A Beginner's Guide to Variational Inference

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5 December 2018

UBD Interview Seminar

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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 $\mathbf{z} = (z_1, \dots, z_m)$.

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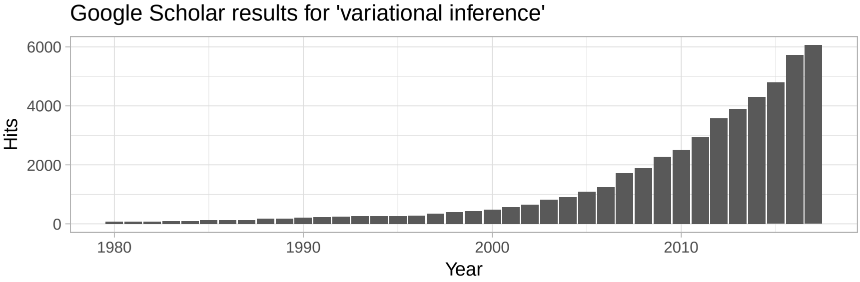
- Variational inference approximates the "posterior" $p(\mathbf{z}|\mathbf{y})$ by a tractably close distribution in the Kullback-Leibler sense.
- Advantages:
  - Computationally fast
  - Convergence easily assessed
  - Works well in practice

In the literature



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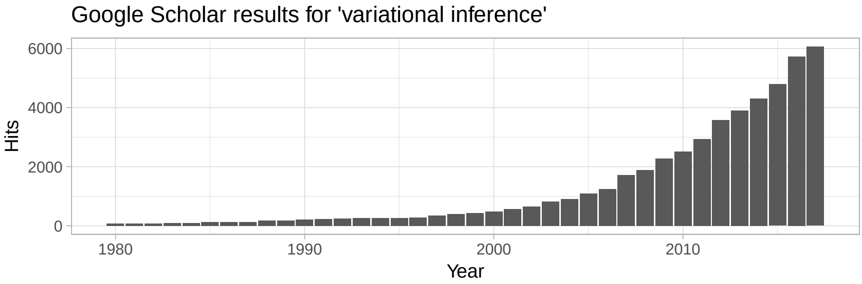

- Well known in machine learning, slowly encroaching other fields.
- Applications (Blei et al., 2017):
  - Computer vision and robotics (image denoising, tracking, recognition)
  - Natural language processing and speech recognition (topic modelling)
  - Social statistics (probit models, latent class models, variable selection)
  - Computational biology (phylogenetic hidden Markov models, population genetics, gene expression analysis)
  - Computational neuroscience (autoregressive processes, hierarchical models, spatial models)

Recommended texts

- D. M. Blei et al. (2017). "Variational Inference: A Review for Statisticians". *J. Am. Stat. Assoc*, 112.518, pp. 859–877
- C. M. Bishop (2006). *Pattern Recognition and Machine Learning*. Springer
- K. P. Murphy (2012). *Machine Learning: A Probabilistic Perspective*. The MIT Press
- M. J. Beal (2003). "Variational algorithms for approximate Bayesian inference". PhD thesis. Gatsby Computational Neuroscience Unit, University College London
- HJ (Oct. 2018). "Regression modelling using priors depending on Fisher information covariance kernels (I-priors)". PhD thesis. London School of Economics and Political Science

Idea

$p(\mathbf{z}|\mathbf{y})$

$q(\mathbf{z})$

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

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

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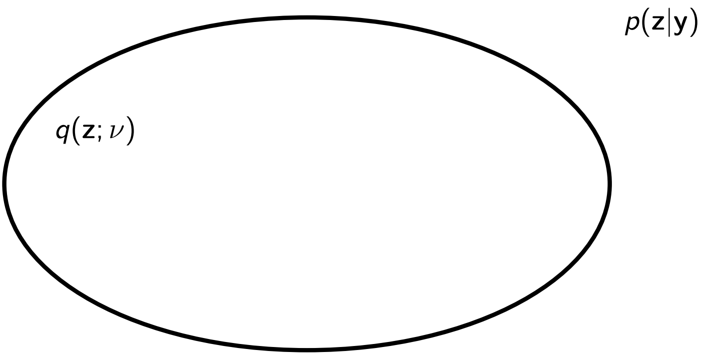

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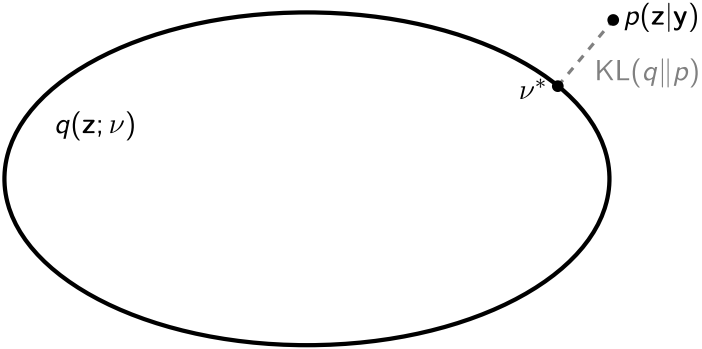

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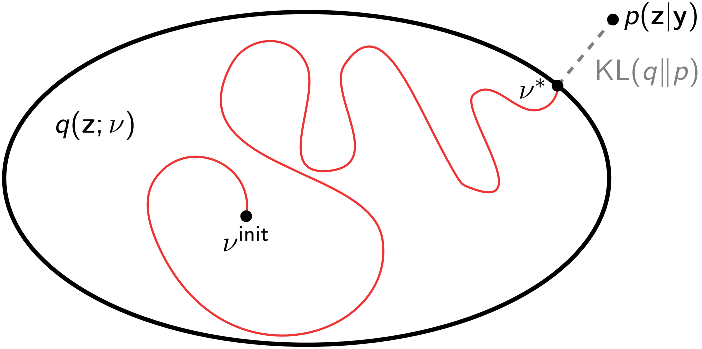

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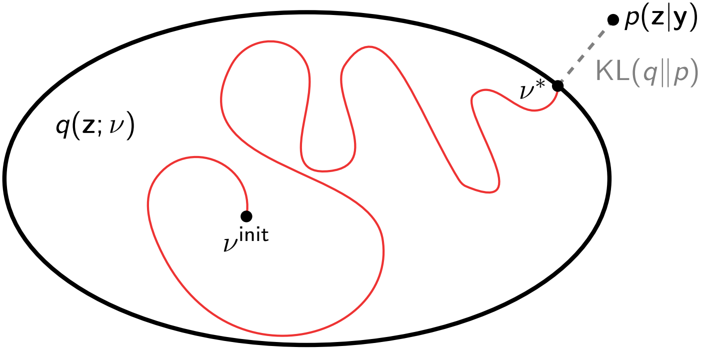

