Approximate Bayesian Inference

Václav Šmídl

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Recapitulation

1. what principle is used in Jeffrey's prior
2. is improper prior $p(\theta) \propto 1$ always non-informative?
3. what is conjugate prior

What is the result of Bayesian inference?

The Bayes rule

$$p(\theta|Y) \propto p(Y|\theta)p(\theta)$$

in practice we appreciate moments, HPD regions:

$$\mathrm{E}(\theta) = \int \theta p(\theta|Y)d\theta \qquad \mathrm{E}(g(\theta)) = \int g(\theta)p(\theta|Y)d\theta$$

$$C : \{\mu \pm 3\sigma\}$$

These are available only for (most of) proper distributions.

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These are available only for (most of) proper distributions.
What if we do not have that?

1. choose different metrics
2. approximate $p(\theta|Y) \approx q(\theta|Y)$
3. combine the above

Alternative results of Bayesian inference

Maximum likelihood (ML): is Bayesian for improper prior $p(\theta) \propto 1$

$$\hat{\theta} = \arg\max p(Y|\theta)$$

Maximum aposteriori (MAP): is a point estimate for prior $p(\theta)$

$$\hat{\theta} = \arg\max p(Y|\theta)p(\theta)$$

Maximum marginal likelihood: is point estimate of a marginal $\theta = [\theta_1, \theta_2]$

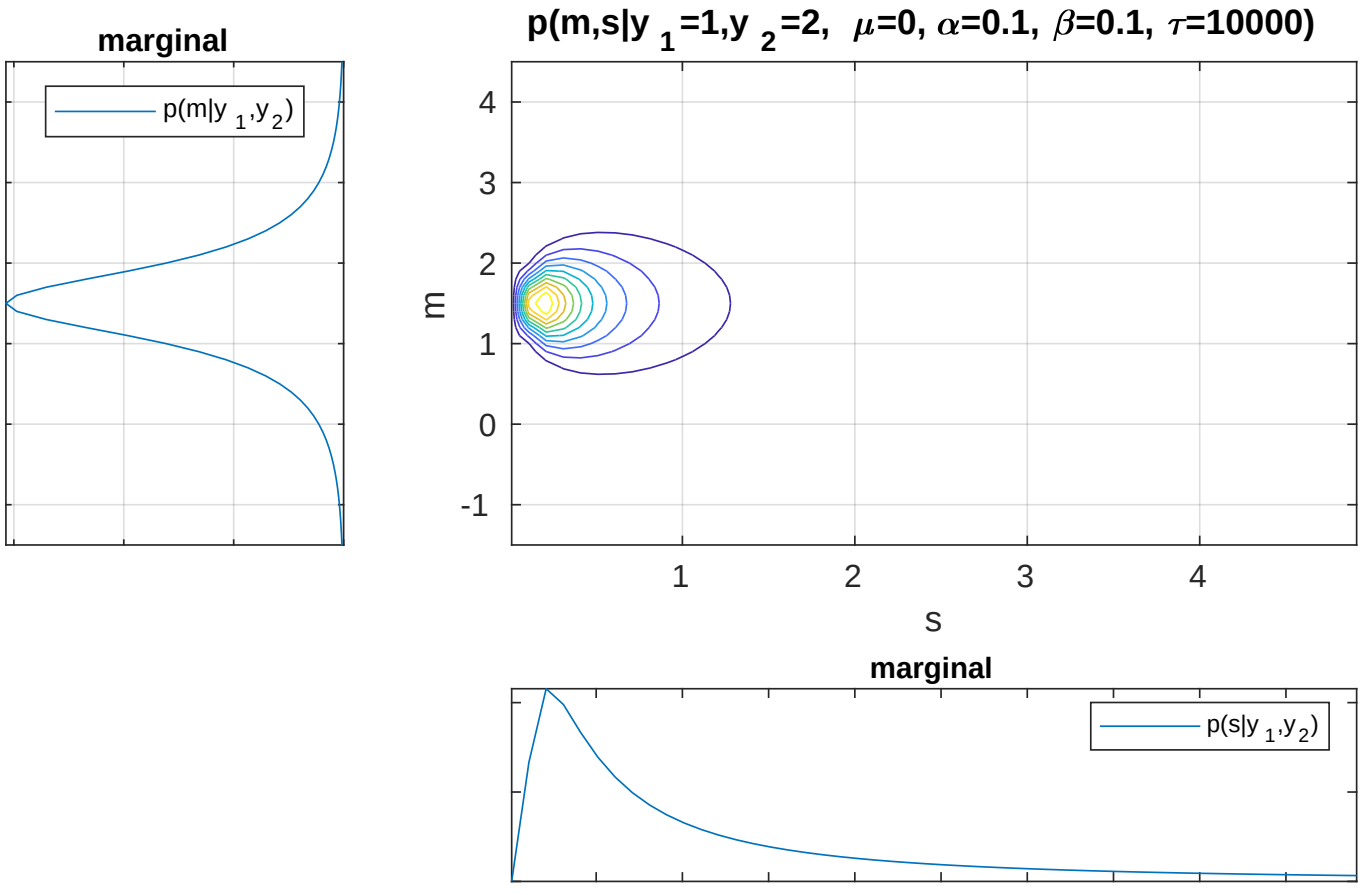
$$\hat{\theta}_1 = \arg\max_{\theta_1} p(\theta_1|Y) = \arg\max_{\theta_1} \int p(\theta_1, \theta_2|Y) d\theta_2$$

