Variational Bayes and beyond: Bayesian inference for big data

Tamara Broderick
ITT Career Development Assistant Professor, MIT

http://www.tamarabroderick.com/tutorials.html
Bayesian inference
Bayesian inference

[Gillon et al 2017]

[Grimm et al 2018]
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[Grimm et al 2018]

[ESO/ L. Calçada M. Kornmesser 2017] [Abbott et al 2016a,b]
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[Gillon et al 2017]

[ESO/ L. Calçada, M. Kornmesser 2017]  [Abbott et al 2016a,b]

[Woodard et al 2017]
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- Analysis goals: Point estimates, coherent uncertainties
- Interpretable, complex, modular; expert information
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- Challenge: fast (compute, user), reliable inference
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- Analysis goals: Point estimates, coherent uncertainties
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- Challenge: fast (compute, user), reliable inference
- Uncertainty doesn’t have to disappear in large data sets
Variational Bayes
Variational Bayes

- Modern problems: often large data, large dimensions
Variational Bayes

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- Variational Bayes can be very fast
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[Blei et al 2003]

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[Blei et al 2003]

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[Airoldi et al 2008]
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[Variational Bayes](Blei et al 2003)
[Airoldi et al 2008]
[Gershman et al 2014]
[Blei et al 2018]
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[Blei et al 2003]

[Stegle et al 2010]

[2018]

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**Variational Bayes**

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Roadmap

• Bayes & Approximate Bayes review
• What is:
  • Variational Bayes (VB)
  • Mean-field variational Bayes (MFVB)
• Why use MFVB?
• When can we trust MFVB?
• Where do we go from here?
Roadmap

- Bayes & Approximate Bayes review
- What is:
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Bayesian inference
Bayesian inference

\[ \theta \]

parameters
Bayesian inference

$p(\theta)$

prior

parameters
Bayesian inference

\[ p(\theta) \]

prior

parameters
Bayesian inference

\[ p(y_{1:N} | \theta)p(\theta) \]

parameters

likelihood prior
Bayesian inference

\[ p(y_{1:N} | \theta) p(\theta) \]

data \quad \text{parameters}

likelihood \quad \text{prior}
Bayesian inference

\[ p(\theta|y_1:N) \propto \theta \cdot p(y_1:N|\theta)p(\theta) \]

posterior likelihood prior

\(\theta\)
Bayesian inference

\[ p(\theta | y_{1:N}) \propto p(y_{1:N} | \theta) p(\theta) \]

posterior likelihood prior

Bayes Theorem
Bayesian inference

\[ p(\theta|y_{1:N}) \propto p(y_{1:N}|\theta)p(\theta) \]

posterior, likelihood, prior
Bayesian inference

\[ p(\theta | y_{1:N}) \propto p(y_{1:N} | \theta) p(\theta) \]

posterior  likelihood  prior

1. Build a model: choose prior & choose likelihood
Bayesian inference

\[ p(\theta|y_{1:N}) \propto p(y_{1:N}|\theta)p(\theta) \]

posterior \quad likelihood \quad prior

1. Build a model: choose prior & choose likelihood
2. Compute the posterior
Bayesian inference

\[ p(\theta|y_{1:N}) \propto p(y_{1:N}|\theta)p(\theta) \]

posterior \hspace{1cm} likelihood \hspace{1cm} prior

1. Build a model: choose prior & choose likelihood
2. Compute the posterior
3. Report a summary, e.g. posterior means and (co)variances
Bayesian inference

\[ p(\theta \mid y_{1:N}) \propto p(y_{1:N} \mid \theta) p(\theta) \]

posterior \quad likelihood \quad prior

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   • Why are steps 2 and 3 hard?
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posterior likelihood prior evidence

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3. Report a summary, e.g. posterior means and (co)variances
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Bayesian inference

\[ p(\theta | y_{1:N}) = \frac{p(y_{1:N} | \theta)p(\theta)}{\int p(y_{1:N}, \theta) d\theta} \]

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Approximate Bayesian Inference
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- Gold standard: Markov Chain Monte Carlo (MCMC) [Bardenet, Doucet, Holmes 2017]
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  - Eventually accurate but can be slow

[Bardenet, Doucet, Holmes 2017]
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Instead: an optimization approach

- Approximate posterior with $q^*$

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  \[ q^* = \arg\min_{q \in Q} f(q(\cdot), p(\cdot|y)) \]
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$$q^* = \arg\min_{q \in Q} \mathbb{E}_{q(\cdot)} f(q(\cdot), p(\cdot | y))$$

[Bardenet, Doucet, Holmes 2017]
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  \[ q^* = \arg\min_{q \in Q} f(q(\cdot), p(\cdot|y)) \]

• Variational Bayes (VB): $f$ is Kullback-Leibler divergence
  \[ KL(q(\cdot)||p(\cdot|y)) \]
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- Variational Bayes (VB): \( f \) is Kullback-Leibler divergence
  
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  KL(q(\cdot) || p(\cdot|y))
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- VB practical success
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Variational Bayes (VB): \( f \) is Kullback-Leibler divergence

\[
KL(q(\cdot)||p(\cdot|y))
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VB practical success: point estimates and prediction

\[\text{[Bardenet, Doucet, Holmes 2017]}\]
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- VB practical success: point estimates and prediction, fast
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  \[ q^* = \arg\min_{q \in Q} f(q(\cdot), p(\cdot|y)) \]

- Variational Bayes (VB): $f$ is Kullback-Leibler divergence
  \[ KL(q(\cdot)||p(\cdot|y)) \]

- VB practical success: point estimates and prediction, fast, streaming, distributed (3.6M Wikipedia, 350K Nature)

[Broderick, Boyd, Wibisono, Wilson, Jordan 2013]

[Bardeanet, Doucet, Holmes 2017]
Why KL?

