A Beginner's Guide to Variational Inference

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Outline

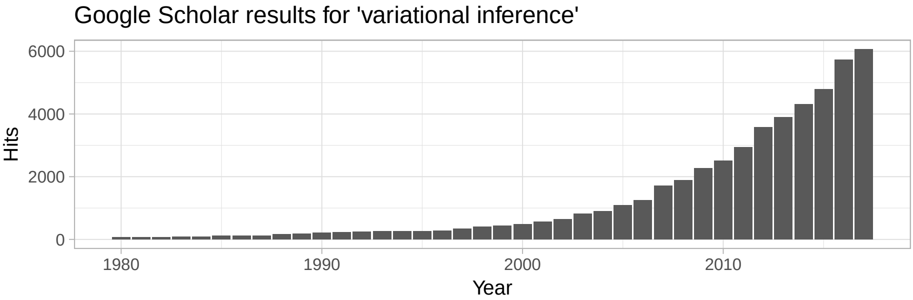
Introduction

- Consider a statistical model where we have observations $\mathbf{y} = (y_1, \dots, y_n)$ and also some latent variables $\mathbf{z} = (z_1, \dots, z_m)$.
- Want to evaluate the intractable integral

$$\mathcal{I} := \int p(\mathbf{y}|\mathbf{z})p(\mathbf{z})\,\mathrm{d}\mathbf{z}$$

  - Bayesian posterior analysis
  - Random effects models
  - Mixture models
- Variational inference approximates the "posterior" $\mathcal{I}$ by a tractably close distribution in the Kullback-Leibler sense.
- Advantages:
  - Computationally fast
  - Convergence easily assessed
  - Works well in practice

In the literature

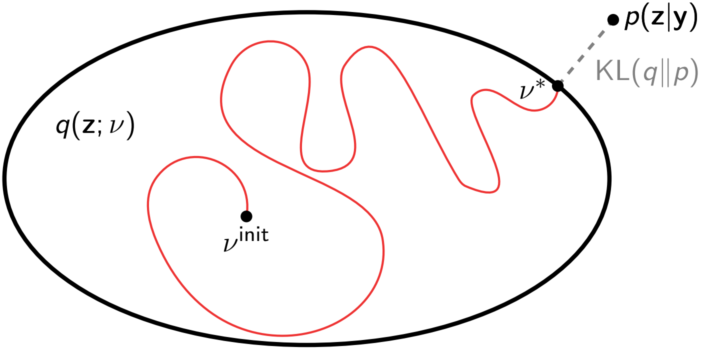


- Well known in the machine learning community.
- In social statistics:
  - E. A. Erosheva et al. (2007). "Describing disability through individual-level mixture models for multivariate binary data". *Ann. Appl. Stat*, 1.2, p. 346
  - J. Grimmer (2010). "An introduction to Bayesian inference via variational approximations". *Political Analysis* 19.1, pp. 32–47
  - Y. S. Wang et al. (2017). "A variational EM method for mixed membership models with multivariate rank data: An analysis of public policy preferences". arXiv: 1512.08731

Recommended texts

- M. J. Beal and Z. Ghahramani (2003). "The variational Bayesian EM algorithm for incomplete data: With application to scoring graphical model structures". In: *Bayesian Statistics 7. Proceedings of the Seventh Valencia International Meeting*. Ed. by J. M. Bernardo et al. Oxford: Oxford University Press, pp. 453–464
- C. M. Bishop (2006). *Pattern Recognition and Machine Learning*. Springer
- K. P. Murphy (2012). *Machine Learning: A Probabilistic Perspective*. The MIT Press
- D. M. Blei et al. (2017). "Variational inference: A review for statisticians". *J. Am. Stat. Assoc*, to appear

Idea



- Minimise Kullback-Leibler divergence (using calculus of variations)

$$\mathrm{KL}(q\|p) = -\int \log \frac{p(\mathbf{z}|\mathbf{y})}{q(\mathbf{z})} q(\mathbf{z})\,\mathrm{d}\mathbf{z}.$$

- **ISSUE**: $\mathrm{KL}(q\|p)$ is intractable.

D. M. Blei (2017). "Variational Inference: Foundations and Innovations". URL: https://simons.berkeley.edu/talks/david-blei-2017-5-1

The Evidence Lower Bound (ELBO)

- Let $q(\mathbf{z})$ be some density function to approximate $p(\mathbf{z}|\mathbf{y})$. Then the log-marginal density can be decomposed as follows:

$$\begin{aligned}
\log p(\mathbf{y}) &= \log p(\mathbf{y},\mathbf{z}) - \log p(\mathbf{z}|\mathbf{y}) \\
&= \int \left\{ \log \frac{p(\mathbf{y},\mathbf{z})}{q(\mathbf{z})} - \log \frac{p(\mathbf{z}|\mathbf{y})}{q(\mathbf{z})} \right\} q(\mathbf{z}) \, d\mathbf{z} \\
&= \mathcal{L}(q) + \mathrm{KL}(q \| p) \\
&\geq \mathcal{L}(q)
\end{aligned}$$

- $\mathcal{L}$ is referred to as the "lower-bound", and it serves as a surrogate function to the marginal.
- Maximising $\mathcal{L}(q)$ is equivalent to minimising $\mathrm{KL}(q \| p)$.
- **ISSUE**: $\mathcal{L}(q)$ is (generally) not convex.

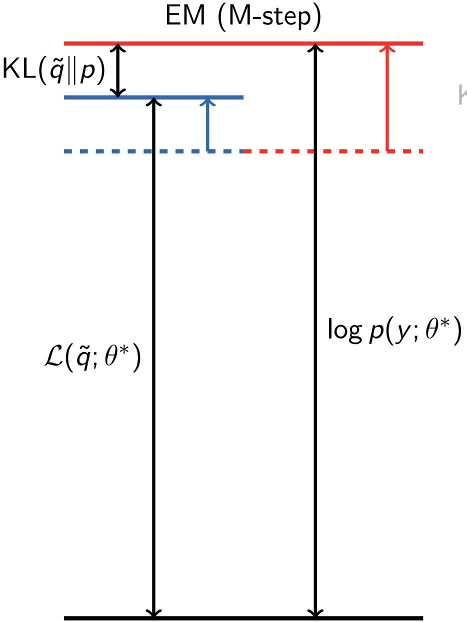
Comparison to the EM algorithm

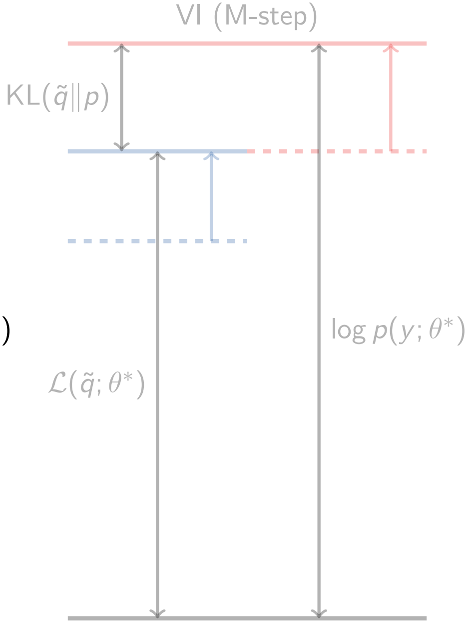
- Suppose for this part, the marginal density $p(\mathbf{y}|\theta)$ depends on parameters θ.
- In the EM algorithm, the true posterior density is used, i.e. $q(\mathbf{z}) \equiv p(\mathbf{z}|\mathbf{y},\theta)$.
- Thus,

