Extending the Bayesian Deep Learning Method MultiSWAG

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Abstract

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Acknowledgements

Any acknowledgements go here.

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Introduction

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Chapter 2

Factor Analysis

2.1 Background

FA is a latent variable model which generates observations $\theta \in \mathbb{R}^d$ as follows. First, a latent vector $\mathbf{h} \in \mathbb{R}^K$, for some $K < d$, is sampled from $p(\mathbf{h}) = \mathcal{N}(\mathbf{0}, \mathbf{I})$. Next, $\mathbf{h}$ is transformed onto a K-dimensional linear subspace of $\mathbb{R}^d$ by left-multiplying it by a *factor loading* matrix $\mathbf{F} \in \mathbb{R}^{d \times K}$. The origin of this subspace is then shifted by adding a bias term $\mathbf{c} \in \mathbb{R}^d$. Finally, the data is perturbed by adding some zero mean Gaussian noise $\varepsilon \in \mathbb{R}^d$ sampled from $\mathcal{N}(\mathbf{0}, \Psi)$, where Ψ is a $d \times d$ diagonal matrix [1]. Putting all this together, an observation $\theta \in \mathbb{R}^d$ is generated according to

$$\theta = \mathbf{F}\mathbf{h} + \mathbf{c} + \varepsilon. \tag{2.1}$$

In this context, an observation θ is the parameter vector of a neural network.

It follows that, given $\mathbf{h}$, the observations θ are Gaussian distributed with mean $\mathbf{F}\mathbf{h} + \mathbf{c}$ and covariance Ψ [1]. Formally,

$$p(\theta|\mathbf{h}) = \mathcal{N}\Big(\mathbf{F}\mathbf{h} + \mathbf{c}, \Psi\Big) = \frac{1}{\sqrt{(2\pi)^d |\Psi|}} \exp\Big(-\frac{1}{2}(\theta - \mathbf{F}\mathbf{h} - \mathbf{c})^\intercal \Psi^{-1} (\theta - \mathbf{F}\mathbf{h} - \mathbf{c})\Big), \tag{2.2}$$

where $|\Psi|$ is the *determinant* of Ψ. From [1], integrating $p(\theta|\mathbf{h})$ over $\mathbf{h}$ gives the marginal distribution

$$p(\theta) = \mathcal{N}\big(\mathbf{c}, \mathbf{F}\mathbf{F}^\intercal + \Psi\big). \tag{2.3}$$

The parameters of the model are $\mathbf{c}, \mathbf{F}$ and Ψ. The value of $\mathbf{c}$ which maximises the likelihood of the observed data is the empirical mean of the observations [1], which in this case is θ_{SWA}. Having set the bias term, an expectation-maximisation (EM) or singular value decomposition (SVD) algorithm can find the maximum likelihood

estimates of $\mathbf{F}$ and Ψ [1]. However, both methods require storing all the observations in memory, making them impractical for high-dimensional data, such as the parameter vectors of deep neural networks. Two alternative online algorithms are presented in Sections 2.2 and 2.3.

2.2 Online Stochastic Gradient Ascent

In situations where learning latent variable models with the classic EM algorithm is slow, [1] suggests optimising the log-likelihood of the model parameters via gradient methods. Since FA is a latent variable model, this approach can be applied here.

In this case, the log-likelihood of the parameters $\mathbf{F}$ and Ψ given the observed data, $\theta_1, \ldots, \theta_T$, is

$$L(\mathbf{F}, \Psi) = \frac{1}{T} \sum_{t=1}^{T} \log p(\theta_t | \mathbf{F}, \Psi). \tag{2.4}$$

The partial derivatives of the log-likelihood with respect to $\mathbf{F}$ and Ψ are therefore

$$\nabla_{\mathbf{F},\Psi} L(\mathbf{F}, \Psi) = \frac{1}{T} \sum_{t=1}^{T} \nabla_{\mathbf{F},\Psi} \log p(\theta_t | \mathbf{F}, \Psi). \tag{2.5}$$

Computing $\nabla_{\mathbf{F},\Psi} L(\mathbf{F}, \Psi)$ in full would require a pass over all observations, $\theta_1, \ldots, \theta_T$. However, a stochastic gradient algorithm can be used instead, as long as the expectation of the sample derivatives is proportional to $\nabla_{\mathbf{F},\Psi} L(\mathbf{F}, \Psi)$. By using $\nabla_{\mathbf{F},\Psi} \log p(\theta_t | \mathbf{F}, \Psi)$, $t = 1, \ldots, T$, as the sample derivatives, this condition clearly holds. Hence, as long as the partial derivatives $\nabla_{\mathbf{F},\Psi} \log p(\theta_t | \mathbf{F}, \Psi)$ can be computed efficiently, they can be used in conjunction with SGD or any of its variants to optimise $\mathbf{F}$ and Ψ online.

By adapting an argument for general latent variable models in [1] to FA, the re-

quired sample derivatives can be written as

$$\begin{aligned}
\nabla_{\mathbf{F},\Psi} \log p(\theta_t|\mathbf{F},\Psi) &= \frac{1}{p(\theta_t|\mathbf{F},\Psi)} \nabla_{\mathbf{F},\Psi} p(\theta_t|\mathbf{F},\Psi) \\
&= \frac{1}{p(\theta_t|\mathbf{F},\Psi)} \nabla_{\mathbf{F},\Psi} \int_{\mathbf{h}_t} p(\theta_t,\mathbf{h}_t|\mathbf{F},\Psi) \\
&= \frac{1}{p(\theta_t|\mathbf{F},\Psi)} \int_{\mathbf{h}_t} \nabla_{\mathbf{F},\Psi} p(\theta_t,\mathbf{h}_t|\mathbf{F},\Psi) \\
&= \frac{1}{p(\theta_t|\mathbf{F},\Psi)} \int_{\mathbf{h}_t} p(\theta_t,\mathbf{h}_t|\mathbf{F},\Psi) \nabla_{\mathbf{F},\Psi} \log p(\theta_t,\mathbf{h}_t|\mathbf{F},\Psi) \\
&= \int_{\mathbf{h}_t} \frac{p(\theta_t,\mathbf{h}_t|\mathbf{F},\Psi)}{p(\theta_t|\mathbf{F},\Psi)} \nabla_{\mathbf{F},\Psi} \log p(\theta_t,\mathbf{h}_t|\mathbf{F},\Psi) \\
&= \int_{\mathbf{h}_t} p(\mathbf{h}_t|\theta_t,\mathbf{F},\Psi) \nabla_{\mathbf{F},\Psi} \log p(\theta_t,\mathbf{h}_t|\mathbf{F},\Psi) \\
&= \mathbb{E}_{p(\mathbf{h}_t|\theta_t,\mathbf{F},\Psi)} \left[\nabla_{\mathbf{F},\Psi} \log p(\theta_t,\mathbf{h}_t|\mathbf{F},\Psi) \right].
\end{aligned} \tag{2.6}$$

This is as far as the derivation in [1] goes. However, given the form of the FA model, it is possible to manipulate the sample derivatives further. In particular, using the fact that $\mathbf{h}_t \sim \mathcal{N}(\mathbf{0},\mathbf{I})$ is independent from $\mathbf{F}$ and Ψ,

$$\begin{aligned}
\nabla_{\mathbf{F},\Psi} \log p(\theta_t,\mathbf{h}_t|\mathbf{F},\Psi) &= \nabla_{\mathbf{F},\Psi} \log \left(p(\theta_t|\mathbf{h}_t,\mathbf{F},\Psi) p(\mathbf{h}_t|\mathbf{F},\Psi) \right) \\
&= \nabla_{\mathbf{F},\Psi} \log \left(p(\theta_t|\mathbf{h}_t,\mathbf{F},\Psi) p(\mathbf{h}_t) \right) \\
&= \nabla_{\mathbf{F},\Psi} \left(\log p(\theta_t|\mathbf{h}_t,\mathbf{F},\Psi) + \log p(\mathbf{h}_t) \right) \\
&= \nabla_{\mathbf{F},\Psi} \log p(\theta_t|\mathbf{h}_t,\mathbf{F},\Psi).
\end{aligned} \tag{2.7}$$

Substituting Equation (2.7) into Equation (2.6),

$$\nabla_{\mathbf{F},\Psi} \log p(\theta_t|\mathbf{F},\Psi) = \mathbb{E}_{p(\mathbf{h}_t|\theta_t,\mathbf{F},\Psi)} \left[\nabla_{\mathbf{F},\Psi} \log p(\theta_t|\mathbf{h}_t,\mathbf{F},\Psi) \right]. \tag{2.8}$$