- Variational Bayes

\[ q^* = \arg\min_{q \in Q} \text{KL} (q(\cdot) || p(\cdot | y)) \]
Why KL?

- Variational Bayes

\[ q^* = \arg\min_{q \in Q} KL \left( q(\cdot) \middle|\middle| p(\cdot | y) \right) \]

\[ KL \left( q(\cdot) \middle|\middle| p(\cdot | y) \right) := \int q(\theta) \log \frac{q(\theta)}{p(\theta | y)} d\theta \]
Why KL?

- Variational Bayes

\[ q^* = \text{argmin}_{q \in Q} \text{KL} (q(\cdot) \| p(\cdot | y)) \]

\[
\text{KL} (q(\cdot) \| p(\cdot | y)) := \int q(\theta) \log \frac{q(\theta)}{p(\theta | y)} d\theta
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\[
= \int q(\theta) \log \frac{q(\theta)p(y)}{p(\theta, y)} d\theta
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Why KL?

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\text{KL} (q(\cdot) || p(\cdot | y)) := \int q(\theta) \log \frac{q(\theta)}{p(\theta | y)} d\theta
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= \int q(\theta) \log \frac{q(\theta)p(y)}{p(\theta, y)} d\theta = \log p(y) - \int q(\theta) \log \frac{p(\theta, y)}{q(\theta)} d\theta
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“Evidence lower bound” (ELBO)
Why KL?

- Variational Bayes

\[ q^* = \text{argmin}_{q \in Q} \text{KL} (q(\cdot) \| p(\cdot | y)) \]

\[
\text{KL} (q(\cdot) \| p(\cdot | y)) \\
:= \int q(\theta) \log \frac{q(\theta)}{p(\theta | y)} d\theta \\
= \int q(\theta) \log \frac{q(\theta)p(y)}{p(\theta, y)} d\theta = \log p(y) - \int q(\theta) \log \frac{p(\theta, y)}{q(\theta)} d\theta
\]

"Evidence lower bound" (ELBO)
Why KL?

- Variational Bayes

\[ q^* = \arg\min_{q \in Q} \text{KL} (q(\cdot) \parallel p(\cdot | y)) \]

\[
\text{KL} (q(\cdot) \parallel p(\cdot | y)) := \int q(\theta) \log \frac{q(\theta)}{p(\theta | y)} \, d\theta
\]

\[
= \int q(\theta) \log \frac{q(\theta)p(y)}{p(\theta, y)} \, d\theta = \log p(y) - \int q(\theta) \log \frac{p(\theta, y)}{q(\theta)} \, d\theta
\]

- \( q^* = \arg\max_{q \in Q} \text{ELBO}(q) \)
Why KL?

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- \( q^* = \text{argmax}_{q \in Q} \text{ELBO}(q) \)

- KL is positive definite  
  [Exercise; cf. Bishop 2006, Sec 1.6.1]

"Evidence lower bound" (ELBO)
Why KL?

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• \( q^* = \text{argmax}_{q \in Q} \text{ELBO}(q) \)

• KL is positive definite \[ \text{Exercise; cf. Bishop 2006, Sec 1.6.1} \]

• KL \( \geq 0 \ \Rightarrow \ \log p(y) \geq \text{ELBO} \)
Why KL?

- Variational Bayes
  
  \[ q^* = \arg\min_{q \in Q} KL (q(\cdot) \| p(\cdot|y)) \]

  \[
  KL (q(\cdot) \| p(\cdot|y))
  := \int q(\theta) \log \frac{q(\theta)}{p(\theta|y)} d\theta
  \]

  \[
  = \int q(\theta) \log \frac{q(\theta)p(y)}{p(\theta, y)} d\theta = \log p(y) - \int q(\theta) \log \frac{p(\theta, y)}{q(\theta)} d\theta
  \]

- \( q^* = \arg\max_{q \in Q} \text{ELBO}(q) \)

- KL is positive definite  [Exercise; cf. Bishop 2006, Sec 1.6.1]

- \( KL \geq 0 \Rightarrow \log p(y) \geq \text{ELBO} \)

- Why KL?
Why KL?