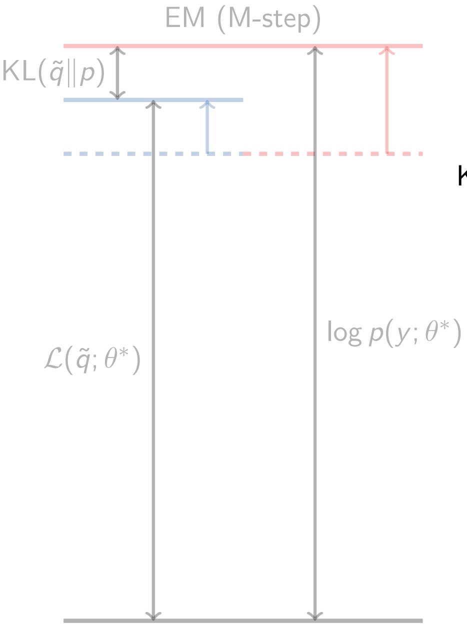
$$\begin{aligned}\log p(\mathbf{y}|\theta) &= \int \left\{ \log \frac{p(\mathbf{y},\mathbf{z}|\theta)}{p(\mathbf{z}|\mathbf{y},\theta)} - \cancel{\log \frac{p(\mathbf{z}|\mathbf{y},\theta)}{p(\mathbf{z}|\mathbf{y},\theta)}} \right\} p(\mathbf{z}|\mathbf{y},\theta^{(t)})\,d\mathbf{z} \\ &= \mathrm{E}_{\theta^{(t)}}[\log p(\mathbf{y},\mathbf{z}|\theta)] - \mathrm{E}_{\theta^{(t)}}[\log p(\mathbf{z}|\mathbf{y},\theta)] \\ &= Q(\theta|\theta^{(t)}) + \text{entropy}.\end{aligned}$$

- Minimising the KL divergence corresponds to the E-step.
- For any θ,

$$\begin{aligned}\log p(\mathbf{y}|\theta) - \log p(\mathbf{y}|\theta^{(t)}) &= Q(\theta|\theta^{(t)}) - Q(\theta^{(t)}|\theta^{(t)}) + \Delta\text{entropy} \\ &\geq Q(\theta|\theta^{(t)}) - Q(\theta^{(t)}|\theta^{(t)}).\end{aligned}$$


EM (M-step)
KL($\tilde{q}\|p$)
$\mathcal{L}(\tilde{q};\theta^*)$
$\log p(y;\theta^*)$


VI (M-step)
KL($\tilde{q}\|p$)
$\mathcal{L}(\tilde{q};\theta^*)$
$\log p(y;\theta^*)$


EM (M-step)
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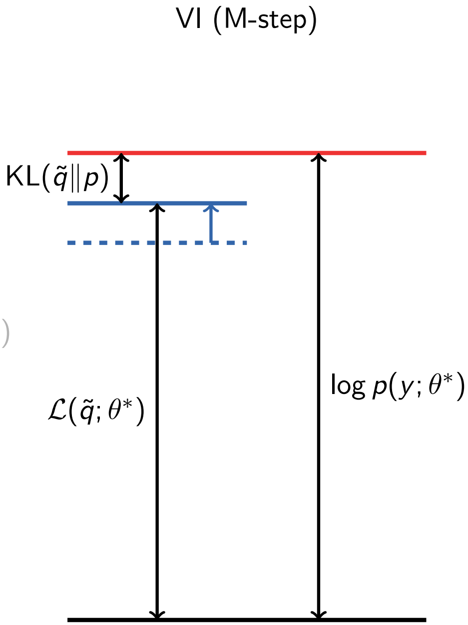

VI (M-step)
KL($\tilde{q}\|p$)
$\mathcal{L}(\tilde{q};\theta^*)$
$\log p(y;\theta^*)$

Factorised distributions (Mean-field theory)

- Maximising $\mathcal{L}$ over all possible q not feasible. Need some restrictions, but only to achieve tractability.
- Suppose we partition elements of $\mathbf{z}$ into M disjoint groups $\mathbf{z} = (\mathbf{z}^{(1)}, \dots, \mathbf{z}^{(M)})$, and assume

$$q(\mathbf{z}) = \prod_{j=1}^{M} q_j(\mathbf{z}^{(j)}).$$

- Under this restriction, the solution to $\arg\max_q \mathcal{L}(q)$ is

$$\tilde{q}_j(\mathbf{z}^{(j)}) \propto \exp\big(\mathrm{E}_{-j}[\log p(\mathbf{y}, \mathbf{z})]\big) \tag{1}$$

  for $j \in \{1, \dots, m\}$.
- In practice, these unnormalised densities are of recognisable form (especially if conjugacy is considered).

Coordinate ascent mean-field variational inference (CAVI)

- The optimal distributions are coupled with another, i.e. each $\tilde{q}_j(\mathbf{z}^{(j)})$ depends on the optimal moments of $\mathbf{z}^{(k)}$, $k \in \{1, \dots, M : k \neq j\}$.
- One way around this to employ an iterative procedure.
- Assess convergence by monitoring the lower bound

$$\mathcal{L}(q) = \mathrm{E}_q[\log p(\mathbf{y}, \mathbf{z})] - \mathrm{E}_q[\log q(\mathbf{z})].$$

Algorithm 1 CAVI

initialise Variational factors $q_j(\mathbf{z}^{(j)})$
while $\mathcal{L}(q)$ not converged **do**
    for $j = 1, \dots, M$ **do**
        $\log q_j(\mathbf{z}^{(j)}) \leftarrow \mathrm{E}_{-j}[\log p(\mathbf{y}, \mathbf{z})] + \text{const.}$ ▷ from (1)
    end for
    $\mathcal{L}(q) \leftarrow \mathrm{E}_q[\log p(\mathbf{y}, \mathbf{z})] - \mathrm{E}_q[\log q(\mathbf{z})]$
end while
return $\tilde{q}(\mathbf{z}) = \prod_{j=1}^M \tilde{q}_j(\mathbf{z}^{(j)})$

