

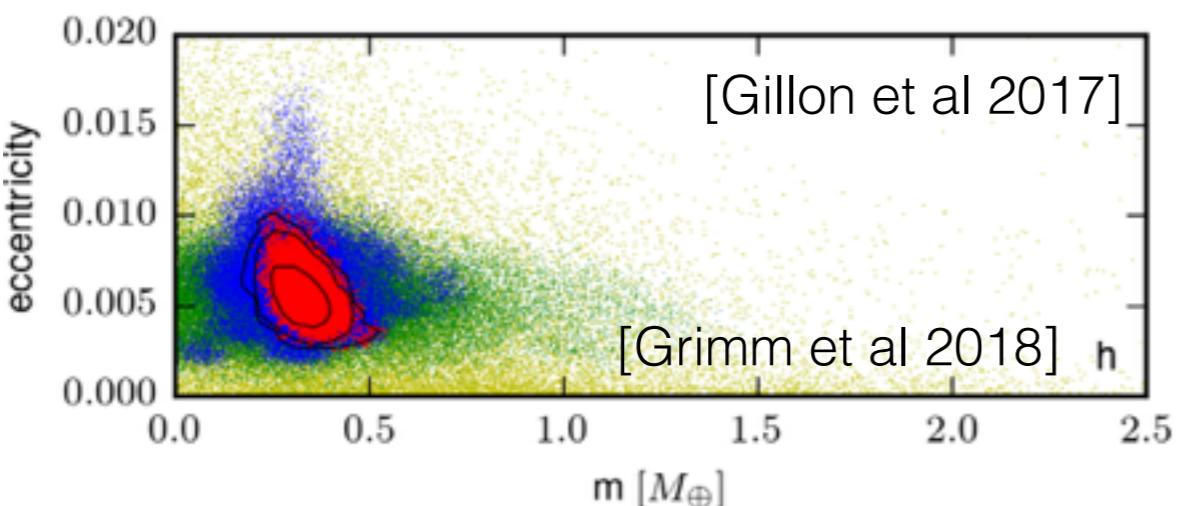


Variational Bayes and beyond: Bayesian inference for big data

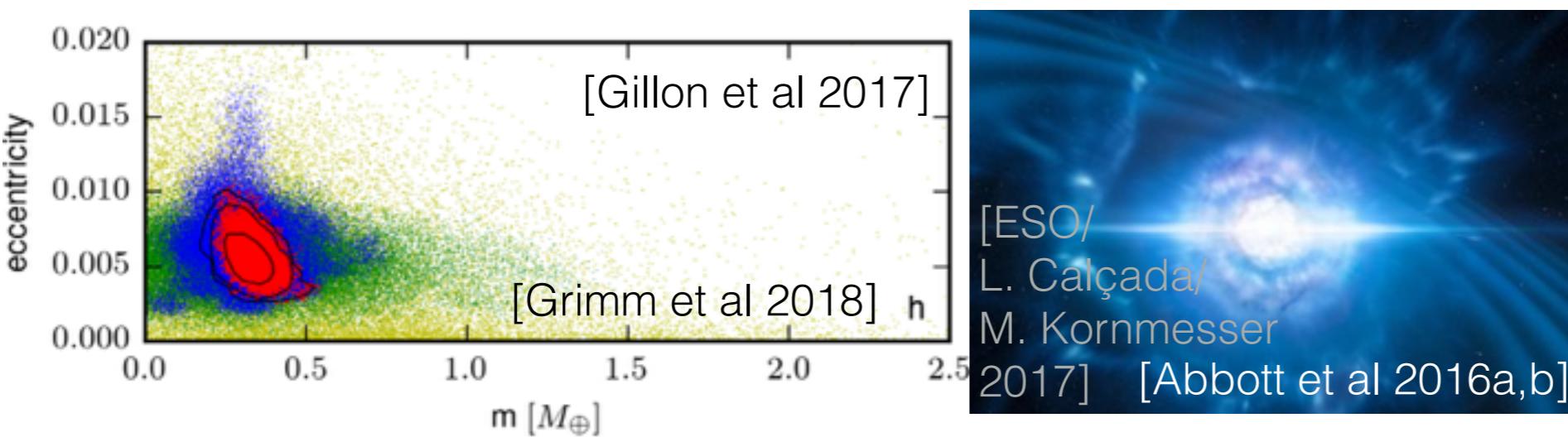
Tamara Broderick
ITT Career Development
Assistant Professor,
MIT

Bayesian inference

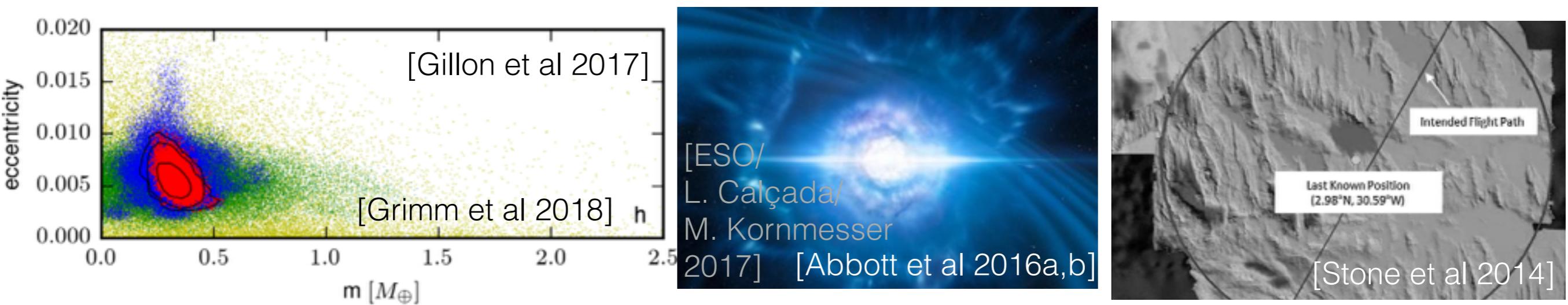
Bayesian inference



Bayesian inference



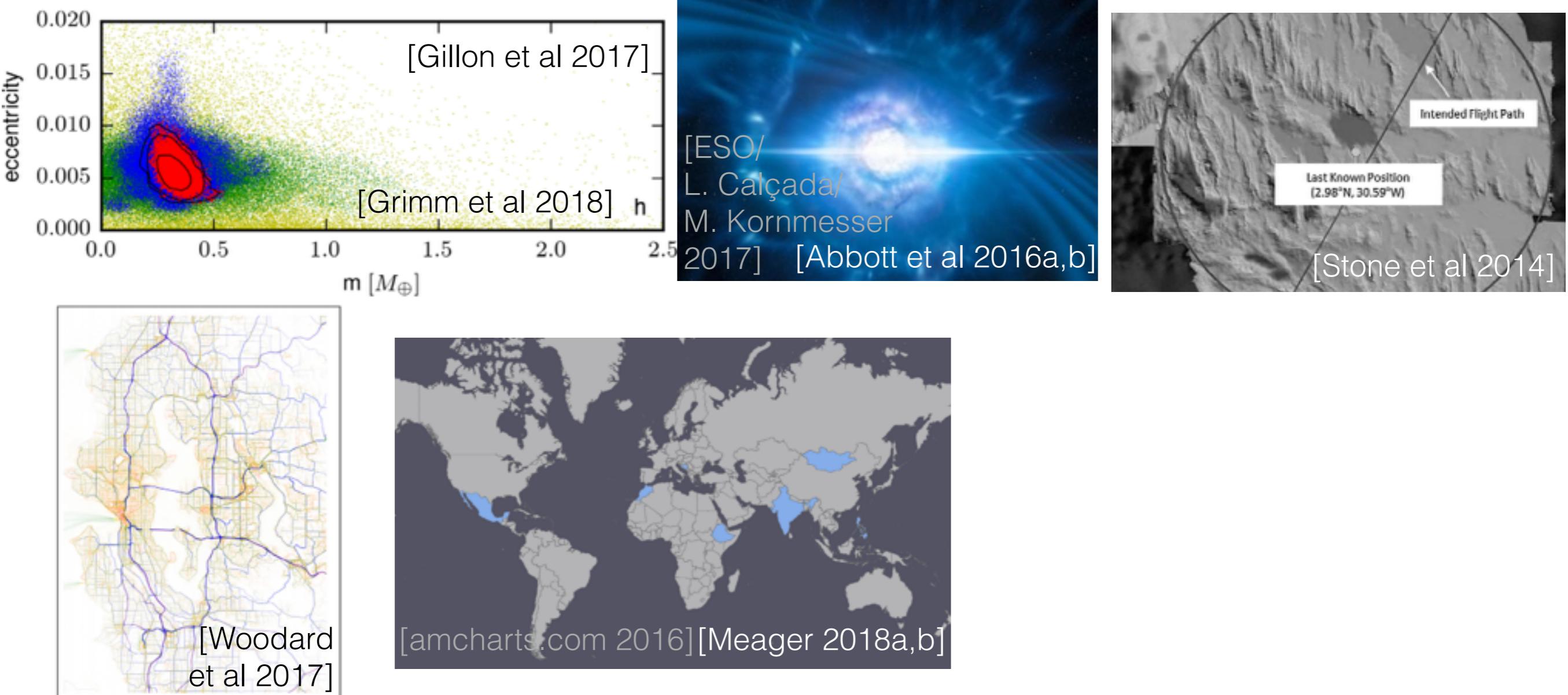
Bayesian inference



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Bayesian inference



Bayesian inference

- Analysis goals: Point estimates, coherent uncertainties
 - Interpretable, complex, modular; expert information



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- Challenge: fast (compute, user), reliable inference

Bayesian inference

- Analysis goals: Point estimates, coherent uncertainties
 - Interpretable, complex, modular; expert information



- 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

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- Variational Bayes can be very fast

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“Arts”	“Budgets”	“Children”	“Education”
NEW	MILLION	CHILDREN	SCHOOL
FILM	TAX	WOMEN	STUDENTS
SHOW	PROGRAM	PEOPLE	SCHOOLS
MUSIC	BUDGET	CHILD	EDUCATION
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ACTRESS	GOVERNMENT	CARE	ELEMENTARY
LOVE	CONGRESS	LIFE	HAITI

[Blei et al
2003]

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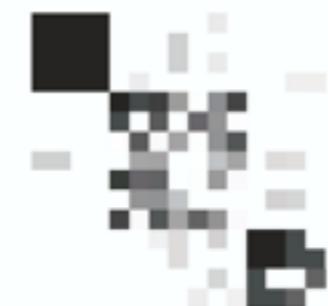
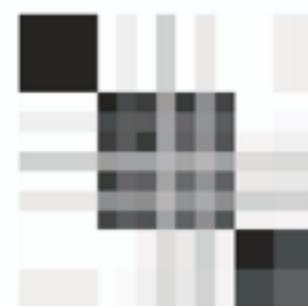
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[Airoldi et al 2008]

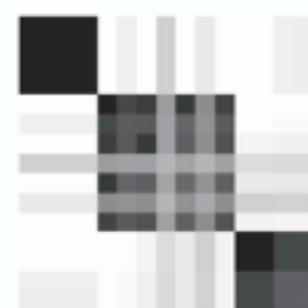
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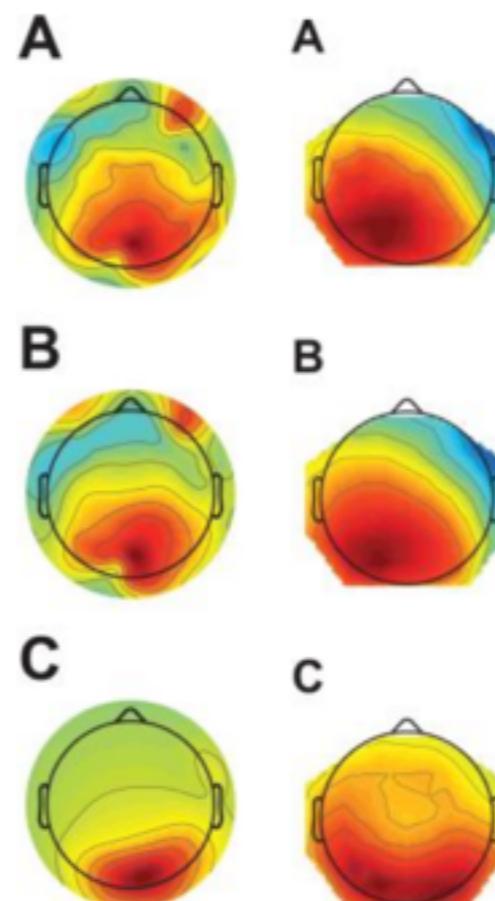
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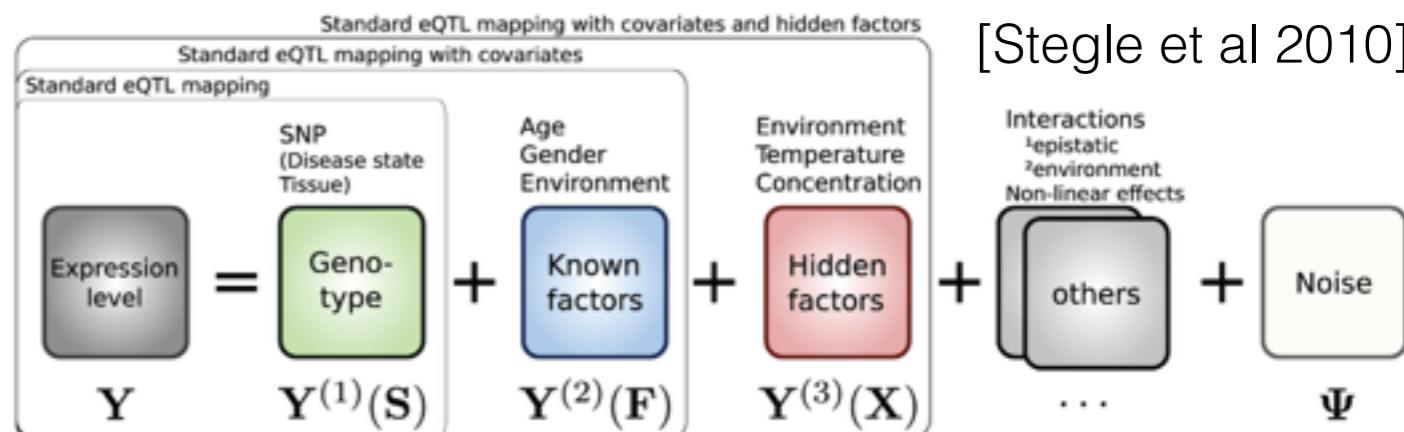
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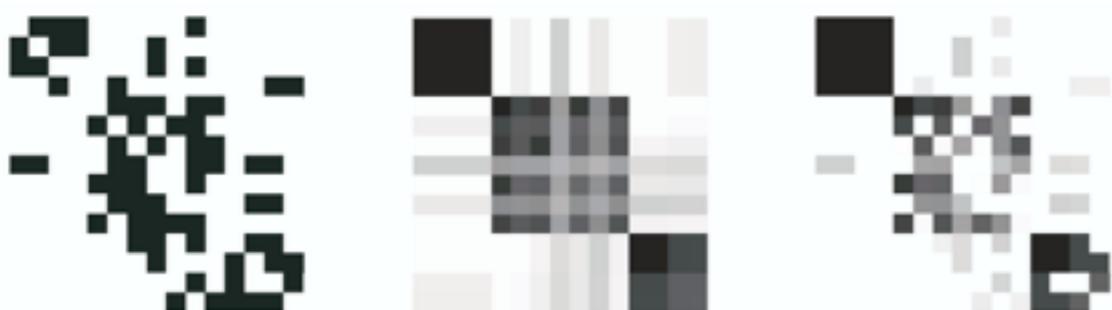
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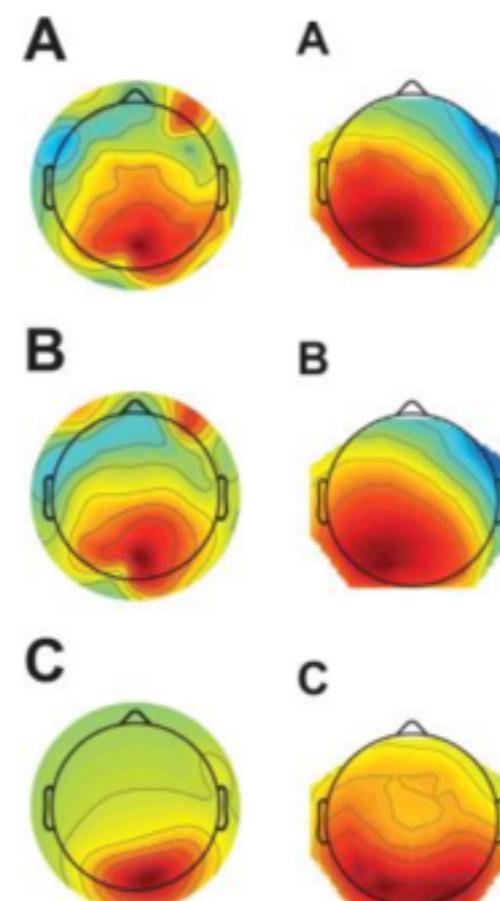
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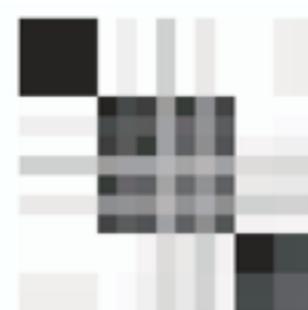
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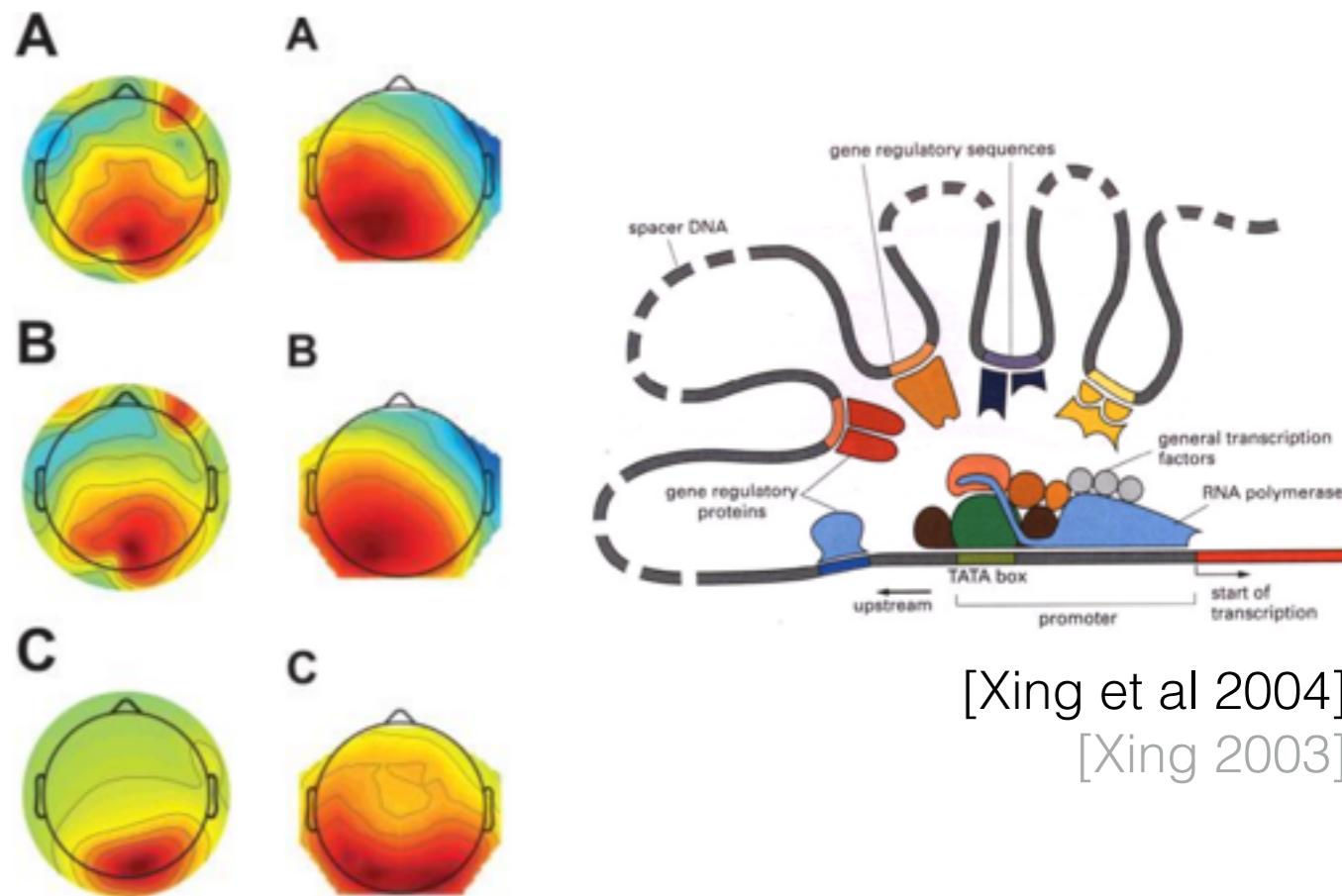
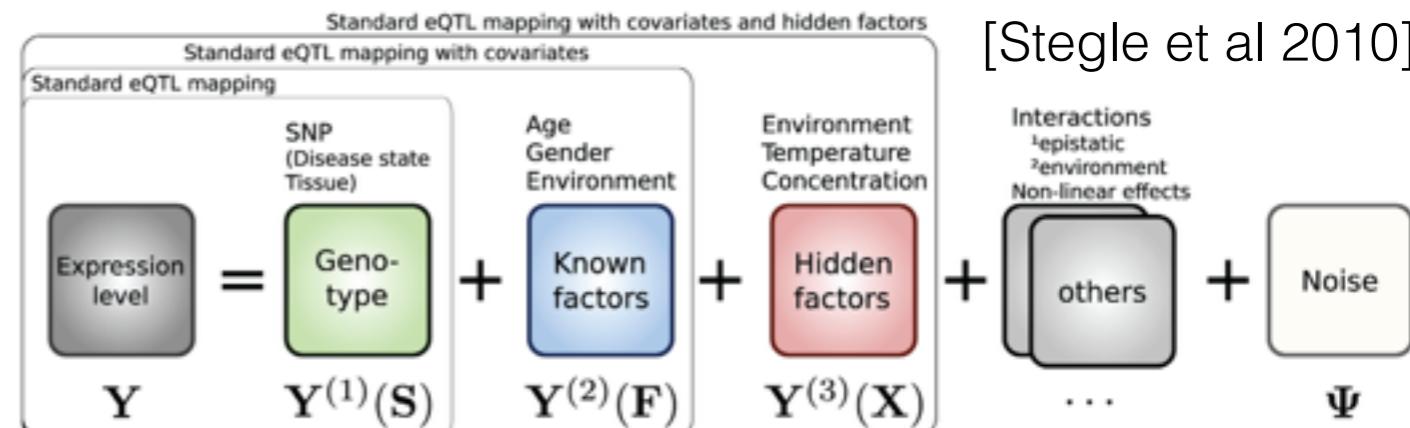
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Roadmap

- 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?

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Bayesian inference

parameters
 θ

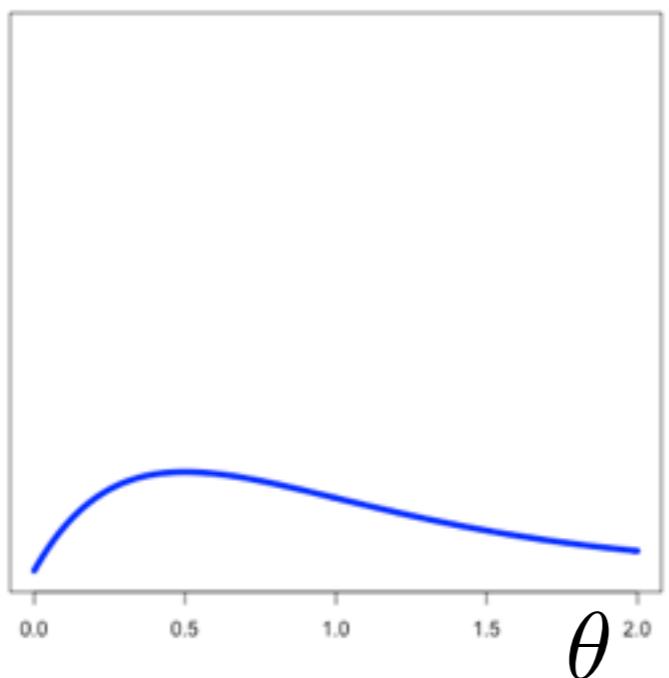
Bayesian inference

parameters
 $p(\theta)$
prior



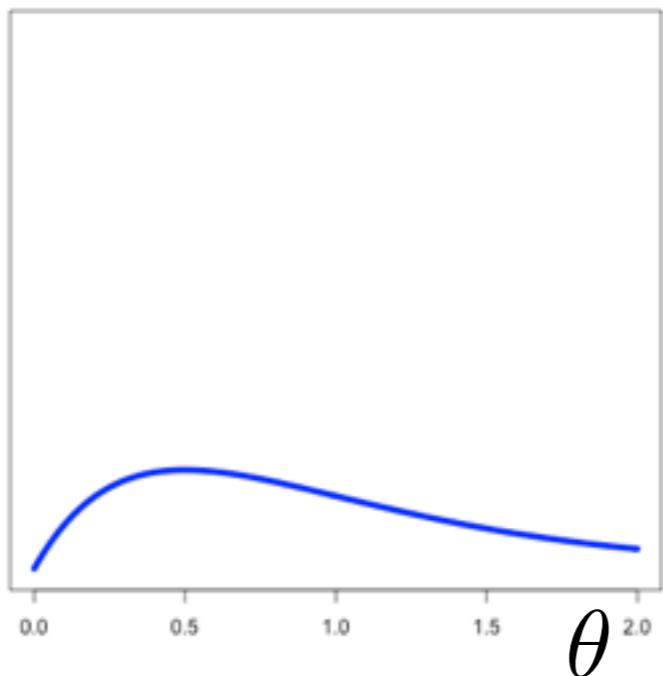
Bayesian inference

parameters
 $p(\theta)$
prior



Bayesian inference

parameters
 $p(y_{1:N} | \theta)p(\theta)$
likelihood prior

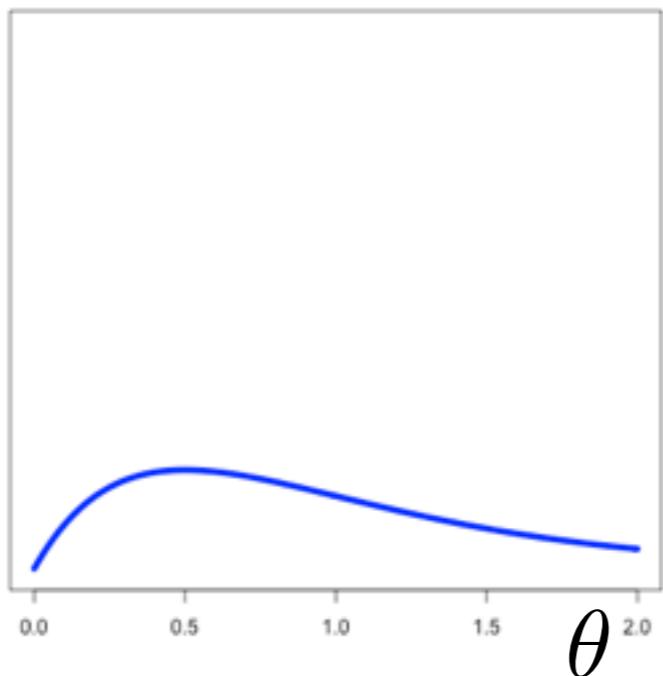


Bayesian inference

data parameters

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

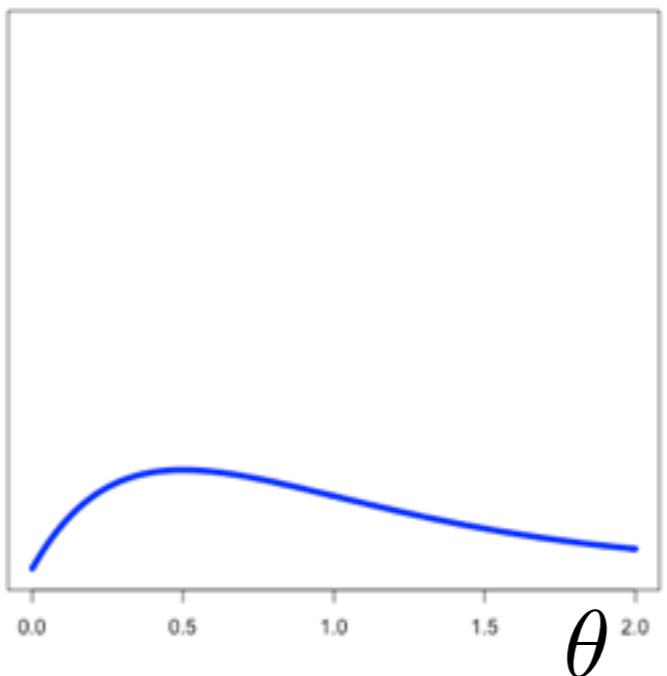
likelihood prior



Bayesian inference

$$p(\theta|y_{1:N}) \propto_{\theta} p(y_{1:N}|\theta)p(\theta)$$

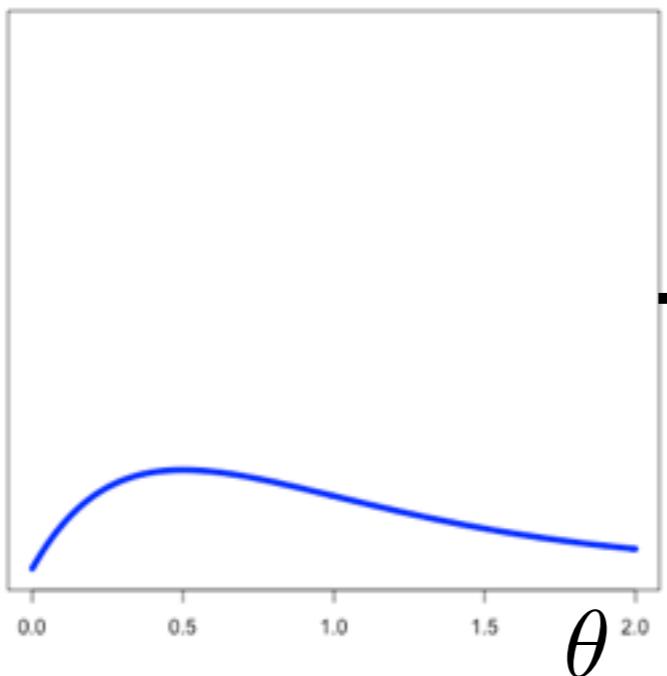
posterior likelihood prior



Bayesian inference

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posterior likelihood prior



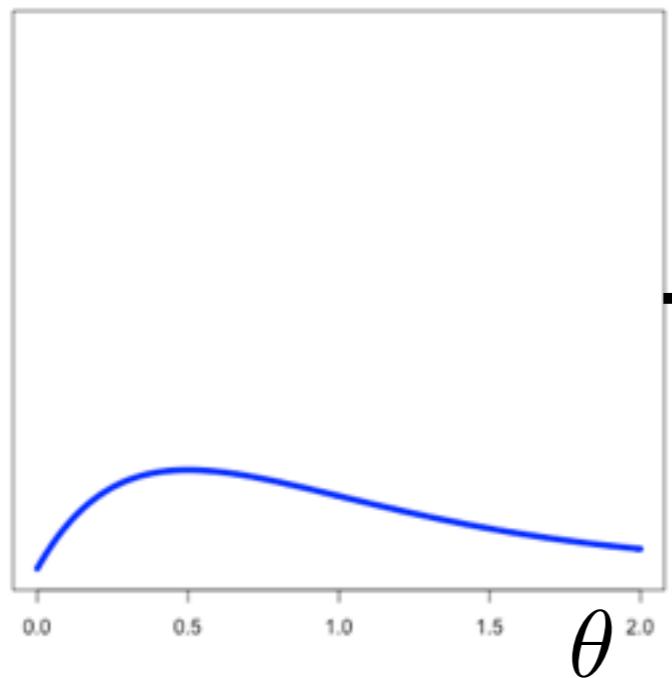
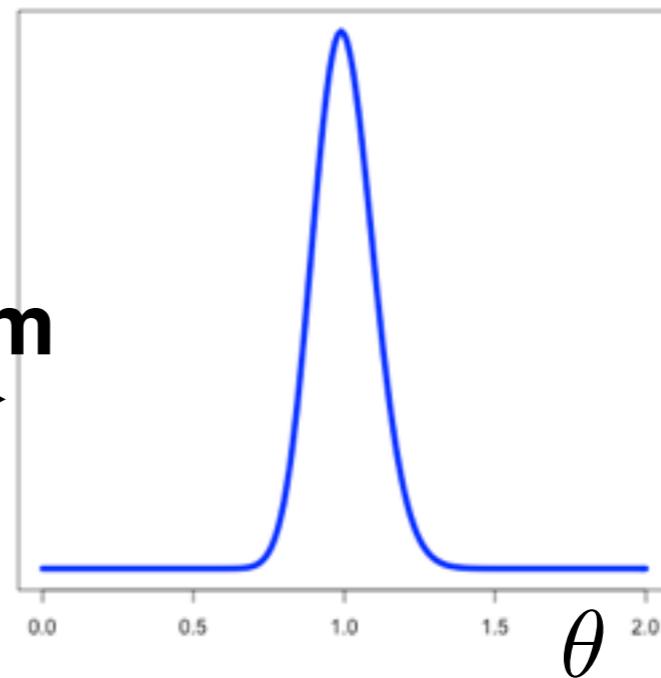
**Bayes
Theorem**



Bayesian inference

$$p(\theta|y_{1:N}) \propto_{\theta} p(y_{1:N}|\theta)p(\theta)$$

posterior likelihood prior

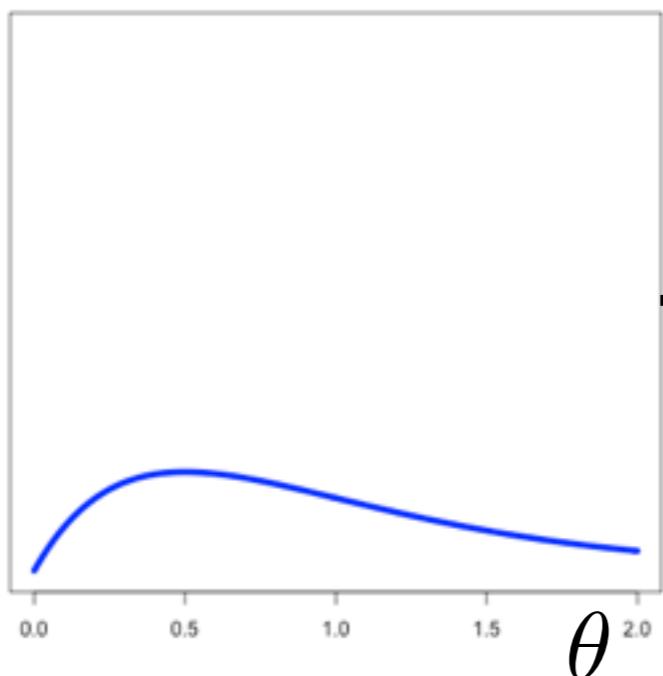


**Bayes
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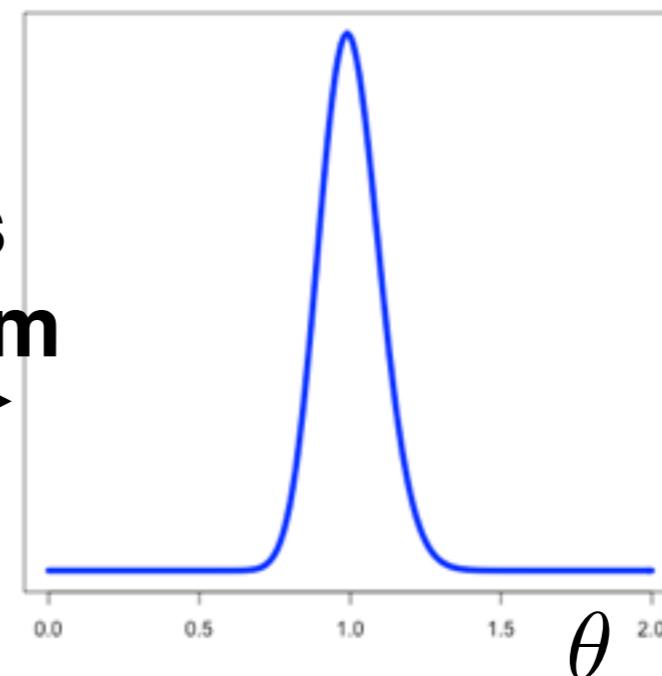
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**Bayes
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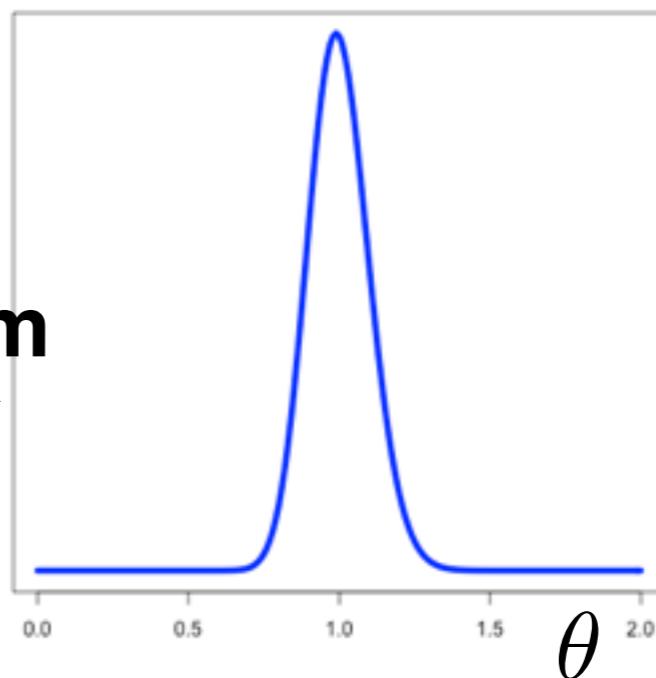


1. Build a model: choose prior & choose likelihood

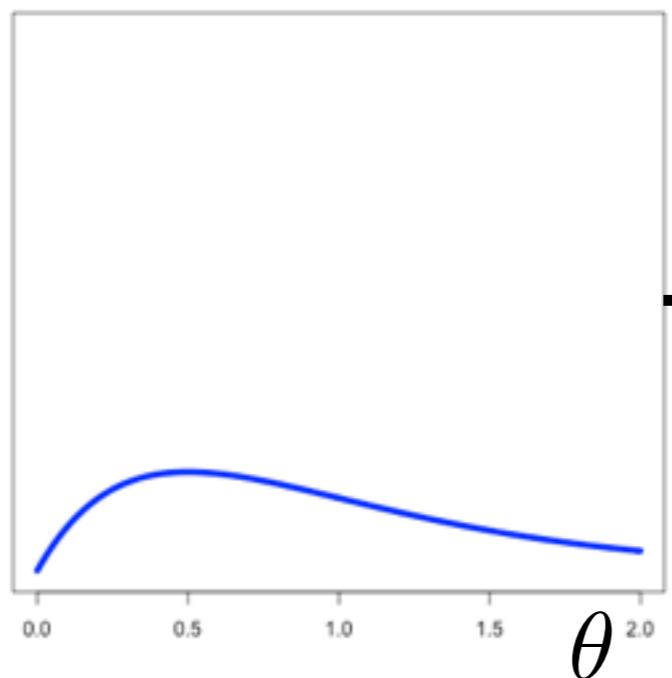
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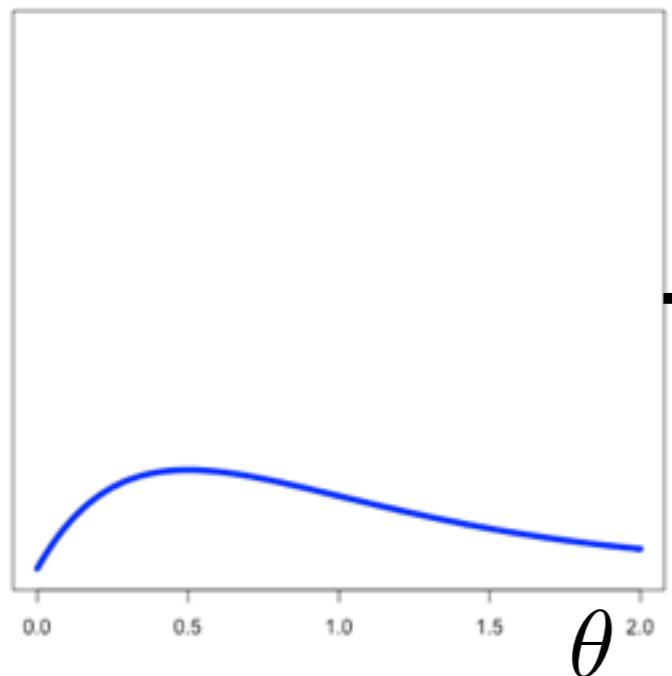
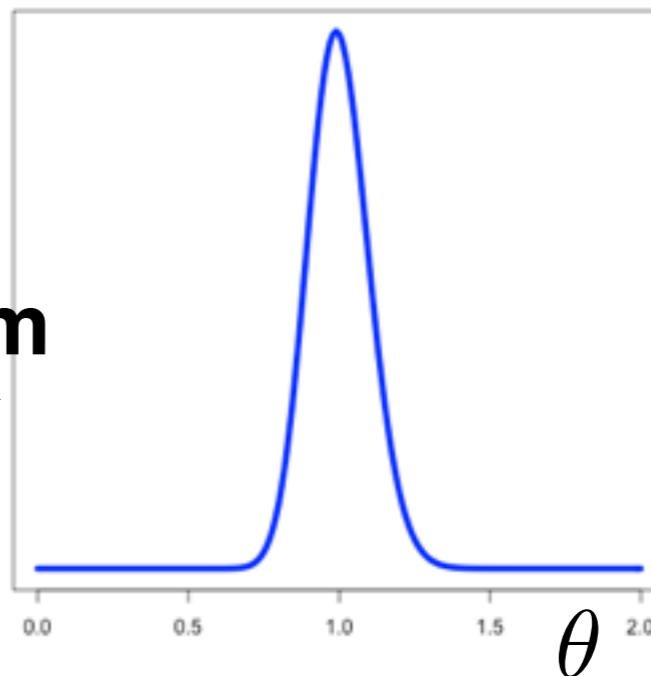


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2. Compute the posterior

Bayesian inference

$$p(\theta|y_{1:N}) \propto_{\theta} p(y_{1:N}|\theta)p(\theta)$$

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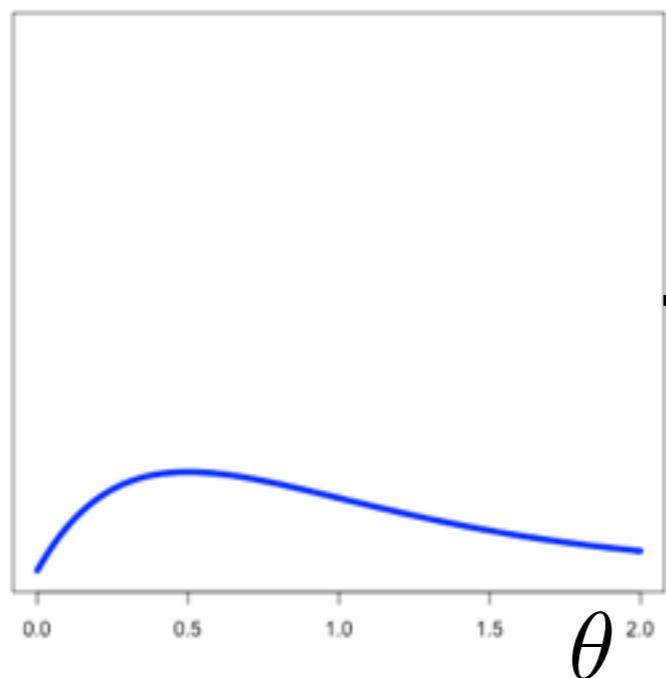
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1. Build a model: choose prior & choose likelihood
2. Compute the posterior
3. Report a summary, e.g. posterior means and (co)variances

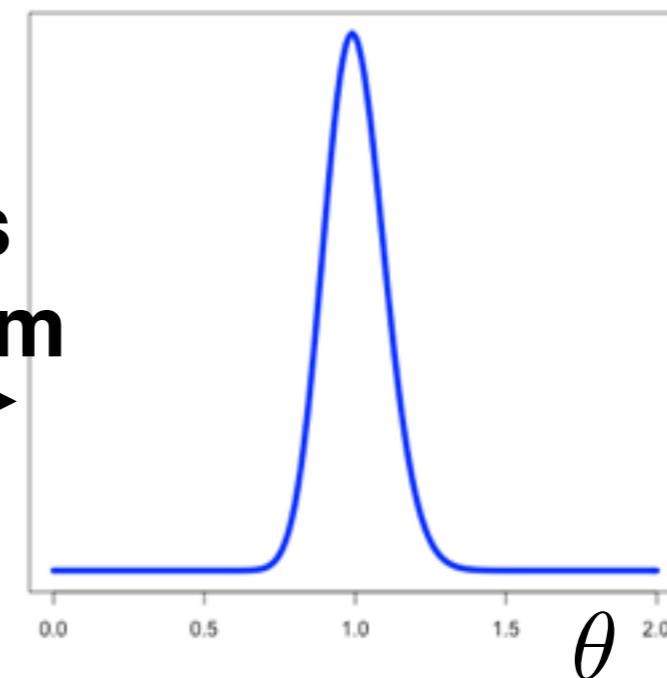
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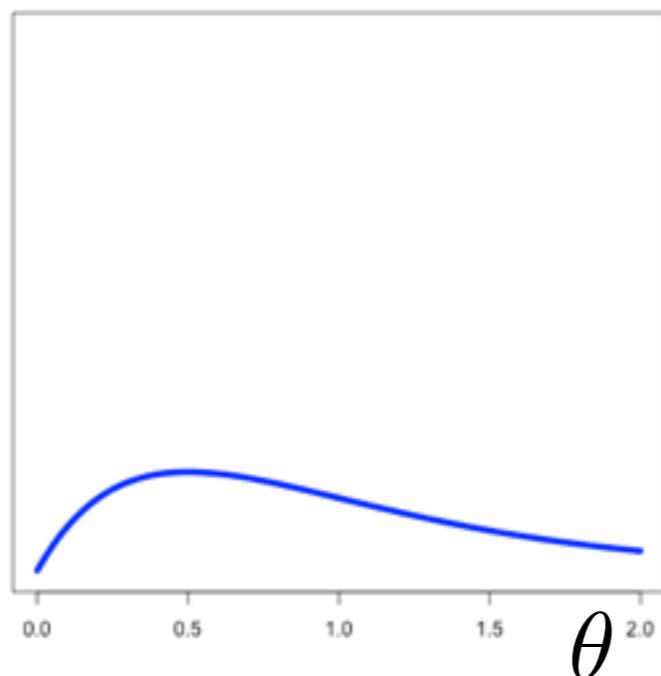


1. Build a model: choose prior & choose likelihood
 2. Compute the posterior
 3. Report a summary, e.g. posterior means and (co)variances
- Why are steps 2 and 3 hard?