Note that $p(\theta_t|\mathbf{h}_t,\mathbf{F},\Psi)$ is just the Gaussian distribution in Equation (2.2), given $\mathbf{F}$ and Ψ. Hence, substituting $\mathbf{c} = \theta_{\text{SWA}}$ into Equation (2.2) and applying the logarithm,

$$\begin{aligned}
\log p(\theta_t|\mathbf{h}_t,\mathbf{F},\Psi) &= -\frac{1}{2}(\theta_t - \mathbf{F}\mathbf{h}_t - \theta_{\text{SWA}})^\intercal \Psi^{-1} (\theta_t - \mathbf{F}\mathbf{h}_t - \theta_{\text{SWA}}) - \frac{1}{2}\log|\Psi| - \frac{d}{2}\log 2\pi \\
&= -\frac{1}{2}(\mathbf{d}_t - \mathbf{F}\mathbf{h}_t)^\intercal \Psi^{-1} (\mathbf{d}_t - \mathbf{F}\mathbf{h}_t) - \frac{1}{2}\log|\Psi| - \frac{d}{2}\log 2\pi,
\end{aligned} \tag{2.9}$$

where $\mathbf{d}_t = \theta_t - \theta_{\text{SWA}}$. This is convenient, since Equation (2.9) can be differentiated with respect to both $\mathbf{F}$ and Ψ. Of course, this requires access to θ_{SWA}, which is not available during training. As a compromise - and following the approach of the SWAG covariance approximation - θ_{SWA} can be replaced by the running average of the neural network's parameter vectors.

2.2.1 Partial derivatives with respect to $\mathbf{F}$

From [3], for any symmetric matrix $\mathbf{W}$,

$$\nabla_{\mathbf{A}}(\mathbf{x}-\mathbf{As})^{\intercal}\mathbf{W}(\mathbf{x}-\mathbf{As}) = -2\mathbf{W}(\mathbf{x}-\mathbf{As})\mathbf{s}^{\intercal}. \tag{2.10}$$

Hence, differentiating Equation (2.9) with respect to $\mathbf{F}$ gives

$$\nabla_{\mathbf{F}} \log p(\theta_t|\mathbf{h}_t,\mathbf{F},\Psi) = \Psi^{-1}(\mathbf{d}_t-\mathbf{F}\mathbf{h}_t)\mathbf{h}_t^{\intercal}. \tag{2.11}$$

It then follows from Equation (2.8) that $\nabla_{\mathbf{F}} \log p(\theta_t|\mathbf{F},\Psi)$ is the expected value of $\Psi^{-1}(\mathbf{d}_t-\mathbf{F}\mathbf{h}_t)\mathbf{h}_t^{\intercal}$ over the distribution $p(\mathbf{h}_t|\theta_t,\mathbf{F},\Psi)$. Letting $\mathbb{E}[\cdot]$ denote $\mathbb{E}_{p(\mathbf{h}_t|\theta_t,\mathbf{F},\Psi)}[\cdot]$ to simplify the notation,

$$\begin{aligned}\nabla_{\mathbf{F}} \log p(\theta_t|\mathbf{F},\Psi) &= \mathbb{E}\left[\Psi^{-1}(\mathbf{d}_t-\mathbf{F}\mathbf{h}_t)\mathbf{h}_t^{\intercal}\right] \\ &= \Psi^{-1}\left(\mathbb{E}\left[\mathbf{d}_t\mathbf{h}_t^{\intercal}\right]-\mathbb{E}\left[\mathbf{F}\mathbf{h}_t\mathbf{h}_t^{\intercal}\right]\right) \\ &= \Psi^{-1}\left(\mathbf{d}_t\mathbb{E}\left[\mathbf{h}_t^{\intercal}\right]-\mathbf{F}\mathbb{E}\left[\mathbf{h}_t\mathbf{h}_t^{\intercal}\right]\right).\end{aligned} \tag{2.12}$$

From the E-step of the EM algorithm for FA in [1], $p(\mathbf{h}_t|\theta_t,\mathbf{F},\Psi) \propto \mathcal{N}(\mathbf{m}_t,\Sigma)$, where

$$\Sigma = (\mathbf{I}+\mathbf{F}^{\intercal}\Psi^{-1}\mathbf{F})^{-1} \quad \text{and} \quad \mathbf{m}_t = \Sigma\mathbf{F}^{\intercal}\Psi^{-1}\mathbf{d}_t. \tag{2.13}$$

Hence, using identities from [3],

$$\mathbb{E}\left[\mathbf{h}_t^{\intercal}\right] = \mathbf{m}_t^{\intercal} \quad \text{and} \quad \mathbb{E}\left[\mathbf{h}_t\mathbf{h}_t^{\intercal}\right] = \Sigma+\mathbf{m}_t\mathbf{m}_t^{\intercal}. \tag{2.14}$$

Finally, substituting Equation (2.14) into Equation (2.12),

$$\nabla_{\mathbf{F}} \log p(\theta_t|\mathbf{F},\Psi) = \Psi^{-1}\left(\mathbf{d}_t\mathbf{m}_t^{\intercal}-\mathbf{F}(\Sigma+\mathbf{m}_t\mathbf{m}_t^{\intercal})\right). \tag{2.15}$$

2.2.2 Partial derivatives with respect to Ψ

In order to differentiate Equation (2.9) with respect to Ψ, it helps to use the fact that Ψ is diagonal. First consider $\mathbf{X}^{-1} = \text{diag}(\frac{1}{x_1},\ldots,\frac{1}{x_d})$ and $\mathbf{a} = (a_1,\ldots,a_d)^{\intercal}$. Then

$$\mathbf{a}^{\intercal}\mathbf{X}^{-1}\mathbf{a} = \sum_{i=1}^{d}\frac{a_i^2}{x_i}, \tag{2.16}$$

and so

$$\frac{\partial}{\partial x_i}\mathbf{a}^{\intercal}\mathbf{X}^{-1}\mathbf{a} = \frac{-a_i^2}{x_i^2} \tag{2.17}$$

for $i = 1, \ldots, d$. Since the partial derivatives of Equation (2.16) with respect to the off-diagonal entries of $\mathbf{X}$ are zero,

$$\begin{aligned} \nabla_{\mathbf{X}}(\mathbf{a}^\intercal \mathbf{X}^{-1}\mathbf{a}) &= \operatorname{diag}\Big(\frac{-a_1^2}{x_1^2}, \ldots, \frac{-a_d^2}{x_d^2}\Big) \\ &= -\operatorname{diag}\big(\operatorname{diag}(\mathbf{X}^{-2}) \odot \mathbf{a}^2\big), \end{aligned} \tag{2.18}$$

where $\odot$ denotes the element-wise matrix product (with broadcasting, if applicable) and the square of a vector is applied element-wise. Also, when applied to a d-length vector, $\operatorname{diag}(\cdot)$ represents the $d \times d$ diagonal matrix with the vector on its diagonal, and when applied to a $d \times d$ matrix, $\operatorname{diag}(\cdot)$ represents the d-length vector consisting of the diagonal entries of the matrix. Substituting $\mathbf{X} = \Psi$ and $\mathbf{a} = \mathbf{d}_t - \mathbf{F}\mathbf{h}_t$, into Equation (2.18),

$$\nabla_{\Psi}(\mathbf{d}_t - \mathbf{F}\mathbf{h}_t)^\intercal \Psi^{-1}(\mathbf{d}_t - \mathbf{F}\mathbf{h}_t) = -\operatorname{diag}\big(\operatorname{diag}(\Psi^{-2}) \odot (\mathbf{d}_t - \mathbf{F}\mathbf{h}_t)^2\big). \tag{2.19}$$

Also, using the identity $\nabla_{\mathbf{X}} \log|\mathbf{X}| = \mathbf{X}^{-\intercal}$ from [3] and the fact that $\Psi^{-\intercal} = \Psi^{-1}$,

$$\nabla_{\Psi} \log|\Psi| = \Psi^{-1}. \tag{2.20}$$

Hence, the partial derivatives of Equation (2.9) with respect to Ψ are

$$\nabla_{\Psi} \log p(\theta_t|\mathbf{h}_t, \mathbf{F}, \Psi) = \frac{1}{2}\operatorname{diag}\big(\operatorname{diag}(\Psi^{-2}) \odot (\mathbf{d}_t - \mathbf{F}\mathbf{h}_t)^2\big) - \frac{1}{2}\Psi^{-1}. \tag{2.21}$$

