

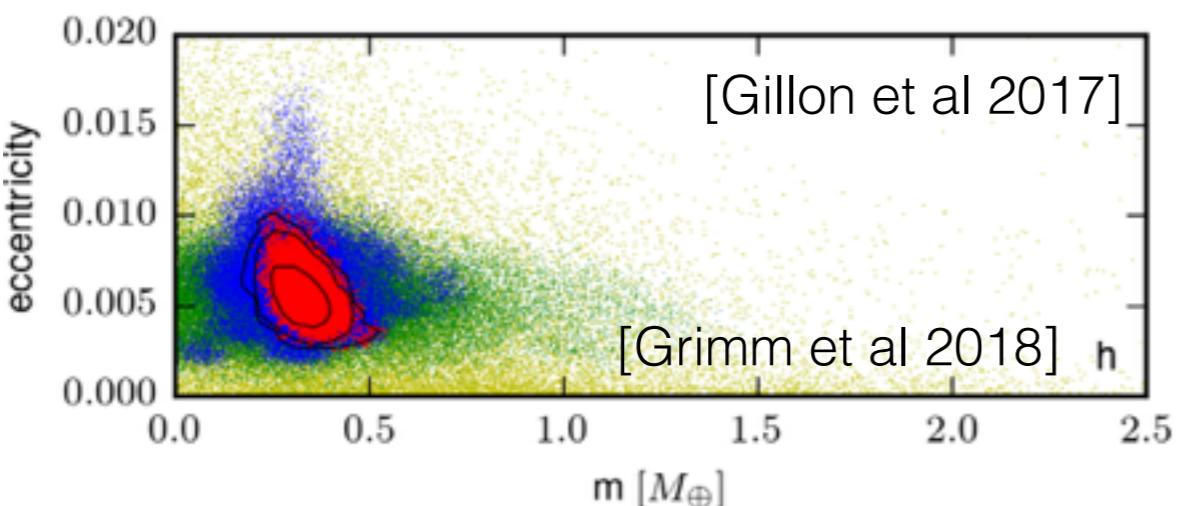


Variational Bayes and beyond: Bayesian inference for big data

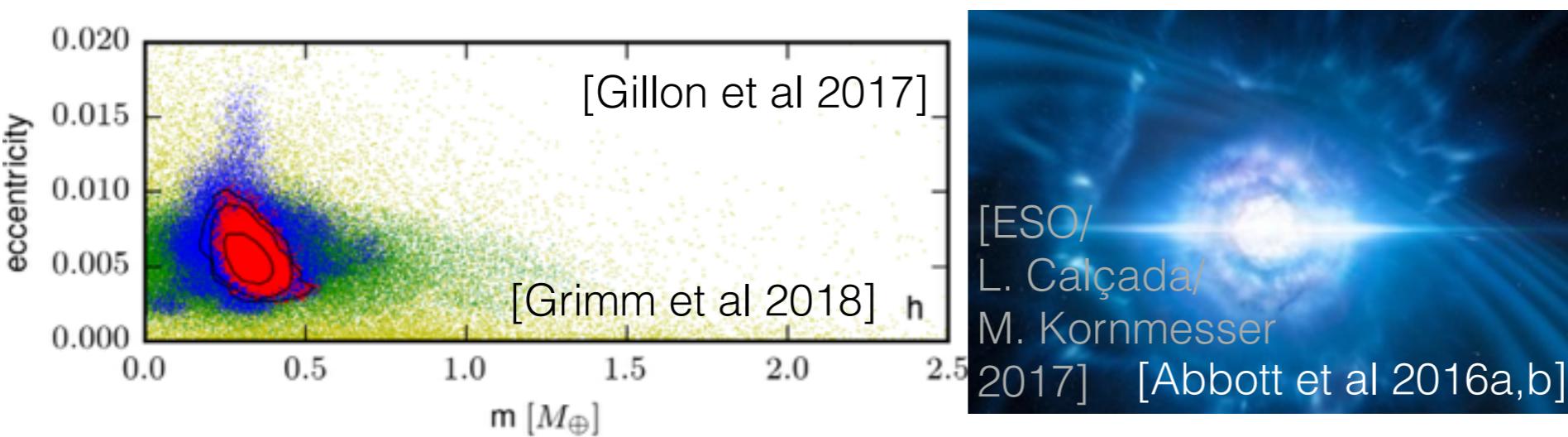
Tamara Broderick
ITT Career Development
Assistant Professor,
MIT

Bayesian inference

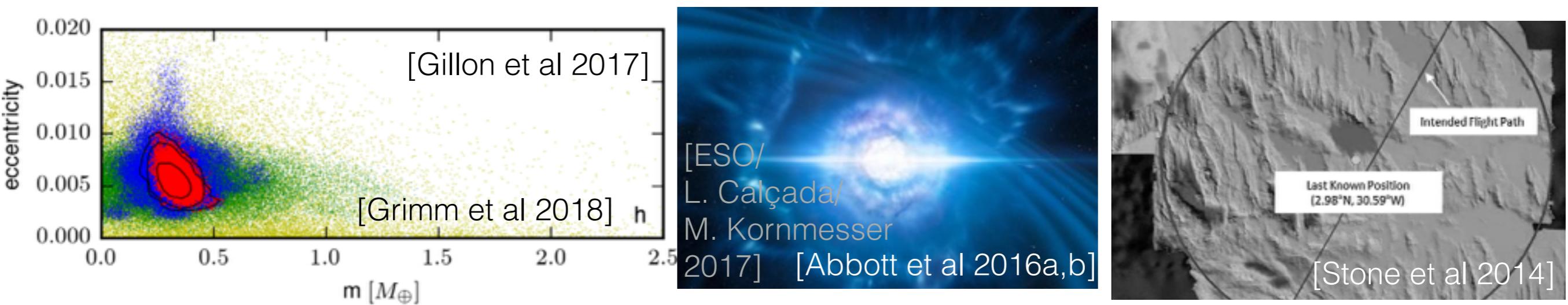
Bayesian inference



Bayesian inference



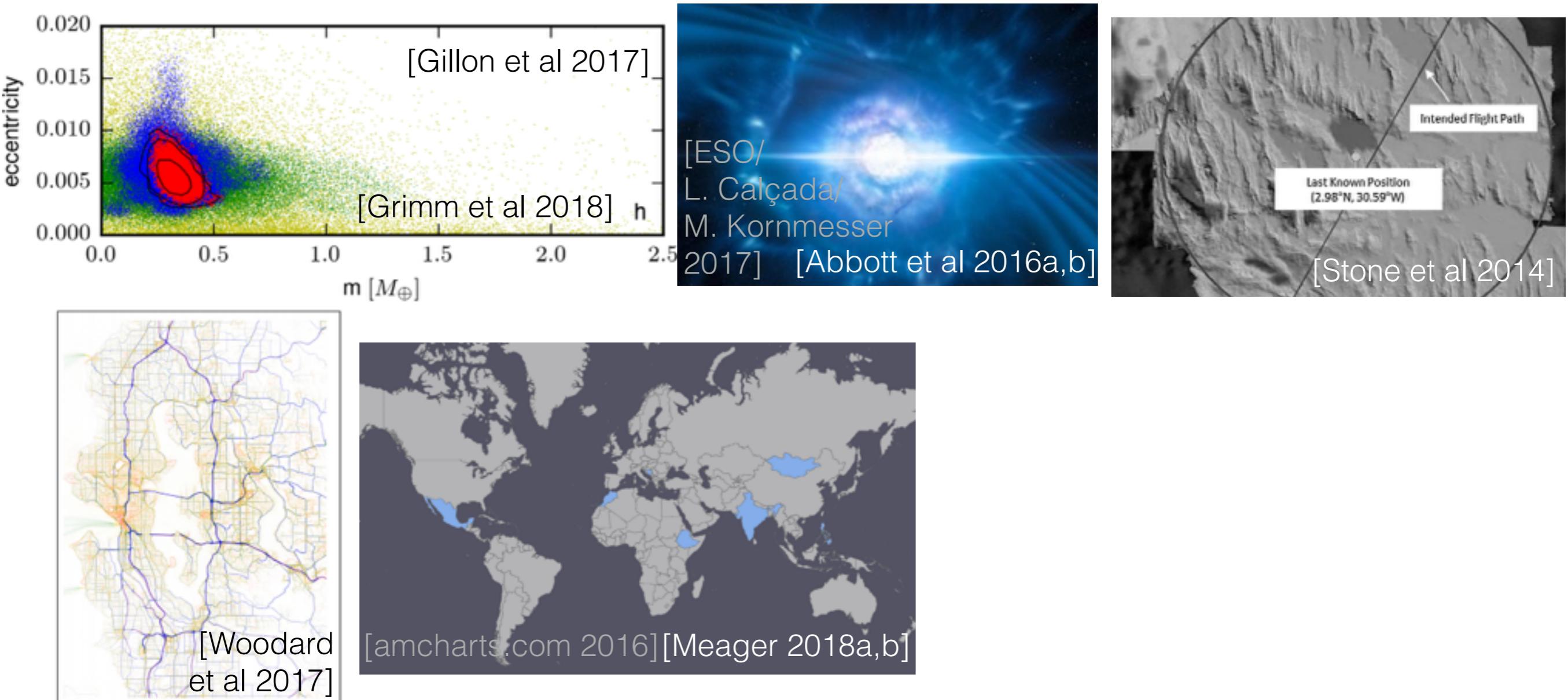
Bayesian inference



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Bayesian inference

- 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

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- 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
MOVIE	BILLION	YEARS	TEACHERS
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LOVE	CONGRESS	LIFE	HAITI

[Blei et al
2003]

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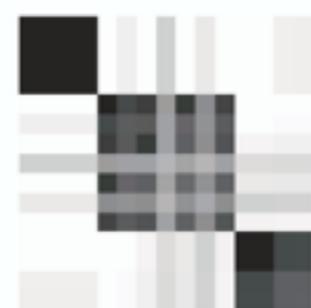
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[Airoldi et al 2008]

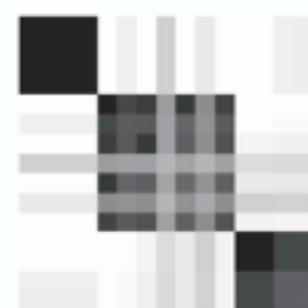
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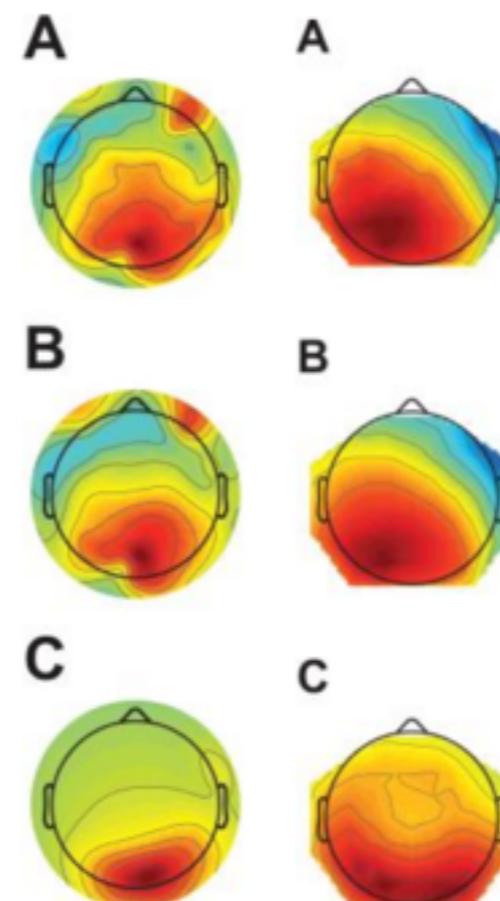
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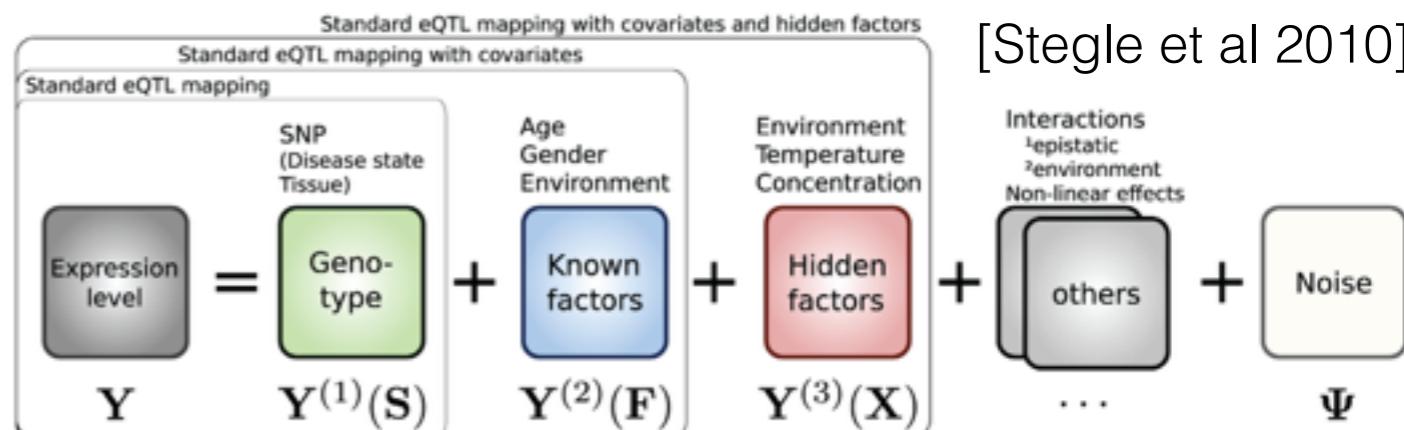
[Blei et al 2018]

Variational Bayes

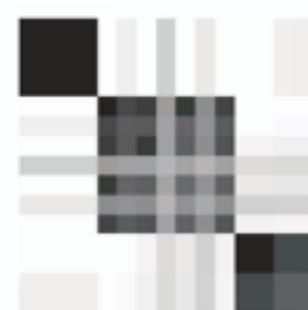
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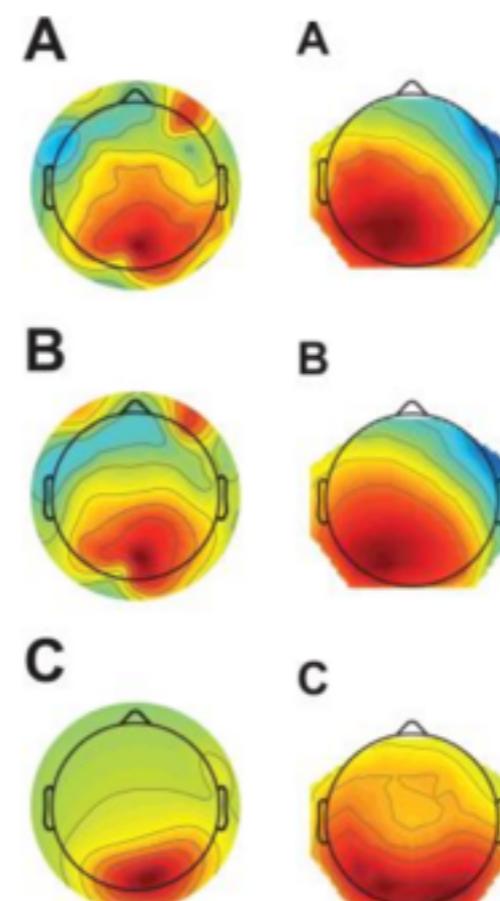
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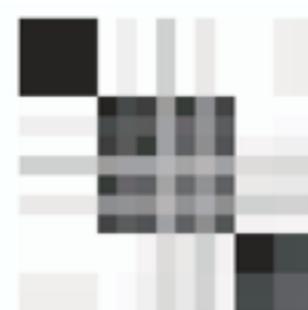
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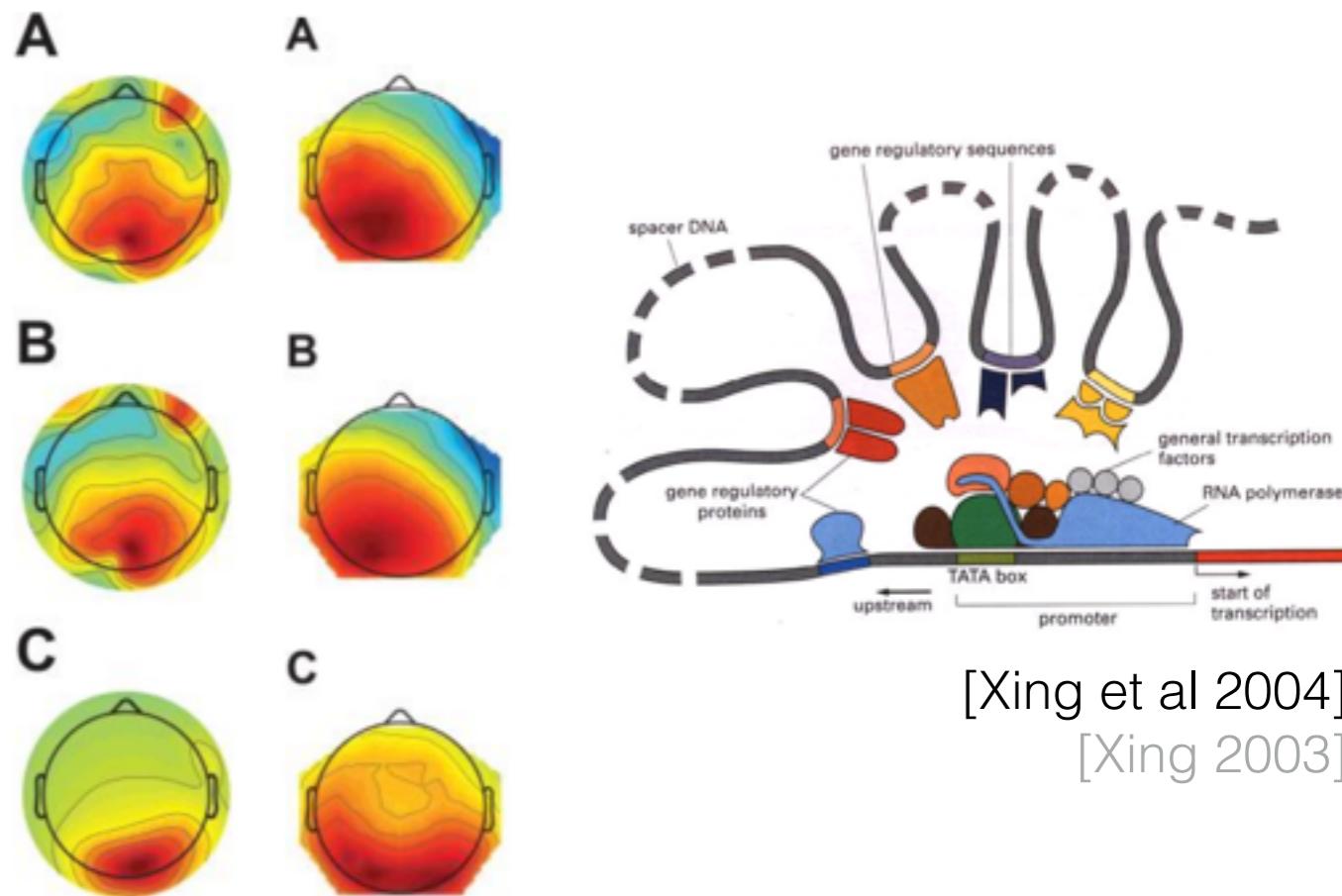
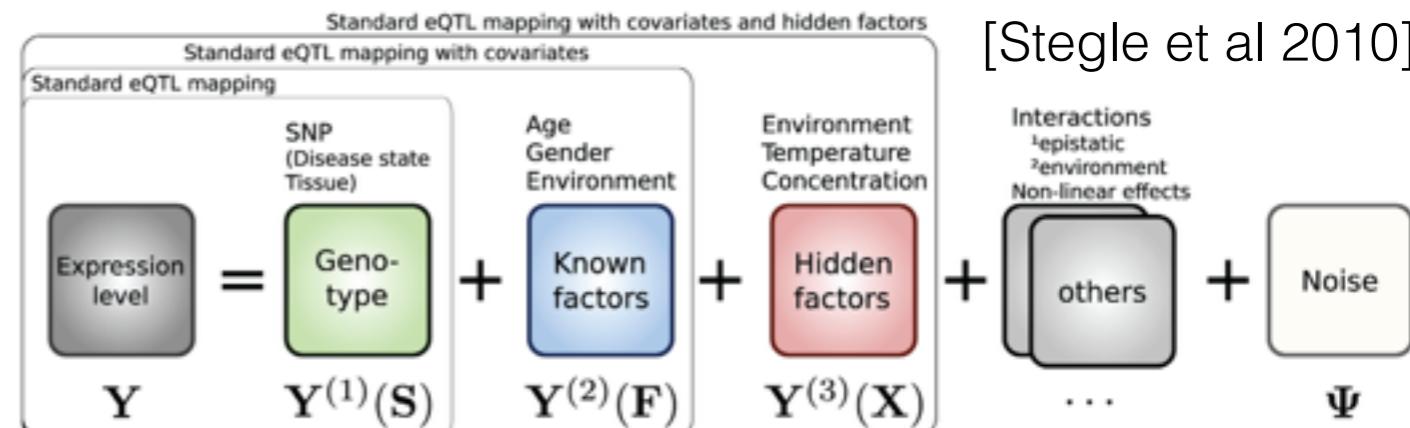
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Roadmap