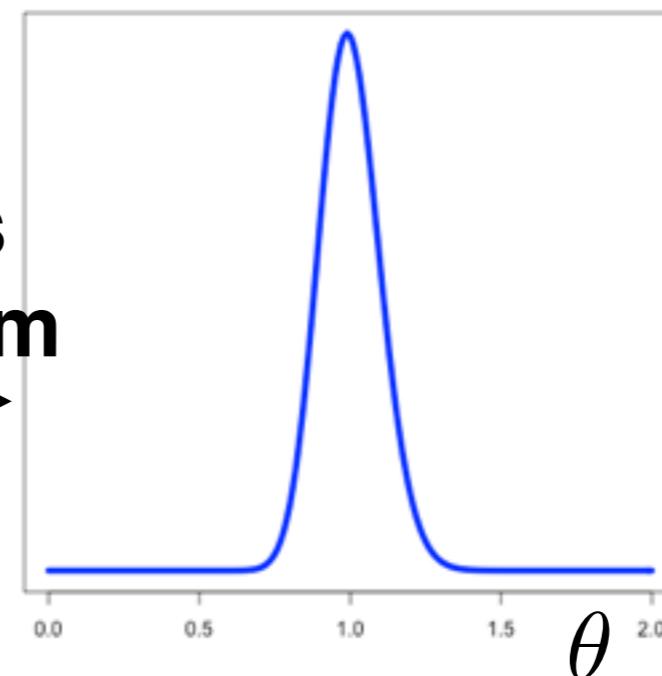
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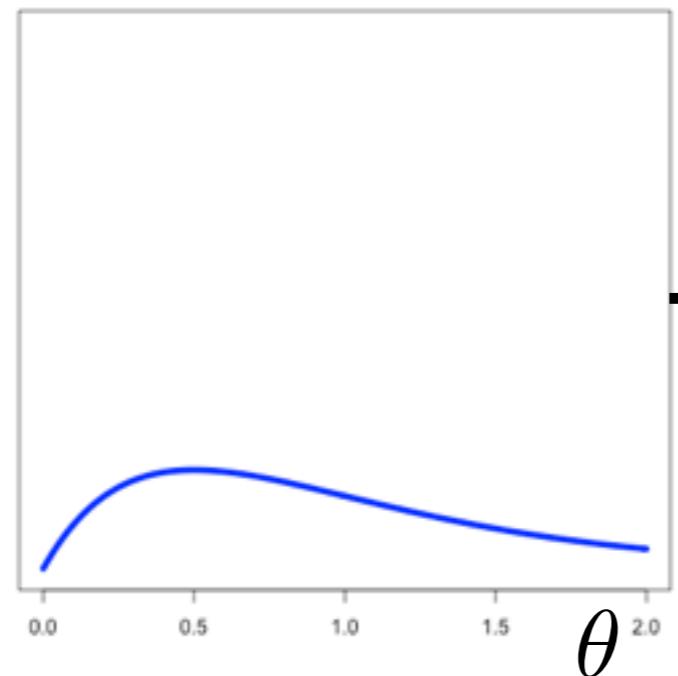
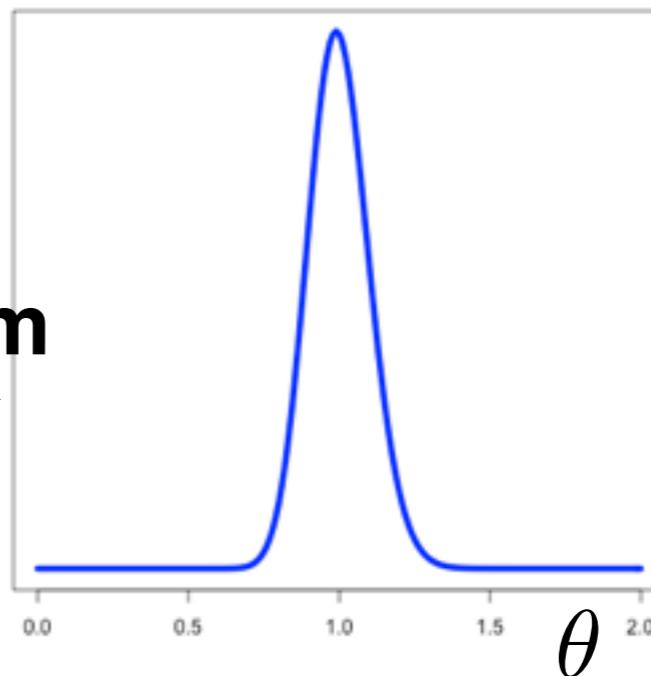


1. Build a model: choose prior & choose likelihood
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- Why are steps 2 and 3 hard?
 - Typically no closed form

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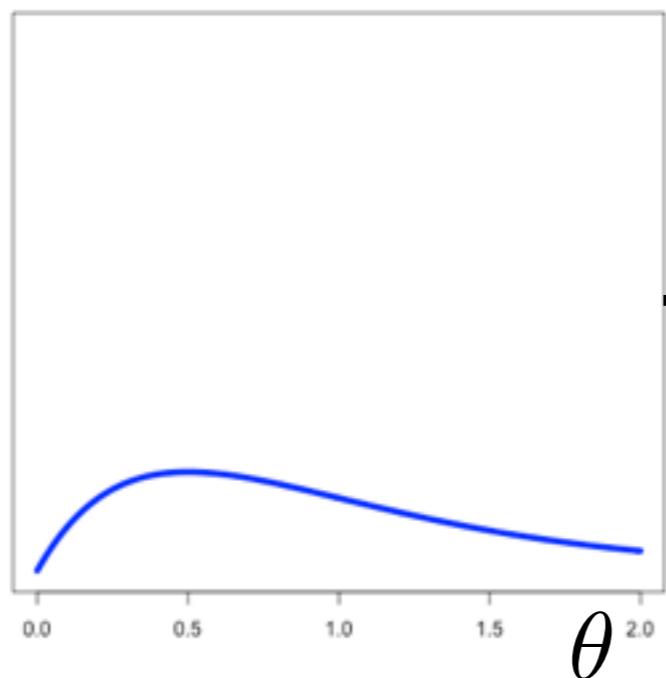


1. Build a model: choose prior & choose likelihood
 2. Compute the posterior
 3. Report a summary, e.g. posterior means and (co)variances
- Why are steps 2 and 3 hard?
 - Typically no closed form, high-dimensional integration

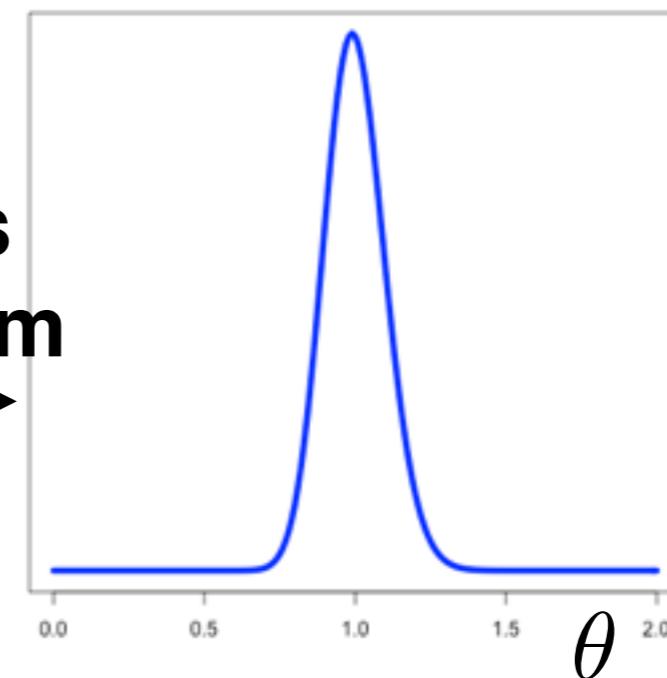
Bayesian inference

$$p(\theta|y_{1:N}) = p(y_{1:N}|\theta)p(\theta)/p(y_{1:N})$$

posterior likelihood prior



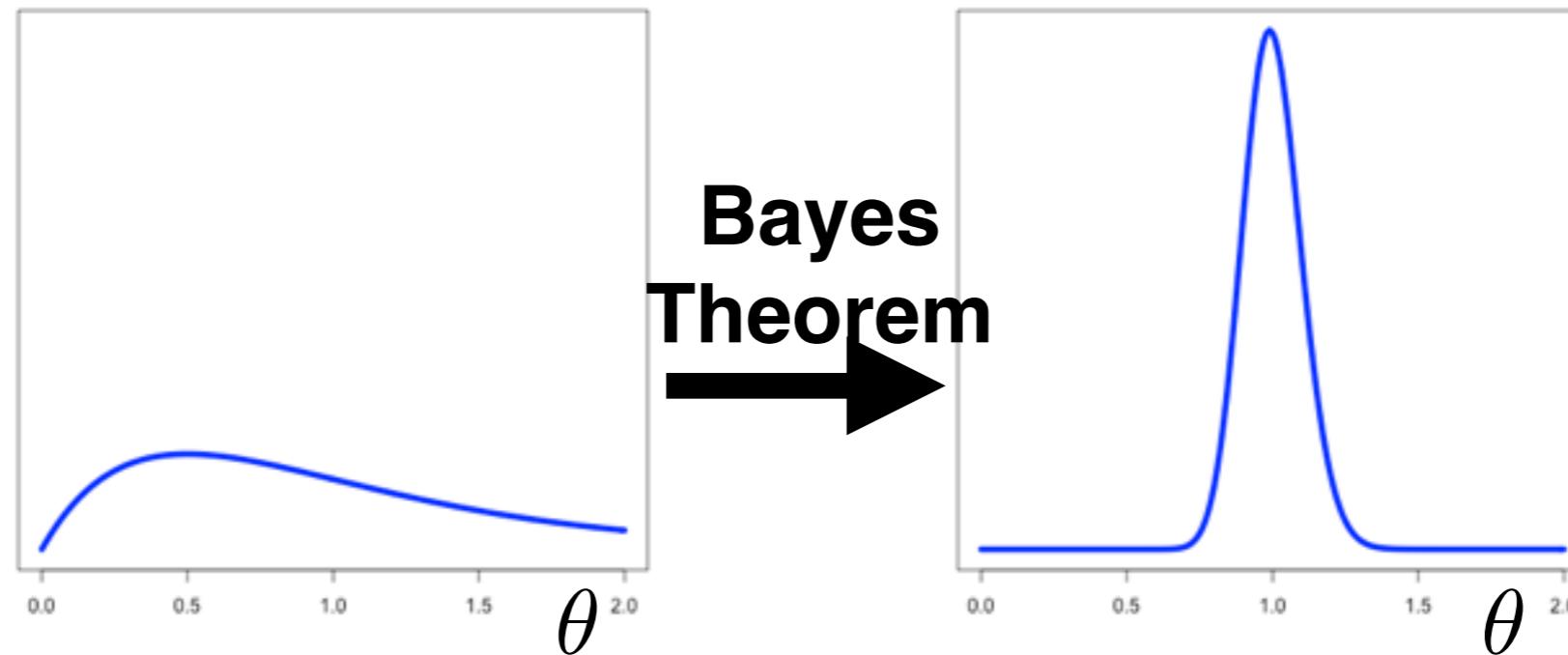
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Bayesian inference

data parameters
 $p(\theta|y_{1:N}) = p(y_{1:N}|\theta)p(\theta)/p(y_{1:N})$
posterior likelihood prior evidence



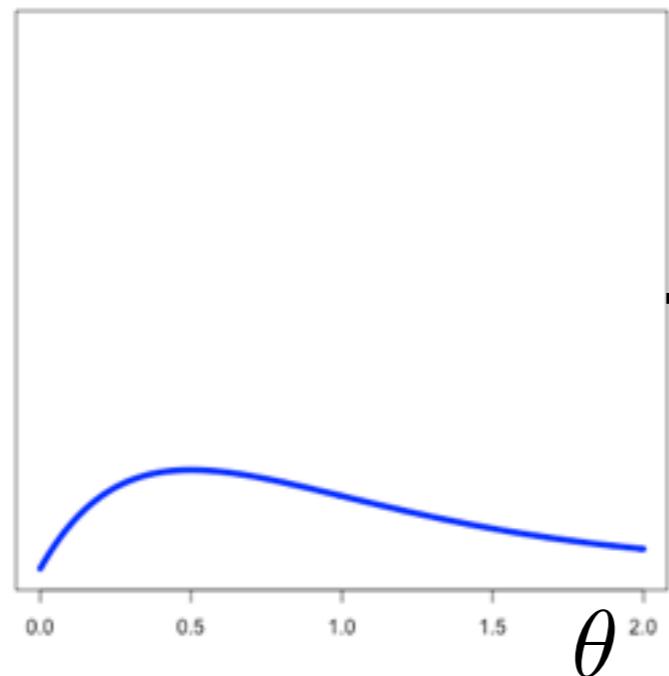
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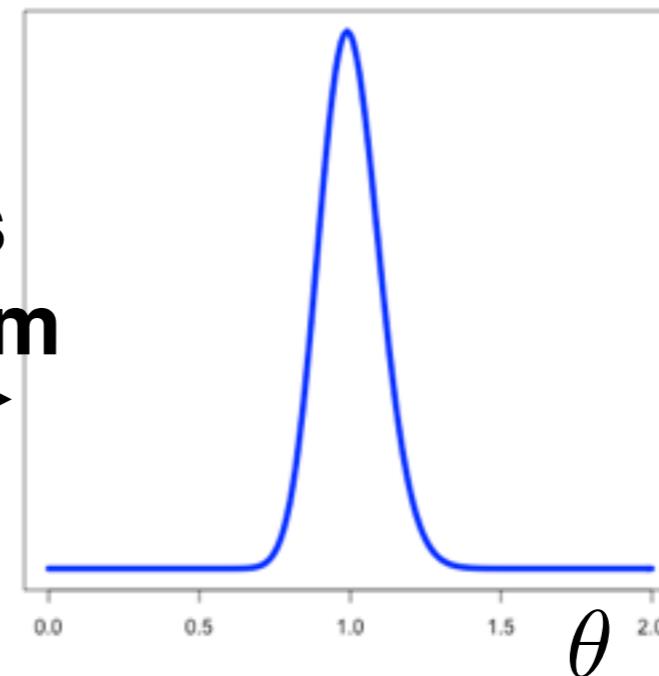
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posterior likelihood prior evidence



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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

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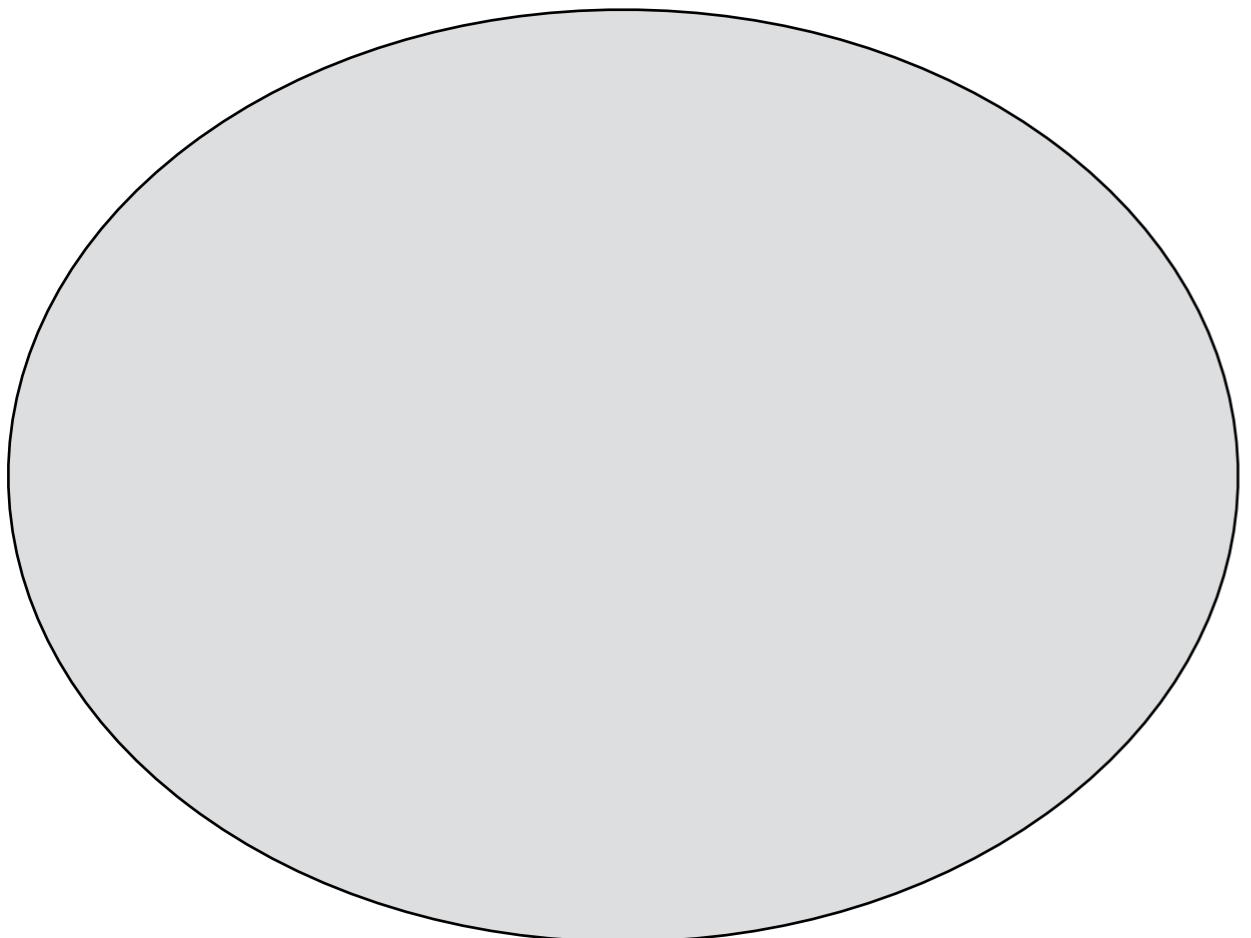
Instead: an optimization approach

- Approximate posterior with q^*

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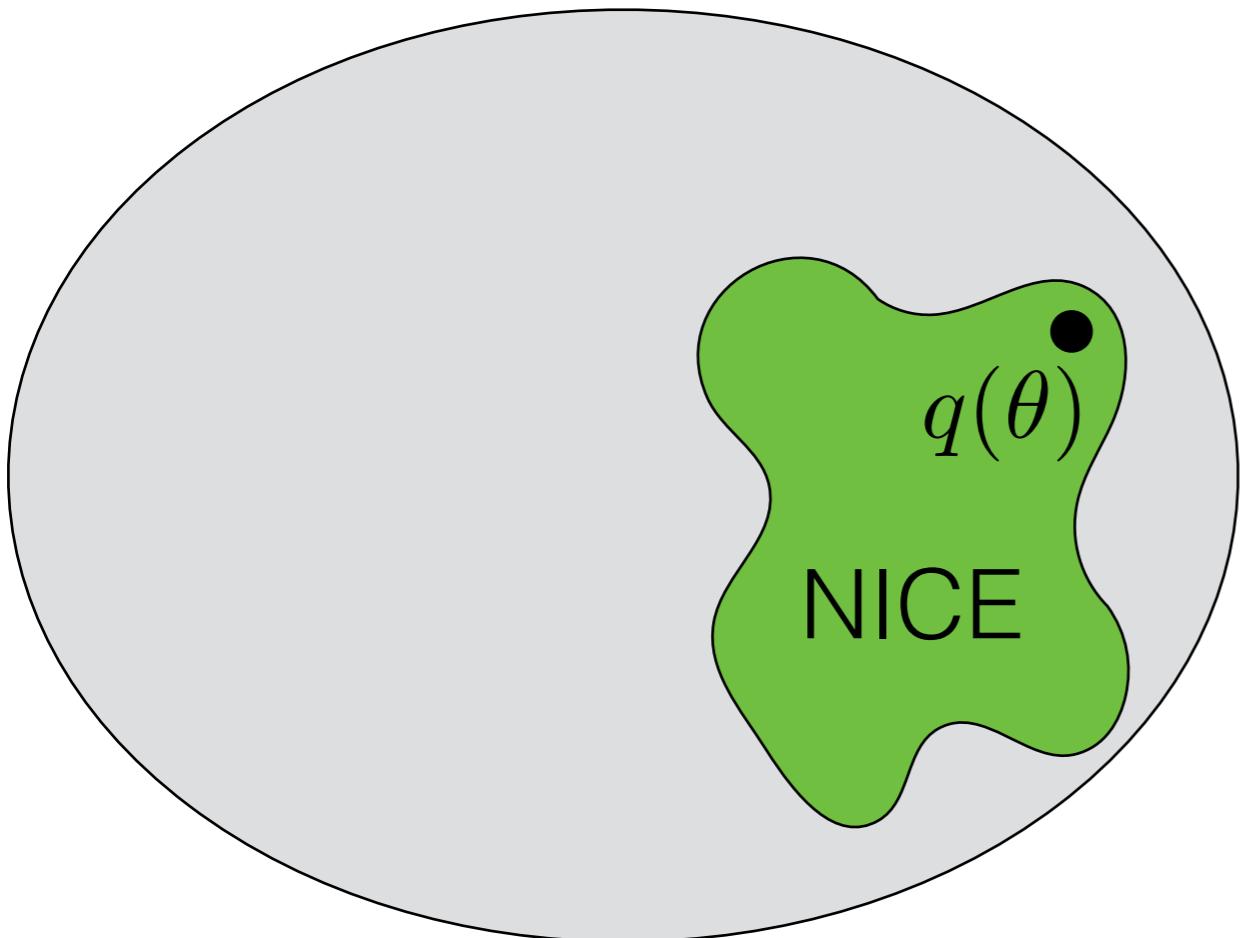
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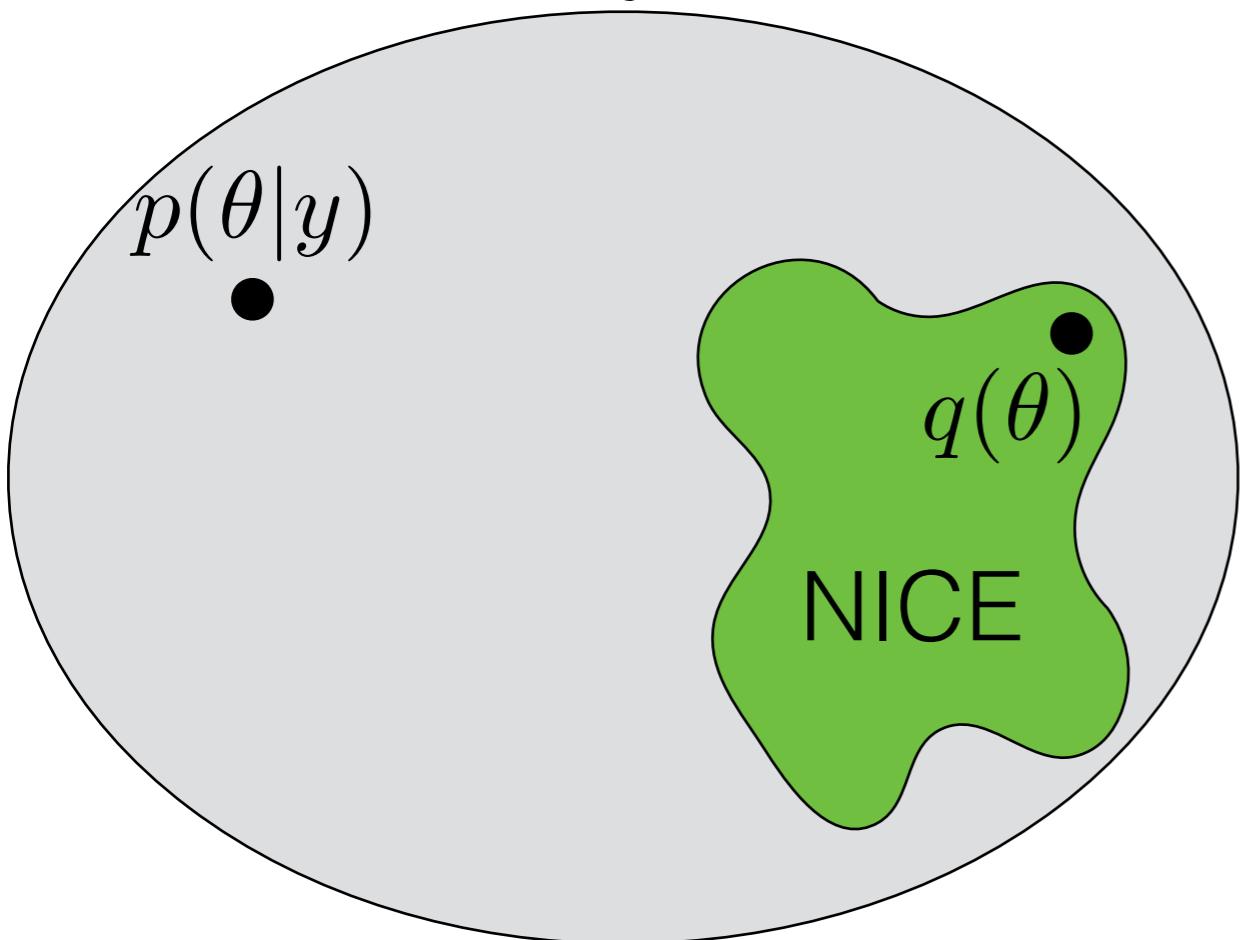
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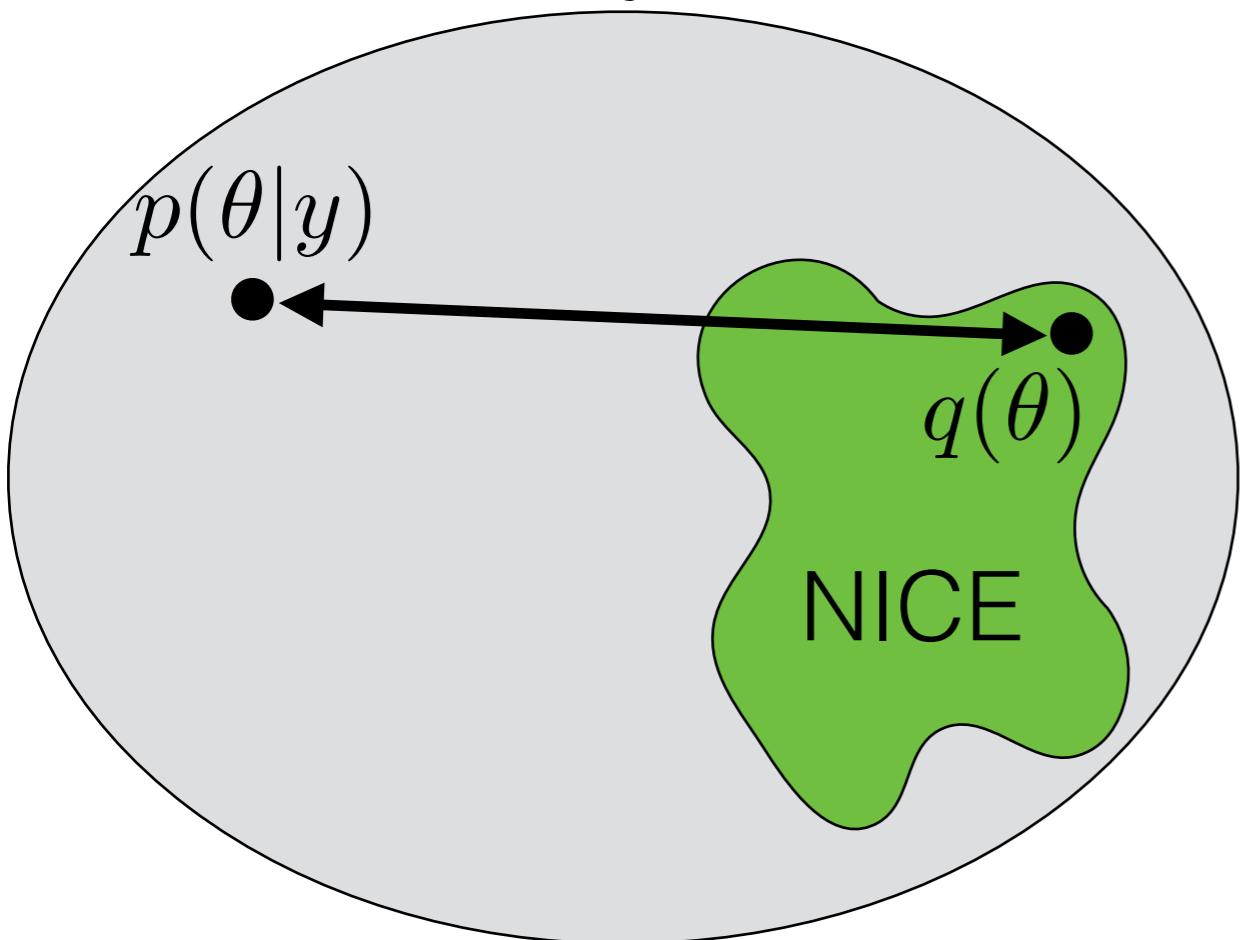
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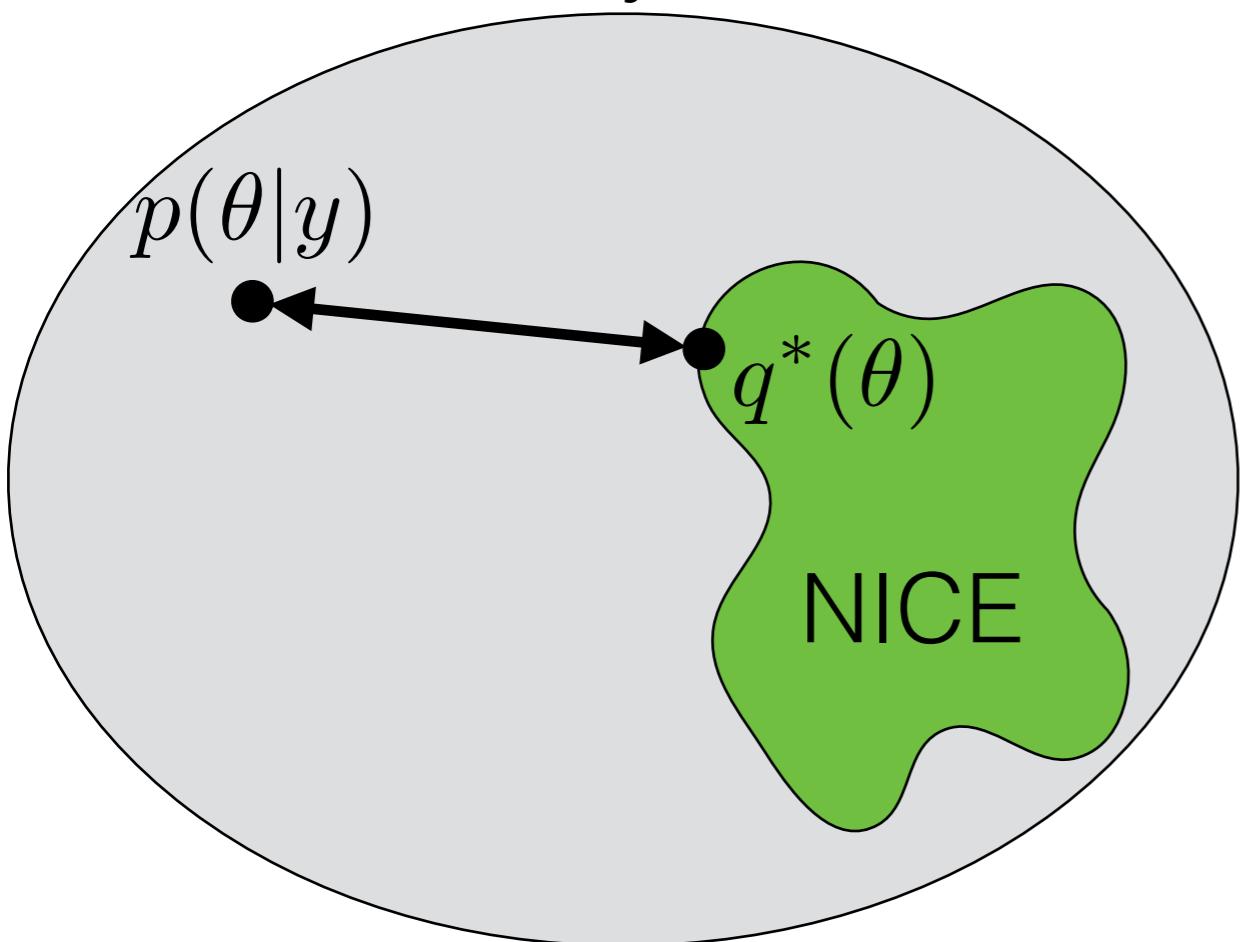
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Approximate Bayesian Inference

[Bardenet,
Doucet,
Holmes
2017]

- Gold standard: Markov Chain Monte Carlo (MCMC)
 - Eventually accurate but can be slow