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$$\mathrm{KL}(q\|p) = -\int \log \frac{p(\mathbf{z}|\mathbf{y})}{q(\mathbf{z})} q(\mathbf{z}) \, d\mathbf{z}.$$

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

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The Evidence Lower Bound (ELBO)

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  - Equality in the bound when $q(\mathbf{z}) \equiv p(\mathbf{z}|\mathbf{y})$, and $\mathrm{KL}(q \| p)$ vanishes

Comparison to the EM algorithm

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Variational inference/Bayes	(Variational) EM algorithm
GOAL: Posterior densities for $(\mathbf{w}, \theta)$	**GOAL**: ML/MAP estimates for θ
Variational approximation for latent variables and parameters $q(\mathbf{w}, \theta) \approx p(\mathbf{w}, \theta \mid \mathbf{y})$	Variational approximation for latent variables only $q(\mathbf{w}) \approx p(\mathbf{w} \mid \mathbf{y})$
Priors required on θ	Priors not necessary for θ
Derivation can be tedious	Derivation less tedious
Inference on θ through (approximate) posterior density $q(\theta)$	Asymptotic distribution of θ not well studied; standard errors for θ not easily obtained

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

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- In practice, these unnormalised densities are of recognisable form (especially if conjugacy is considered).

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Algorithm 4 CAVI

1: **initialise** Variational factors $q_j(\mathbf{z}_{[j]})$
2: **while** $\mathcal{L}(q)$ not converged **do**
3:     **for** $j = 1, \dots, M$ **do**
4:         $\log q_j(\mathbf{z}_{[j]}) \leftarrow \mathrm{E}_{-j}[\log p(\mathbf{y}, \mathbf{z})] + \text{const.}$ ▷ from (1)
5:     **end for**
6:     $\mathcal{L}(q) \leftarrow \mathrm{E}_q[\log p(\mathbf{y}, \mathbf{z})] - \mathrm{E}_q[\log q(\mathbf{z})]$
7: **end while**
8: **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}

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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} \\
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$$\log \tilde{q}_\mu(\mu) = \mathrm{E}_\psi[\log p(\mathbf{y}|\mu,\psi)] + \mathrm{E}_\psi[\log p(\mu|\psi)] + \text{const.}$$

$$\log \tilde{q}_\psi(\psi) = \mathrm{E}_\mu[\log p(\mathbf{y}|\mu,\psi)] + \mathrm{E}_\mu[\log p(\mu|\psi)] + \log p(\psi) + \text{const.}$$

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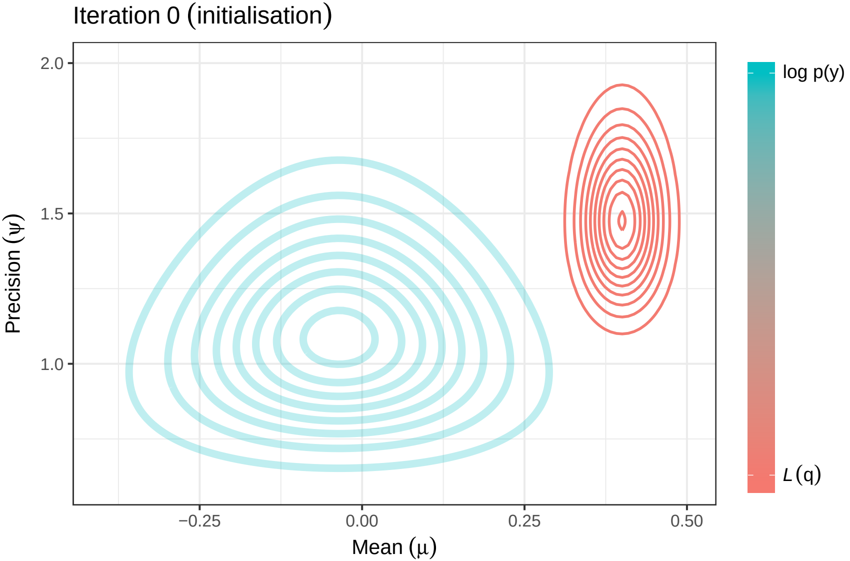
$$\tilde{a} = a_0 + \frac{n}{2} \qquad \tilde{b} = b_0 + \frac{1}{2}\,\mathrm{E}_q\left[\textstyle\sum_{i=1}^n (y_i - \mu)^2 + \kappa_0(\mu - \mu_0)^2\right]$$

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



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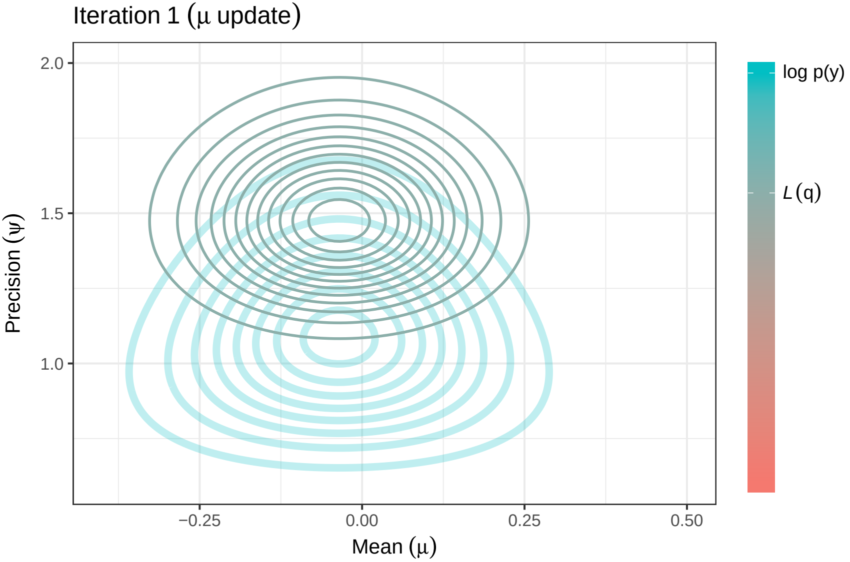