Again, letting $\mathbb{E}[\cdot]$ denote $\mathbb{E}_{p(\mathbf{h}_t|\theta_t,\mathbf{F},\Psi)}[\cdot]$, it follows from Equation (2.8) that

$$\begin{aligned} 2 \cdot \nabla_{\Psi} \log p(\theta_t|\mathbf{F}, \Psi) &= \mathbb{E}\big[\operatorname{diag}\big(\operatorname{diag}(\Psi^{-2}) \odot (\mathbf{d}_t - \mathbf{F}\mathbf{h}_t)^2\big) - \Psi^{-1}\big] \\ &= \operatorname{diag}\Big(\mathbb{E}\big[\operatorname{diag}(\Psi^{-2}) \odot (\mathbf{d}_t - \mathbf{F}\mathbf{h}_t)^2\big]\Big) - \mathbb{E}\big[\Psi^{-1}\big] \\ &= \operatorname{diag}\Big(\operatorname{diag}(\Psi^{-2}) \odot \mathbb{E}\big[(\mathbf{d}_t - \mathbf{F}\mathbf{h}_t)^2\big]\Big) - \Psi^{-1}. \end{aligned} \tag{2.22}$$

Now, expanding the expectation inside Equation (2.22) and substituting in the expressions from Equation (2.14),

$$\begin{aligned} \mathbb{E}\big[(\mathbf{d}_t - \mathbf{F}\mathbf{h}_t)^2\big] &= \mathbb{E}\big[\mathbf{d}_t \odot \mathbf{d}_t\big] - 2\mathbb{E}\big[\mathbf{d}_t \odot (\mathbf{F}\mathbf{h}_t)\big] + \mathbb{E}\big[(\mathbf{F}\mathbf{h}_t) \odot (\mathbf{F}\mathbf{h}_t)\big] \\ &= \mathbf{d}_t \odot \mathbf{d}_t - 2\mathbf{d}_t \odot \big(\mathbf{F}\mathbb{E}\big[\mathbf{h}_t\big]\big) + \mathbb{E}\big[\operatorname{diag}(\mathbf{F}\mathbf{h}_t\mathbf{h}_t^\intercal\mathbf{F}^\intercal)\big] \\ &= \mathbf{d}_t \odot \mathbf{d}_t - 2\mathbf{d}_t \odot (\mathbf{F}\mathbf{m}_t) + \operatorname{diag}\big(\mathbb{E}\big[\mathbf{F}\mathbf{h}_t\mathbf{h}_t^\intercal\mathbf{F}^\intercal\big]\big) \\ &= \mathbf{d}_t \odot \mathbf{d}_t - 2\mathbf{d}_t \odot (\mathbf{F}\mathbf{m}_t) + \operatorname{diag}\big(\mathbf{F}\mathbb{E}\big[\mathbf{h}_t\mathbf{h}_t^\intercal\big]\mathbf{F}^\intercal\big) \\ &= \mathbf{d}_t \odot \mathbf{d}_t - 2\mathbf{d}_t \odot (\mathbf{F}\mathbf{m}_t) + \operatorname{diag}\big(\mathbf{F}(\Sigma + \mathbf{m}_t\mathbf{m}_t^\intercal)\mathbf{F}^\intercal\big). \end{aligned} \tag{2.23}$$

Finally, substituting Equation (2.23) into Equation (2.22) and rearranging,

$$\nabla_{\Psi} \log p(\theta_t|\mathbf{F},\Psi) = \operatorname{diag}\left(\frac{1}{2}\operatorname{diag}(\Psi^{-2}) \odot \Big(\mathbf{d}_t \odot \mathbf{d}_t - 2\mathbf{d}_t \odot (\mathbf{F}\mathbf{m}_t) + \operatorname{diag}\big(\mathbf{F}(\Sigma + \mathbf{m}_t\mathbf{m}_t^{\intercal})\mathbf{F}^{\intercal}\big)\Big)\right) - \frac{1}{2}\Psi^{-1}. \tag{2.24}$$

2.2.3 Practical implementation

In practice, storing the full $d \times d$ covariance matrix Ψ (or its inverse) would be infeasible for high-dimensional $\theta_t \in \mathbb{R}^d$. However, since Ψ is diagonal and the partial derivatives of the log-likelihood with respect to the off-diagonal are always zero, it suffices to work with the diagonal entries only. All occurrences of $d \times d$ matrices can then be removed from the gradient calculations.

First, note that the partial derivatives with respect to both $\mathbf{F}$ and Ψ depend on $\mathbf{m}_t$ and Σ from Equation (2.13), which themselves depend on Ψ^{-1}. Let $\psi = \operatorname{diag}(\Psi)$ and $\psi^{-n} = \operatorname{diag}(\Psi^{-n})$ for $n \in \mathbb{N}^+$. Then

$$\mathbf{F}^{\intercal}\Psi^{-1} = (\mathbf{F} \odot \psi^{-1})^{\intercal}. \tag{2.25}$$

Now, setting $\mathbf{C} = (\mathbf{F} \odot \psi^{-1})^{\intercal}$ and substituting into Equation (2.13), it follows that

$$\Sigma = (\mathbf{I} + \mathbf{C}\mathbf{F})^{-1} \quad \text{and} \quad \mathbf{m}_t = \Sigma\mathbf{C}\mathbf{d}_t. \tag{2.26}$$

These more efficient values can then be used in Equation (2.15), which itself can be simplified to

$$\nabla_{\mathbf{F}} \log p(\theta_t|\mathbf{F},\Psi) = \psi^{-1} \odot \big(\mathbf{d}_t\mathbf{m}_t^{\intercal} - \mathbf{F}(\Sigma + \mathbf{m}_t\mathbf{m}_t^{\intercal})\big). \tag{2.27}$$

Also, the partial derivatives with respect to Ψ in Equation (2.24) can be re-written with respect to ψ, as

$$\nabla_{\psi} \log p(\theta_t|\mathbf{F},\Psi) = \frac{1}{2}\psi^{-2} \odot \Big(\mathbf{d}_t \odot \mathbf{d}_t - 2\mathbf{d}_t \odot (\mathbf{F}\mathbf{m}_t) + \operatorname{sum}\big((\mathbf{F}(\Sigma + \mathbf{m}_t\mathbf{m}_t^{\intercal})) \odot \mathbf{F},\ \dim = 1\big)\Big) - \frac{1}{2}\psi^{-1}, \tag{2.28}$$

where $\operatorname{sum}(\cdot,\ \dim = 1)$ denotes the operation of summing along the rows of a matrix.

One final point is that the elements of ψ must be positive, since they represent variances. One way to achieve this is by using the re-parameterisation $\psi = \exp\beta$ for

some unconstrained parameter $\beta \in \mathbb{R}^d$. Then the gradient updates can be performed on β instead of ψ. Using the chain rule from calculus,

$$\begin{aligned}\nabla_\beta \log p(\theta_t|\mathbf{F},\Psi) &= \nabla_\psi \log p(\theta_t|\mathbf{F},\Psi) \odot \nabla_\beta \exp\beta \\ &= \nabla_\psi \log p(\theta_t|\mathbf{F},\Psi) \odot \exp\beta \\ &= \nabla_\psi \log p(\theta_t|\mathbf{F},\Psi) \odot \psi,\end{aligned} \tag{2.29}$$

where $\nabla_\psi \log p(\theta_t|\mathbf{F},\Psi)$ is given in Equation (2.28).

Pseudo code for online stochastic gradient ascent (SGA) for FA is given in Algorithm 1.

