A Beginner's Guide to Variational Inference

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Outline

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Idea

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Mean-field distributions

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2 Examples

Univariate Gaussian Gaussian mixtures

Discussion

Exponential families
Zero-forcing vs Zero-avoiding
Quality of approximation
Advanced topics

Introduction

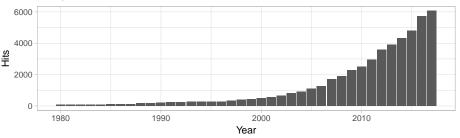
- Consider a statistical model where we have observations $\mathbf{y} = (y_1, \dots, y_n)$ and also some latent variables $\mathbf{z} = (z_1, \dots, z_m)$.
- Want to evaluate the intractable integral

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

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

In the literature

Google Scholar results for 'variational inference'

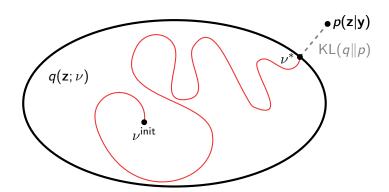


- Well known in the machine learning community.
- In social statistics:
 - E. A. Erosheva et al. (2007). "Describing disability through individual-level mixture models for multivariate binary data". Ann. Appl. Stat, 1.2, p. 346
 - ▶ J. Grimmer (2010). "An introduction to Bayesian inference via variational 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)

$$\mathsf{KL}(q\|p) = -\int \log rac{p(\mathsf{z}|\mathsf{y})}{q(\mathsf{z})} q(\mathsf{z}) \, \mathsf{dz}.$$

• **ISSUE**: 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(z) be some density function to approximate p(z|y). Then the log-marginal density can be decomposed as follows:

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

- \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 $\mathsf{KL}(q||p)$.
- ISSUE: 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,

$$\log p(\mathbf{y}|\theta) = \int \left\{ \log \frac{p(\mathbf{y}, \mathbf{z}|\theta)}{p(\mathbf{z}|\mathbf{y}, \theta)} - \log \frac{p(\mathbf{z}|\mathbf{y}, \theta)}{p(\mathbf{z}|\mathbf{y}, \theta)} \right\} p(\mathbf{z}|\mathbf{y}, \theta^{(t)}) d\mathbf{z}$$

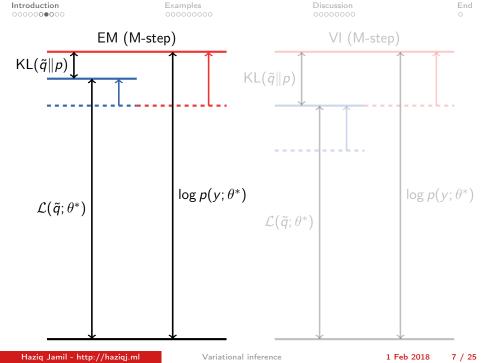
$$= \mathsf{E}_{\theta^{(t)}}[\log p(\mathbf{y}, \mathbf{z}|\theta)] - \mathsf{E}_{\theta^{(t)}}[\log p(\mathbf{z}|\mathbf{y}, \theta)]$$

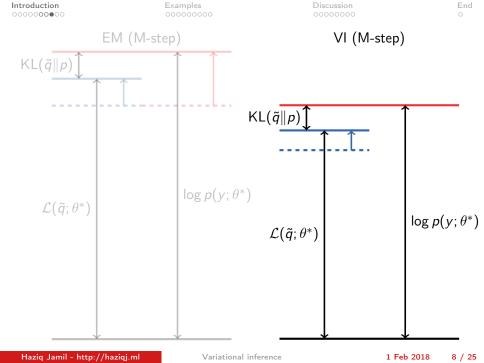
$$= Q(\theta|\theta^{(t)}) + \text{entropy}.$$

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

$$\log p(\mathbf{y}|\theta) - \log p(\mathbf{y}|\theta^{(t)}) = Q(\theta|\theta^{(t)}) - Q(\theta^{(t)}|\theta^{(t)}) + \Delta \text{entropy}$$

$$\geq Q(\theta|\theta^{(t)}) - Q(\theta^{(t)}|\theta^{(t)}).$$





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 z into M disjoint groups $z = (z^{(1)}, \dots, z^{(M)})$, and assume

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

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

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

for $i \in \{1, ..., m\}$.