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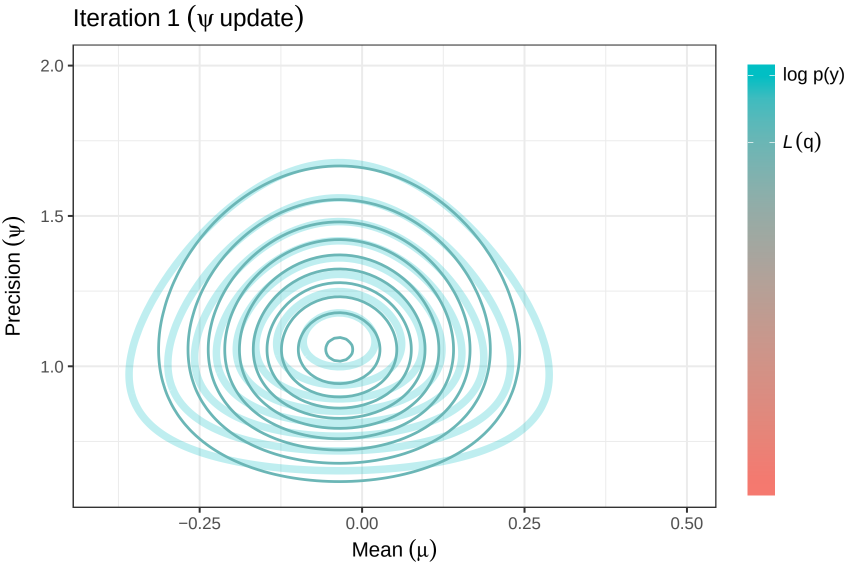

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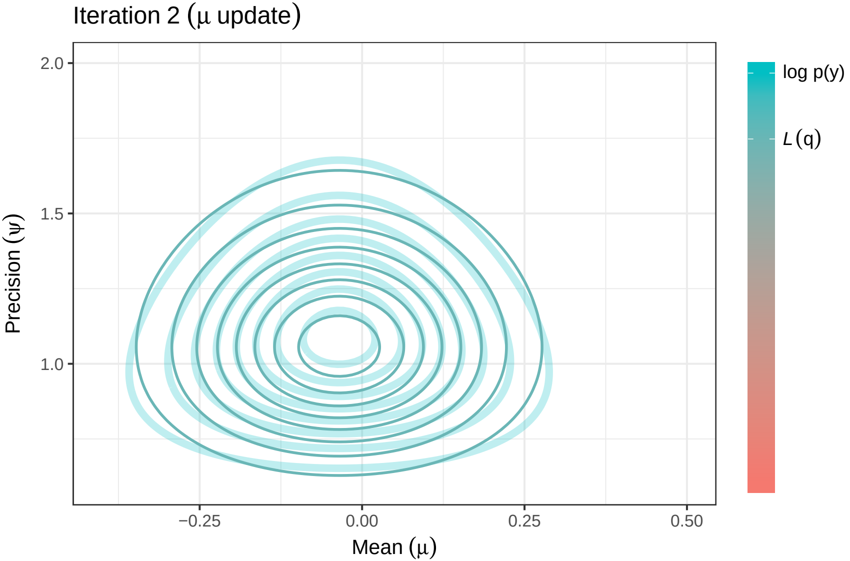

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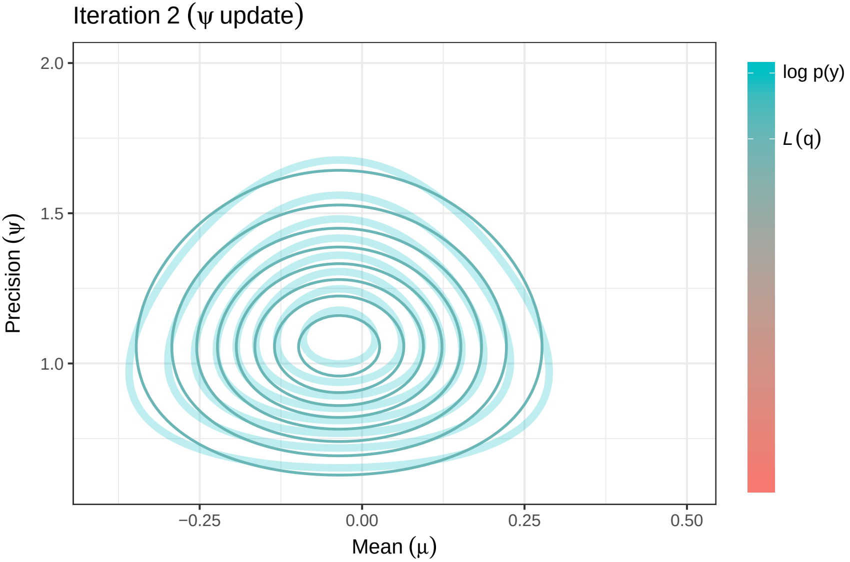


Comparison of solutions

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

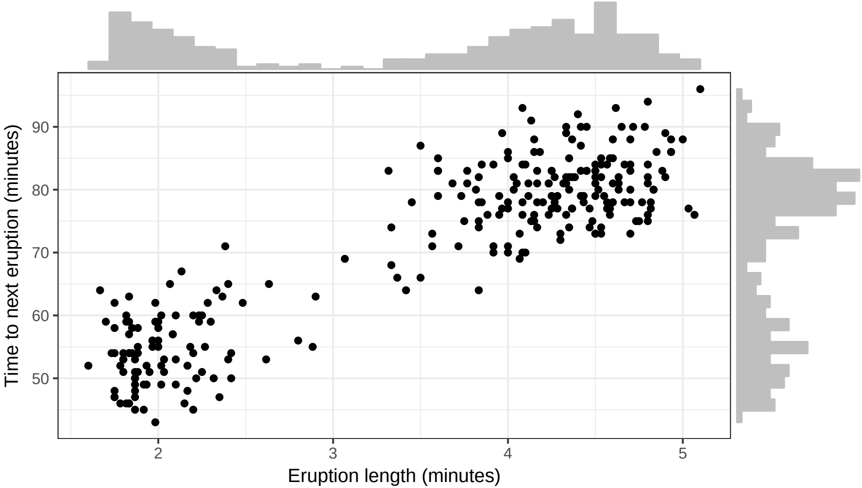
$$\mu|\psi \sim \mathrm{N}\left(\frac{\kappa_0\mu_0 + n\bar{y}}{\kappa_0 + n}, \frac{1}{(\kappa_0 + n)\psi}\right)$$

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

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

- $\mathrm{Cov}(\mu, \psi) = 0$ 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)



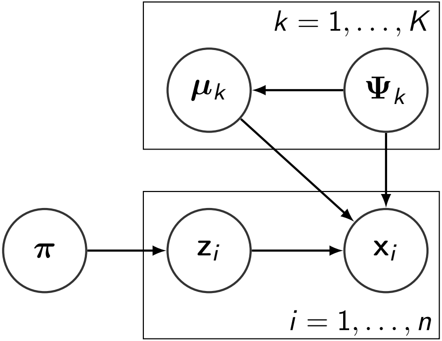
- Let $\mathbf{x}_i \in \mathbb{R}^d$ and assume $\mathbf{x}_i \overset{\text{iid}}{\sim} \sum_{k=1}^{K} \pi_k \, \mathrm{N}_d(\boldsymbol{\mu}_k, \boldsymbol{\Psi}_k^{-1})$ for $i = 1, \dots, n$.