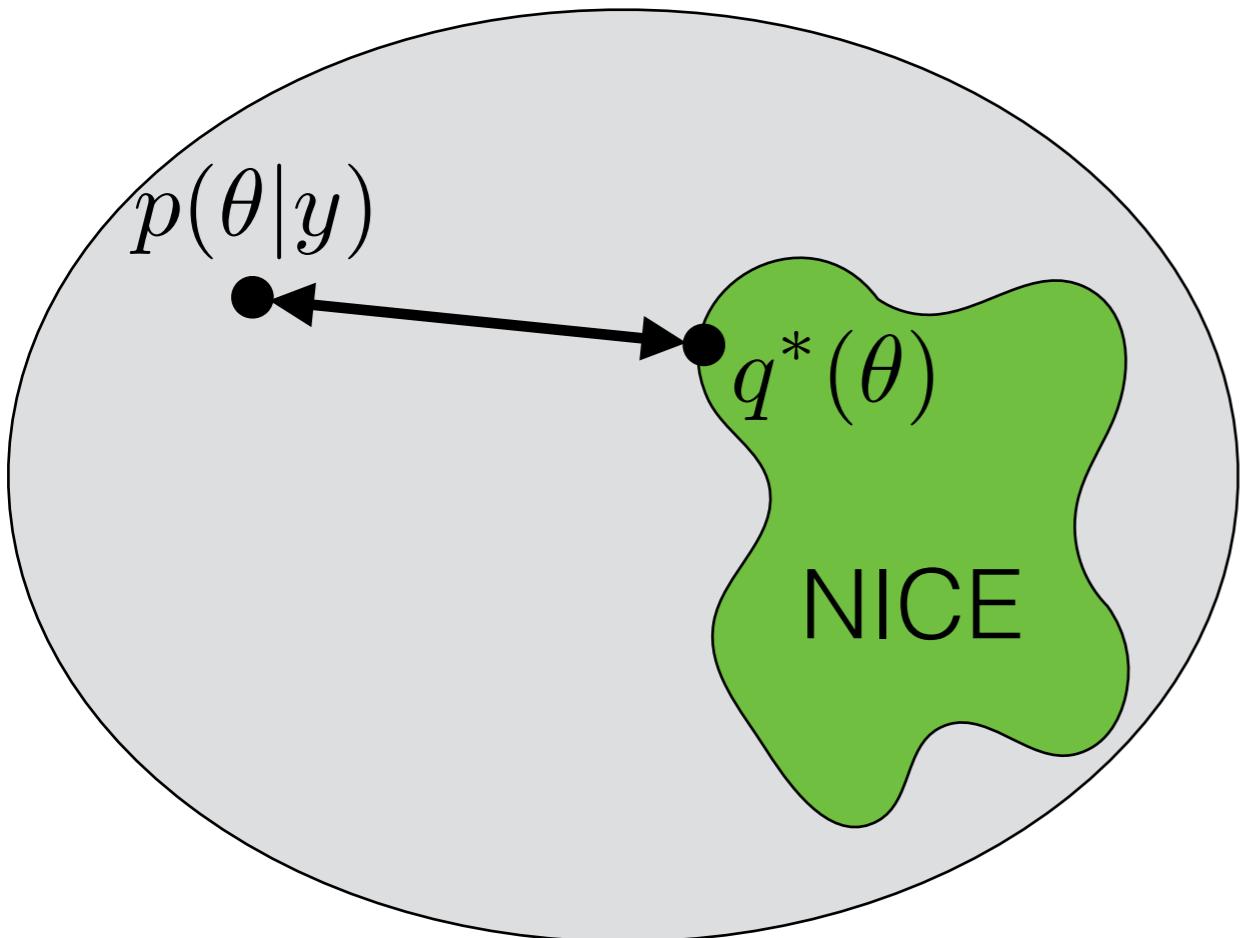


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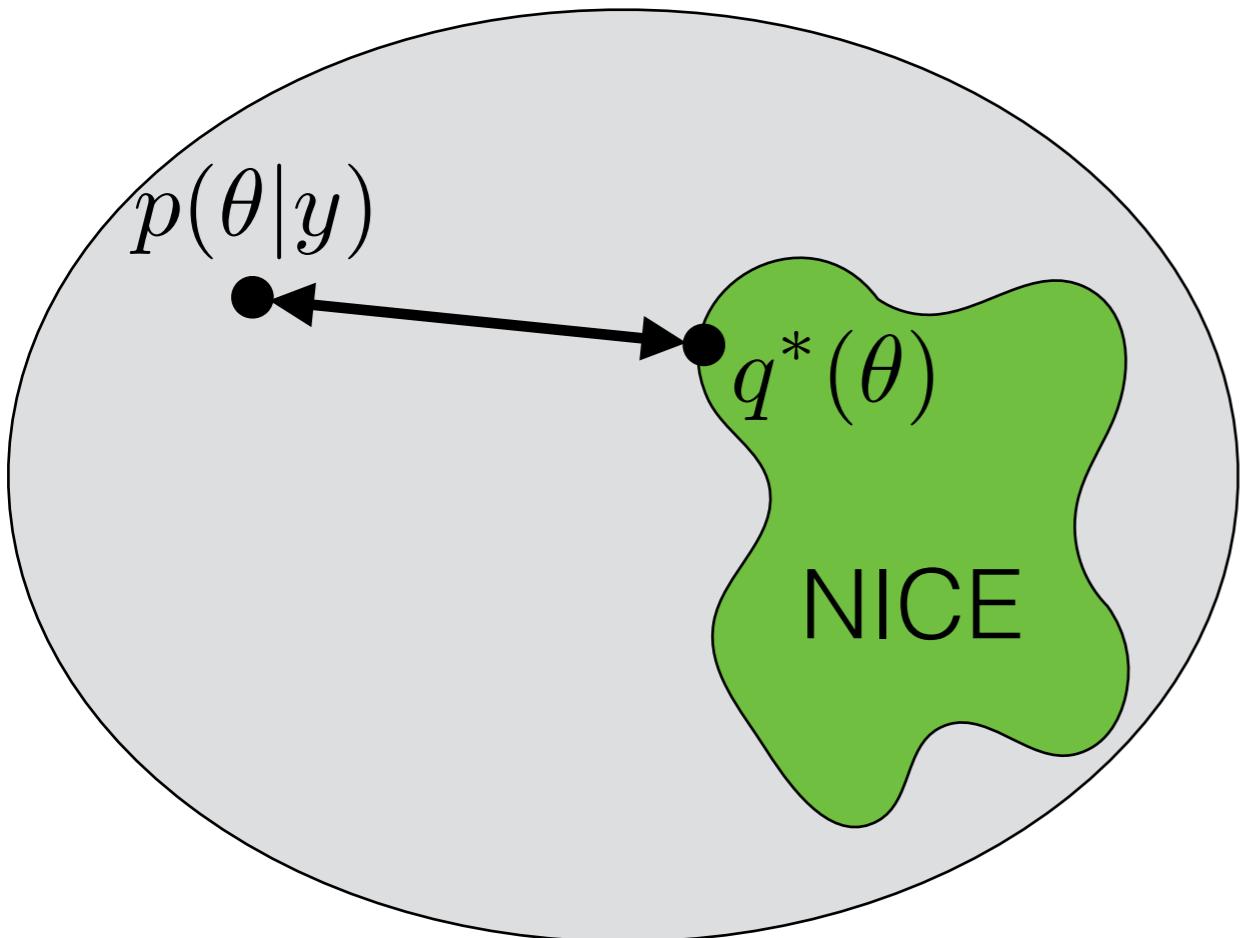
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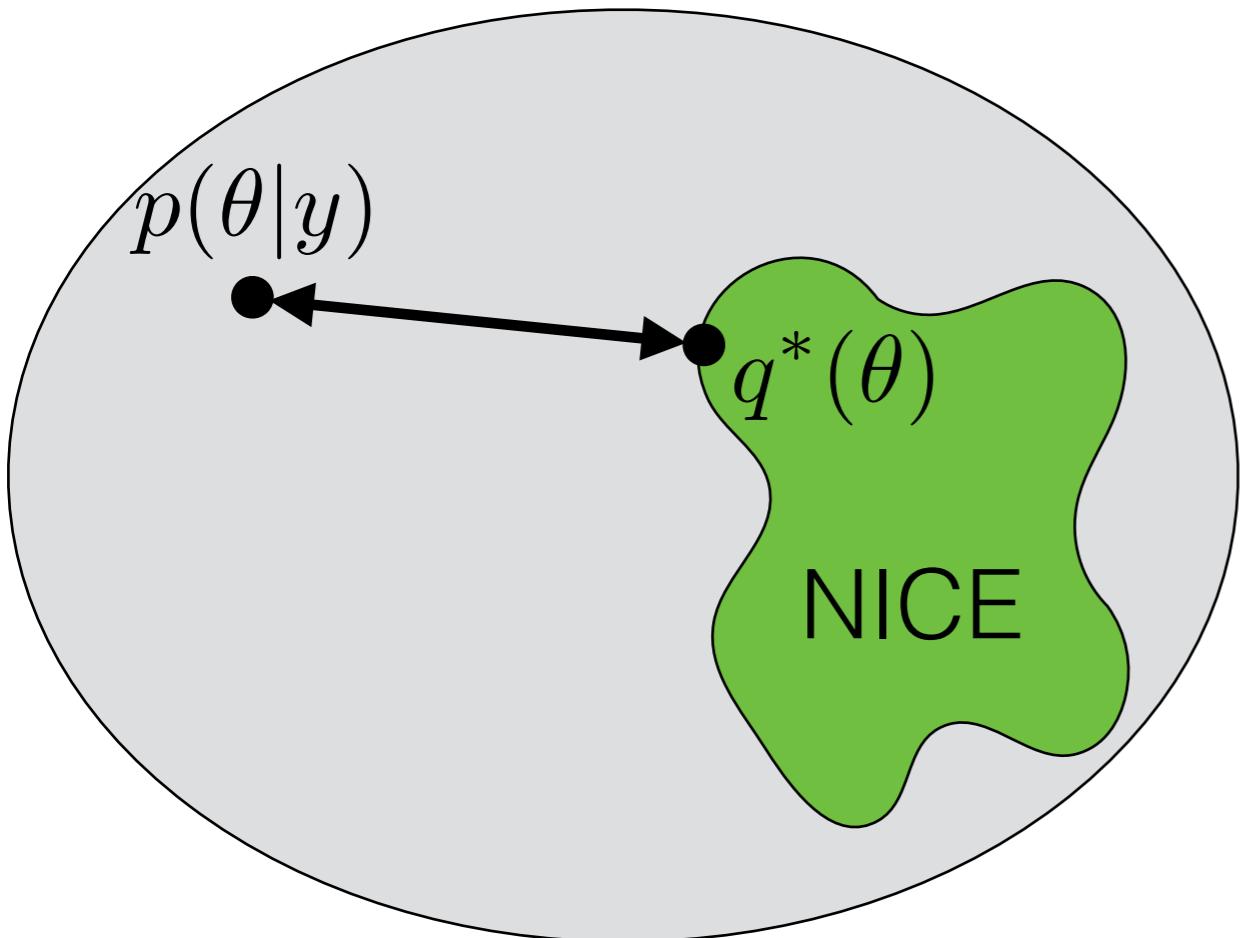
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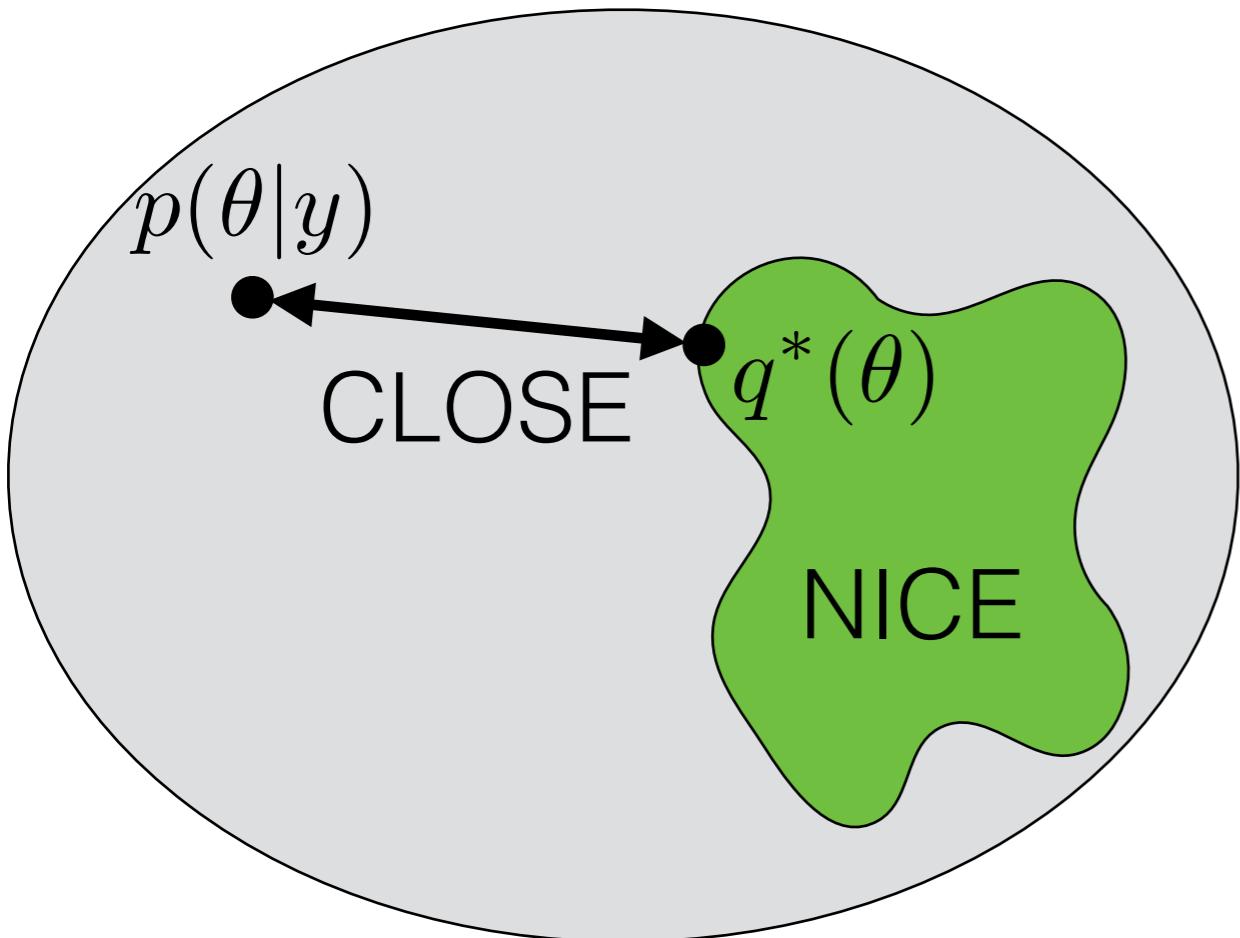
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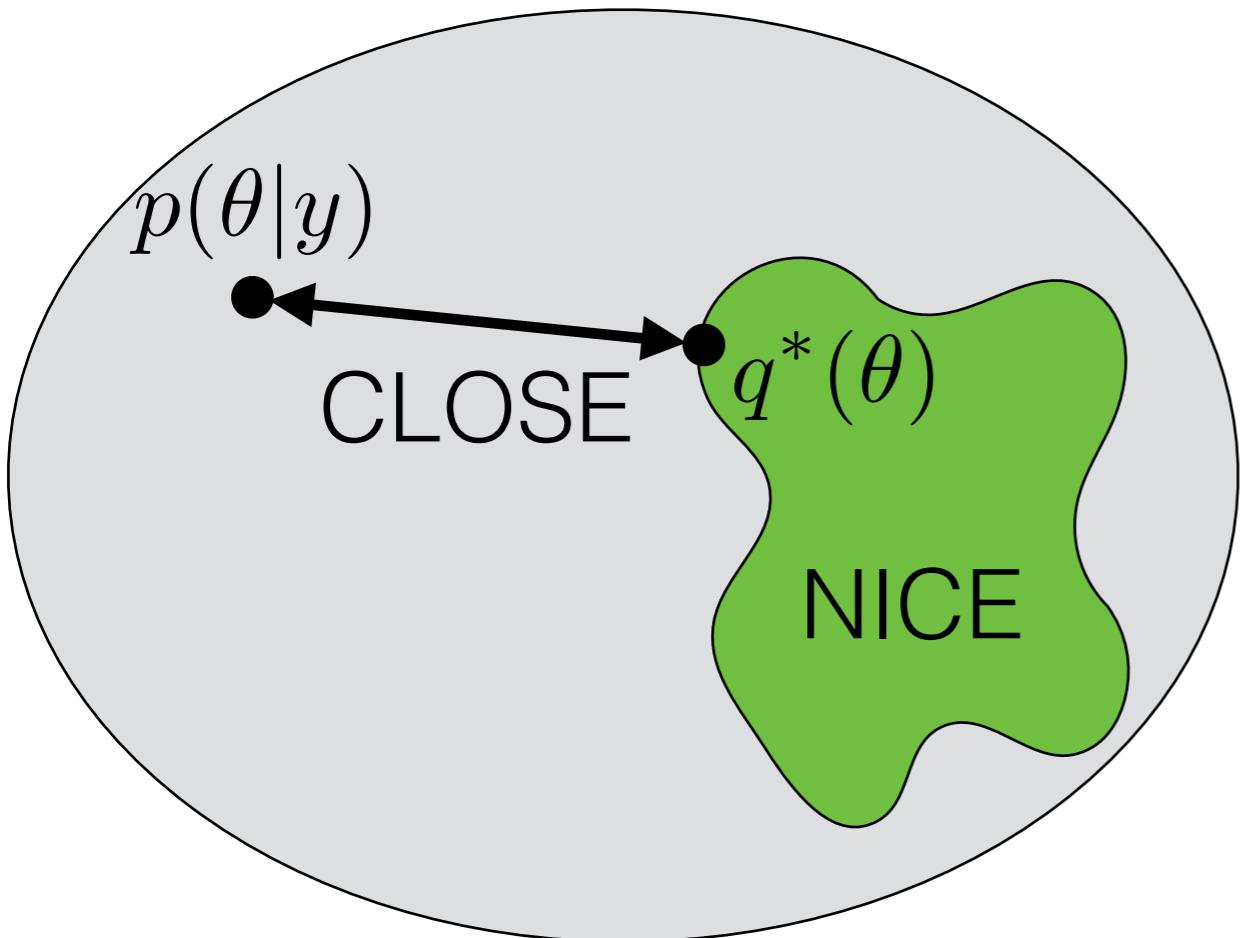
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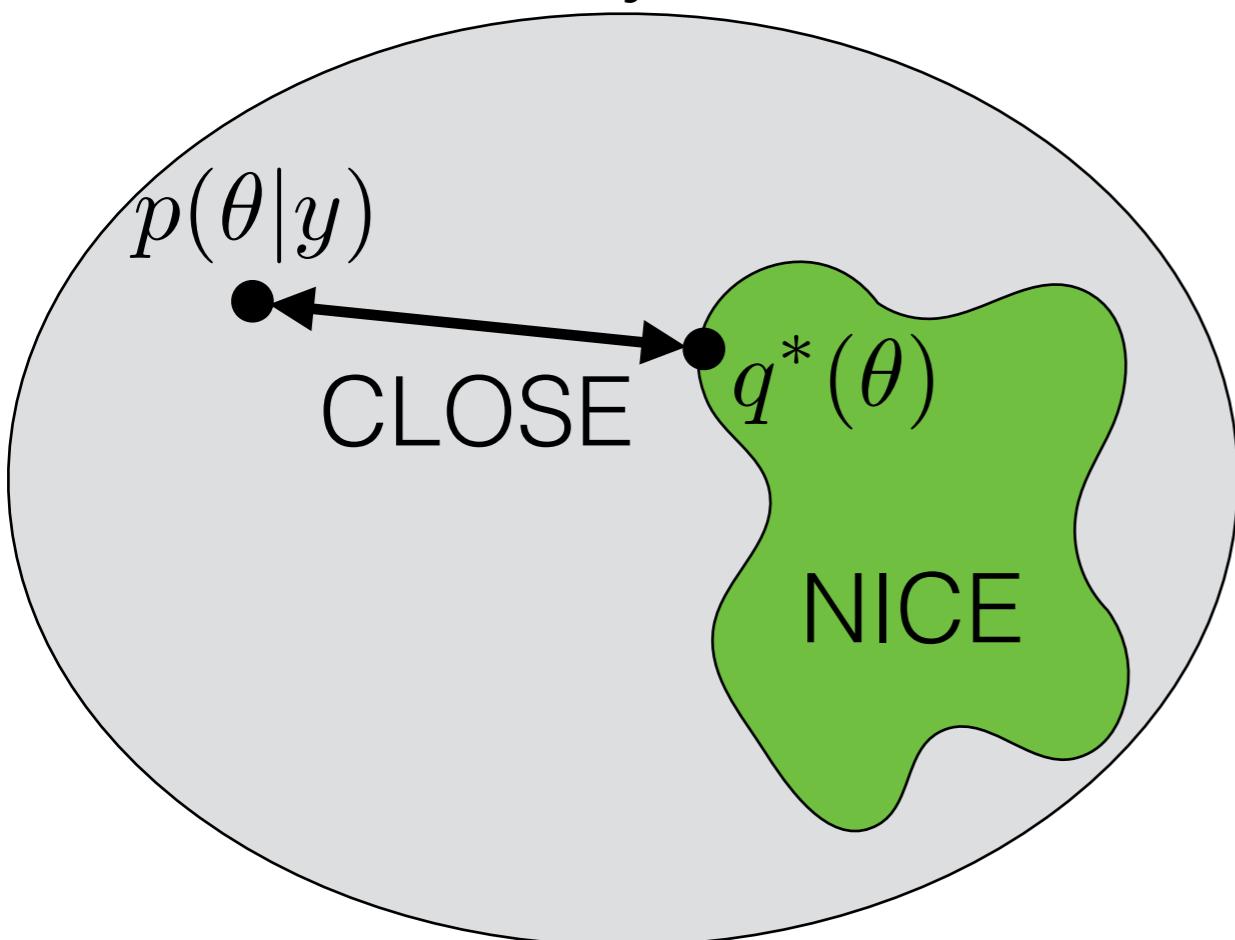
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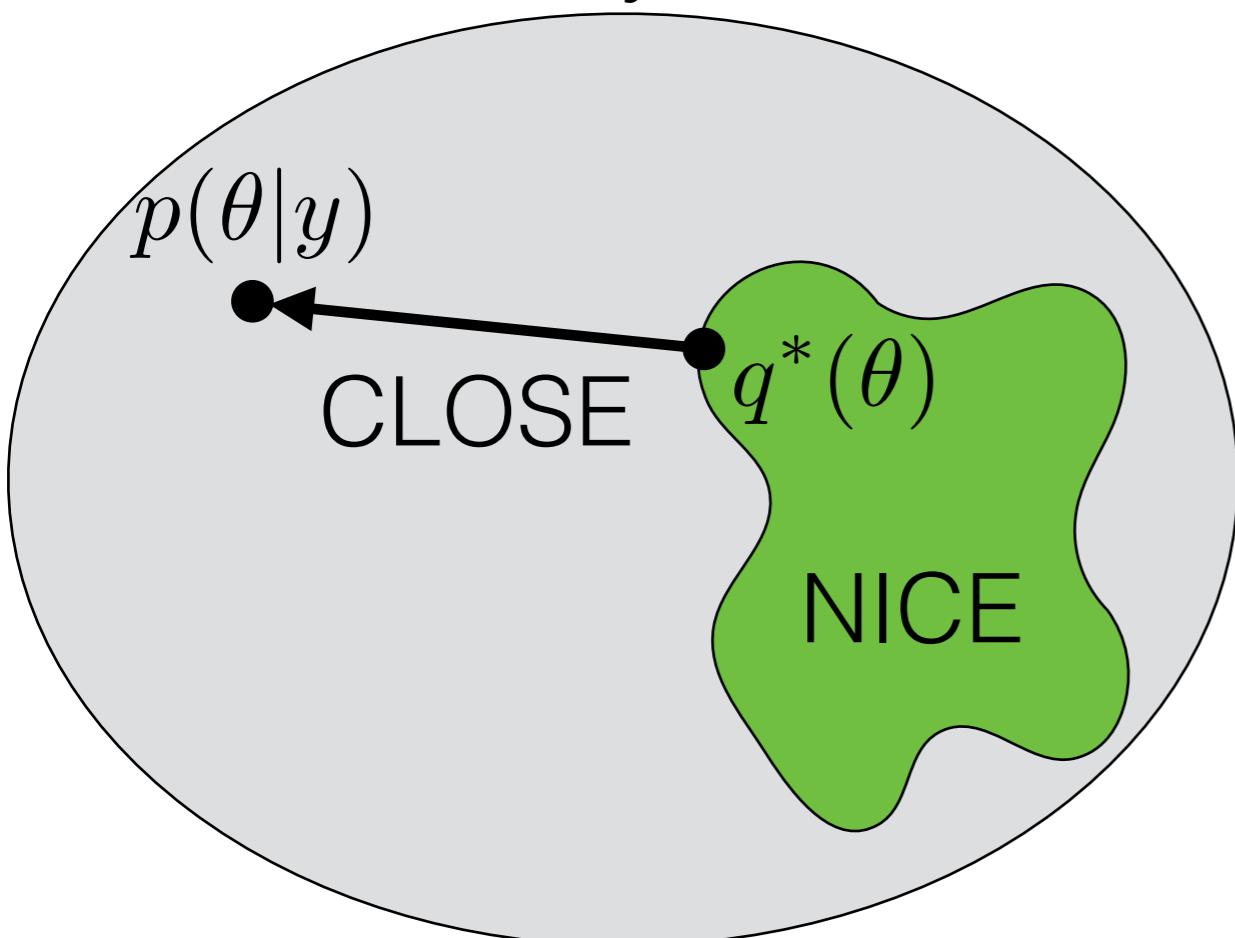
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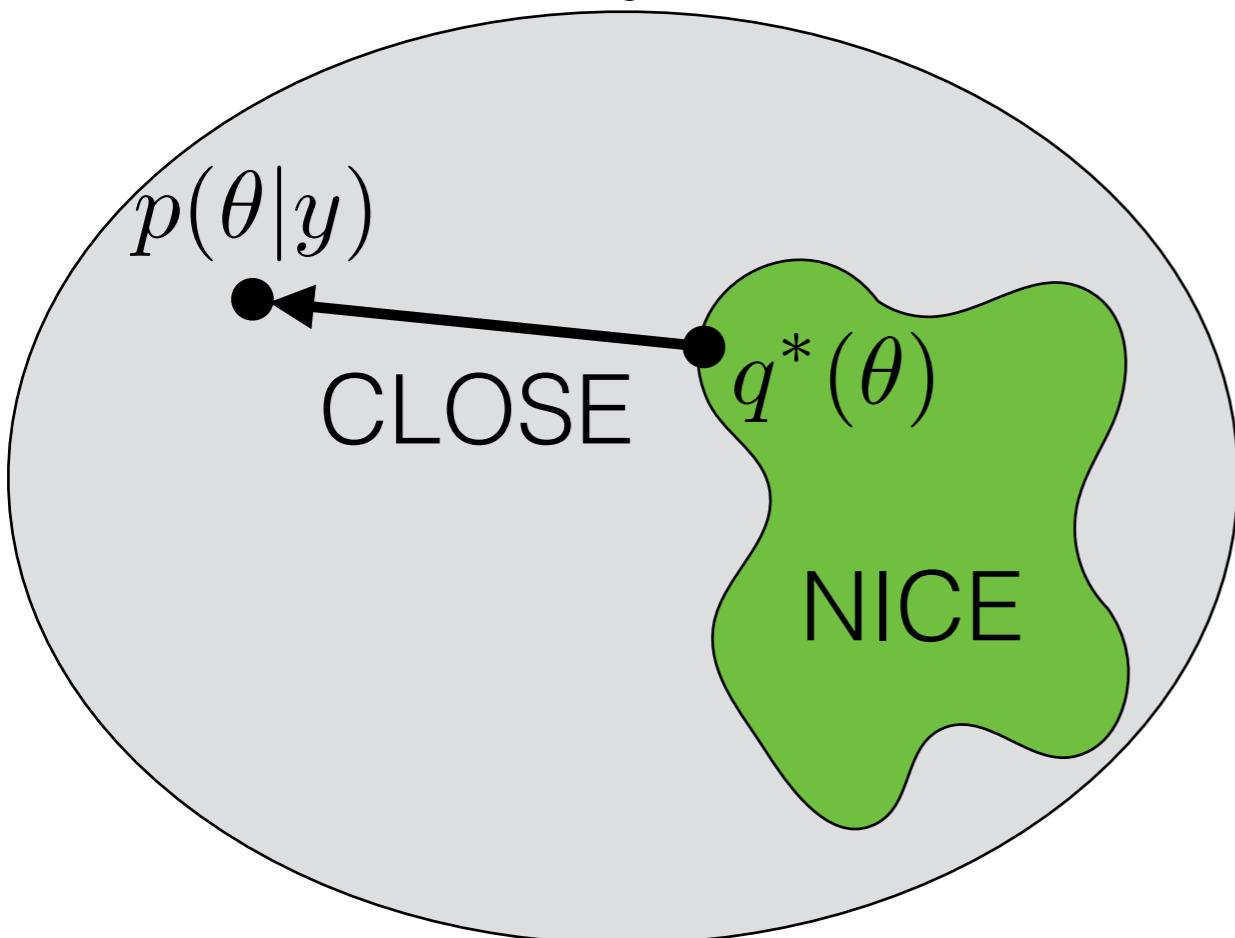
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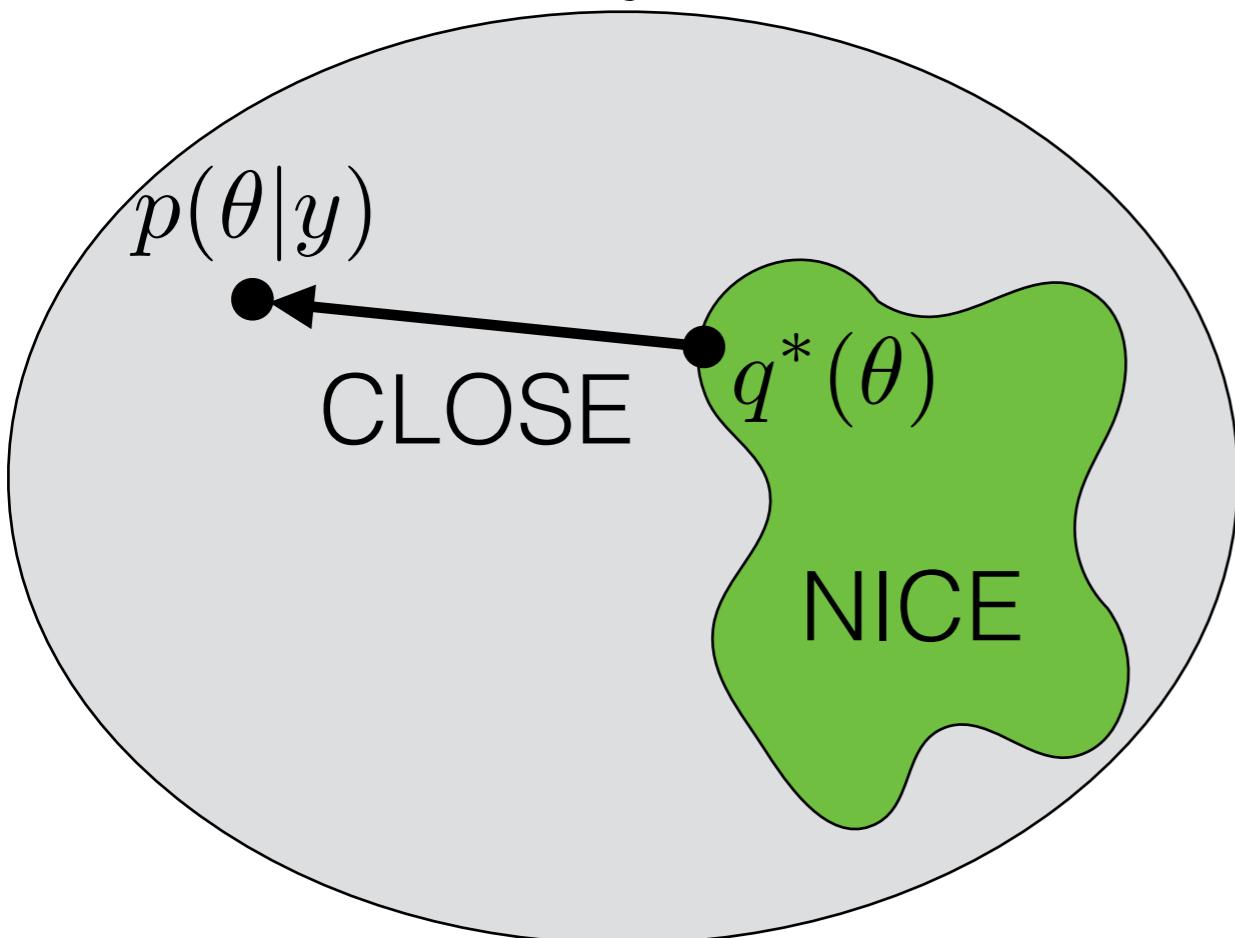
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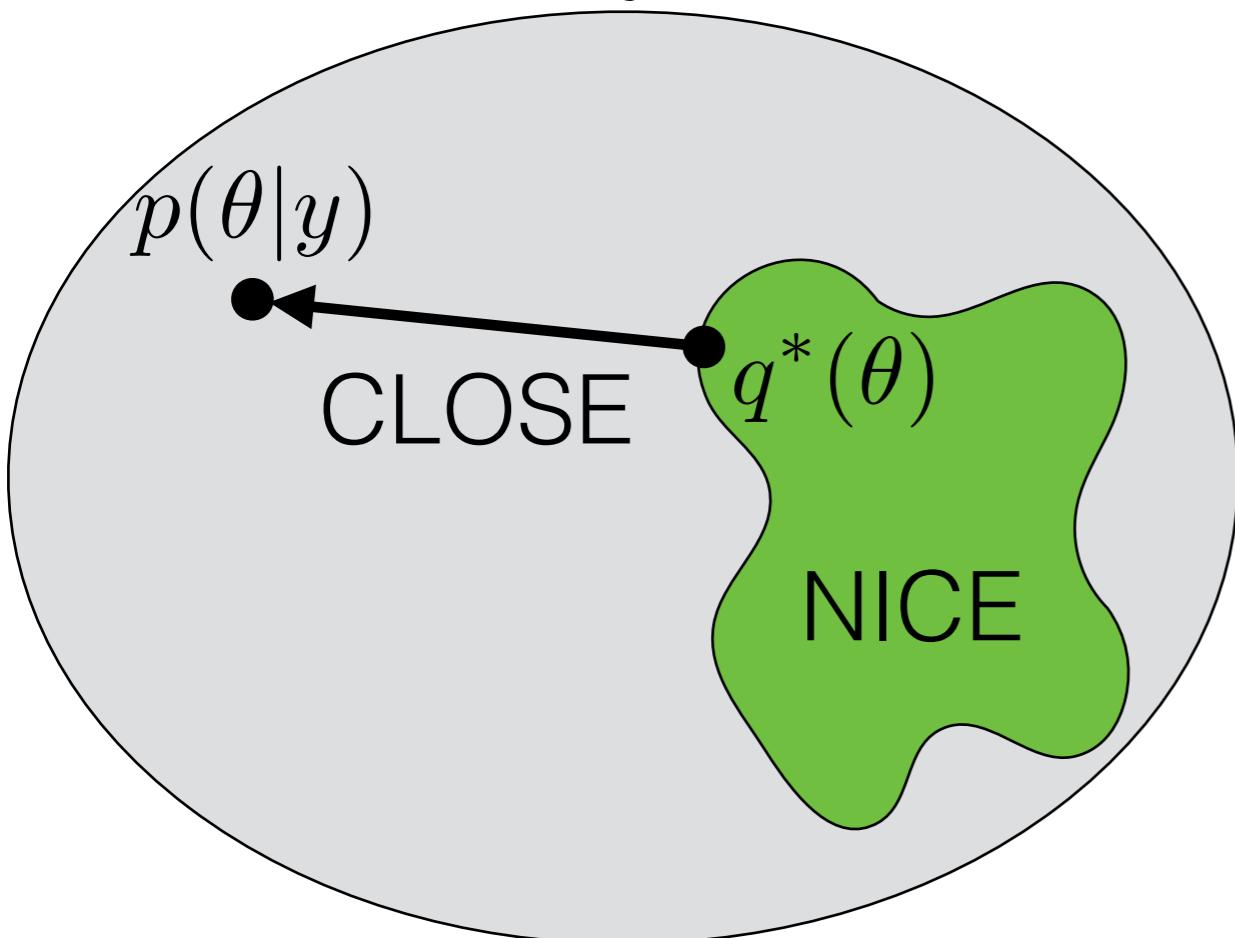
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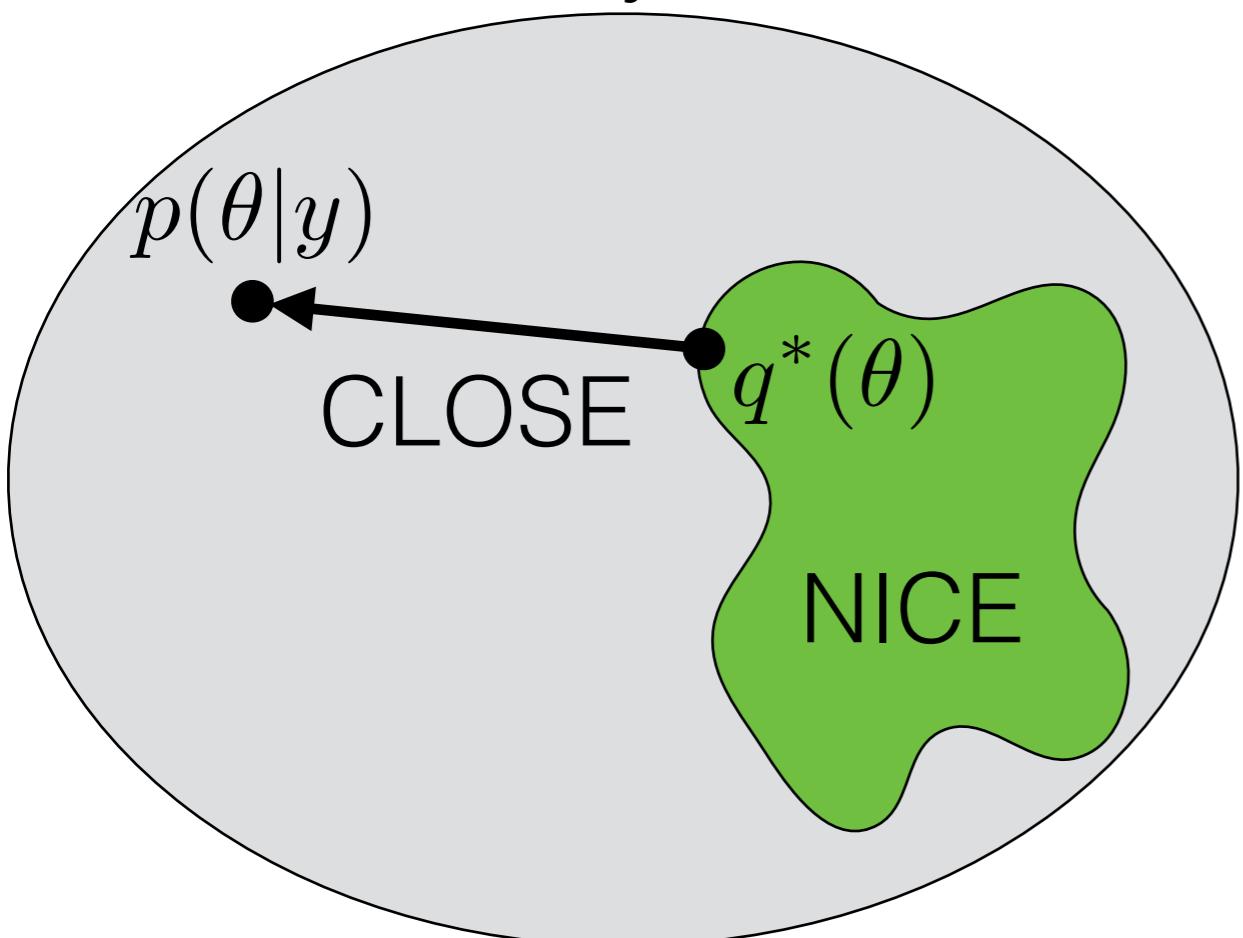
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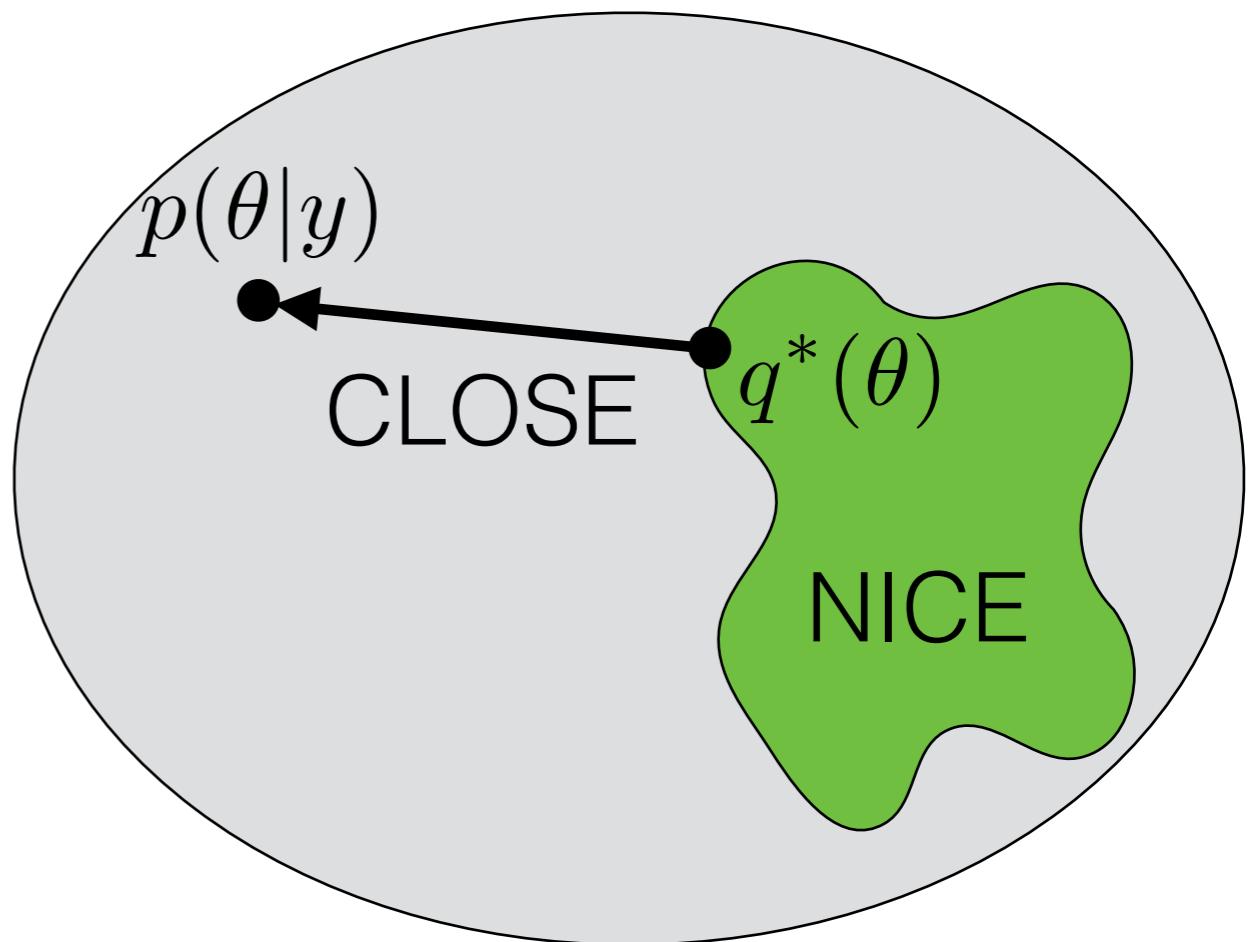
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$$KL(q(\cdot)||p(\cdot|y))$$
- VB practical success: point estimates and prediction, fast, streaming, distributed (3.6M Wikipedia, 350K Nature)

Why KL?

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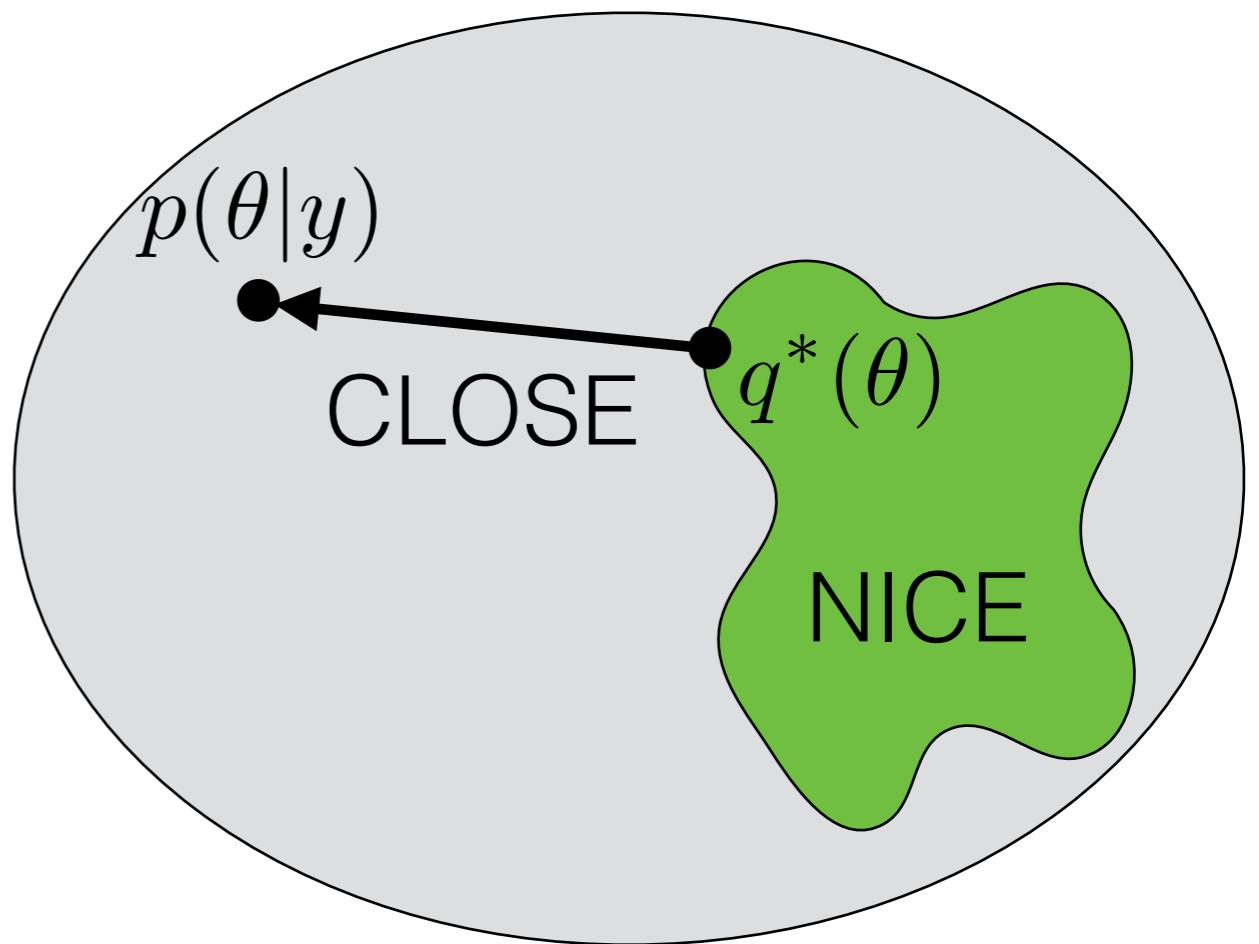
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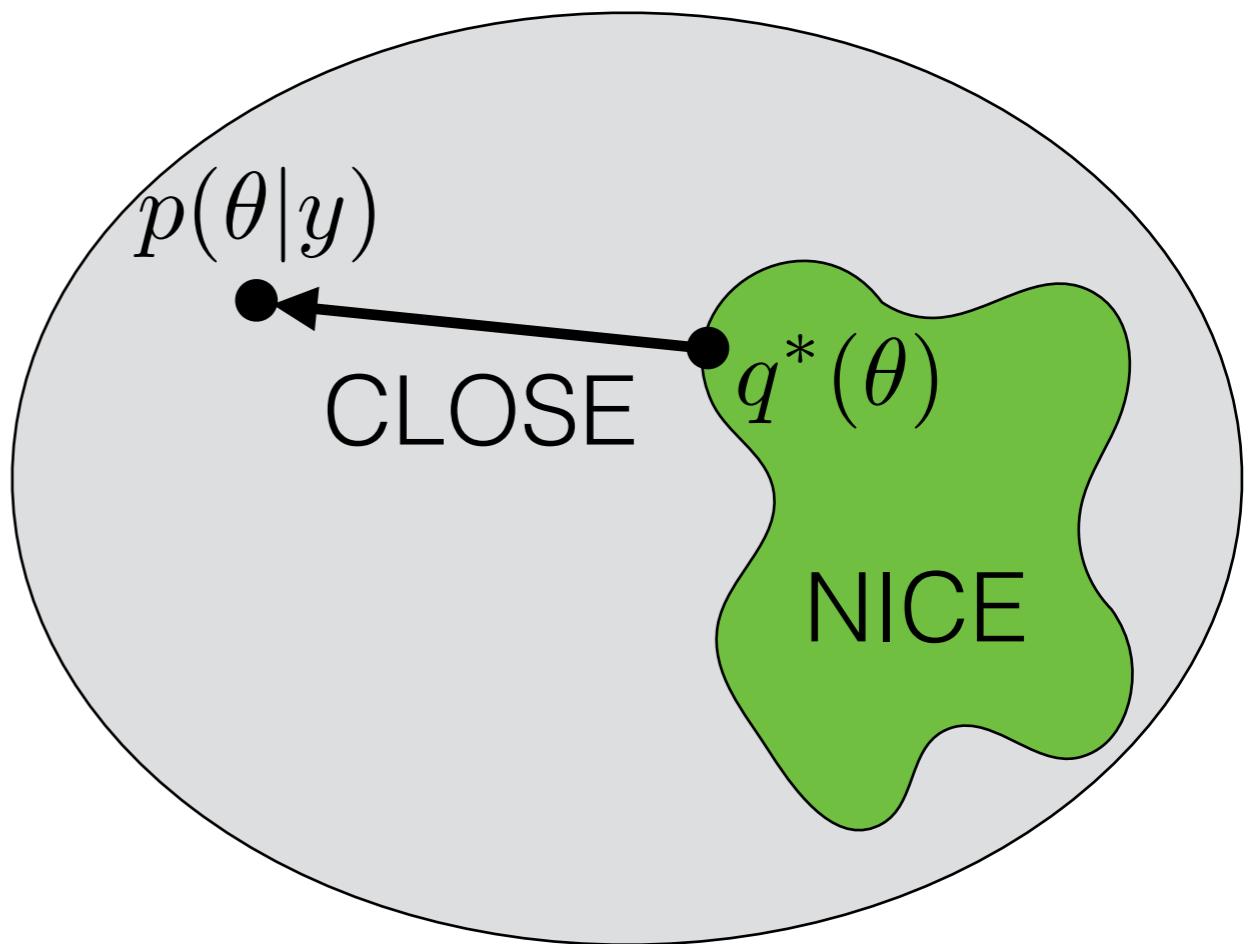
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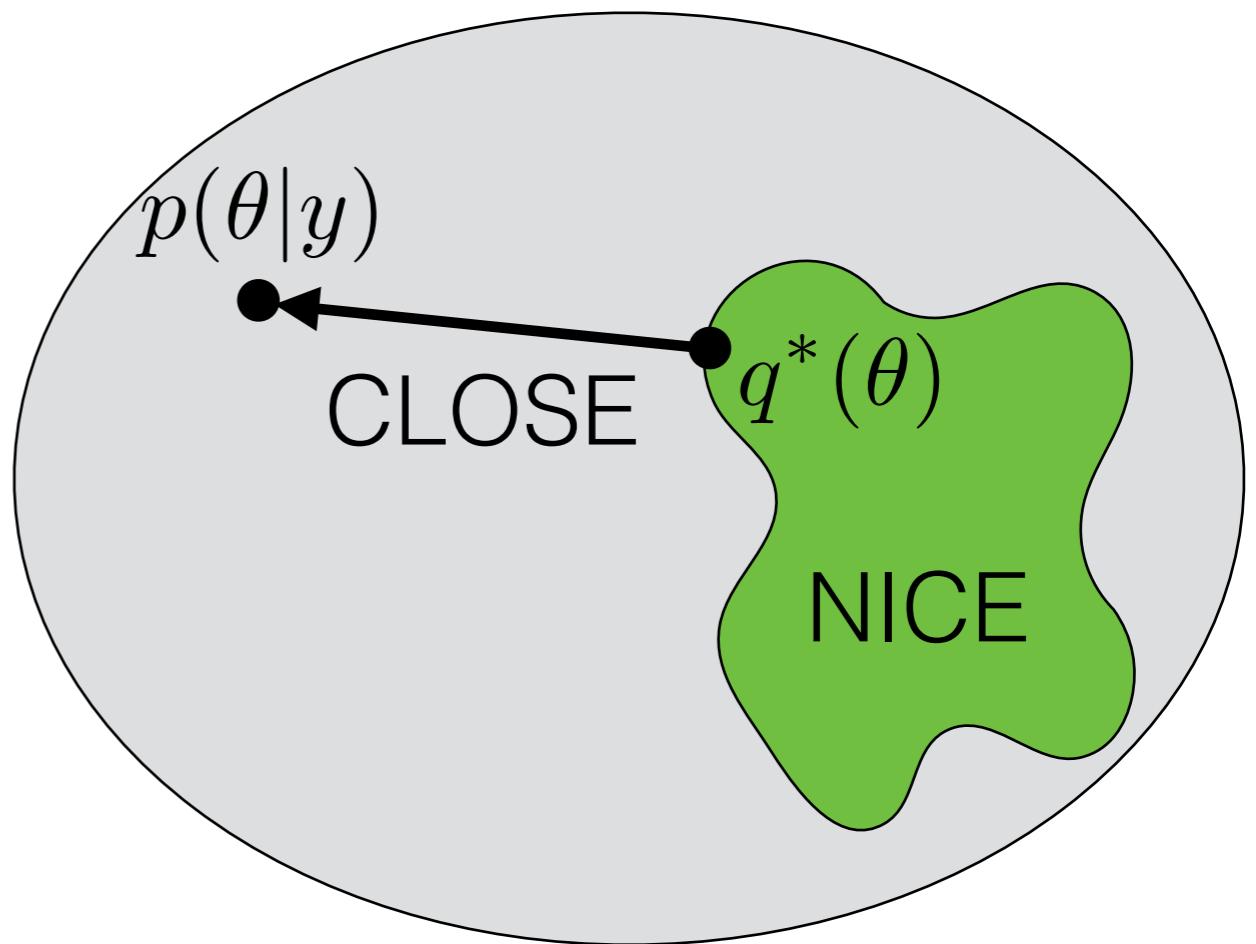
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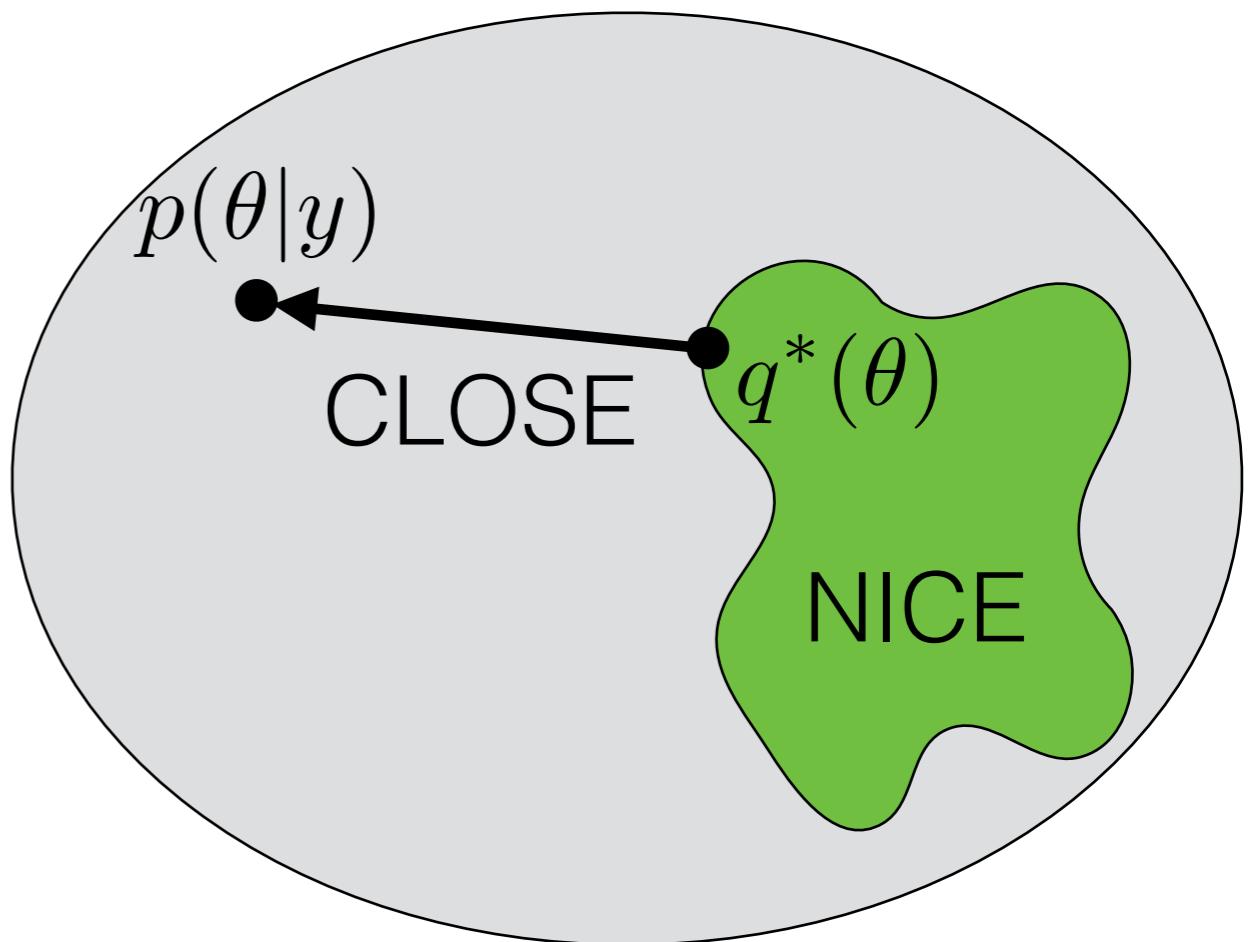
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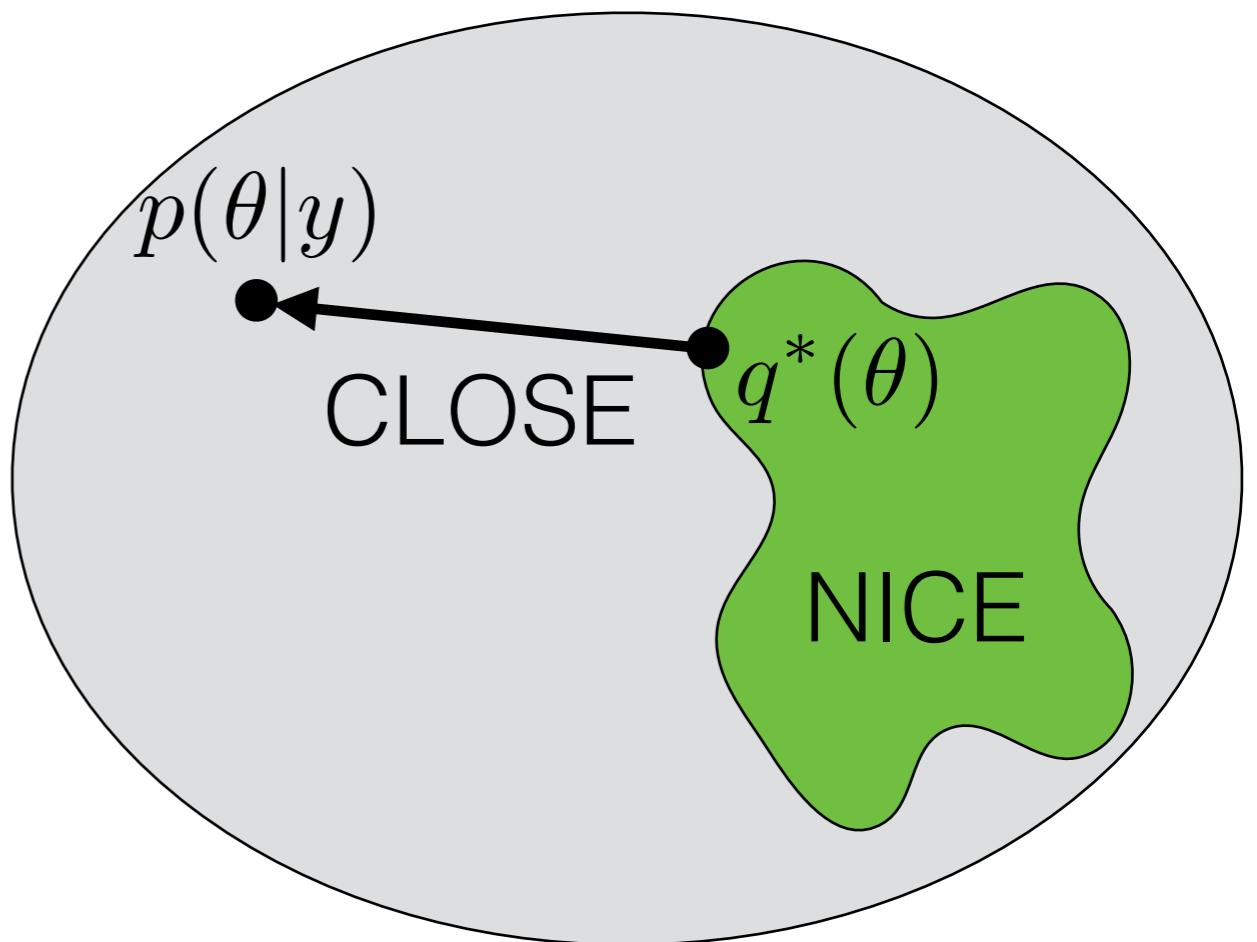
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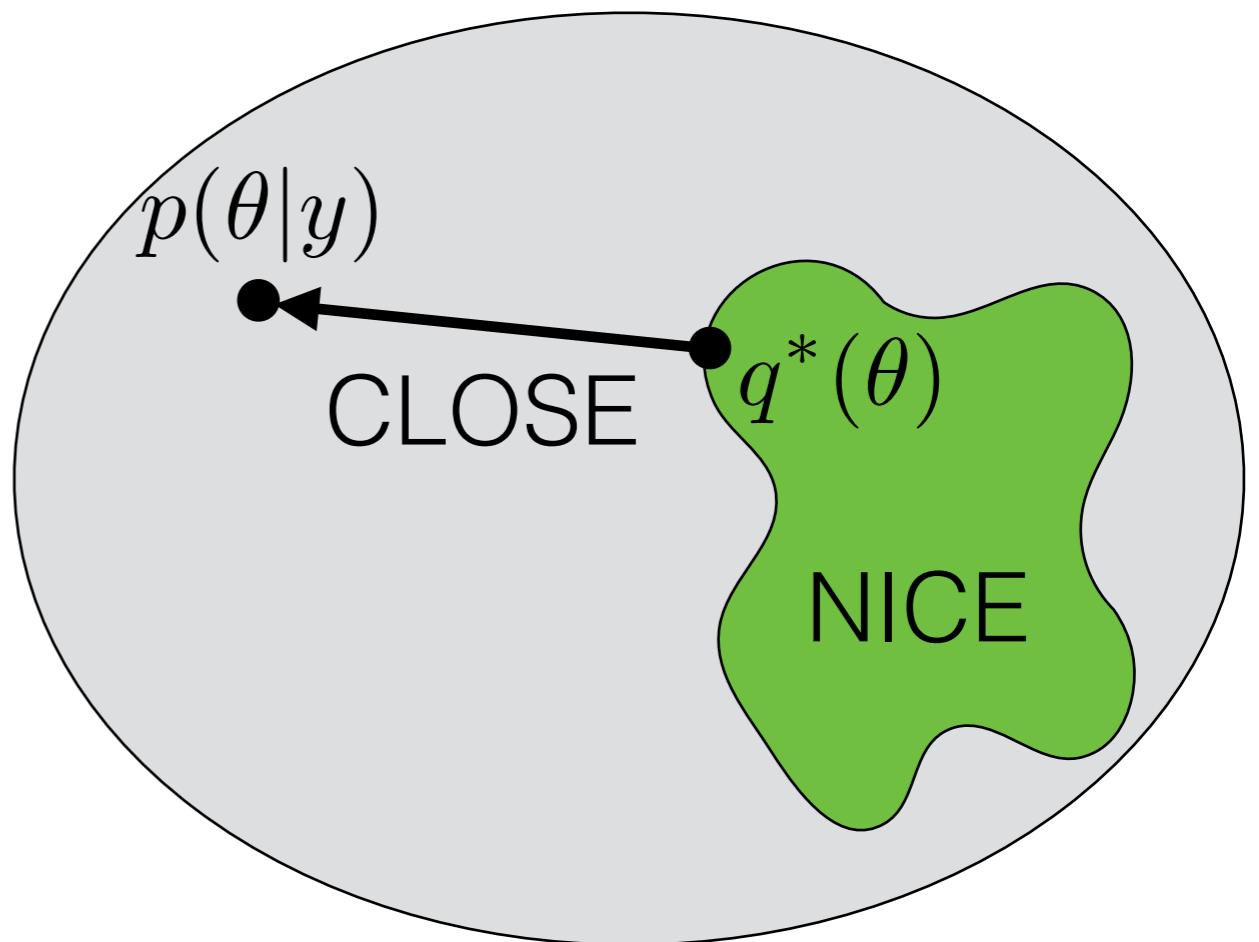
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“Evidence lower bound” (ELBO)