Estimation of a 1-dim Gaussian mean and variance

- **GOAL**: Bayesian inference of mean μ and variance ψ^{-1}

$$
\begin{aligned}
y_i &\overset{\text{iid}}{\sim} \mathrm{N}(\mu, \psi^{-1}) && \text{Data} \\
\mu|\psi &\sim \mathrm{N}\left(\mu_0, (\kappa_0\psi)^{-1}\right) && \text{Priors} \\
\psi &\sim \Gamma(a_0, b_0) \\
i &= 1, \dots, n
\end{aligned}
$$

- Substitute $p(\mu, \psi|\mathbf{y})$ with the mean-field approximation

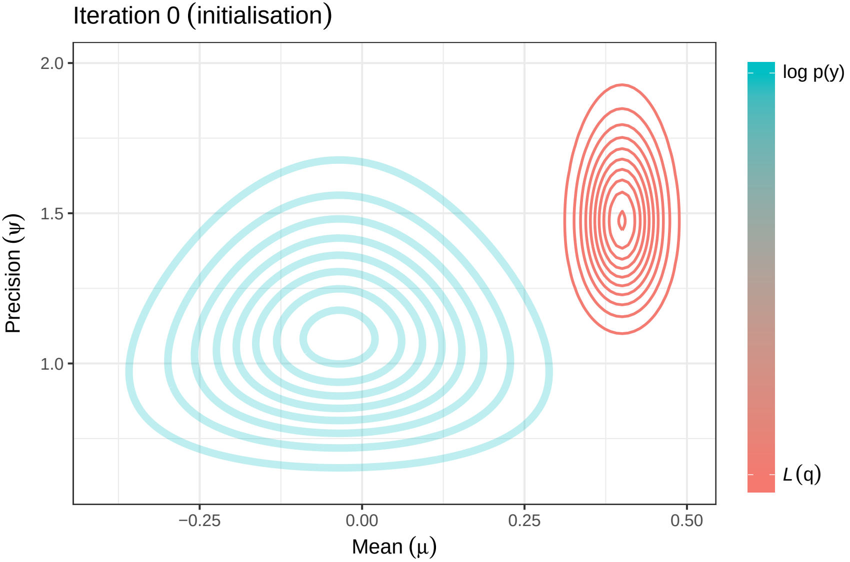
$$q(\mu, \psi) = q_\mu(\mu) q_\psi(\psi).$$

- From (1), we can work out the solutions

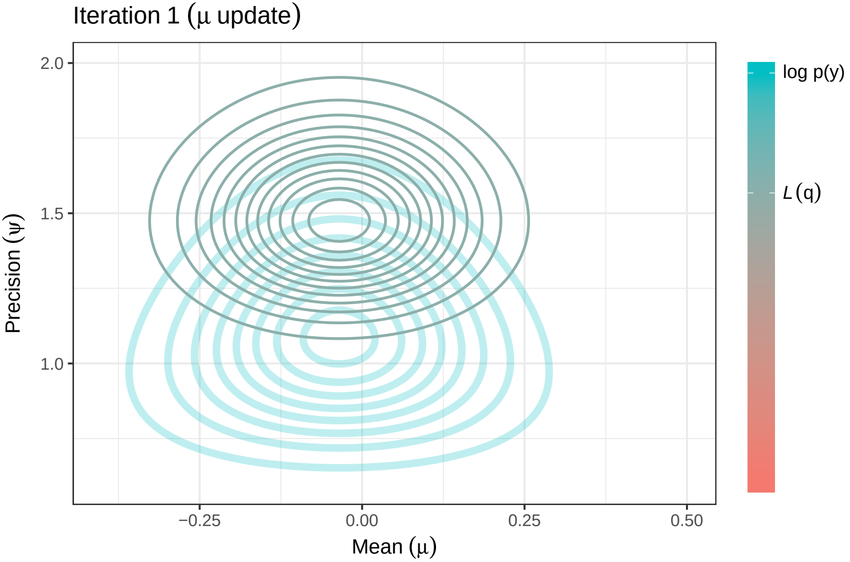
$$\tilde{q}_\mu(\mu) \equiv \mathrm{N}\left(\frac{\kappa_0\mu_0 + n\bar{y}}{\kappa_0 + n}, \frac{1}{(\kappa_0 + n)\,\mathrm{E}_q[\psi]}\right) \quad \text{and} \quad \tilde{q}_\psi(\psi) \equiv \Gamma(\tilde{a}, \tilde{b})$$

$$\tilde{a} = a_0 + \frac{n}{2} \qquad \tilde{b} = b_0 + \frac{1}{2}\mathrm{E}_q\left[\textstyle\sum_{i=1}^n (y_i - \mu)^2 + \kappa_0(\mu - \mu_0)^2\right]$$

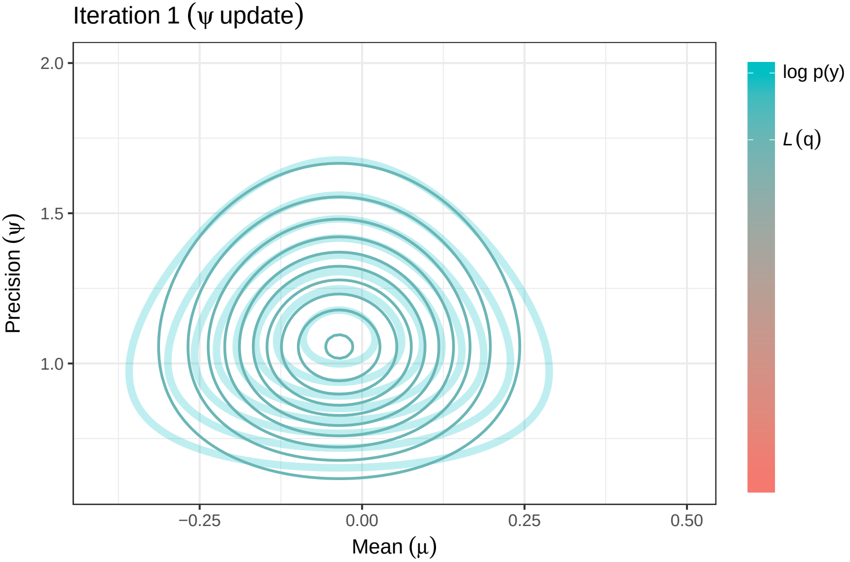
Estimation of a 1-dim Gaussian mean and variance (cont.)