Gaussian mixture model

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

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

Gaussian mixture model



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

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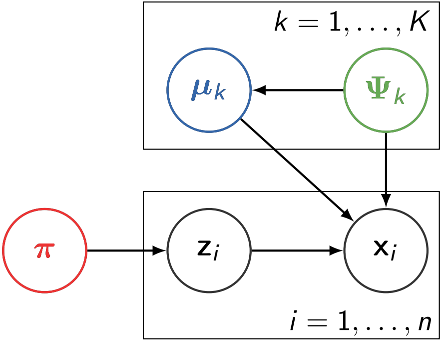

$$
\begin{aligned}
&p(\mathbf{x}, \mathbf{z}, \boldsymbol{\pi}, \boldsymbol{\mu}, \boldsymbol{\Psi}) \\
&= p(\mathbf{x}|\mathbf{z}, \boldsymbol{\mu}, \boldsymbol{\Psi}) p(\mathbf{z}|\boldsymbol{\pi}) \\
&\quad \times p(\boldsymbol{\pi}) p(\boldsymbol{\mu}|\boldsymbol{\Psi}) p(\boldsymbol{\Psi}) \\
&=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

Variational inference for GMM

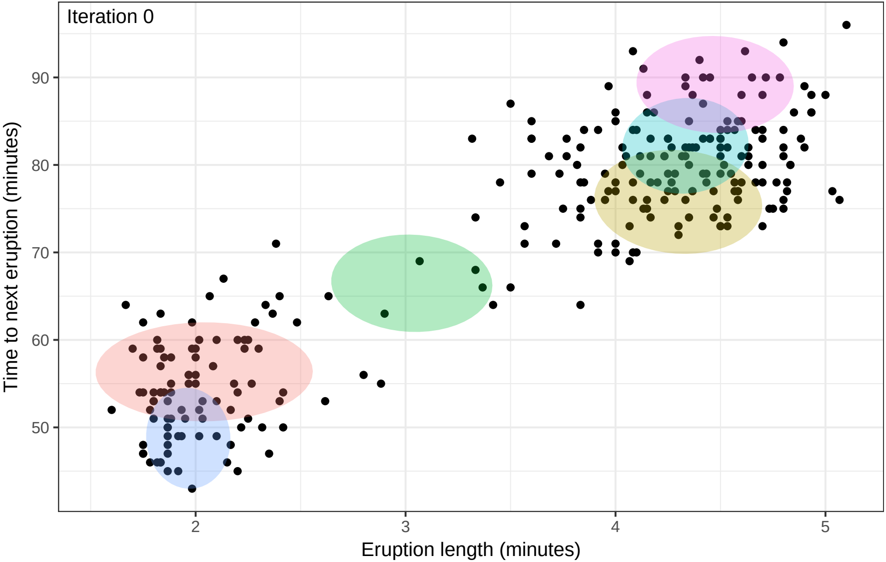
- Assume the mean-field posterior density

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

Algorithm 5 CAVI for GMM details

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



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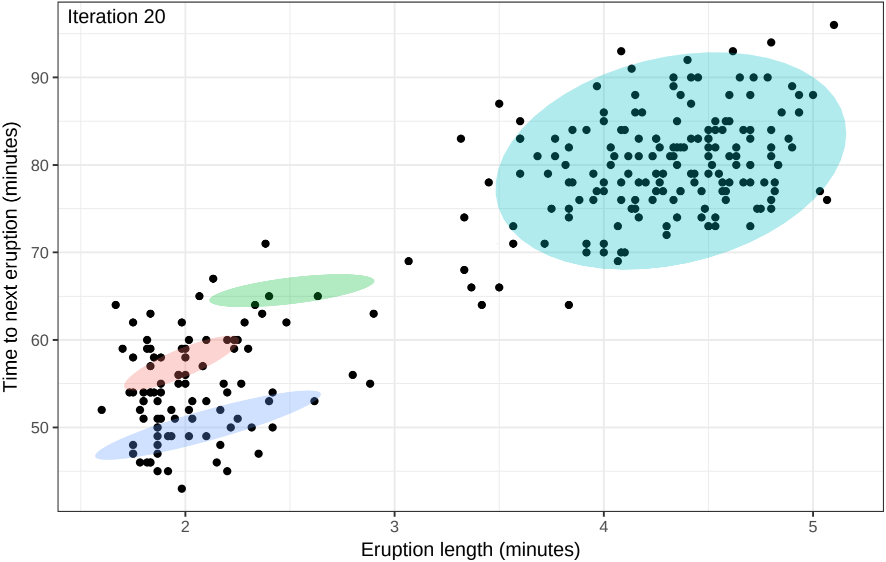

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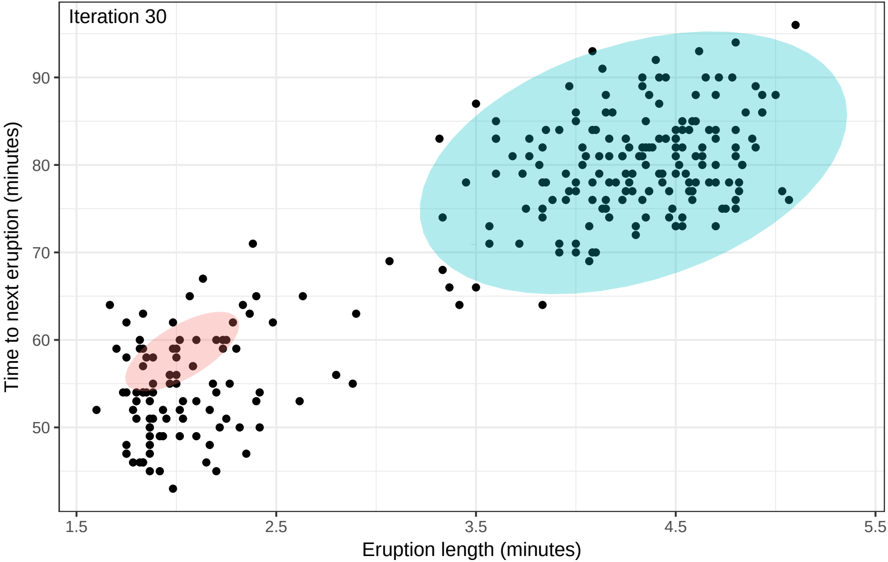