Algorithm 1 Online Stochastic Gradient Ascent for Factor Analysis

Input: Observation dimension d, latent dimension K, learning rate $\alpha > 0$

Initialise $\mathbf{F} \in \mathbb{R}^{d\times K}$, $\psi > \mathbf{0} \in \mathbb{R}^d$, $\overline{\theta}_0 = \mathbf{0}^d$
$\beta \leftarrow \log\psi$
for $t = 1,\ldots,T$ **do**
    Sample observation $\theta_t \in \mathbb{R}^d$
    $\overline{\theta}_t \leftarrow \overline{\theta}_{t-1} + \frac{1}{t}\left(\overline{\theta}_t - \overline{\theta}_{t-1}\right)$
    $\mathbf{d}_t \leftarrow \theta_t - \overline{\theta}_t$
    $\mathbf{C} \leftarrow (\mathbf{F} \odot \psi^{-1})^\intercal$ (with broadcasting)
    $\Sigma \leftarrow (\mathbf{I} + \mathbf{CF})^{-1}$
    $\mathbf{m}_t \leftarrow \Sigma\mathbf{C}\mathbf{d}_t$
    Compute $\nabla_\mathbf{F} \log p(\theta_t|\mathbf{F},\Psi)$ according to Equation (2.27)
    Compute $\nabla_\beta \log p(\theta_t|\mathbf{F},\Psi)$ according to Equation (2.29)
    $\mathbf{F} \leftarrow \mathbf{F} + \alpha\nabla_\mathbf{F} \log p(\theta_t|\mathbf{F},\Psi)$
    $\beta \leftarrow \beta + \alpha\nabla_\beta \log p(\theta_t|\mathbf{F},\Psi)$
    $\psi \leftarrow \exp\beta$
end for
$\theta_{\text{SWA}} \leftarrow \overline{\theta}_T$
return $\theta_{\text{SWA}}, \mathbf{F}, \psi$

2.3 Online Expectation-Maximisation

The classic EM algorithm for FA iteratively optimises the log-likelihood of $\mathbf{F}$ and Ψ by alternating "E" and "M" steps until convergence. Using properties of the Kullback-

Leibler divergence, it can be shown that

$$L(\mathbf{F}, \Psi) \geq -\sum_{t=1}^{T} \mathbb{E}_{q(\mathbf{h}_t|\theta_t)}\big[\log q(\mathbf{h}_t|\theta_t)\big] + \sum_{t=1}^{T} \mathbb{E}_{q(\mathbf{h}_t|\theta_t)}\big[\log p(\mathbf{h}_t, \theta_t|\mathbf{F}, \Psi)\big], \tag{2.30}$$

where the first and second terms on the right-hand side are called the *entropy* and *energy*, respectively, and $q(\mathbf{h}_t|\theta_t)$, $t = 1, \ldots, T$, are known as the *variational* distributions [1]. The EM algorithm optimises this lower bound on the log-likelihood with respect to $\mathbf{F}$, Ψ and also $q(\mathbf{h}_t|\theta_t)$, hence the name "variational distributions". The idea is that, by pushing up the lower bound, the log-likelihood $L(\mathbf{F}, \Psi)$ will hopefully increase as well. In fact, it is guaranteed that each iteration of EM does not decrease $L(\mathbf{F}, \Psi)$, which again follows from the properties of the Kullback-Leibler divergence [1].

2.3.1 E-step

In the batch E-step, $\mathbf{F}$ and Ψ are fixed and Equation (2.30) is maximised with respect to $q(\mathbf{h}_t|\theta_t)$, $t = 1, \ldots, T$. From [1], the optimal variational distributions are

$$q(\mathbf{h}_t|\theta_t) = p(\mathbf{h}_t|\theta_t, \mathbf{F}, \Psi) \propto \mathcal{N}(\mathbf{m}_t, \Sigma), \tag{2.31}$$

where $\mathbf{m}_t$ and Σ are given in Equation (2.26). Note that this optimisation can be performed separately for each θ_t as it is sampled, using the estimates of $\mathbf{F}$ and Ψ on iteration t. However, in batch EM all $q(\mathbf{h}_t|\theta_t)$ are updated on every iteration. This is clearly not possible in an online algorithm which discards θ_t before sampling θ_{t+1}. Therefore, as a compromise, in the online version each $q(\mathbf{h}_t|\theta_t)$ will be computed once only, on iteration t, and held fixed thereafter. The only other detail is that the batch algorithm uses θ_{SWA} to compute $\mathbf{m}_t$. As θ_{SWA} is not available during training, it will be replaced by the running average of the neural network's parameter vectors, as in the online SGA algorithm from Section 2.2.

2.3.2 M-step

In the batch M-step, $q(\mathbf{h}_t|\theta_t)$, $t = 1, \ldots, T$, are fixed and Equation (2.30) is maximised with respect to $\mathbf{F}$ and Ψ. From [1], the optimal values are

$$\mathbf{F} = \mathbf{A}\mathbf{H}^{-1}, \tag{2.32}$$

where

$$\mathbf{A} = \frac{1}{T}\sum_{t=1}^{T} \mathbf{d}_t \mathbf{m}_t^\intercal \quad \text{and} \quad \mathbf{H} = \Sigma + \frac{1}{T}\sum_{t=1}^{T} \mathbf{m}_t \mathbf{m}_t^\intercal, \tag{2.33}$$

and

$$\Psi = \operatorname{diag}\left(\operatorname{diag}\left(\frac{1}{T}\sum_{t=1}^{T}\mathbf{d}_t\mathbf{d}_t^\intercal - 2\mathbf{F}\mathbf{A}^\intercal + \mathbf{F}\mathbf{H}\mathbf{F}^\intercal\right)\right). \tag{2.34}$$

Note that this optimisation involves summing over $t = 1,\ldots,T$. Moreover, on each iteration all components of the sums in Equation (2.33) and Equation (2.34) are updated. As in the E-step, updating all components is not possible in an online algorithm. Therefore, in the online version these sums will be updated incrementally on each iteration.

2.3.3 Practical implementation

Let $\overline{\mathbf{A}}_t$ and $\overline{\mathbf{H}}_t$ be the estimates of $\mathbf{A}$ and $\mathbf{H}$ from Equation (2.33), respectively, after iteration t of online EM. That is,

$$\overline{\mathbf{A}}_t = \frac{1}{t}\sum_{i=1}^{t}\mathbf{d}_i\mathbf{m}_i^\intercal \quad \text{and} \quad \overline{\mathbf{H}}_t = \Sigma + \frac{1}{t}\sum_{i=1}^{t}\mathbf{m}_i\mathbf{m}_i^\intercal. \tag{2.35}$$

Then the estimates of $\mathbf{F}$ and Ψ on iteration t become

$$\mathbf{F} = \overline{\mathbf{A}}_t\overline{\mathbf{H}}_t^{-1} \tag{2.36}$$

and

$$\Psi = \operatorname{diag}\left(\operatorname{diag}\left(\frac{1}{t}\sum_{i=1}^{t}\mathbf{d}_i\mathbf{d}_i^\intercal - 2\mathbf{F}\overline{\mathbf{A}}_t^\intercal + \mathbf{F}\overline{\mathbf{H}}_t\mathbf{F}^\intercal\right)\right). \tag{2.37}$$

As in the online SGA algorithm from Section 2.2, it suffices to work with $\psi = \operatorname{diag}(\Psi)$ instead of Ψ. The diagonal entries of Equation (2.37) can be computed more efficiently as

$$\begin{aligned}\psi &= \frac{1}{t}\sum_{i=1}^{t}\mathbf{d}_i^2 - 2\cdot\operatorname{sum}\big(\mathbf{F}\odot\overline{\mathbf{A}}_t,\ \dim = 1\big) + \operatorname{sum}\big((\mathbf{F}\overline{\mathbf{H}}_t)\odot\mathbf{F},\ \dim = 1\big)\\ &= \frac{1}{t}\sum_{i=1}^{t}\mathbf{d}_i^2 + \operatorname{sum}\big((\mathbf{F}\overline{\mathbf{H}}_t)\odot\mathbf{F} - 2\mathbf{F}\odot\overline{\mathbf{A}}_t,\ \dim = 1\big).\end{aligned} \tag{2.38}$$

(TODO: check whether this can be negative). All that remains to complete the online algorithm is to define the incremental update rules for $\overline{\mathbf{A}}_t$ and $\overline{\mathbf{H}}_t$. Both are similar, and

for $\overline{\mathbf{A}}_t$ the derivation is

$$\begin{aligned}
\overline{\mathbf{A}}_t &= \frac{1}{t}\sum_{i=1}^{t}\mathbf{d}_i\mathbf{m}_i^\intercal \\
&= \frac{1}{t}\left(\sum_{i=1}^{t-1}\mathbf{d}_i\mathbf{m}_i^\intercal + \mathbf{d}_t\mathbf{m}_t^\intercal\right) \\
&= \frac{1}{t}\left(\frac{t-1}{t-1}\sum_{i=1}^{t-1}\mathbf{d}_i\mathbf{m}_i^\intercal + \mathbf{d}_t\mathbf{m}_t^\intercal\right) \\
&= \frac{1}{t}\left(t\cdot\frac{1}{t-1}\sum_{i=1}^{t-1}\mathbf{d}_i\mathbf{m}_i^\intercal - \frac{1}{t-1}\sum_{i=1}^{t-1}\mathbf{d}_i\mathbf{m}_i^\intercal + \mathbf{d}_t\mathbf{m}_t^\intercal\right) \\
&= \frac{1}{t}\left(t\overline{\mathbf{A}}_{t-1} - \overline{\mathbf{A}}_{t-1} + \mathbf{d}_t\mathbf{m}_t^\intercal\right) \\
&= \overline{\mathbf{A}}_{t-1} + \frac{1}{t}\left(\mathbf{d}_t\mathbf{m}_t^\intercal - \overline{\mathbf{A}}_{t-1}\right).
\end{aligned} \tag{2.39}$$

Pseudo code for online EM for FA is given in Algorithm 2.