Empirical Bayes (EB): is a method of inferring $\theta = [\theta_1, \theta_2]$

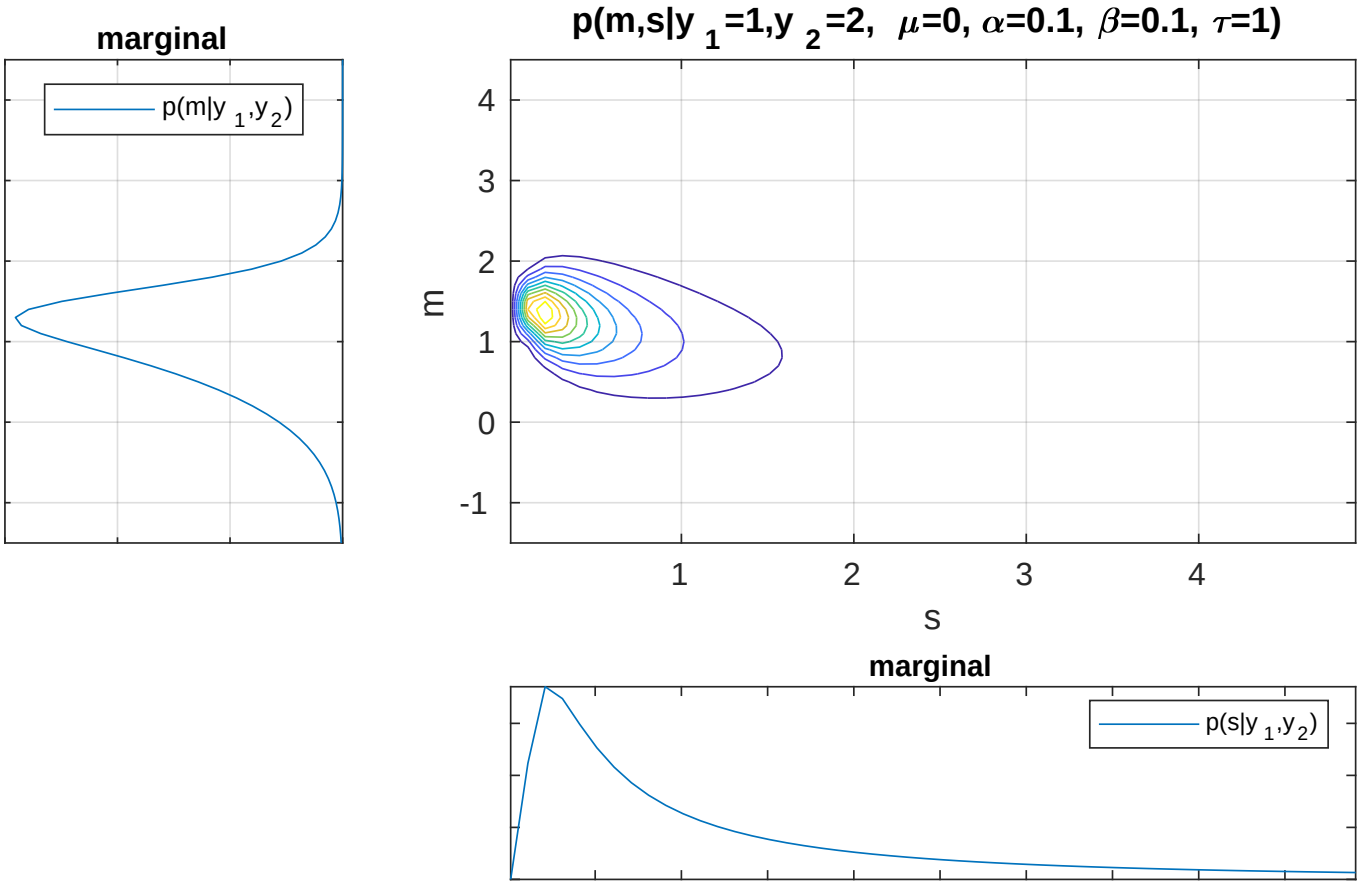
$$p(\theta_1|Y) \approx p(\theta_1|Y, \theta_2^*)$$