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

parameters
 θ

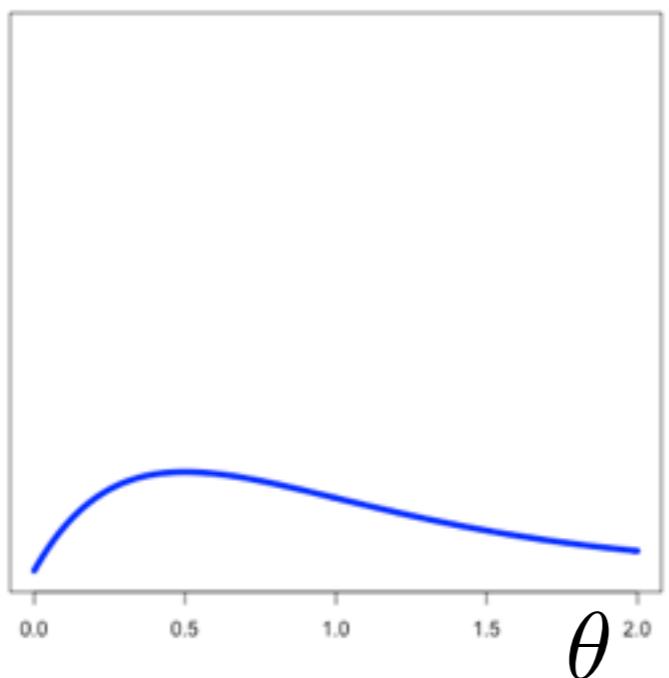
Bayesian inference

parameters
 $p(\theta)$
prior



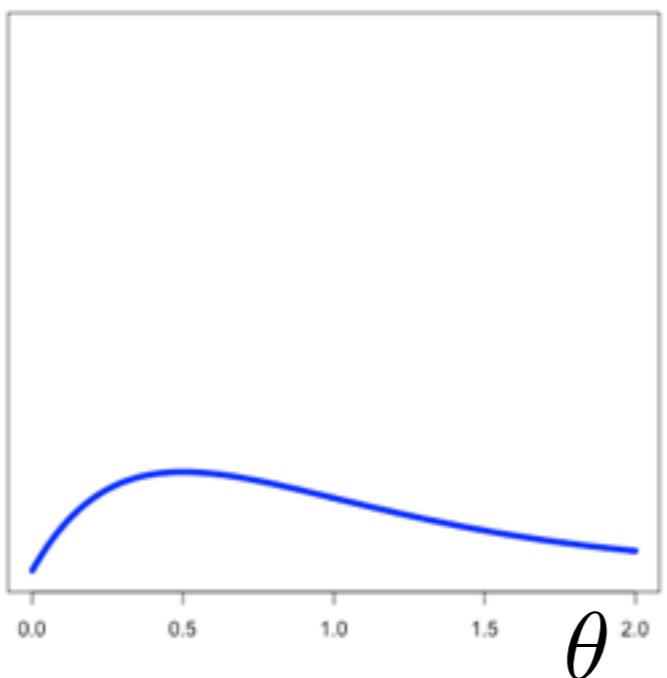
Bayesian inference

parameters
 $p(\theta)$
prior



Bayesian inference

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

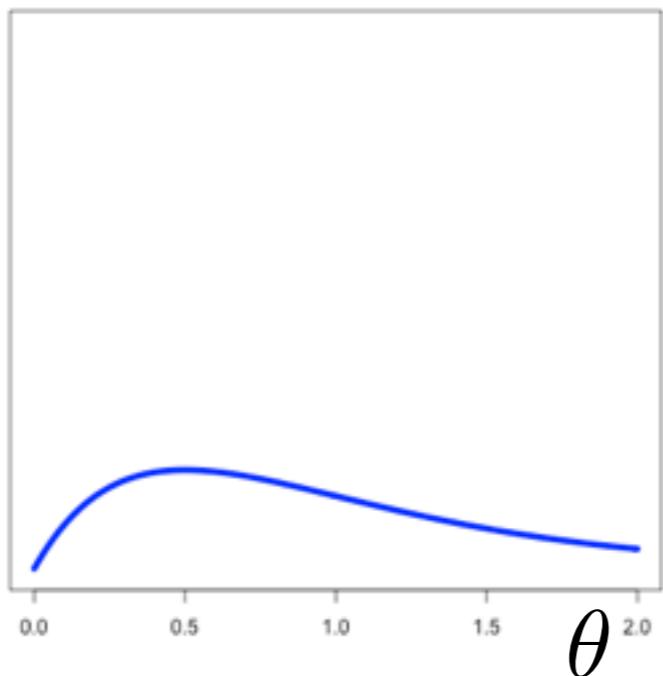


Bayesian inference

data parameters

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

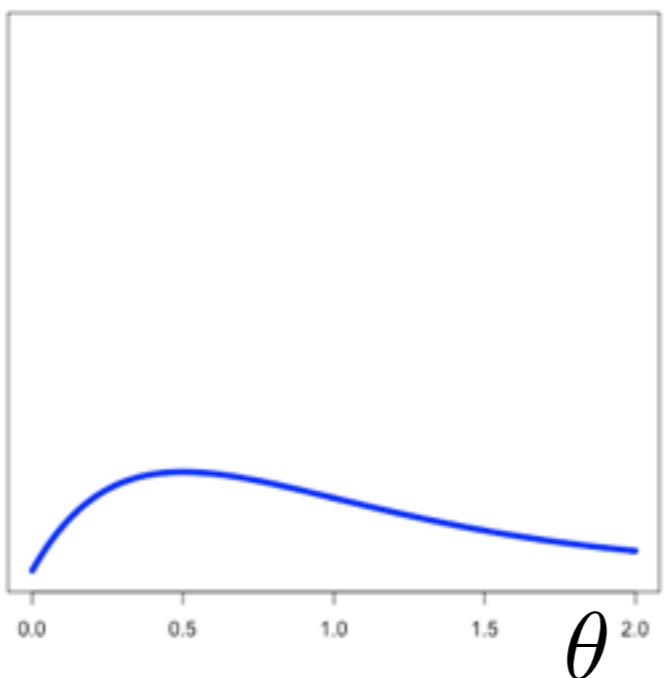
likelihood prior



Bayesian inference

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

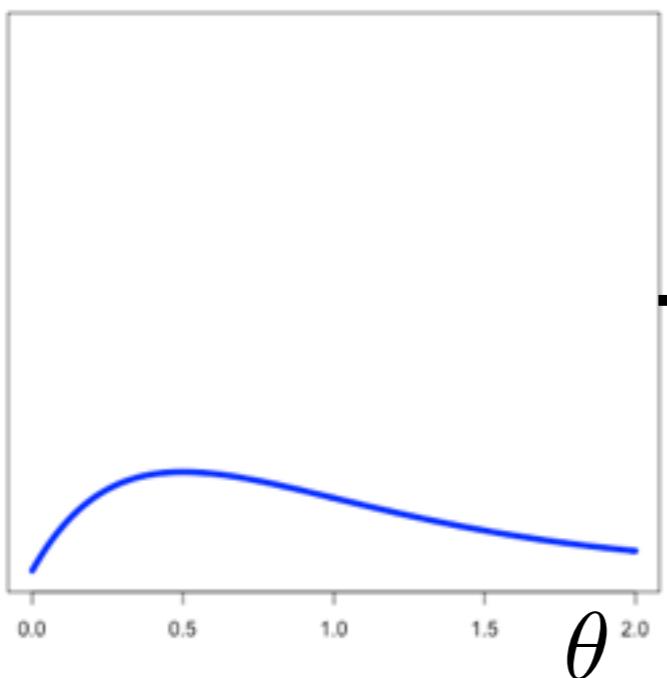
posterior likelihood prior



Bayesian inference

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posterior likelihood prior

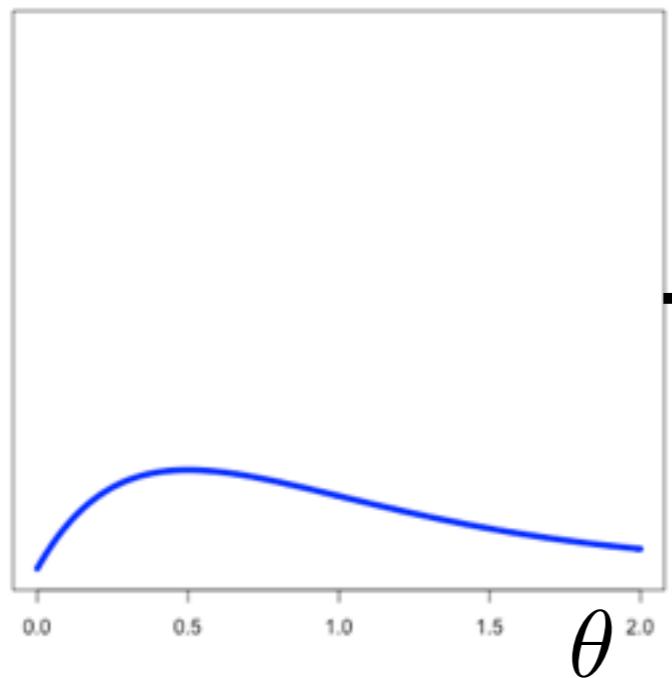
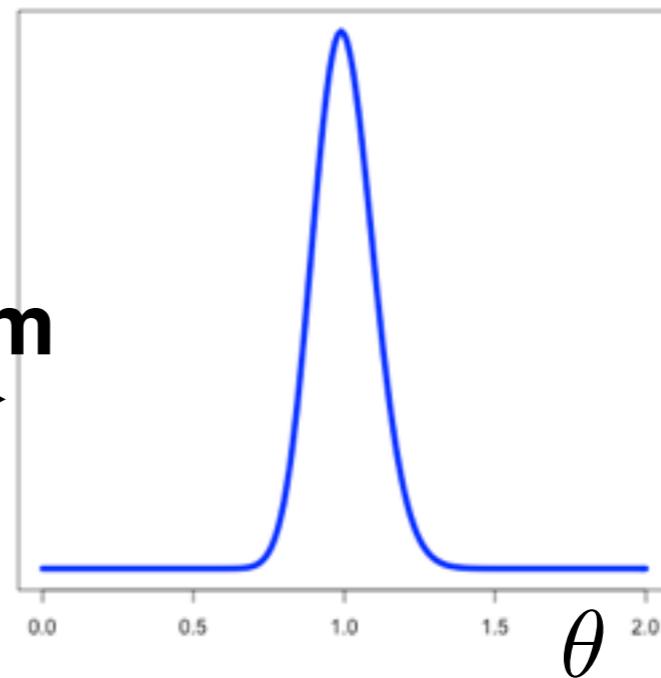


**Bayes
Theorem**
→

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posterior likelihood prior

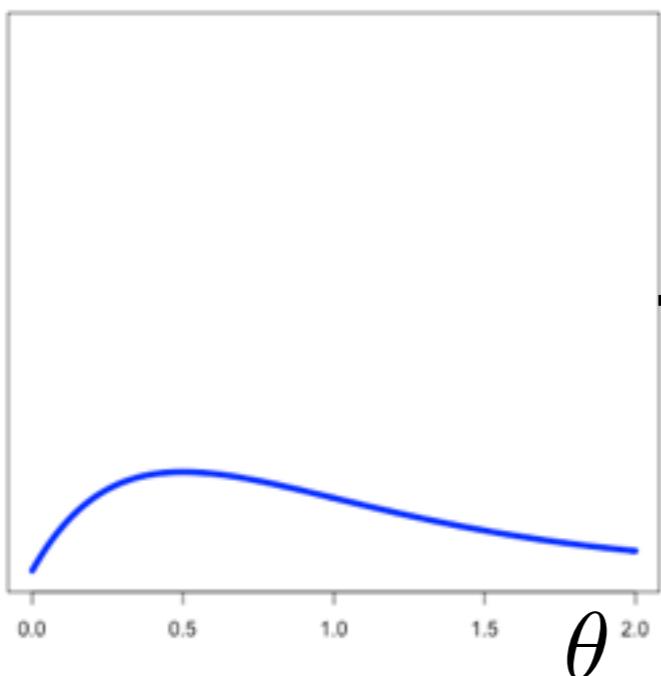


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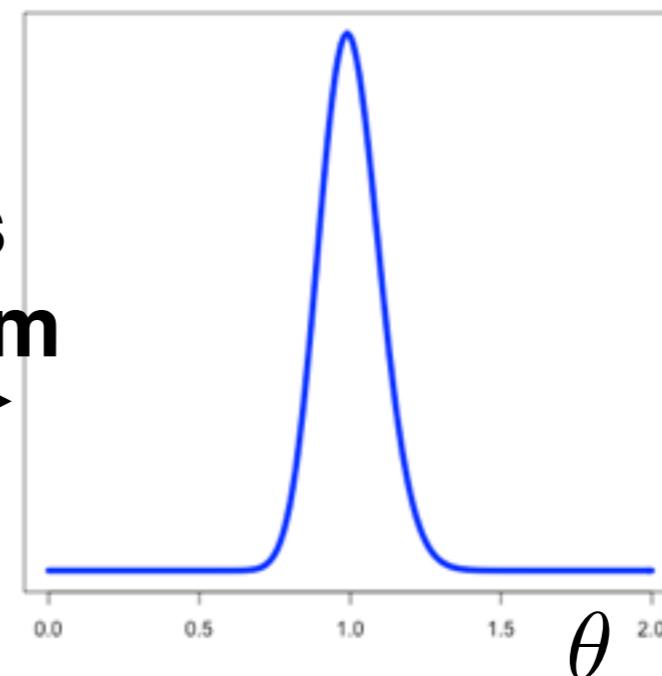
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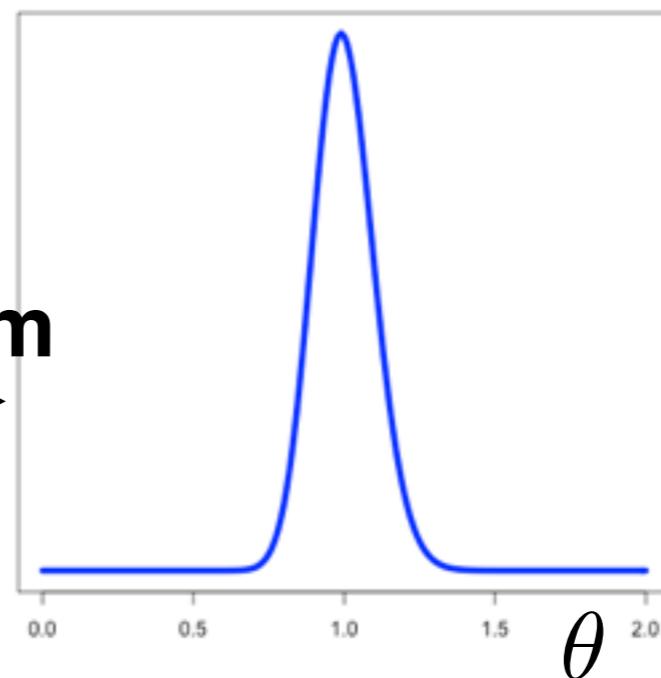