Algorithm 2 Online Expectation-Maximisation for Factor Analysis

Input: Observation dimension d, latent dimension K

Initialise $\mathbf{F} \in \mathbb{R}^{d\times K}$, $\boldsymbol{\psi} > \mathbf{0} \in \mathbb{R}^d$
Initialise $\overline{\boldsymbol{\theta}}_0 = \mathbf{0}^d, \overline{\mathbf{A}}_0 = \mathbf{0}^{d\times K}, \overline{\mathbf{B}}_0 = \mathbf{0}^{K\times K}, \overline{\mathbf{d}^2}_0 = \mathbf{0}^d$
for $t = 1,\ldots,T$ **do**
    Sample observation $\boldsymbol{\theta}_t \in \mathbb{R}^d$
    $\overline{\boldsymbol{\theta}}_t \leftarrow \overline{\boldsymbol{\theta}}_{t-1} + \frac{1}{t}\left(\overline{\boldsymbol{\theta}}_t - \overline{\boldsymbol{\theta}}_{t-1}\right)$
    $\mathbf{d}_t \leftarrow \boldsymbol{\theta}_t - \overline{\boldsymbol{\theta}}_t$
    $\mathbf{C} \leftarrow (\mathbf{F}\odot\boldsymbol{\psi}^{-1})^\intercal$ (with broadcasting)
    $\Sigma \leftarrow (\mathbf{I} + \mathbf{C}\mathbf{F})^{-1}$
    $\mathbf{m}_t \leftarrow \Sigma\mathbf{C}\mathbf{d}_t$
    $\overline{\mathbf{B}}_t \leftarrow \overline{\mathbf{B}}_{t-1} + \frac{1}{t}(\mathbf{m}_t\mathbf{m}_t^\intercal - \overline{\mathbf{B}}_{t-1})$
    $\overline{\mathbf{H}}_t \leftarrow \Sigma + \overline{\mathbf{B}}_t$
    $\overline{\mathbf{A}}_t \leftarrow \overline{\mathbf{A}}_{t-1} + \frac{1}{t}(\mathbf{d}_t\mathbf{m}_t^\intercal - \overline{\mathbf{A}}_{t-1})$
    $\mathbf{F} \leftarrow \overline{\mathbf{A}}_t\overline{\mathbf{H}}_t^{-1}$
    $\overline{\mathbf{d}^2}_t \leftarrow \overline{\mathbf{d}^2}_{t-1} + \frac{1}{t}(\mathbf{d}_t^2 - \overline{\mathbf{d}^2}_{t-1})$
    $\boldsymbol{\psi} \leftarrow \overline{\mathbf{d}^2}_t + \mathrm{sum}\left((\mathbf{F}\overline{\mathbf{H}}_t)\odot\mathbf{F} - 2\mathbf{F}\odot\overline{\mathbf{A}}_t,\ \mathrm{dim} = 1\right)$
end for
$\boldsymbol{\theta}_{\mathrm{SWA}} \leftarrow \overline{\boldsymbol{\theta}}_T$
return $\boldsymbol{\theta}_{\mathrm{SWA}}, \mathbf{F}, \boldsymbol{\psi}$

2.4 Factors and Noise Initialisation

One detail missing from Algorithms 1 and 2 is how $\mathbf{F}$ and ψ are initialised. Suppose $\mathbf{F}$ is initialised with ones on its diagonal and zeros everywhere else. That is,

$$\mathbf{F} = \begin{bmatrix} \mathbf{I} \\ \mathbf{0} \end{bmatrix} \in \mathbb{R}^{d \times K}, \tag{2.40}$$

where $\mathbf{I} \in \mathbb{R}^{K \times K}$ and $\mathbf{0} \in \mathbb{R}^{(d-K) \times K}$. Then for $\mathbf{h} \in \mathbb{R}^K$, the product $\mathbf{Fh} \in \mathbb{R}^d$ is just the vector formed by appending $d-K$ zeros onto the end of $\mathbf{h}$. In order to increase the initial diversity of $\mathbf{Fh}$, noise is added to the off-diagonal entries of $\mathbf{F}$. That is, $\mathbf{F}$ is initialised as

$$\mathbf{F} = \begin{bmatrix} 1 & \nu_{1,2} & \cdots & \nu_{1,K} \\ \nu_{2,1} & 1 & & \nu_{2,K} \\ \vdots & & \ddots & \vdots \\ \nu_{K,1} & \nu_{K,2} & \cdots & 1 \\ \nu_{K+1,1} & \nu_{K+1,2} & \cdots & \nu_{K+1,K} \\ \vdots & \vdots & \vdots & \vdots \\ \nu_{d,1} & \nu_{d,2} & \cdots & \nu_{d,K} \end{bmatrix}, \tag{2.41}$$

where $\nu_{i,j} \sim \mathcal{N}(0, \sigma^2)$ for some small σ, which is a hyperparameter.

From Equation (2.3), the full covariance matrix of a FA model is $\mathbf{F}\mathbf{F}^\intercal + \Psi$, where $\Psi = \operatorname{diag}(\psi)$. To ensure that neither $\mathbf{F}\mathbf{F}^\intercal$ nor Ψ dominates in the initial covariance matrix, the initial entries of ψ are set equal to the maximum diagonal value of $\mathbf{F}\mathbf{F}^\intercal$. That is,

$$\psi = (s, s, \ldots, s)^\intercal \in \mathbb{R}^d, \quad s = \max\big(\operatorname{diag}(\mathbf{F})\big). \tag{2.42}$$

2.5 Experiments

2.5.1 Methodology

The aim of these experiments is to test how well the online FA algorithms from Section 2 are able to fit observations sampled from actual FA models. The form of a FA model is given in Equation (2.3). In particular, it has parameters $\mathbf{c}, \mathbf{F}$ and Ψ. The maximum likelihood estimate of $\mathbf{c}$, given the data, is just the empirical mean of the sampled observations [1]. This is computed exactly in both online FA algorithms (Algorithms 1 and 2) by maintaining a running average of the observations. The other parameters, $\mathbf{F}$ and Ψ, appear in the FA model as part of the full covariance matrix, $\mathbf{F}\mathbf{F}^\intercal + \Psi$. Note

that right-multiplying $\mathbf{F}$ by any orthogonal matrix $\mathbf{A} \in \mathbb{R}^{K \times K}$ will result in the exact same covariance [1], since

$$(\mathbf{FA})(\mathbf{FA})^\intercal + \Psi = \mathbf{FAA}^\intercal\mathbf{F}^\intercal + \Psi = \mathbf{FF}^\intercal + \Psi. \tag{2.43}$$

Hence, the maximum likelihood estimate of $\mathbf{F}$ is not unique. However, the maximum likelihood estimate of $\mathbf{FF}^\intercal + \Psi$ (TODO: include citation) is unique. Therefore, a covariance matrix of an online FA model, fit to samples from the true FA model, can be directly compared to the true covariance matrix.