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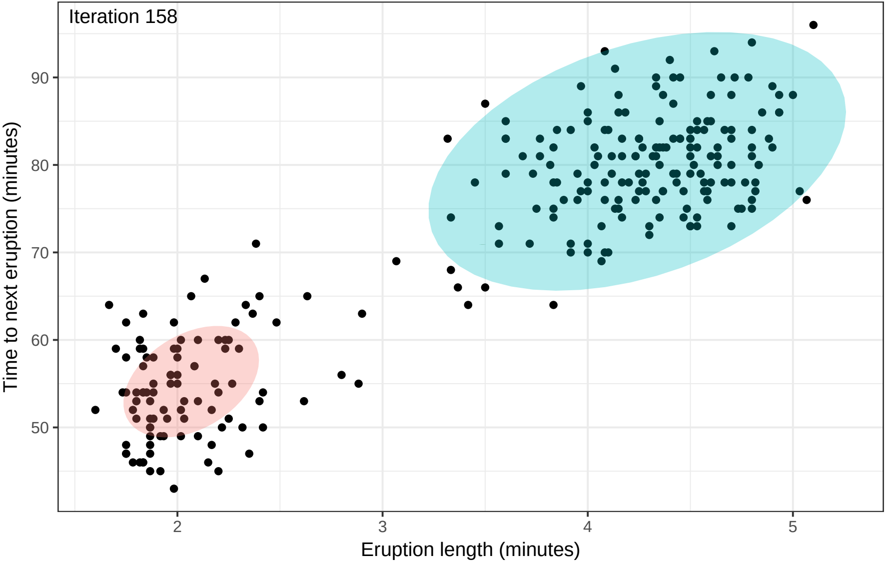

Final thoughts on variational GMM

- 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:

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

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- Then, from (1),

$$\begin{aligned}
\tilde{q}_j(\mathbf{z}^{(j)}) &\propto \exp\big(\operatorname{E}_{-j}[\log p(\mathbf{z}^{(j)}|\mathbf{z}_{-j},\mathbf{y})]\big) \\
&= \exp\Big(\log h(\mathbf{z}^{(j)}) + \operatorname{E}[\eta_j(\mathbf{z}_{-j},\mathbf{y})] \cdot \mathbf{z}^{(j)} - \operatorname{E}[A(\eta_j)]\Big) \\
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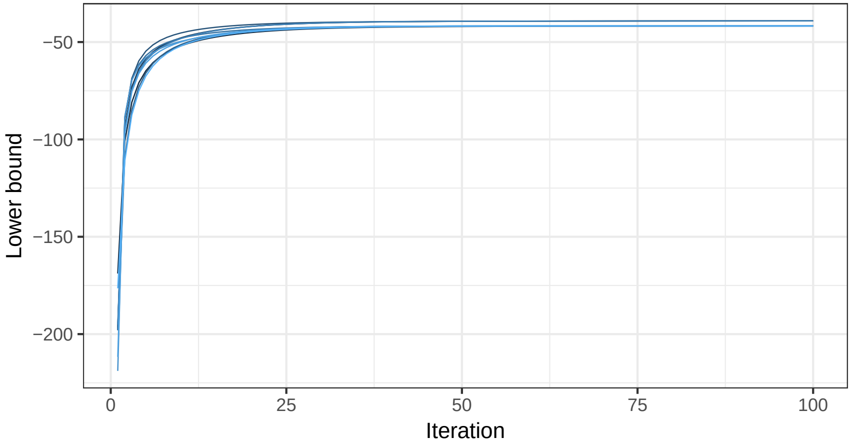
- C.f. Gibbs conditional densities.
- **ISSUE**: What if not in exponential family? Importance sampling or Metropolis sampling.

Non-convexity of ELBO



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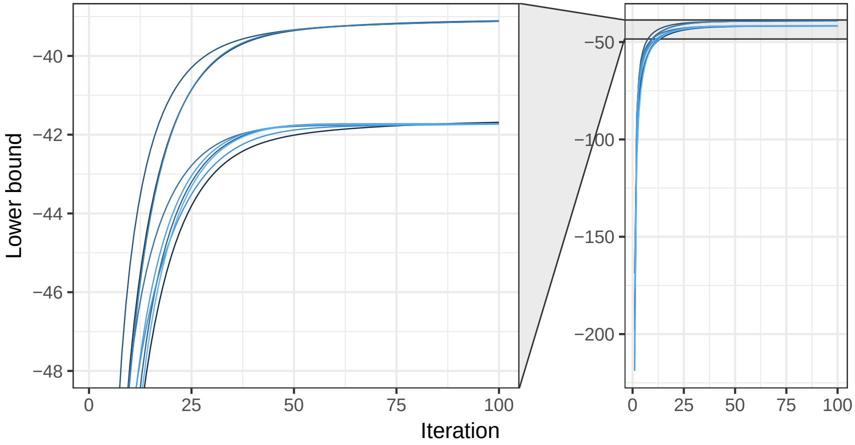

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Zero-forcing vs Zero-avoiding

- 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*).
- What about other measures of closeness?

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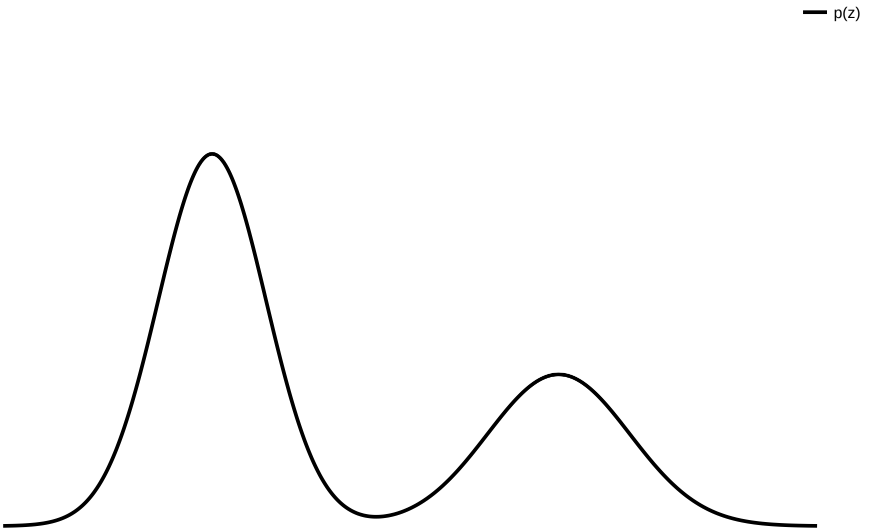
- What about other measures of closeness? For instance,

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

- 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.)



