathcal{GP}(f, \mu^{\boldsymbol{\theta}}, k^{\boldsymbol{\theta}}) = \mathcal{GP}(f; m_{\text{post}}^{\boldsymbol{\theta}}, V_{\text{post}}^{\boldsymbol{\theta}}) \cdot \mathcal{N}(\boldsymbol{y}; \mu^{\boldsymbol{\theta}}(X), \Lambda^{\boldsymbol{\theta}} + k^{\boldsymbol{\theta}}(X, X))$$

ML / MAP in Practice

Finding the "best fit" θ in Gaussian models

[e.g. DJC MacKay, *The evidence framework applied to classification networks*, 1992]

$$
\begin{aligned}
\hat{\boldsymbol{\theta}} &= \arg\max_{\boldsymbol{\theta}} p(\boldsymbol{y} \mid \boldsymbol{x}, \boldsymbol{\theta}) = \arg\max_{\boldsymbol{\theta}} \int \mathcal{N}(\boldsymbol{y}; f(X), \Lambda_\theta) \cdot \mathcal{N}(f_X, \mu_X, k_{XX})\, df_X \\
&= \arg\max_{\boldsymbol{\theta}} \mathcal{N}(\boldsymbol{y}; \mu_X; k_{XX} + \Lambda_\theta) \int \mathcal{N}(f_X; \mu_{y,X}, v_{y,XX})\, df_X \\
&= \arg\max_{\boldsymbol{\theta}} \mathcal{N}(\boldsymbol{y}; \quad \mu_X^\theta, \quad k_{XX}^\theta + \Lambda^\theta) \\
&= \arg\max_{\boldsymbol{\theta}} \log \mathcal{N}(\boldsymbol{y}; \quad \mu_X^\theta, \quad k_{XX}^\theta + \Lambda^\theta) \\
&= \arg\min_{\boldsymbol{\theta}} -\log \mathcal{N}(\boldsymbol{y}; \quad \mu_X^\theta, \quad k_{XX}^\theta + \Lambda^\theta) \\
&= \arg\min_{\boldsymbol{\theta}} \frac{1}{2} \left(\underbrace{(\boldsymbol{y} - \mu_X^\theta)^\intercal \left(k_{XX}^\theta + \Lambda^\theta\right)^{-1} (\boldsymbol{y} - \phi_X^{\boldsymbol{\theta}\,\intercal} \mu)}_{\text{square error}} + \underbrace{\log \left| k_{XX}^\theta + \Lambda^\theta \right|}_{\text{model complexity / \textbf{Occam factor}}} \right) + \frac{N}{2} \log 2\pi
\end{aligned}
$$

Numquam ponenda est pluralitas sine necessitate.
Plurality must never be posited without necessity.

William of Occam
(1285 (Occam, Surrey)–1349 (Munich, Bavaria))
stained-glass window by Lawrence Lee

The Evidence framework beyond GP regression

Laplace approximations yield approximate evidences.

- For general likelihoods, the evidence $p(\boldsymbol{y} \mid \boldsymbol{\theta}) = \int p(\boldsymbol{y} \mid \boldsymbol{f}, \boldsymbol{\theta}) p(\boldsymbol{f} \mid \boldsymbol{\theta})\, d\boldsymbol{f}$ will be intractable
- If we approximate it with a Gaussian by a Laplace approximation, we need to be careful with the constant term. Say we have found $\boldsymbol{f}^* = \arg\max \log p(\boldsymbol{f} \mid \boldsymbol{y})$ and $\Psi = -\nabla\nabla \log p(\boldsymbol{f} \mid \boldsymbol{y})$. Then

$$\begin{aligned}
p(\boldsymbol{y} \mid \boldsymbol{\theta}) &= \int p(\boldsymbol{y} \mid \boldsymbol{f}) p(\boldsymbol{f})\, d\boldsymbol{f} \\
&\approx \int \exp\left(\log p(\boldsymbol{y} \mid \boldsymbol{f}^*) + \log p(\boldsymbol{f}^*) - \frac{1}{2}(\boldsymbol{f} - \boldsymbol{f}^*)\Psi(\boldsymbol{f} - \boldsymbol{f}^*)\right) d\boldsymbol{f} \\
&= p(\boldsymbol{y} \mid \boldsymbol{f}^*) p(\boldsymbol{f}^*) \cdot (2\pi)^{D/2} |\Psi|^{1/2}
\end{aligned}$$

- If the prior happens to be Gaussian $p(\boldsymbol{f}) = \mathcal{N}(\boldsymbol{f}; \boldsymbol{m}, K)$, we get

$$\log p(\boldsymbol{y} \mid \boldsymbol{\theta}) \approx \log p(\boldsymbol{y} \mid \boldsymbol{f}^*) - \frac{1}{2}(\boldsymbol{f}^* - \boldsymbol{m}) K^{-1} (\boldsymbol{f}^* - \boldsymbol{m}) - \frac{1}{2} \log |B|$$

with $|B| = |K| \cdot |K^{-1} + \underbrace{\nabla\nabla^\intercal \log p(\boldsymbol{y} \mid \boldsymbol{f}^*)}_{=:W}|^{-1} = |I + K \cdot W|$.