Since the covariance matrices have shape $d \times d$, memory requirements dictate that d, the observation dimension, cannot be too large. Therefore, a value of $d = 1000$ was used in all experiments in this section. Two different latent dimensions were tested, namely $K = 10$ and $K = 100$. Since computing the maximum likelihood estimate of $\mathbf{c} \in \mathbb{R}^d$ is trivial, in all experiments the entries of $\mathbf{c}$ were simply sampled independently from a standard normal distribution. Each factor loading matrix $\mathbf{F}$ was generated in such a way that its columns spanned the K-dimensional latent space and the conditioning number of the resultant covariance matrix could be controlled. This was achieved by finding the first K eigenvectors of a symmetric positive semi-definite matrix $\mathbf{M} \in \mathbb{R}^{d \times d}$, and then setting the columns of $\mathbf{F}$ equal to these eigenvectors multiplied by a vector $\mathbf{s} > \mathbf{0} \in \mathbb{R}^d$ (element-wise). By construction, the K eigenvectors are linearly independent and therefore span the latent space, and scaling them by $\mathbf{s}$ affects the conditioning number of $\mathbf{FF}^\intercal$. The conditioning number can be controlled by specifying the range of $\mathbf{s}$, or alternatively, the range of $\mathbf{s}^2$, which is called the *spectrum*. In each experiment the spectrum was sampled from a uniform distribution with one of the following ranges: $[0,1]$, $[1,10]$ or $[10,100]$. Finally, the diagonal entries of Ψ were sampled from a uniform distribution with upper bound equal to the maximum value of $\mathbf{s}^2$. This is consistent with the FA assumption that an observation, $\theta = \mathbf{Fh} + \mathbf{c} + \varepsilon$, is generated by corrupting the signal $\mathbf{Fh} + \mathbf{c}$ with some random noise $\varepsilon \sim \mathcal{N}(\mathbf{0}, \Psi)$ (TODO: this paragraph is a bit wooly. Talk to Michael about what is going on here and maybe add some citations). The full details of how FA models were generated are given in Algorithm 3.

Having generated a FA model, observations were sampled according to Equation (2.1). Using the data, the parameters of the model were then estimated by three separate FA algorithms: online SGA (Algorithm 1), online EM (Algorithm 2) and the scikit-learn `FactorAnalysis` estimator [2]. The scikit-learn implementation is based on the batch SVD algorithm from [1] and should in theory find the maximum likeli-

Algorithm 3 Generate a Factor Analysis Model

Input: Observation dimension d, latent dimension K, spectrum range $[a,b]$

1: Generate $\mathbf{c} \in \mathbb{R}^d$ by sampling entries independently from $\mathcal{N}(0,1)$
2: Generate $\mathbf{A} \in \mathbb{R}^{d\times d}$ by sampling entries independently from $\mathcal{N}(0,1)$
3: $\mathbf{M} \leftarrow \mathbf{A}\mathbf{A}^\intercal$
4: Compute the K eigenvectors, $\mathbf{v}_1,\ldots,\mathbf{v}_K \in \mathbb{R}^d$, corresponding to the K largest eigenvalues of $\mathbf{M}$
5: Construct the matrix $\mathbf{V}_K \in \mathbb{R}^{d\times K}$ with columns $\mathbf{v}_1,\ldots,\mathbf{v}_K$
6: Generate $\mathbf{s}^2 \in \mathbb{R}^d$ by sampling entries independently from $\mathcal{U}(a,b)$
7: $\mathbf{s} \leftarrow \sqrt{\mathbf{s}^2}$ (square root is applied element-wise)
8: $\mathbf{F} \leftarrow \mathbf{V}_K \odot \mathbf{s}$ (with broadcasting)
9: $s_{max} \leftarrow \max(\mathbf{s}^2)$ (largest element of $\mathbf{s}^2$)
10: Generate $\psi \in \mathbb{R}^d$ by sampling entries independently from $\mathcal{U}(0,s_{max})$
11: $\Psi \leftarrow \mathrm{diag}(\psi)$
12: **return** $\mathbf{c},\mathbf{F},\Psi$

hood parameters of the model, given the data. Each algorithm was tested on samples of varying size, from 200 up to 100,000 observations. The latent dimension of each approximate model was set to the true latent dimension K. All other hyperparameters of the scikit-learn algorithm were set to their default values. For both online algorithms, $\mathbf{F}$ and Ψ were initialised according to Equations (2.41) and (2.42) with $\sigma = 0.1$, and online SGA ran with a learning rate of 0.001. Each experiment was repeated ten times. In each trial a different random seed was used for generating the true FA model and also initialising the parameters of the online algorithms.

2.5.2 Results

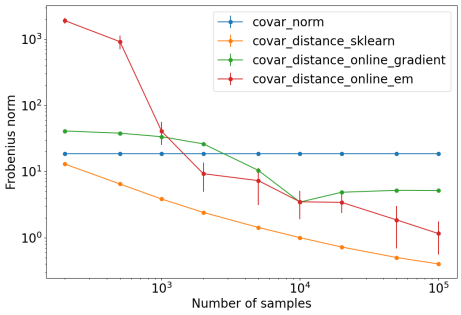
Figure 2.1 shows the distance between the true covariance matrix of each FA model and the corresponding estimated covariance matrix of each learning algorithm, as a function of the number of samples used to fit the approximate models. The distance between two matrices is measured by the Frobenius norm (also sometimes called the Euclidean norm) of the difference between the two matrices. To give a sense of the size of the distance, the Frobenius norm of the true covariance matrix is also show on each plot.

In the first row of the figure are the results corresponding to FA models whose

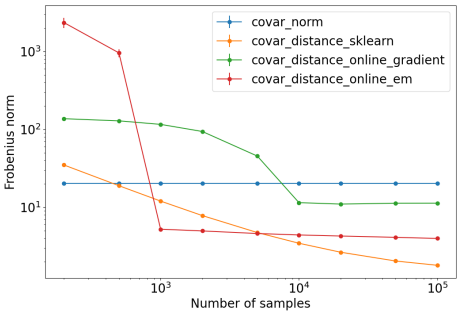
factor loading matrices were generated with a spectrum range of $[0,1]$. In this case, for both $K = 10$ and $K = 100$, online EM generally approximates the true covariance matrix better than online SGA, except when the number of samples is less than 1000. When $K = 10$, the scikit-learn approximation is best for all samples sizes. The same is true for $K = 100$, except when the sample size is between 1000 and 2000.

In the second row of the figure are the results corresponding to a spectrum range of $[1,10]$. When $K = 10$, online SGA consistently gets closer to the true covariance matrix that online EM for all sample sizes. When $K = 100$, online SGA is better for sample sizes less than or equal to 500 and greater than or equal to 20,000, whereas online EM is better for the other intermediate sample sizes. The scikit-learn approximation is again always superior when $K = 10$, and for $K = 100$ except when the sample size is between 1000 and 2000. For a spectrum range of $[10,100]$ the results are very similar, as shown in the third row of the figure.

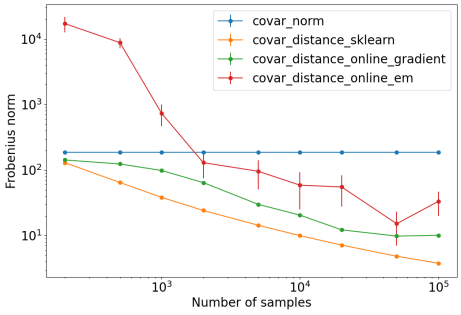
Figure 2.2 shows the log-likelihood of the true and approximate FA models for the same combinations of observation dimension, latent dimension, spectrum range and sample size. In general, for sample sizes of 10,000 and above, the log-likelihood of all three approximate model is very similar to the log-likelihood of the true model. In the case of online EM, the log-likelihood is very close to that of the true model even for very small sample sizes. In contrast, online SGA needs around 5,000 to 10,000 samples to increase the log-likelihood to a similar value. For small samples sizes, the model learned by the scikit-learn algorithm actually has greater log-likelihood than the true model.