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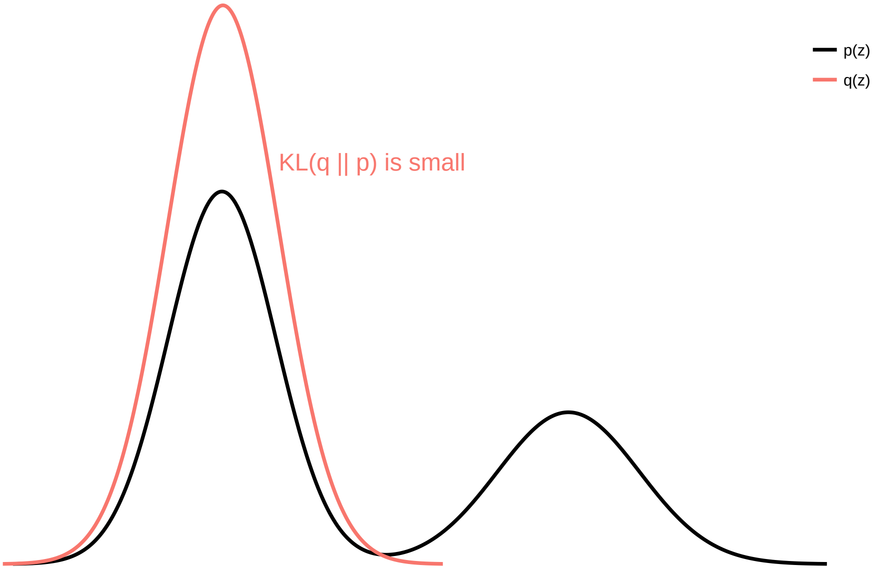

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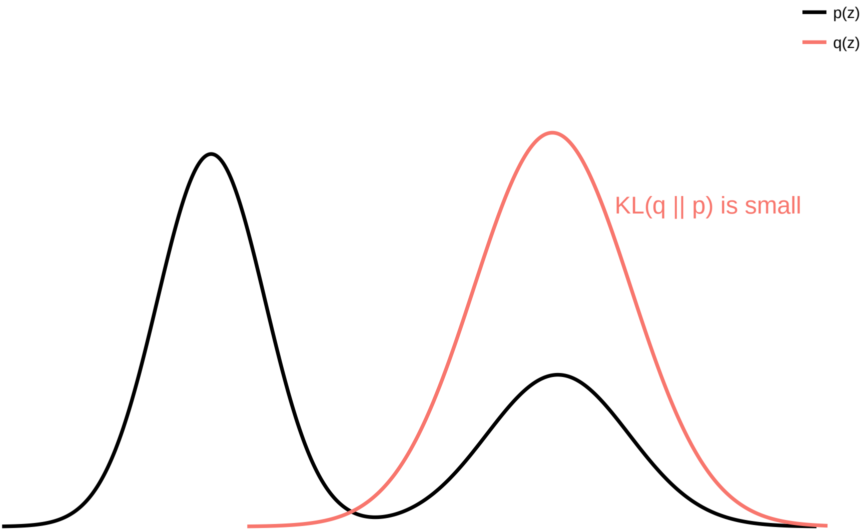

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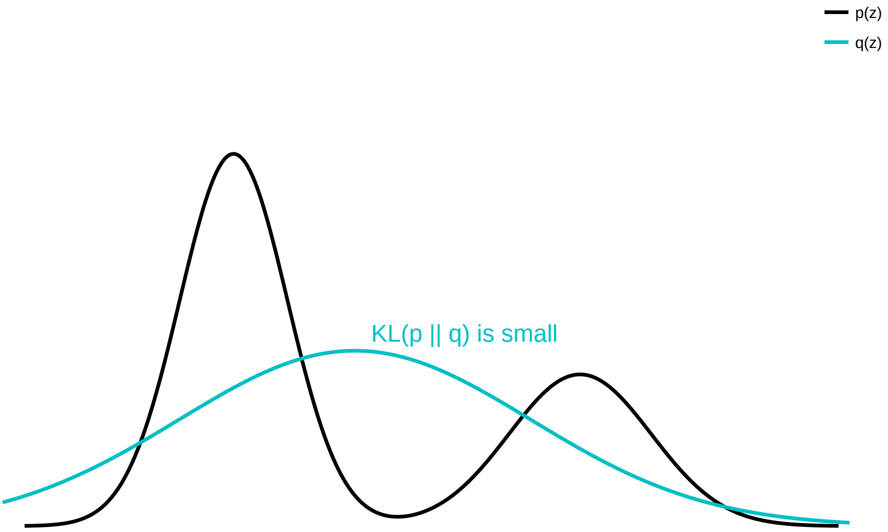
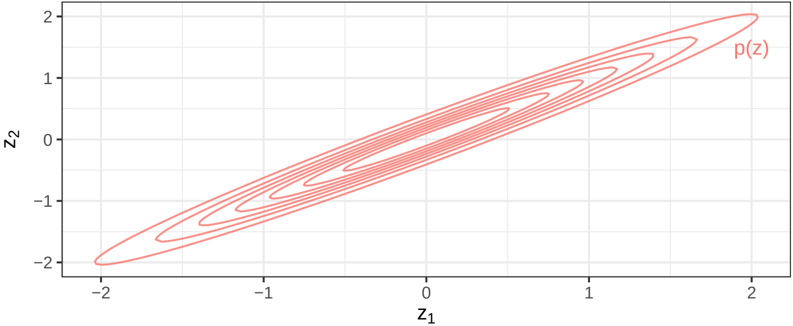


Distortion of higher order moments



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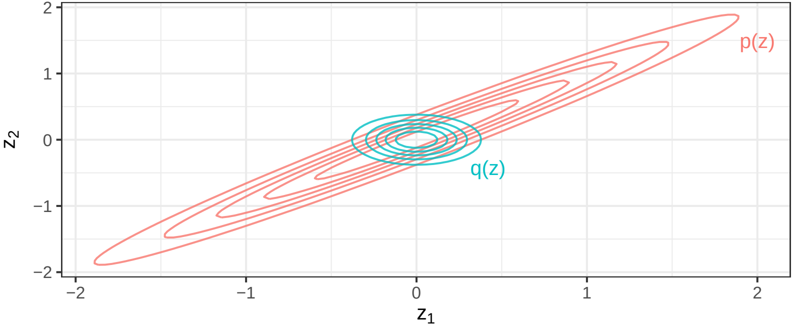

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and by definition, $\mathrm{Cov}(z_1, z_2) = 0$ under $\tilde{q}$.