1. Build a model: choose prior & choose likelihood

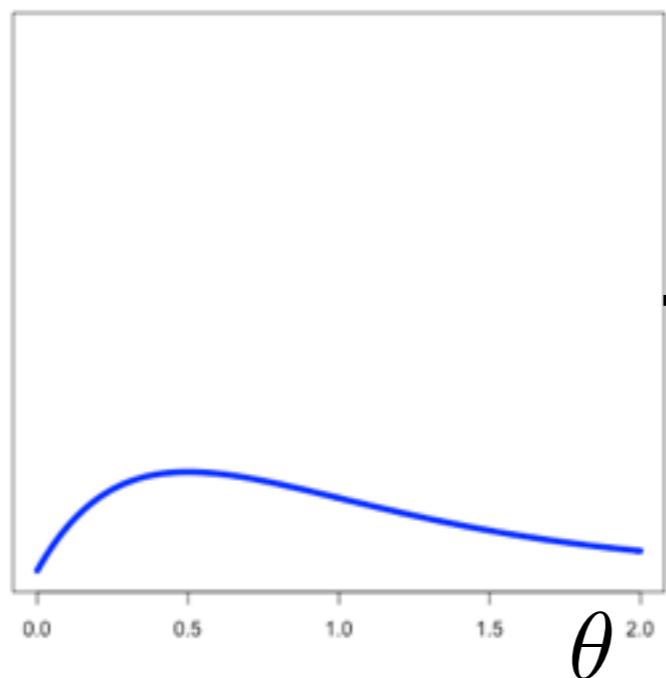
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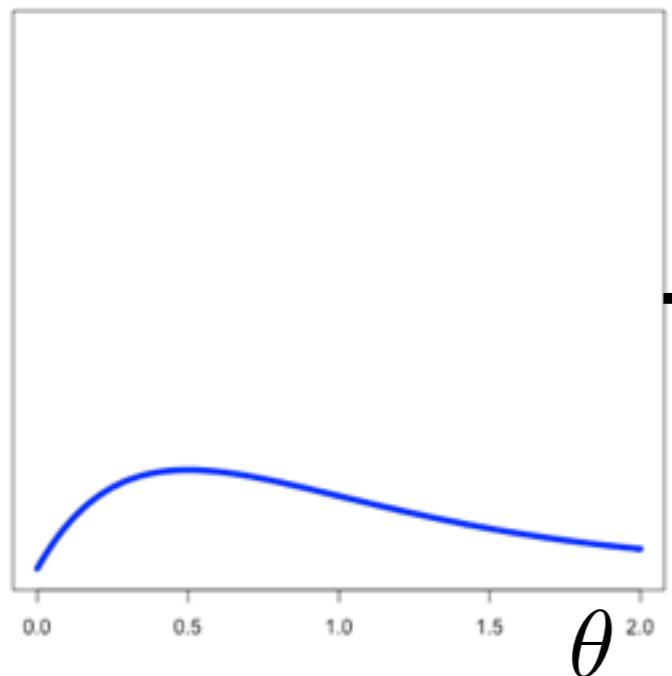
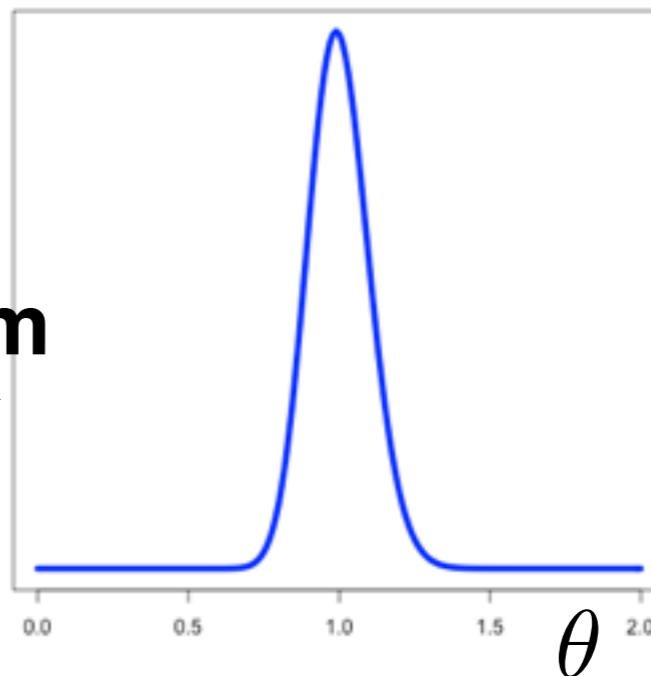


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2. Compute the posterior

Bayesian inference

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

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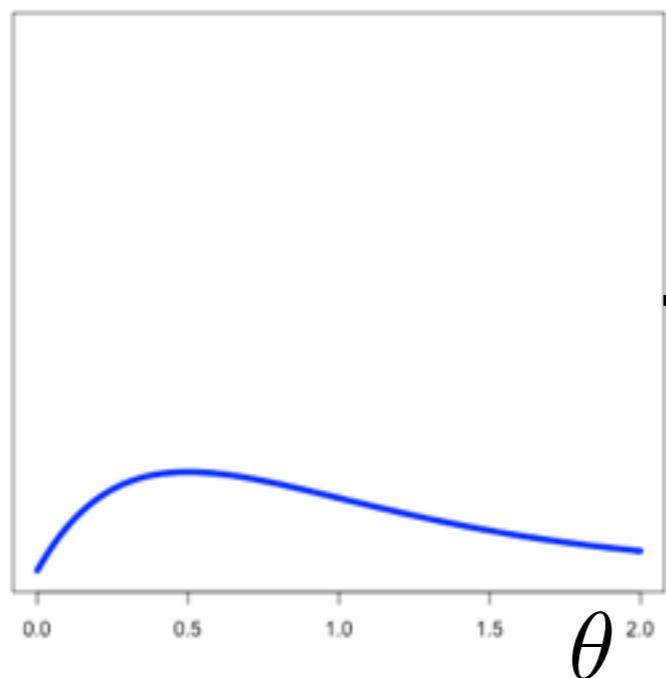
**Bayes
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1. Build a model: choose prior & choose likelihood
2. Compute the posterior
3. Report a summary, e.g. posterior means and (co)variances

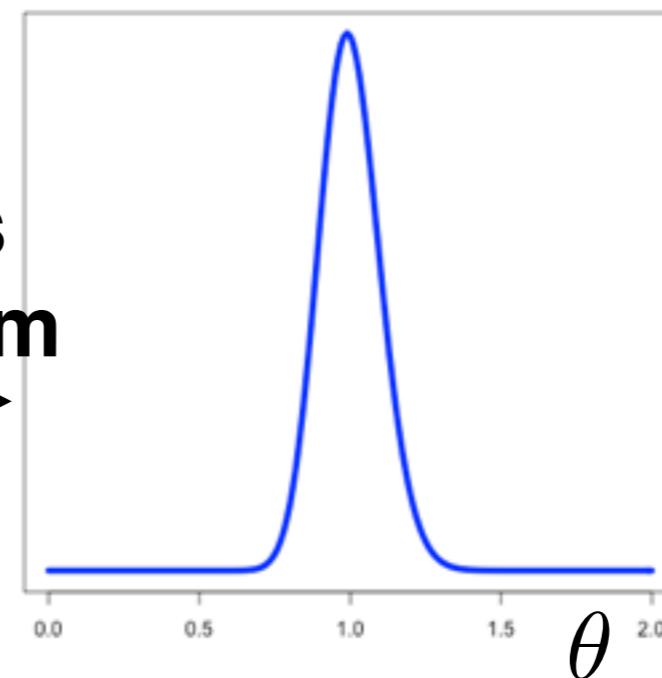
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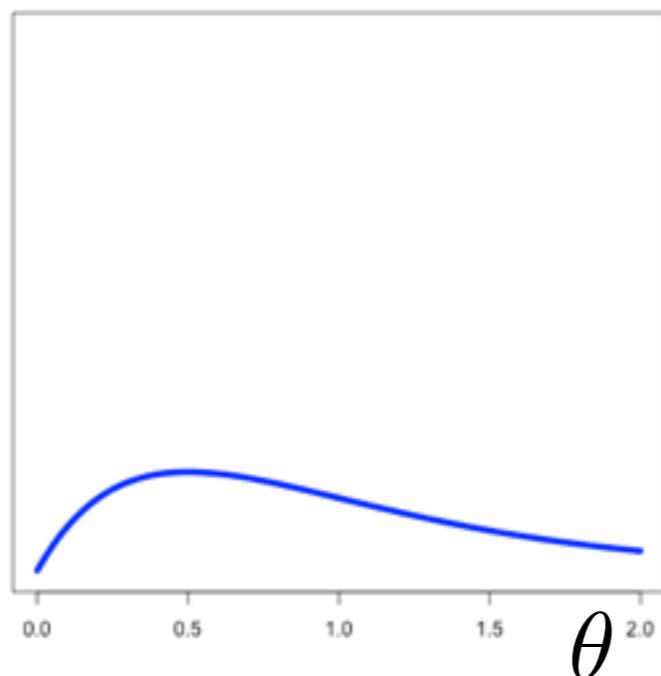


1. Build a model: choose prior & choose likelihood
 2. Compute the posterior
 3. Report a summary, e.g. posterior means and (co)variances
- Why are steps 2 and 3 hard?

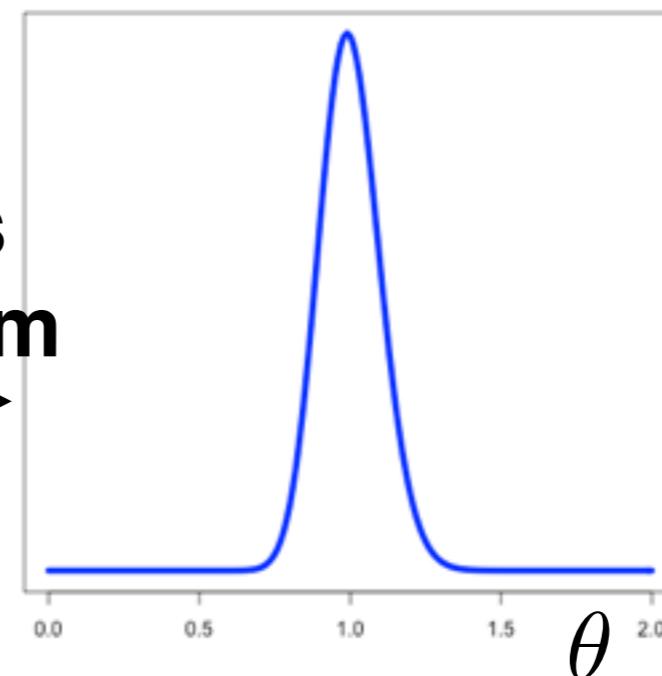
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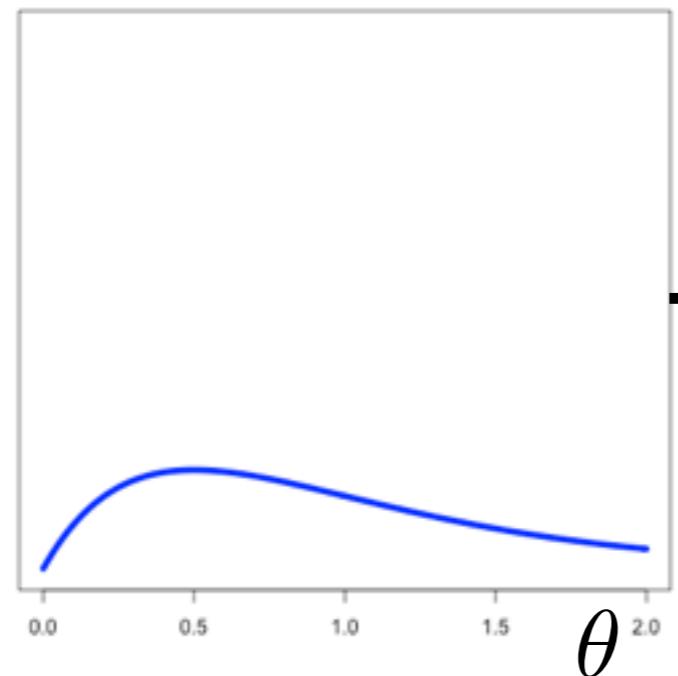
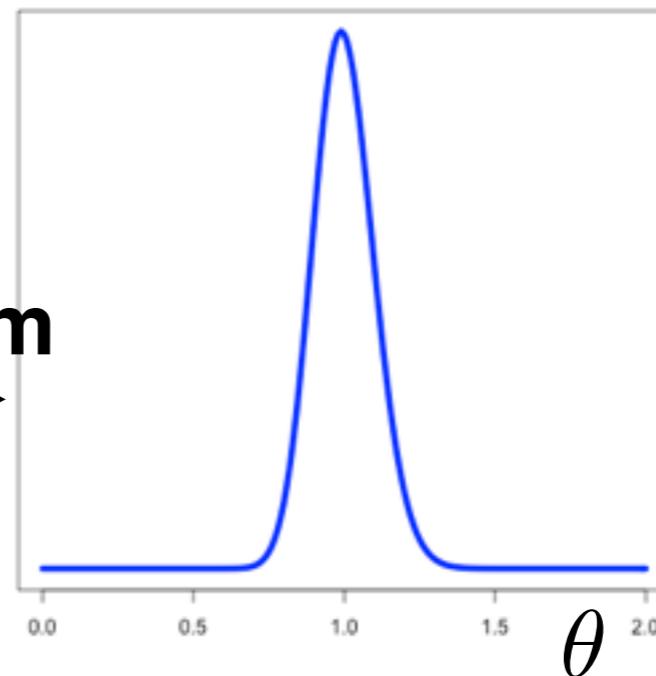


1. Build a model: choose prior & choose likelihood
 2. Compute the posterior
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- Why are steps 2 and 3 hard?
 - Typically no closed form

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posterior likelihood prior

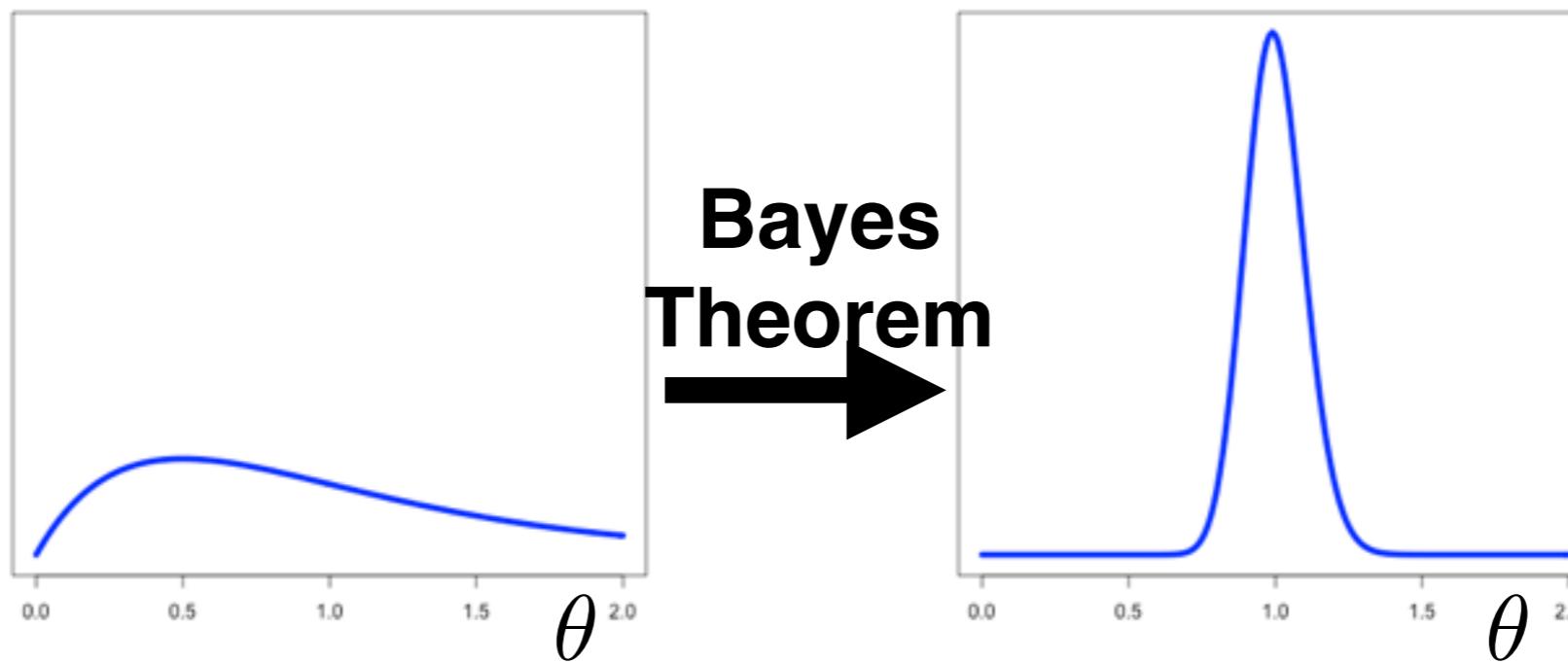


1. Build a model: choose prior & choose likelihood
 2. Compute the posterior
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- Why are steps 2 and 3 hard?
 - Typically no closed form, high-dimensional integration

Bayesian inference

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

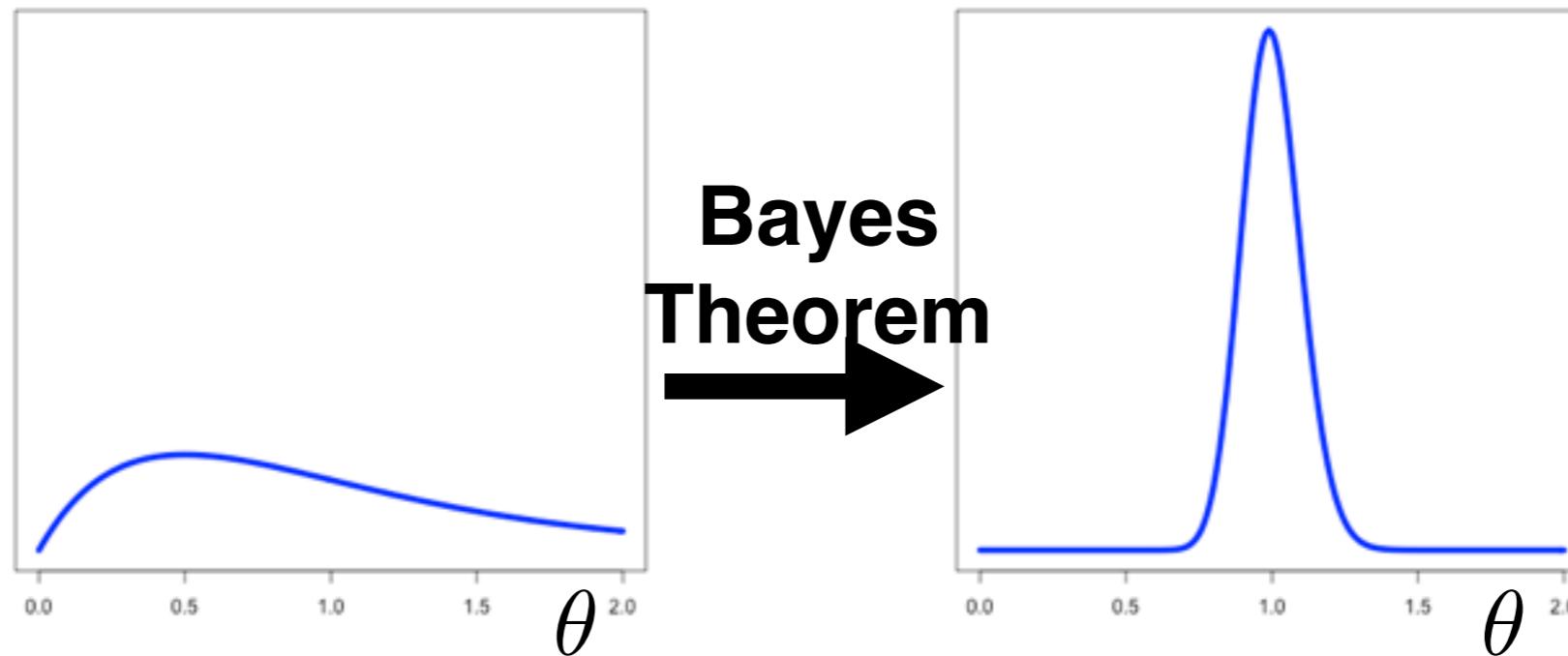
posterior likelihood prior



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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