- Variational Bayes
  \[ q^* = \text{argmin}_{q \in Q} \text{KL} (q(\cdot) \| p(\cdot | y)) \]

\[
\text{KL} (q(\cdot) \| p(\cdot | y))
\]

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- \[ q^* = \text{argmax}_{q \in Q} \text{ELBO}(q) \]

- KL is positive definite \[ \text{Exercise; cf. Bishop 2006, Sec 1.6.1} \]

- KL \[ \geq 0 \Rightarrow \log p(y) \geq \text{ELBO} \]

- Why KL (in this direction)?
Variational Bayes

$q^* = \arg\min_{q \in Q} KL \left( q(\cdot) \| p(\cdot | y) \right)$
Variational Bayes

\[ q^* = \arg\min_{q \in Q} KL (q(\cdot)||p(\cdot|y)) \]

Choose “NICE” distributions
Variational Bayes

\[ q^* = \arg\min_{q \in \mathcal{Q}} \text{KL} (q(\cdot) || p(\cdot | y)) \]

Choose “NICE” distributions

\[ p(\theta | y) \]

CLOSE

\[ q^*(\theta) \]

NICE
Variational Bayes

\[ q^* = \arg\min_{q \in Q} KL(q(\cdot) \| p(\cdot | y)) \]

Choose “NICE” distributions
Variational Bayes

\[ q^* = \arg\min_{q \in Q} KL (q(\cdot) \| p(\cdot | y)) \]

Choose “NICE” distributions

- Mean-field variational Bayes (MFVB)

\[ Q_{MFVB} := \left\{ q : q(\theta) = \prod_{j=1}^{J} q_j(\theta_j) \right\} \]
Variational Bayes

$$q^* = \arg\min_{q \in Q} KL (q(\cdot) \| p(\cdot|y))$$

Choose “NICE” distributions

- Mean-field variational Bayes (MFVB)

$$Q_{MFVB} := \left\{ q : q(\theta) = \prod_{j=1}^{J} q_j(\theta_j) \right\}$$

- Often also exponential family
Variational Bayes

\[ q^* = \arg\min_{q \in Q} \text{KL} (q(\cdot) || p(\cdot | y)) \]

Choose “NICE” distributions

- Mean-field variational Bayes (MFVB)

\[ Q_{MFVB} := \left\{ q : q(\theta) = \prod_{j=1}^{J} q_j(\theta_j) \right\} \]

- Often also exponential family
- Not a modeling assumption
Variational Bayes

\[ q^* = \arg\min_{q \in Q} KL (q(\cdot) \| p(\cdot | y)) \]

Choose “NICE” distributions

- Mean-field variational Bayes (MFVB)

\[
Q_{\text{MFVB}} := \left\{ q : q(\theta) = \prod_{j=1}^{J} q_j(\theta_j) \right\}
\]

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- Not a modeling assumption

[Bishop 2006]
Variational Bayes

\[ q^* = \arg\min_{q \in Q} KL(q(\cdot) \| p(\cdot | y)) \]

Choose “NICE” distributions

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Now we have an optimization problem; how to solve it?
Variational Bayes

\[ q^* = \arg\min_{q \in Q} \text{KL} (q(\cdot) || p(\cdot|y)) \]

Choose “NICE” distributions

- Mean-field variational Bayes (MFVB)

\[ Q_{MFVB} := \left\{ q : q(\theta) = \prod_{j=1}^{J} q_j(\theta_j) \right\} \]

- Often also exponential family
- \textit{Not} a modeling assumption

Now we have an optimization problem; how to solve it?

- One option: Coordinate descent in \( q_1, \ldots, q_J \)
Approximate Bayesian inference
Approximate Bayesian inference

Use $q^*$ to approximate $p(\cdot | y)$
Approximate Bayesian inference

Use $q^*$ to approximate $p(\cdot | y)$

Optimization

$q^* = \arg\min_{q \in Q} f(q(\cdot), p(\cdot | y))$
Approximate Bayesian inference

Use $q^*$ to approximate $p(\cdot | y)$

Optimization

$$q^* = \arg\min_{q \in Q} f(q(\cdot), p(\cdot | y))$$

Variational Bayes

$$q^* = \arg\min_{q \in Q} KL(q(\cdot) || p(\cdot | y))$$
Approximate Bayesian inference

Use $q^*$ to approximate $p(\cdot | y)$

Optimization
$q^* = \arg\min_{q \in \mathcal{Q}} f(q(\cdot), p(\cdot | y))$

Variational Bayes
$q^* = \arg\min_{q \in \mathcal{Q}} KL(q(\cdot) || p(\cdot | y))$

Mean-field variational Bayes
$q^* = \arg\min_{q \in \mathcal{Q}_{MFVB}} KL(q(\cdot) || p(\cdot | y))$
Approximate Bayesian inference

Use $q^*$ to approximate $p(\cdot|y)$

Optimization

$q^* = \arg\min_{q \in Q} f(q(\cdot), p(\cdot|y))$

Variational Bayes

$q^* = \arg\min_{q \in Q} KL(q(\cdot)||p(\cdot|y))$

Mean-field variational Bayes

$q^* = \arg\min_{q \in Q_{MFVB}} KL(q(\cdot)||p(\cdot|y))$
Approximate Bayesian inference

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$q^* = \arg\min_{q \in Q} f(q(\cdot), p(\cdot|y))$

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- Coordinate descent
Approximate Bayesian inference

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Optimization

$q^* = \arg\min_{q \in Q} f(q(\cdot), p(\cdot|y))$

Variational Bayes

$q^* = \arg\min_{q \in Q} KL(q(\cdot) || p(\cdot|y))$

Mean-field variational Bayes

$q^* = \arg\min_{q \in Q_\text{MFVB}} KL(q(\cdot) || p(\cdot|y))$

- Coordinate descent
- Stochastic variational inference (SVI) [Hoffman et al 2013]
Approximate Bayesian inference