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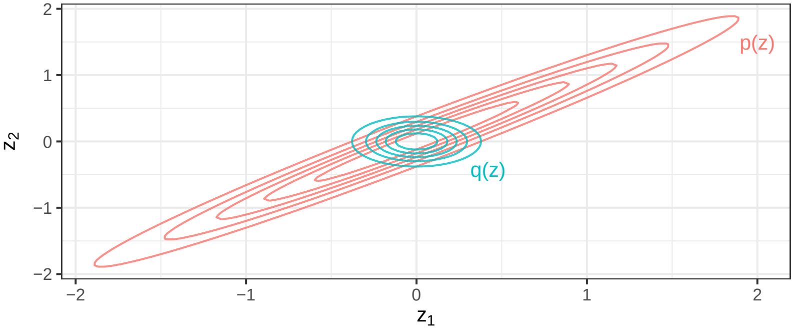

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  and by definition, $\mathrm{Cov}(z_1, z_2) = 0$ under $\tilde{q}$.
- This leads to underestimation of variances (widely reported in the literature—Zhao and Marriott, 2013).

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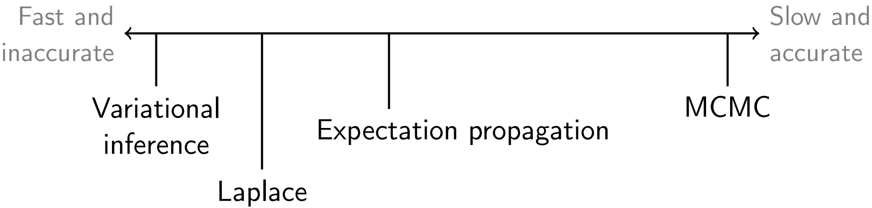
- Speed trumps accuracy?



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:

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

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  - 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

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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)

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- 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.

back

Comparison to the EM algorithm

- In addition to latent variables $\mathbf{z}$, typically there are unknown parameters θ to be estimated.
  - Frequentist estimation: θ is fixed
  - Bayesian estimation: $\theta \sim p(\theta)$ is random
- Consider θ fixed. Maximising the (marginal) log-likelihood directly

$$\arg\max_\theta \ \log \left\{ \int \overbrace{p(\mathbf{y}|\mathbf{z},\theta)p(\mathbf{z}|\theta)}^{p(\mathbf{y},\mathbf{z})} \, \mathrm{d}\mathbf{z} \right\}$$

  is difficult. However, if somehow the latent variables were known, then the problem may become easier.
- Given initial values $\theta^{(0)}$, the EM algorithm cycles through
  - **E-step**: Compute $Q(\theta|\theta^{(t)}) := \mathrm{E}_{\mathbf{z}}[\log p(\mathbf{y},\mathbf{z}|\theta) \,|\, \mathbf{y}, \theta^{(t)}]$
  - **M-step**: $\theta^{(t+1)} \leftarrow \arg\max_\theta Q(\theta|\theta^{(t)})$

  for $t = 1, 2, \ldots$ until convergence.

back

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 $p(\mathbf{y}) = \int e^{Q(\mathbf{f})} \, \mathrm{d}\mathbf{f}$. 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 $\tilde{\mathbf{f}}$.

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

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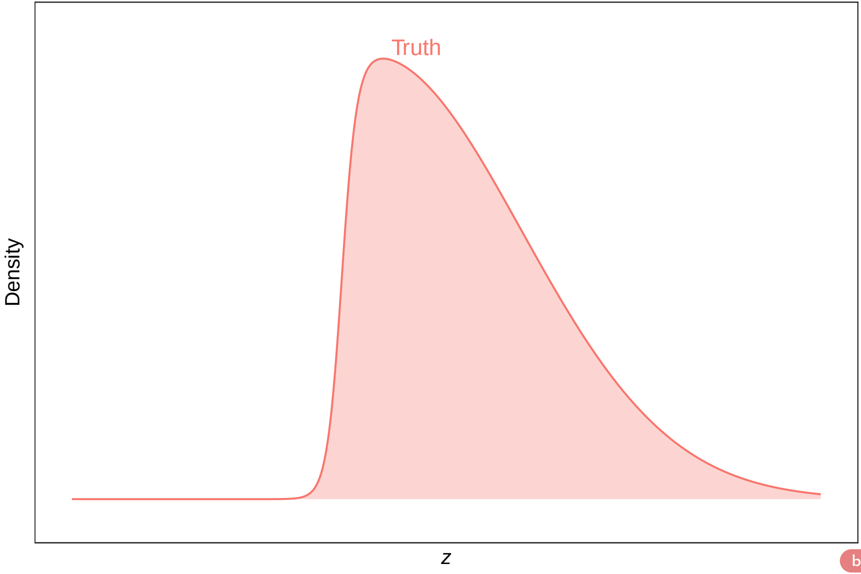
Comparison of approximations (density)



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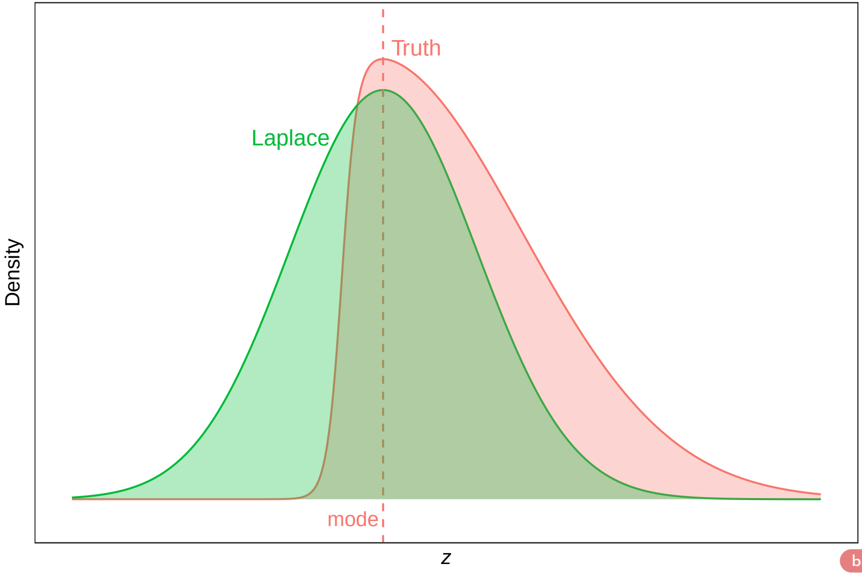