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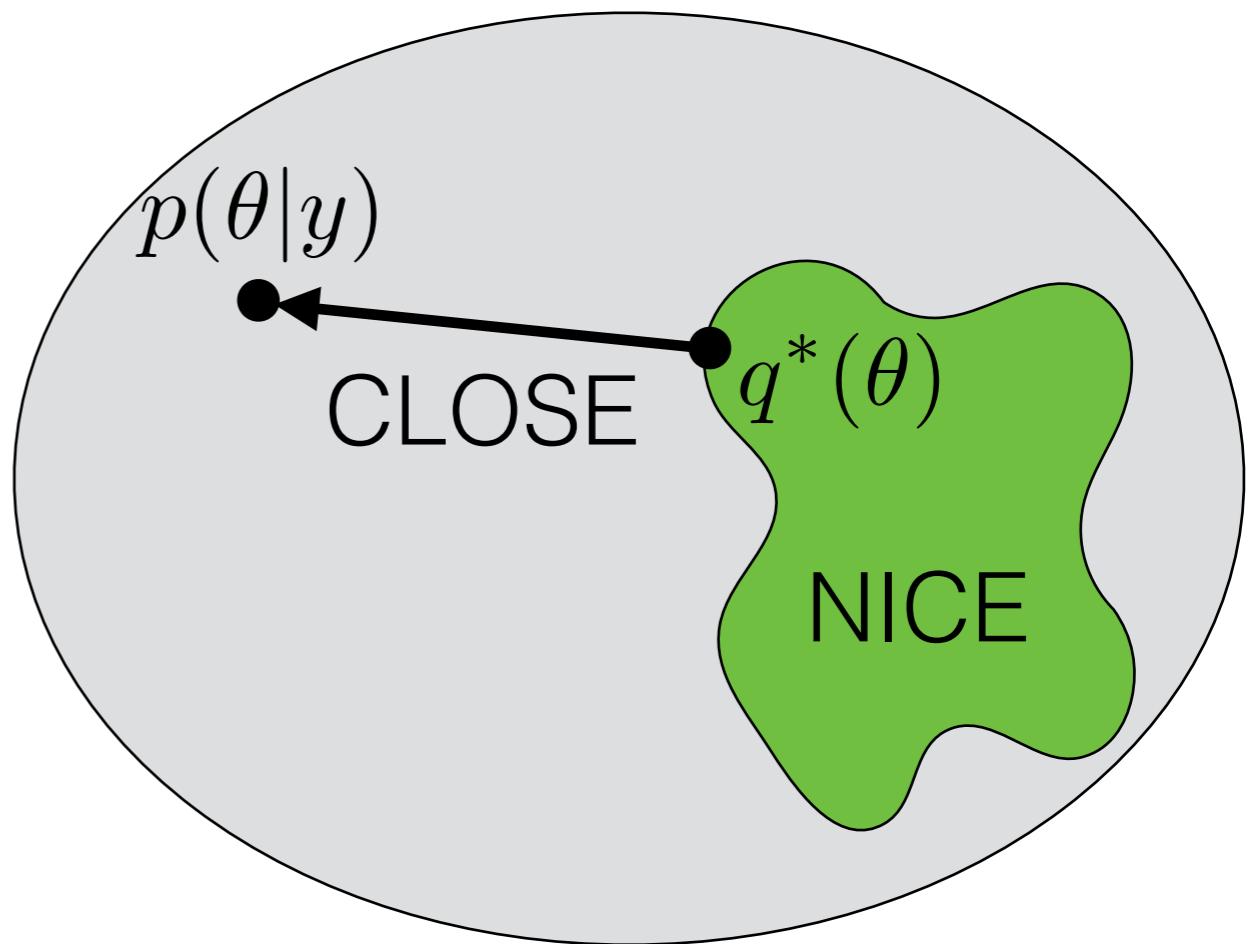
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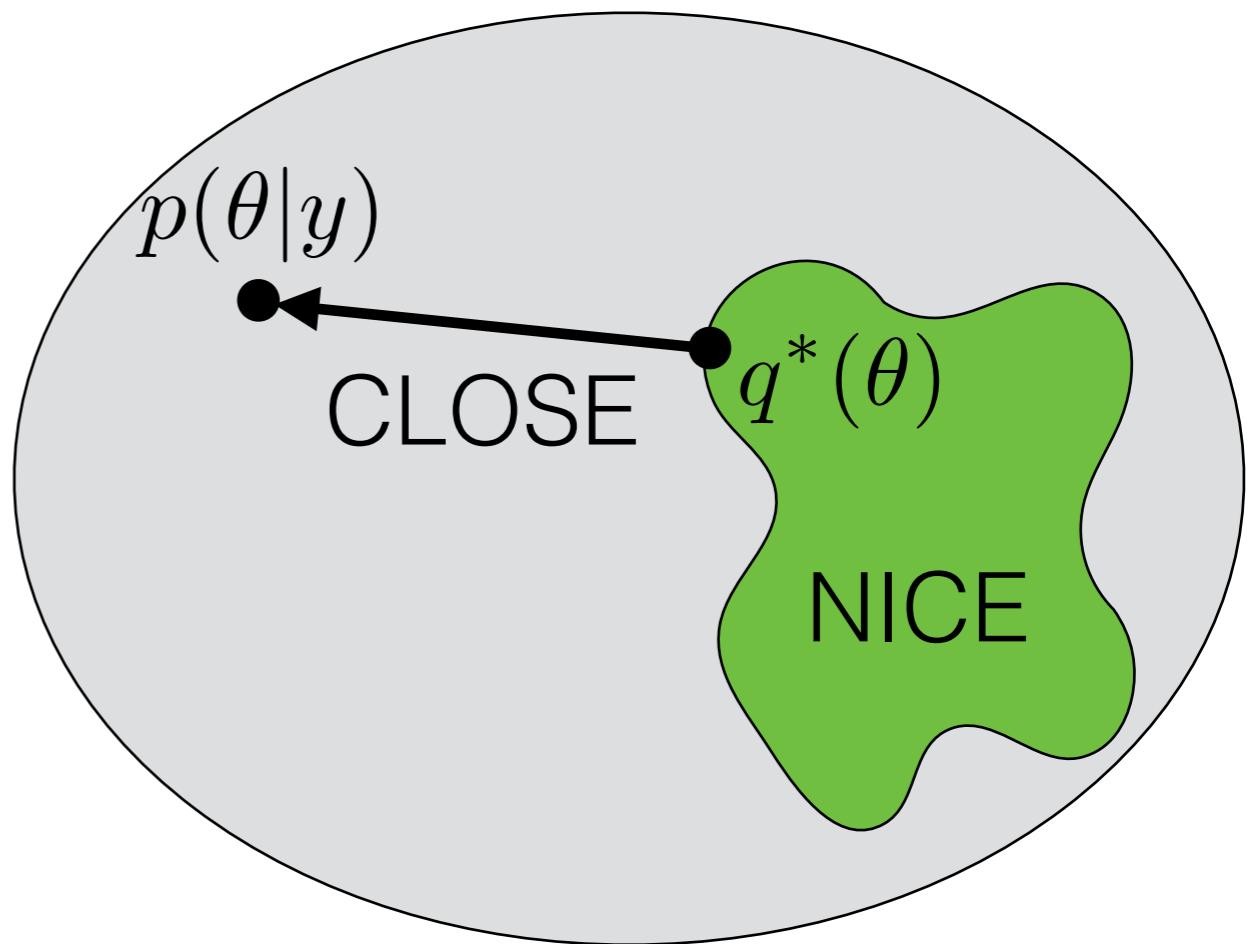
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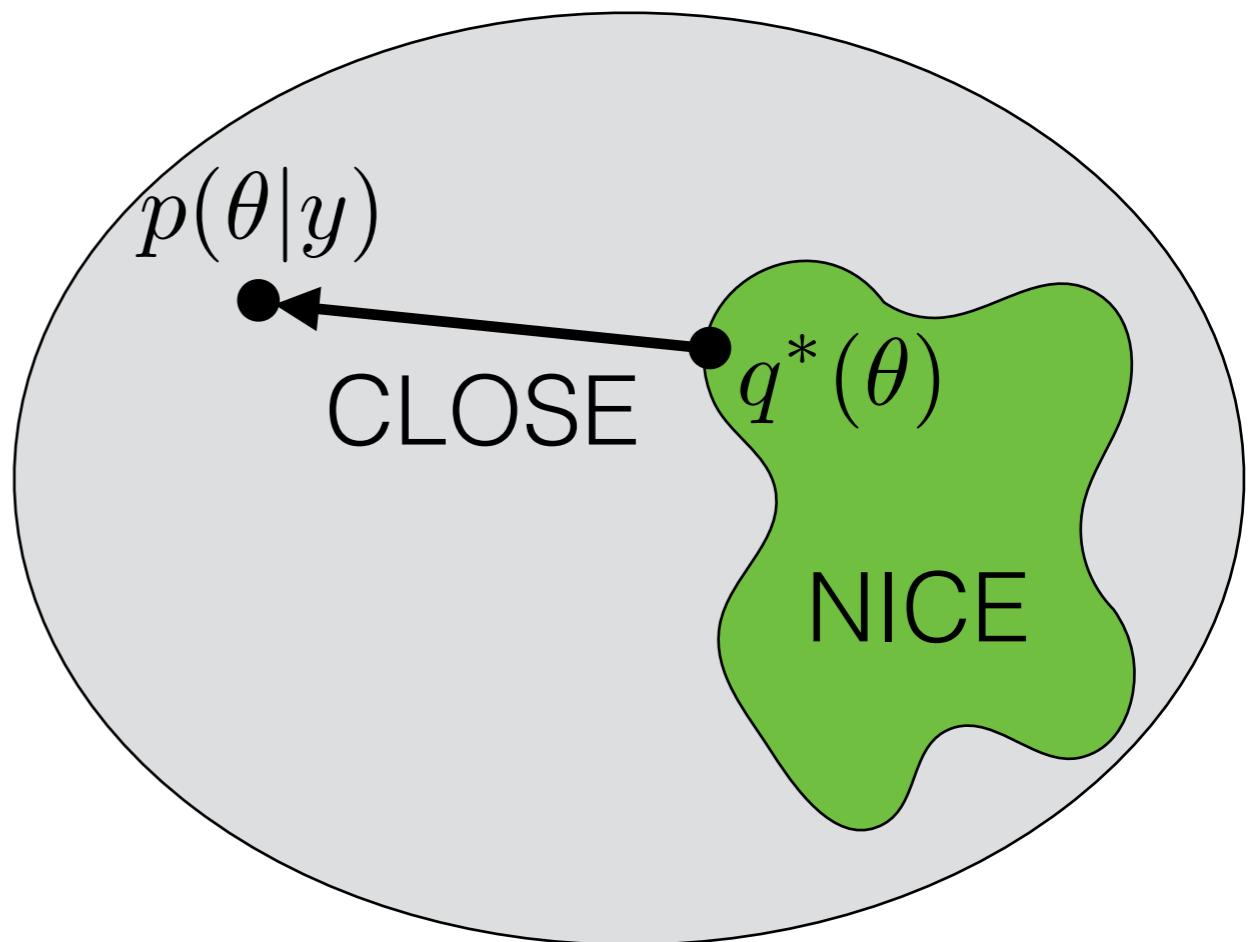
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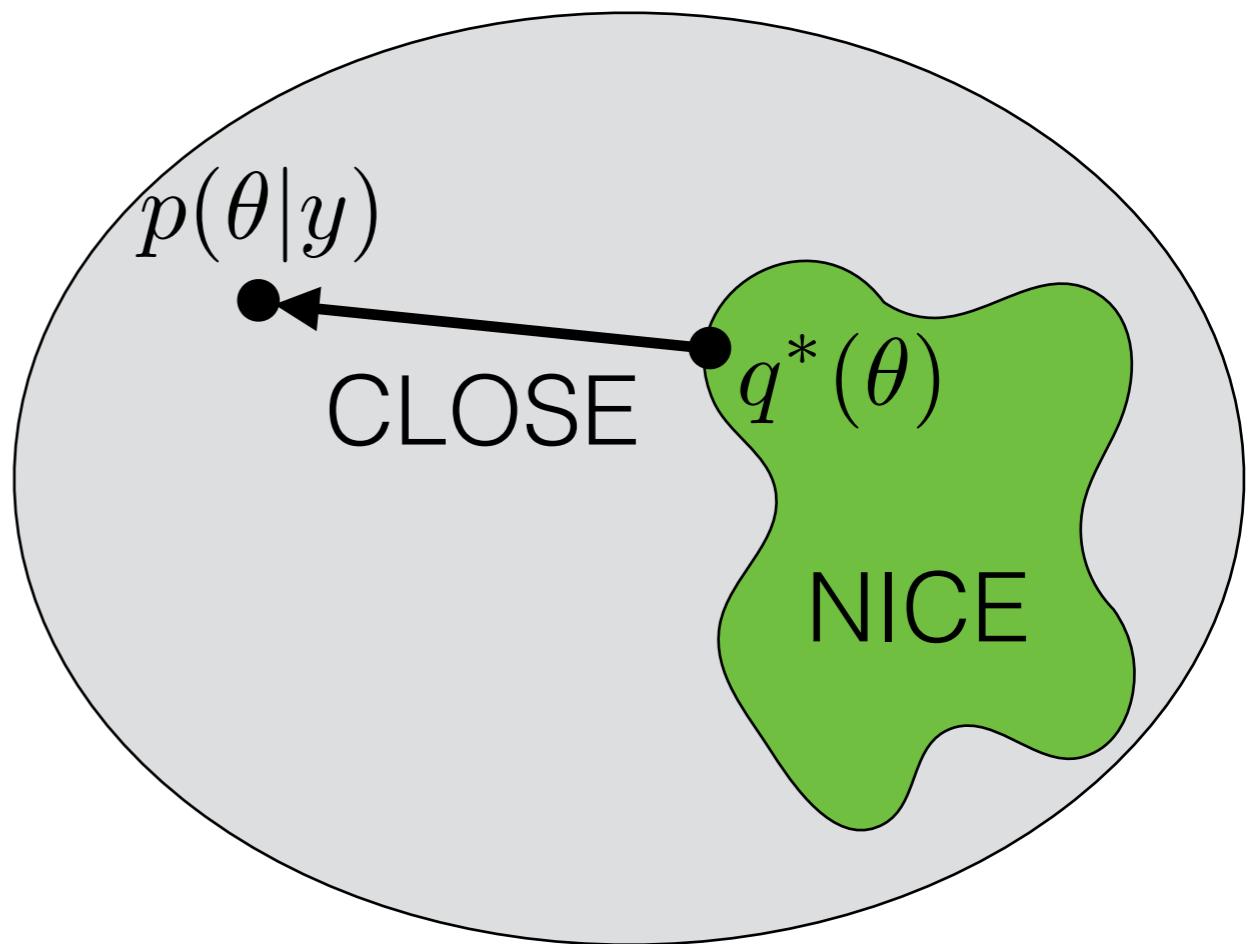
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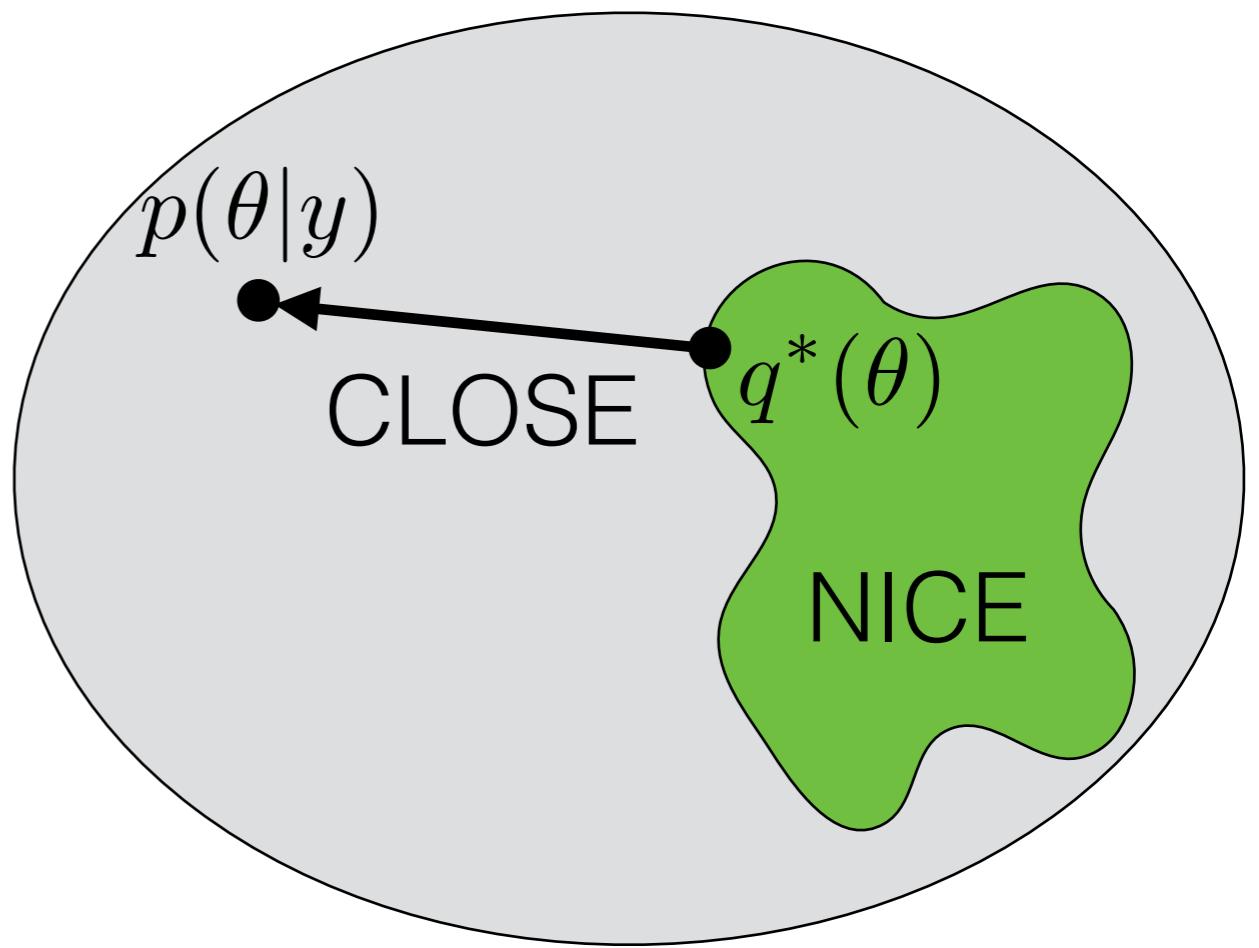
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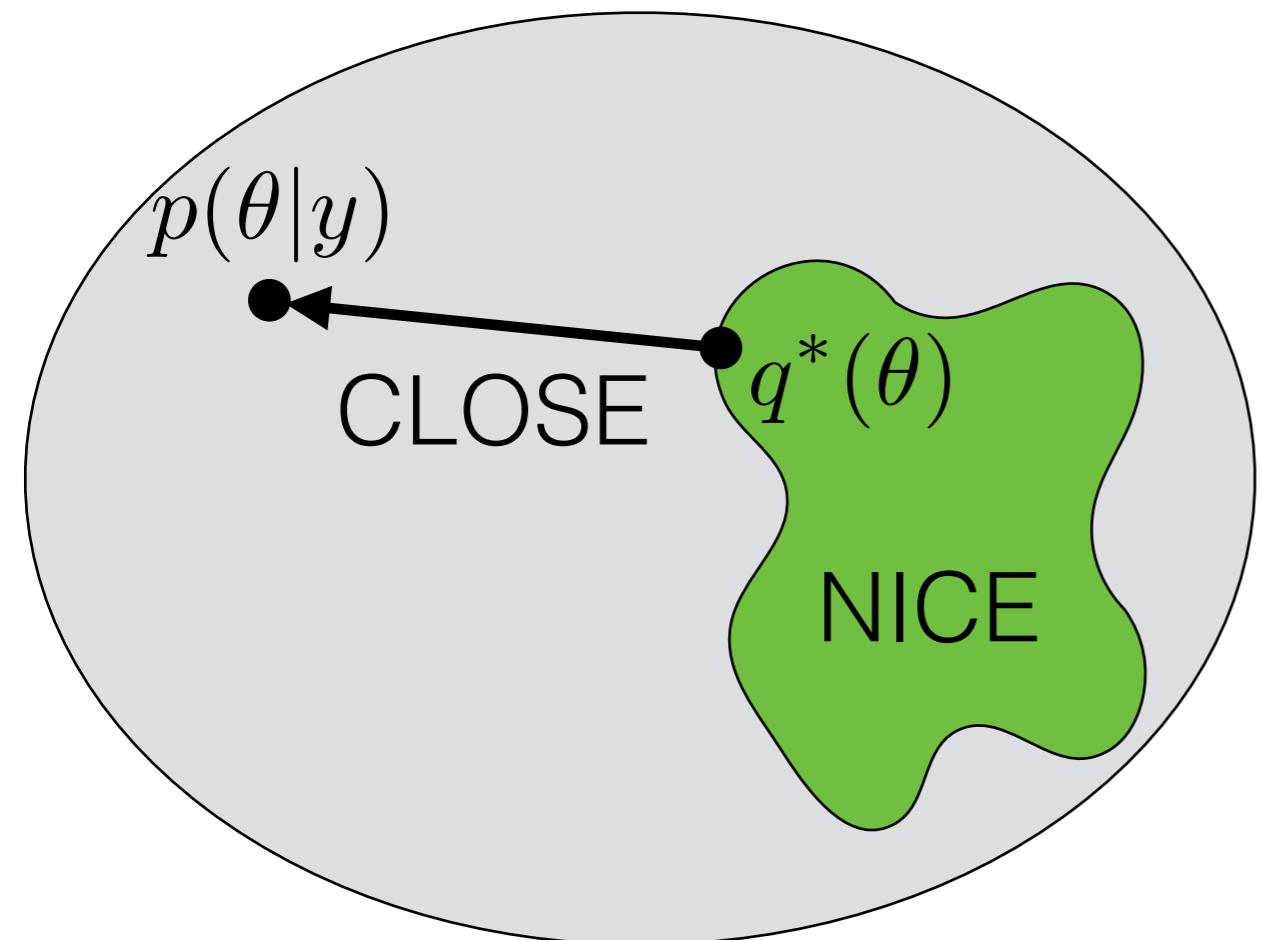
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- Why KL (in this direction)?

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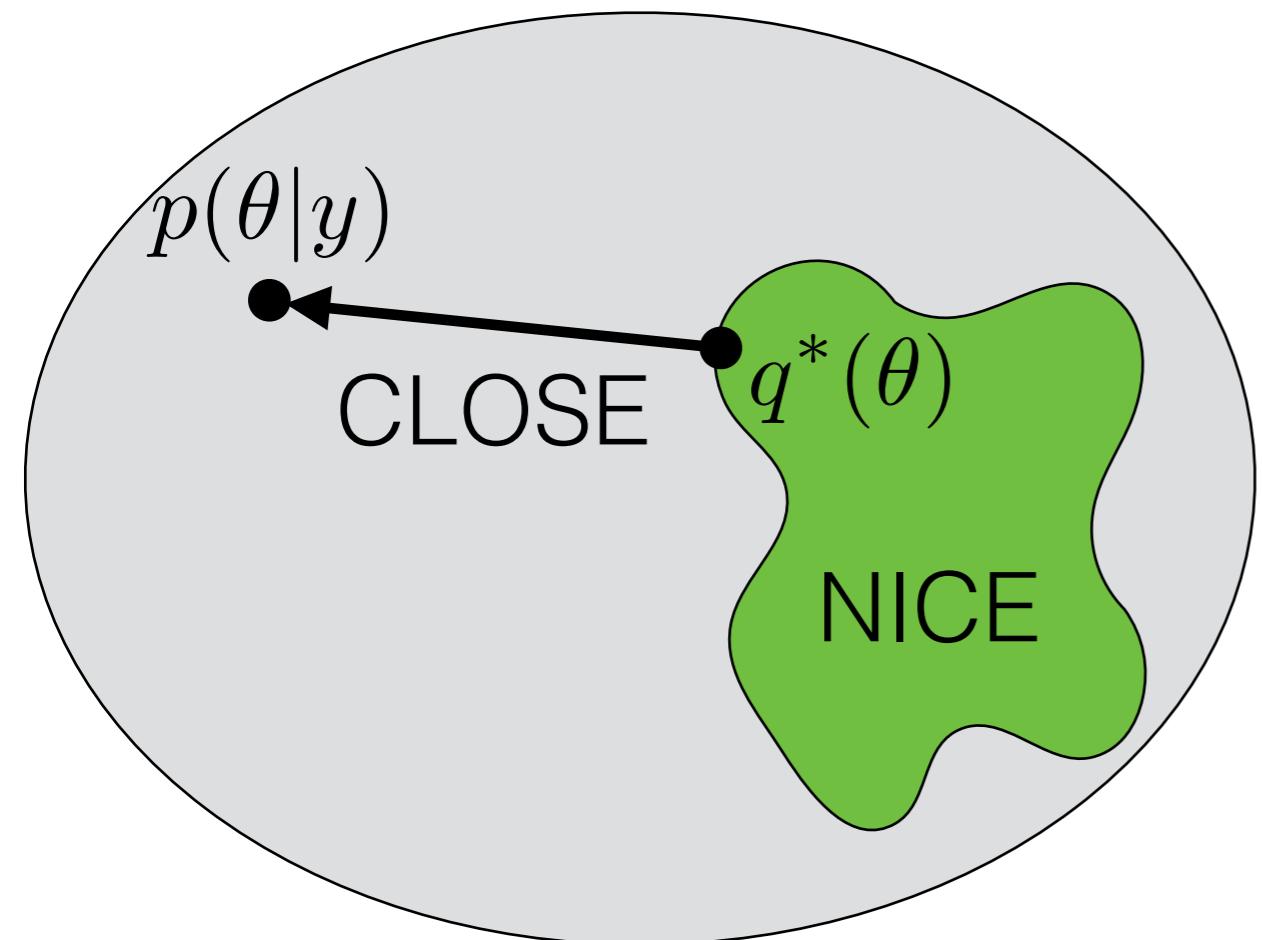
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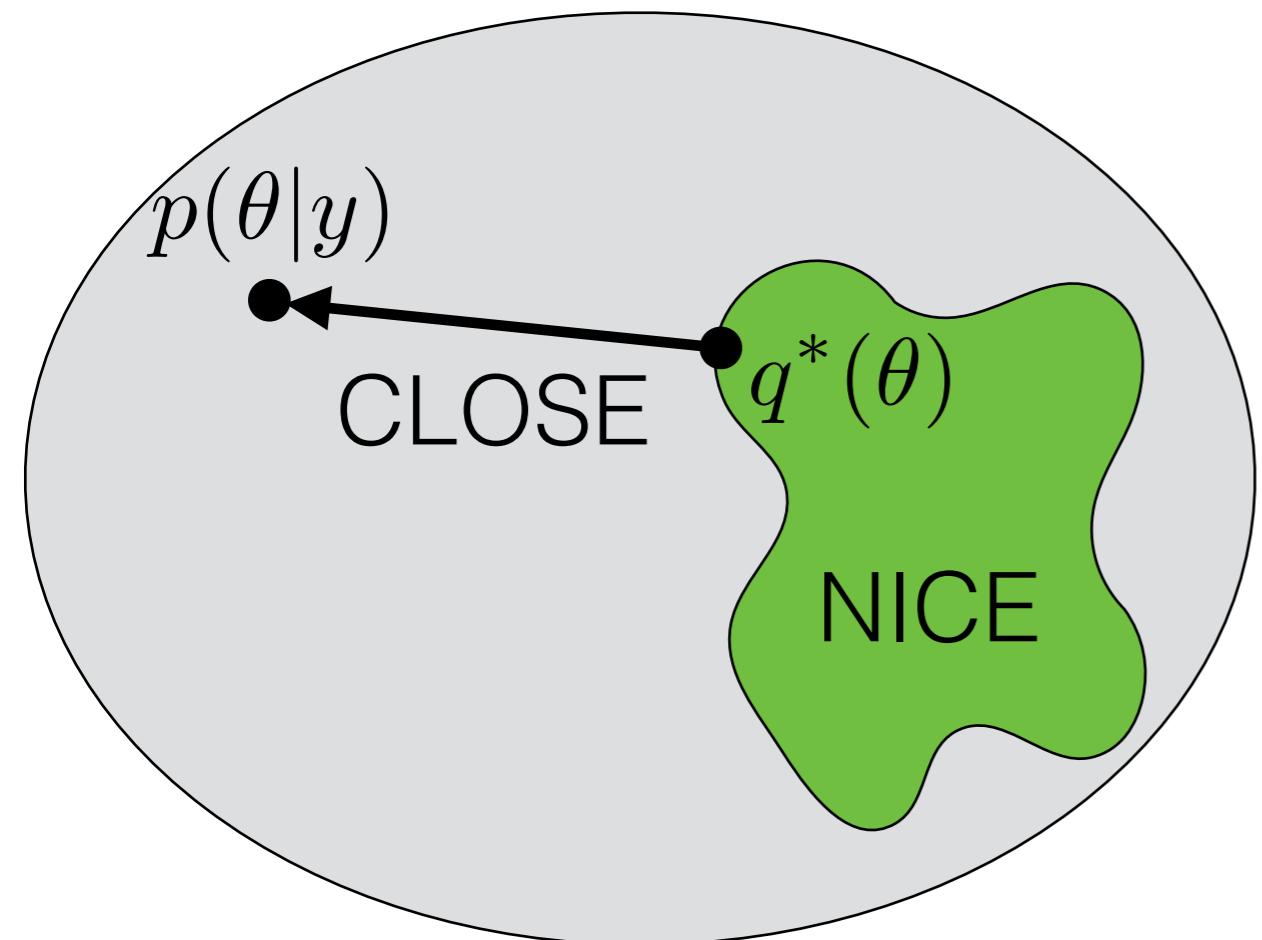
Choose “NICE” distributions



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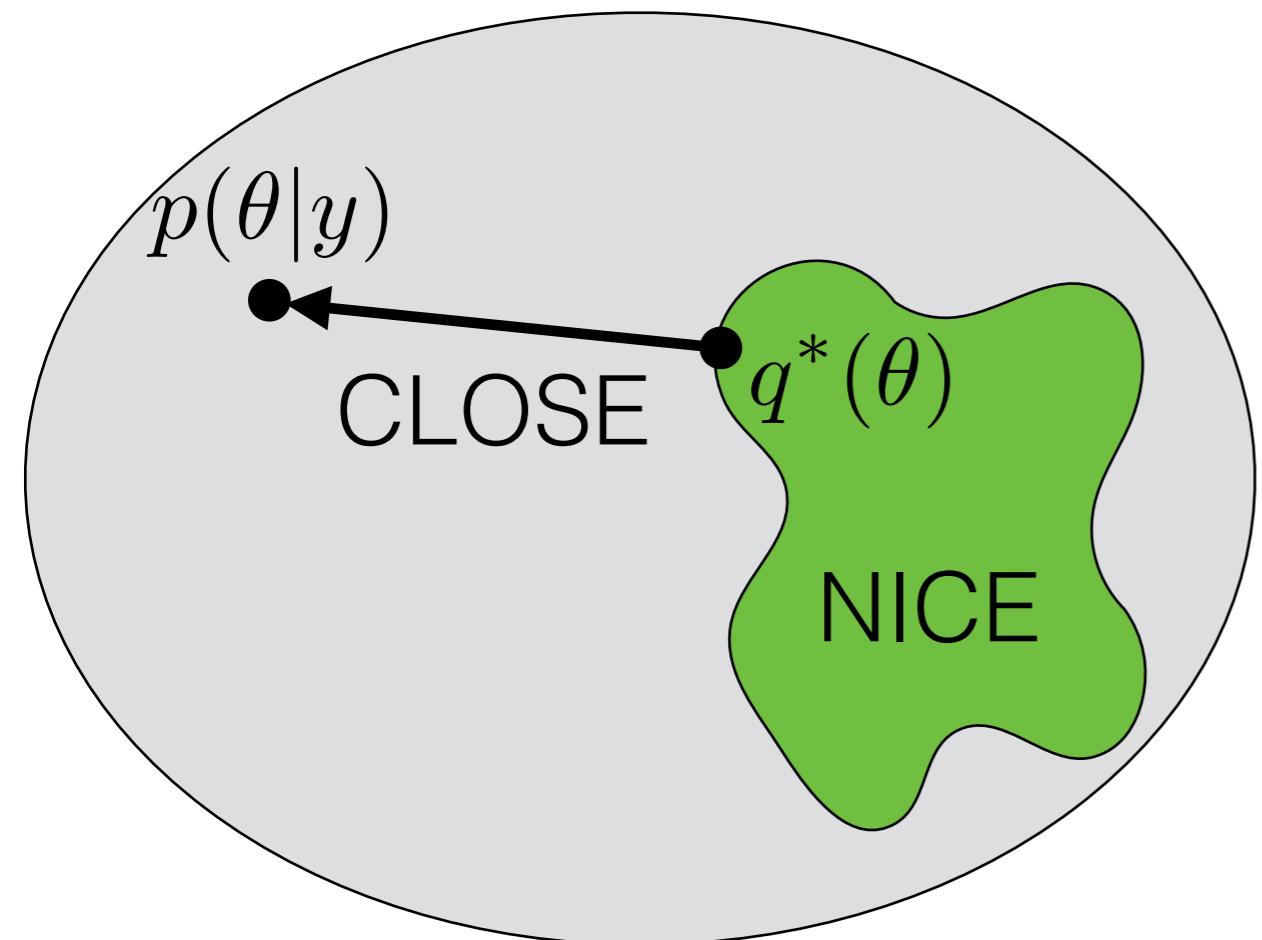
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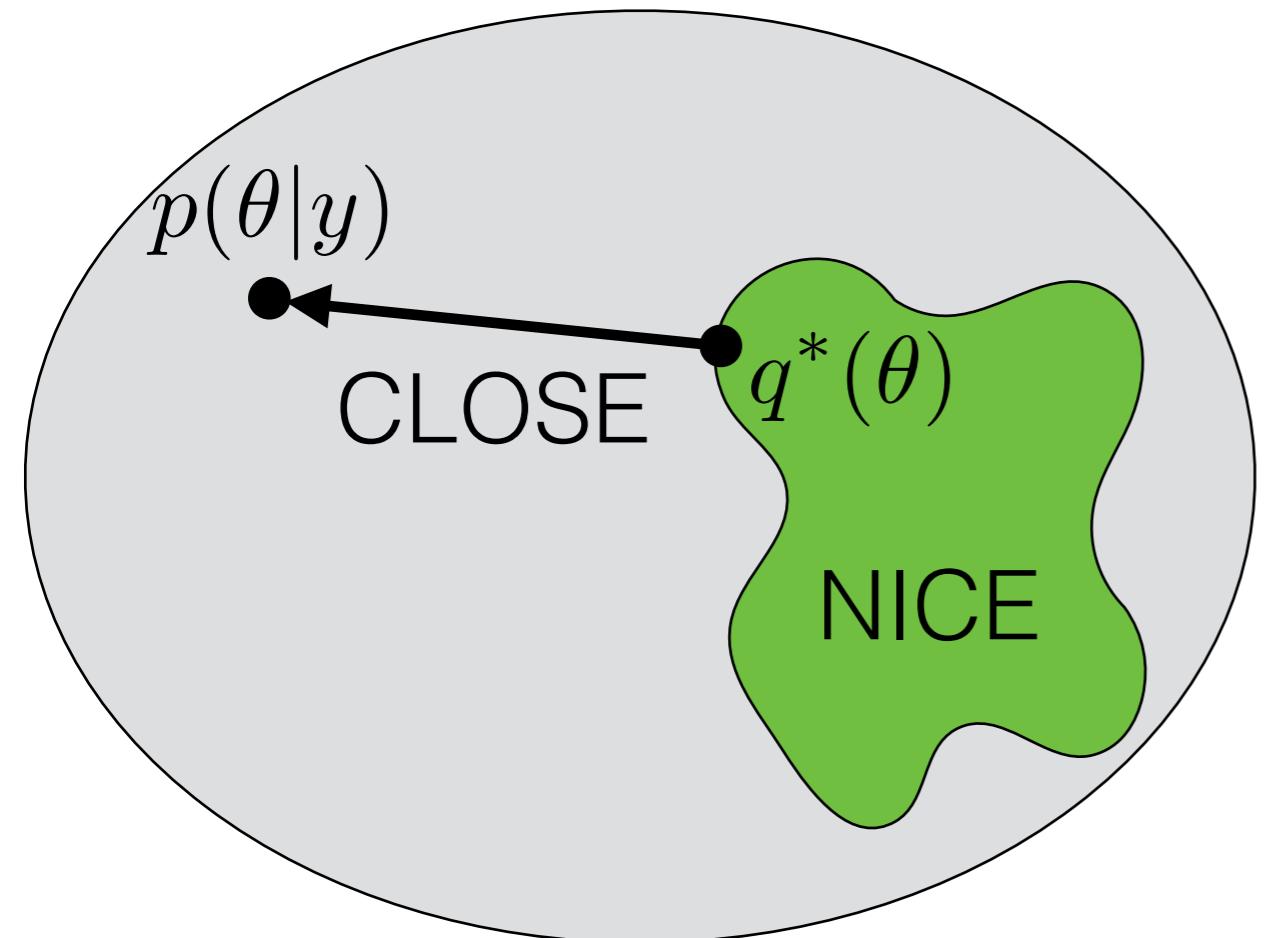
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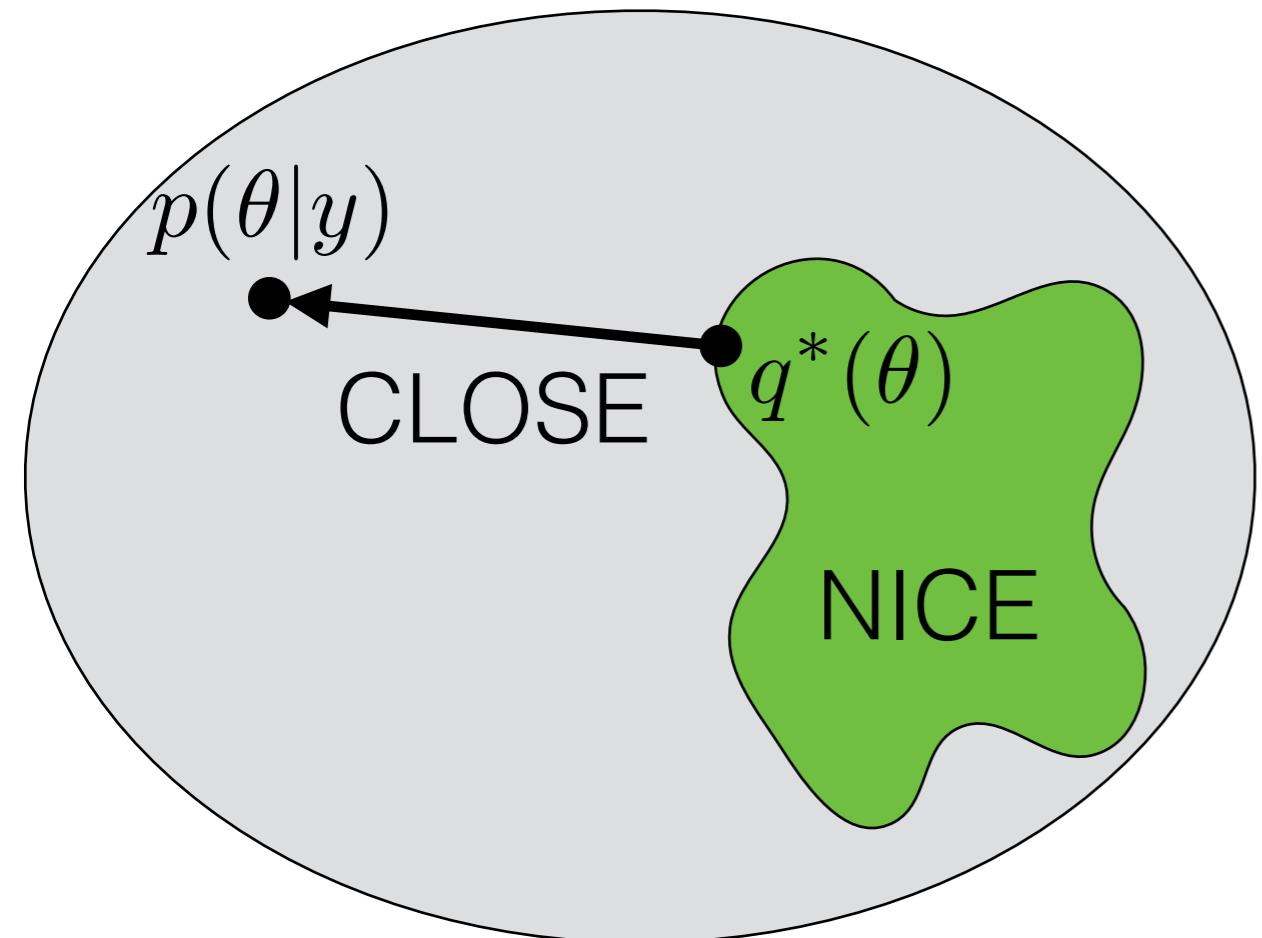
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- Mean-field variational Bayes (MFVB)

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

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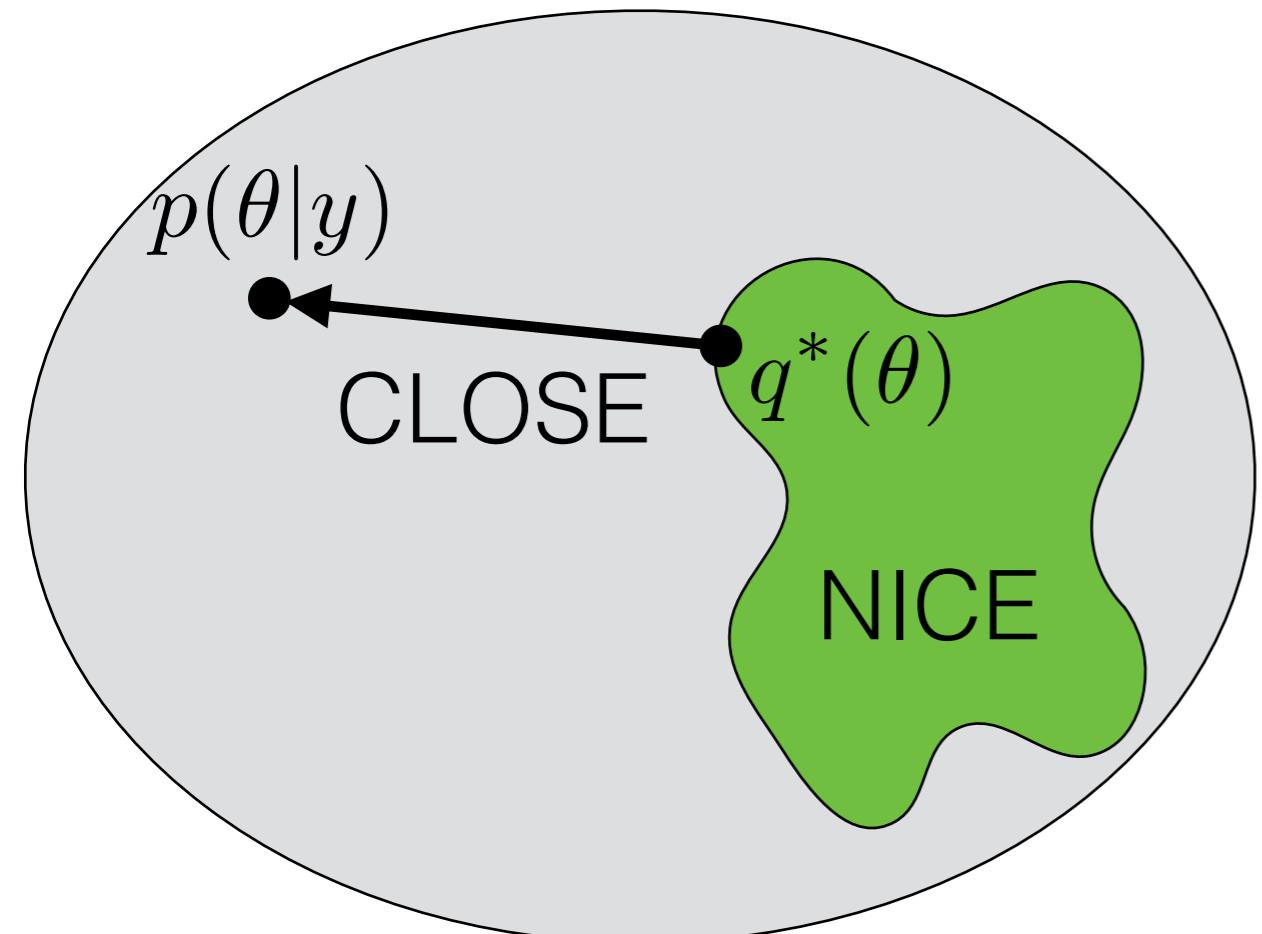
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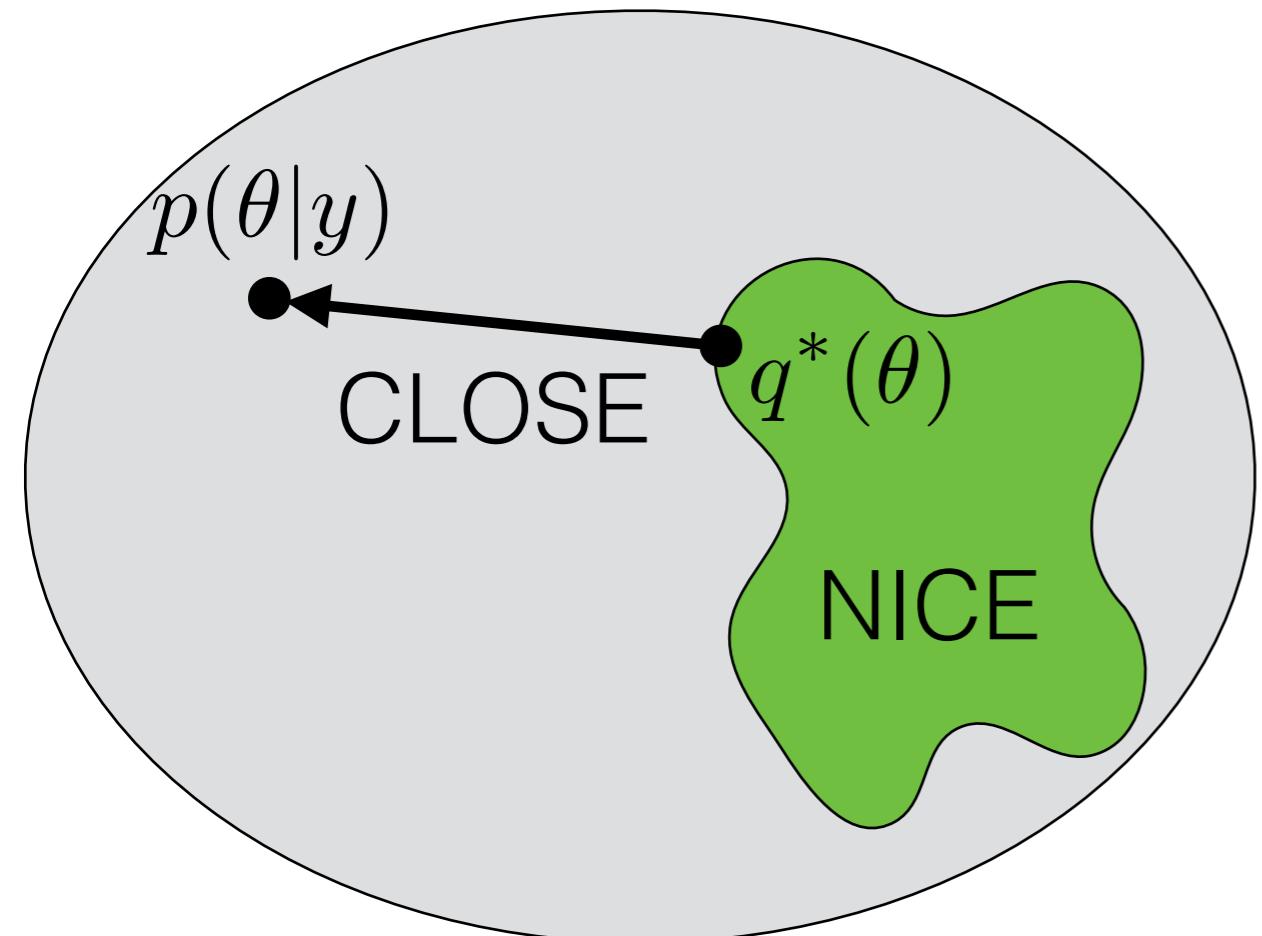
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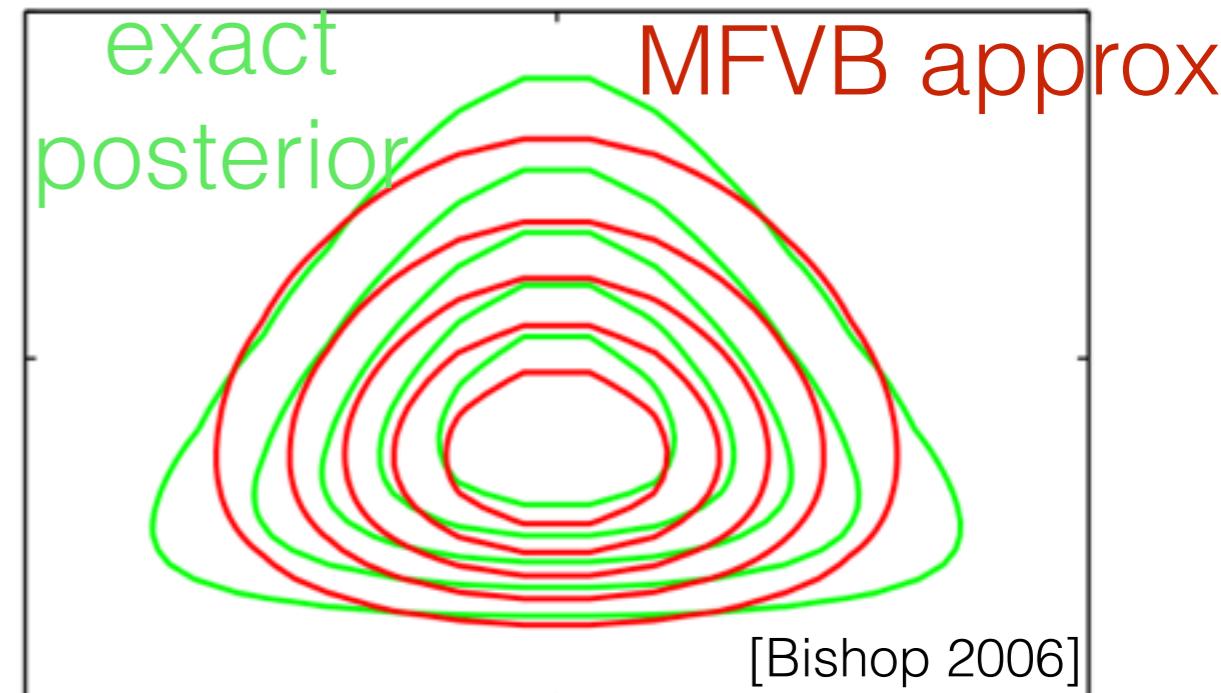


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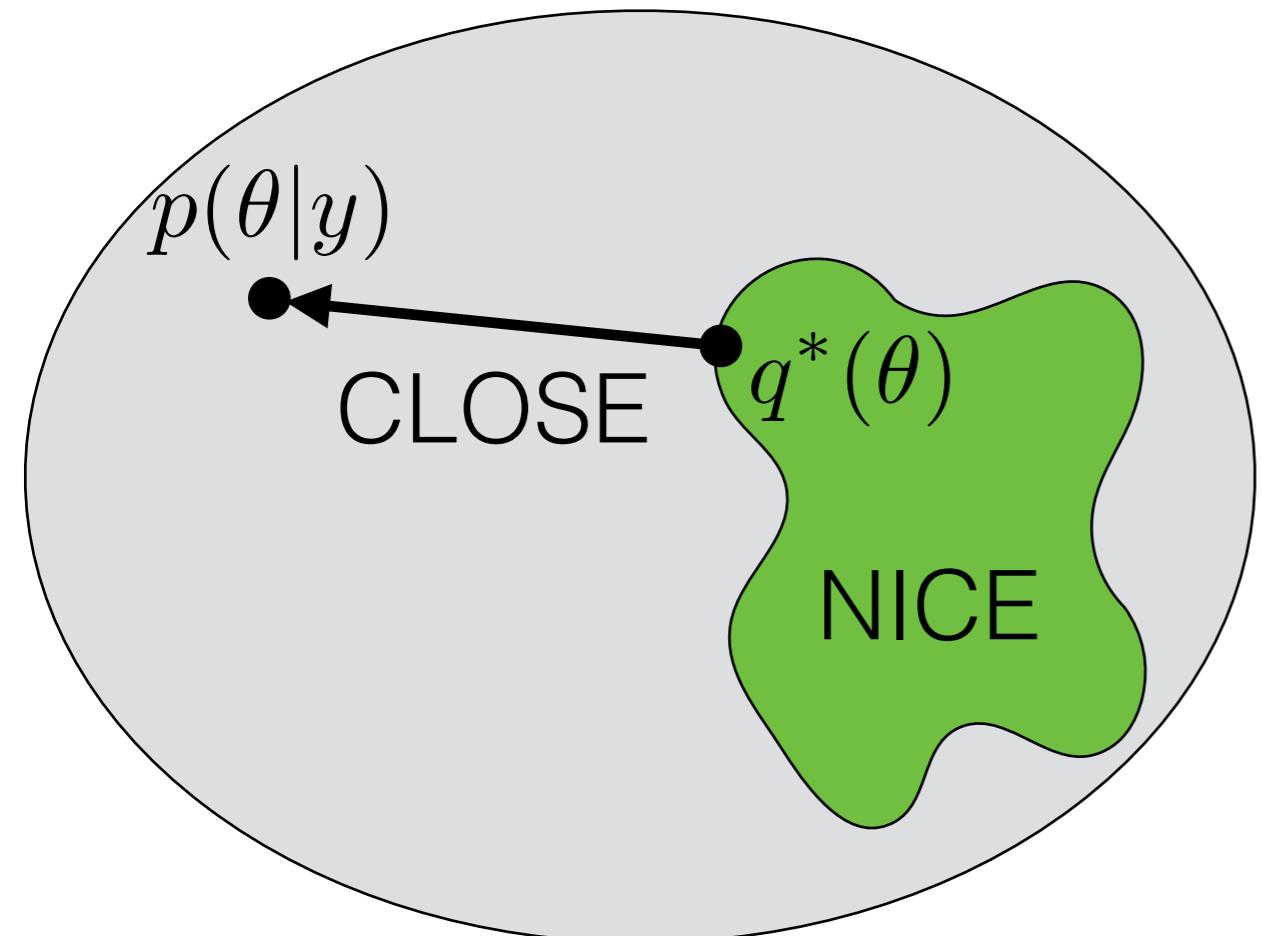
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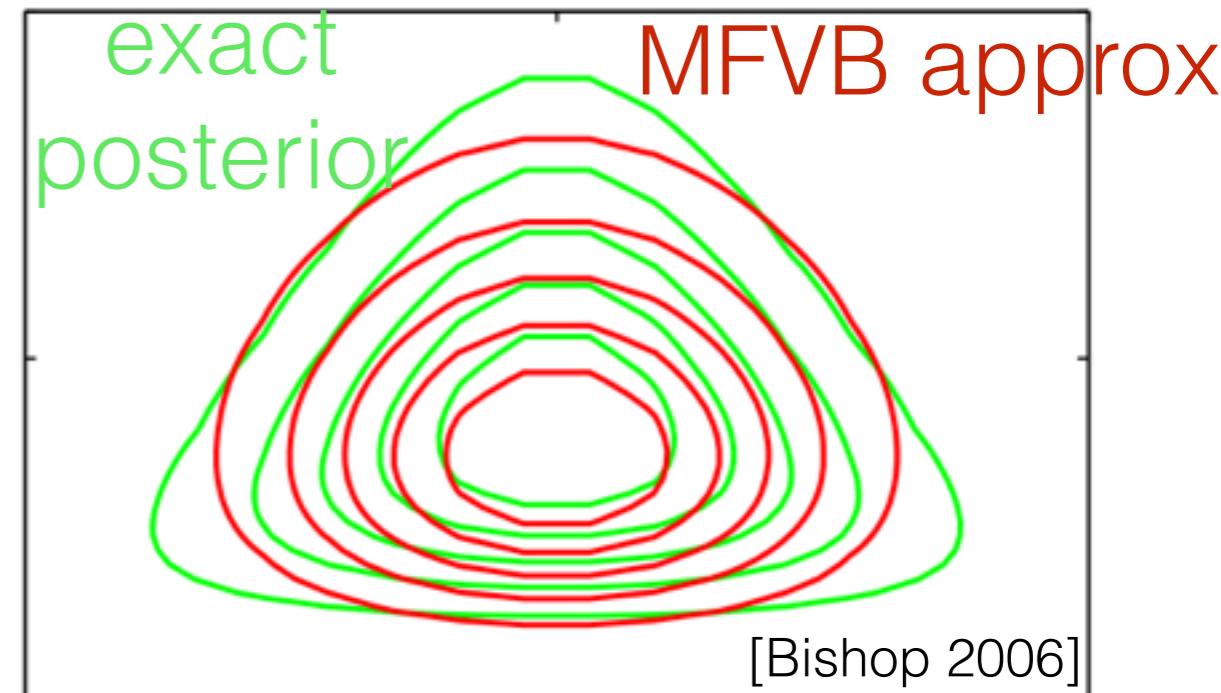
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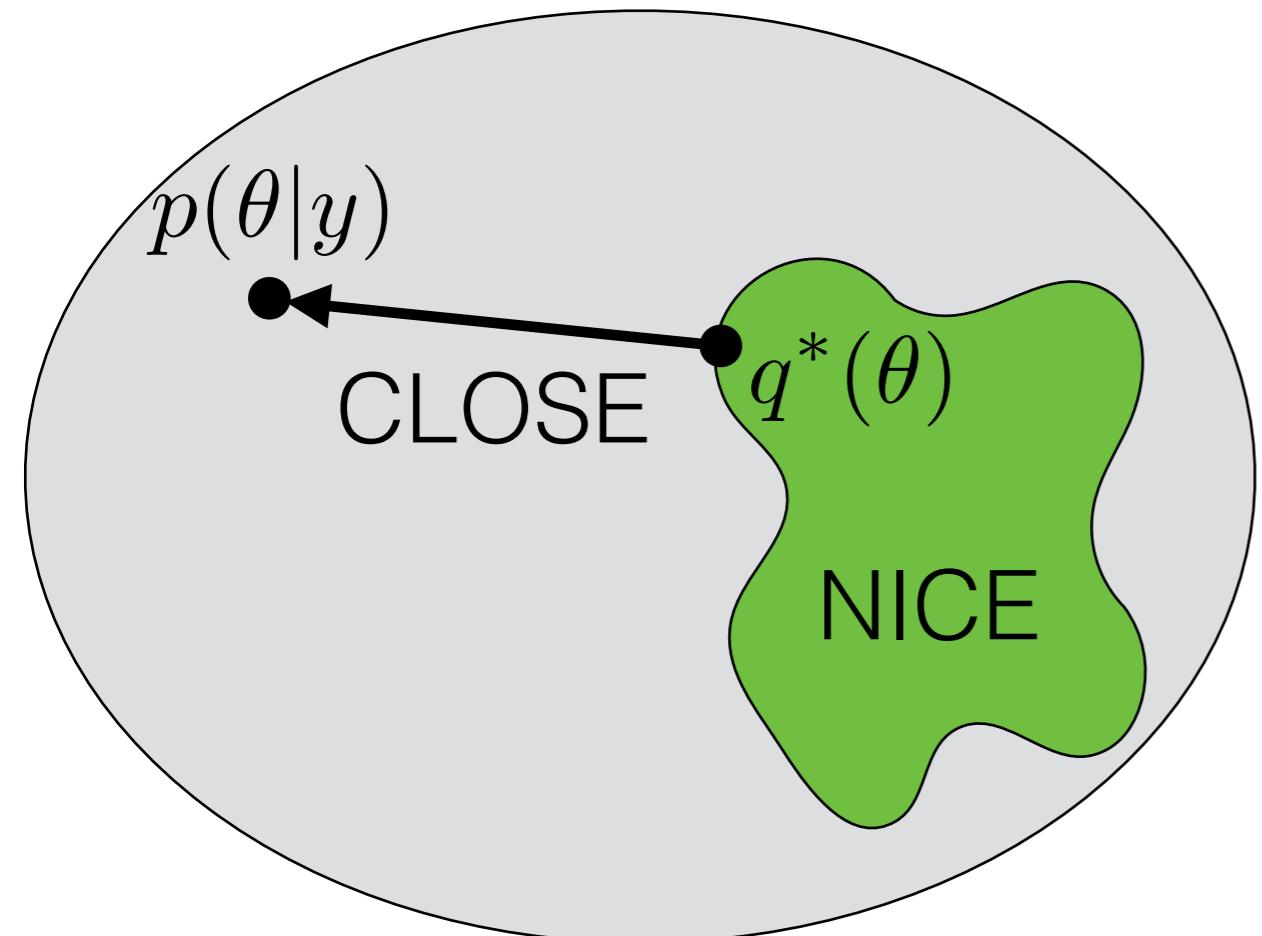
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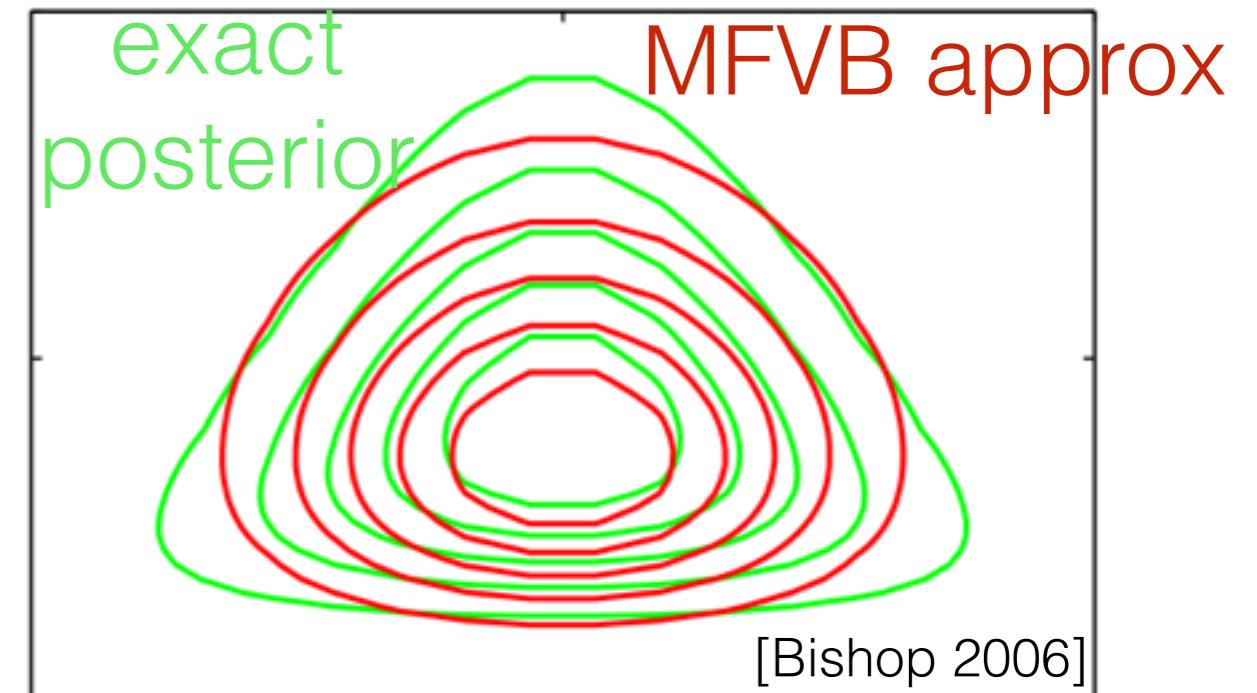
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- One option: Coordinate descent in q_1, \dots, q_J



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

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

Approximate Bayesian inference

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

Optimization

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

Variational Bayes

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

Mean-field variational Bayes

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

- 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?