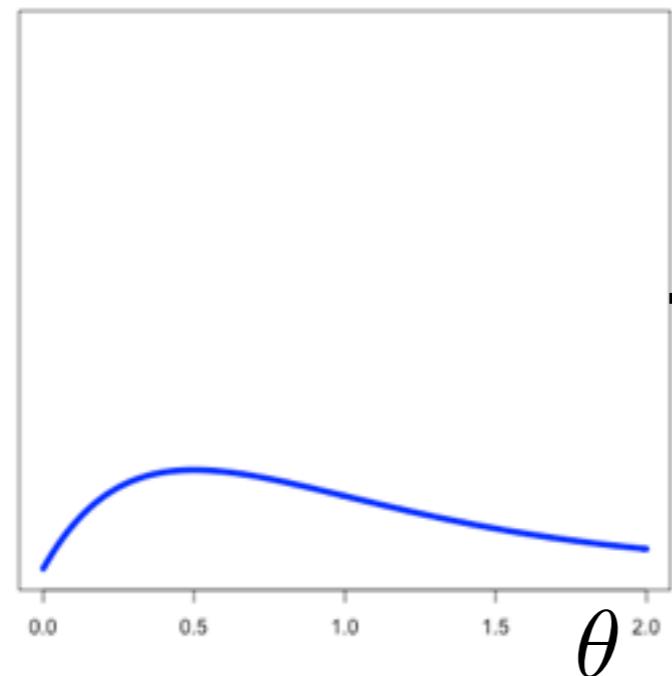
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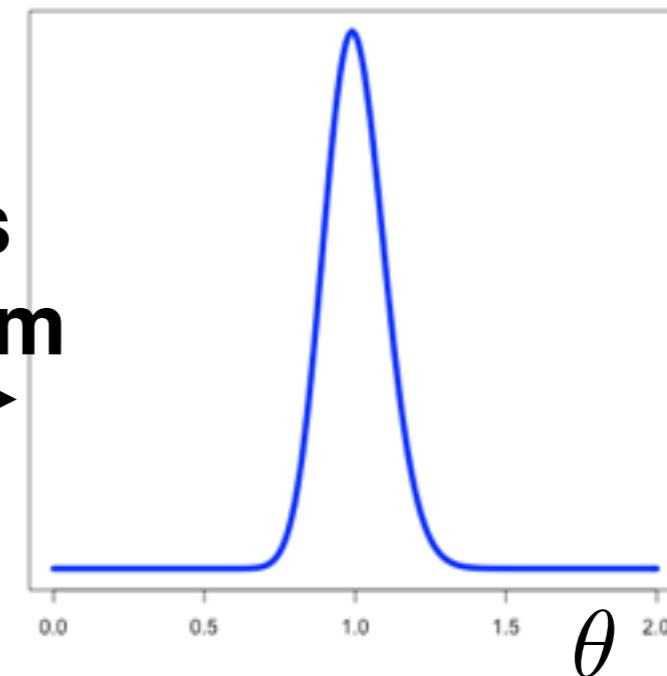
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posterior likelihood prior evidence



**Bayes
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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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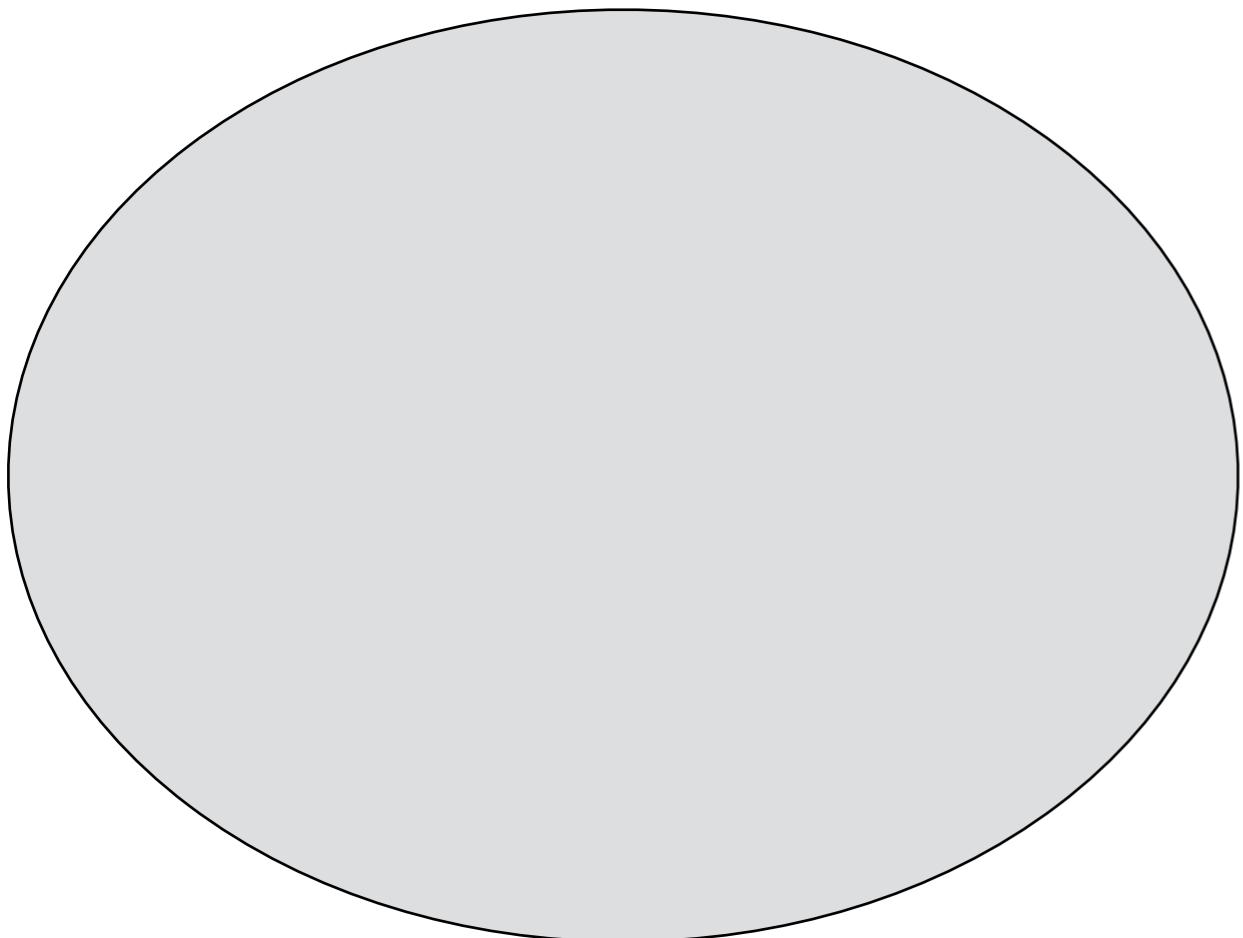
Instead: an optimization approach

- Approximate posterior with q^*

Approximate Bayesian Inference

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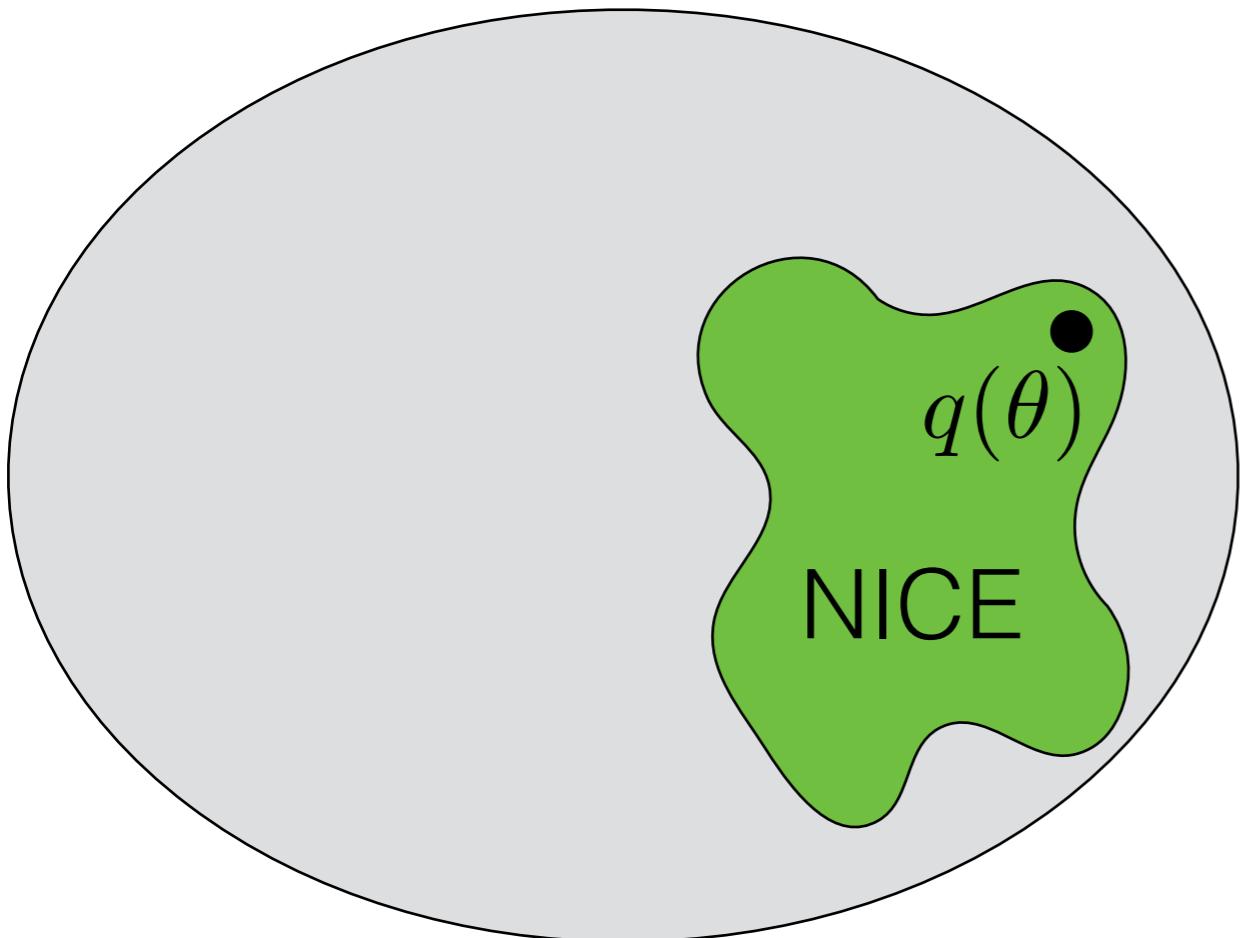
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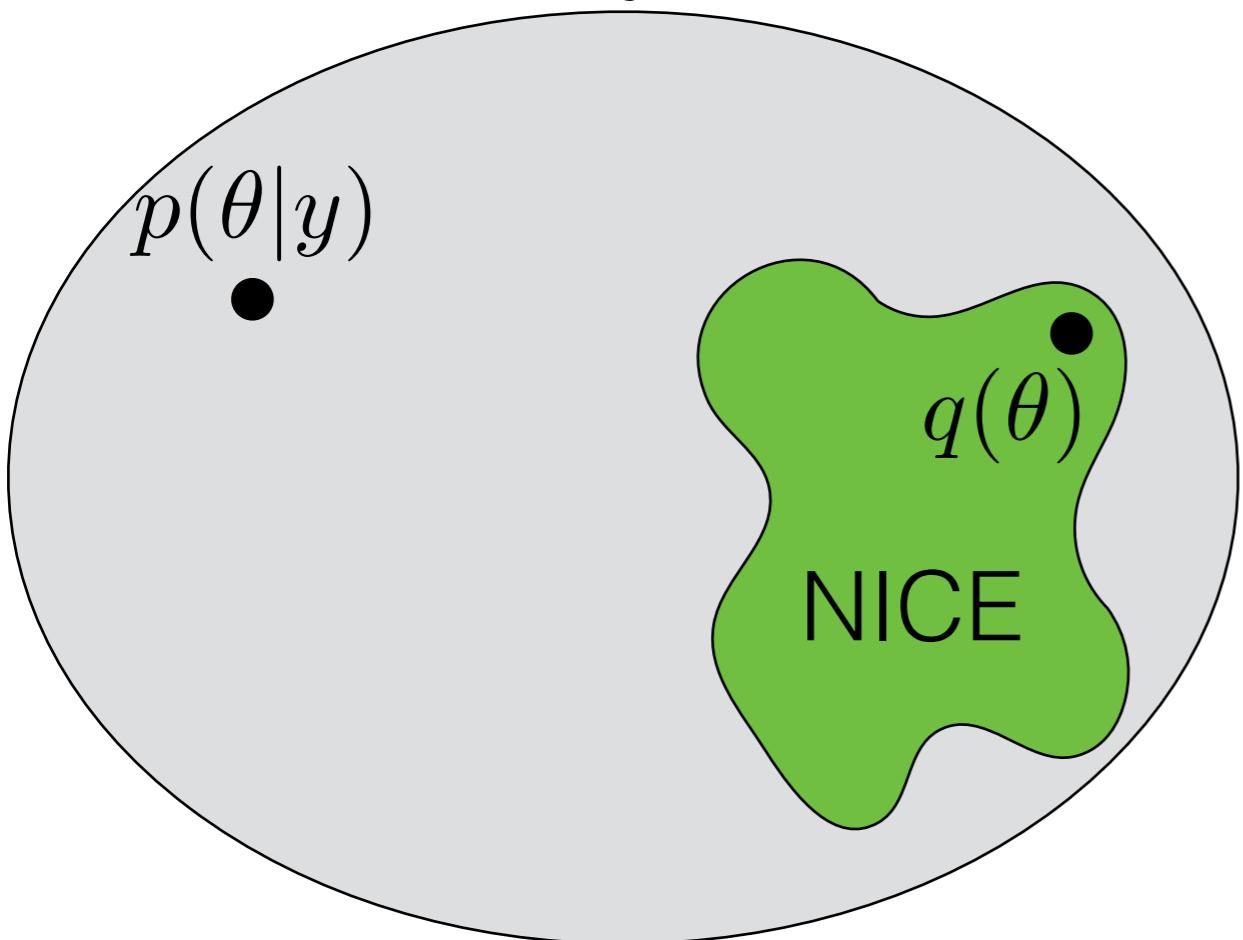
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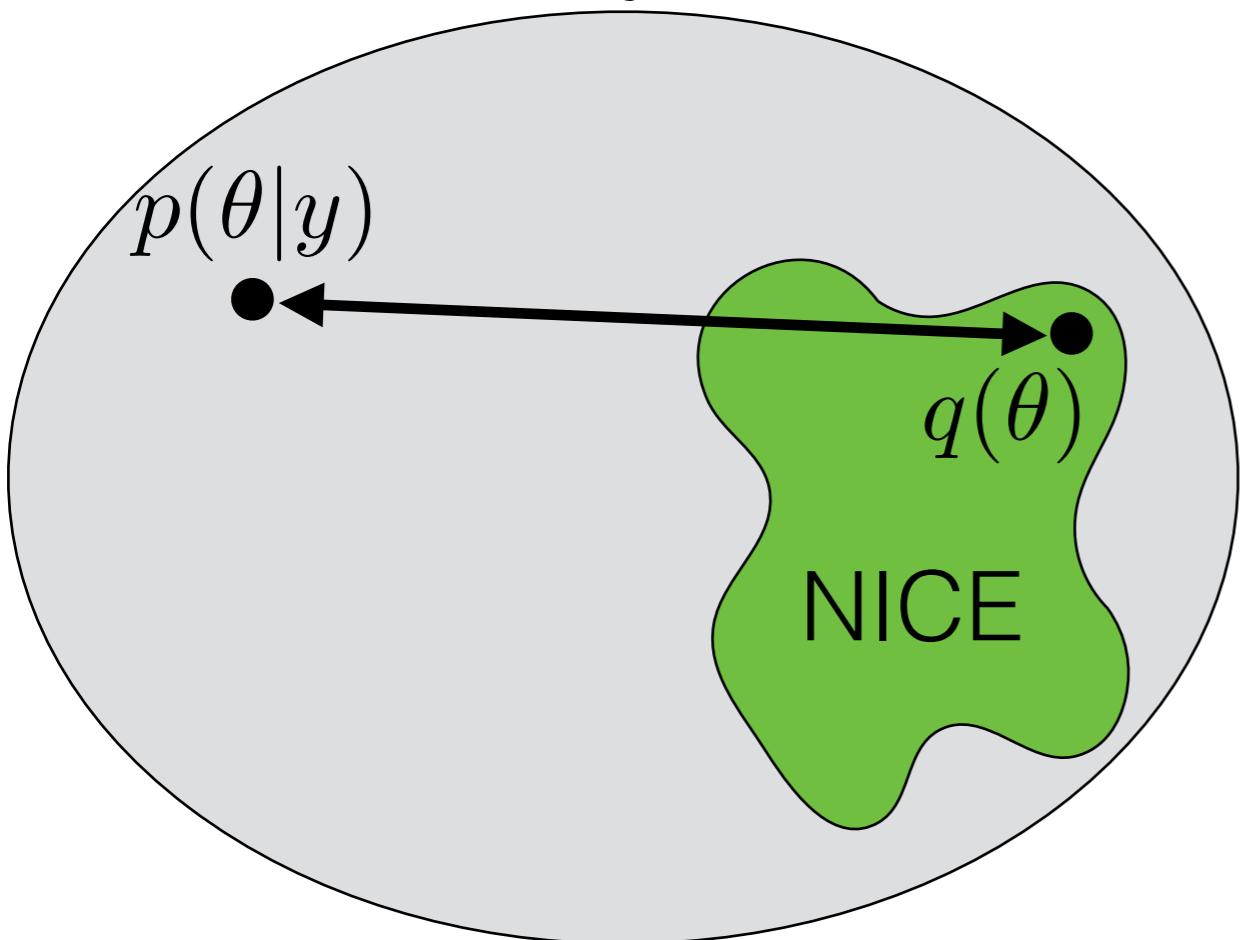
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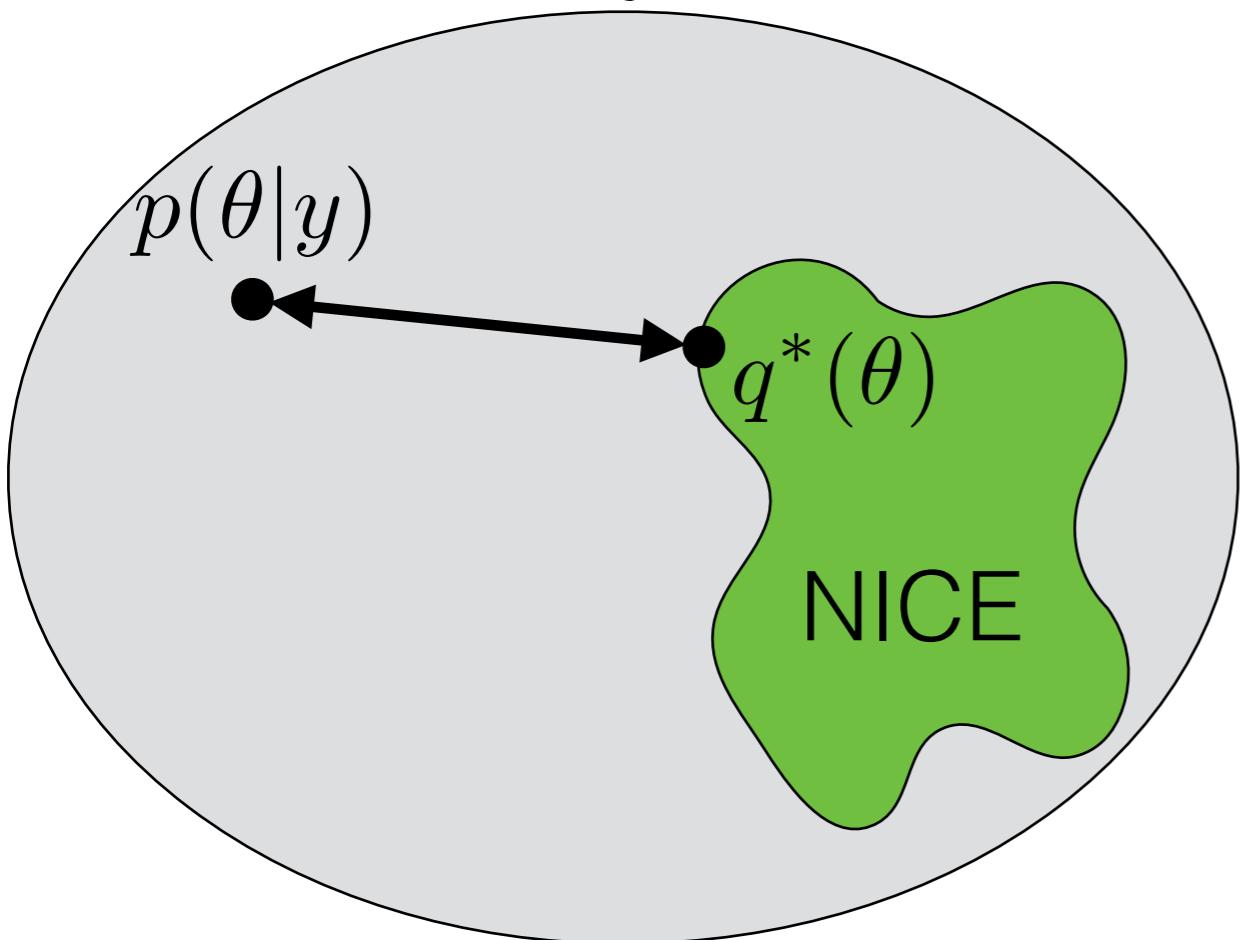
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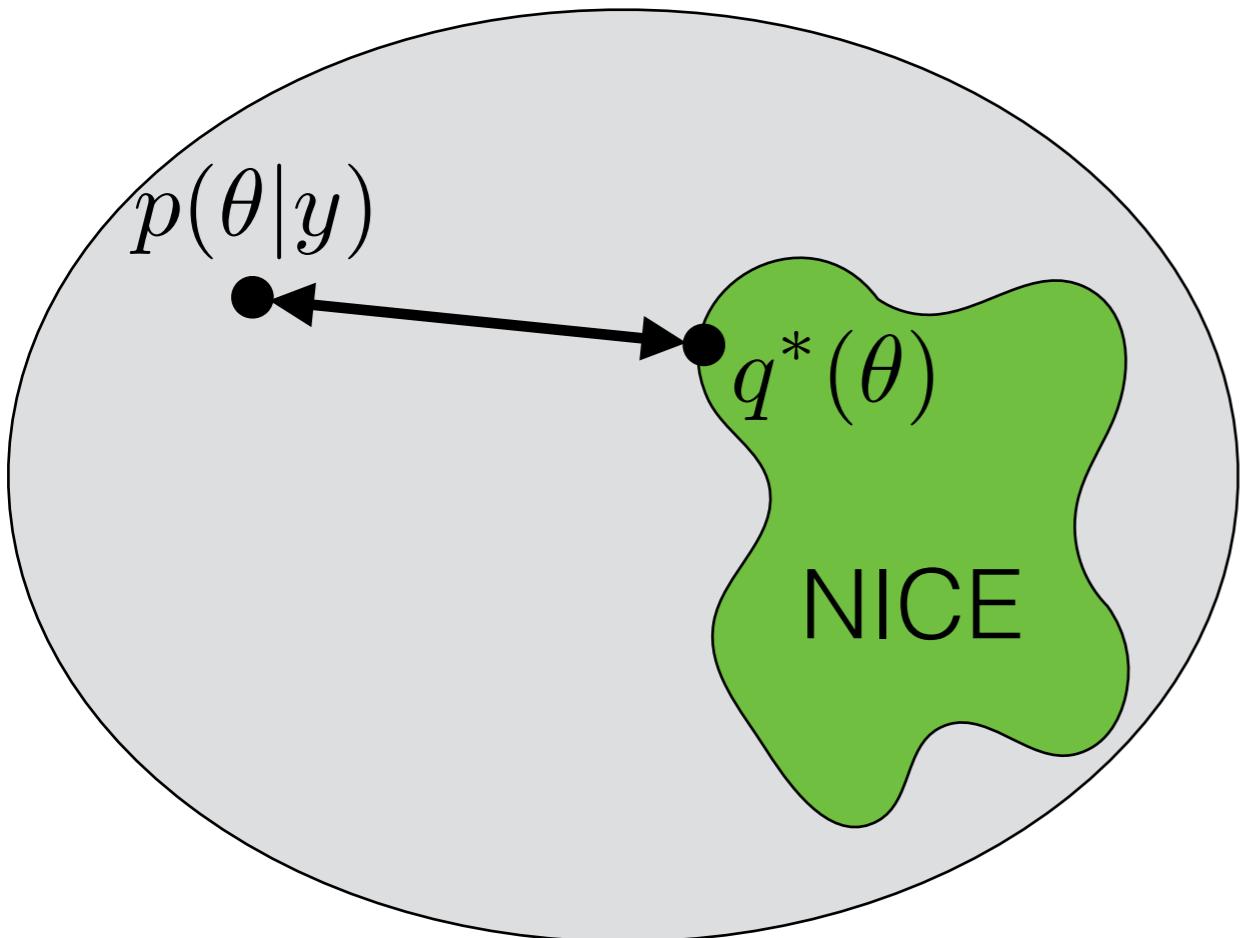