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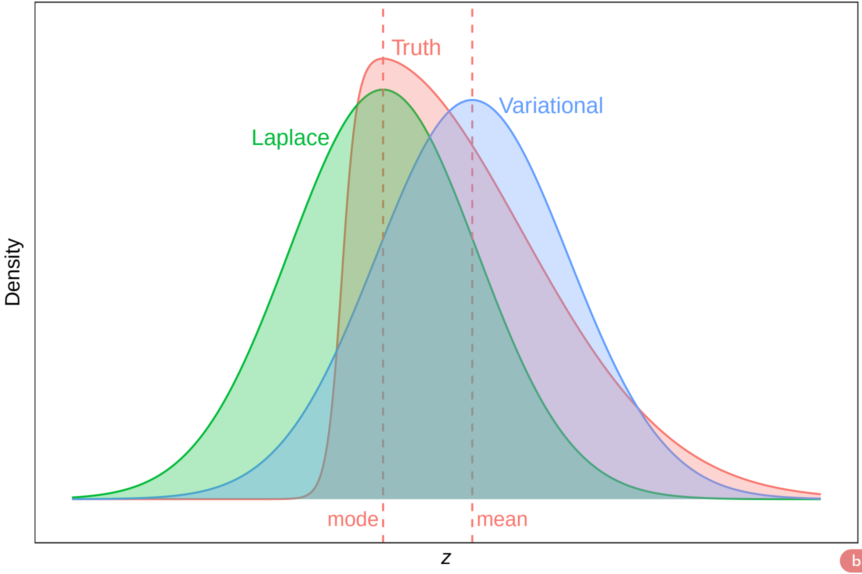

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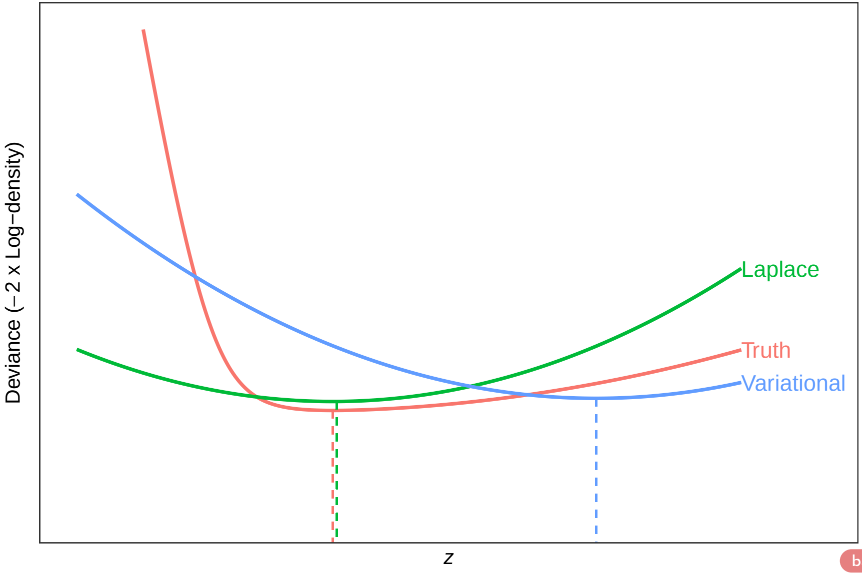
Comparison of approximations (deviance)



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Variational solutions to Gaussian mixture model

Variational M-step

$$\tilde{q}(\mathbf{z}) = \prod_{i=1}^{n} \prod_{k=1}^{K} r_{ik}^{z_{ik}}, \qquad r_{ik} = \rho_{ik} \Big/ \sum_{k=1}^{K} \rho_{ik}$$

$$\log \rho_{ik} = \mathrm{E}[\log \pi_k] + \frac{1}{2} \mathrm{E}\left[\log |\boldsymbol{\Psi}_k| \right] - \frac{d}{2} \log 2\pi$$
$$- \frac{1}{2} \mathrm{E}\left[(\mathbf{x}_i - \boldsymbol{\mu}_k)^\top \boldsymbol{\Psi}_k (\mathbf{x}_i - \boldsymbol{\mu}_k) \right]$$

Variational E-step

$$\tilde{q}(\pi_1, \ldots, \pi_K) = \mathrm{Dir}_K(\boldsymbol{\pi}|\tilde{\boldsymbol{\alpha}}), \qquad \tilde{\alpha}_k = \alpha_{0k} + \textstyle\sum_{i=1}^{n} r_{ik}$$

$$\tilde{q}(\boldsymbol{\mu}, \boldsymbol{\Psi}) = \prod_{k=1}^{K} \mathrm{N}_d \left(\boldsymbol{\mu}_k | \tilde{\mathbf{m}}_k, (\tilde{\kappa}_k \boldsymbol{\Psi}_k)^{-1} \right) \mathrm{Wis}_d(\boldsymbol{\Psi}_k | \tilde{\mathbf{W}}_k, \tilde{\nu}_k)$$

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Variational solutions to Gaussian mixture model (cont.)

$$\tilde{\kappa}_k = \kappa_0 + \textstyle\sum_{i=1}^n r_{ik}$$

$$\tilde{\mathbf{m}}_k = (\kappa_0 \mathbf{m}_0 + \textstyle\sum_{i=1}^n r_{ik}\mathbf{x}_i)/\tilde{\kappa}_k$$

$$\mathbf{W}_k^{-1} = \mathbf{W}_0^{-1} + \sum_{i=1}^n r_{ik}(\mathbf{x}_i - \bar{\mathbf{x}}_k)(\mathbf{x}_i - \bar{\mathbf{x}}_k)^\top$$

$$\bar{\mathbf{x}}_k = \sum_{i=1}^n r_{ik}\mathbf{x}_i \Big/ \sum_{i=1}^n r_{ik}$$

$$\nu_k = \nu_0 + \textstyle\sum_{i=1}^n r_{ik}$$

Also useful

$$\mathrm{E}\left[(\mathbf{x}_i - \boldsymbol{\mu}_k)^\top \boldsymbol{\Psi}_k (\mathbf{x}_i - \boldsymbol{\mu}_k)\right] = d/\tilde{\kappa}_k + \nu_k(\mathbf{x}_i - \tilde{\mathbf{m}}_k)^\top \tilde{\mathbf{W}}_k (\mathbf{x}_i - \tilde{\mathbf{m}}_k)$$

$$\mathrm{E}[\log \pi_k] = \textstyle\sum_{i=1}^d \psi\left(\frac{\nu_k + 1 - i}{2}\right) + d\log 2 + \log|\tilde{\mathbf{W}}_k|$$

$$\mathrm{E}\left[\log|\boldsymbol{\Psi}_k|\right] = \psi(\tilde{\alpha}_k) - \psi\left(\textstyle\sum_{k=1}^K \tilde{\alpha}_k\right), \qquad \psi(\cdot) \text{ is the digamma function}$$

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