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- Bayes & Approximate Bayes review
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Midge wing length

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



[CSIRO 2004]

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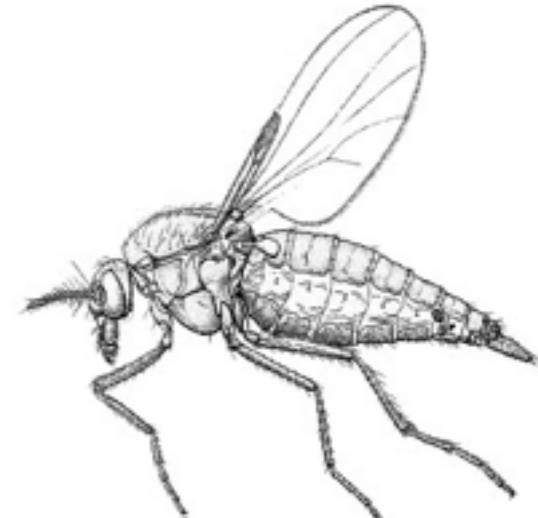
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“variational parameters”

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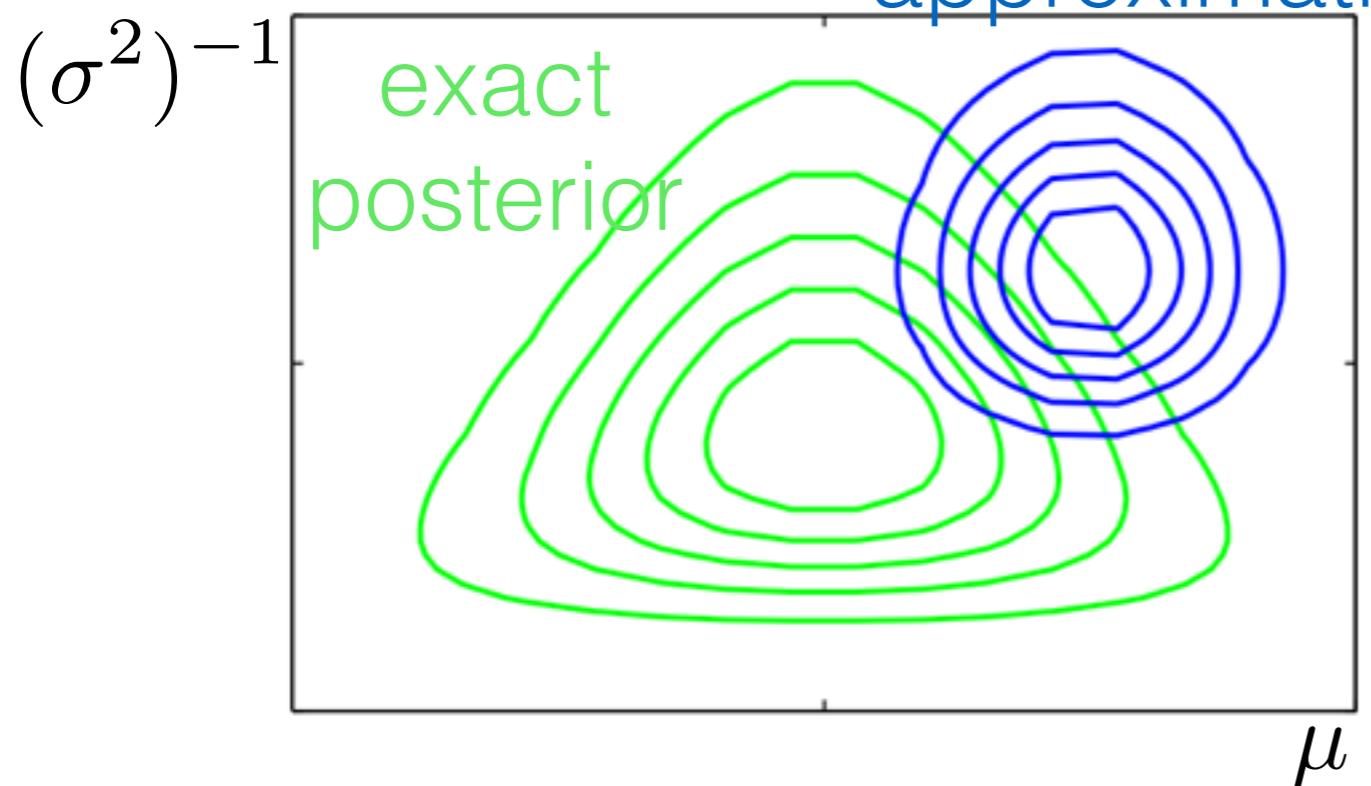
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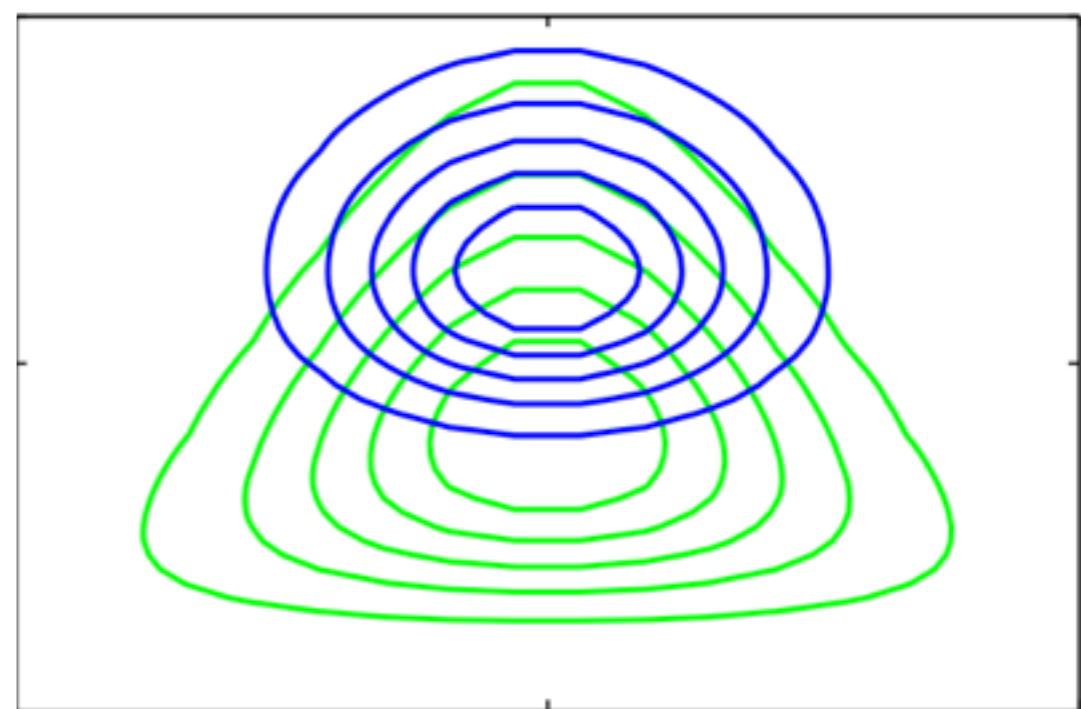
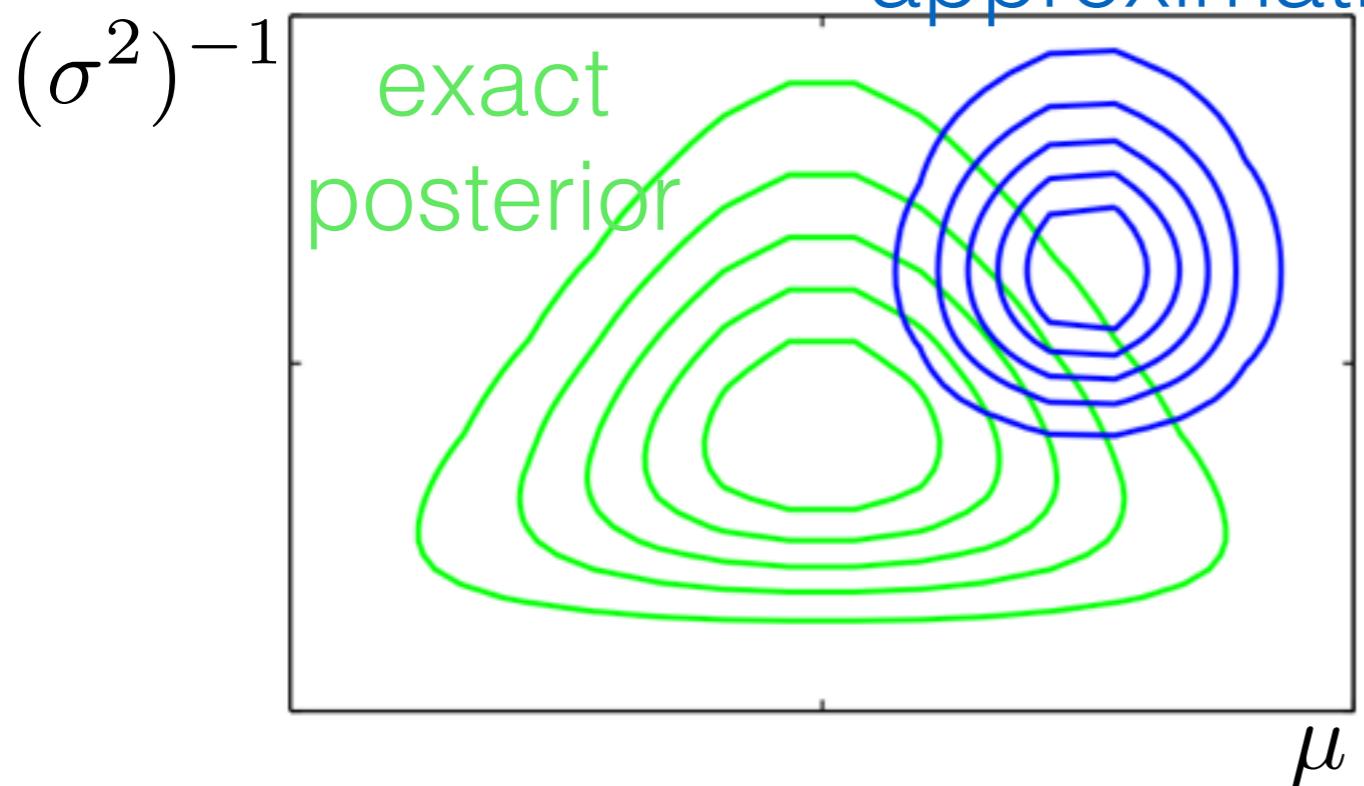
$$q^*(\mu) = N(\mu | m_\mu, \rho_\mu^2) \quad q^*((\sigma^2)^{-1}) = \text{Gamma}((\sigma^2)^{-1} | a_\sigma, b_\sigma)$$

- Iterate: $(m_\mu, \rho_\mu^2) = f(a_\sigma, b_\sigma)$ “variational parameters”
 $(a_\sigma, b_\sigma) = g(m_\mu, \rho_\mu^2)$

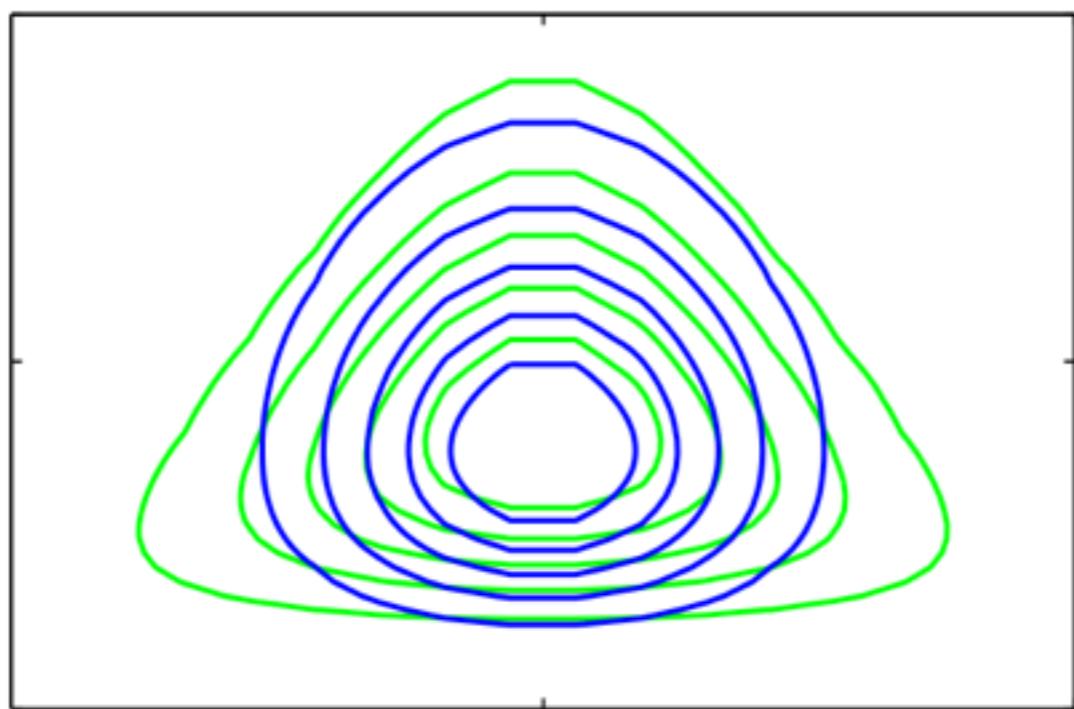
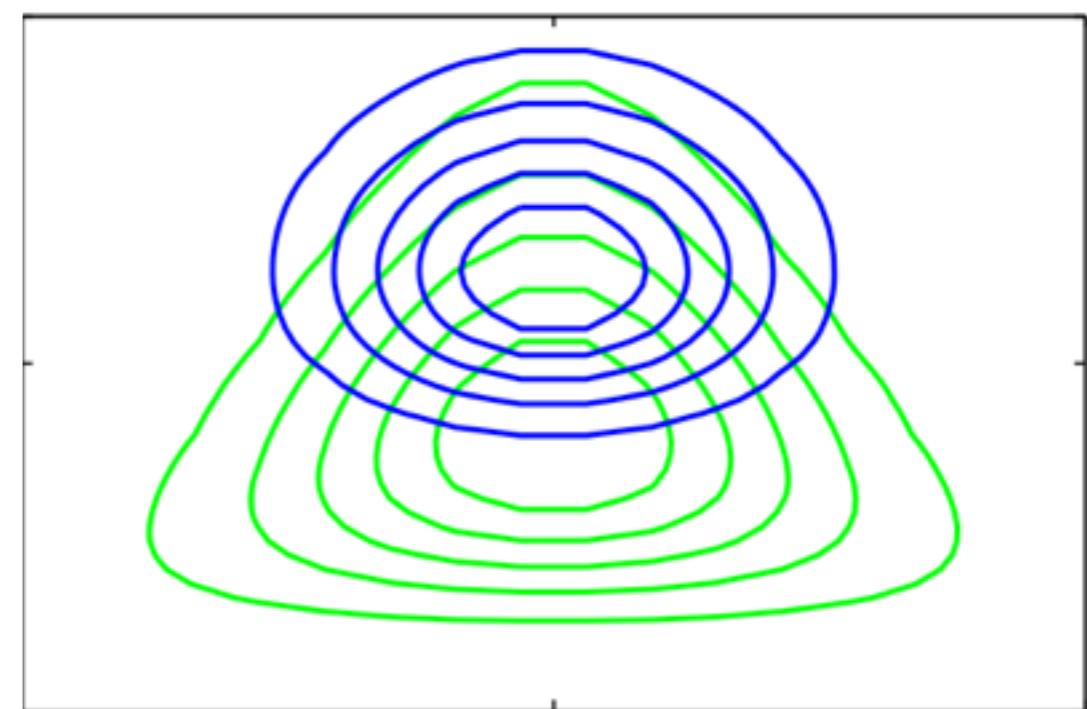
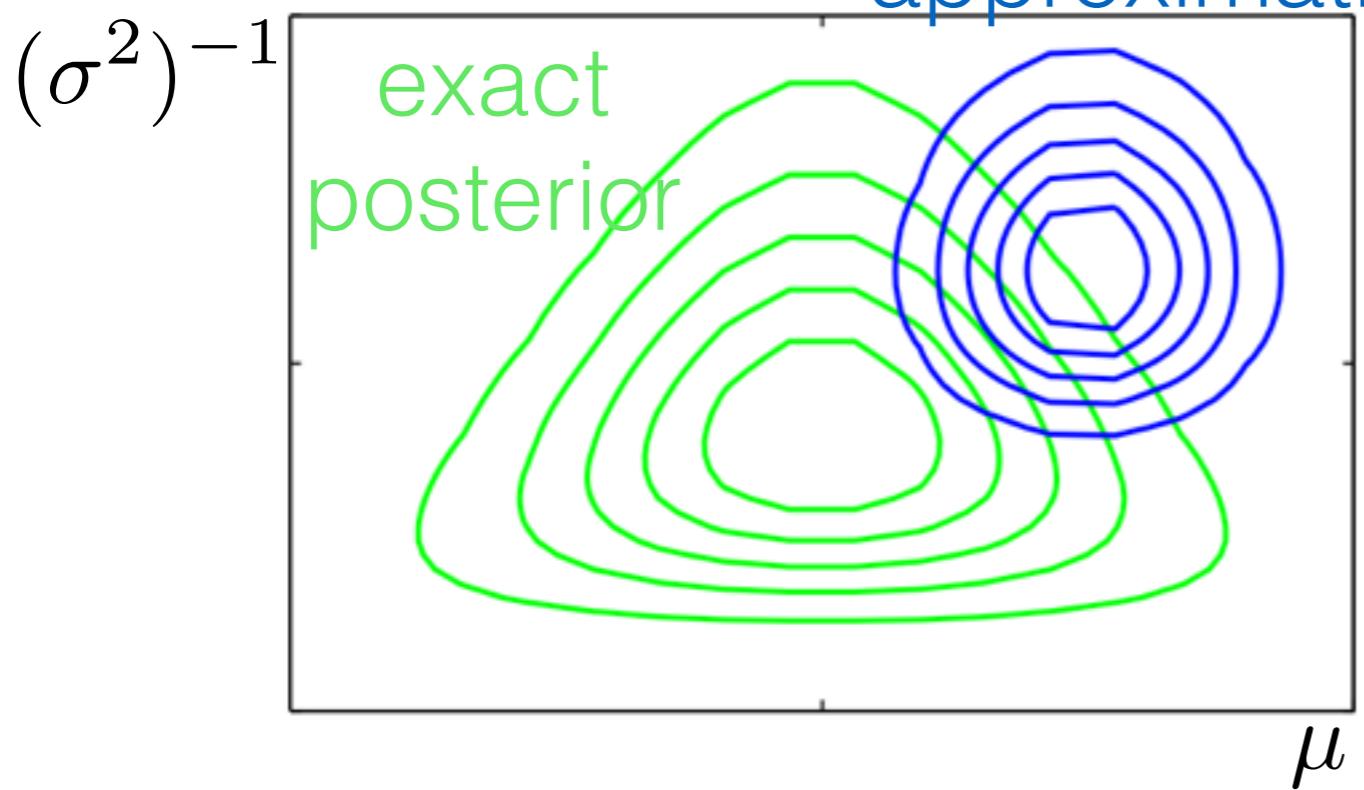
Midge wing length approximation



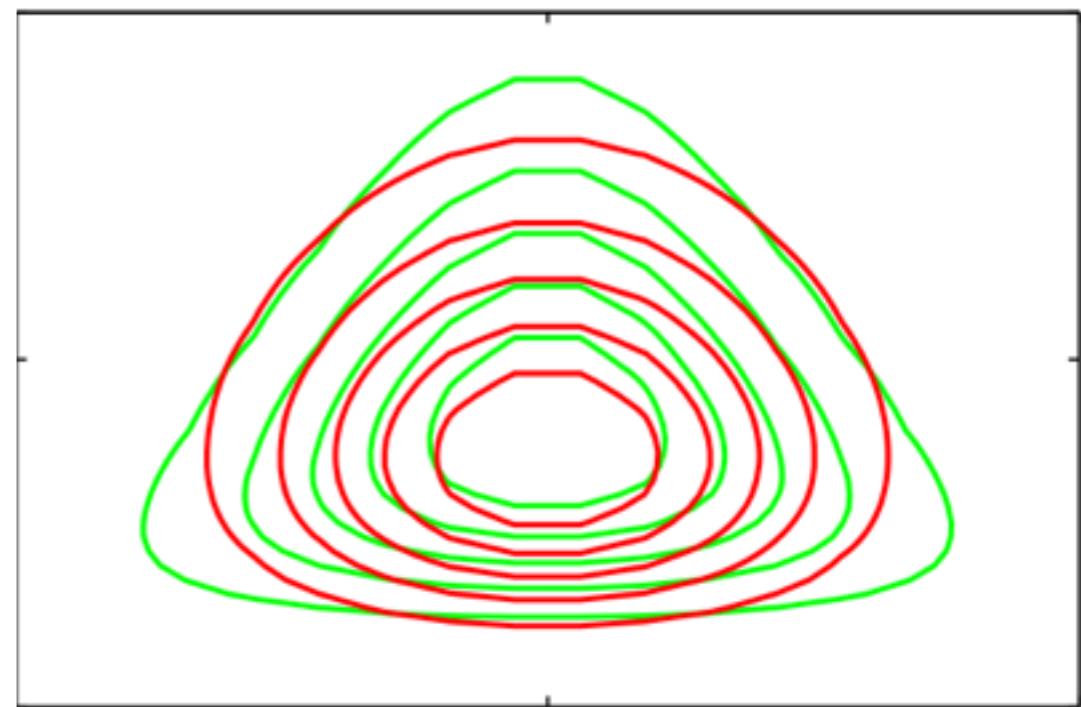
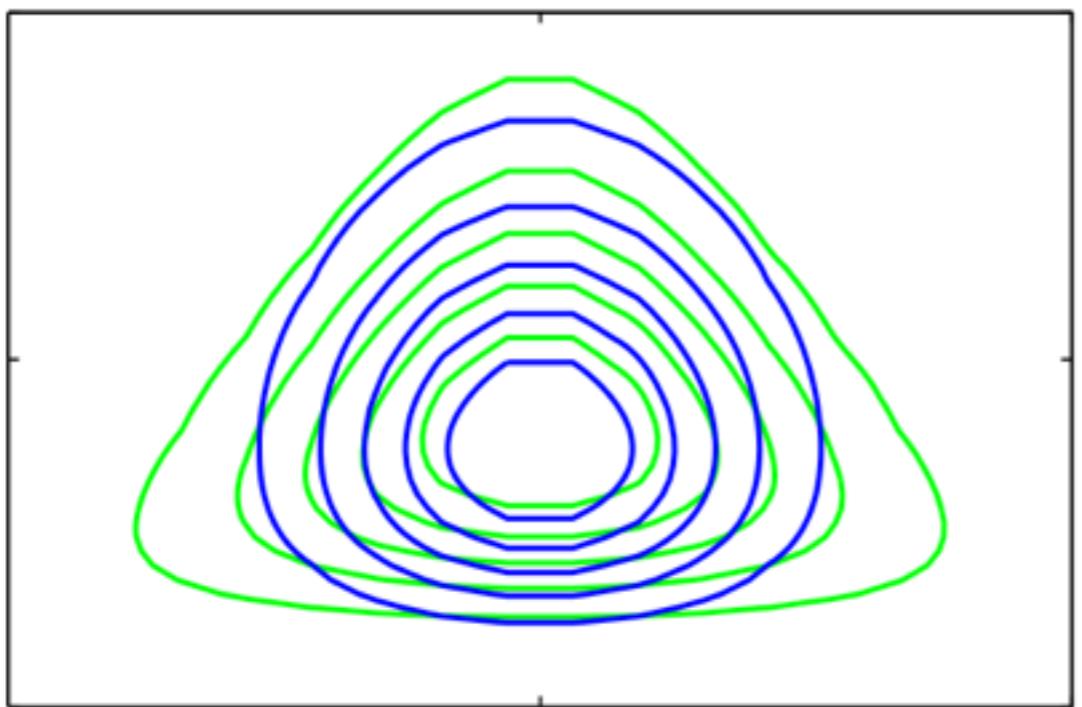
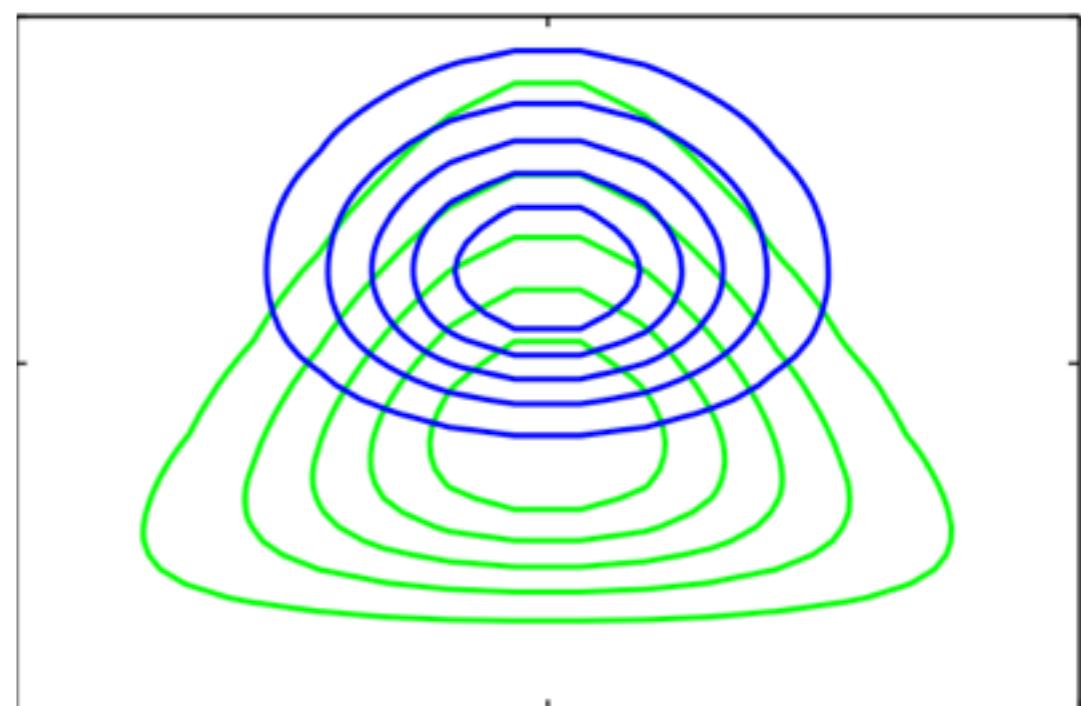
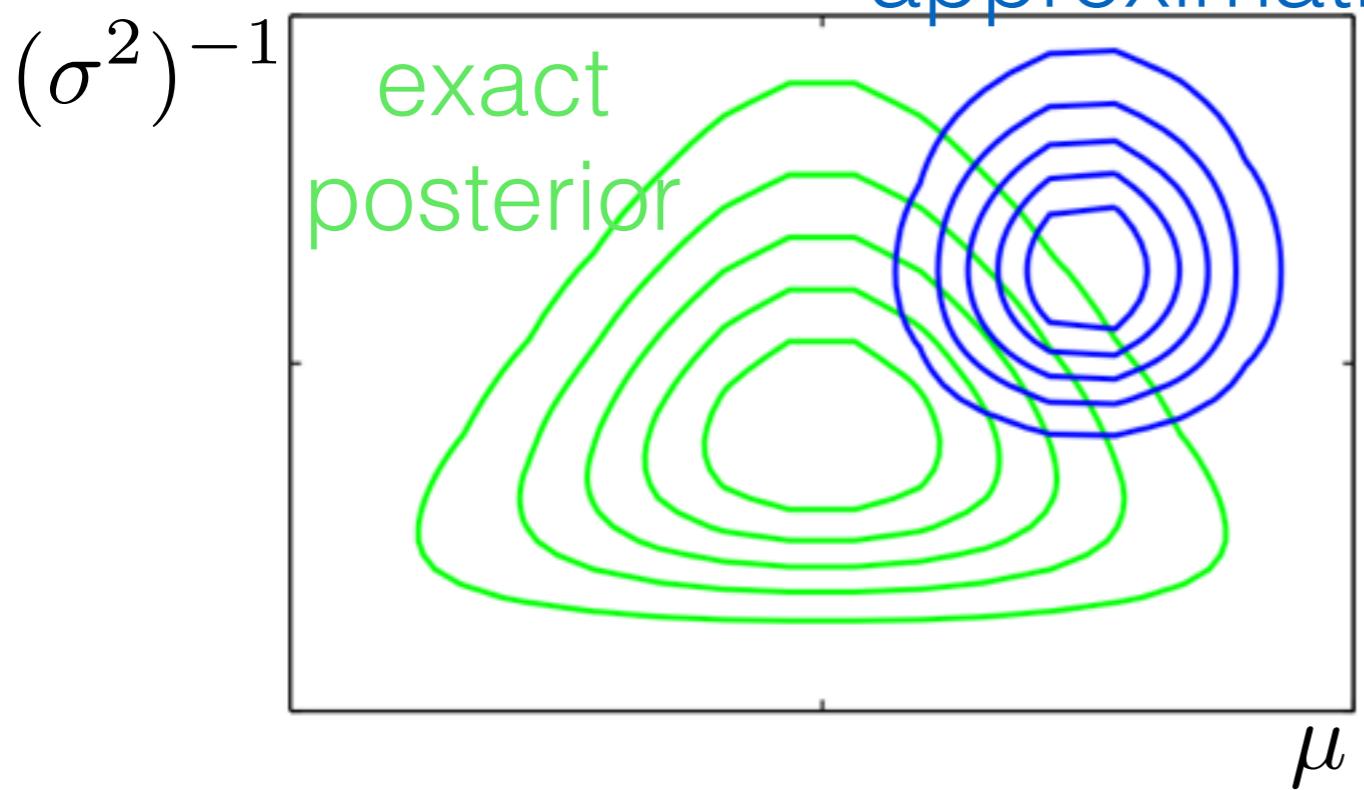
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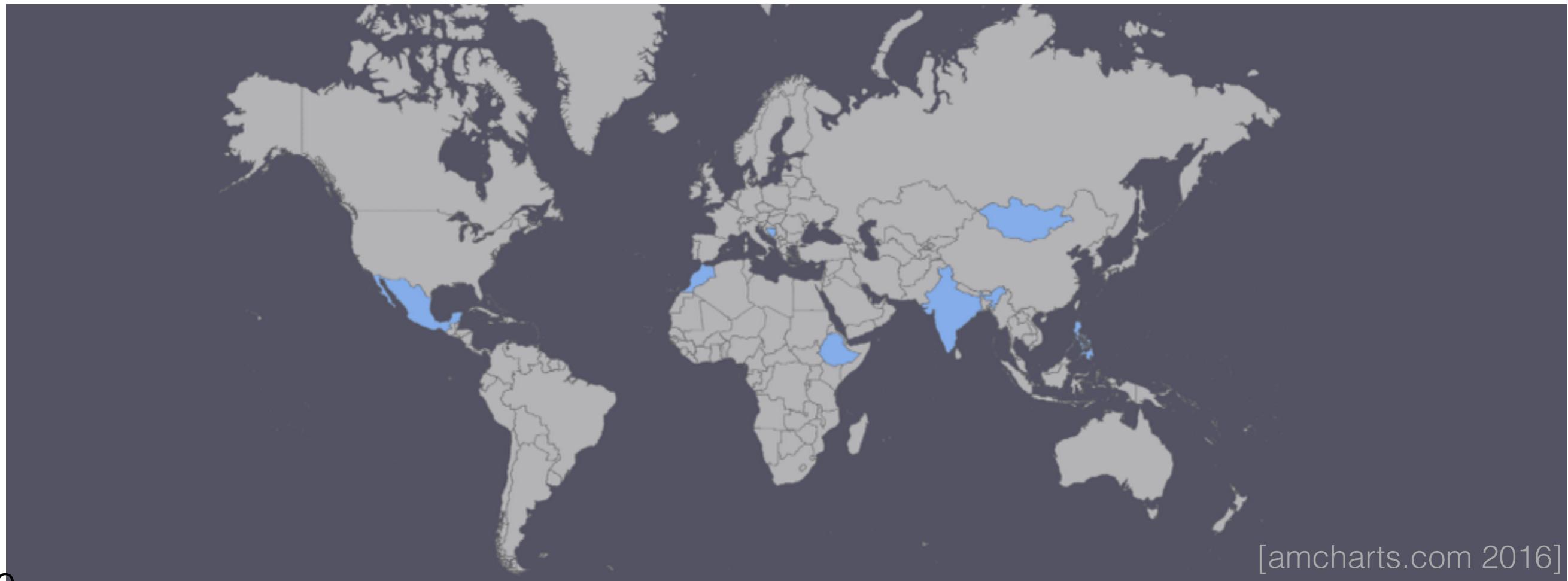
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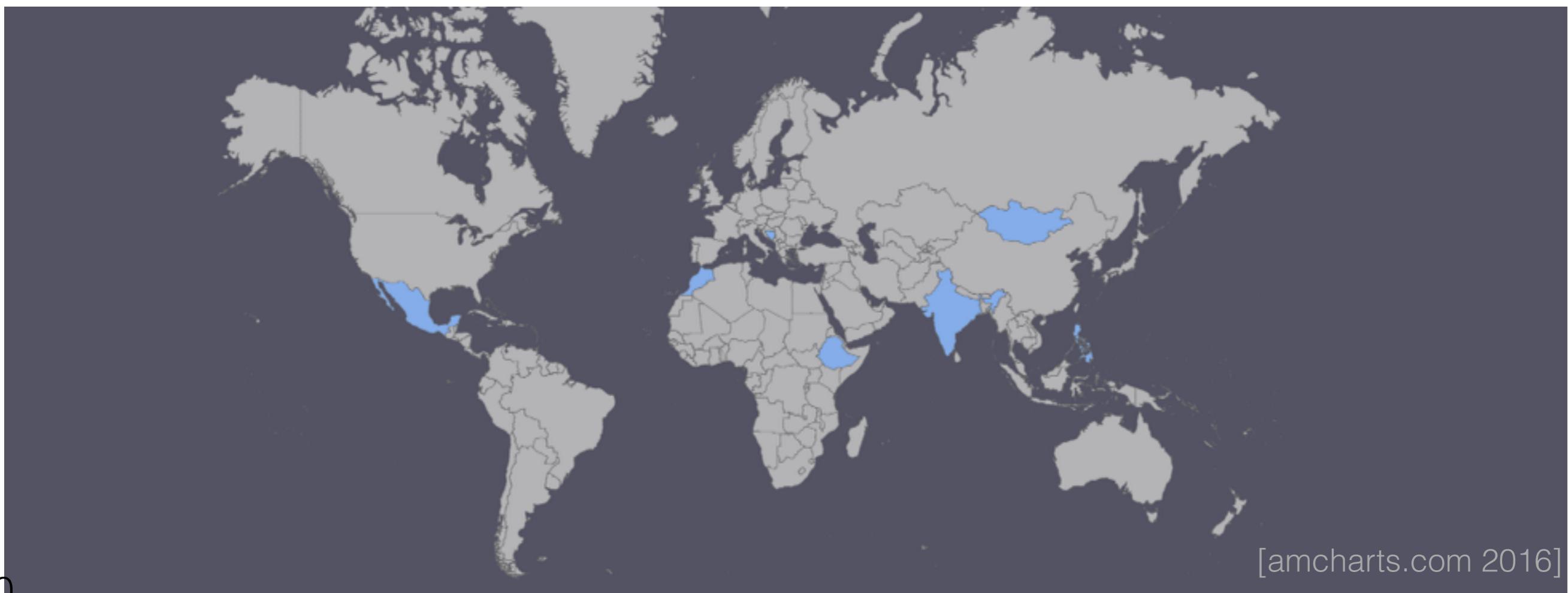


Microcredit Experiment



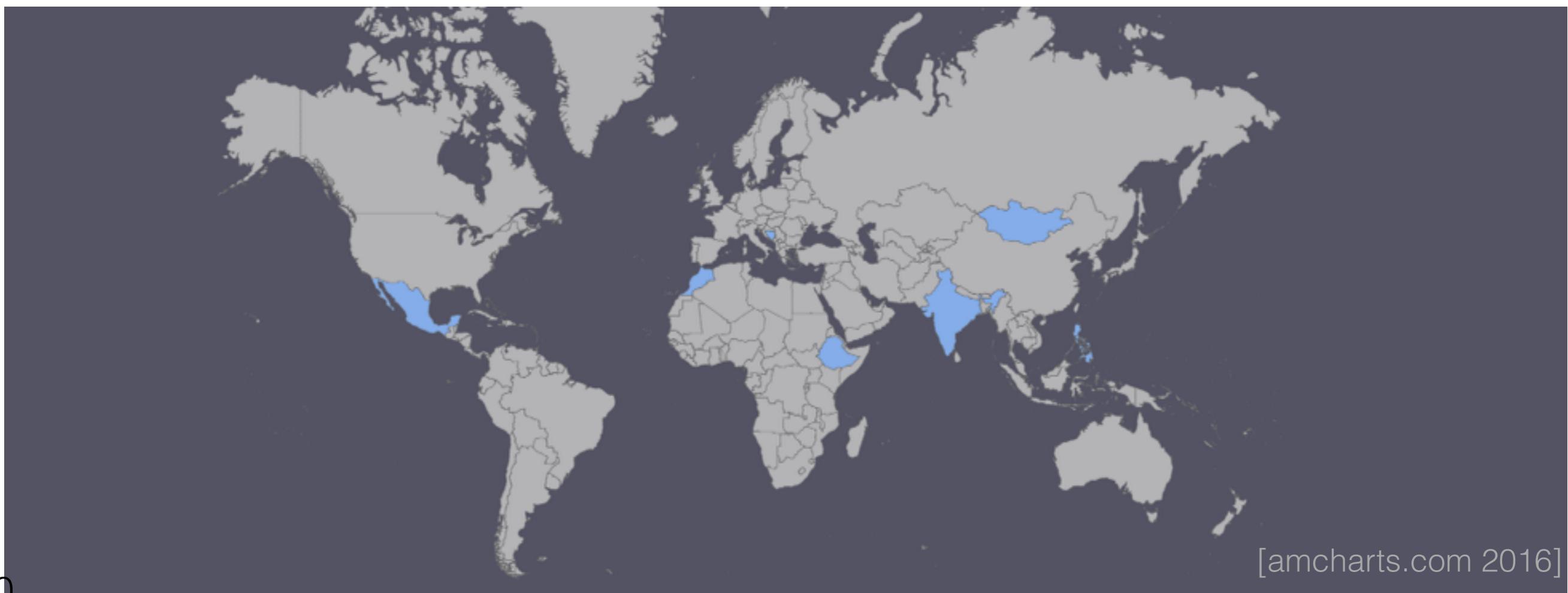
Microcredit Experiment

- Simplified from Meager (2018a)
- $K = 7$ microcredit trials (Mexico, Mongolia, Bosnia, India, Morocco, Philippines, Ethiopia)



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 profit

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profit $\rightarrow y_{kn}$

1 if microcredit $\rightarrow T_{kn}\tau_k$

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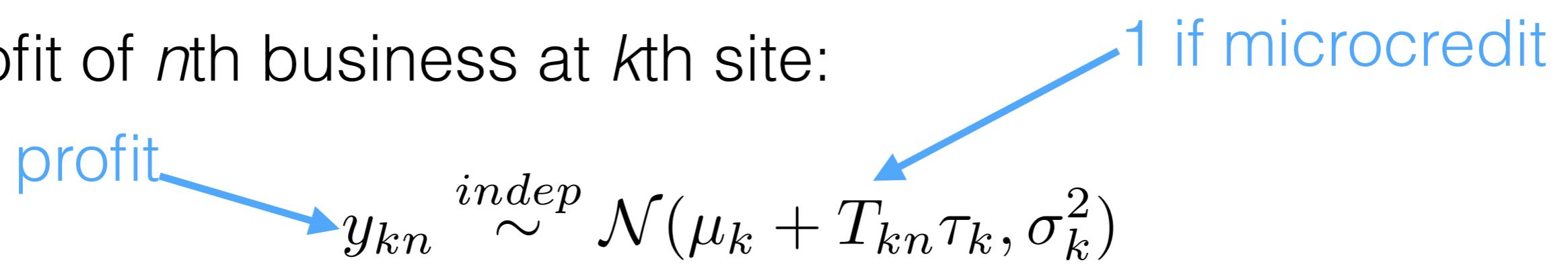
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- Priors and hyperpriors:

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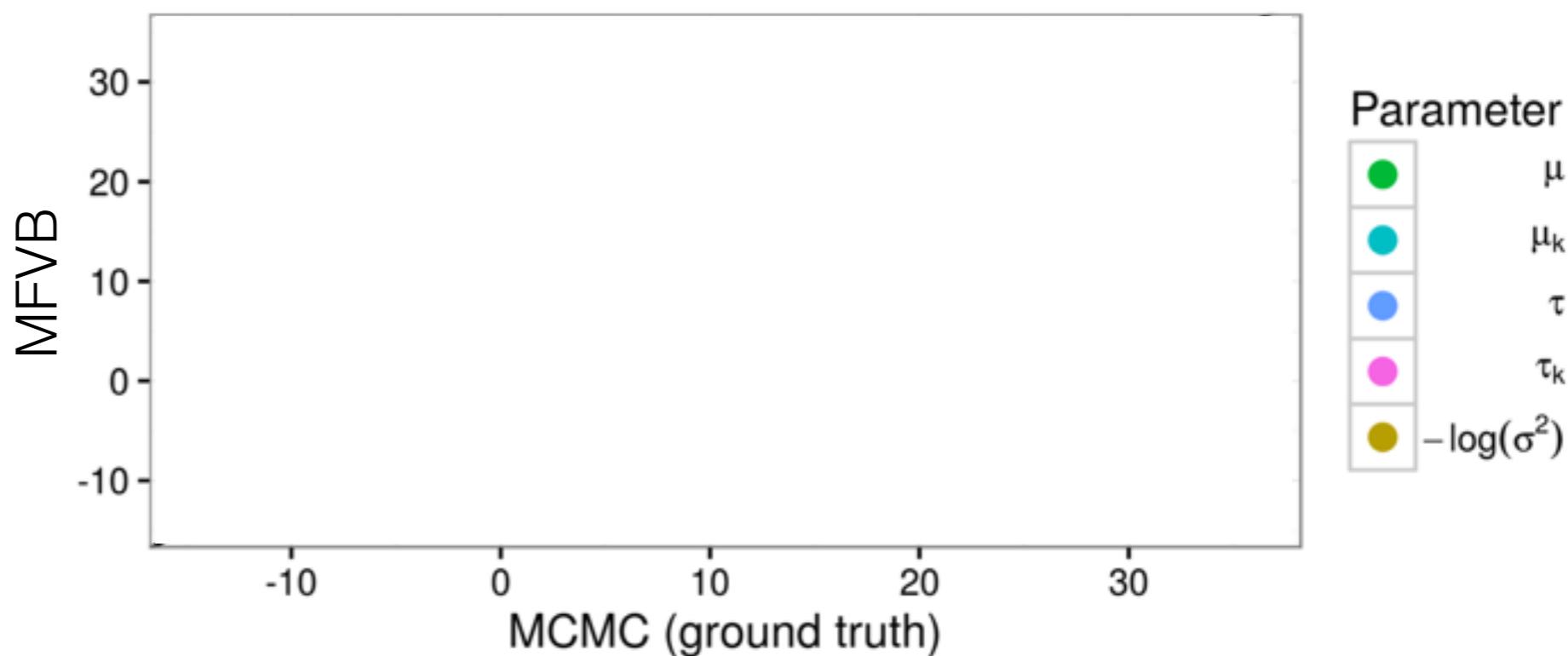
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$$\sigma_k^{-2} \stackrel{iid}{\sim} \Gamma(a, b)$$

$$C \sim \text{Sep\&LKJ}(\eta, c, d)$$

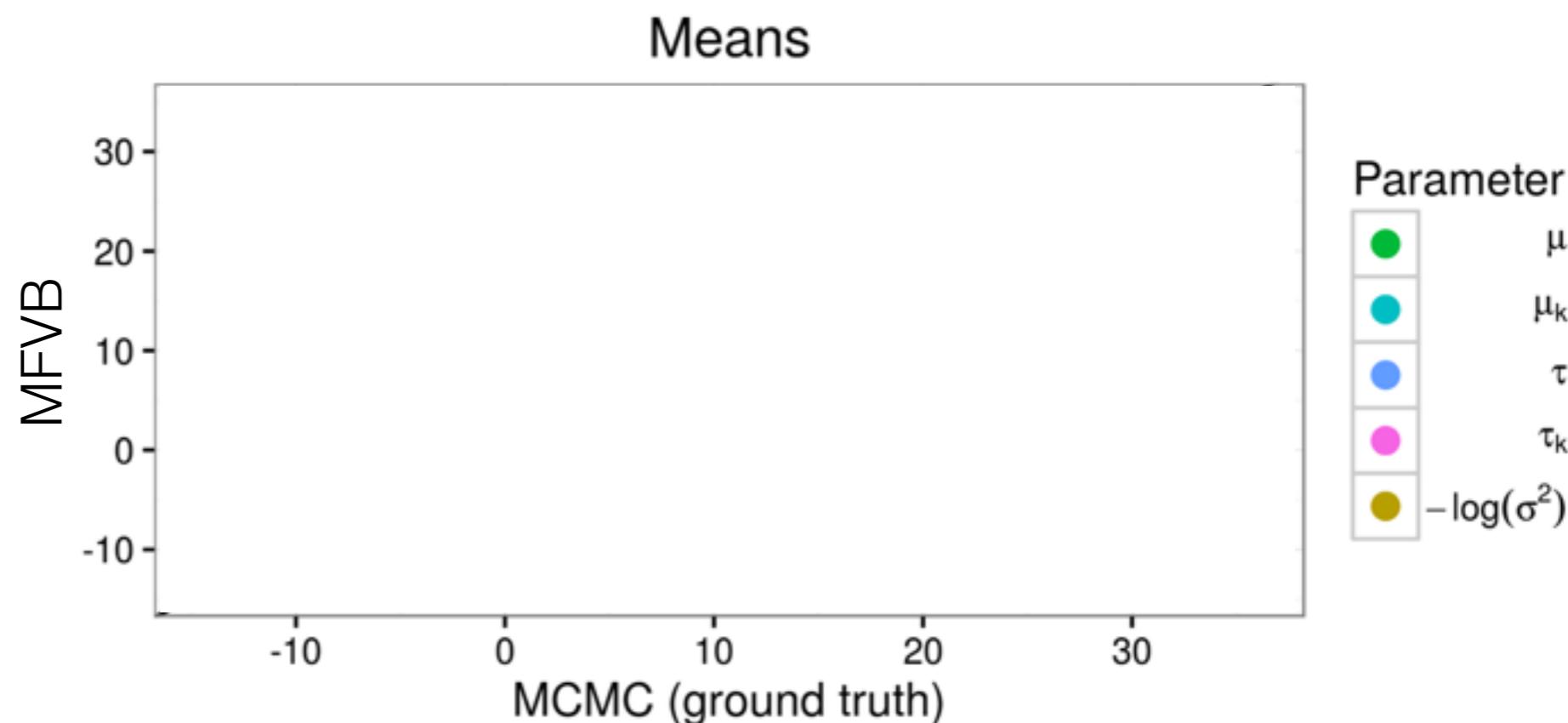
Microcredit

Means



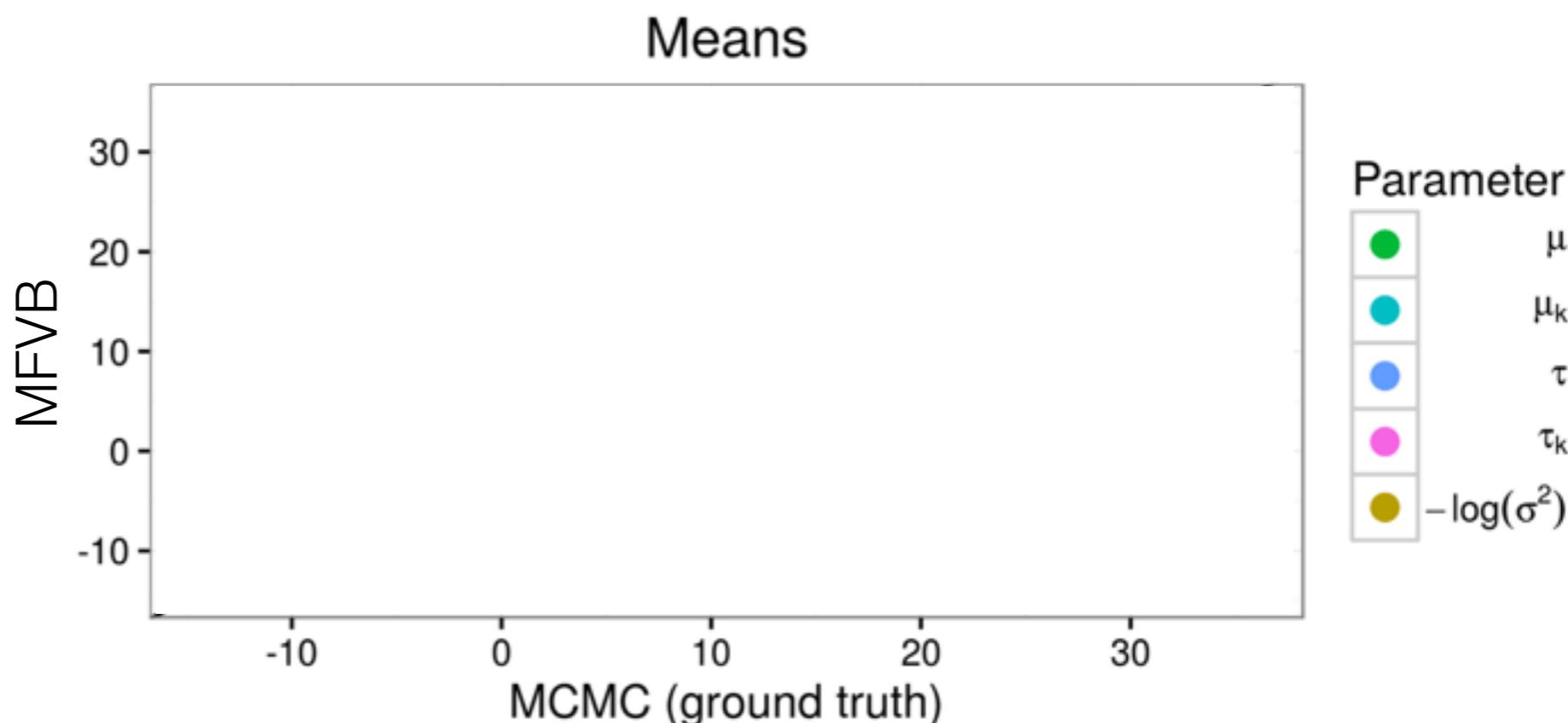
Microcredit

- One set of 2500 MCMC draws:
45 minutes



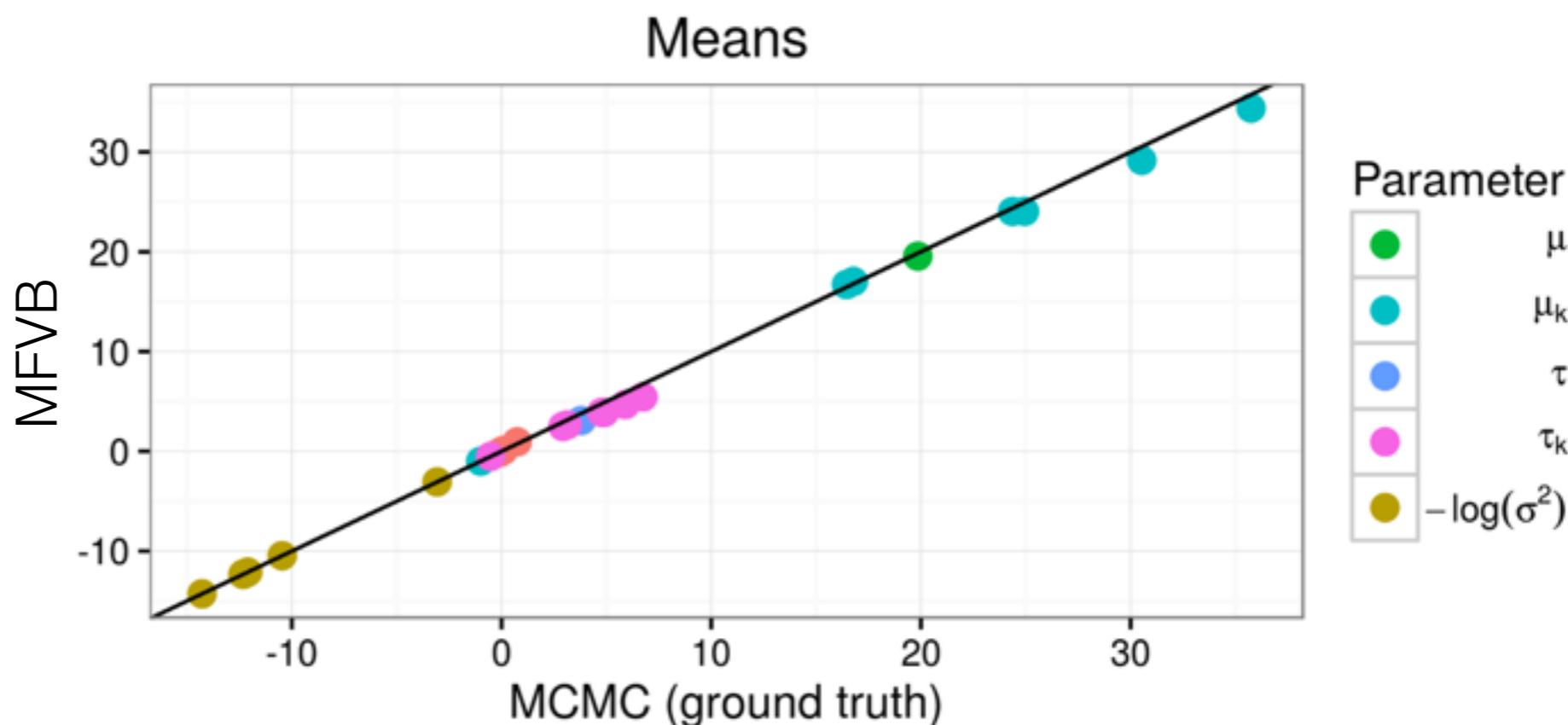
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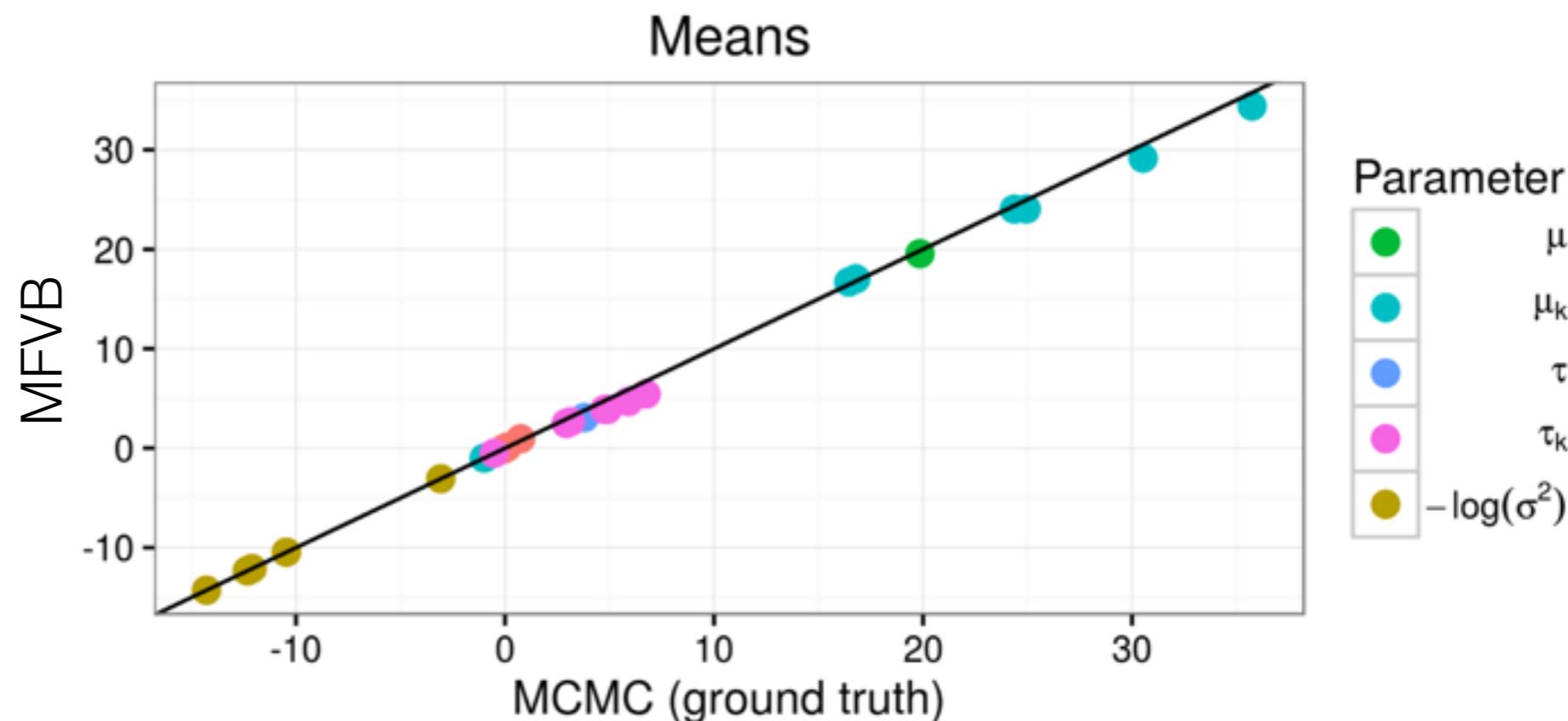
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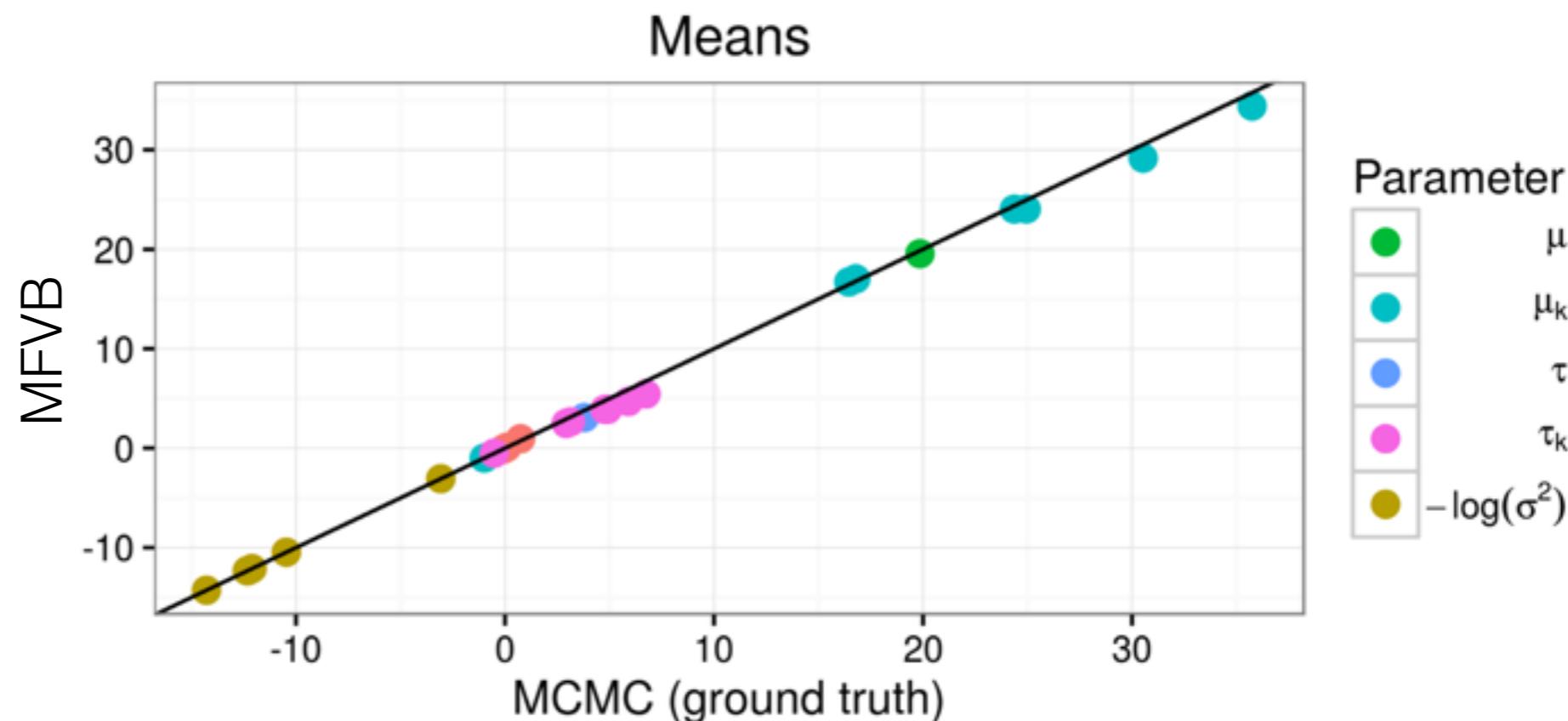


Criteo Online Ads Experiment

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

Microcredit

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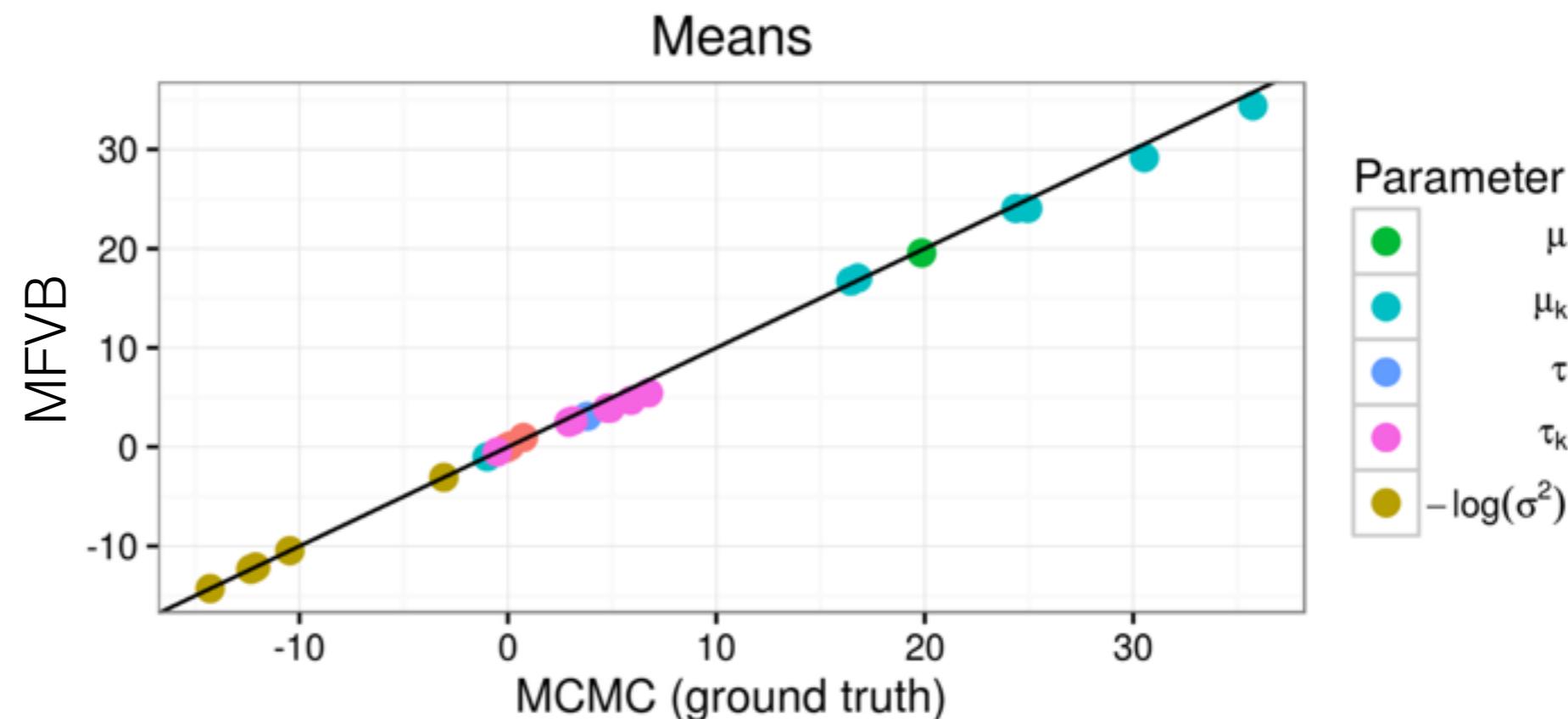


Criteo Online Ads Experiment

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Criteo Online Ads Experiment

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- Q: How predictive of conversion are different features?
- Logistic GLMM; $N = 61,895$ subset to compare to MCMC

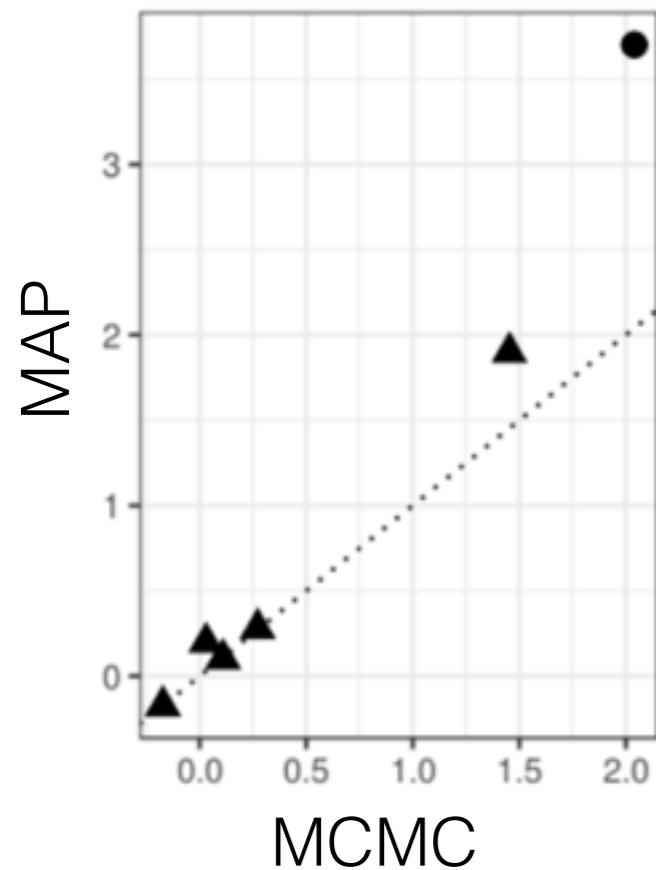
Criteo Online Ads Experiment

Criteo Online Ads Experiment

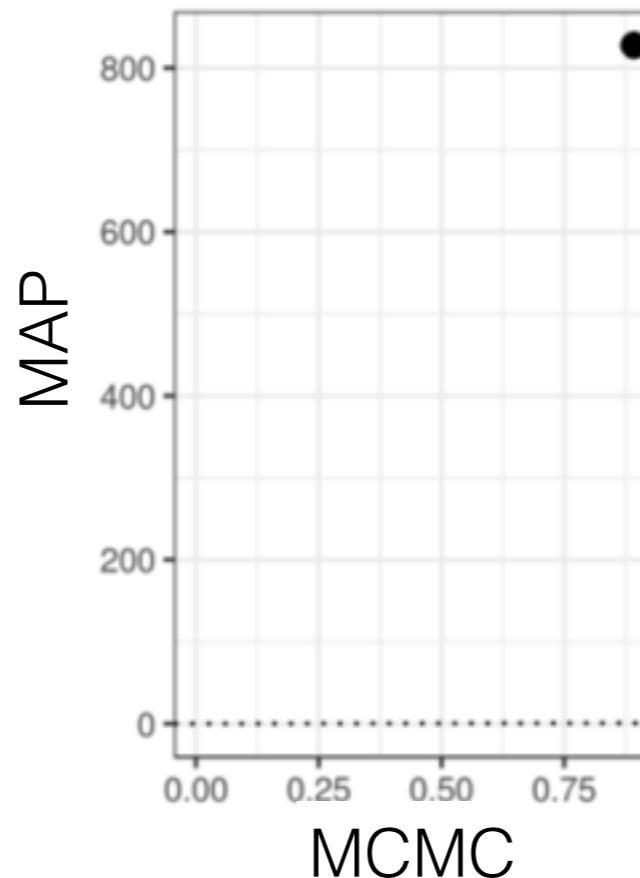
- MAP: **12 s**

Criteo Online Ads Experiment

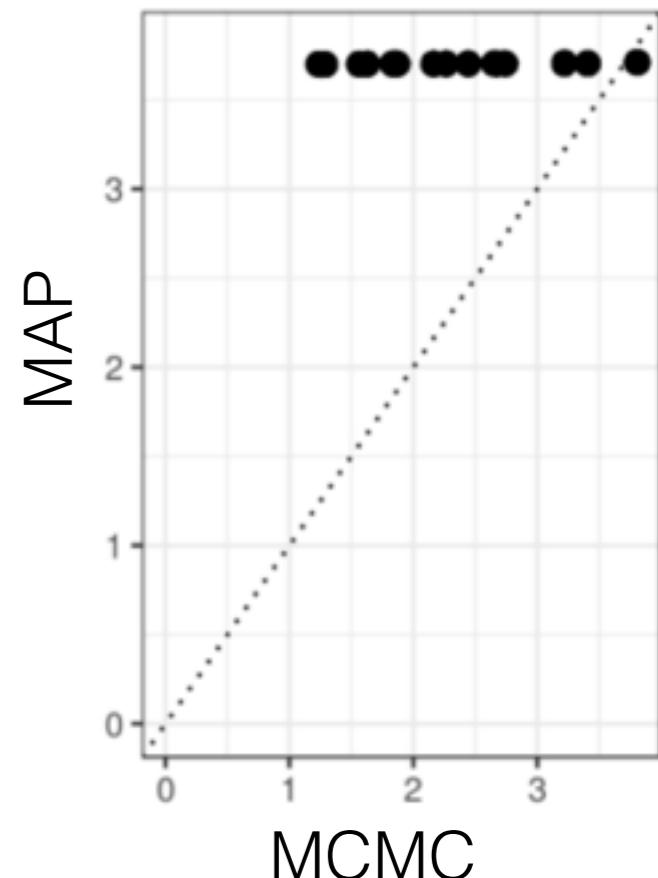
Global parameters ($-\tau$)



Global parameter τ



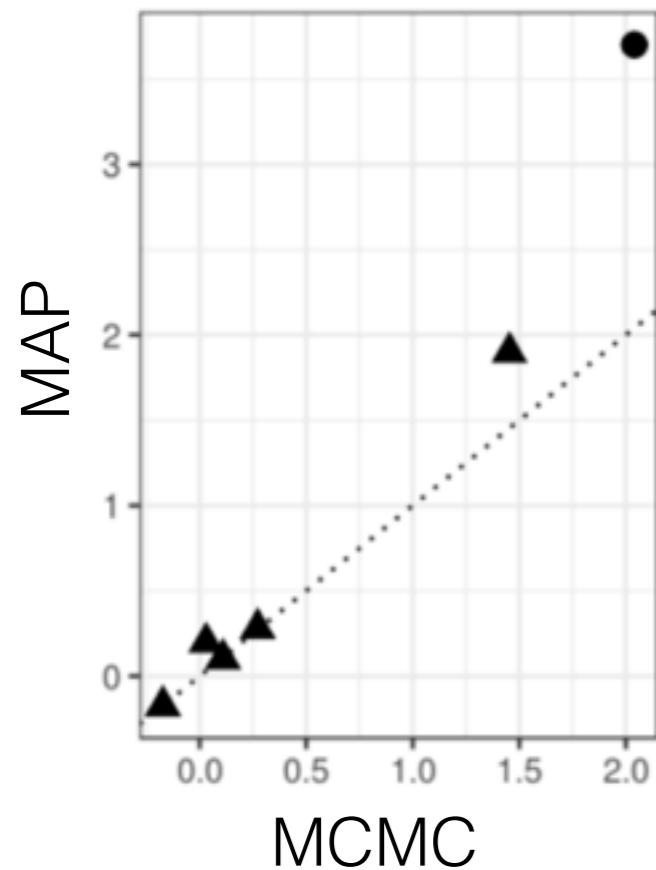
Local parameters



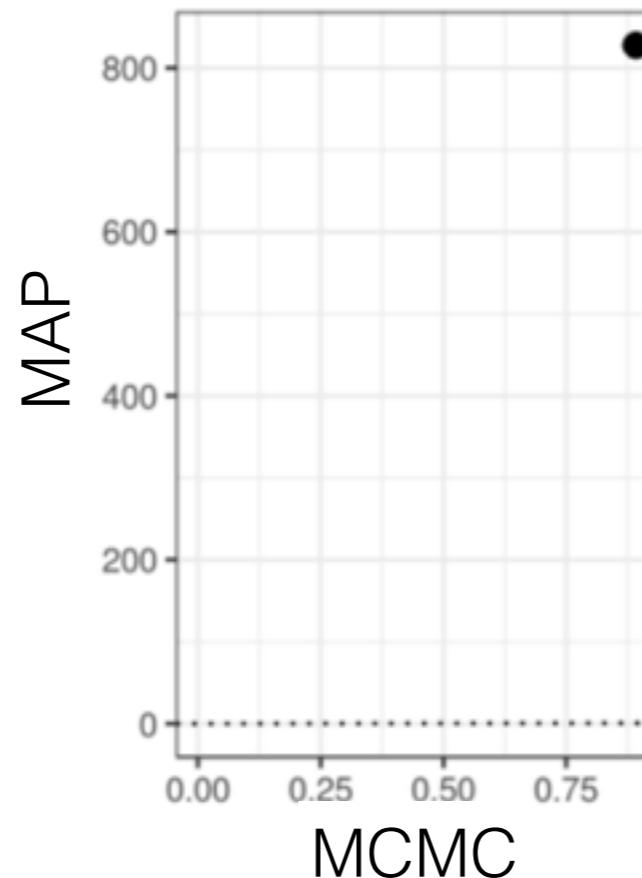
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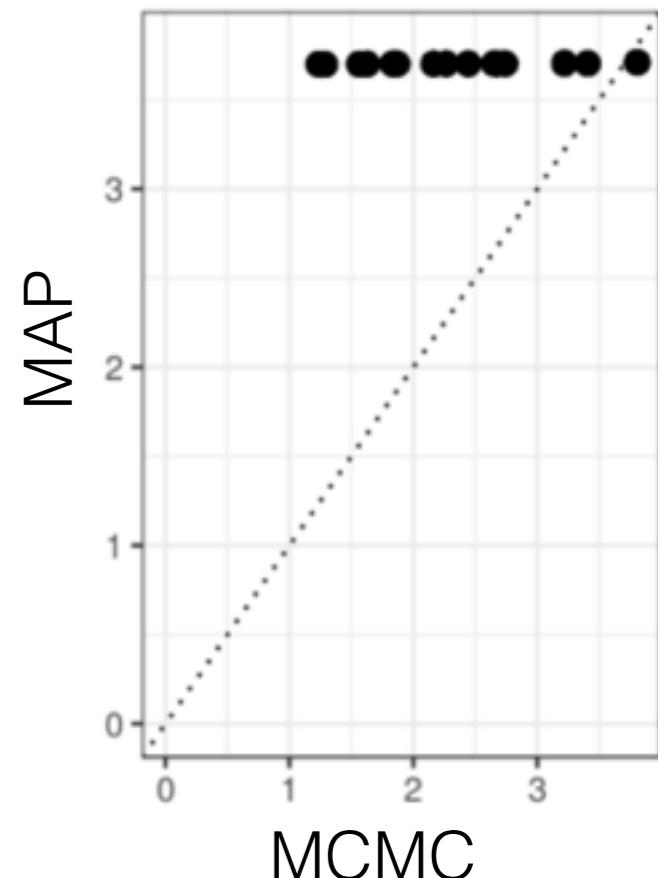
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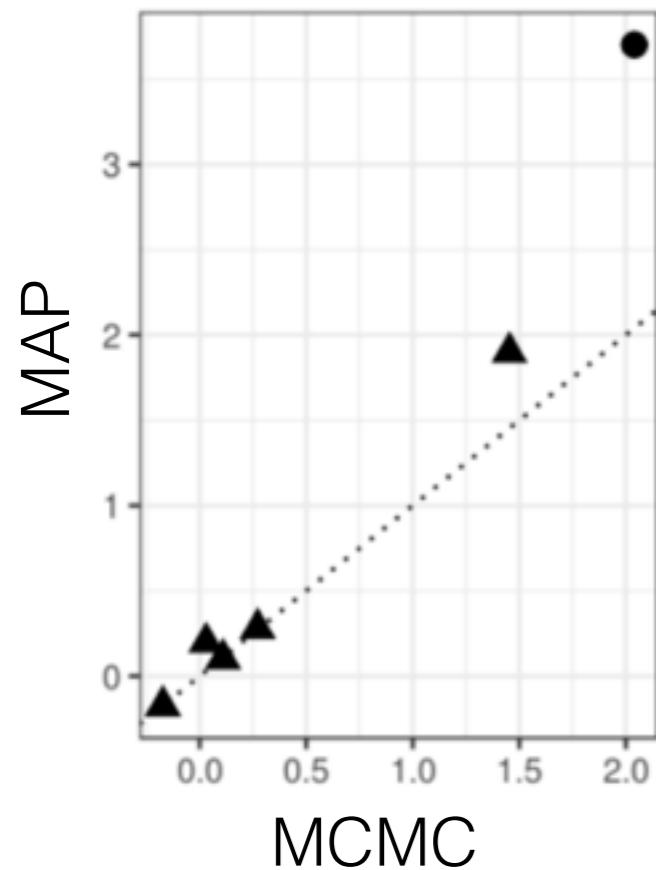
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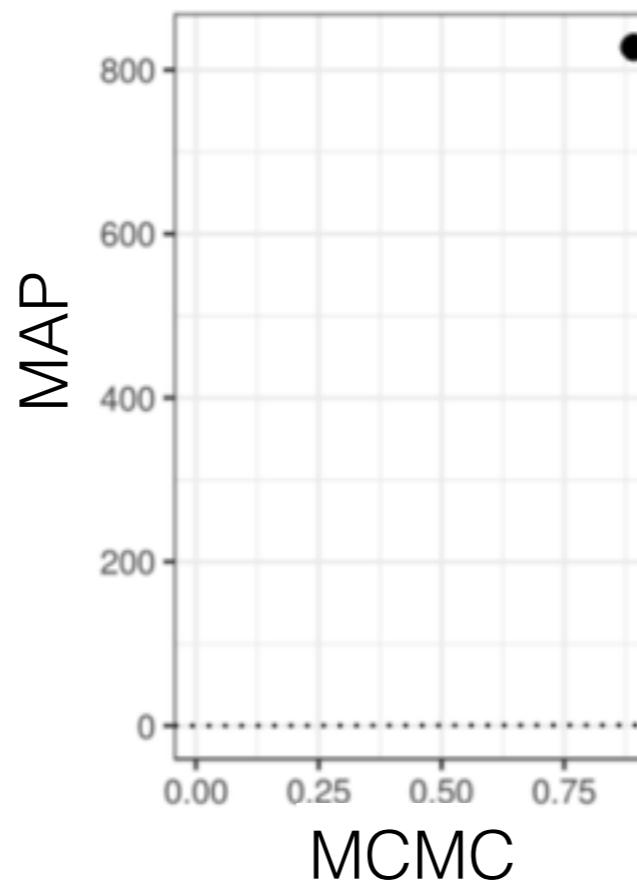
- MAP: **12 s**
- MFVB: **57 s**

Criteo Online Ads Experiment

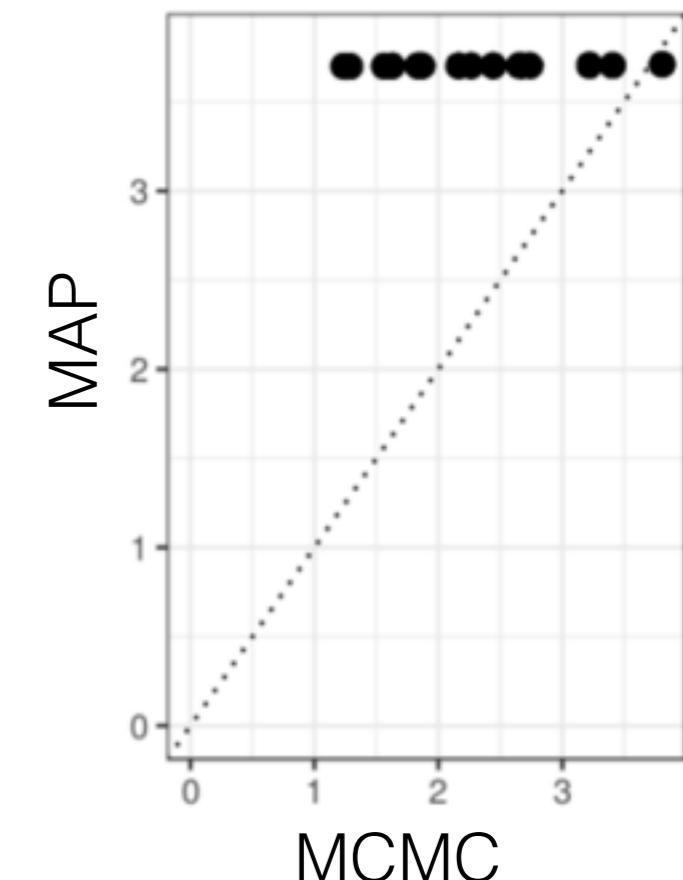
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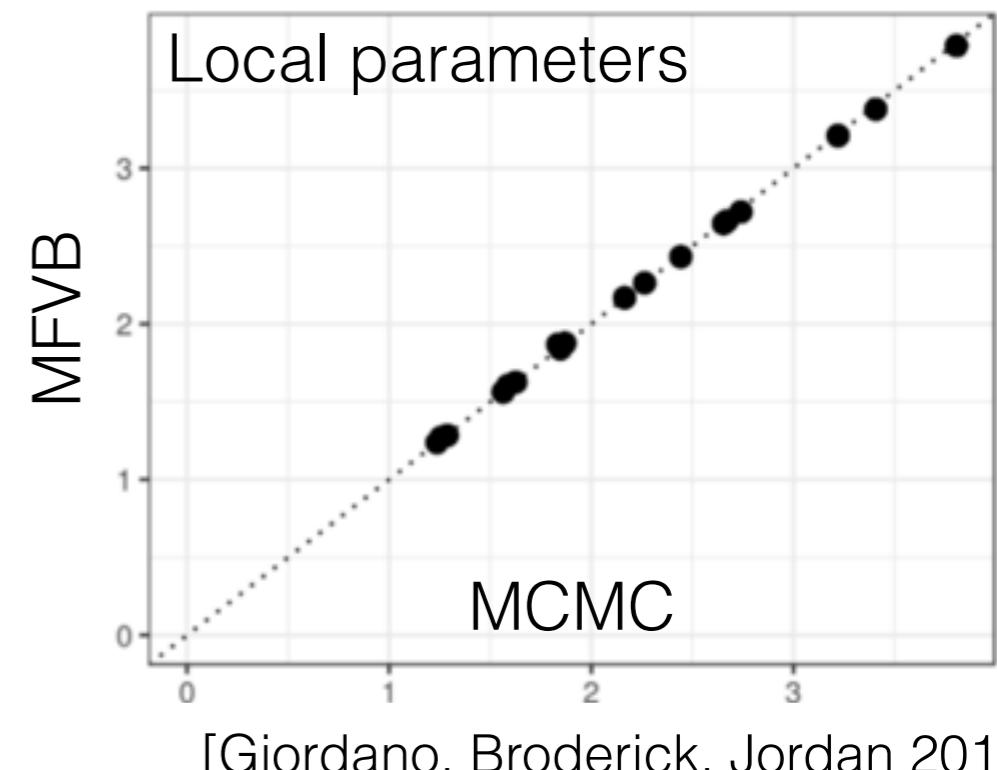
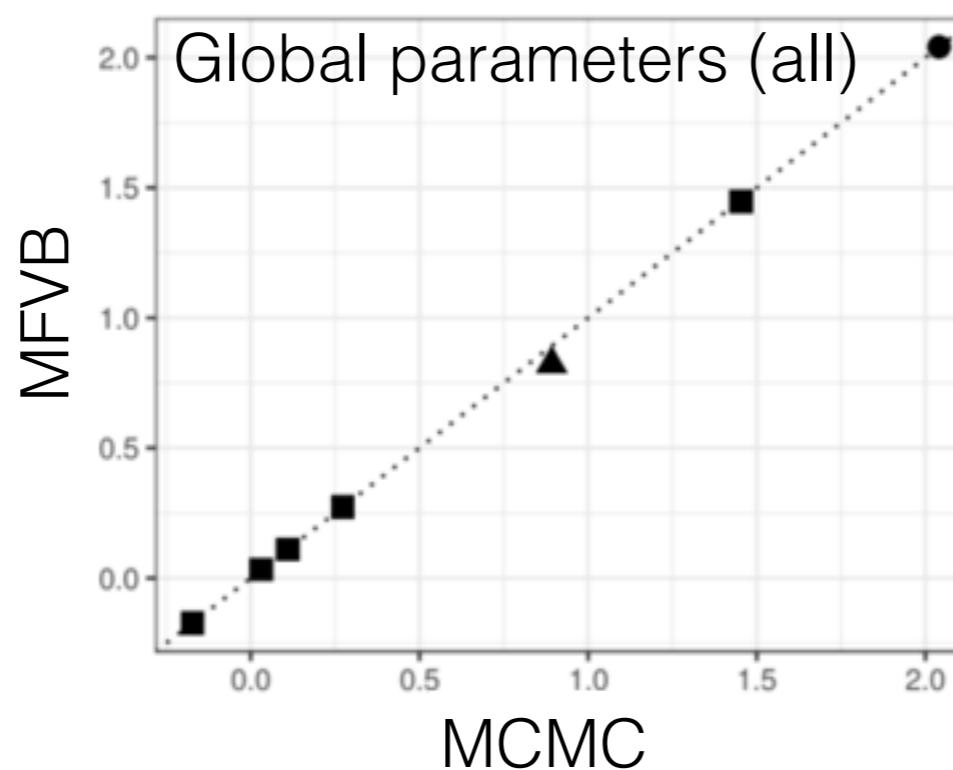
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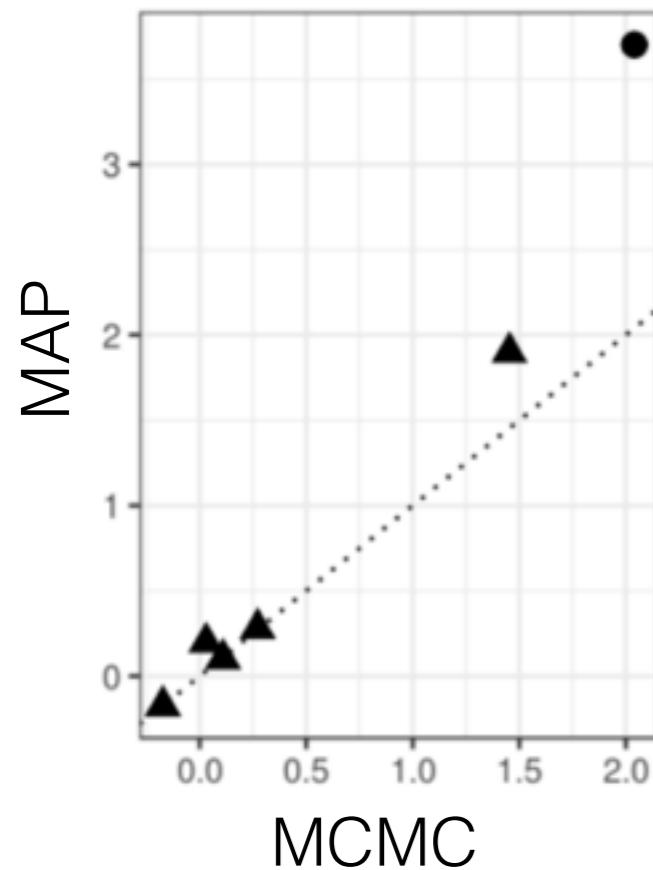


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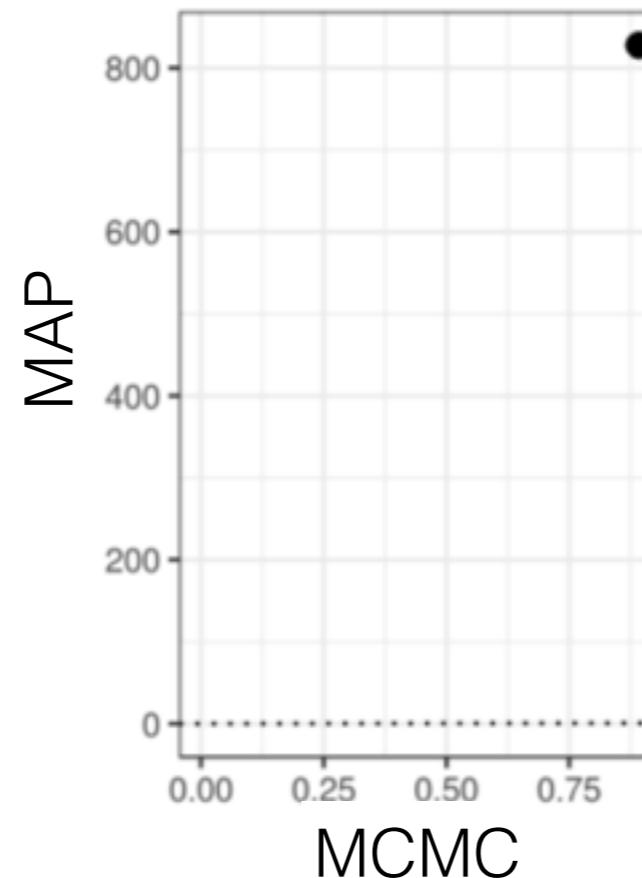


Criteo Online Ads Experiment

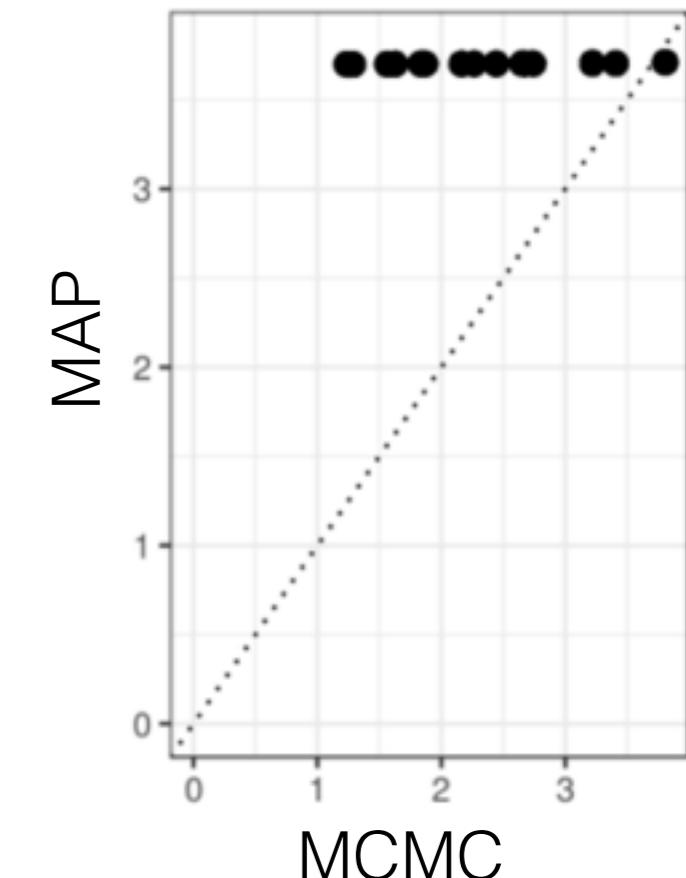
Global parameters ($-\tau$)



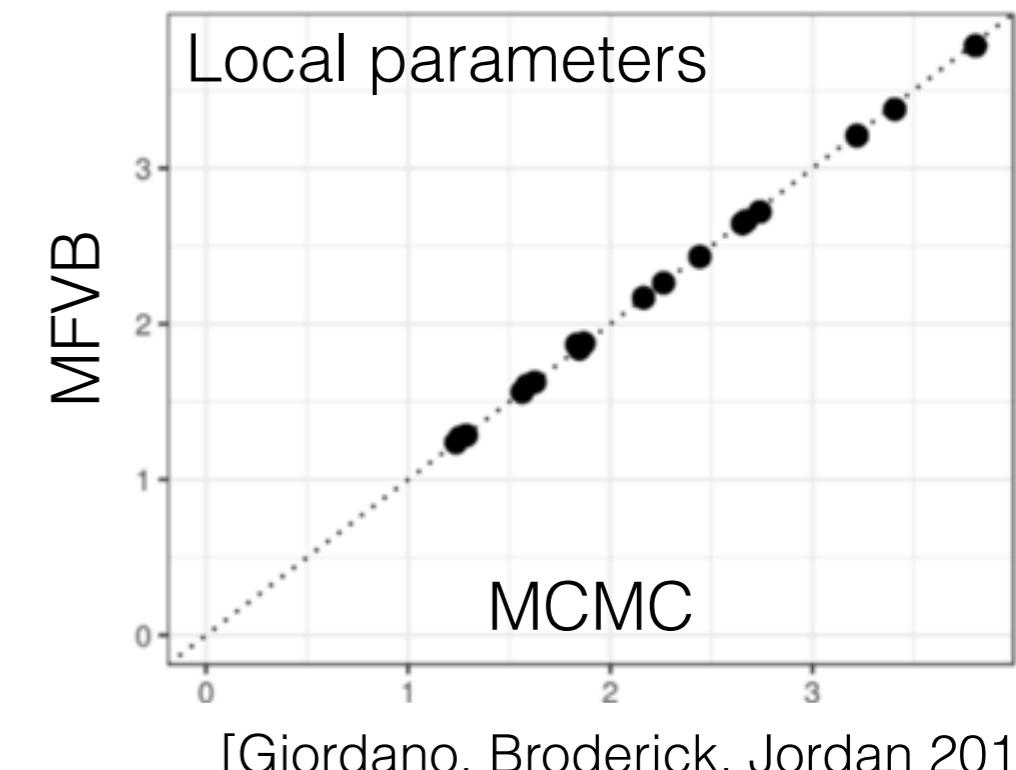
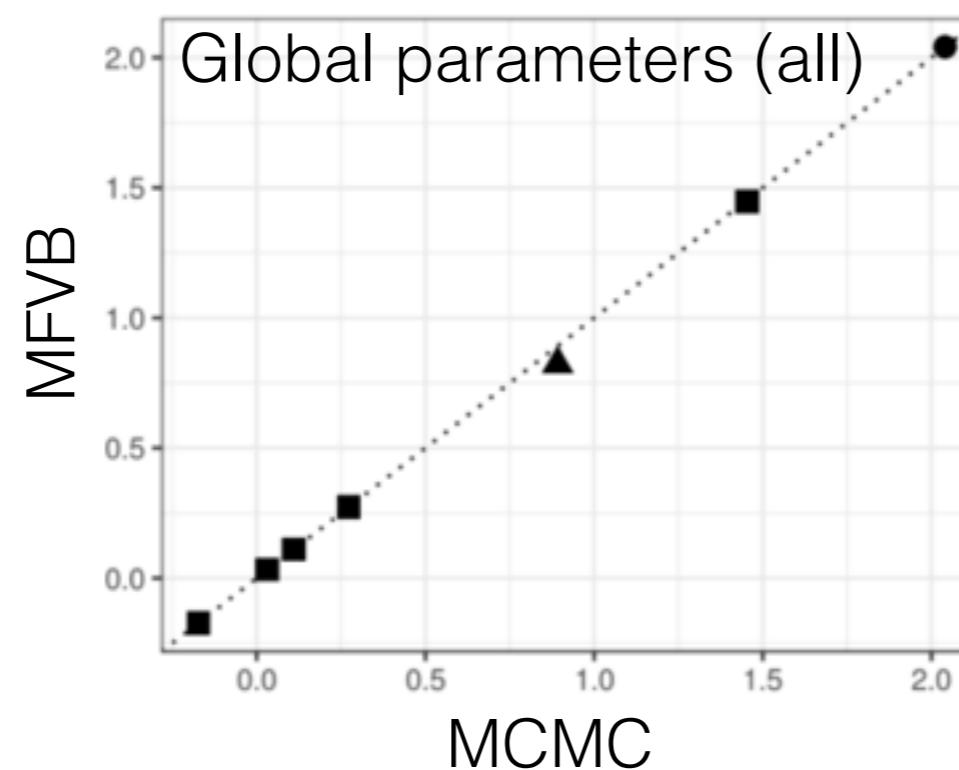
Global parameter τ