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

Introduction

Coordinate ascent mean-field variational inference (CAVI)

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

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

Algorithm 1 CAVI

- 1: **initialise** Variational factors $q_i(\mathbf{z}^{(j)})$
- 2: while $\mathcal{L}(q)$ not converged do
- for $j = 1, \ldots, M$ do 3:
- $\log q_i(\mathbf{z}^{(j)}) \leftarrow \mathsf{E}_{-i}[\log p(\mathbf{y}, \mathbf{z})] + \mathsf{const.}$ ⊳ from (1) 4.
- end for 5:
- $\mathcal{L}(q) \leftarrow \mathsf{E}_q[\log p(\mathsf{y},\mathsf{z})] \mathsf{E}_q[\log q(\mathsf{z})]$
- 7. end while
- 8: return $\tilde{q}(z) = \prod_{i=1}^{M} \tilde{q}_i(z^{(j)})$

- Introduction
- 2 Examples
- 3 Discussion

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

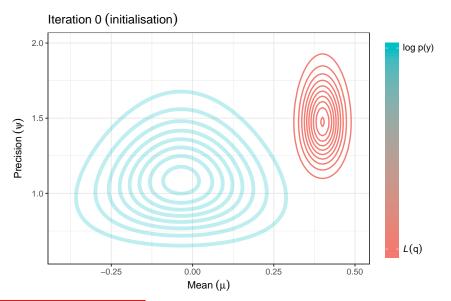
$$y_i \stackrel{\mathsf{iid}}{\sim} \mathsf{N}(\mu, \psi^{-1})$$
 Data $\mu | \psi \sim \mathsf{N} \left(\mu_0, (\kappa_0 \psi)^{-1} \right)$ $\psi \sim \mathsf{\Gamma}(a_0, b_0)$ Priors $i = 1, \dots, n$

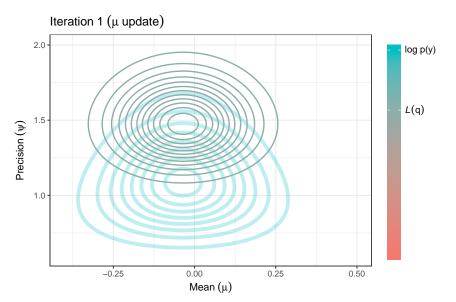
• Substitute $p(\mu, \psi|\mathbf{y})$ with the mean-field approximation

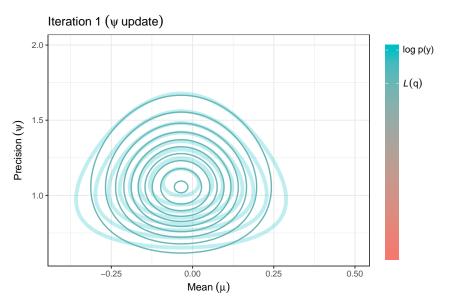
$$q(\mu,\psi)=q_{\mu}(\mu)q_{\psi}(\psi).$$

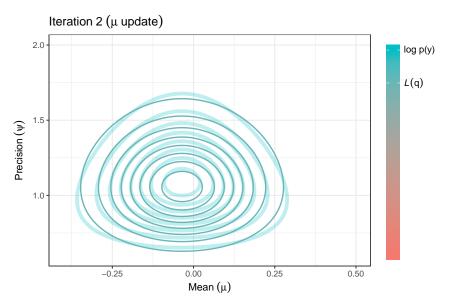
• From (1), we can work out the solutions

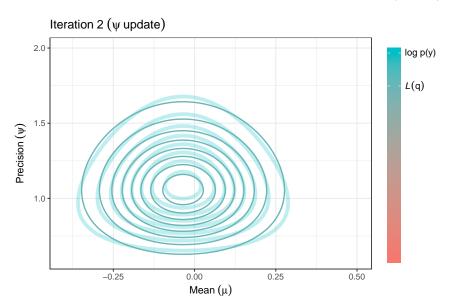
$$ilde{q}_{\mu}(\mu) \equiv \mathsf{N}\left(rac{\kappa_0\mu_0 + nar{y}}{\kappa_0 + n}, rac{1}{(\kappa_0 + n)\,\mathsf{E}_q[\psi]}
ight) \quad \mathsf{and} \quad ilde{q}_{\psi}(\psi) \equiv \Gamma(ilde{a}, ilde{b})$$
 $ilde{a} = a_0 + rac{n}{2} \qquad \qquad ilde{b} = b_0 + rac{1}{2}\,\mathsf{E}_q\left[\sum_{i=1}^n (y_i - \mu)^2 + \kappa_0(\mu - \mu_0)^2\right]$