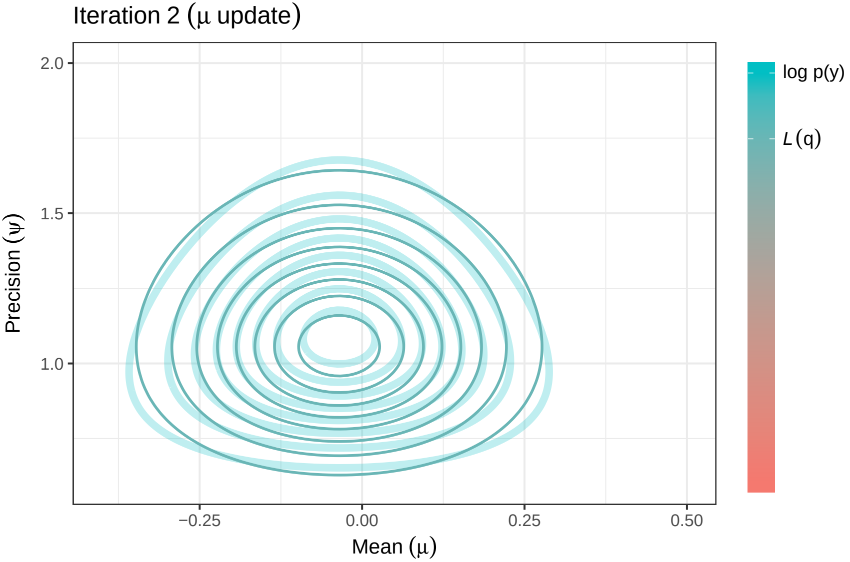
Estimation of a 1-dim Gaussian mean and variance (cont.)



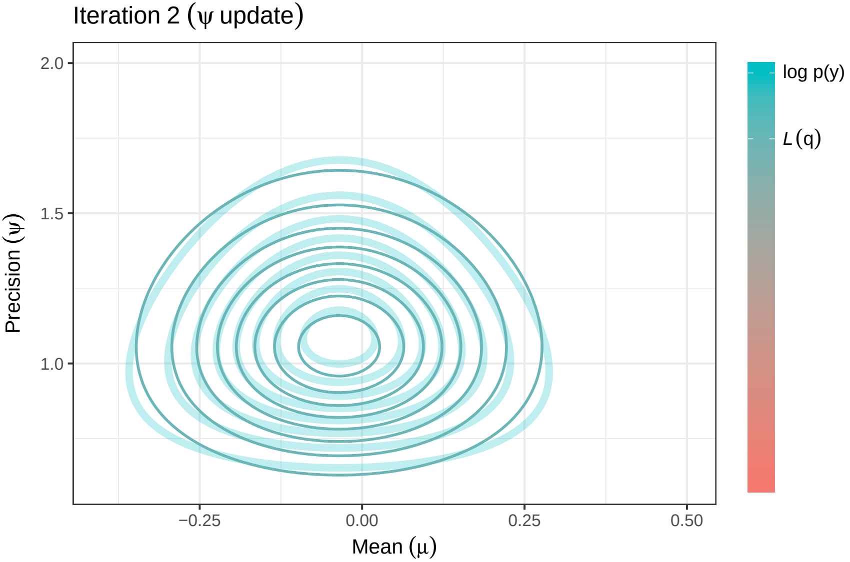
Estimation of a 1-dim Gaussian mean and variance (cont.)



Estimation of a 1-dim Gaussian mean and variance (cont.)



Estimation of a 1-dim Gaussian mean and variance (cont.)



Comparison of solutions

Variational posterior

$$\mu \sim \mathrm{N}\left(\frac{\kappa_0\mu_0 + n\bar{y}}{\kappa_0 + n}, \frac{1}{(\kappa_0 + n)\,\mathrm{E}[\psi]}\right)$$

$$\psi \sim \Gamma\left(a_0 + \frac{n}{2}, b_0 + \frac{1}{2}c\right)$$

$$c = \mathrm{E}\left[\sum_{i=1}^{n}(y_i - \mu)^2 + \kappa_0(\mu - \mu_0)^2\right]$$

True posterior

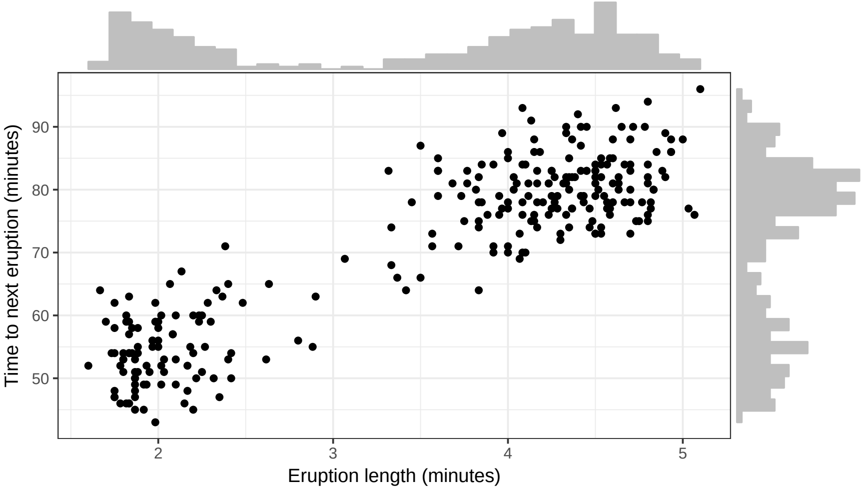
$$\mu|\psi \sim \mathrm{N}\left(\frac{\kappa_0\mu_0 + n\bar{y}}{\kappa_0 + n}, \frac{1}{(\kappa_0 + n)\psi}\right)$$

$$\psi \sim \Gamma\left(a_0 + \frac{n}{2}, b_0 + \frac{1}{2}c'\right)$$

$$c' = \sum_{i=1}^{n}(y_i - \bar{y})^2 + \frac{\kappa_0}{\kappa_0 + n}(\bar{y} - \mu_0)^2$$

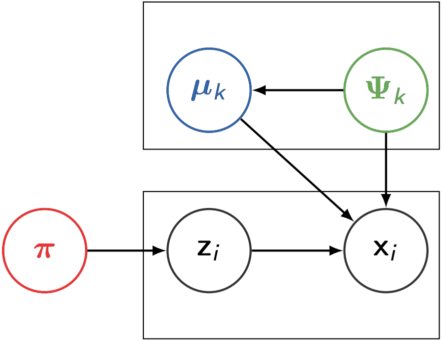
- $\mathrm{Cov}(\mu, \psi) = 0$ by design in VI solutions.
- For this simple example, it is possible to decouple and solve explicitly.
- VI solutions leads to unbiased MLE if $\kappa_0 = \mu_0 = a_0 = b_0 = 0$.

Gaussian mixture model (Old Faithful data set)



- Let $\mathbf{x}_i \in \mathbb{R}^d$ and assume $\mathbf{x}_i \overset{\text{iid}}{\sim} \sum_{k=1}^{K} \pi_k \, \mathrm{N}_d(\boldsymbol{\mu}_k, \boldsymbol{\Psi}_k^{-1})$ for $i = 1, \dots, n$.