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- Gold standard: Markov Chain Monte Carlo (MCMC)
 - Eventually accurate but can be slow



Instead: an optimization approach

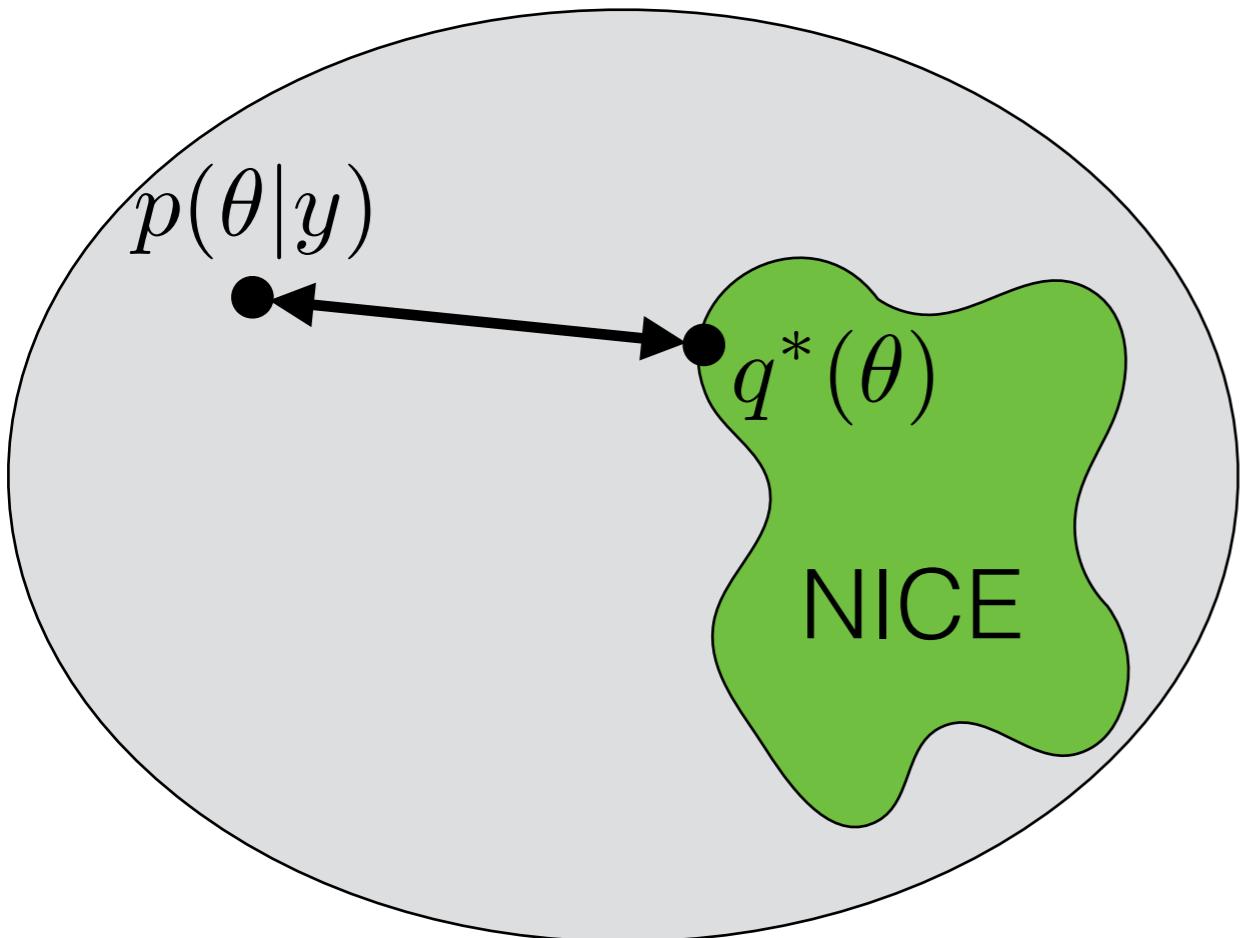
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Approximate Bayesian Inference