Local parameters



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



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
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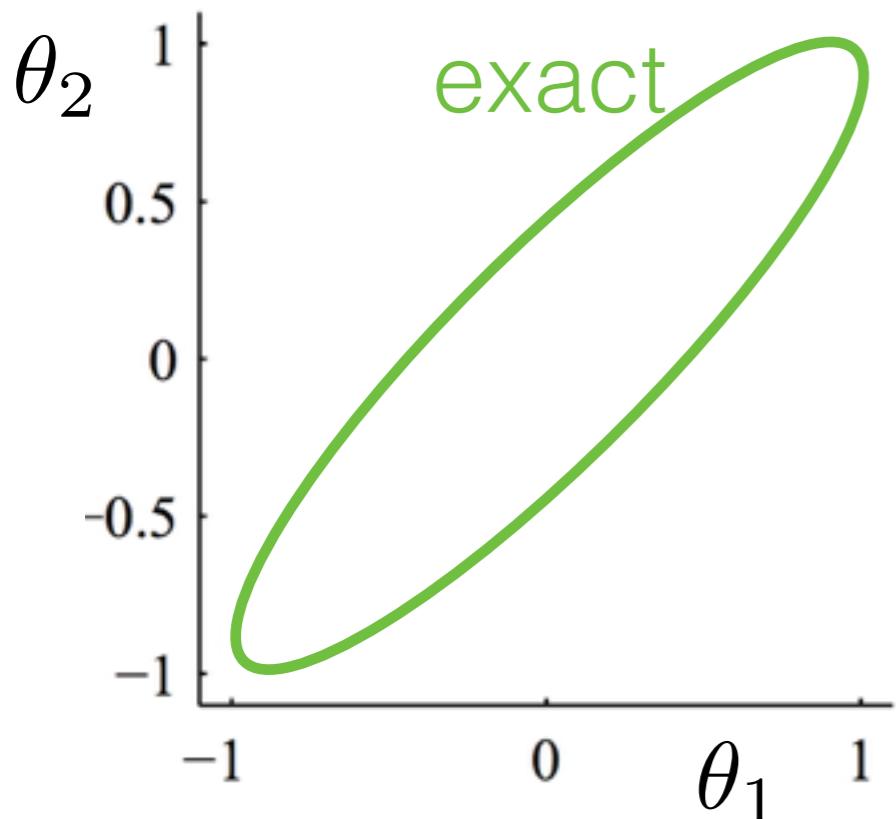
What about uncertainty?

$$KL(q||p(\cdot|x)) = \int_{\theta} q(\theta) \log \frac{q(\theta)}{p(\theta|x)} d\theta$$
$$q(\theta) = \prod_{j=1}^J q_j(\theta_j)$$

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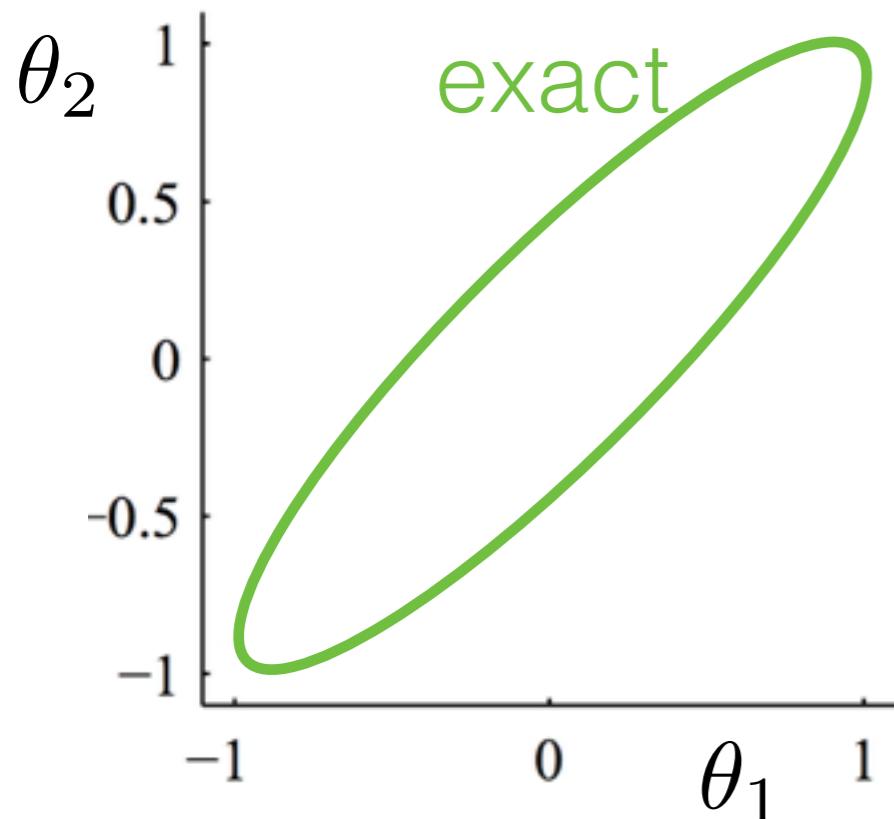


[Turner & Sahani
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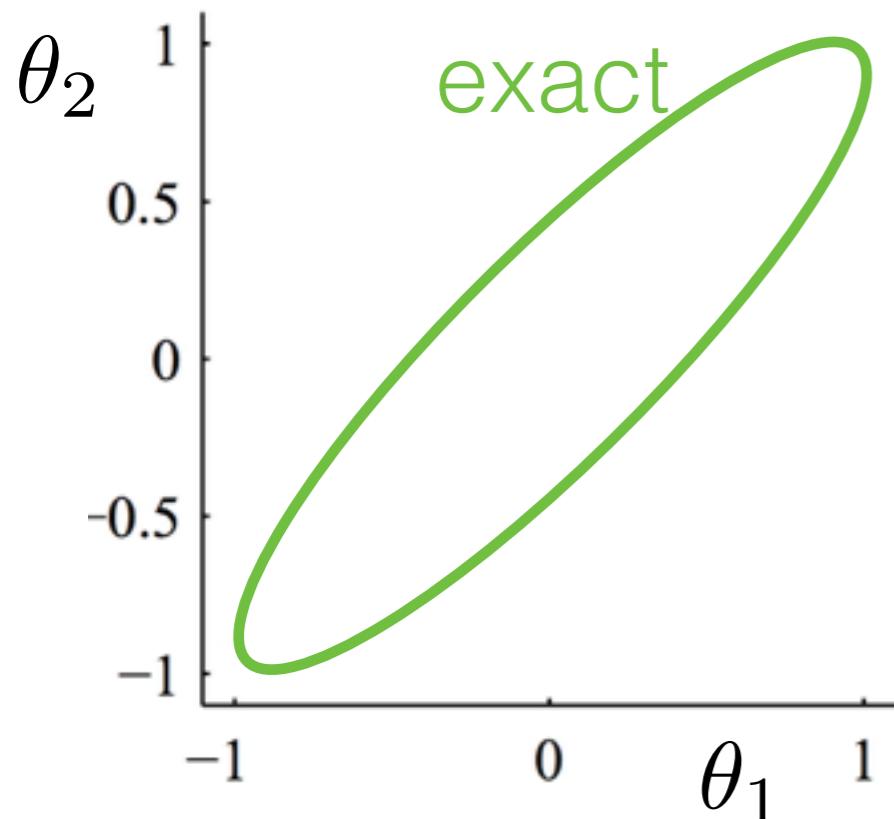
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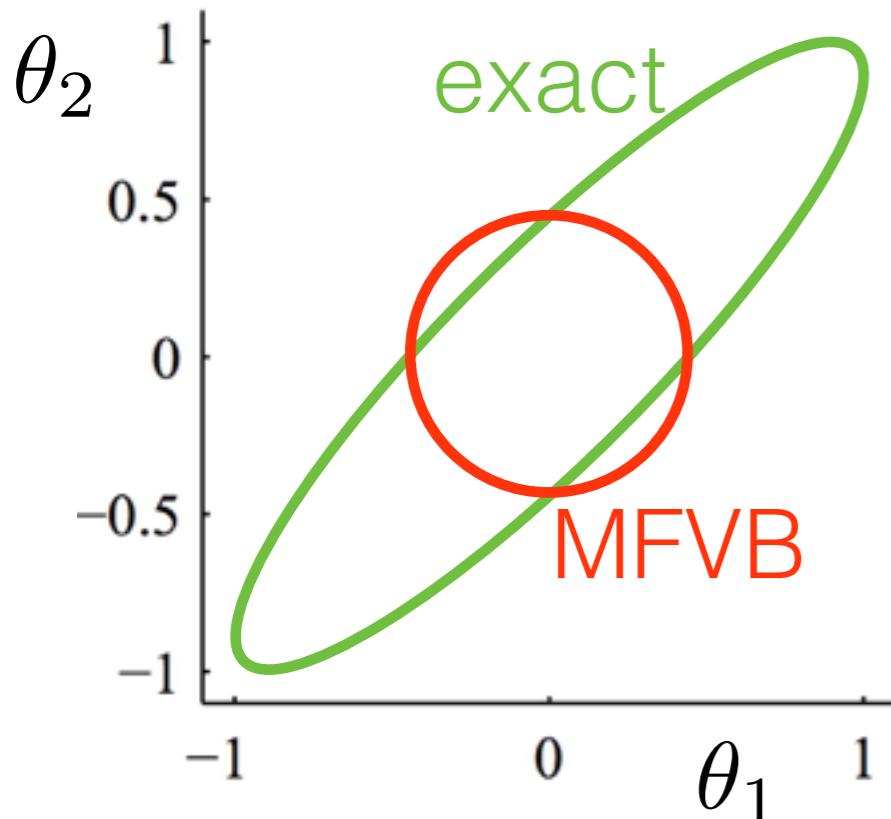
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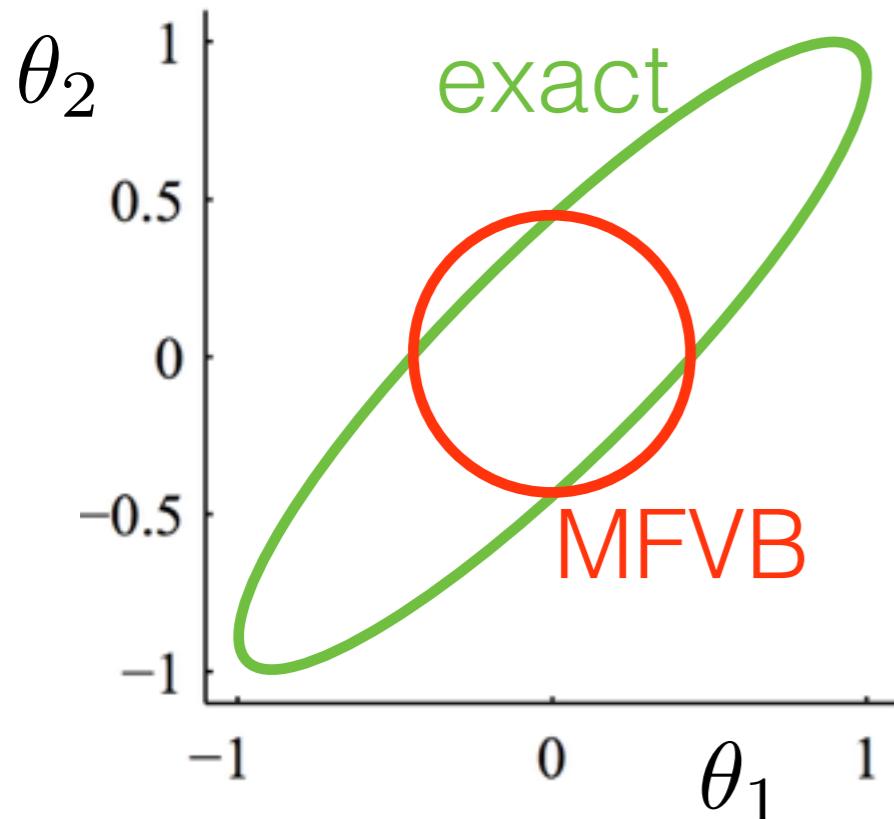
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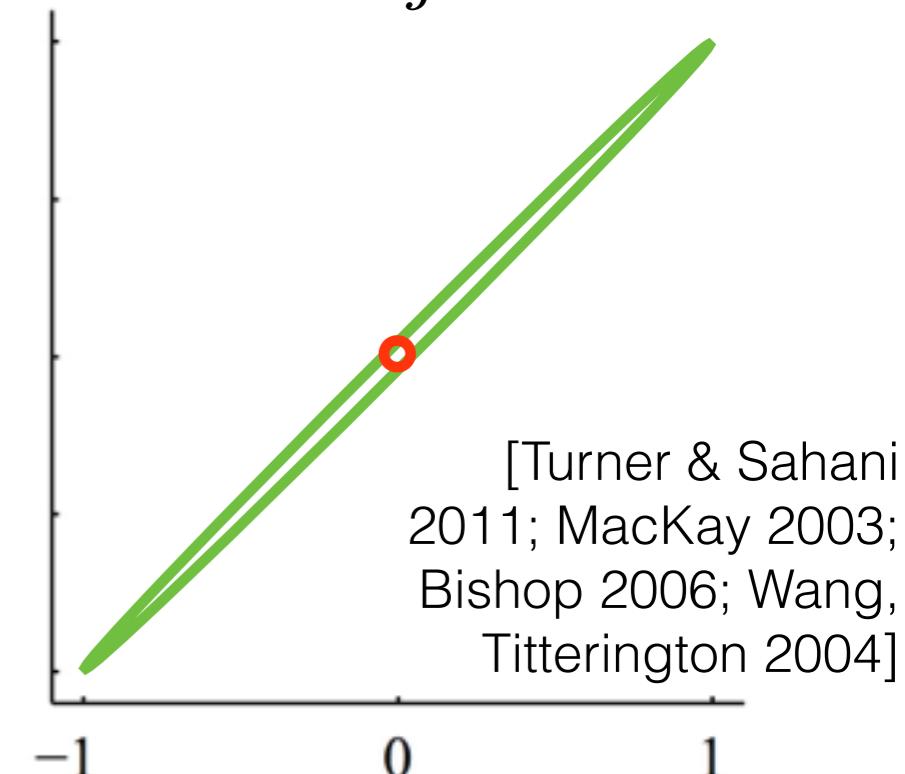
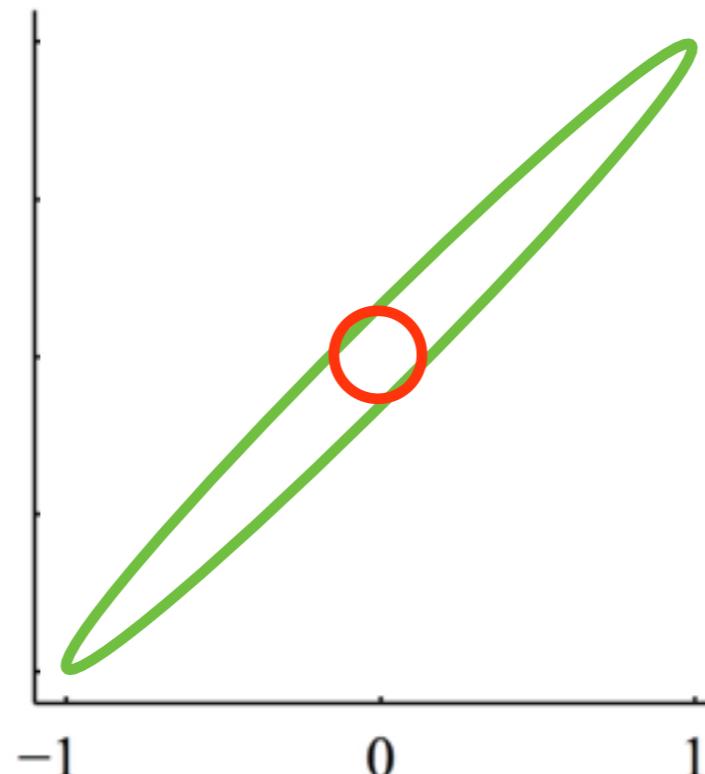
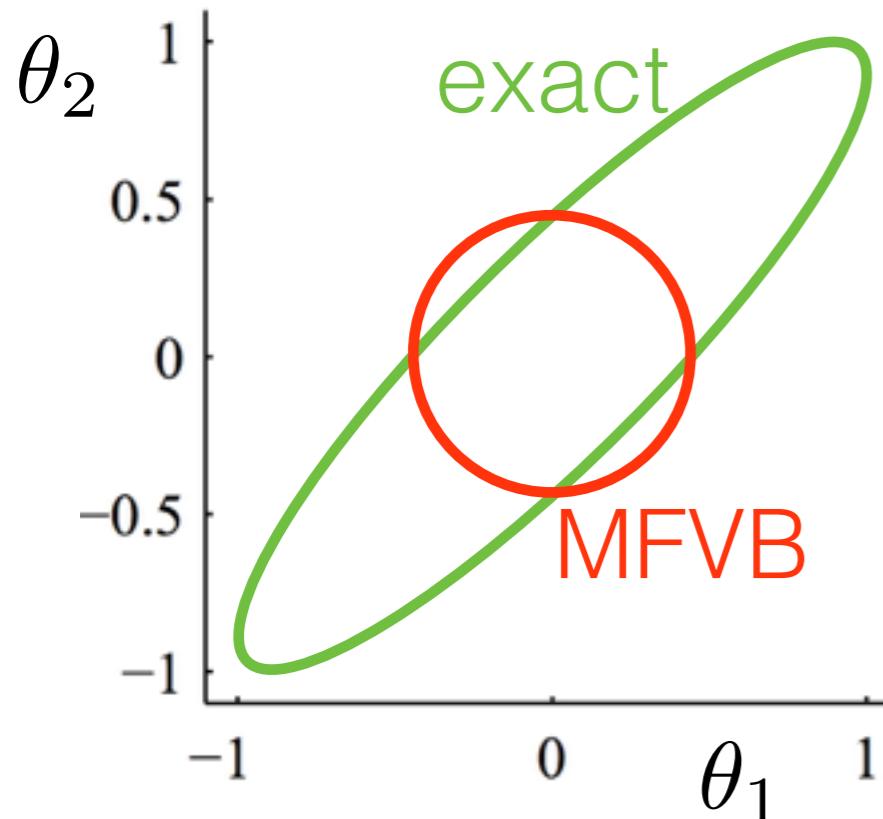
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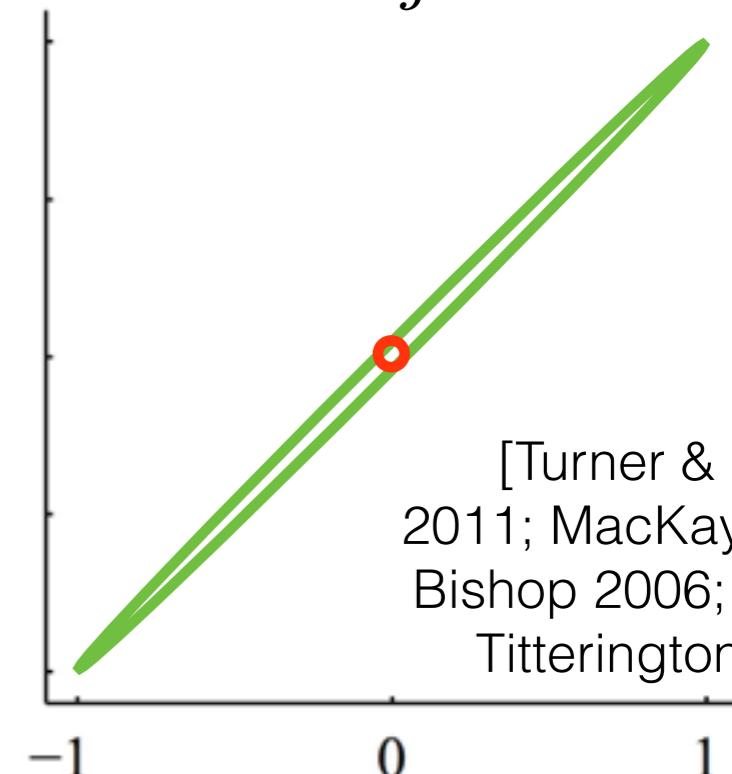
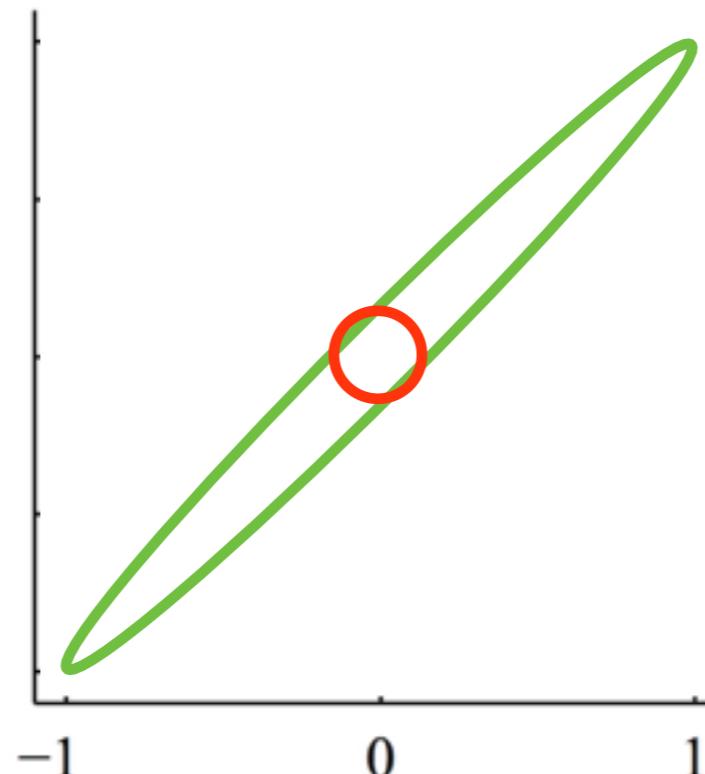
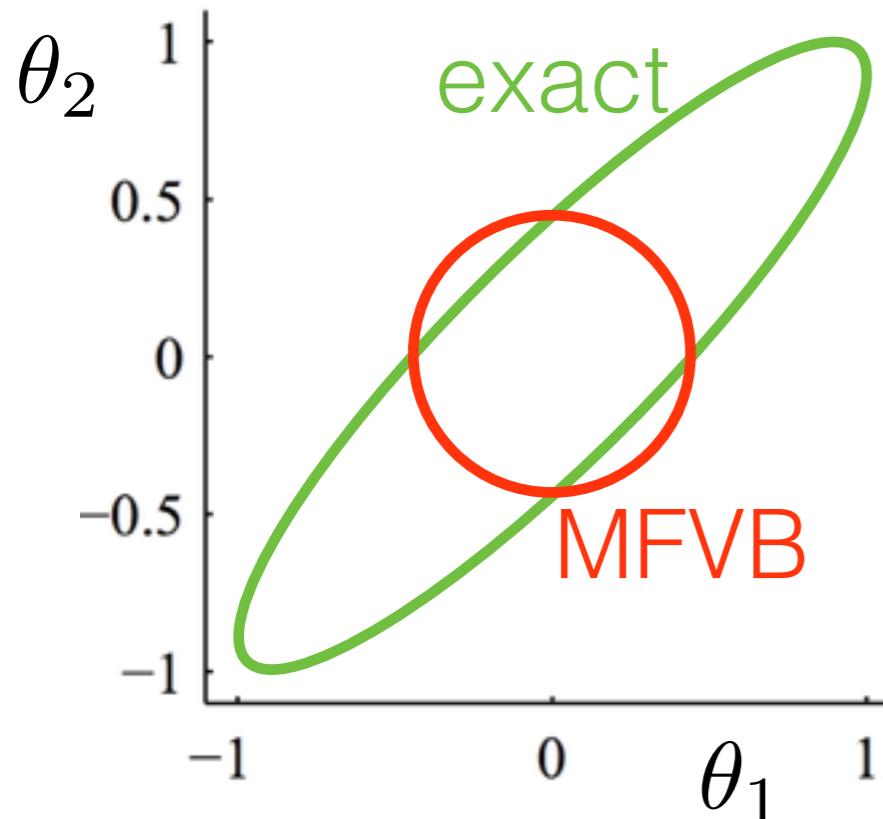


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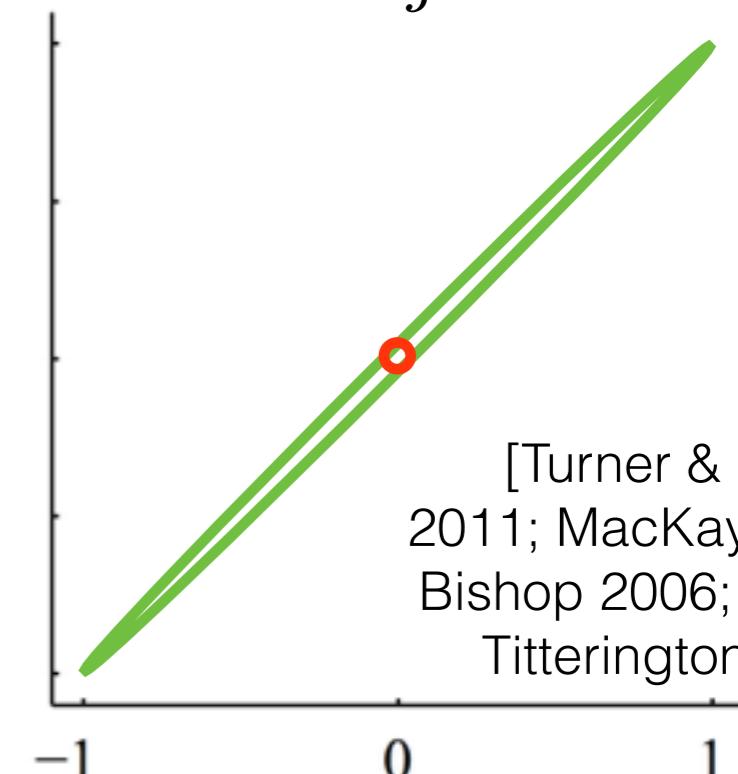
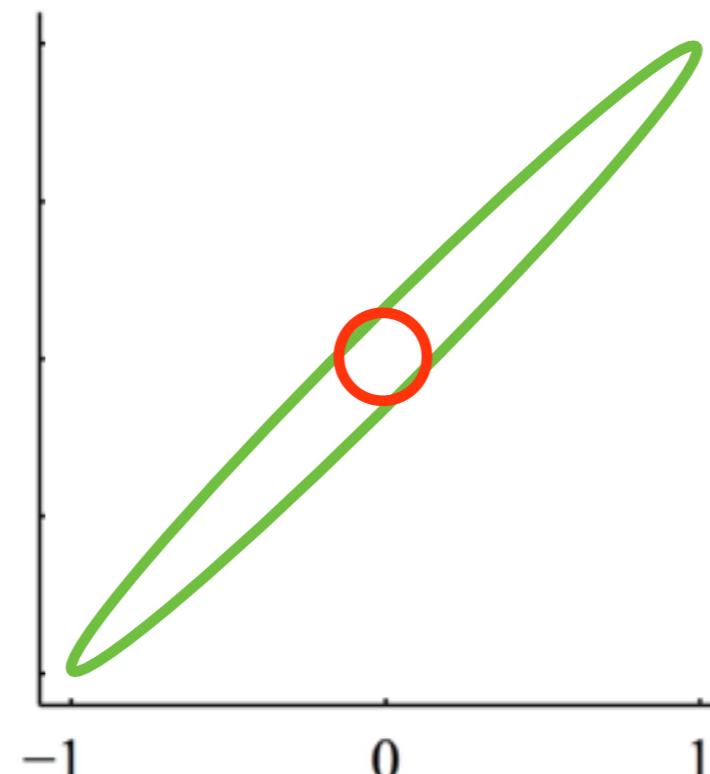
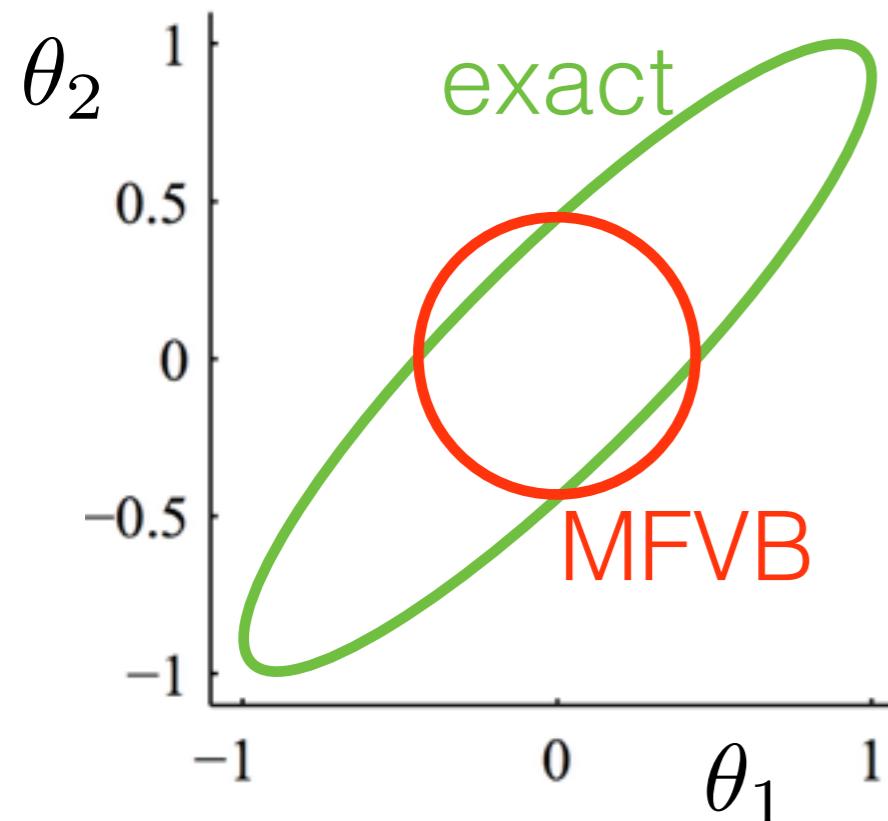


- Underestimates variance (sometimes severely)
- No covariance estimates
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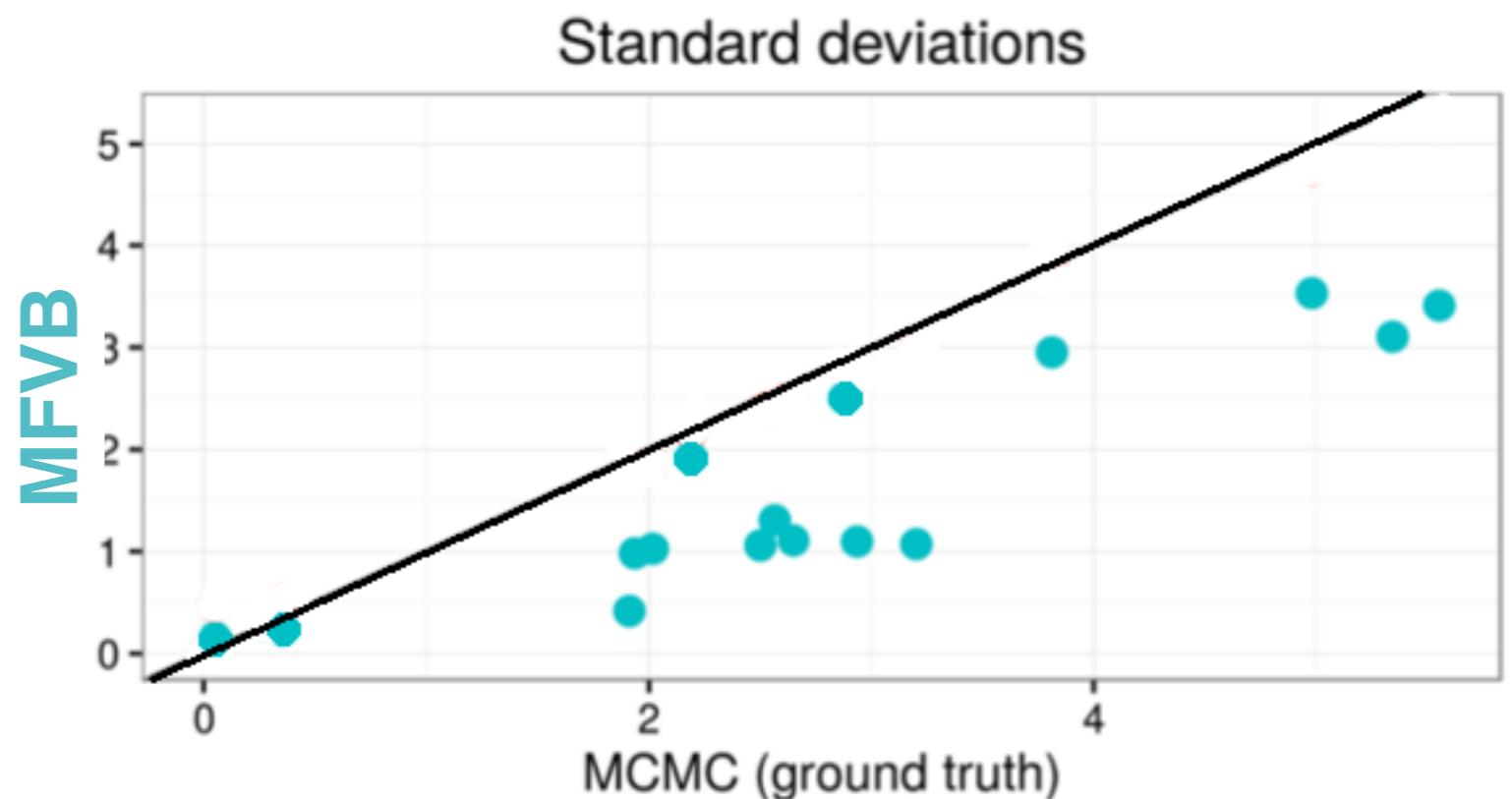
- Underestimates variance (sometimes severely)
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- Exercise: derive exact (closed) form of q^*

What about uncertainty?

- Microcredit

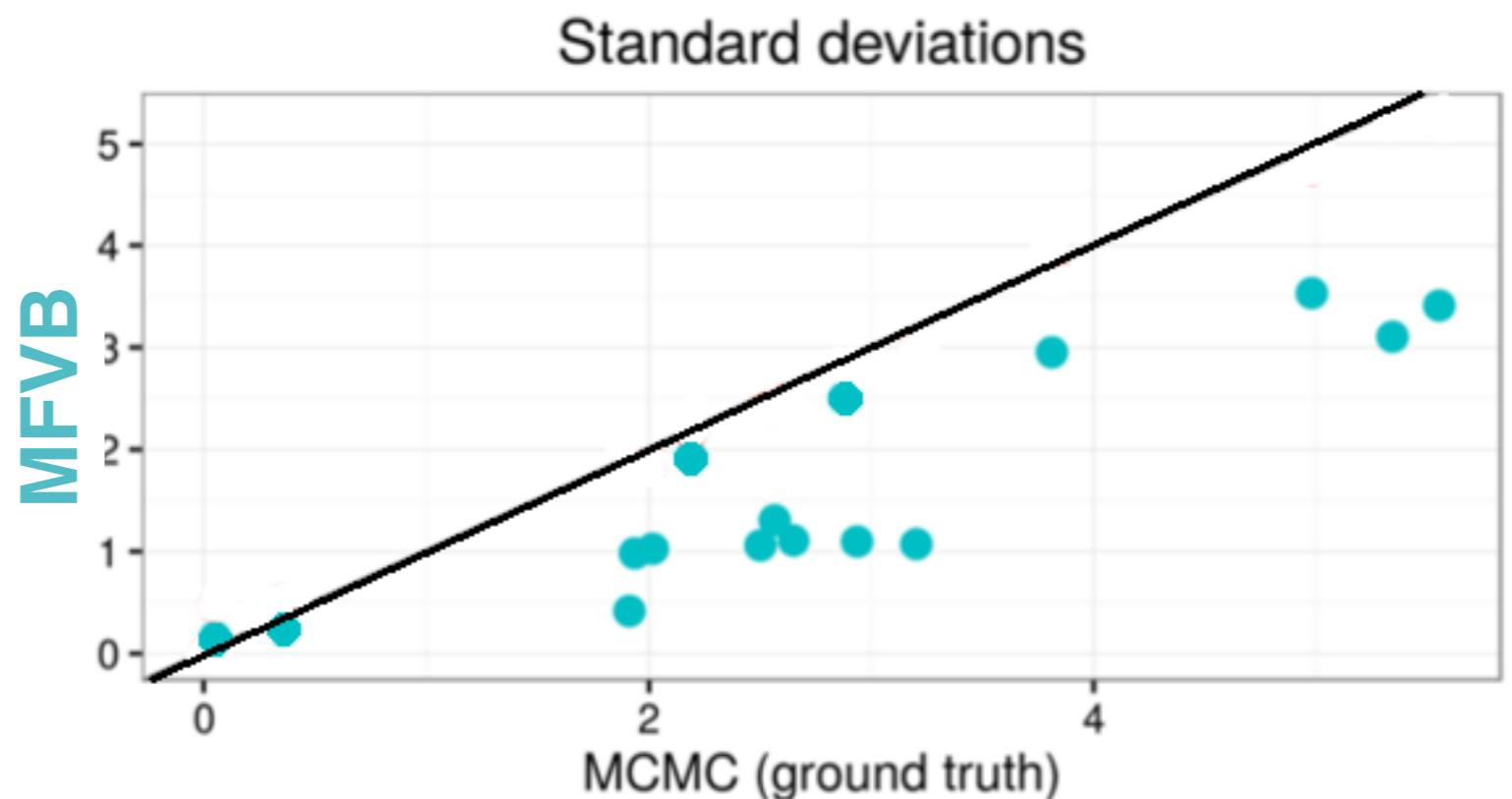
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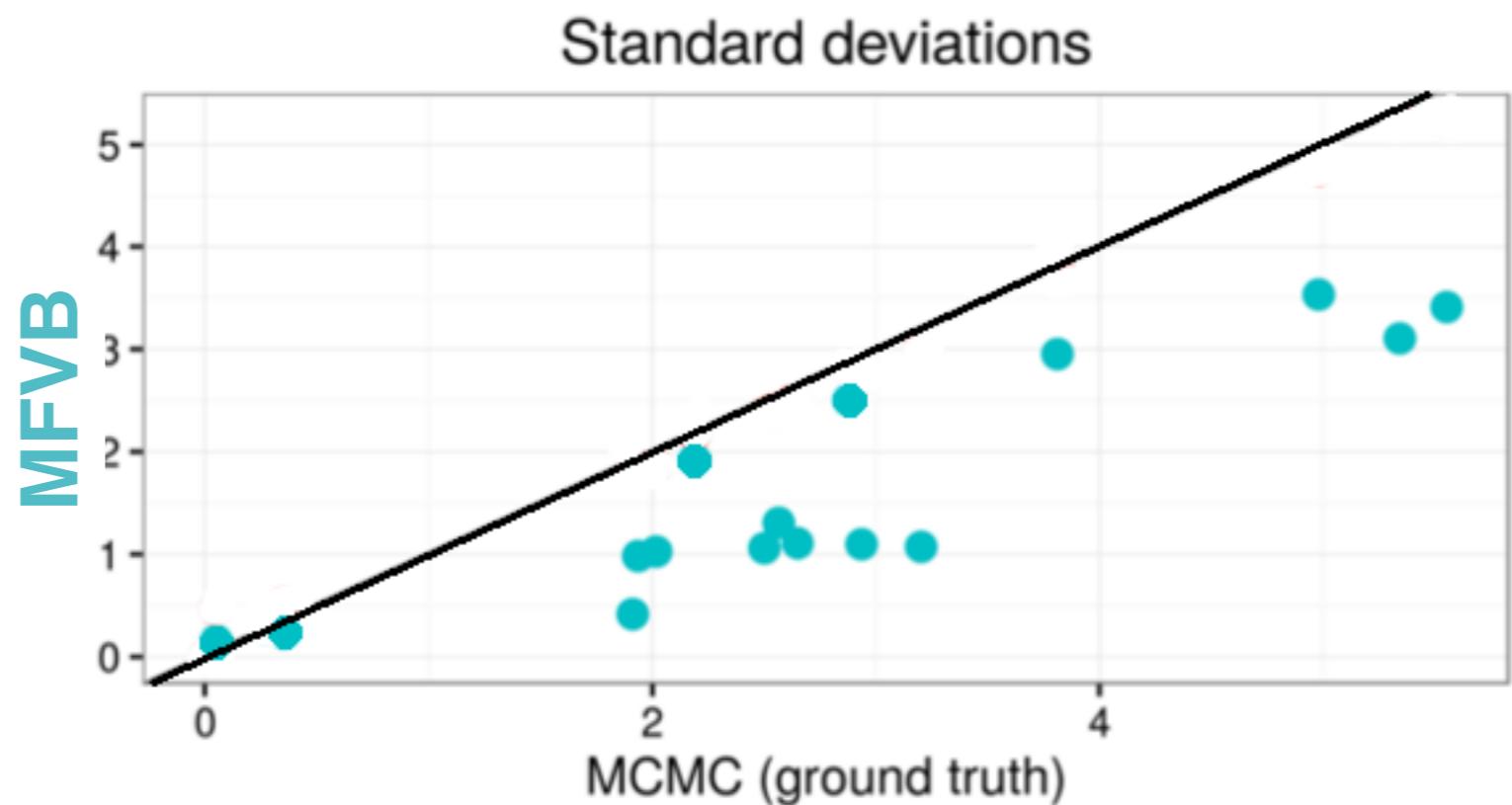
What about uncertainty?

- Microcredit effect
- τ mean:
3.08 USD PPP



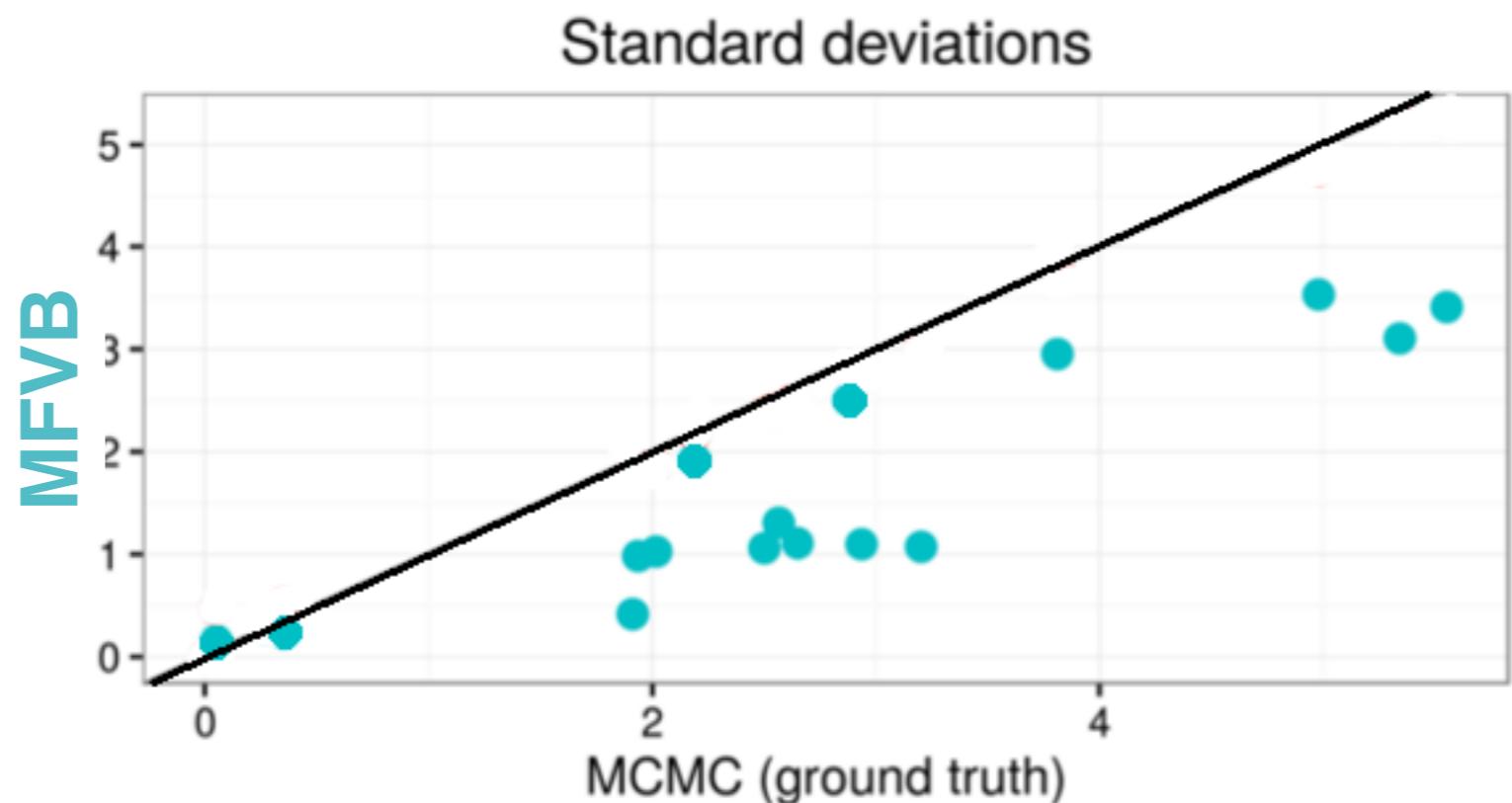
What about uncertainty?