Use $q^*$ to approximate $p(\cdot|y)$

Optimization

$$q^* = \text{argmin}_{q \in Q} f(q(\cdot), p(\cdot|y))$$

Variational Bayes

$$q^* = \text{argmin}_{q \in Q} KL(q(\cdot)||p(\cdot|y))$$

Mean-field variational Bayes

$$q^* = \text{argmin}_{q \in Q_{MFVB}} KL(q(\cdot)||p(\cdot|y))$$

- Coordinate descent
- Stochastic variational inference (SVI) [Hoffman et al 2013]
- Automatic differentiation variational inference (ADVI) [Kucukelbir et al 2015, 2017]
Roadmap

• Bayes & Approximate Bayes review
• What is:
  • Variational Bayes (VB)
  • Mean-field variational Bayes (MFVB)
• Why use MFVB?
• When can we trust MFVB?
• Where do we go from here?
Roadmap

• Bayes & Approximate Bayes review
• What is:
  • Variational Bayes (VB)
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• Why use MFVB?
• When can we trust MFVB?
• Where do we go from here?
Midge wing length

• Catalogued midge wing lengths (mm) \( y = (y_1, \ldots, y_N) \)
Midge wing length

- Catalogued midge wing lengths (mm) \( y = (y_1, \ldots, y_N) \)

- Model:
  \[
p(y|\theta) : \quad y_n \overset{iid}{\sim} \mathcal{N}(\mu, \sigma^2), \quad n = 1, \ldots, N
  \]
Midge wing length

- Catalogued midge wing lengths (mm) $y = (y_1, \ldots, y_N)$
- Parameters of interest: population mean and variance $\theta = (\mu, \sigma^2)$
- Model:
  
  $p(y|\theta) : \quad y_n \overset{iid}{\sim} \mathcal{N}(\mu, \sigma^2), \quad n = 1, \ldots, N$
Midge wing length

- Catalogued midge wing lengths (mm) \( y = (y_1, \ldots, y_N) \)
- Parameters of interest: population mean and variance
- Model:
  \[ p(y|\theta) : \quad y_n \overset{iid}{\sim} \mathcal{N}(\mu, \sigma^2), \quad n = 1, \ldots, N \]
  \[ p(\theta) : \quad (\sigma^2)^{-1} \sim \text{Gamma}(a_0, b_0) \]
  \[ \mu|\sigma^2 \sim \mathcal{N}(\mu_0, \lambda_0\sigma^2) \]
Midge wing length

- Catalogued midge wing lengths (mm) \( y = (y_1, \ldots, y_N) \)
- Parameters of interest: population mean and variance
- Model:
  \[
  p(y|\theta) : \quad y_n \overset{iid}{\sim} N(\mu, \sigma^2), \quad n = 1, \ldots, N
  
  p(\theta) : \quad (\sigma^2)^{-1} \sim \text{Gamma}(a_0, b_0)
  
  \mu|\sigma^2 \sim N(\mu_0, \lambda_0\sigma^2)
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Midge wing length

- Catalogued midge wing lengths (mm) \( y = (y_1, \ldots, y_N) \)
- Parameters of interest: population mean and precision \( \theta = (\mu, \tau) \)
- Model:
  \[
  p(y|\theta): \quad y_n \overset{iid}{\sim} \mathcal{N}(\mu, \sigma^2), \quad n = 1, \ldots, N
  \]
  \[
  p(\theta): \quad (\sigma^2)^{-1} \sim \text{Gamma}(a_0, b_0)
  \]
  \[
  \mu | \sigma^2 \sim \mathcal{N}(\mu_0, \lambda_0 \sigma^2)
  \]

[Hoff 2009; Grogan, Wirth 1981; MacKay 2003; Bishop 2006]
Midge wing length

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  \[
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Midge wing length

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- Parameters of interest: population mean and precision
- Model:
  \[
  \begin{align*}
  p(y|\theta) & : y_n \overset{iid}{\sim} \mathcal{N}(\mu, \tau^{-1}), & n = 1, \ldots, N \\
  p(\theta) & : \tau \sim \text{Gamma}(a_0, b_0) \\
  \mu | \tau & \sim \mathcal{N}(\mu_0, (\rho_0 \tau)^{-1})
  \end{align*}
  \]
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• Exercise: check \( p(\mu, \tau|y) \neq f_1(\mu, y)f_2(\tau, y) \)
Midge wing length

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  \mu | \tau \sim \mathcal{N}(\mu_0, (\rho_0 \tau)^{-1})
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  \[
  q^*(\mu, \tau) = q^*_\mu(\mu)q^*_\tau(\tau) = \arg\min_{q \in Q_{MFVB}} KL(q(\cdot)||p(\cdot|y))
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Midge wing length

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  \]
- Coordinate descent (derivation shortly) [Bishop 2006, Sec 10.1.3]
Midge wing length

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- Parameters of interest: population mean and precision \( \theta = (\mu, \tau) \)
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  q^*_\mu(\mu) = \mathcal{N}(\mu|\mu_N, \rho_N^{-1}) \quad q^*_\tau(\tau) = \text{Gamma}(\tau|a_N, b_N)
  \]
Midge wing length

- Catalogued midge wing lengths (mm) \( y = (y_1, \ldots, y_N) \)
- Parameters of interest: population mean and precision \( \theta = (\mu, \tau) \)