A special option: The EM algorithm

Maximizing model Evidence

<u>The general recipe</u> for hyperparameter inference:
Consider a model with **parameters** $\boldsymbol{\theta}$, **observed data** $\boldsymbol{y}$ and **latent variables** z

- Ideally, we would like to maximize the **marginal (log-) likelihood (evidence)**

$$\log p(\boldsymbol{y} \mid \boldsymbol{\theta}) = \log \left(\int p(\boldsymbol{y}, z \mid \boldsymbol{\theta})\, dz \right) \qquad (\star)$$

- if we can not do this integral, we can try **Laplace** (as above). This is nearly always *possible* (if $\log p(\boldsymbol{y} \mid \boldsymbol{z})$ is twice differentiable), bu it is fundamentally an approximation.
- however, *in some cases*, we may be able to compute the Expectation **of the "complete data" log likelihood** (for a fixed value $\boldsymbol{\theta}_*$)

$$q(\boldsymbol{\theta}, \boldsymbol{\theta}_*) = \int p(z \mid \boldsymbol{y}, \boldsymbol{\theta}_*) \log p(\boldsymbol{y}, z \mid \boldsymbol{\theta})\, dz$$

and then Maximize $q(\boldsymbol{\theta}, \boldsymbol{\theta}_*)$ **with respect to** $\boldsymbol{\theta}$. This can be easier than $(\star)$ because the log "simplifies things" (e.g. turns products into sums, thus factors into components).

The EM Algorithm

Dempster, Laird, Rubin, *Maximum likelihood from incomplete data via the EM algorithm*, RSS B **39** (1) 1977, 1–38

Definition: The **Expectation Maximizatiion (EM)** algorithm:
Consider a model with **parameters** $\boldsymbol{\theta}$, **observed data** $\boldsymbol{y}$ and **latent variables** $\boldsymbol{z}$.

```
while not converged, do:
```

E compute the **Expected complete data log-likelihood**

$$q(\boldsymbol{\theta}, \boldsymbol{\theta}_t) = \int p(\boldsymbol{z} \mid \boldsymbol{y}, \boldsymbol{\theta}_t) \log p(\boldsymbol{y}, \boldsymbol{z} \mid \boldsymbol{\theta}) \, dz$$

M Set θ_{t+1} to **Maximize** $\boldsymbol{\theta}_{t+1} = \arg\max_{\boldsymbol{\theta}} q(\boldsymbol{\theta}, \boldsymbol{\theta}_{t+1})$.

We will see on Thursday why this is a meaningful thing to do.

Example: EM for Gauss-Markov Models

completed in this week's exercise

Consider the Gauss-Markov Model with $\boldsymbol{z} := [\boldsymbol{x}_t]_{t=0,\dots,T}$ and $\boldsymbol{\theta} := (A, Q, H, R)$.

$$p(\boldsymbol{z}, \boldsymbol{y} \mid \boldsymbol{\theta}) = p(\boldsymbol{x}_0) \prod_{t=1}^{T} p(\boldsymbol{x}_t \mid \boldsymbol{x}_{t-1}, \boldsymbol{\theta}) p(\boldsymbol{y}_t \mid \boldsymbol{x}_t, \boldsymbol{\theta}) = \mathcal{N}(\boldsymbol{x}_0; m_0, P_0) \prod_{t=1}^{T} \mathcal{N}(\boldsymbol{x}_t; A\boldsymbol{x}_{t-1}, Q) \mathcal{N}(\boldsymbol{y}_t, H\boldsymbol{x}_t, R)$$

Here it is actually possible to compute $p(\boldsymbol{y} \mid \boldsymbol{\theta})$ (see last lectures), but that term can only be maximized numerically. Instead, notice that the complete-data log-likelihood neatly separates into local terms

$$\log p(\boldsymbol{z}, \boldsymbol{y} \mid \boldsymbol{\theta}) = \log \mathcal{N}(\boldsymbol{x}_0) + \sum_{t=1}^{T} \log \mathcal{N}(\boldsymbol{x}_t; A\boldsymbol{x}_{t-1}, Q) + \sum_{t=1}^{T} \log \mathcal{N}(\boldsymbol{y}_t; H\boldsymbol{x}_t, R)$$

And the expectation of a log-Gaussian is easy to compute, because

$$\int (W\boldsymbol{x} - \boldsymbol{\mu})^\intercal \Sigma^{-1} (W\boldsymbol{x} - \boldsymbol{\mu}) \cdot \mathcal{N}(\boldsymbol{x}; \boldsymbol{m}, V)\, d\boldsymbol{x} = (\boldsymbol{\mu} - W\boldsymbol{m})^\intercal \Sigma^{-1} (\boldsymbol{\mu} - W\boldsymbol{m}) + \operatorname{tr}(W^\intercal \Sigma^{-1} W V)$$

Rest: Homework.

Summary:

- The *Evidence* in Bayes' theorem is the *marginal likelihood* of the model

$$p(\mathbf{y} \mid \theta) = \int p(\mathbf{y}, \mathbf{z} \mid \theta)\, d\mathbf{z}$$

- In principle it provides the "next level" for Bayesian inference on θ. But it is often intractable.
- Laplace approximations provide a *general, approximate* way to approximate the Evidence
- in *some* models, the **EM** algorithm offers a tractable iterative solution.

Please cite this course, as

```
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