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Doucet,
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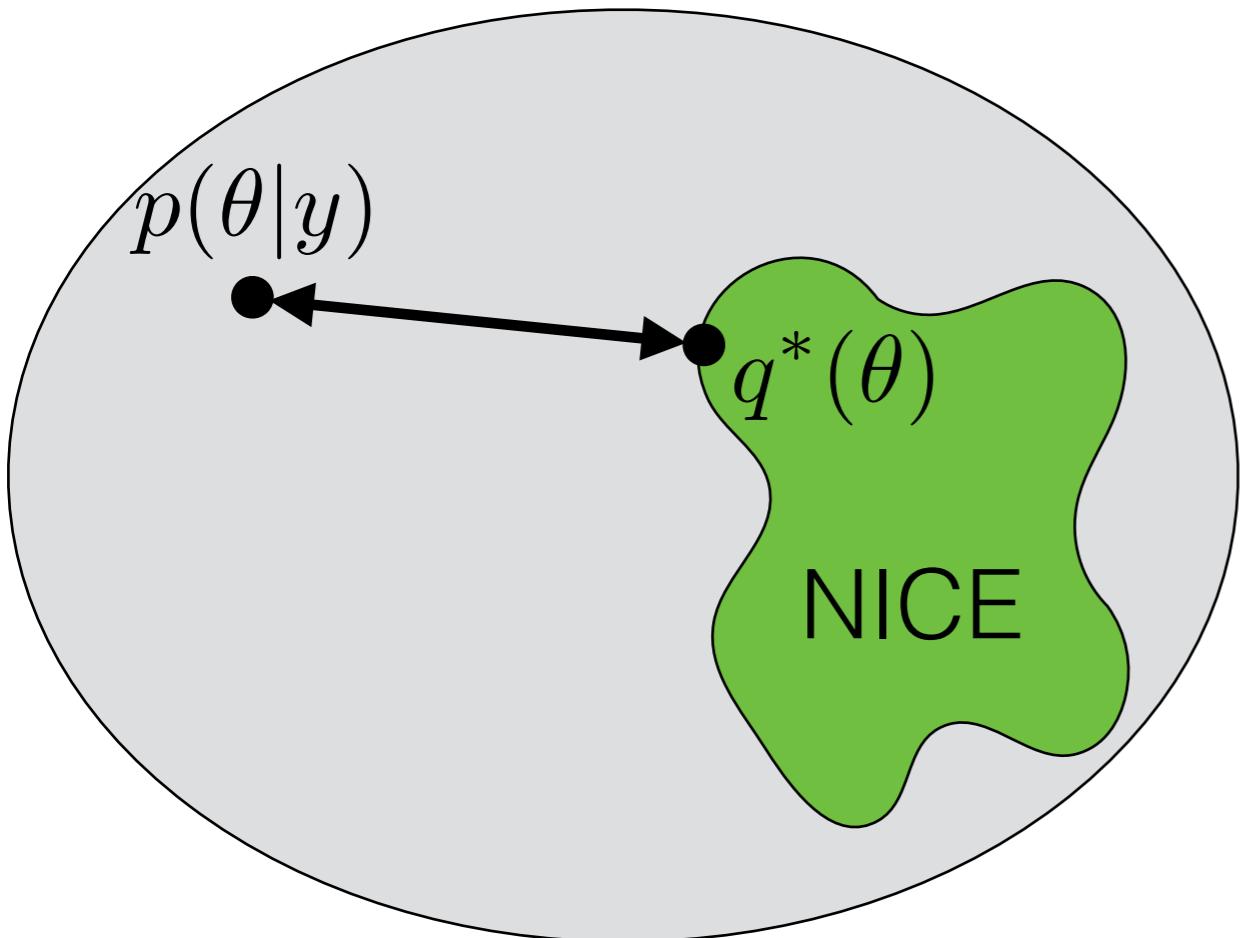
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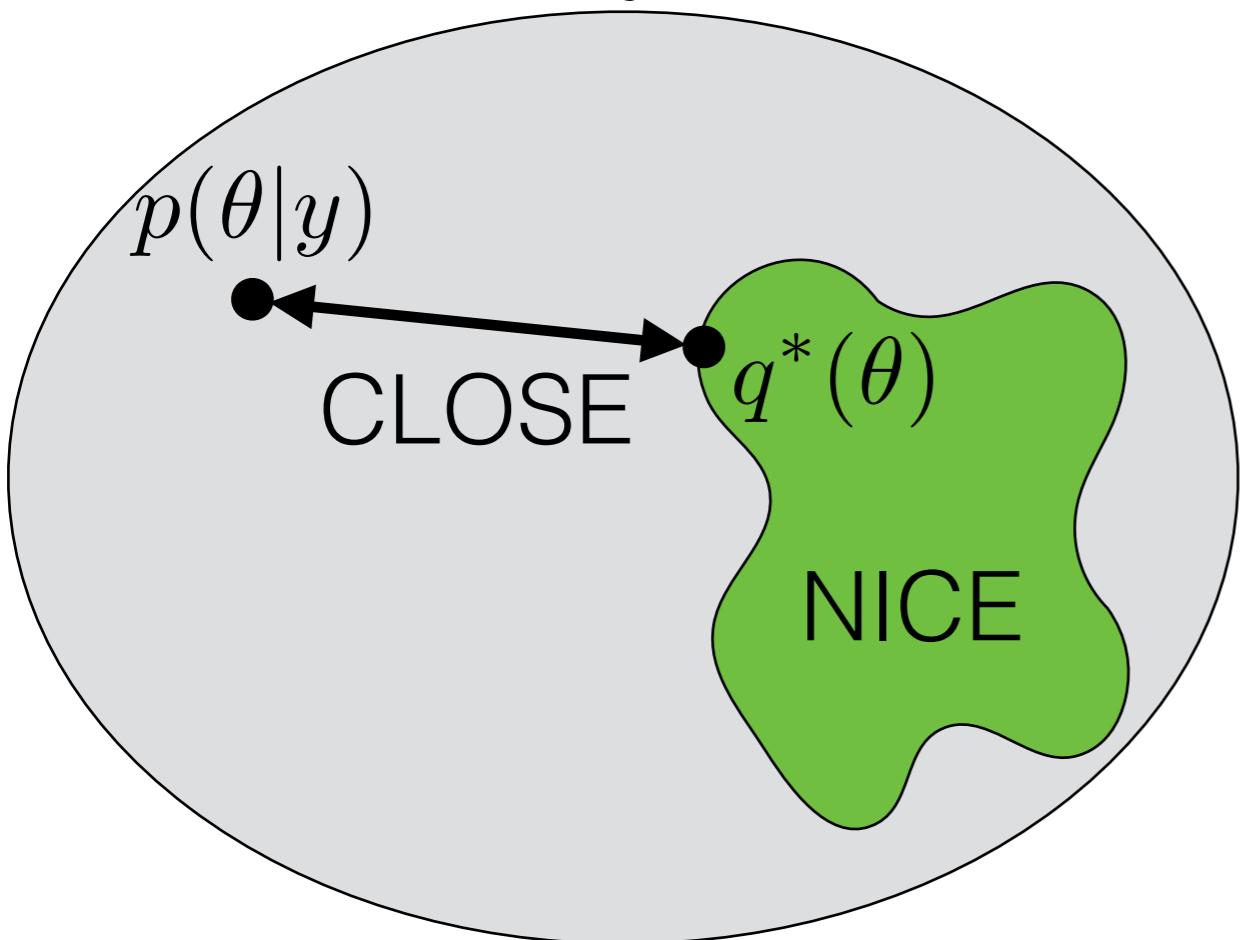
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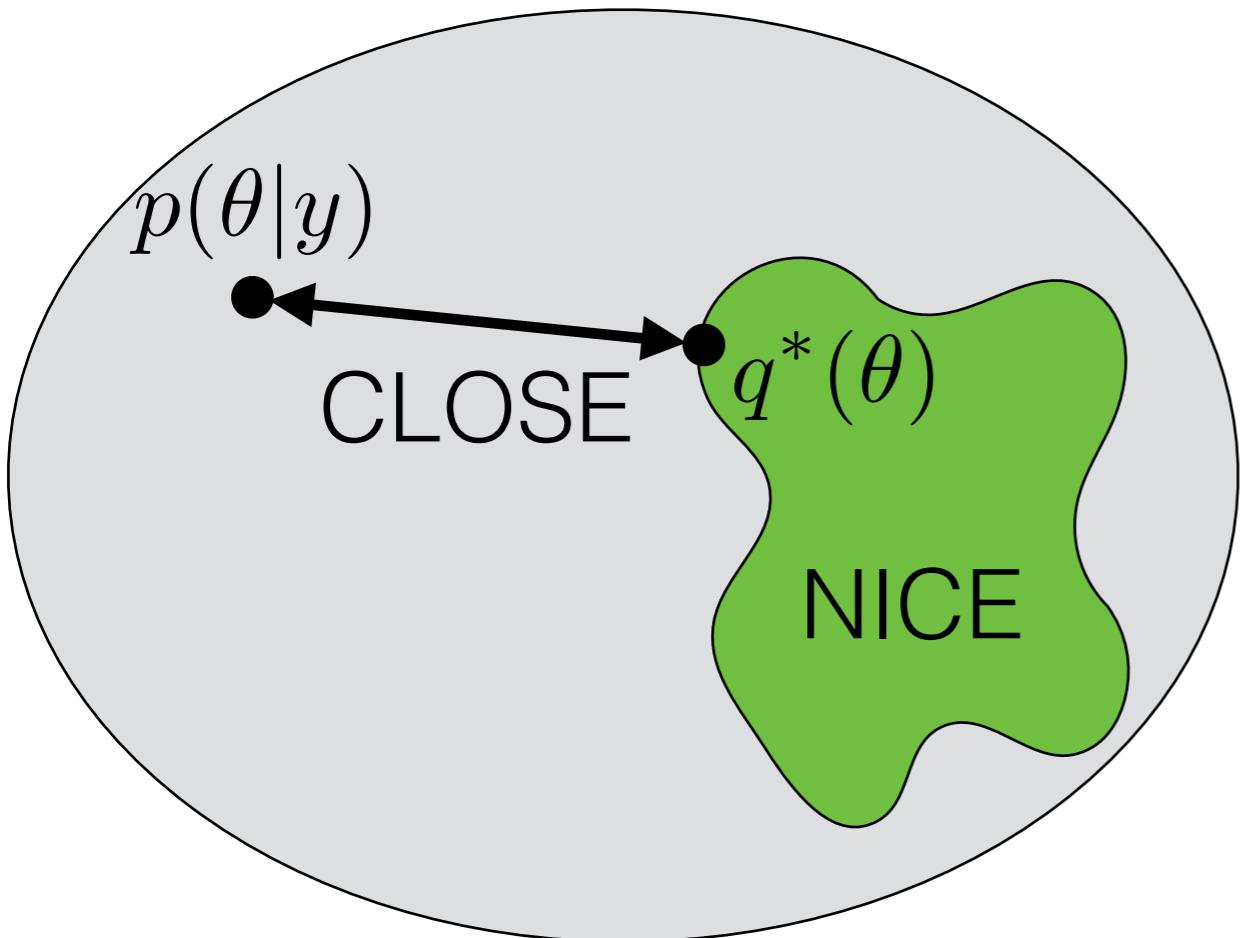
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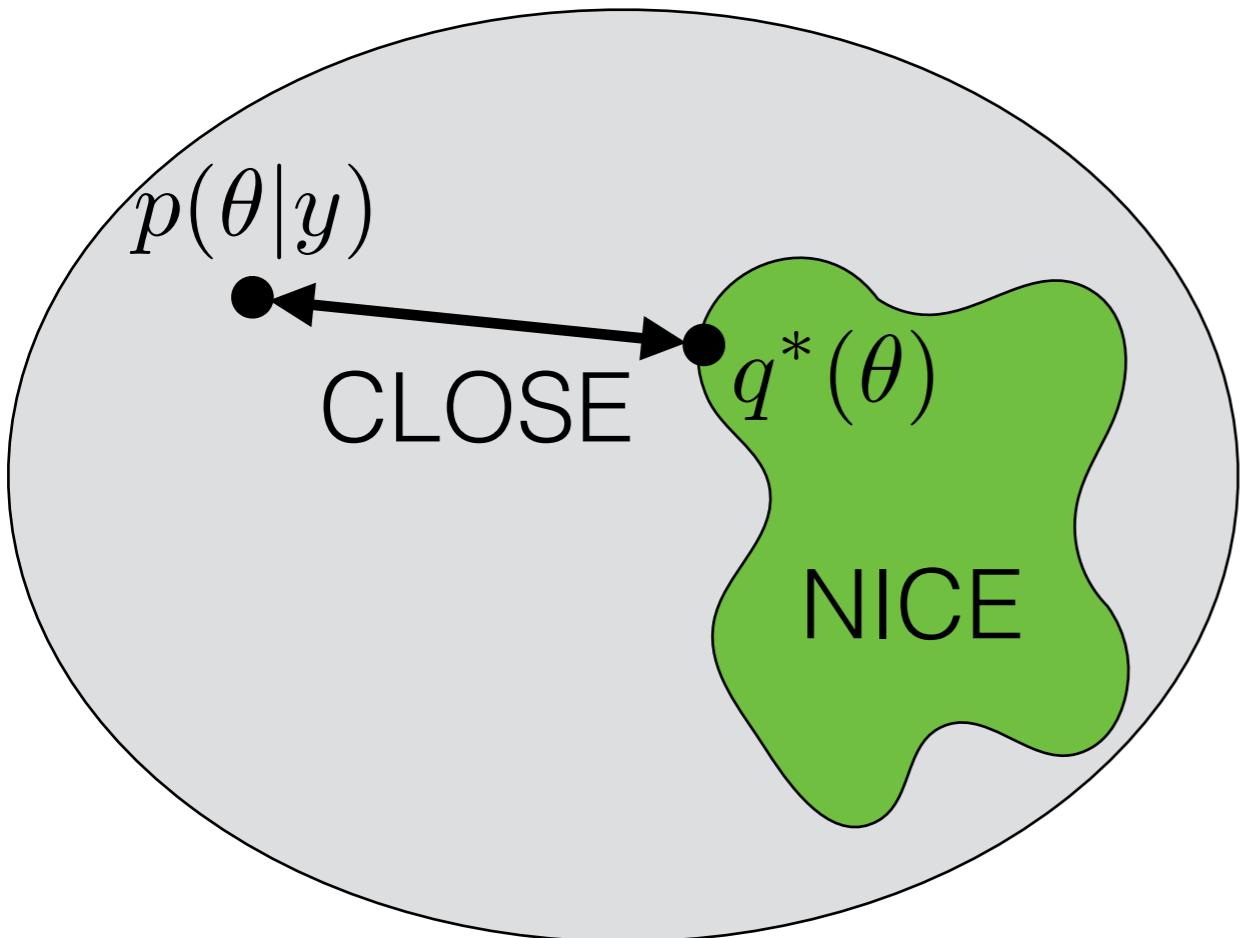
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[board]

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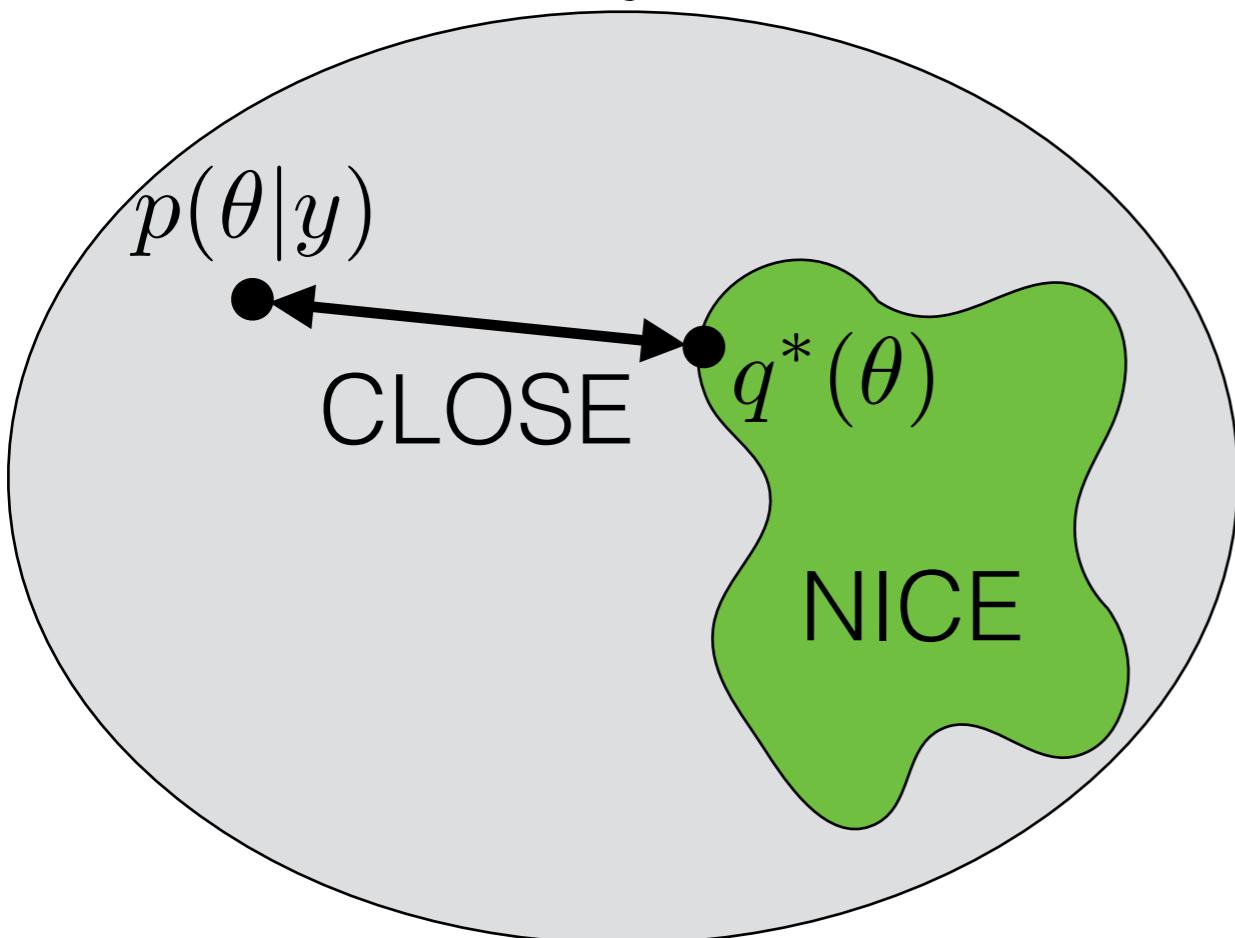
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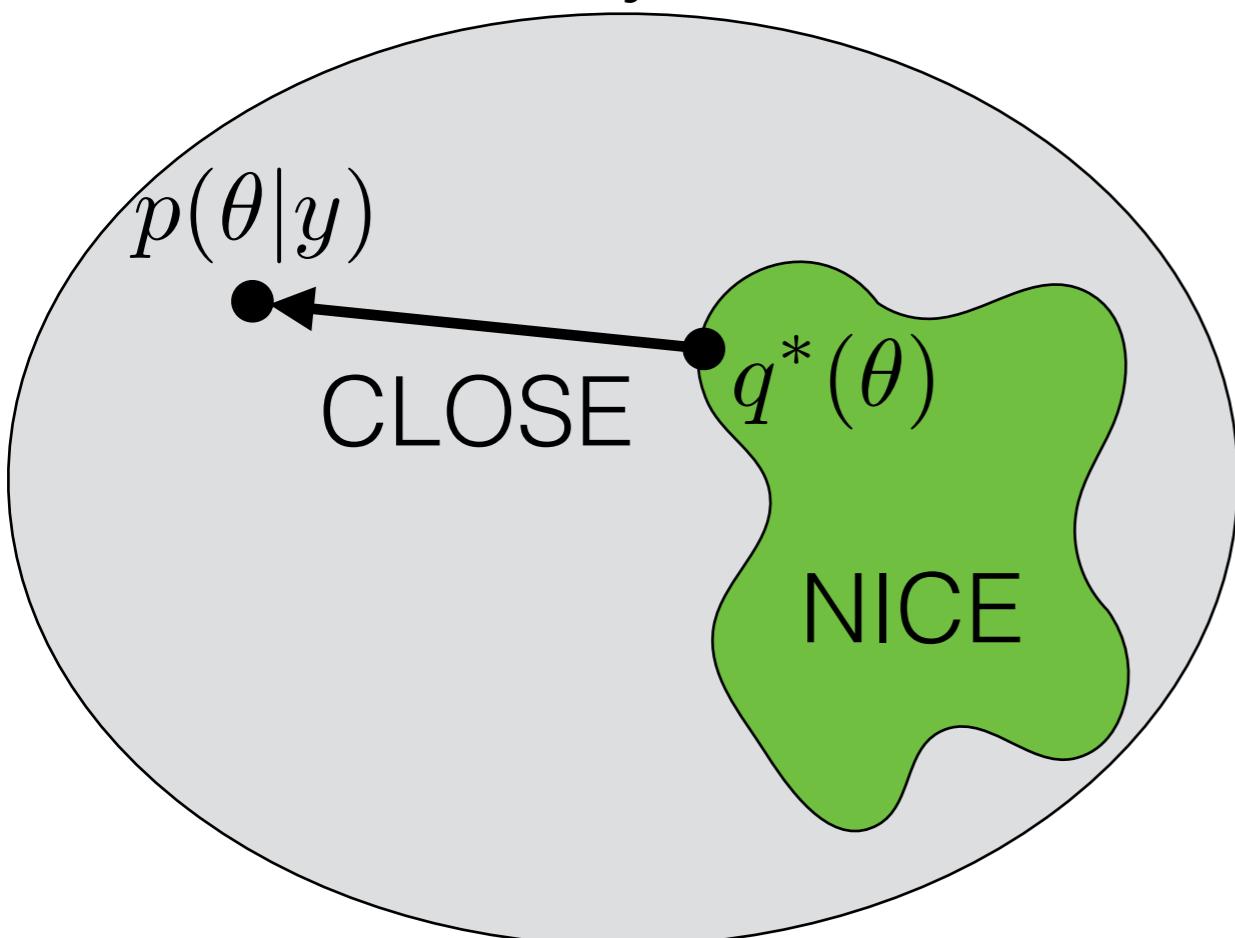
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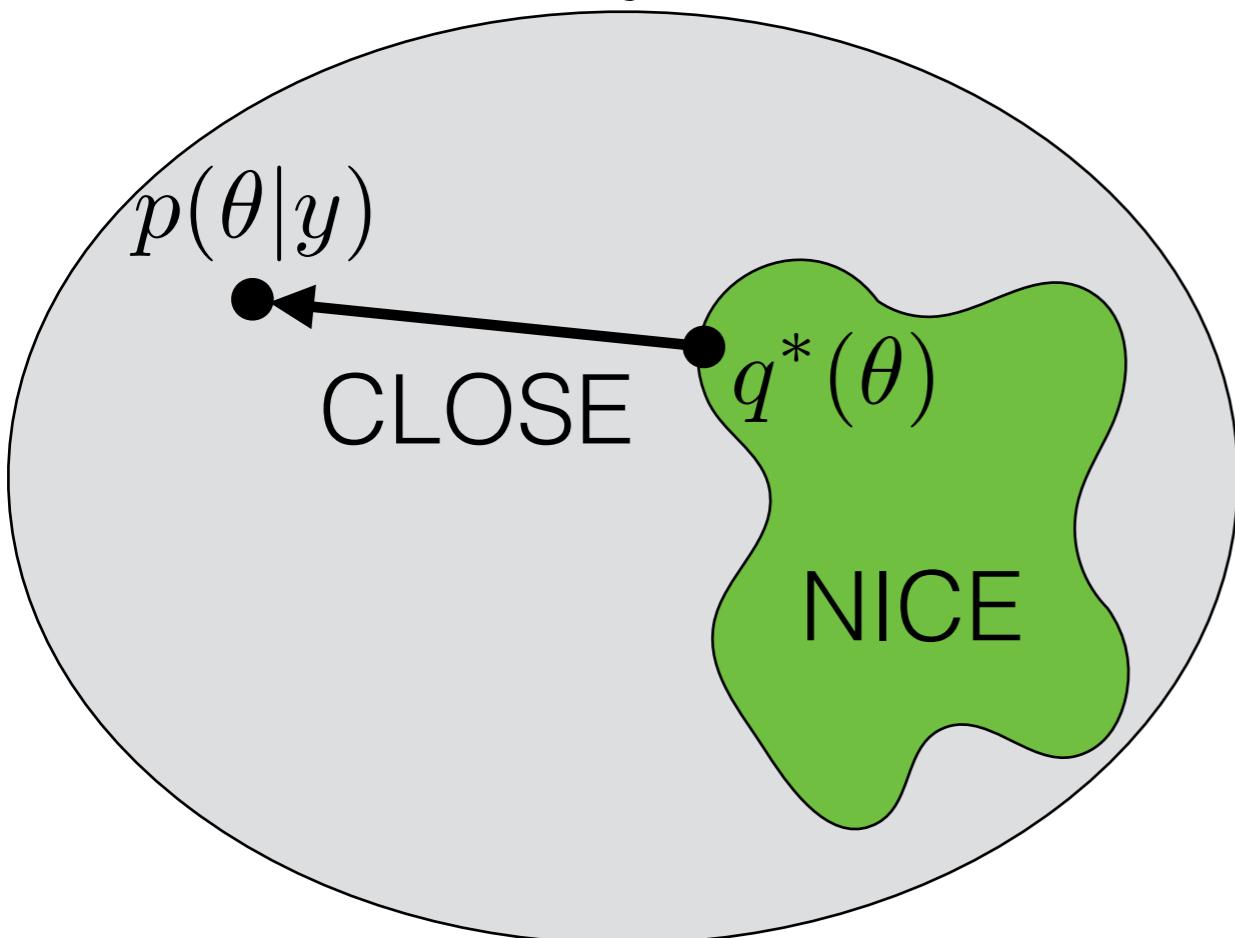
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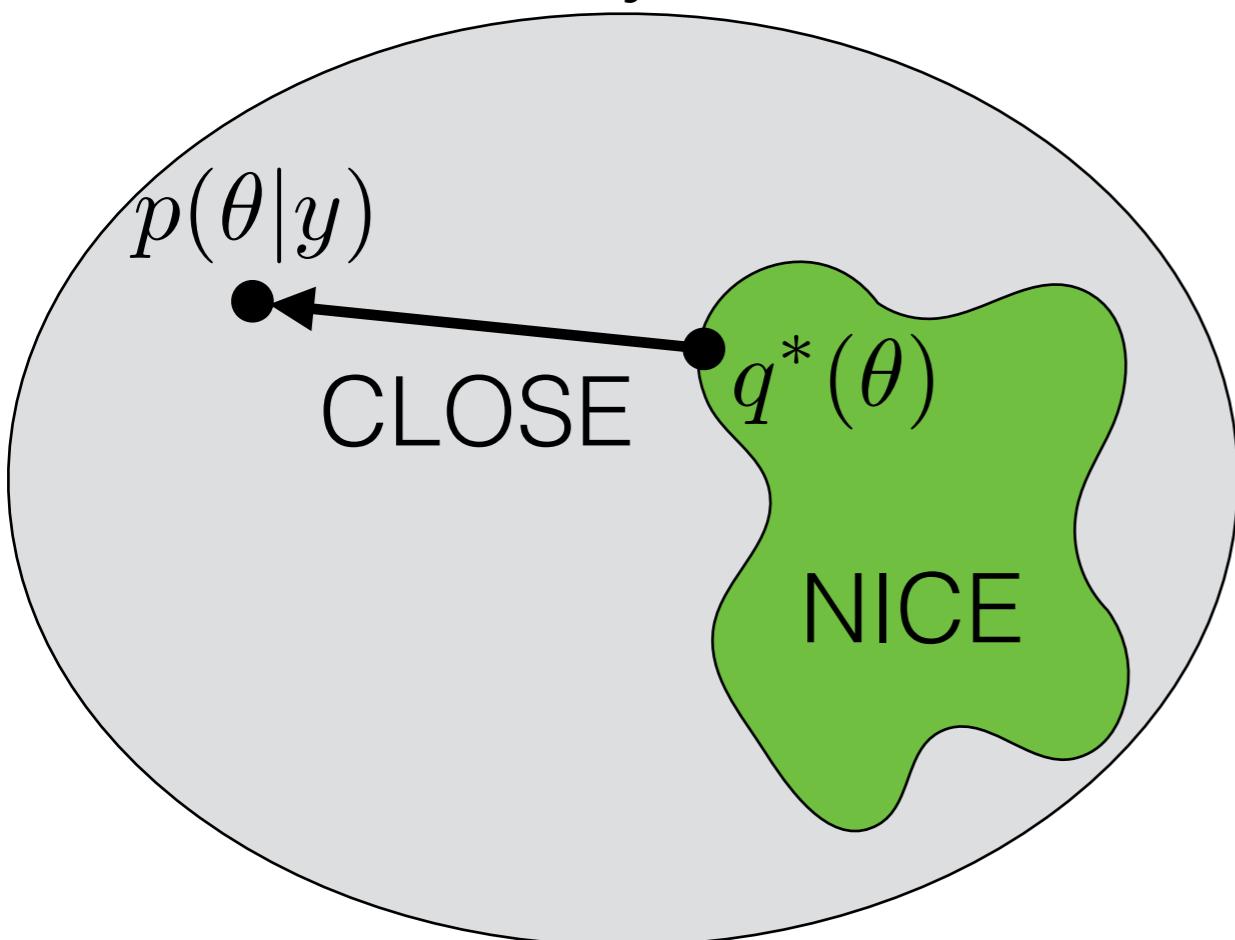
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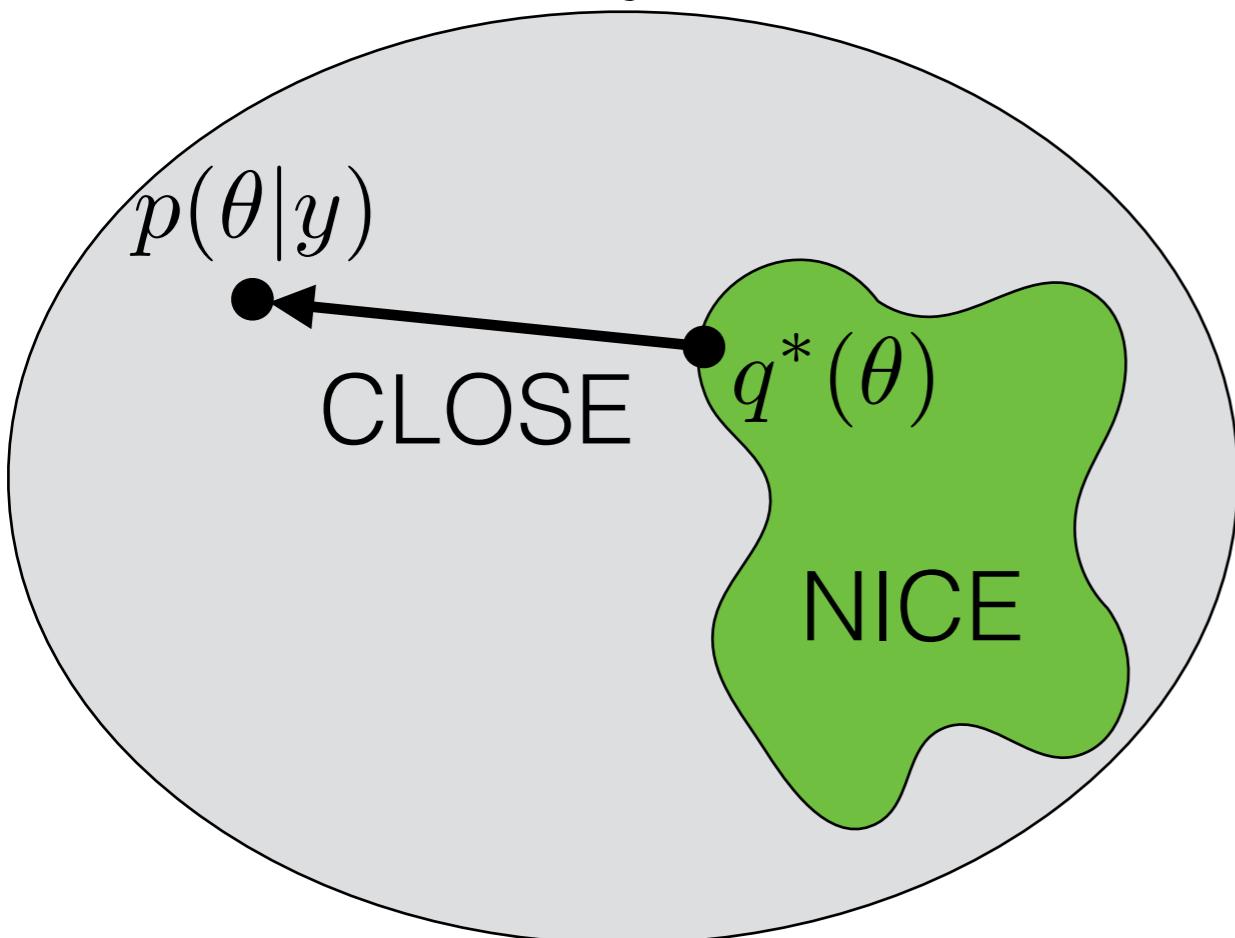
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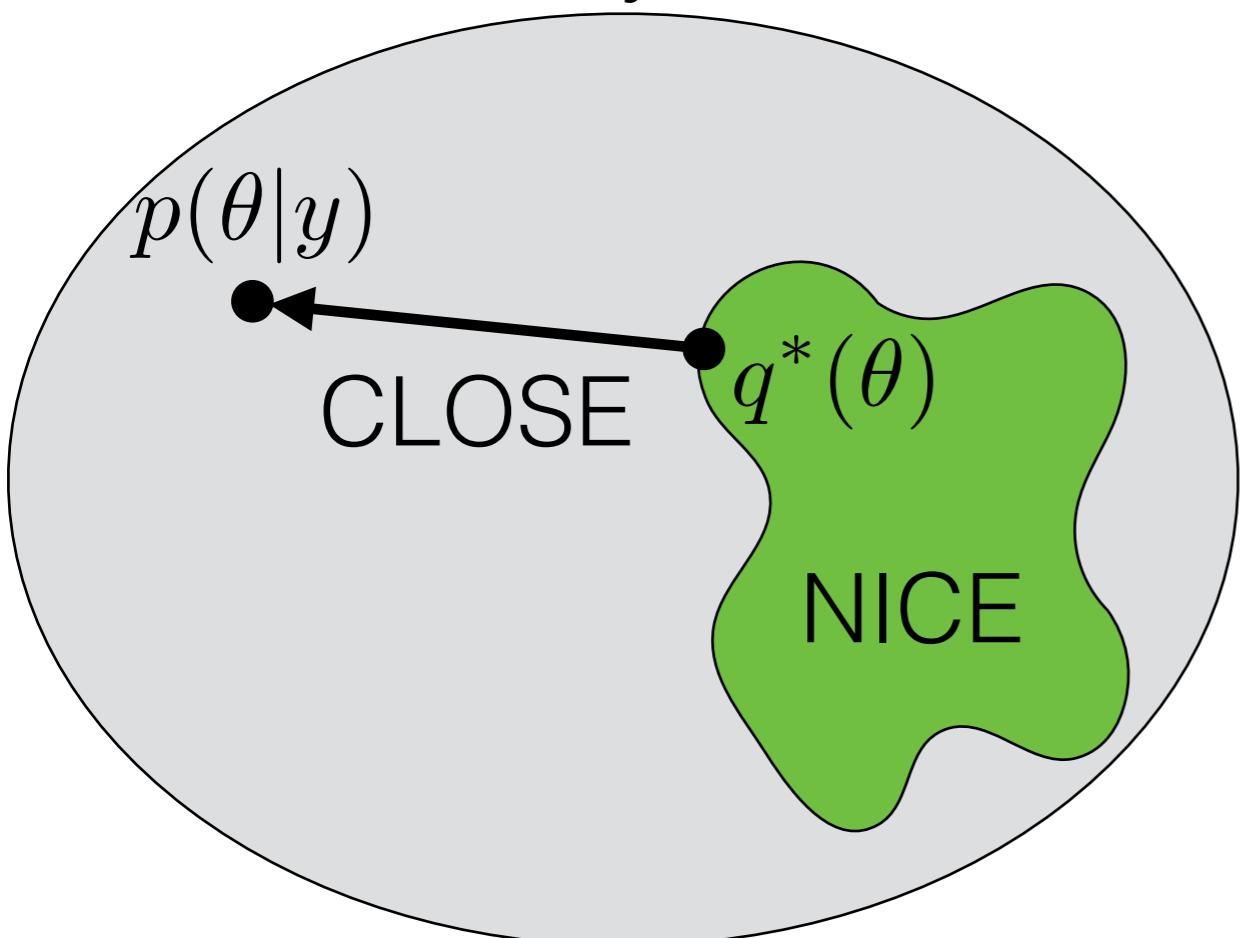
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Approximate Bayesian Inference