Comparison of solutions

Variational posterior

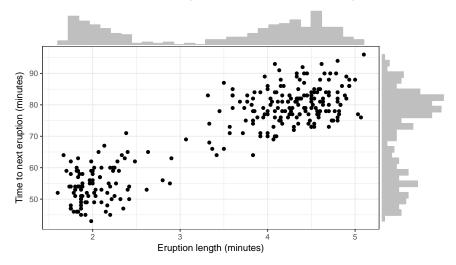
$$\mu \sim N\left(\frac{\kappa_0\mu_0 + n\bar{y}}{\kappa_0 + n}, \frac{1}{(\kappa_0 + n)E[\psi]}\right)$$
 $\psi \sim \Gamma\left(a_0 + \frac{n}{2}, b_0 + \frac{1}{2}c\right)$
 $c = E\left[\sum_{i=1}^n (y_i - \mu)^2 + \kappa_0(\mu - \mu_0)^2\right]$

True posterior

$$\begin{split} \mu|\psi &\sim \mathsf{N}\left(\frac{\kappa_0\mu_0 + n\bar{y}}{\kappa_0 + n}, \frac{1}{(\kappa_0 + n)\psi}\right)\\ \psi &\sim \Gamma\left(a_0 + \frac{n}{2}, b_0 + \frac{1}{2}c'\right)\\ c' &= \sum_{n=0}^{n} (y_i - \bar{y})^2 + \frac{\kappa_0}{\kappa_0 + n}(\bar{y} - \mu_0)^2 \end{split}$$

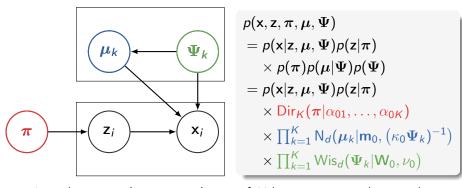
- $Cov(\mu, \psi) = 0$ by design in VI solutions.
- For this simple example, it is possible to decouple and solve explicitly.
- VI solutions leads to unbiased MLE if $\kappa_0 = \mu_0 = a_0 = b_0 = 0$.

Gaussian mixture model (Old Faithful data set)



• Let $x_i \in \mathbb{R}^d$ and assume $x_i \stackrel{\mathsf{iid}}{\sim} \sum_{k=1}^K \pi_k \, \mathsf{N}_d(\boldsymbol{\mu}_k, \boldsymbol{\Psi}_k^{-1})$ 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 $z = \{z_1, \dots, z_n\}$ are observed along with $x = \{x_1, \dots, x_n\}$,

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

Variational inference for GMM

Assume the mean-field posterior density

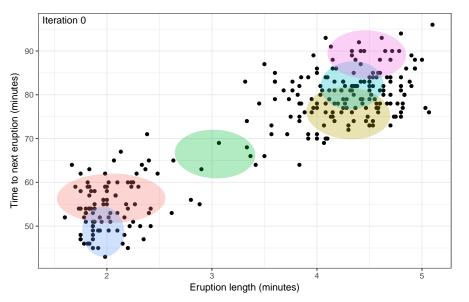
$$egin{aligned} q(\mathsf{z},\pi,\mu,\Psi) &= q(\mathsf{z})q(\pi,\mu,\Psi) \ &= q(\mathsf{z})q(\pi)q(\mu|\Psi)q(\Psi). \end{aligned}$$

Algorithm 2 CAVI for GMM

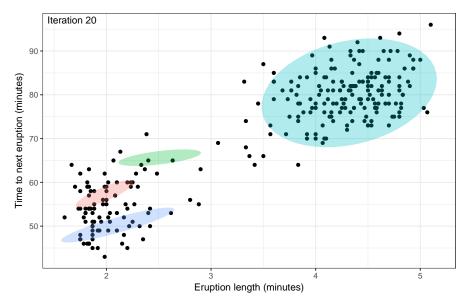
details

- 1: initialise Variational factors q(z), $q(\pi)$ and $q(\mu, \Psi)$
- 2: while $\mathcal{L}(q)$ not converged do
- 3: $q(z_{ik}) \leftarrow \text{Bern}(\cdot)$
- 4: $q(\pi) \leftarrow \mathsf{Dir}_{\mathcal{K}}(\cdot)$
- 5: $q(\mu|\Psi) \leftarrow \mathsf{N}_d(\cdot,\cdot)$
- 6: $q(\Psi) \leftarrow \mathsf{Wis}_d(\cdot, \cdot)$
- 7: $\mathcal{L}(q) \leftarrow \mathsf{E}_q[\log p(\mathsf{x},\mathsf{z},\pi,\mu,\Psi)] \mathsf{E}_q[\log q(\mathsf{z},\pi,\mu,\Psi)]$
- 8: end while
- 9: return $ilde{q}(\mathsf{z},\pi,\mu,\Psi) = ilde{q}(\mathsf{z}) ilde{q}(\pi) ilde{q}(\mu|\Psi) ilde{q}(\Psi)$

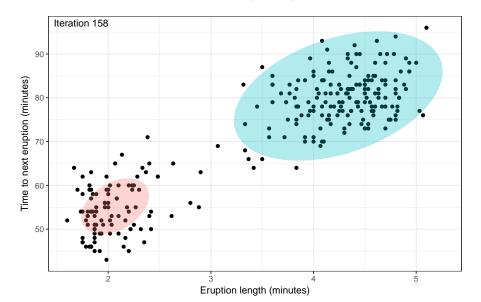
Variational inference for GMM (cont.)