where $\theta_2^* = \arg\max_{\theta_2} p(\theta_2|Y)$.

Example


marginal
p(m|y 1,y 2)
p(m,s|y 1=1,y 2=2, μ=0, α=0.1, β=0.1, τ=10000)
m
s
4
3
2
1
0
-1
1
2
3
4
marginal
p(s|y 1,y 2)

Example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m
s
4
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2
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3
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EM algorithm classical form

Splits unknown vector into two parts:

1. quantity of interest θ (e.g. mean m)
2. missing data z (e.g. variance s)

General concept of missing data:

- nuisance parameter – we do not really care about it
- missing data – if we knew it, the solution would be easy
- latent variable

EM algorithm

General EM algorithm [Dempster, Laird, Rubin, 1977]. Maximum likelihood estimate:

$$\hat{\theta} = \arg\max_{\theta} \int p(Y|\theta, z)p(z)dz,$$

can be (approximately) found by alternating:

E-step: $q(\theta|\theta^{(i)}) = \int \log p(Y, z|\theta)p(z|\theta^{(i)}, Y)dz$

M-step: $\theta^{(i+1)} = \arg\max_{\theta} q(\theta|\theta^{(i)})$

where $^{(i)}$ is the iteration index, starting from initial condition $\theta^{(1)}$. Necessary condition:

- we need to be able to compute

$$p(z|\theta^{(i)}, Y) = \frac{p(Y, z|\theta^{(i)})}{p(Y|\theta^{(i)})}$$

Toy example: $\theta = m$, $z = s$

Necessary condition:

$$p(z|\theta^{(i)}, Y) \equiv p(s|m^{(i)}, Y)$$

already done:

$$\begin{aligned} & p(s|m, y_1, y_2, \mu, \alpha, \beta, \tau) \\ & \quad \propto \frac{1}{s^{\alpha_0+2}} \exp\left(-\frac{1}{2}\frac{(m-y_1)^2}{s} - \frac{1}{2}\frac{(m-y_2)^2}{s} - \frac{\beta_0}{s}\right) \\ & \quad = i\mathcal{G}(\underbrace{\alpha_0+1}_{\alpha}, \underbrace{0.5(m-y_1)^2 + 0.5(m-y_2)^2 + \beta_0}_{\beta}) \\ & \quad = i\mathcal{G}(\alpha, \beta) \end{aligned}$$