Gaussian mixture model



$$
\begin{aligned}
&p(\mathbf{x}, \mathbf{z}, \boldsymbol{\pi}, \boldsymbol{\mu}, \boldsymbol{\Psi}) \\
&= p(\mathbf{x}|\mathbf{z}, \boldsymbol{\mu}, \boldsymbol{\Psi}) p(\mathbf{z}|\boldsymbol{\pi}) \\
&\quad \times p(\boldsymbol{\pi}) p(\boldsymbol{\mu}|\boldsymbol{\Psi}) p(\boldsymbol{\Psi}) \\
&= p(\mathbf{x}|\mathbf{z}, \boldsymbol{\mu}, \boldsymbol{\Psi}) p(\mathbf{z}|\boldsymbol{\pi}) \\
&\quad \times \operatorname{Dir}_K(\boldsymbol{\pi}|\alpha_{01}, \dots, \alpha_{0K}) \\
&\quad \times \textstyle\prod_{k=1}^K \mathrm{N}_d\big(\boldsymbol{\mu}_k|\mathbf{m}_0, (\kappa_0 \boldsymbol{\Psi}_k)^{-1}\big) \\
&\quad \times \textstyle\prod_{k=1}^K \operatorname{Wis}_d(\boldsymbol{\Psi}_k|\mathbf{W}_0, \nu_0)
\end{aligned}
$$

- Introduce $\mathbf{z}_i = (z_{i1}, \dots, z_{iK})$, a 1-of-$K$ binary vector, where each $z_{ik} \sim \operatorname{Bern}(\pi_k)$.
- Assuming $\mathbf{z} = \{\mathbf{z}_1, \dots, \mathbf{z}_n\}$ are observed along with $\mathbf{x} = \{\mathbf{x}_1, \dots, \mathbf{x}_n\}$,

$$p(\mathbf{x}|\mathbf{z}, \boldsymbol{\mu}, \boldsymbol{\Psi}) = \prod_{i=1}^n \prod_{k=1}^K \mathrm{N}_d(\mathbf{x}_i|\boldsymbol{\mu}_k, \boldsymbol{\Psi}_k^{-1})^{z_{ik}}.$$

Variational inference for GMM

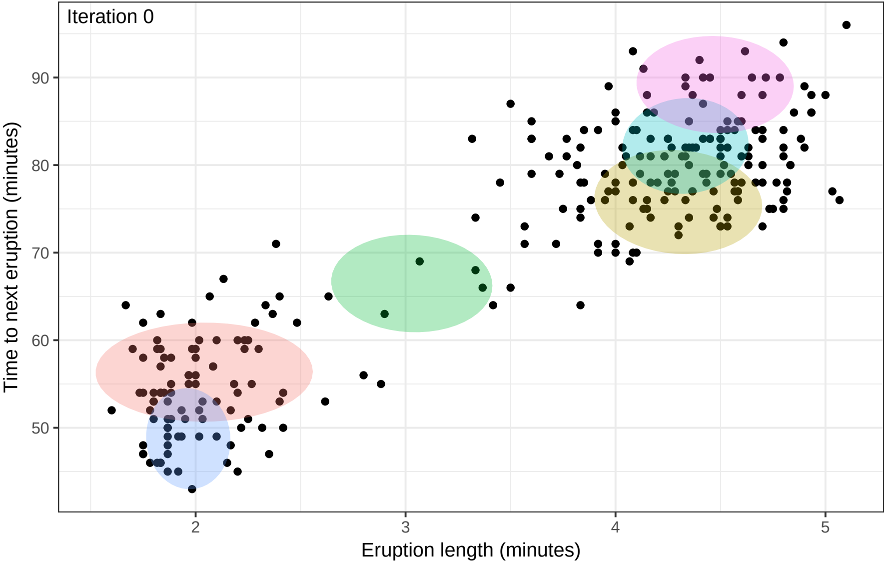
- Assume the mean-field posterior density

$$\begin{aligned} q(\mathbf{z}, \boldsymbol{\pi}, \boldsymbol{\mu}, \boldsymbol{\Psi}) &= q(\mathbf{z}) q(\boldsymbol{\pi}, \boldsymbol{\mu}, \boldsymbol{\Psi}) \\ &= q(\mathbf{z}) q(\boldsymbol{\pi}) q(\boldsymbol{\mu}|\boldsymbol{\Psi}) q(\boldsymbol{\Psi}). \end{aligned}$$

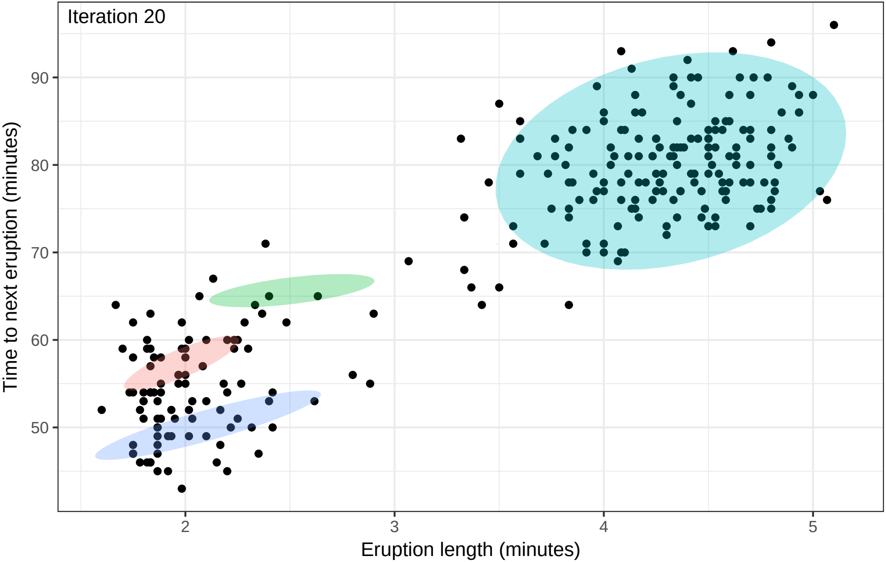
Algorithm 2 CAVI for GMM

initialise Variational factors $q(\mathbf{z})$, $q(\boldsymbol{\pi})$ and $q(\boldsymbol{\mu}, \boldsymbol{\Psi})$
while $\mathcal{L}(q)$ not converged **do**
    $q(z_{ik}) \leftarrow \mathrm{Bern}(\cdot)$
    $q(\boldsymbol{\pi}) \leftarrow \mathrm{Dir}_K(\cdot)$
    $q(\boldsymbol{\mu}|\boldsymbol{\Psi}) \leftarrow \mathrm{N}_d(\cdot, \cdot)$
    $q(\boldsymbol{\Psi}) \leftarrow \mathrm{Wis}_d(\cdot, \cdot)$
    $\mathcal{L}(q) \leftarrow \mathrm{E}_q[\log p(\mathbf{x}, \mathbf{z}, \boldsymbol{\pi}, \boldsymbol{\mu}, \boldsymbol{\Psi})] - \mathrm{E}_q[\log q(\mathbf{z}, \boldsymbol{\pi}, \boldsymbol{\mu}, \boldsymbol{\Psi})]$
end while
return $\tilde{q}(\mathbf{z}, \boldsymbol{\pi}, \boldsymbol{\mu}, \boldsymbol{\Psi}) = \tilde{q}(\mathbf{z}) \tilde{q}(\boldsymbol{\pi}) \tilde{q}(\boldsymbol{\mu}|\boldsymbol{\Psi}) \tilde{q}(\boldsymbol{\Psi})$