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.

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Exponential families

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

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

• Then, from (1),

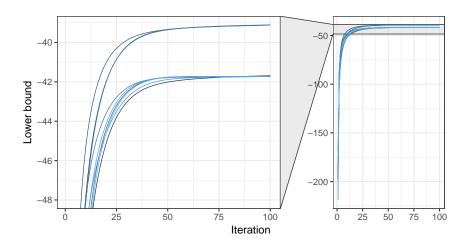
$$\begin{split} \tilde{q}_{j}(\mathbf{z}^{(j)}) &\propto \exp\left(\mathsf{E}_{-j}[\log p(\mathbf{z}^{(j)}|\mathbf{z}_{-j},\mathbf{y})]\right) \\ &= \exp\left(\log h(\mathbf{z}^{(j)}) + \mathsf{E}[\eta_{j}(\mathbf{z}_{-j},\mathbf{y})] \cdot \mathbf{z}^{(j)} - \mathsf{E}[A(\eta_{j})]\right) \\ &\propto h(\mathbf{z}^{(j)}) \exp\left(\mathsf{E}[\eta_{j}(\mathbf{z}_{-j},\mathbf{y})] \cdot \mathbf{z}^{(j)}\right) \end{split}$$

is also in the same exponential family.

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

Discussion

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:

$$\mathsf{KL}(q\|p) = \int \log rac{q(\mathsf{z})}{p(\mathsf{z}|\mathsf{y})} q(\mathsf{z}) \, \mathsf{dz}$$

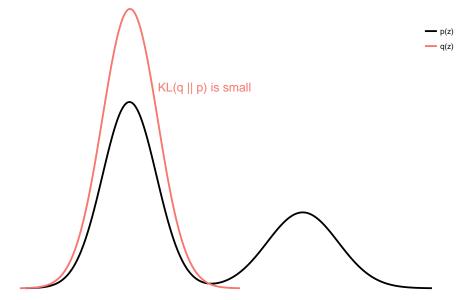
- KL(q||p) is large when $p(\mathbf{z}|\mathbf{y})$ is close to zero, unless $q(\mathbf{z})$ is also close to zero (*zero-forcing*).
- ISSUE: What about other measures of closeness? For instance,

$$\mathsf{KL}(p\|q) = \int \log rac{p(\mathsf{z}|\mathsf{y})}{q(\mathsf{z}|\mathsf{y})} p(\mathsf{z}|\mathsf{y}) \, \mathsf{dz}.$$

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

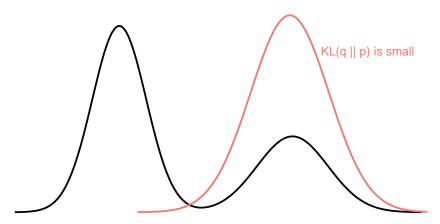
End

Zero-forcing vs Zero-avoiding (cont.)



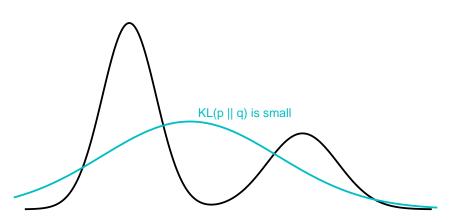
Zero-forcing vs Zero-avoiding (cont.)



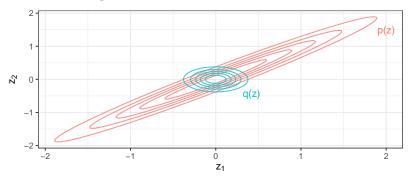


Zero-forcing vs Zero-avoiding (cont.)