E-step: $\theta = m$, $z = s$

Proxy distribution

$$q(m|m^{(i)}) = \int \log p(y_1, y_2, m, s) p(s|m^{(i)}|Y) ds$$
$$= \mathrm{E}_{p(s|m^{(i)},Y)}(\log p(y_1, y_2, m, s))$$

using

$$p(y_1, y_2, m, s) \propto \frac{1}{s} \exp\left(-\frac{1}{2}\frac{(m-y_1)^2}{s} - \frac{1}{2}\frac{(m-y_2)^2}{s} - \frac{1}{2}\frac{(m-\mu)^2}{\tau}\right)$$

$$\log p(y_1, y_2, m, s) = c + \log s - \frac{1}{2}\frac{(m-y_1)^2}{s} - \frac{1}{2}\frac{(m-y_2)^2}{s} - \frac{1}{2}\frac{(m-\mu)^2}{\tau},$$

$$q(m|m^{(i)}) = c - \frac{1}{2}\mathrm{E}(\frac{1}{s})\left[(m-y_1)^2 + (m-y_2)^2\right] - \frac{1}{2}\frac{(m-\mu)^2}{\tau}$$

$$\mathrm{E}(\frac{1}{s}) = \frac{\alpha}{\beta} \qquad \hat{s} = \frac{\beta}{\alpha}$$

$$q(m|m^{(i)}) = c - \frac{1}{2}\left[\frac{(m-y_1)^2}{\hat{s}} + \frac{(m-y_2)^2}{\hat{s}}\right] - \frac{1}{2}\frac{(m-\mu)^2}{\tau}$$

M-step

New point estimate $m^{(i+1)} = \arg\max_m q(m|m^{(i)})$

1. set first derivative equal to 0
2. completion of squares

$$m^{(i+1)} = \left(\frac{1}{\tau} + \frac{2}{\hat{s}}\right)^{-1} \left(\frac{\mu}{\tau} + \frac{y_1 + y_2}{\hat{s}}\right),$$

based on $\hat{s}$ estimate of conditional.
Algorithm:

1. set $i = 1$, choose $m^{(1)}$
2. compute

$$\alpha = \alpha_0 + 1,$$
$$\beta = 0.5(m^{(i)} - y_1)^2 + 0.5(m^{(i)} - y_2)^2 + \beta_0$$

3. Recompute $m^{(i+1)}$

Homework assignment

Note: meaning of variables can be swapped. E-step over m and M-step on s.

Working code for EM estimation of toy problem:

1. $\hat{m} = \arg\max p(m|y_1, y_2)$ (2 points)
2. $\hat{s} = \arg\max p(s|y_1, y_2)$ (8 points)

Distributional approximations

Principles of approximations:

Laplace Approximation: by Taylor approximation

$$\log p(\theta) \approx \log p(\hat{\theta}) + [\nabla \log p(\hat{\theta})]^T(\theta - \hat{\theta}) - \frac{1}{2}(\theta - \hat{\theta})H(\theta - \hat{\theta})$$

$$H = -\nabla\nabla \log p(\hat{\theta})$$

Divergence Minimization: approximation by optimization

Monte Carlo: approximation by sampling

Divergence minimization

We seek best approximation of intractable distribution $p(\theta)$ in the chosen class of parametric functions, $q(\theta|)$, such that

$$\theta^* = \arg\min_{\theta} D(p, q),$$

where $D(p, q)$ is a statistical divergence.