[Bardenet,
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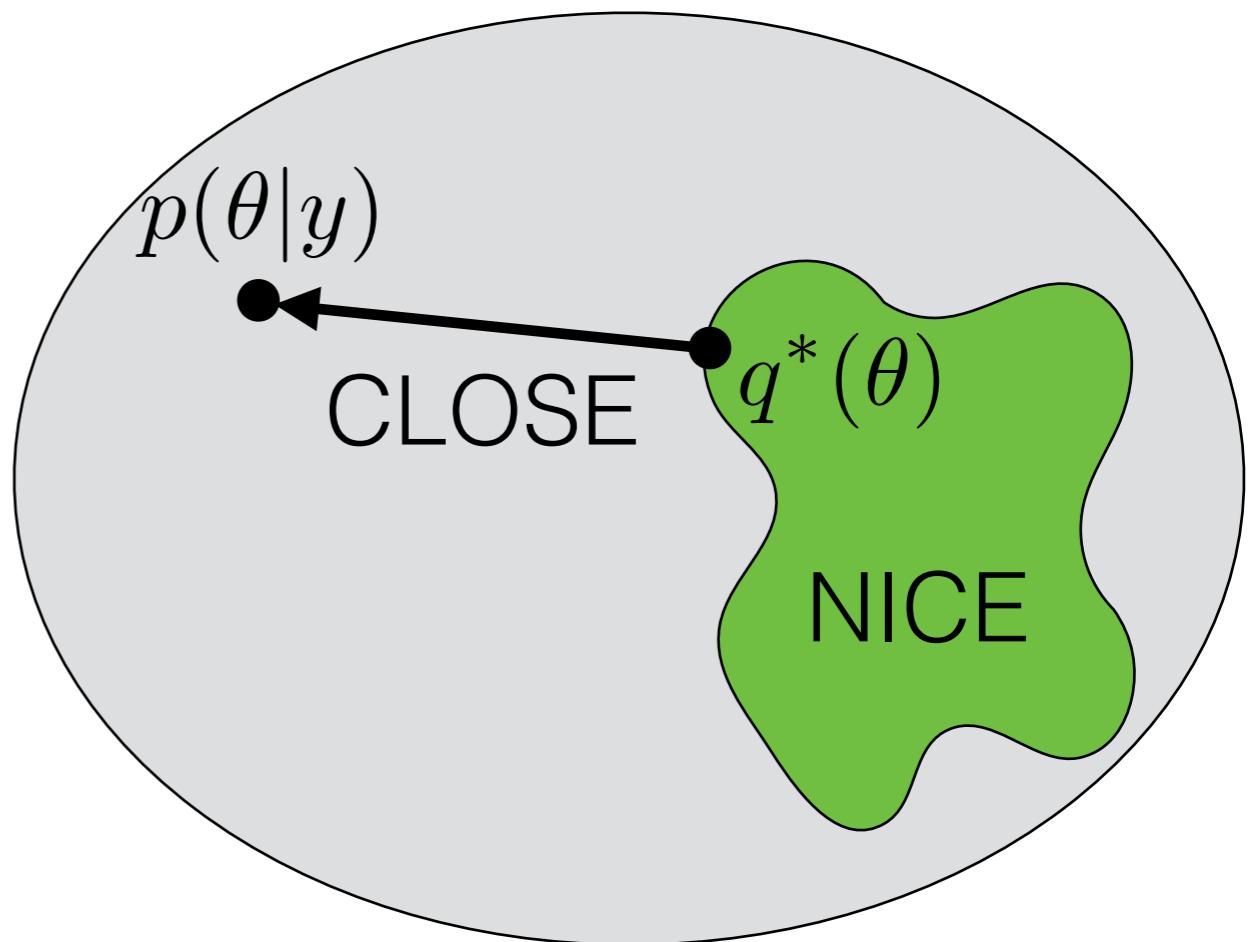
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- Variational Bayes (VB): f is Kullback-Leibler divergence
$$KL(q(\cdot)||p(\cdot|y))$$
- VB practical success: point estimates and prediction, fast, streaming, distributed (3.6M Wikipedia, 350K Nature)

Why KL?