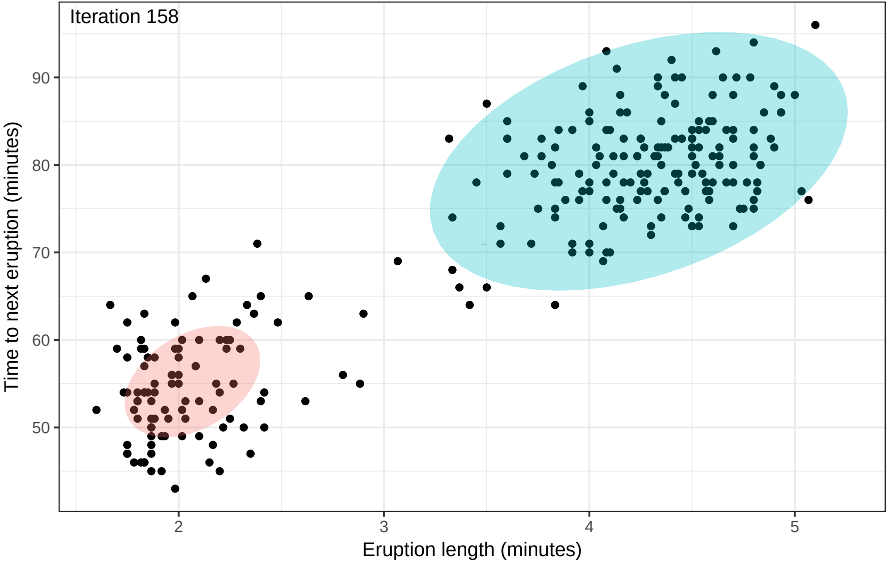
Variational inference for GMM (cont.)



Variational inference for GMM (cont.)



Variational inference for GMM (cont.)



Final thoughts on variational GMM

- Similar algorithm to the EM, and therefore similar computational time.
- Can extend to mixture of bernoullis a.k.a. latent class analysis.
- **PROS**:
  - Automatic selection of number of mixture components.
  - Less pathological special cases compared to EM solutions because regularised by prior information.
  - Less sensitive to number of parameters/components.
- **CONS**:
  - Hyperparameter tuning.

Exponential families

- For the mean-field variational method, suppose that each complete conditional is in the exponential family:

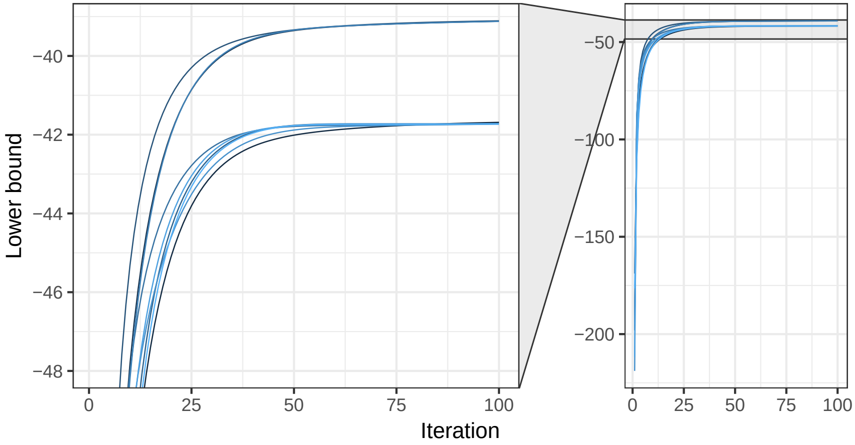
$$p(\mathbf{z}^{(j)}|\mathbf{z}_{-j},\mathbf{y}) = h(\mathbf{z}^{(j)}) \exp\big(\eta_j(\mathbf{z}_{-j},\mathbf{y})\cdot\mathbf{z}^{(j)} - A(\eta_j)\big).$$

- Then, from (1),

$$\begin{aligned}\tilde{q}_j(\mathbf{z}^{(j)}) &\propto \exp\big(\,\mathrm{E}_{-j}[\log p(\mathbf{z}^{(j)}|\mathbf{z}_{-j},\mathbf{y})]\big)\\ &= \exp\Big(\log h(\mathbf{z}^{(j)}) + \mathrm{E}[\eta_j(\mathbf{z}_{-j},\mathbf{y})]\cdot\mathbf{z}^{(j)} - \mathrm{E}[A(\eta_j)]\Big)\\ &\propto h(\mathbf{z}^{(j)}) \exp\Big(\mathrm{E}[\eta_j(\mathbf{z}_{-j},\mathbf{y})]\cdot\mathbf{z}^{(j)}\Big)\end{aligned}$$

  is also in the same exponential family.
- C.f. Gibbs conditional densities.
- **ISSUE**: What if not in exponential family? Importance sampling or Metropolis sampling.

Non-convexity of ELBO



- CAVI only guarantees converges to a local optimum.
- Multiple local optima may exist.

Zero-forcing vs Zero-avoiding

- Back to the KL divergence:

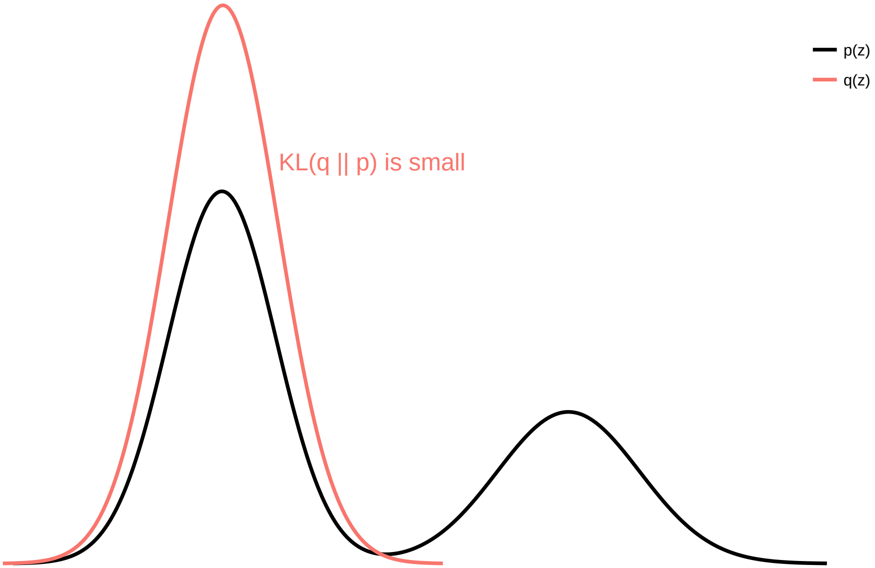
$$\mathrm{KL}(q\|p) = \int \log \frac{q(\mathbf{z})}{p(\mathbf{z}|\mathbf{y})} q(\mathbf{z}) \, \mathrm{d}\mathbf{z}$$