Model:

\[
p(y|\theta) : \quad y_n \overset{iid}{\sim} \mathcal{N}(\mu, \tau^{-1}), \quad n = 1, \ldots, N
\]

\[
p(\theta) : \quad \tau \sim \text{Gamma}(a_0, b_0)
\]

\[
\mu|\tau \sim \mathcal{N}(\mu_0, (\rho_0 \tau)^{-1})
\]

Exercise: check \( p(\mu, \tau|y) \neq f_1(\mu, y) f_2(\tau, y) \)

MFVB approximation:

\[
q^*(\mu, \tau) = q^*_\mu(\mu) q^*_\tau(\tau) = \arg\min_{q \in Q_{\text{MFVB}}} KL(q(\cdot)||p(\cdot|y))
\]

Coordinate descent (derivation shortly) \([\text{Bishop 2006, Sec 10.1.3}]\)

\[
q^*_\mu(\mu) = \mathcal{N}(\mu|\mu_N, \rho_N^{-1}) \quad q^*_\tau(\tau) = \text{Gamma}(\tau|a_N, b_N)
\]

"variational parameters"
Midge wing length

- Catalogued midge wing lengths (mm) \( y = (y_1, \ldots, y_N) \)
- Parameters of interest: population mean and precision \( \theta = (\mu, \tau) \)
- Model:
  \[
p(y|\theta) : \quad y_n \sim \mathcal{N}(\mu, \tau^{-1}), \quad n = 1, \ldots, N
  \]
  \[
p(\theta) : \quad \tau \sim \text{Gamma}(a_0, b_0)
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  \]
- Coordinate descent (derivation shortly) \( \text{[Bishop 2006, Sec 10.1.3]} \)
  \[
  q^*_\mu(\mu) = \mathcal{N}(\mu|\mu_N, \rho_N^{-1}) \quad q^*_\tau(\tau) = \text{Gamma}(\tau|a_N, b_N)
  \]
  - Iterate: \( (\mu_N, \rho_N) = f(a_N, b_N) \)
  \[
  (a_N, b_N) = g(\mu_N, \rho_N)
  \]

[Hoff 2009; Grogan, Wirth 1981; MacKay 2003; Bishop 2006]
Midge wing length

- Catalogued midge wing lengths (mm) \( y = (y_1, \ldots, y_N) \)
- Parameters of interest: population mean and precision \( \theta = (\mu, \tau) \)
- Model (conjugate prior): [Exercise: find the posterior]
  \[
p(y|\theta) : \quad y_n \sim \mathcal{N}(\mu, \tau^{-1}), \quad n = 1, \ldots, N
  \]
  \[
p(\theta) : \quad \tau \sim \text{Gamma}(a_0, b_0)
  \]
  \[
  \mu|\tau \sim \mathcal{N}(\mu_0, (\rho_0 \tau)^{-1})
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- Exercise: check \( p(\mu, \tau|y) \neq f_1(\mu, y)f_2(\tau, y) \)
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  q^*_\mu(\mu) = \mathcal{N}(\mu|\mu_N, \rho_N^{-1}) \quad q^*_\tau(\tau) = \text{Gamma}(\tau|a_N, b_N)
  \]
  \[
  \text{Iterate:} \quad (\mu_N, \rho_N) = f(a_N, b_N) \quad (a_N, b_N) = g(\mu_N, \rho_N) \quad \text{“variational parameters”}
  \]

[Hoff 2009; Grogan, Wirth 1981; MacKay 2003; Bishop 2006]
Midge wing length approximation

exact posterior

$\tau$ $\mu$
Midge wing length approximation

exact posterior

Midge wing length approximation

exact posterior

\[ \tau \]

\[ \mu \]
Midge wing length approximation

exact posterior

[Bishop 2006]
Midge wing length

- Catalogued midge wing lengths (mm) \( y = (y_1, \ldots, y_N) \)
- Parameters of interest: population mean and precision \( \theta = (\mu, \tau) \)
- Model:
  \[
p(y|\theta) : \quad y_n \sim i.i.d. \mathcal{N}(\mu, \tau^{-1}), \quad n = 1, \ldots, N
  \]
  \[
p(\theta) : \quad \tau \sim \text{Gamma}(a_0, b_0)
  \]
  \[
  \mu|\tau \sim \mathcal{N}(\mu_0, (\rho_0\tau)^{-1})
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- Exercise: check \( p(\mu, \tau|y) \neq f_1(\mu, y)f_2(\tau, y) \)
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  \[q^*(\mu, \tau) = q^*_\mu(\mu)q^*_\tau(\tau) = \text{argmin}_{q \in Q_{MFVB}} KL(q(\cdot)||p(\cdot|y))\]
- Coordinate descent (derivation shortly) \[\text{[Bishop 2006, Sec 10.1.3]}\]
  \[
  q^*_\mu(\mu) = \mathcal{N}(\mu|\mu_N, \rho_N^{-1}) \quad q^*_\tau(\tau) = \text{Gamma}(\tau|a_N, b_N)
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- Iterate:
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  (\mu_N, \rho_N) = f(a_N, b_N)
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  \]
  \[\text{“variational parameters”}\]
Midge wing length

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- Parameters of interest: population mean and precision \( \theta = (\mu, \tau) \)
- Model:
  \[
p(y|\theta) : \quad y_n \overset{iid}{\sim} \mathcal{N}(\mu, \tau^{-1}), \quad n = 1, \ldots, N
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  \]
  - Iterate: \((\mu_N, \rho_N) = f(a_N, b_N)\) \hspace{1cm} “variational parameters”
  \[
  (a_N, b_N) = g(\mu_N, \rho_N)
  \]

\[\text{[board]}\]

\[\text{[CSIRO 2004]}\]
Midge wing length

approximation

exact posterior

\[ \tau \]

\[ \mu \]