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Variational Bayes:

1. conditional independence $q(\theta_1, \theta_2) = q(\theta_1)q(\theta_2)$,
2. (reverse) Kullback-Leibler. $\mathrm{KL}(q||p) \neq \mathrm{KL}(p||q)$

Kullback Leibler divergence

Measure of divergence between two probability densities

$$KL(q||p) = E_q\left(\log \frac{q}{p}\right)$$

Not a metric!

$$E_q\left(\log \frac{q}{p}\right) \neq E_p\left(\log \frac{p}{q}\right)$$

also known as relative/free entropy

$$KL(q||p) = E_q\left(\log q\right) - E_q\left(\log p\right)$$

with properties:

1. $KL(q||p) \geq 0$,
2. $KL(q||p) = 0, \iff q = p$

EM algorithm is a divergence minimization problem

Approximation of posterior $p(\theta_1, \theta_2|Y)$ under constraints

$$q(\theta_1, \theta_2|Y) = q(\theta_1|Y, S_1)\delta(\theta_2 - \hat{\theta}_2)$$

reaches minimum of the KL

$$S_1, \hat{\theta}_2 = \arg\min_{S_1, \hat{\theta}_2} KL(q||p)$$

at points:

$$q(\theta_1|Y, S_1) \propto p(\theta_1|Y, \hat{\theta}_2)$$
$$\hat{\theta}_2 = \arg\max E_{q(\theta_1)} \left[\log p(Y, \theta_1, \theta_2)\right].$$

EM algorithm is a coordinate descent solution of this optimization.

Variational Bayes

Is a divergence minimization technique with

$$q^* = \arg\min_q KL(q||p) = \arg\min_q E_q\left(\log\frac{q}{p}\right)$$

$$q(\theta_1, \theta_2) = q(\theta_1|Y)q(\theta_2|Y).$$

which allows free-form optimization.

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$$q^* = \arg\min_q KL(q||p) = \arg\min_q E_q\left(\log\frac{q}{p}\right)$$
$$q(\theta_1, \theta_2) = q(\theta_1|Y)q(\theta_2|Y).$$

which allows free-form optimization.
Result:

$$q(\theta_1|Y) \propto \exp\left(E_{q(\theta_2)}\left[\log p(Y, \theta_1, \theta_2)\right]\right)$$
$$q(\theta_2|Y) \propto \exp\left(E_{q(\theta_1)}\left[\log p(Y, \theta_1, \theta_2)\right]\right)$$

which is a set of implicit functions.

- Proportionality above allows to use $p(Y, \theta_1, \theta_2)$ in place of $p(\theta_1, \theta_2|Y)$
- Variational EM algorithm (E-E algorithm).

E-step: m of the toy problem

Proxy distribution

$$q(m) = \mathrm{E}_{q(s)}(\log p(y_1, y_2, m, s))$$

using

$$p(y_1, y_2, m, s) \propto \frac{1}{s}\frac{1}{s^{\alpha_0+1}} \exp\left(-\frac{1}{2}\frac{(m-y_1)^2}{s} - \frac{1}{2}\frac{(m-y_2)^2}{s} - \frac{1}{2}\frac{(m-\mu)^2}{\tau} - \frac{\beta_0}{s}\right)$$

$$\log p(y_1, y_2, m, s) \propto (\alpha_0+2)\log s - \frac{1}{2}\frac{(m-y_1)^2}{s} - \frac{1}{2}\frac{(m-y_2)^2}{s} - \frac{1}{2}\frac{(m-\mu)^2}{\tau} - \frac{\beta_0}{s},$$

$$\propto -\frac{1}{2}\mathrm{E}\left(\frac{1}{s}\right)\left[(m-y_1)^2 + (m-y_2)^2\right] - \frac{1}{2}\frac{(m-\mu)^2}{\tau}$$

$$\propto -\frac{1}{2}\left[\frac{(m-y_1)^2}{\hat{s}} + \frac{(m-y_2)^2}{\hat{s}}\right] - \frac{1}{2}\frac{(m-\mu)^2}{\tau}$$

$$q(m) = \mathcal{N}\left(m; \left(\frac{1}{\tau} + \frac{2}{\hat{s}}\right)^{-1}\left(\frac{\mu}{\tau} + \frac{y_1+y_2}{\hat{s}}\right), \left(\frac{1}{\tau} + \frac{2}{\hat{s}}\right)^{-1}\right)$$