- $\mathrm{KL}(q\|p)$ is large when $p(\mathbf{z}|\mathbf{y})$ is close to zero, unless $q(\mathbf{z})$ is also close to zero (*zero-forcing*).
- **ISSUE**: What about other measures of closeness? For instance,

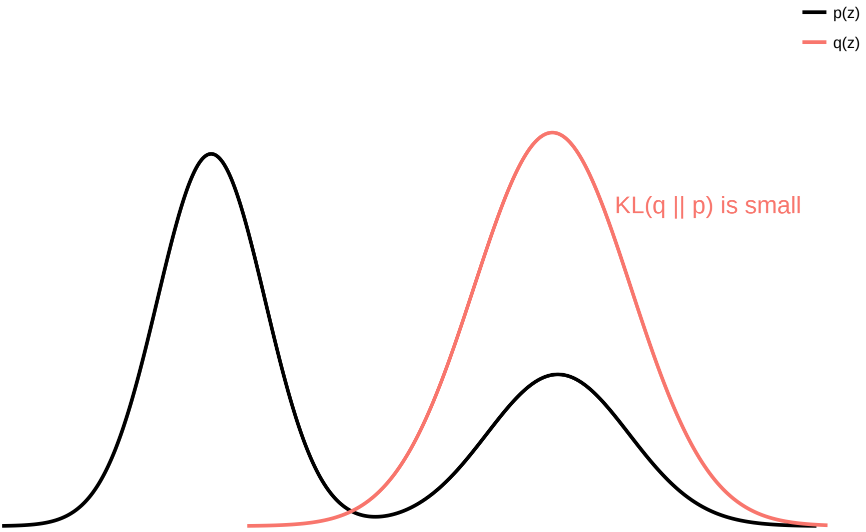
$$\mathrm{KL}(p\|q) = \int \log \frac{p(\mathbf{z}|\mathbf{y})}{q(\mathbf{z}|\mathbf{y})} p(\mathbf{z}|\mathbf{y}) \, \mathrm{d}\mathbf{z}.$$

- This gives the Expectation Propagation (EP) algorithm.
- It is *zero-avoiding*, because $\mathrm{KL}(p\|q)$ is small when both $p(\mathbf{z}|\mathbf{y})$ and $q(\mathbf{z})$ are non-zero.

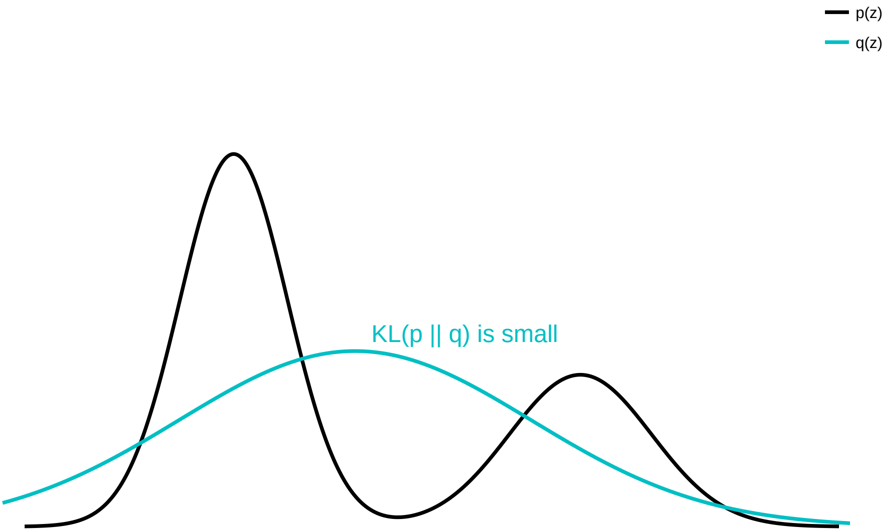
Zero-forcing vs Zero-avoiding (cont.)



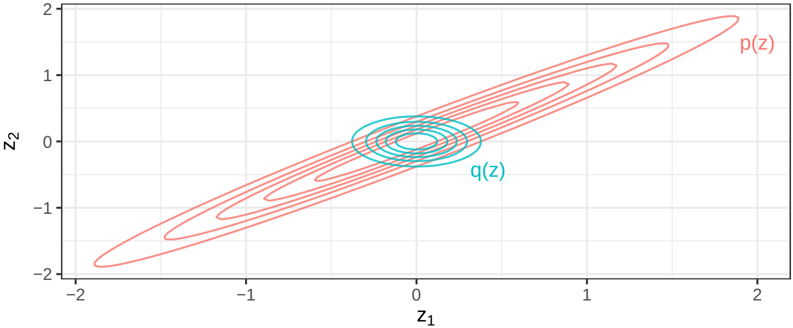
Zero-forcing vs Zero-avoiding (cont.)



Zero-forcing vs Zero-avoiding (cont.)



Distortion of higher order moments



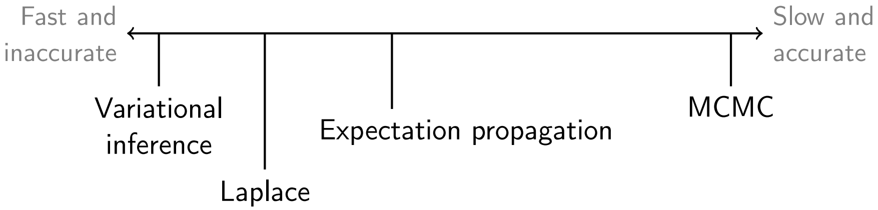
- Consider $\mathbf{z} = (z_1, z_2)^\top \sim \mathrm{N}_2(\boldsymbol{\mu}, \boldsymbol{\Psi}^{-1})$, $\mathrm{Cov}(z_1, z_2) \neq 0$.
- Approximating $p(\mathbf{z})$ by $q(\mathbf{z}) = q(z_1)q(z_2)$ yields

$$\tilde{q}(z_1) = \mathrm{N}(z_1 | \mu_1, \boldsymbol{\Psi}_{11}^{-1}) \quad \text{and} \quad \tilde{q}(z_2) = \mathrm{N}(z_2 | \mu_2, \boldsymbol{\Psi}_{22}^{-1})$$

  and by definition, $\mathrm{Cov}(z_1, z_2) = 0$ under $\tilde{q}$.
- This leads to underestimation of variances (widely reported in the literature—Zhao and Marriott 2013).

Quality of approximation

- Variational inference converges to a different optimum than ML, except for certain models (Gunawardana and Byrne 2005).
- But not much can be said about the quality of approximation.
- Statistical properties not well understood—what is its statistical profile relative to the exact posterior?
- Speed trumps accuracy?