[Bishop 2006]
Microcredit Experiment
Microcredit Experiment

• Simplified from Meager (2018a)
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• $K = 7$ microcredit trials (Mexico, Mongolia, Bosnia, India, Morocco, Philippines, Ethiopia)
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$$y_{kn}$$
Microcredit Experiment

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- $K = 7$ microcredit trials (Mexico, Mongolia, Bosnia, India, Morocco, Philippines, Ethiopia)
- $N_k$ businesses in $k$th site ($\sim 900$ to $\sim 17K$)
- Profit of $n$th business at $k$th site:

$$y_{kn} \overset{indep}{\sim} \mathcal{N}(\mu_k + T_{kn}, \tau_k)$$
Microcredit Experiment

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- $K = 7$ microcredit trials (Mexico, Mongolia, Bosnia, India, Morocco, Philippines, Ethiopia)
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profit

$1$ if microcredit
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- Profit of $n$th business at $k$th site:

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y_{kn} \sim \mathcal{N}(\mu_k + T_{kn} \tau_k, \sigma_k^2)
\]

profit \[1 \text{ if microcredit}\]
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- $N_k$ businesses in $k$th site ($\sim 900$ to $\sim 17K$)
- Profit of $n$th business at $k$th site:
  \[ y_{kn} \sim \text{iid} \mathcal{N}(\mu_k + T_{kn}\tau_k, \sigma_k^2) \]
- Priors and hyperpriors:

1 if microcredit
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\[
y_{kn} \overset{\text{iid}}{\sim} \mathcal{N}(\mu_k + T_{kn}\tau_k, \sigma_k^2)
\]

• Priors and hyperpriors:

\[
\begin{pmatrix}
\mu_k \\
\tau_k
\end{pmatrix} \overset{\text{iid}}{\sim} \mathcal{N}\left(\begin{pmatrix}
\mu \\
\tau
\end{pmatrix}, C\right)
\]
Microcredit Experiment

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\tau
\end{pmatrix}, C\right)
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\[
\sigma_k^{-2} \overset{iid}{\sim} \Gamma(a, b)
\]
Microcredit Experiment

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• Priors and hyperpriors:
  \[
  \begin{align*}
  \left( \begin{array}{c}
  \mu_k \\
  \tau_k
  \end{array} \right) & \overset{iid}{\sim} \mathcal{N}\left( \left( \begin{array}{c}
  \mu \\
  \tau
  \end{array} \right), C \right) \\
  \left( \begin{array}{c}
  \mu \\
  \tau
  \end{array} \right) & \overset{iid}{\sim} \mathcal{N}\left( \left( \begin{array}{c}
  \mu_0 \\
  \tau_0
  \end{array} \right), \Lambda^{-1} \right) \\
  \sigma_k^{-2} & \overset{iid}{\sim} \Gamma(a, b) \\
  C & \sim \text{Sep&LKJ}(\eta, c, d)
  \end{align*}
  \]
Microcredit

MFVB: How will we know if it’s working?
Microcredit

Means

Parameter
- \mu
- \mu_k
- \tau
- \tau_k
- \log(\sigma^2)

MFVB vs. MCMC (ground truth)
Microcredit

- *One set* of 2500 MCMC draws: 45 minutes

[Giordano, Broderick, Meager, Huggins, Jordan 2016]
Microcredit

- **One set of 2500 MCMC draws:** 45 minutes
- **MFVB optimization:** <1 min
Microcredit

- *One set* of 2500 MCMC draws: *45 minutes*
- MFVB optimization: *<1 min*
Microcredit

- One set of 2500 MCMC draws: 45 minutes
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Criteo Online Ads Experiment

- Click-through conversion prediction
- Q: Will a customer (e.g.) buy a product after clicking?

[Giordano, Broderick, Meager, Huggins, Jordan 2016]
Microcredit

- One set of 2500 MCMC draws: 45 minutes
- MFVB optimization: <1 min

Criteo Online Ads Experiment

- Click-through conversion prediction
- Q: Will a customer (e.g.) buy a product after clicking?
- Q: How predictive of conversion are different features?

[Giordano, Broderick, Meager, Huggins, Jordan 2016]
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- *One set of 2500 MCMC draws: 45 minutes*
- MFVB optimization: <1 min

Criteo Online Ads Experiment

- Click-through conversion prediction
- Q: Will a customer (e.g.) buy a product after clicking?
- Q: How predictive of conversion are different features?
- Logistic GLMM

[Giordano, Broderick, Meager, Huggins, Jordan 2016; Giordano, Broderick, Jordan 2017]
**Microcredit**

- **One set of 2500 MCMC draws:** 45 minutes
- **MFVB optimization:** <1 min

**Criteo Online Ads Experiment**

- Click-through conversion prediction
- Q: Will a customer (e.g.) buy a product after clicking?
- Q: How predictive of conversion are different features?
- Logistic GLMM; \( N = 61,895 \) subset to compare to MCMC

[Giordano, Broderick, Meager, Huggins, Jordan 2016; Giordano, Broderick, Jordan 2017]
Criteo Online Ads Experiment
Criteo Online Ads Experiment