E-step: s

Proxy distribution

$$q(s) = \mathrm{E}_{q(m)}(\log p(y_1, y_2, m, s))$$

using

$$p(y_1, y_2, m, s) \propto \frac{1}{s}\frac{1}{s^{\alpha_0+1}} \exp\left(-\frac{1}{2}\frac{(m-y_1)^2}{s} - \frac{1}{2}\frac{(m-y_2)^2}{s} - \frac{1}{2}\frac{(m-\mu)^2}{\tau} - \frac{\beta_0}{s}\right)$$

$$\log p(y_1, y_2, m, s) = -(\alpha_0+2)\log s - \frac{1}{2}\frac{(m-y_1)^2}{s} - \frac{1}{2}\frac{(m-y_2)^2}{s} - \frac{1}{2}\frac{(m-\mu)^2}{\tau} - \frac{\beta_0}{s},$$

$$\begin{aligned}
\mathrm{E}_{q(m)}(\log p(y_1, \cdot)) &= -(\alpha_0+2)\log s - \frac{1}{2s}\mathrm{E}_{q(m)}\left[(m-y_1)^2 + (m-y_2)^2\right] - \frac{\beta_0}{s} \\
&= -(\alpha_0+2)\log s - \frac{1}{2s}\mathrm{E}_{q(m)}\left[(m^2 - 2my_1 + y_2 + m^2 - 2y_2 m + y_2\right] \\
q(s) &= i\mathcal{G}(\alpha, \beta), \\
\alpha &= \alpha_0 + 1, \\
\beta &= 0.5\mathrm{E}(m^2) - \mathrm{E}(m)(y_1 + y_2) + 0.5(y_1 + y_2) + \beta_0
\end{aligned}$$

Toy: Variational Bayes

Factors:

$$q(m) = \mathcal{N}\left(m; \left(\frac{1}{\tau} + \frac{2}{\hat{s}}\right)^{-1}\left(\frac{\mu}{\tau} + \frac{y_1 + y_2}{\hat{s}}\right), \left(\frac{1}{\tau} + \frac{2}{\hat{s}}\right)^{-1}\right)$$

$$q(s) = i\mathcal{G}\left(\alpha_0 + 1, \mathrm{E}(m^2) - \mathrm{E}(m)(y_1 + y_2) + 0.5(y_1 + y_2) + \beta_0\right)$$