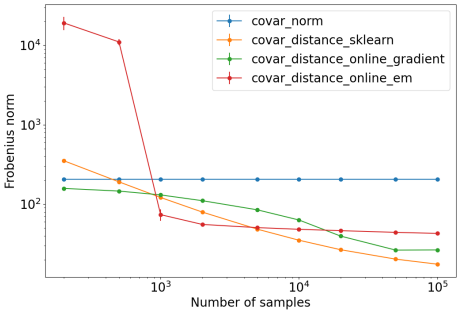
(a) $d = 1000$, $K = 10$, $\mathbf{s}^2 \sim \mathcal{U}(0, 1)$



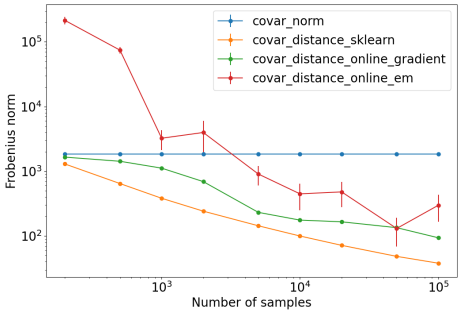
(b) $d = 1000$, $K = 100$, $\mathbf{s}^2 \sim \mathcal{U}(0, 1)$



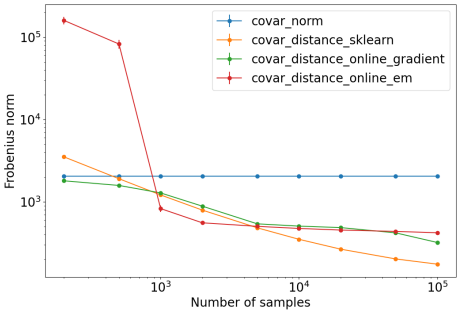
(c) $d = 1000$, $K = 10$, $\mathbf{s}^2 \sim \mathcal{U}(1, 10)$



(d) $d = 1000$, $K = 100$, $\mathbf{s}^2 \sim \mathcal{U}(1, 10)$

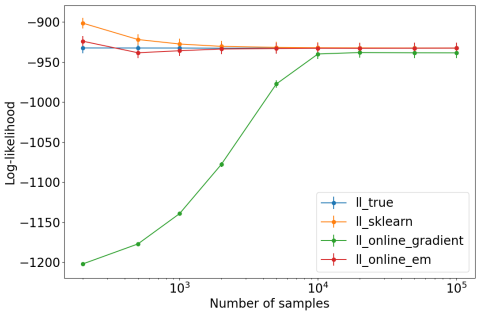


(e) $d = 1000$, $K = 10$, $\mathbf{s}^2 \sim \mathcal{U}(10, 100)$

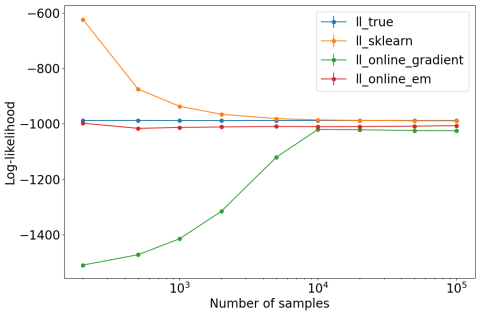


(f) $d = 1000$, $K = 100$, $\mathbf{s}^2 \sim \mathcal{U}(10, 100)$

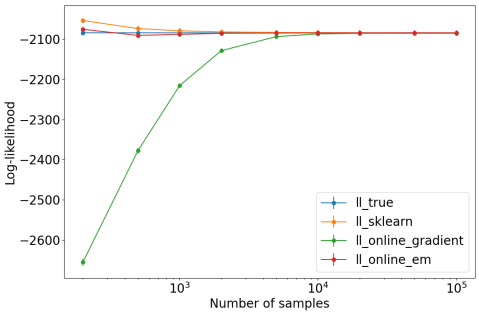
Figure 2.1: The distance of the estimated FA covariance matrices from the true covariance matrix as a function of the number of samples used to learn the models. The blue line shows the Frobenius norm of the true covariance matrix, while the orange, green and red lines shown the Frobenius norm of the difference between the true covariance matrix and the estimated covariance matrix for the scikit-learn batch algorithm, online SGA and online EM, respectively. Each data point shows the mean value over ten trials with different random seeds, and standard error bars are also plotted. In all experiments the observation dimension was $d = 1000$. The different plots correspond to different combinations of the latent dimension K and the range of the spectrum $\mathbf{s}^2$.



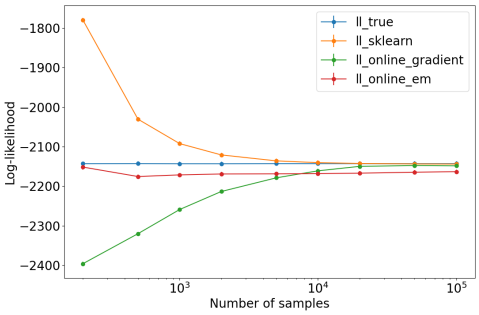
(a) $d = 1000$, $K = 10$, $\mathbf{s}^2 \sim \mathcal{U}(0, 1)$



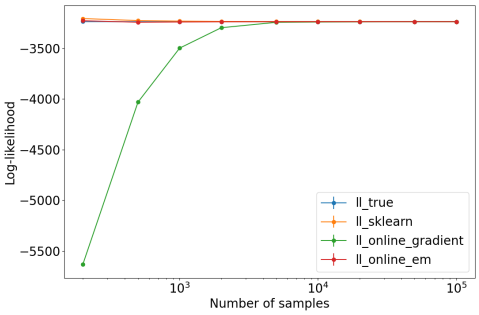
(b) $d = 1000$, $K = 100$, $\mathbf{s}^2 \sim \mathcal{U}(0, 1)$



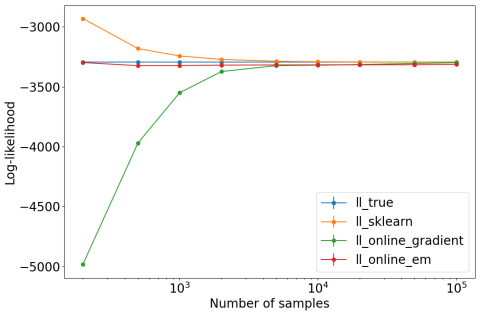
(c) $d = 1000$, $K = 10$, $\mathbf{s}^2 \sim \mathcal{U}(1, 10)$



(d) $d = 1000$, $K = 100$, $\mathbf{s}^2 \sim \mathcal{U}(1, 10)$



(e) $d = 1000$, $K = 10$, $\mathbf{s}^2 \sim \mathcal{U}(10, 100)$



(f) $d = 1000$, $K = 100$, $\mathbf{s}^2 \sim \mathcal{U}(10, 100)$

Figure 2.2: The log-likelihood of the true and estimated FA models. The blue line shows the log-likelihood of the true FA model, while the orange, green and red lines shown the log-likelihood of the models estimated by the scikit-learn batch algorithm, online SGA and online EM, respectively. Each data point shows the mean value over ten trials with different random seeds, and standard error bars are also plotted. In all experiments the observation dimension was $d = 1000$. The different plots correspond to different combinations of the latent dimension K and the range of the spectrum $\mathbf{s}^2$.

Chapter 3

Bayesian Linear Regression

3.1 Background

A linear regression model is a mapping from vector inputs $\mathbf{x} \in \mathbb{R}^d$ to scalar outputs $y \in \mathbb{R}$ via an affine transformation. Given a set of observed input-output pairs, $\mathcal{D} = \{(\mathbf{x}_n, y_n)\}_{n=1}^N$, it is assumed that each output is generated according to

$$y_n = \theta^\intercal \mathbf{x}_n + \varepsilon \tag{3.1}$$

for some unknown $\theta \in \mathbb{R}^d$. The underlying signal, $\theta^\intercal \mathbf{x}_n$, is corrupted by additive noise,

$$\varepsilon \sim \mathcal{N}(0, \sigma^2), \tag{3.2}$$

for some $\sigma > 0$ [1]. The model is often written with an explicit bias term, but this can be absorbed into θ by adding a constant of one to the input, leading to the expression in Equation (3.1).