- MAP: 12 s
Criteo Online Ads Experiment

- **MAP:** 12 s

[Giordano, Broderick, Jordan 2017]
Criteo Online Ads Experiment

Global parameters (-τ)

Global parameter τ

Local parameters

• MAP: **12 s**
• MFVB: **57 s**

[Giordano, Broderick, Jordan 2017]
Criteo Online Ads Experiment

- MAP: 12 s
- MFVB: 57 s
Criteo Online Ads Experiment

- MAP: **12 s**
- MFVB: **57 s**
- MCMC (5K samples): 21,066 s (5.85 h)

[Giordano, Broderick, Jordan 2017]
Roadmap

• Bayes & Approximate Bayes review
• What is:
  • Variational Bayes (VB)
  • Mean-field variational Bayes (MFVB)
• Why use MFVB?
• When can we trust MFVB?
• Where do we go from here?
Roadmap

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Variational Bayes and beyond: Bayesian inference for big data

Tamara Broderick
ITT Career Development
Assistant Professor,
MIT

http://www.tamarabroderick.com/tutorials.html
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Approximate Bayesian inference

Use $q^*$ to approximate $p(\cdot | y)$

Optimization

$q^* = \arg\min_{q \in Q} f(q(\cdot), p(\cdot | y))$

Variational Bayes

$q^* = \arg\min_{q \in Q} KL(q(\cdot) || p(\cdot | y))$

Mean-field variational Bayes

$q^* = \arg\min_{q \in Q_{MFVB}} KL(q(\cdot) || p(\cdot | y))$

- Coordinate descent
- Stochastic variational inference (SVI) [Hoffman et al 2013]
- Automatic differentiation variational inference (ADVI) [Kucukelbir et al 2015, 2017]
Criteo Online Ads Experiment

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What about uncertainty?

$$KL(q || p(\cdot | y)) = \int_\theta q(\theta) \log \frac{q(\theta)}{p(\theta | y)} d\theta$$

$$q(\theta) = \prod_{j=1}^{J} q_j(\theta_j)$$
What about uncertainty?

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[Turner & Sahani 2011; MacKay 2003; Bishop 2006; Wang, Titterington 2004]
What about uncertainty?

\[ KL(q||p(\cdot|y)) = \int_{\theta} q(\theta) \log \frac{q(\theta)}{p(\theta|y)} d\theta \]

\[ q(\theta) = \prod_{j=1}^{J} q_j(\theta_j) \]

- Conjugate linear regression

[Turner & Sahani 2011; MacKay 2003; Bishop 2006; Wang, Titterington 2004]
What about uncertainty?

$$KL(q \| p(\cdot \mid y)) = \int_\theta q(\theta) \log \frac{q(\theta)}{p(\theta \mid y)} d\theta$$

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- Conjugate linear regression
- Bayesian central limit theorem

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[Exercise: derive the MFVB-CA steps. Hint: use precision matrix.]
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- Underestimates variance (sometimes severely)
- Conjugate linear regression
- Bayesian central limit theorem

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[Turner & Sahani 2011; MacKay 2003; Bishop 2006; Wang, Titterington 2004]
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$$KL(q||p(\cdot|y)) = \int \theta q(\theta) \log \frac{q(\theta)}{p(\theta|y)} d\theta$$

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- Underestimates variance (sometimes severely)

- Conjugate linear regression

- Bayesian central limit theorem

[Exercise: derive the MFVB-CA steps. Hint: use precision matrix.]
What about uncertainty?

- Underestimates variance (sometimes severely)
- No covariance estimates
- Conjugate linear regression
- Bayesian central limit theorem

\[ KL(q||p(\cdot|y)) = \int_{\theta} q(\theta) \log \frac{q(\theta)}{p(\theta|y)} d\theta \]

\[ q(\theta) = \prod_{j=1}^{J} q_j(\theta_j) \]

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What about uncertainty?

• Microcredit
What about uncertainty?

- Microcredit
What about uncertainty?

- Microcredit effect
- τ mean: 3.08 USD PPP

[Giordano, Broderick, Meager, Huggins, Jordan 2016]
What about uncertainty?

- Microcredit effect
  - $\tau$ mean: 3.08 USD PPP
  - $\tau$ std dev: 1.83 USD PPP

[Giordano, Broderick, Meager, Huggins, Jordan 2016]
What about uncertainty?

• Microcredit effect
• $\tau$ mean: 3.08 USD PPP
• $\tau$ std dev: 1.83 USD PPP
• Mean is 1.68 std dev from 0

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- Microcredit effect
  - $\tau$ mean: 3.08 USD PPP
  - $\tau$ std dev: 1.83 USD PPP
  - Mean is 1.68 std dev from 0

- Criteo online ads experiment

[Giordano, Broderick, Meager, Huggins, Jordan 2016; Giordano, Broderick, Jordan 2017]
What about means?