with

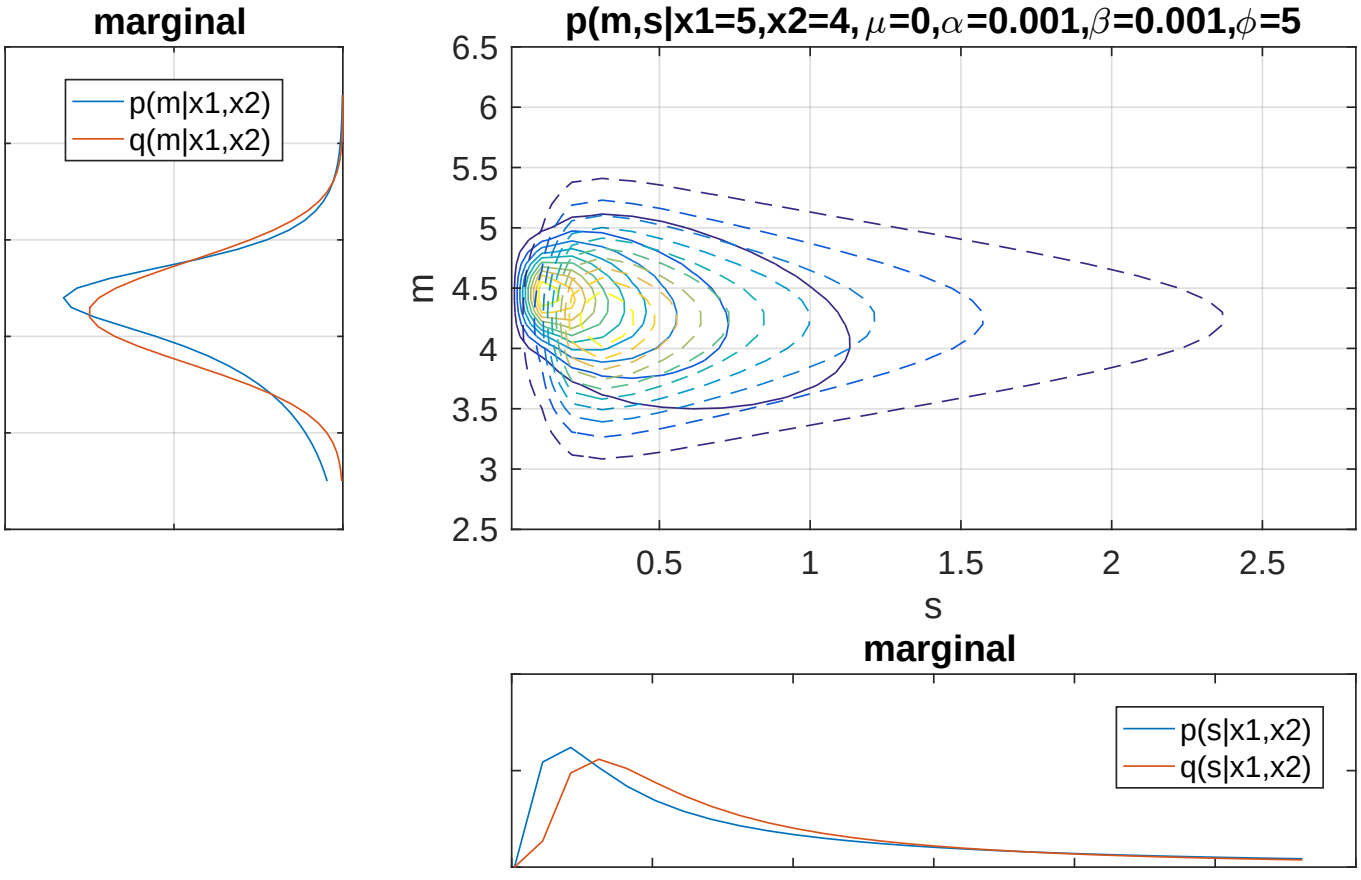
$$\hat{s} = \frac{\mathrm{E}(m^2) - \mathrm{E}(m)(y_1 + y_2) + 0.5(y_1 + y_2) + \beta_0}{\alpha_0 + 1},$$

$$\mathrm{E}(m) = \left(\frac{1}{\tau} + \frac{2}{\hat{s}}\right)^{-1}\left(\frac{\mu}{\tau} + \frac{y_1 + y_2}{\hat{s}}\right),$$

$$\mathrm{E}(m^2) = \mathrm{E}(m)^2 + \left(\frac{1}{\tau} + \frac{2}{\hat{s}}\right)^{-1},$$

which needs to be (Iterated).

Toy: Variational Bayes Iterations



Homework assignment

1. Working code for Variational Bayes estimation of the toy problem (5 points).

$$p(m, s|\tau, Y)$$

2. Working code for Variational Bayes estimation of

$$p(m, \tau|s, Y)$$