— p(z) — q(z)



Distortion of higher order moments



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

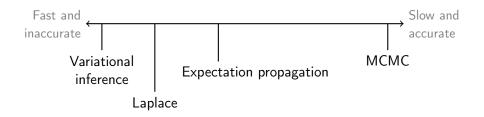
$$ilde{q}(z_1) = \mathsf{N}(z_1|\mu_1, \Psi_{11}^{-1}) \ \ \mathsf{and} \ \ ilde{q}(z_2) = \mathsf{N}(z_2|\mu_2, \Psi_{22}^{-1})$$

and by definition, $Cov(z_1, z_2) = 0$ 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:

$$\mathcal{I} = \int \exp i t(x^{\top} \beta) p(\beta) d\beta \ge \int f(x^{\top} \beta, \xi) p(\beta) d\beta.$$

- Stochastic variational inference
 - 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!

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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References II

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References III

- Wang, Y. S., R. Matsueda, and E. A. Erosheva (2017). "A variational EM method for mixed membership models with multivariate rank data: An analysis of public policy preferences". arXiv: 1512.08731.
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4 Additional material

The variational principle Laplace's method Solutions to Gaussian mixture

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

$$\underset{\theta}{\operatorname{arg\,max}} p(\theta) =: \hat{\theta}$$

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

Using variational calculus, we can solve

$$\operatorname{arg\,max}_{p} \mathcal{H}(p) =: \tilde{p}$$

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

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 ${\bf A}=-{\sf D}^2 Q({\bf f})$ being the negative Hessian of Q evaluated at $\tilde{{\bf f}}$.

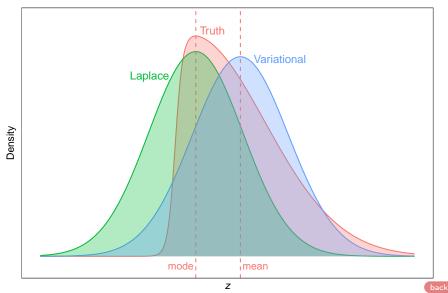
• The posterior $p(\mathbf{f}|\mathbf{y})$ is approximated by $N(\tilde{\mathbf{f}}, \mathbf{A}^{-1})$, and the marginal by

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

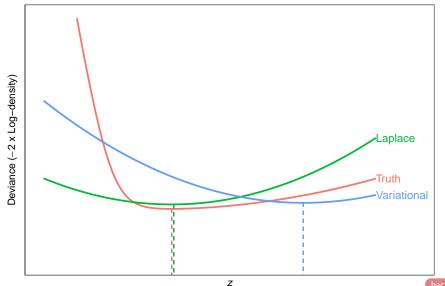
• Won't scale with large *n*; difficult to find modes in high dimensions.

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

Comparison of approximations (density)



Comparison of approximations (deviance)



Variational solutions to Gaussian mixture model

Variational M-step

$$\begin{split} \tilde{q}(\mathbf{z}) &= \prod_{i=1}^n \prod_{k=1}^K r_{ik}^{z_{ik}}, \quad r_{ik} = \rho_{ik} / \sum_{k=1}^K \rho_{ik} \\ \log \rho_{ik} &= \mathsf{E}[\log \pi_k] + \frac{1}{2} \, \mathsf{E}\left[\log |\Psi_k|\right] - \frac{d}{2} \log 2\pi \\ &- \frac{1}{2} \, \mathsf{E}\left[(\mathbf{x}_i - \boldsymbol{\mu}_k)^\top \Psi_k (\mathbf{x}_i - \boldsymbol{\mu}_k)\right] \end{split}$$

Variational E-step

$$ilde{q}(\pi_1, \dots, \pi_K) = \operatorname{Dir}_K(\boldsymbol{\pi}|\tilde{\boldsymbol{lpha}}), \quad ilde{lpha}_k = lpha_{0k} + \sum_{i=1}^n r_{ik}$$

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

Variational solutions to Gaussian mixture model (cont.)

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

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

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

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

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

Also useful

$$\begin{aligned} \mathsf{E}\left[(\mathsf{x}_i - \boldsymbol{\mu}_k)^\top \boldsymbol{\Psi}_k (\mathsf{x}_i - \boldsymbol{\mu}_k)\right] &= d/\tilde{\kappa}_k + \nu_k (\mathsf{x}_i - \tilde{\mathsf{m}}_k)^\top \tilde{\mathsf{W}}_k (\mathsf{x}_i - \tilde{\mathsf{m}}_k) \\ \mathsf{E}[\log \pi_k] &= \sum_{i=1}^d \psi\left(\frac{\nu_k + 1 - i}{2}\right) + d\log 2 + \log |\tilde{\mathsf{W}}_k| \\ \mathsf{E}\left[\log |\boldsymbol{\Psi}_k|\right] &= \psi(\tilde{\alpha}_k) - \psi\left(\sum_{k=1}^K \tilde{\alpha}_k\right) \end{aligned}$$