Advanced topics

- Local variational bounds
  - Not using the mean-field assumption.
  - Instead, find a bound for the marginalising integral $\mathcal{I}$.
  - Used for Bayesian logistic regression as follows:

$$\mathcal{I} = \int \operatorname{expit}(x^\top \beta) p(\beta) \, \mathrm{d}\beta \geq \int f(x^\top \beta, \xi) p(\beta) \, \mathrm{d}\beta.$$

- Stochastic variational inference
  - VI on its own doesn't offer much computational advantages.
  - Use ideas from stochastic optimisation—gradient based improvement of ELBO from subsamples of the data.
  - Scales to massive data.
- Black box variational inference
  - Beyond exponential families and model-specific derivations.

End

Thank you!

Slides and source code are made available at: http://socialstats.haziqj.ml

References I

Beal, M. J. and Z. Ghahramani (2003). "The variational Bayesian EM algorithm for incomplete data: With application to scoring graphical model structures". In: *Bayesian Statistics 7*. Proceedings of the Seventh Valencia International Meeting. Ed. by J. M. Bernardo, A. P. Dawid, J. O. Berger, M. West, D. Heckerman, M. Bayarri, and A. F. Smith. Oxford: Oxford University Press, pp. 453–464.

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The variational principle

- Name derived from calculus of variations which deals with maximising or minimising functionals.

Functions	$p : \theta \mapsto \mathbb{R}$	(standard calculus)
Functionals	$\mathcal{H} : p \mapsto \mathbb{R}$	(variational calculus)

- Using standard calculus, we can solve

$$\arg\max_{\theta} p(\theta) =: \hat{\theta}$$

  e.g. p is a likelihood function, and $\hat{\theta}$ is the ML estimate.

- Using variational calculus, we can solve

$$\arg\max_{p} \mathcal{H}(p) =: \tilde{p}$$

  e.g. $\mathcal{H}$ is the entropy $\mathcal{H} = -\int p(x) \log p(x) \, dx$, and $\tilde{p}$ is the entropy maximising distribution.

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Laplace's method

- Interested in $p(\mathbf{f}|\mathbf{y}) \propto p(\mathbf{y}|\mathbf{f})p(\mathbf{f}) =: e^{Q(\mathbf{f})}$, with normalising constant $p(\mathbf{y}) = \int e^{Q(\mathbf{f})} \, d\mathbf{f}$. The Taylor expansion of Q about its mode $\tilde{\mathbf{f}}$

$$Q(\mathbf{f}) \approx Q(\tilde{\mathbf{f}}) - \frac{1}{2}(\mathbf{f} - \tilde{\mathbf{f}})^\top \mathbf{A}(\mathbf{f} - \tilde{\mathbf{f}})$$

  is recognised as the logarithm of an unnormalised Gaussian density, with $\mathbf{A} = -\mathrm{D}^2 Q(\mathbf{f})$ being the negative Hessian of Q evaluated at $\tilde{\mathbf{f}}$.

- The posterior $p(\mathbf{f}|\mathbf{y})$ is approximated by $\mathrm{N}(\tilde{\mathbf{f}}, \mathbf{A}^{-1})$, and the marginal by

$$p(\mathbf{y}) \approx (2\pi)^{n/2} |\mathbf{A}|^{-1/2} p(\mathbf{y}|\tilde{\mathbf{f}}) p(\tilde{\mathbf{f}})$$

- Won't scale with large n; difficult to find modes in high dimensions.

R. Kass and A. Raftery (1995). "Bayes Factors". *Journal of the American Statistical Association* 90.430, pp. 773–795, §4.1, pp.777-778.

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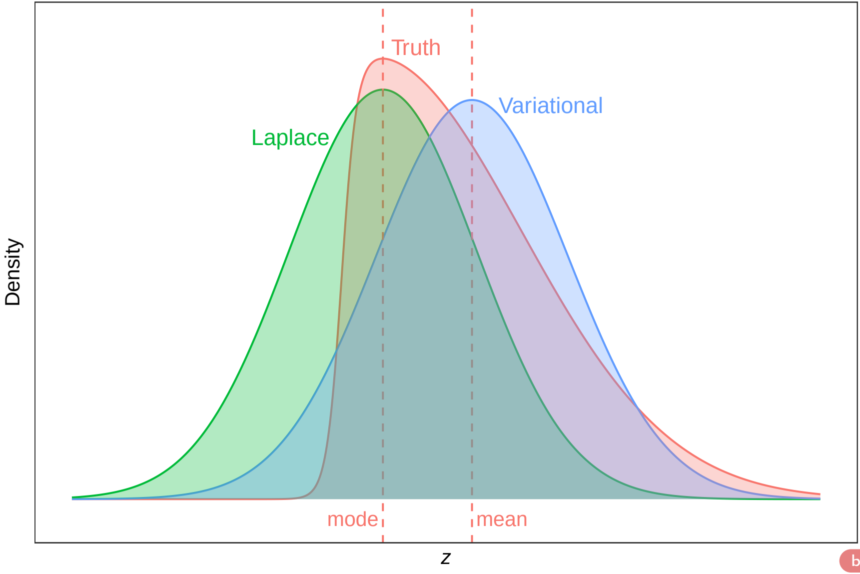
Comparison of approximations (density)



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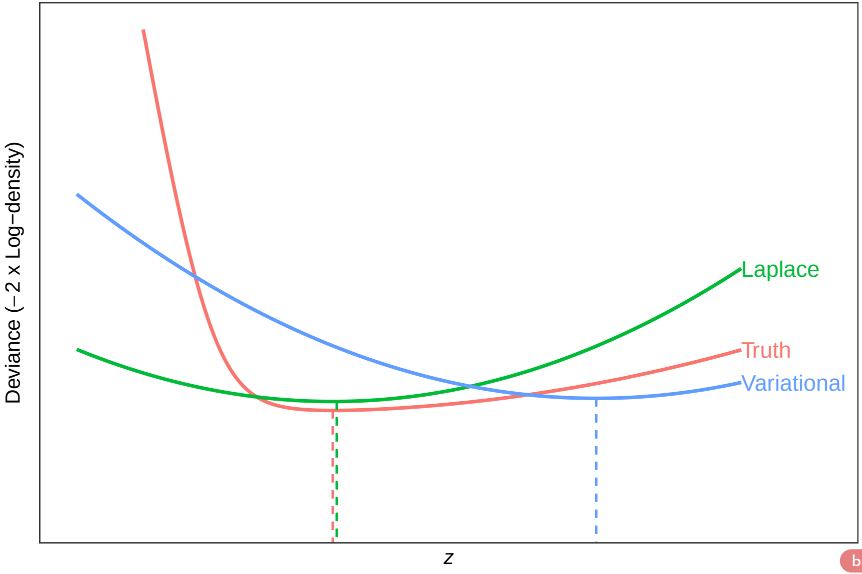
Comparison of approximations (deviance)



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