3.1.1 Computing the Posterior

Due to the additive noise, each y_n is a random variable, conditioned on $\mathbf{x}_n$ and θ. Since ε is Gaussian distributed, the conditional pdf of y_n is

$$p(y_n|\theta, \mathbf{x}_n) = \mathcal{N}\big(\theta^\intercal \mathbf{x}_n, \sigma^2\big) = \frac{1}{\sqrt{2\pi\sigma^2}} \exp\Big(-\frac{1}{2\sigma^2}\big(y_n - \theta^\intercal \mathbf{x}_n\big)^2\Big). \tag{3.3}$$

Assuming that the observations in $\mathcal{D}$ are independent and identically distributed, the log-likelihood of θ having generated the data is

$$\begin{aligned}\log p(\mathcal{D}|\theta) &= \sum_{n=1}^{N} \left[\log p(y_n|\theta, \mathbf{x}_n) + \log p(\mathbf{x}_n)\right] \\ &= \sum_{n=1}^{N} \left[-\frac{1}{2}\log 2\pi\sigma^2 - \frac{1}{2\sigma^2}\left(y_n - \theta^\intercal \mathbf{x}_n\right)^2\right] + \sum_{n=1}^{N} \log p(\mathbf{x}_n) \\ &= -\frac{1}{2\sigma^2}\sum_{n=1}^{N}\left(y_n - \theta^\intercal \mathbf{x}_n\right)^2 - \frac{N}{2}\log\sigma^2 - \frac{N}{2}\log 2\pi + \sum_{n=1}^{N} \log p(\mathbf{x}_n) \\ &= -\frac{\beta}{2}\sum_{n=1}^{N}\left(y_n - \theta^\intercal \mathbf{x}_n\right)^2 + \frac{N}{2}\log\beta + \text{constant},\end{aligned} \tag{3.4}$$

where $\beta = \frac{1}{\sigma^2}$ [1]. In Bayesian linear regression, a prior distribution for θ is also specified. A common choice is

$$p(\theta) = \mathcal{N}\left(\mathbf{0}, \alpha^{-1}\mathbf{I}\right) = \left(\frac{\alpha}{2\pi}\right)^{\frac{d}{2}} \exp\left(-\frac{\alpha}{2}\theta^\intercal\theta\right) \tag{3.5}$$

for some $\alpha > 0$, called the *precision* [1]. Applying the logarithm,

$$\begin{aligned}\log p(\theta) &= \frac{d}{2}\log\frac{\alpha}{2\pi} - \frac{\alpha}{2}\theta^\intercal\theta \\ &= -\frac{\alpha}{2}\theta^\intercal\theta + \frac{d}{2}\log\alpha + \text{constant}.\end{aligned} \tag{3.6}$$

Now, using Bayes' rule and Equation (3.4) and Equation (3.6), it follows that the log-posterior distribution of θ for fixed α and β is

$$\begin{aligned}\log p(\theta|\mathcal{D}) &= \log\frac{p(\mathcal{D}|\theta)p(\theta)}{p(\mathcal{D})} \\ &= \log p(\mathcal{D}|\theta) + \log p(\theta) - \log p(\mathcal{D}) \\ &= -\frac{\beta}{2}\sum_{n=1}^{N}\left(y_n - \theta^\intercal \mathbf{x}_n\right)^2 - \frac{\alpha}{2}\theta^\intercal\theta + \text{constant} \\ &= -\frac{\beta}{2}\sum_{n=1}^{N}\left(y_n^2 - 2y_n\theta^\intercal\mathbf{x}_n + (\theta^\intercal\mathbf{x}_n)^2\right) - \frac{\alpha}{2}\theta^\intercal\theta + \text{constant} \\ &= -\frac{\beta}{2}\sum_{n=1}^{N} y_n^2 + \beta\sum_{n=1}^{N} y_n\theta^\intercal\mathbf{x}_n - \frac{\beta}{2}\sum_{n=1}^{N}\theta^\intercal\mathbf{x}_n\mathbf{x}_n^\intercal\theta - \frac{\alpha}{2}\theta^\intercal\theta + \text{constant} \\ &= \left(\beta\sum_{n=1}^{N} y_n\mathbf{x}_n\right)^\intercal\theta - \frac{1}{2}\theta^\intercal\left(\alpha\mathbf{I} + \beta\sum_{n=1}^{N}\mathbf{x}_n\mathbf{x}_n^\intercal\right)\theta + \text{constant} \\ &= \mathbf{b}^\intercal\theta - \frac{1}{2}\theta^\intercal\mathbf{A}\theta + \text{constant},\end{aligned} \tag{3.7}$$

where

$$\mathbf{A} = \alpha\mathbf{I} + \beta\sum_{n=1}^{N}\mathbf{x}_n\mathbf{x}_n^\intercal \quad \text{and} \quad \mathbf{b} = \beta\sum_{n=1}^{N} y_n\mathbf{x}_n. \tag{3.8}$$

Now, using a result from [1] to complete the square of Equation (3.7),

$$\begin{aligned}\log p(\theta|\mathcal{D}) &= -\frac{1}{2}\big(\theta-\mathbf{A}^{-1}\mathbf{b}\big)^{\mathsf{T}}\mathbf{A}\big(\theta-\mathbf{A}^{-1}\mathbf{b}\big)+\frac{1}{2}\mathbf{b}^{\mathsf{T}}\mathbf{A}^{-1}\mathbf{b}+\text{constant}\\ &= -\frac{1}{2}\big(\theta-\mathbf{A}^{-1}\mathbf{b}\big)^{\mathsf{T}}\mathbf{A}\big(\theta-\mathbf{A}^{-1}\mathbf{b}\big)+\text{constant}\\ &= -\frac{1}{2}\big(\theta-\mathbf{m}\big)^{\mathsf{T}}\mathbf{S}^{-1}\big(\theta-\mathbf{m}\big)+\text{constant},\end{aligned} \tag{3.9}$$

where

$$\mathbf{m}=\mathbf{A}^{-1}\mathbf{b} \quad \text{and} \quad \mathbf{S}=\mathbf{A}^{-1}. \tag{3.10}$$

Hence, the posterior distribution of θ is

$$p(\theta|\mathcal{D})=\mathcal{N}(\mathbf{m},\mathbf{S}). \tag{3.11}$$

3.1.2 Estimating the Posterior Online

Since the posterior of the linear regression parameter vector can be computed in closed form, the ability of the online FA algorithms to learn the posterior can be evaluated in this case. For a linear regression model trained via SGD, Algorithms 1 and 2 can both be used to fit a Gaussian posterior distribution to the iterates, $\theta_1,\ldots,\theta_T$, encountered along the SGD trajectory. The mean and covariance of the learned distributions can then be compared directly to the ground truth. Recall, however, that the posterior distribution in Equation (3.11) refers to specific values of α and β. The parameter β is $\frac{1}{\sigma^2}$, where σ is the standard deviation of the outputs y_n in Equation (3.3). This can be estimated by calculating the empirical standard deviation of $\{y_n\}_{n=1}^N$.

The precision α is a user-defined parameter which controls the complexity of the model. In Equation (3.7), the log-posterior of θ was written as

$$\log p(\theta|\mathcal{D}) = -\frac{\beta}{2}\sum_{n=1}^{N}\big(y_n-\theta^{\mathsf{T}}\mathbf{x}_n\big)^2-\frac{\alpha}{2}\theta^{\mathsf{T}}\theta+\text{constant}. \tag{3.12}$$

Hence, the maximum *a posteriori* (MAP) estimate of θ is that which maximises

$$-\frac{\beta}{2}\sum_{n=1}^{N}\big(y_n-\theta^{\mathsf{T}}\mathbf{x}_n\big)^2-\frac{\alpha}{2}\theta^{\mathsf{T}}\theta. \tag{3.13}$$

Since $\beta>0$, it is equivalent to minimise this expression scaled by $-\frac{2}{\beta}$, that is,

$$\sum_{n=1}^{N}\big(y_n-\theta^{\mathsf{T}}\mathbf{x}_n\big)^2+\frac{\alpha}{\beta}\theta^{\mathsf{T}}\theta. \tag{3.14}$$

This objective function is analogous to the L2-regularised training loss often used in non-Bayesian linear regression [1], which is

$$\sum_{n=1}^{N} \left(y_n - \theta^\intercal \mathbf{x}_n\right)^2 + \lambda \theta^\intercal \theta \tag{3.15}$$

for some $\lambda > 0$. Setting $\lambda = \frac{\alpha}{\beta}$, the optimal θ found by L2-regularised linear regression is the same as the MAP estimate of θ in Bayesian linear regression with prior $p(\theta) = \mathcal{N}\left(\mathbf{0}, \alpha^{-1}\mathbf{I}\right)$. This means that, given data $\mathcal{D}$ and a particular value of α, the posterior distribution of θ can be estimated by fitting an online FA model to the SGD iterates sampled while minimising Equation (3.15) with $\lambda = \frac{\alpha}{\beta}$.

3.2 Experiments

3.2.1 Methodology

3.2.2 Results

Chapter 4

Conclusions

4.1 Final Reminder

The body of your dissertation, before the references and any appendices, *must* finish by page 40. The introduction, after preliminary material, should have started on page 1.

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