- Model for relational data with covariates
- When 1000+ nodes, MCMC > 1 day  
  [Fosdick 2013, Ch 4]

![Graph showing comparison between MFVB and MCMC means](Fosdick 2013, Ch 4, Fig 4.3)
Posterior means: revisited

- Want to predict college GPA $y_n$
Posterior means: revisited

- Want to predict college GPA \( y_n \)
- Collect: standardized test scores (e.g., SAT, ACT) \( x_n \)
Posterior means: revisited

- Want to predict college GPA $y_n$
- Collect: standardized test scores (e.g., SAT, ACT) $x_n$
- Collect: regional test scores $r_n$
Posterior means: revisited

• Want to predict college GPA $y_n$
• Collect: standardized test scores (e.g., SAT, ACT) $x_n$
• Collect: regional test scores $r_n$
• Model: $y_n|\beta, z, \sigma^2 \overset{indep}{\sim} \mathcal{N}(\beta^T x_n + z_{k(n)} r_n, \sigma^2)$
Posterior means: revisited

• Want to predict college GPA \( y_n \)
• Collect: standardized test scores (e.g., SAT, ACT) \( x_n \)
• Collect: regional test scores \( r_n \)
• Model: 
\[
y_n \mid \beta, z, \sigma^2 \overset{\text{iid}}{\sim} \mathcal{N}(\beta^T x_n + z_k(n) r_n, \sigma^2)
\]
\[
z_k \mid \rho^2 \overset{\text{iid}}{\sim} \mathcal{N}(0, \rho^2)
\]
\[
\beta \sim \mathcal{N}(0, \Sigma)
\]
\[
(\sigma^2)^{-1} \sim \text{Gamma}(a_{\sigma^2}, b_{\sigma^2})
\]
\[
(\rho^2)^{-1} \sim \text{Gamma}(a_{\rho^2}, b_{\rho^2})
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[Giordano, Broderick, Jordan 2015]
Posterior means: revisited

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- Model: 
  $$ y_n | \beta, z, \sigma^2 \overset{\text{indep}}{\sim} \mathcal{N}(\beta^T x_n + z_{k(n)} r_n, \sigma^2) $$
  $$ z_k | \rho^2 \overset{iid}{\sim} \mathcal{N}(0, \rho^2) $$
  $$ \beta \sim \mathcal{N}(0, \Sigma) $$
  $$ (\sigma^2)^{-1} \sim \text{Gamma}(a_{\sigma^2}, b_{\sigma^2}) $$
  $$ (\rho^2)^{-1} \sim \text{Gamma}(a_{\rho^2}, b_{\rho^2}) $$

- Data simulated from model (3 data sets, 300 data points):

[Giordano, Broderick, Jordan 2015]
Posterior means: revisited

- Want to predict college GPA \( y_n \)
- Collect: standardized test scores (e.g., SAT, ACT) \( x_n \)
- Collect: regional test scores \( r_n \)
- Model:
  \[
  y_n | \beta, z, \sigma^2 \overset{\text{indep}}{\sim} N(\beta^T x_n + z_{k(n)} r_n, \sigma^2)
  \]
  \[
  z_k | \rho^2 \overset{\text{iid}}{\sim} N(0, \rho^2)
  \]
  \[
  \rho^2 \sim Gamma(a_{\rho^2}, b_{\rho^2})
  \]
  \[
  \beta \sim N(0, \Sigma)
  \]
  \[
  \sigma^2 \sim Gamma(a_{\sigma^2}, b_{\sigma^2})
  \]
  \[
  \rho^2 \sim Gamma(a_{\rho^2}, b_{\rho^2})
  \]

- Data simulated from model (100 data sets, 300 data points):

[Giordano, Broderick, Jordan 2015]
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What can we do?

• Reliable diagnostics
What can we do?

• Reliable diagnostics
• KL vs ELBO
What can we do?

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What can we do?

- Reliable diagnostics
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[Gorham, Mackey 2015, 2017; Chwialkowski, Strathmann, Gretton 2016; Jitkrittum et al 2017; Talts et al 2018; Yao et al 2018, etc.]

“Yes, but did it work? Evaluating variational inference” ICML 2018
What can we do?

• Reliable diagnostics
• KL vs ELBO

[Gojmer, Mackey 2015, 2017; Chwialkowski, Strathmann, Gretton 2016; Jitkrittum et al 2017; Talts et al 2018; Yao et al 2018, etc.]

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“...closest nice distr.
“Yes, but did it work? Evaluating variational inference” ICML 2018

- Richer “nice” set; alternative divergences
What can we do?

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• KL vs ELBO
  [Gorham, Mackey 2015, 2017; Chwialkowski, Strathmann, Gretton 2016; Jitkrittum et al 2017; Talts et al 2018; Yao et al 2018, etc.]

  “Yes, but did it work? Evaluating variational inference” ICML 2018

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  [Turner, Sahani 2011]
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- Richer “nice” set; alternative divergences
  [Turner, Sahani 2011]
  [Huggins, Kasprzak, Campbell, Broderick, 2018]

Optimize: closest nice distr.
What can we do?

- Reliable diagnostics
- KL vs ELBO
  [Gorham, Mackey 2015, 2017; Chwialkowski, Strathmann, Gretton 2016; Jitkrittum et al 2017; Talts et al 2018; Yao et al 2018, etc.]

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- Corrections [next]
What can we do?

• Reliable diagnostics

• KL vs ELBO

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• Richer “nice” set; alternative divergences

  [Turner, Sahani 2011]
  [Huggins, Kasprzak, Campbell, Broderick, 2018]

• Corrections [next]

• Theoretical guarantees on finite-data quality [next]
What to read next

Textbooks and Reviews


More Experiments

References (1/6)


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