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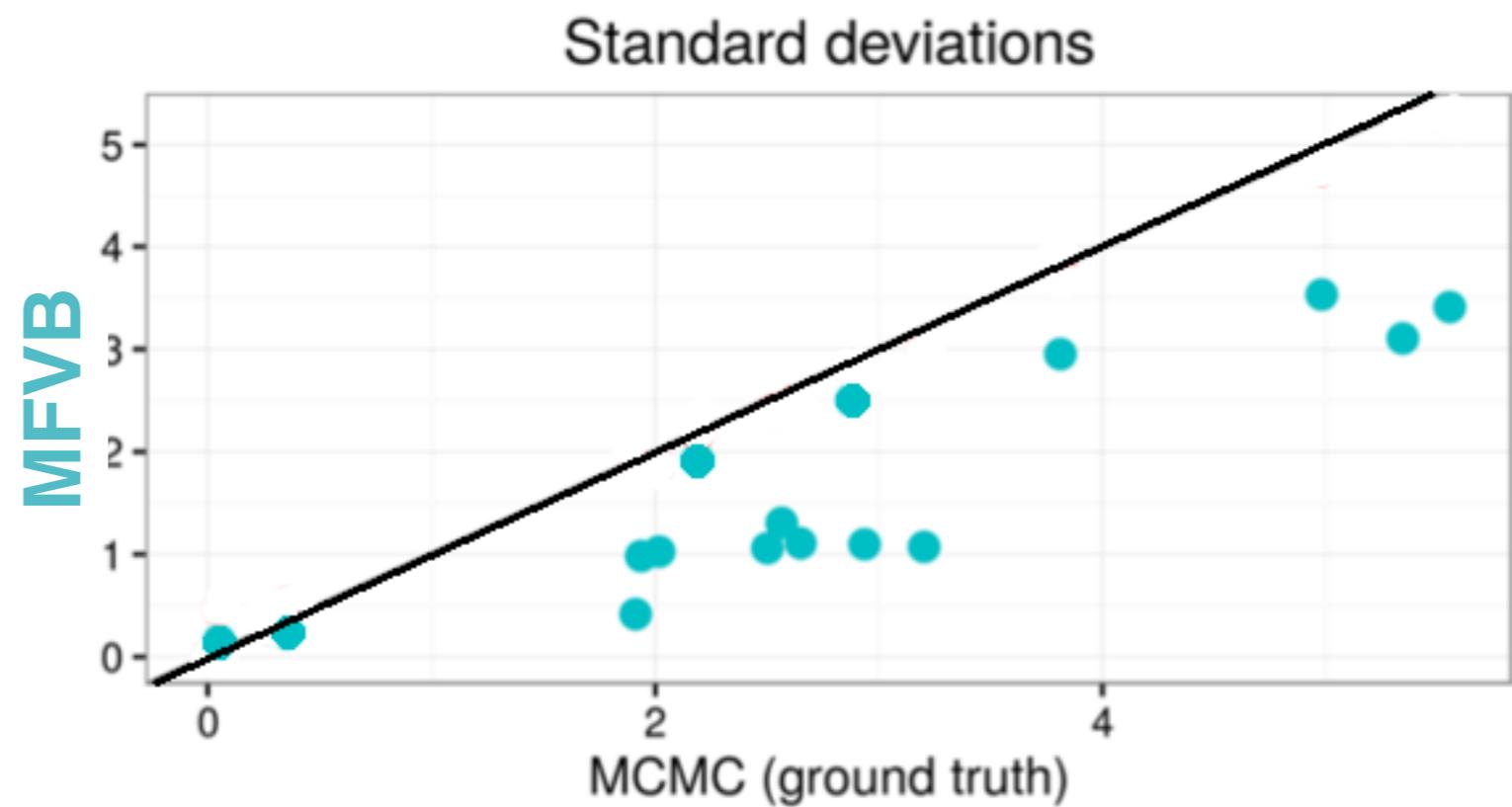
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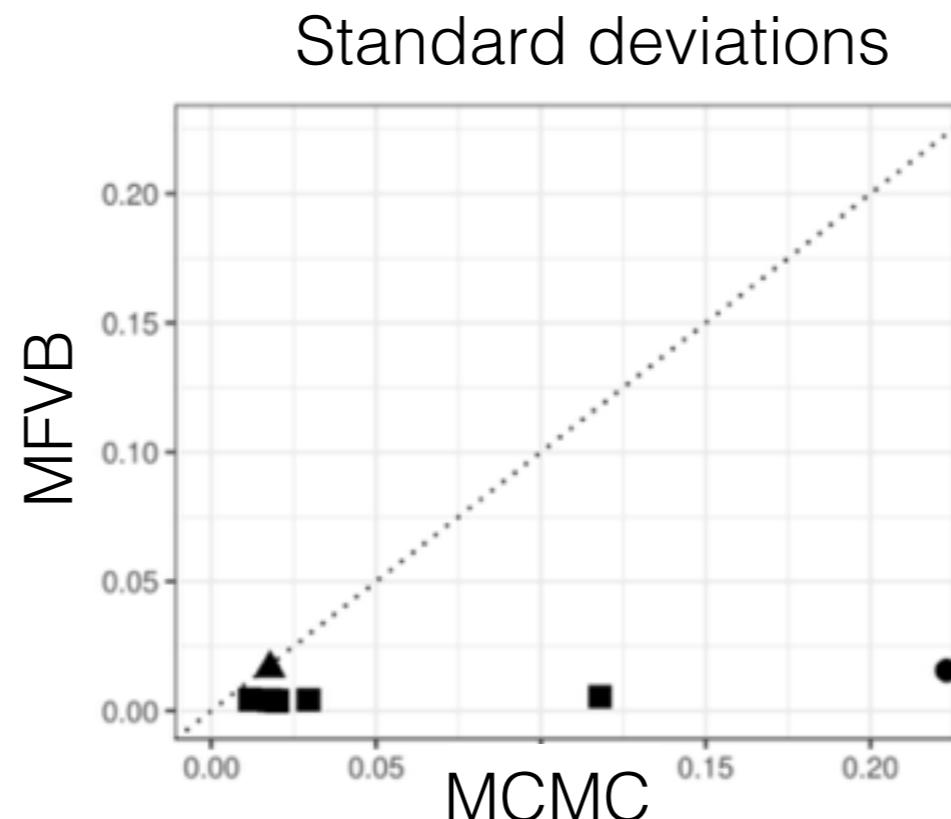


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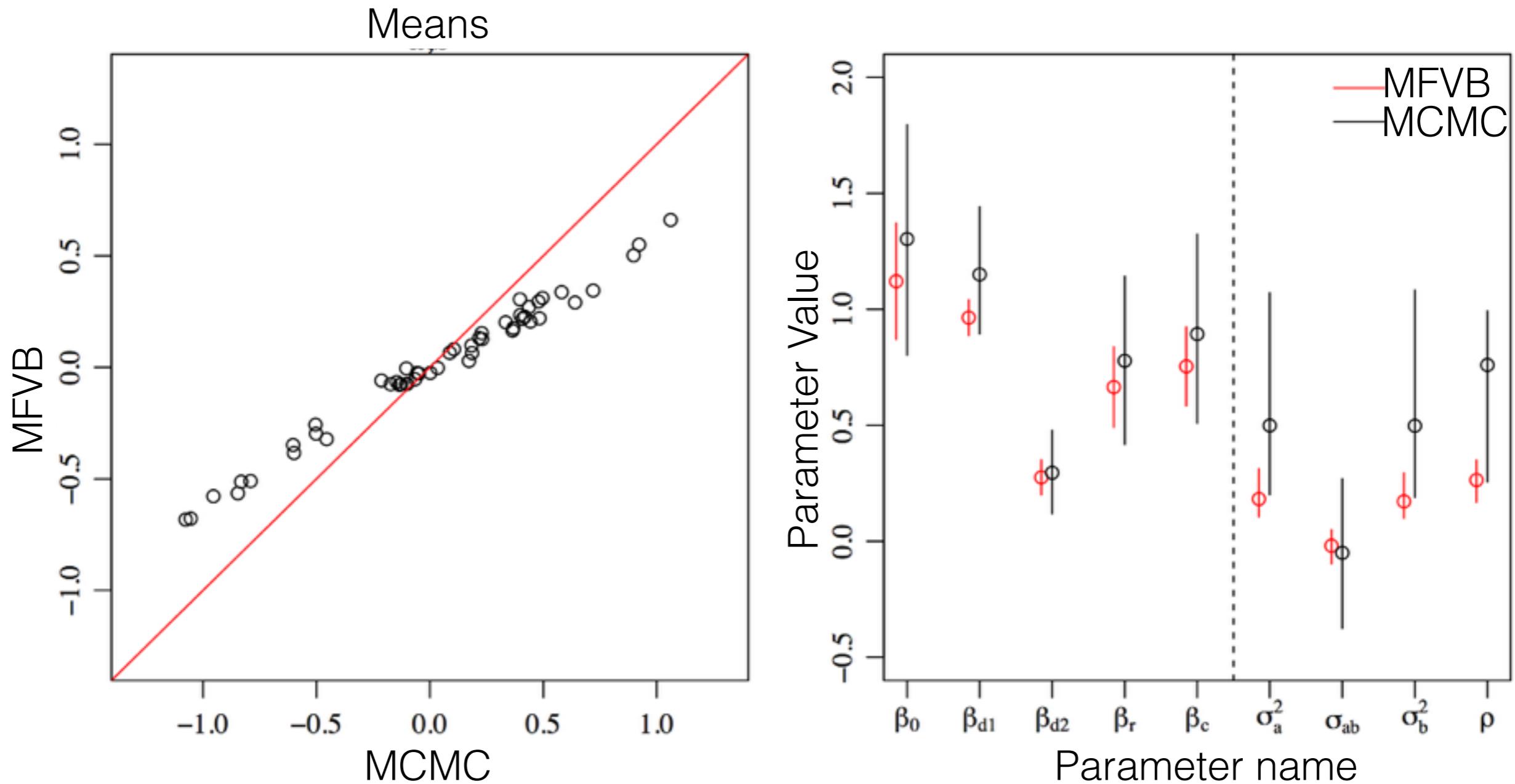
- Criteo
online ads
experiment



What about means?

- Model for relational data with covariates
- 1000+ nodes; MCMC > 1 day

[Fosdick 2013, Ch 4]



[Fosdick 2013, Ch 4, Fig 4.3]

Posterior means: revisited

- Want to predict college GPA y_n

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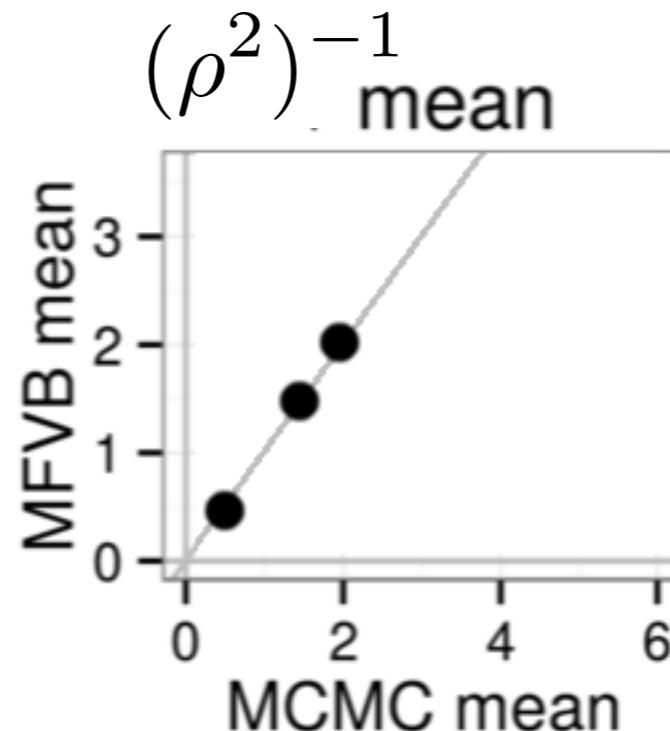
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 $\beta \sim \mathcal{N}(0, \Sigma) \quad (\rho^2)^{-1} \sim \text{Gamma}(a_{\rho^2}, b_{\rho^2})$

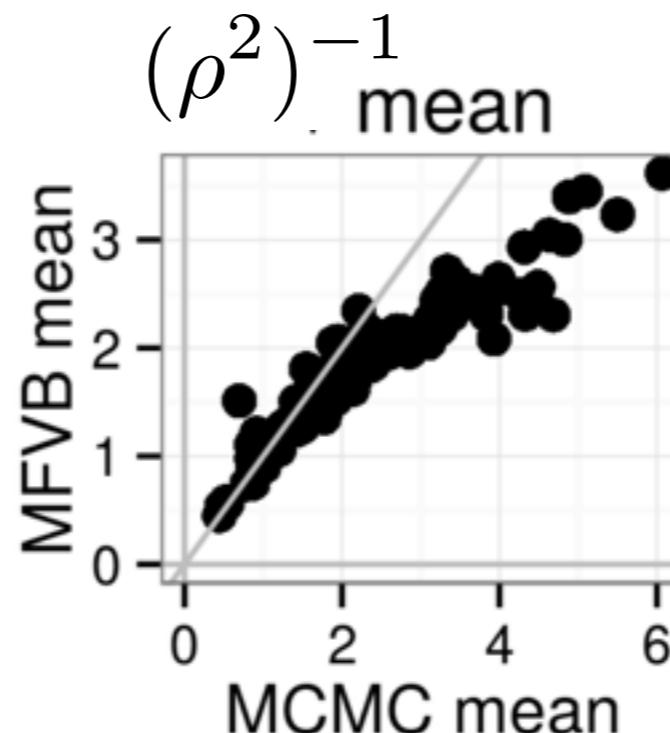
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- Data simulated from model (100 data sets, 300 data points):



What can we do?

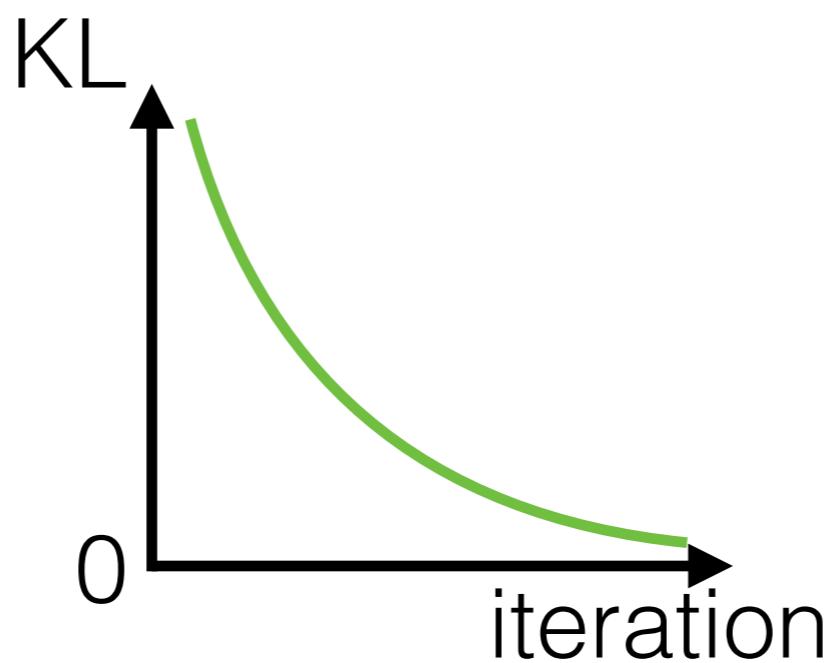
- Reliable diagnostics

What can we do?

- Reliable diagnostics
 - KL vs ELBO

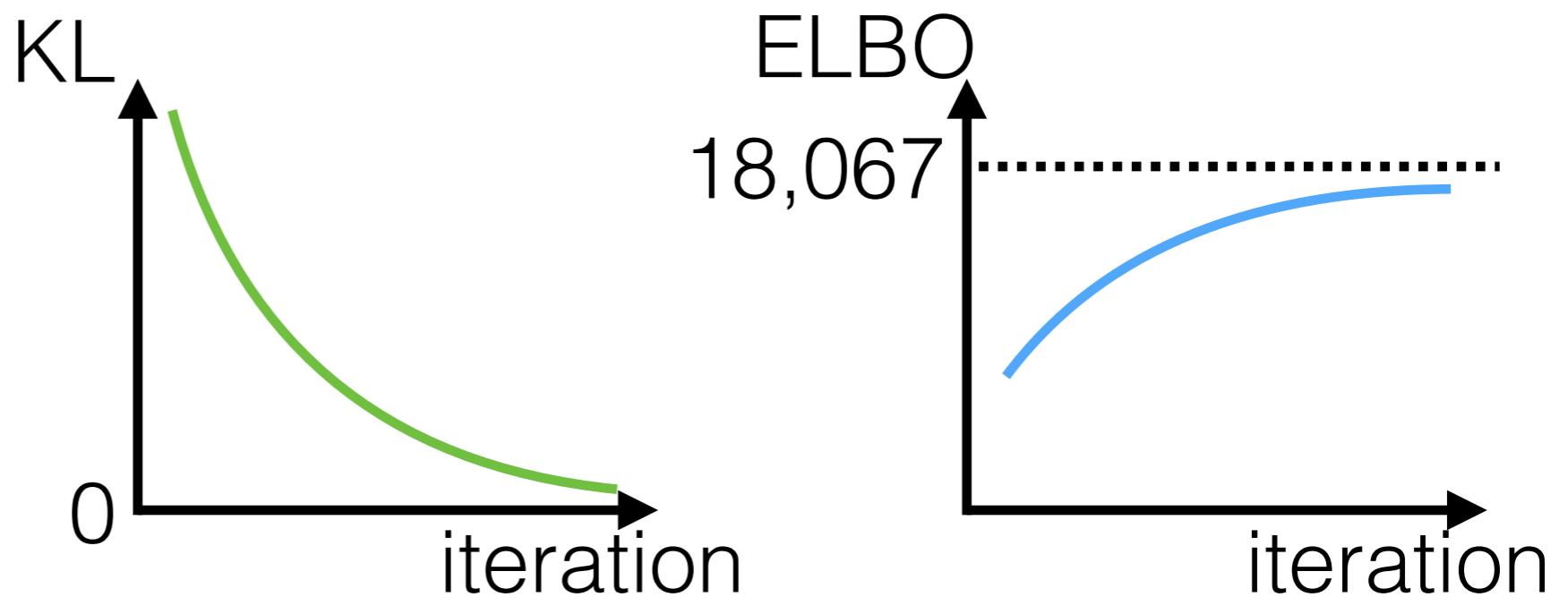
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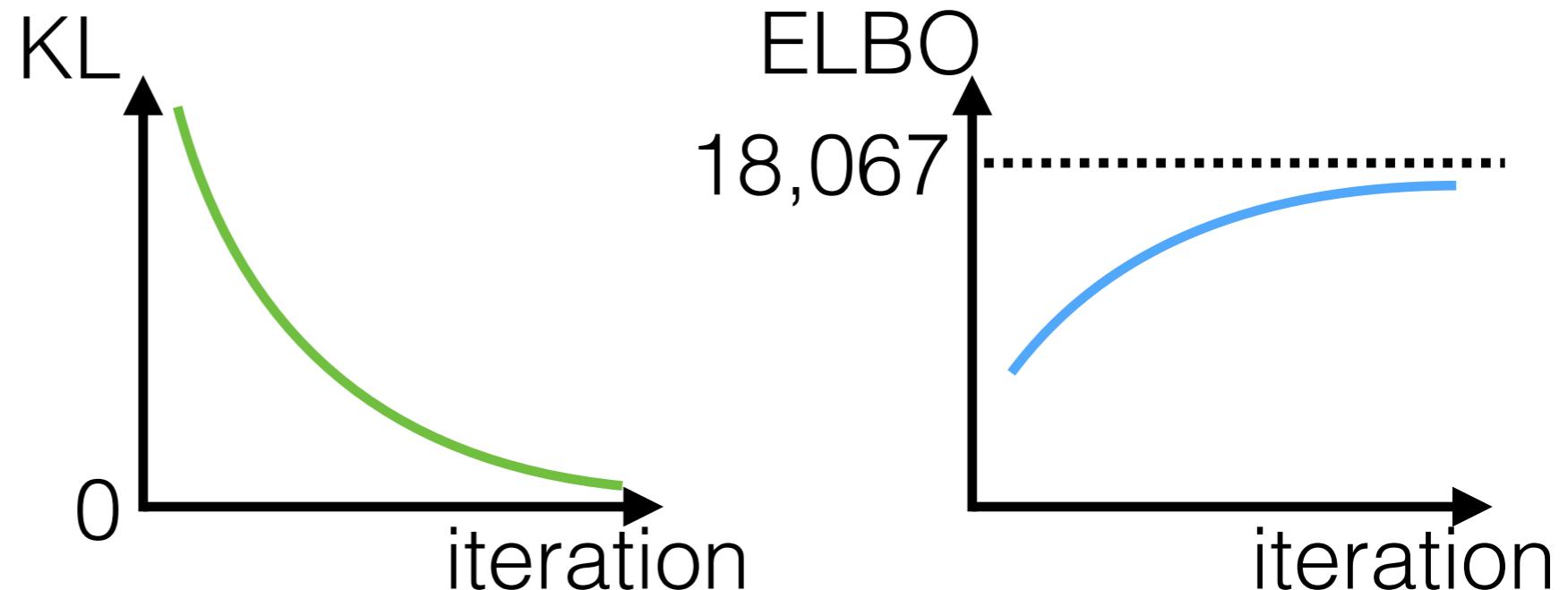
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What can we do?

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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.]

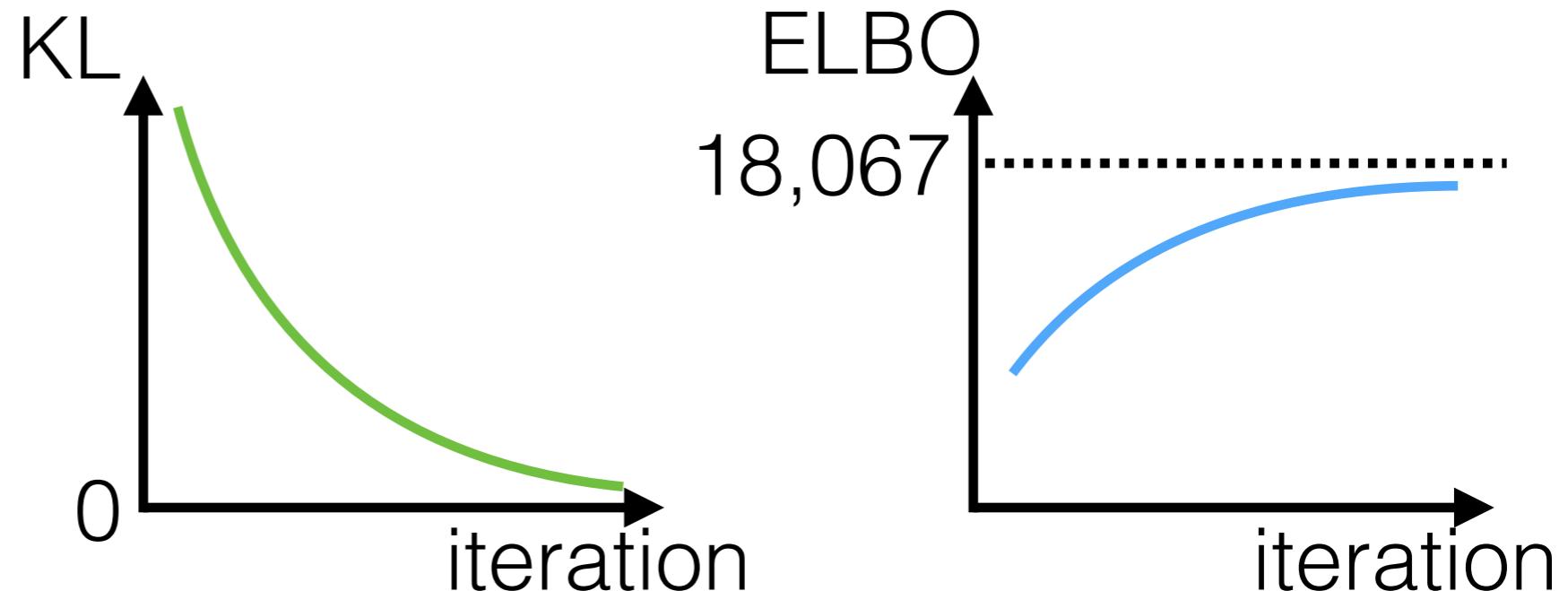


→ “Yes, but did it work? Evaluating variational inference” ICML Wedn 5pm

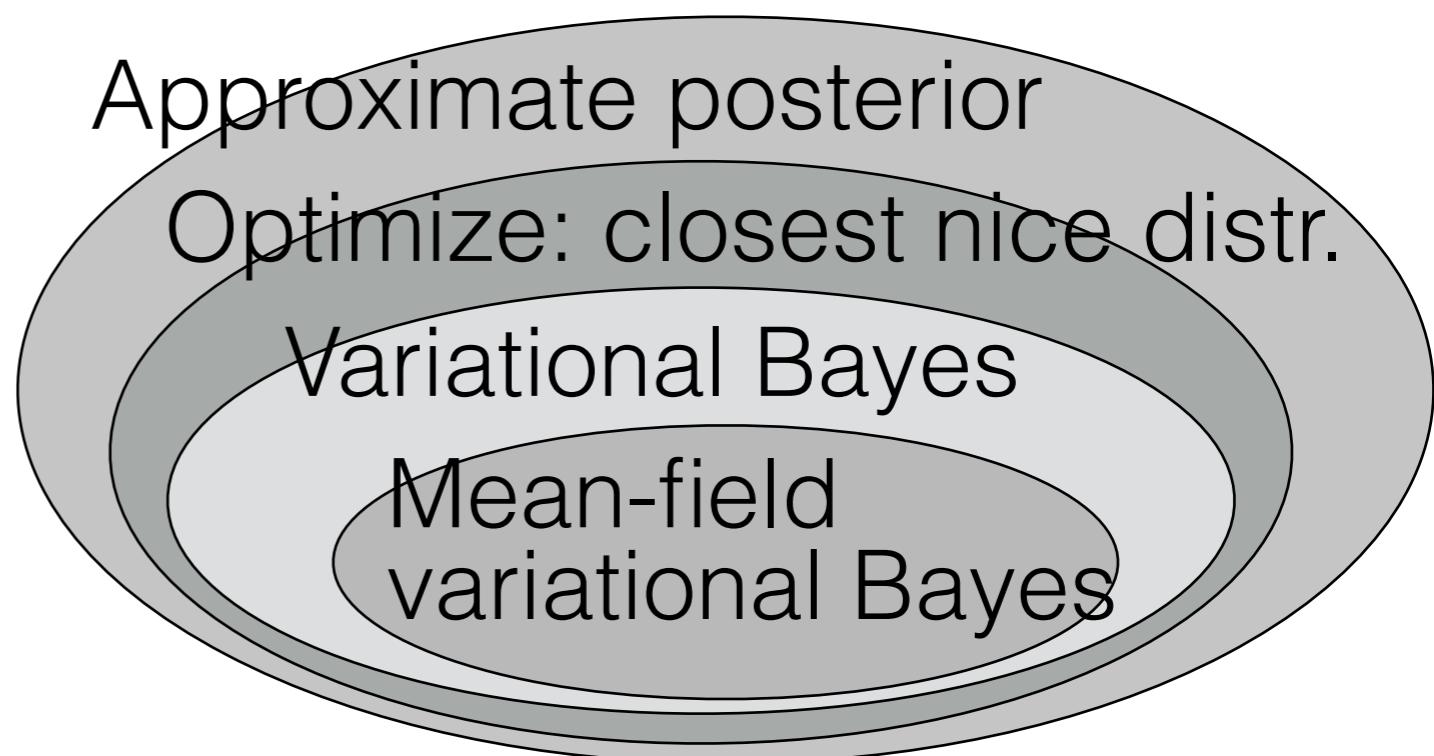
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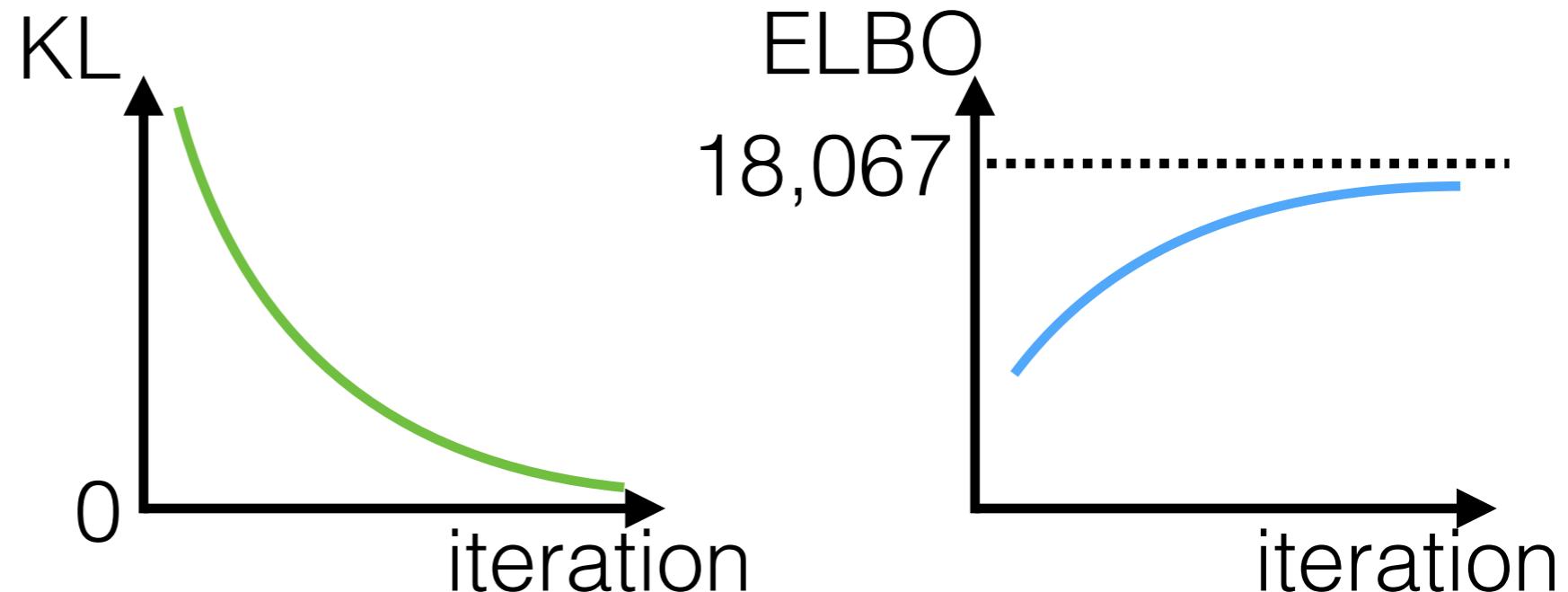
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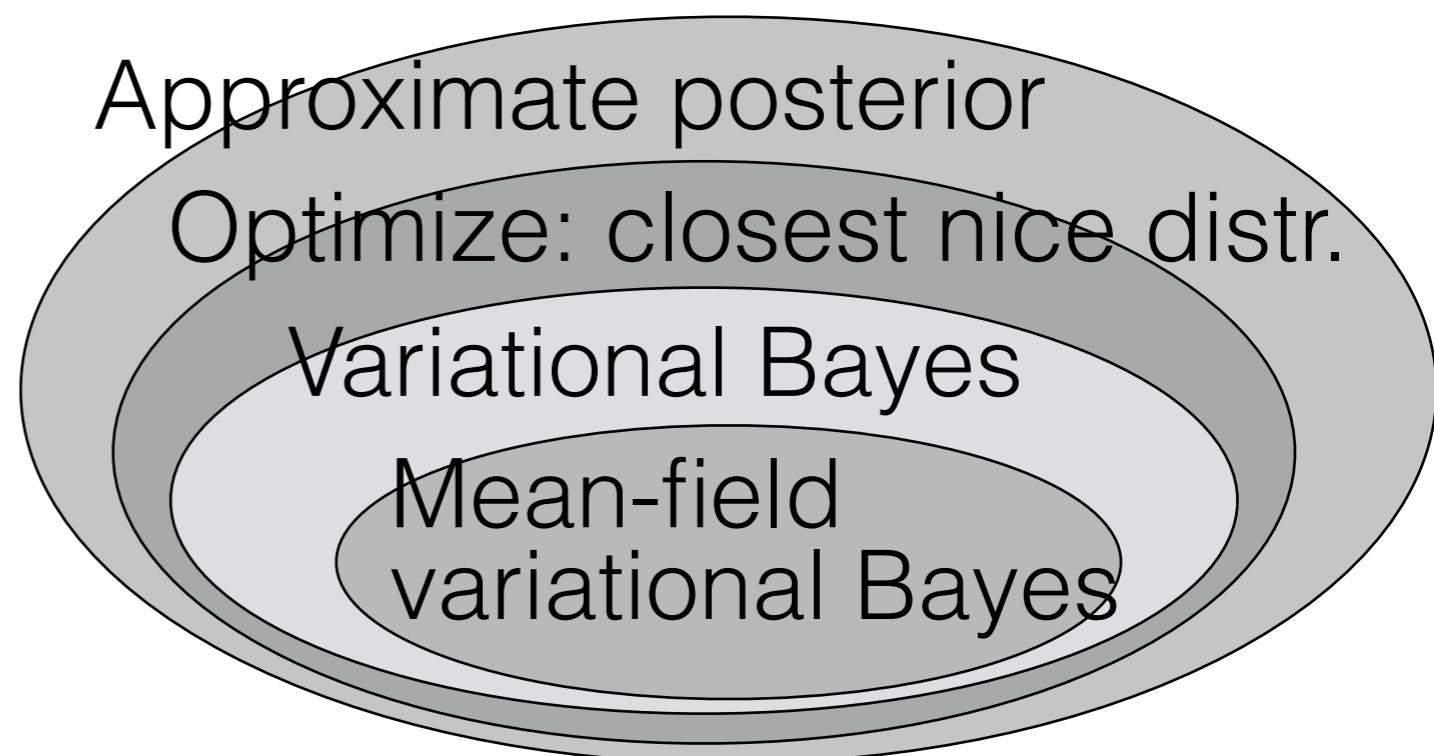
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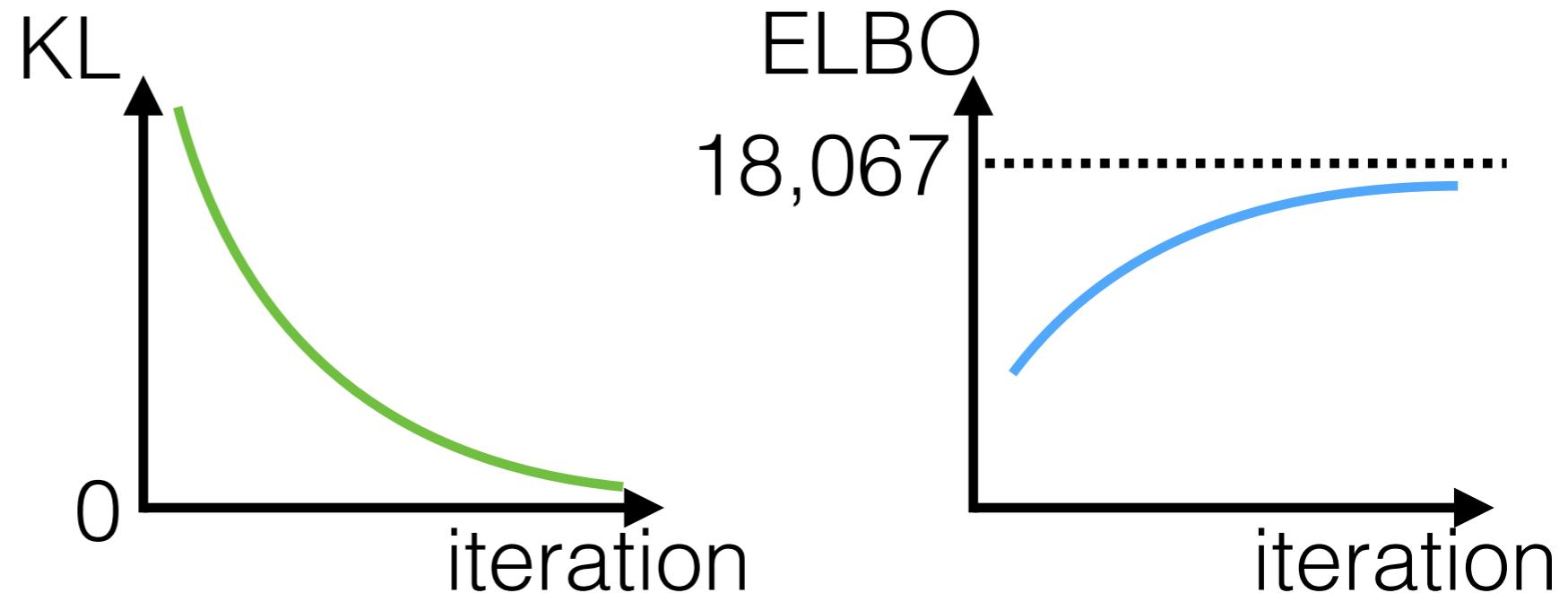
- “Yes, but did it work? Evaluating variational inference” ICML Wedn 5pm
- Richer “nice” set; alternative divergences



What can we do?

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 - KL vs ELBO

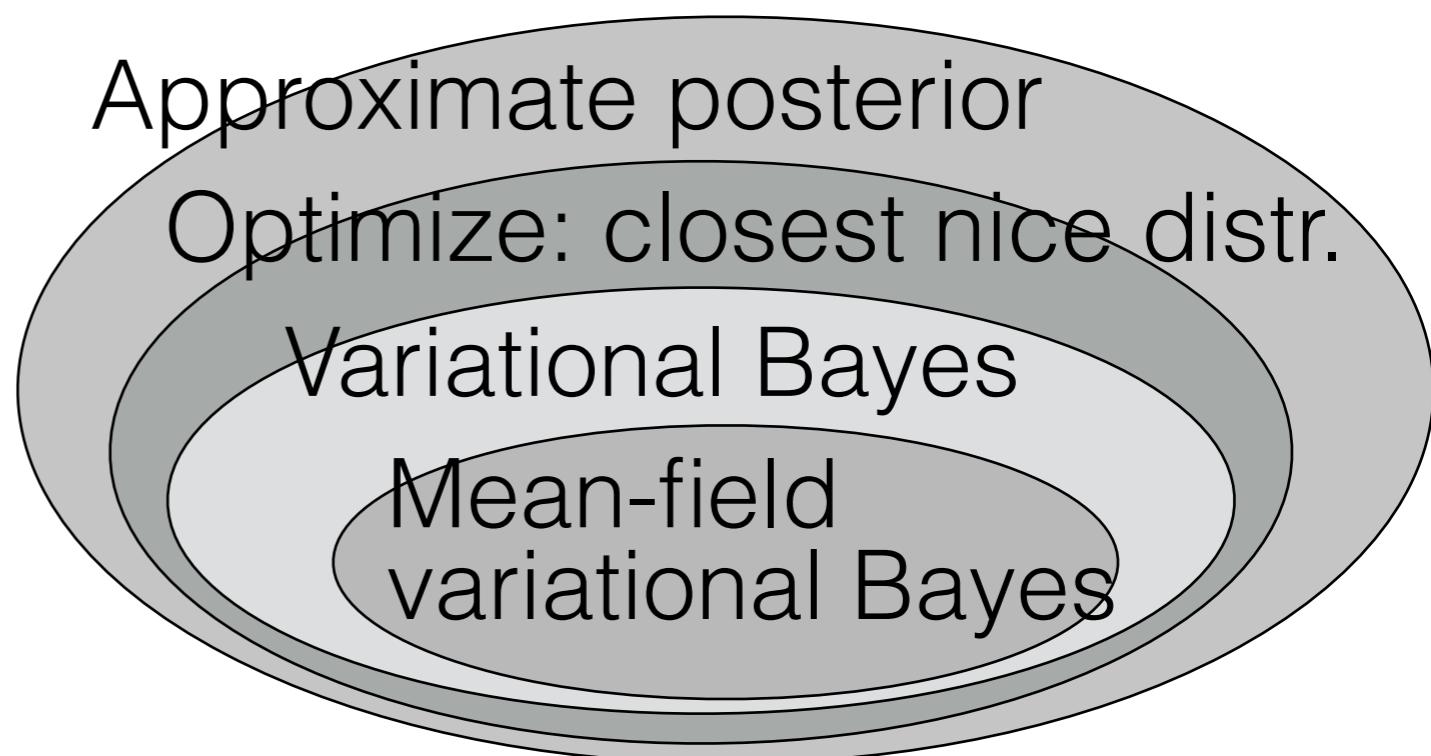
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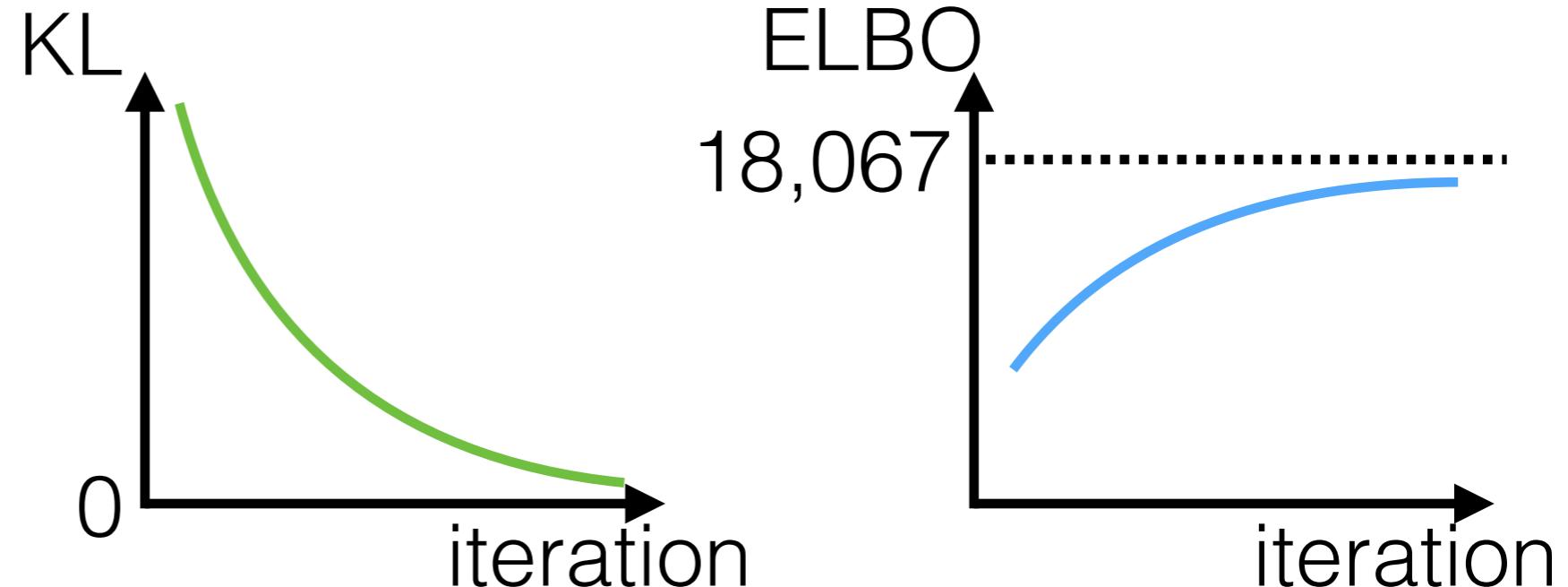
[Turner, Sahani 2011]



What can we do?

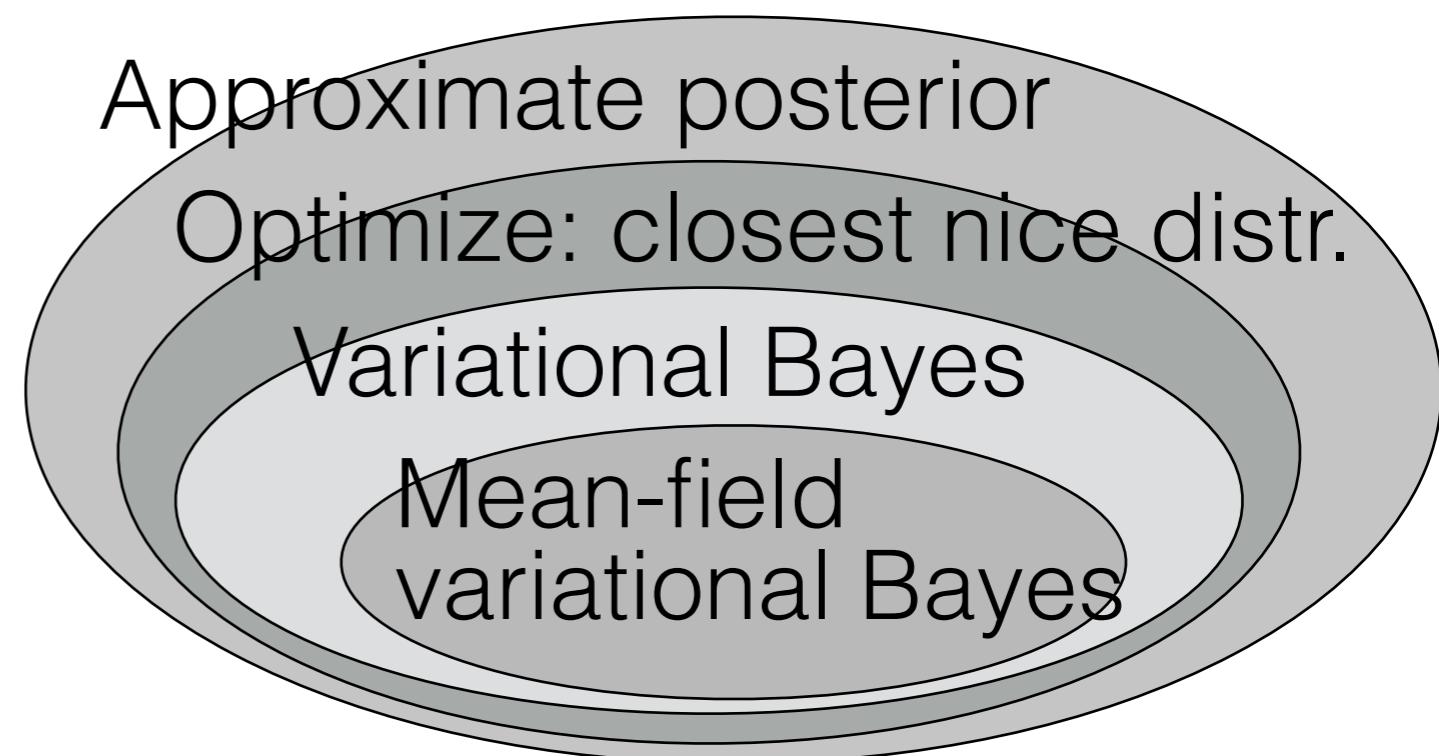
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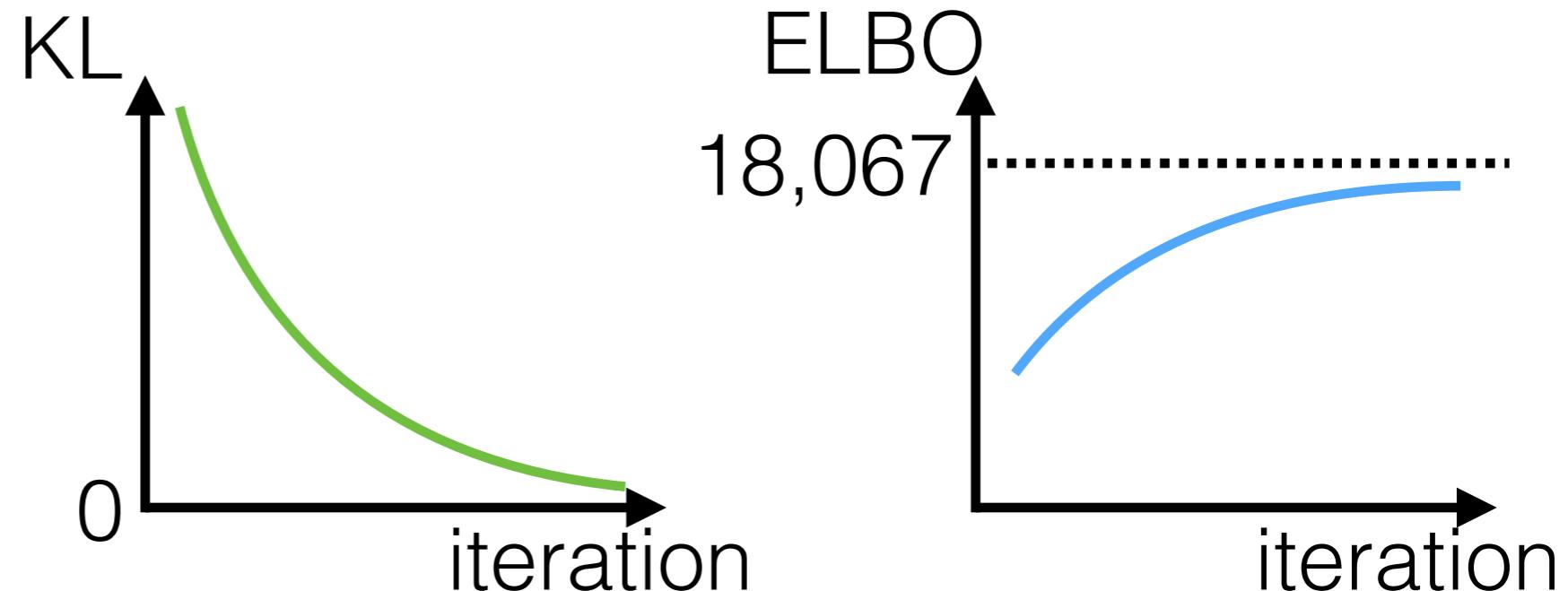
- Richer “nice” set; alternative divergences
[Turner, Sahani 2011]
- Theoretical guarantees on finite-data quality



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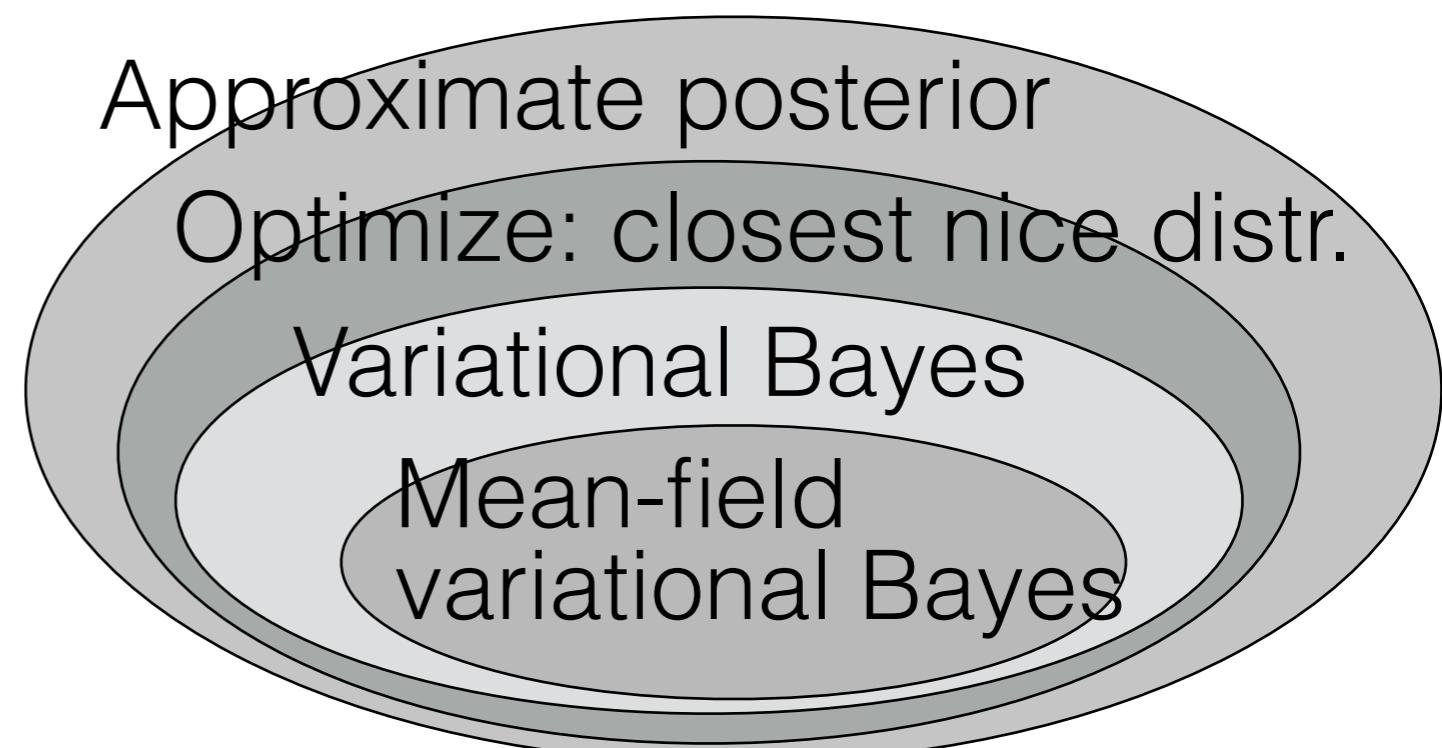


→ “Yes, but did it work? Evaluating variational inference” ICML Wedn 5pm

- Richer “nice” set; alternative divergences

[Turner, Sahani 2011]

- Theoretical guarantees on finite-data quality
 - Data summarization



What to read next

- Textbooks and Reviews
 - Bishop. *Pattern Recognition and Machine Learning*, Ch 10. 2006.
 - Blei, Kucukelbir, McAuliffe. Variational inference: A review for statisticians, *JASA* 2016.
 - MacKay. *Information Theory, Inference, and Learning Algorithms*, Ch 33. 2003.
 - Murphy. *Machine Learning: A Probabilistic Perspective*, Ch 21. 2012.
 - Ormerod, Wand. Explaining Variational Approximations. *Amer Stat* 2010.
 - Turner, Sahani. Two problems with variational expectation maximisation for time-series models. In *Bayesian Time Series Models*, 2011.
 - Wainwright, Jordan. Graphical models, exponential families, and variational inference. *Foundations and Trends in Machine Learning*, 2008.
- More Experiments
 - RJ Giordano, T Broderick, and MI Jordan. Linear response methods for accurate covariance estimates from mean field variational Bayes. *NIPS* 2015.
 - RJ Giordano, T Broderick, R Meager, J Huggins, and MI Jordan. Fast robustness quantification with variational Bayes. *ICML Data4Good Workshop* 2016.
 - RJ Giordano, T Broderick, and MI Jordan. Covariances, robustness, and variational Bayes, 2017. Under review. ArXiv:1709.02536.

See end of Part II slides for full reference list.