- Variational Bayes

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



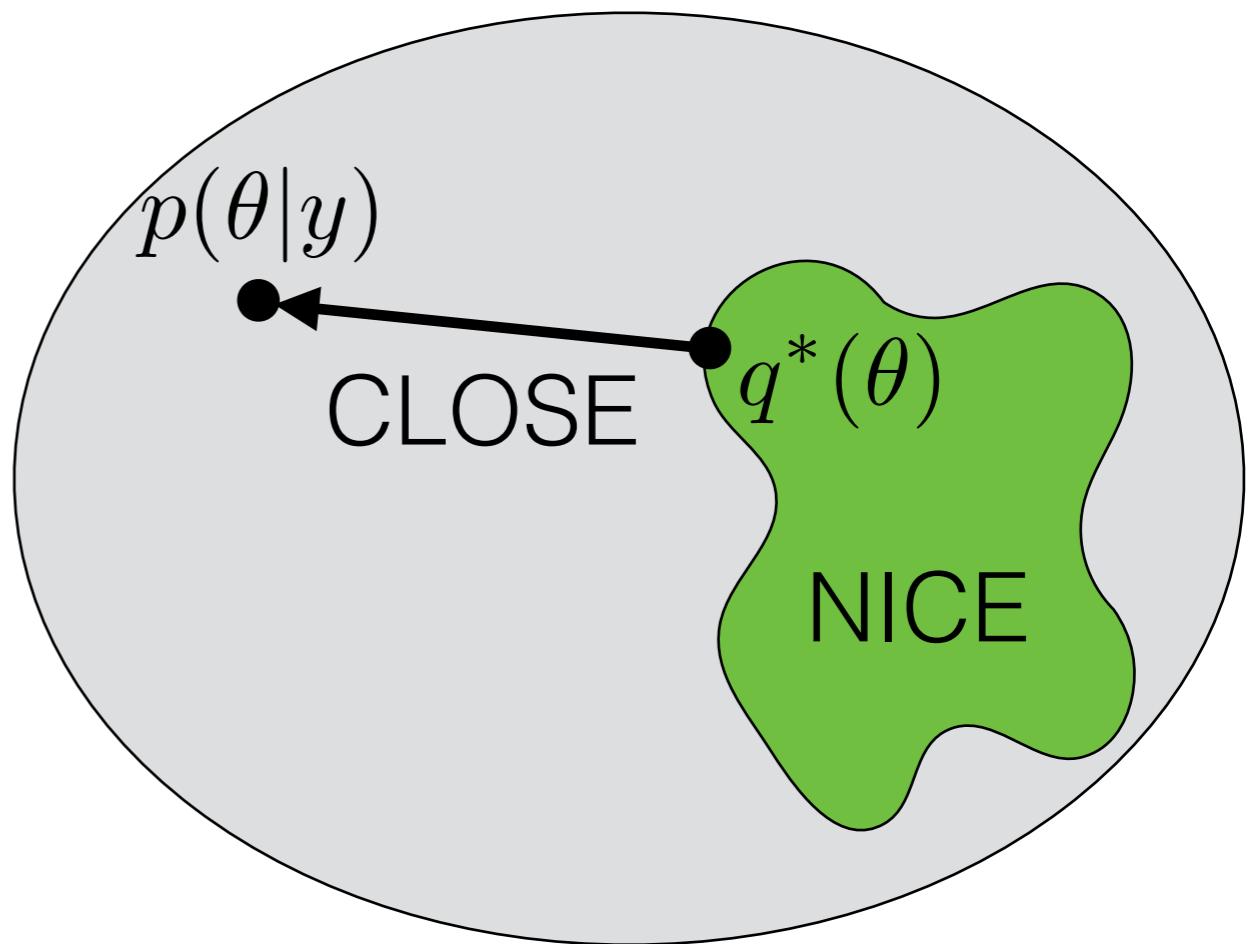
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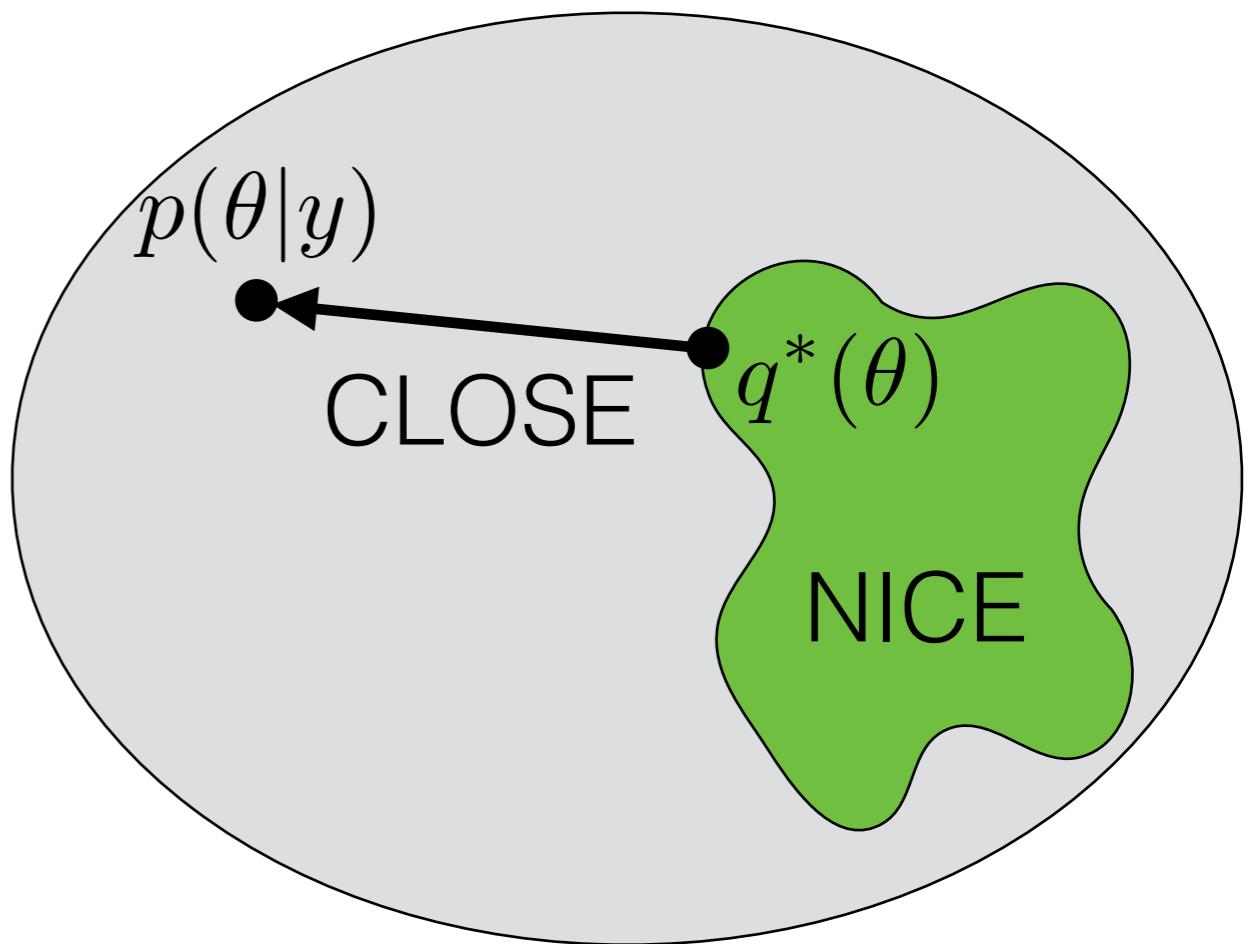
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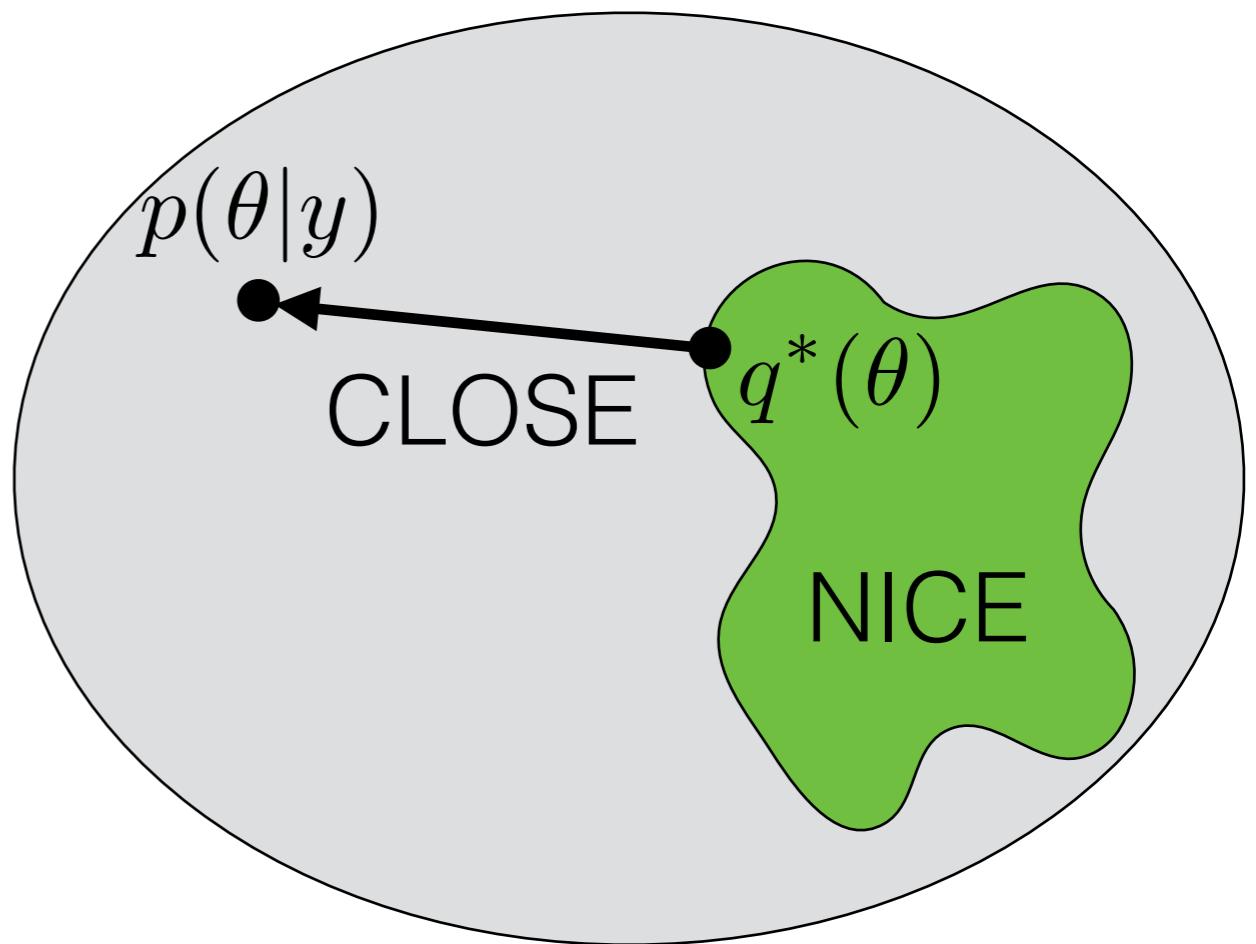
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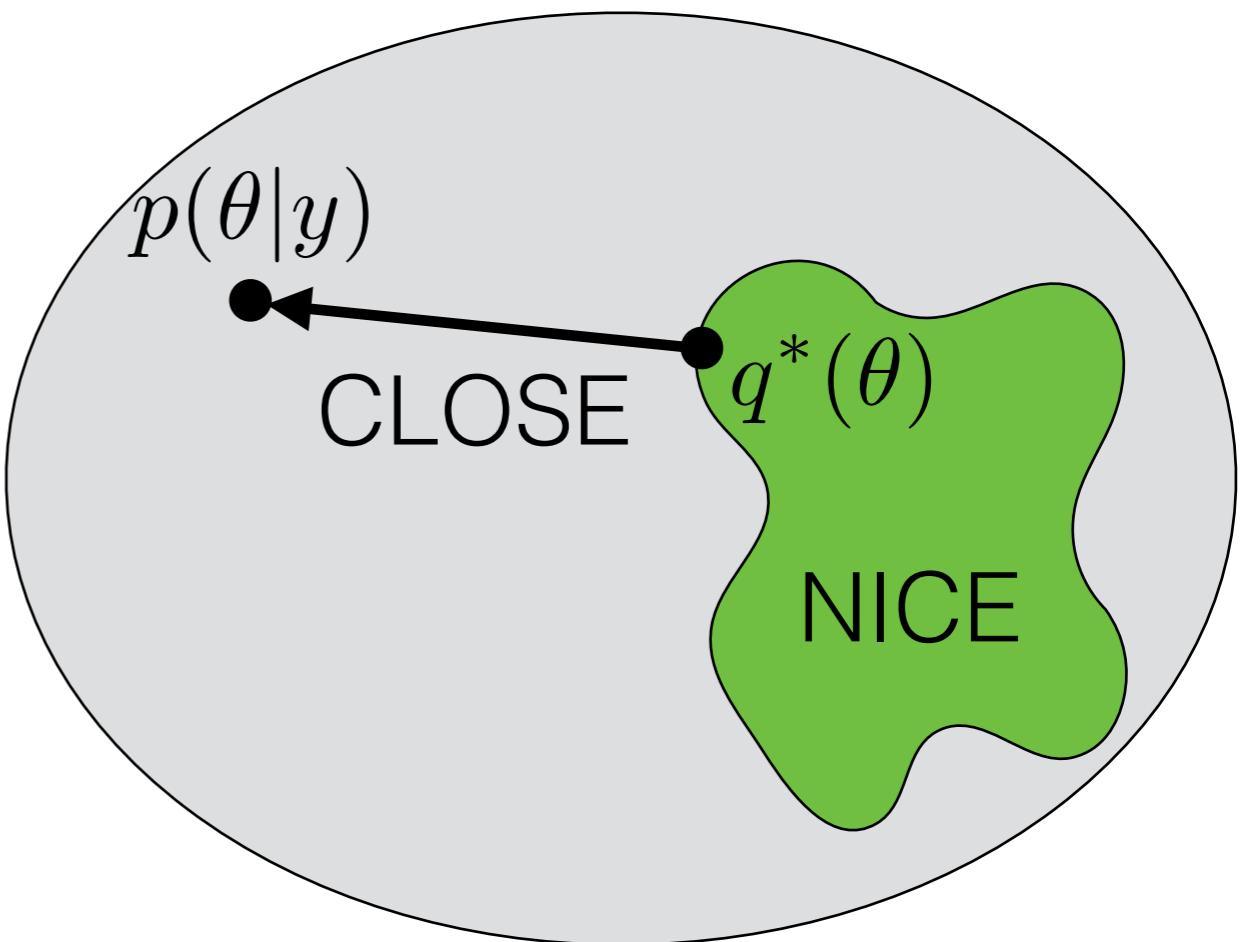
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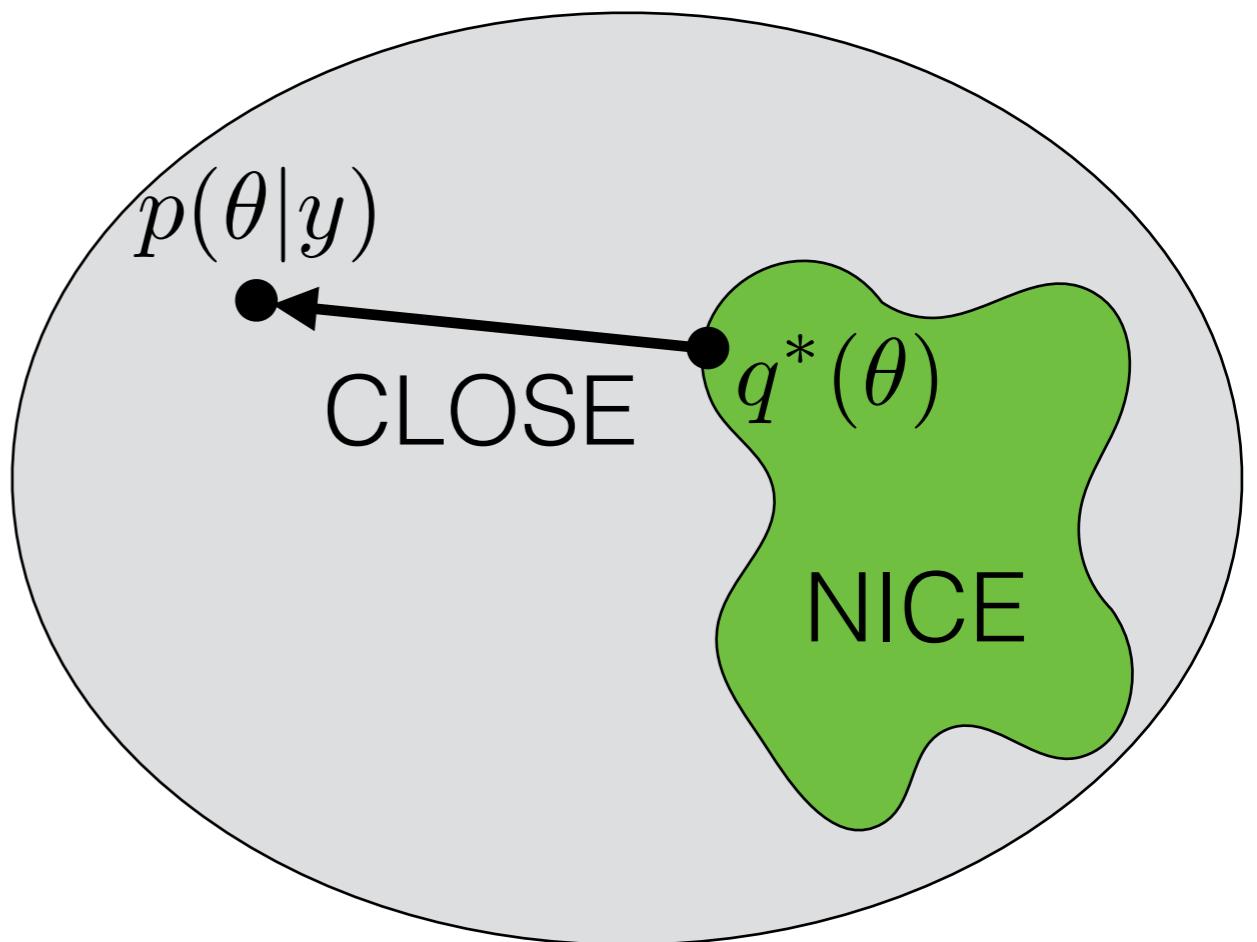
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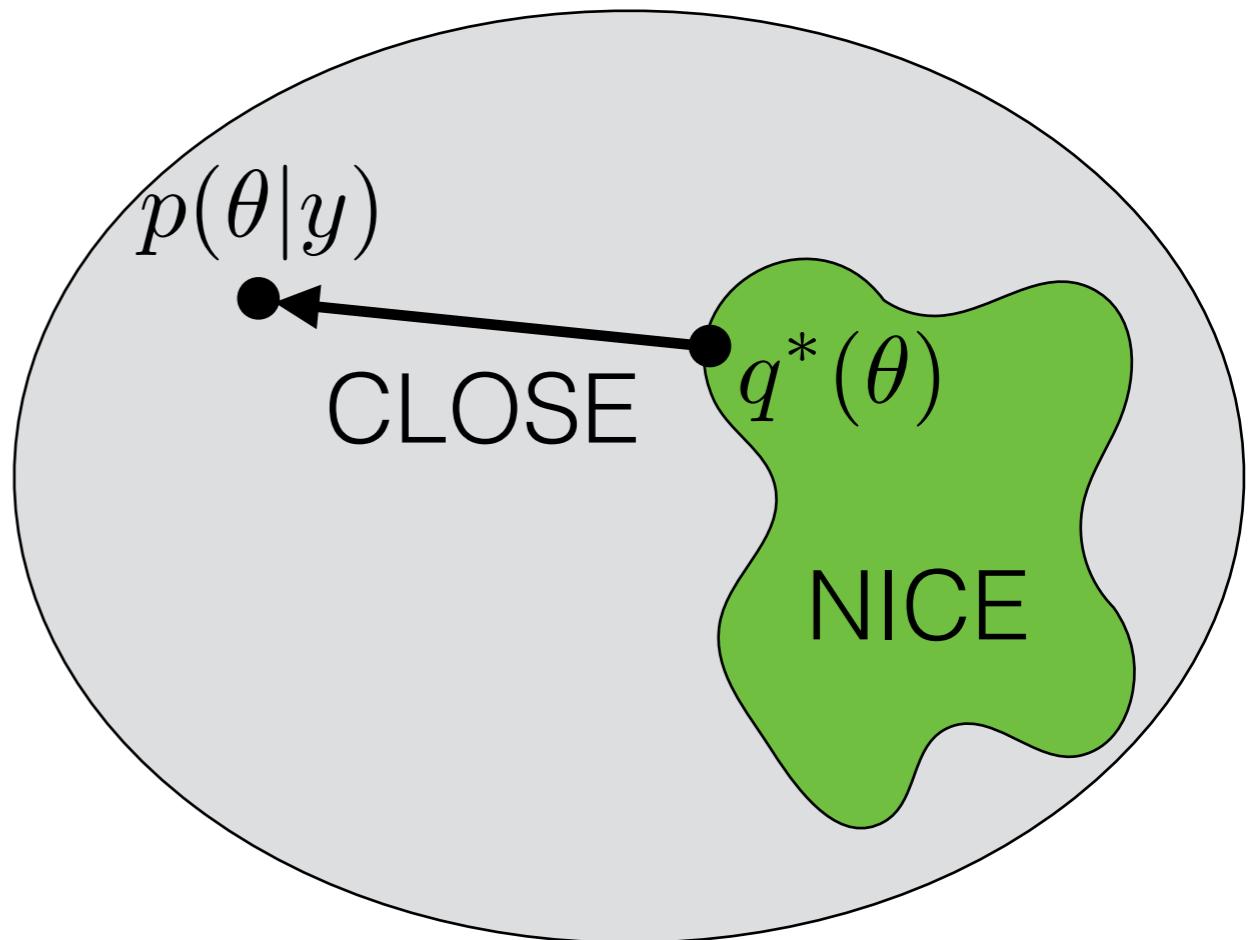
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“Evidence lower bound” (ELBO)

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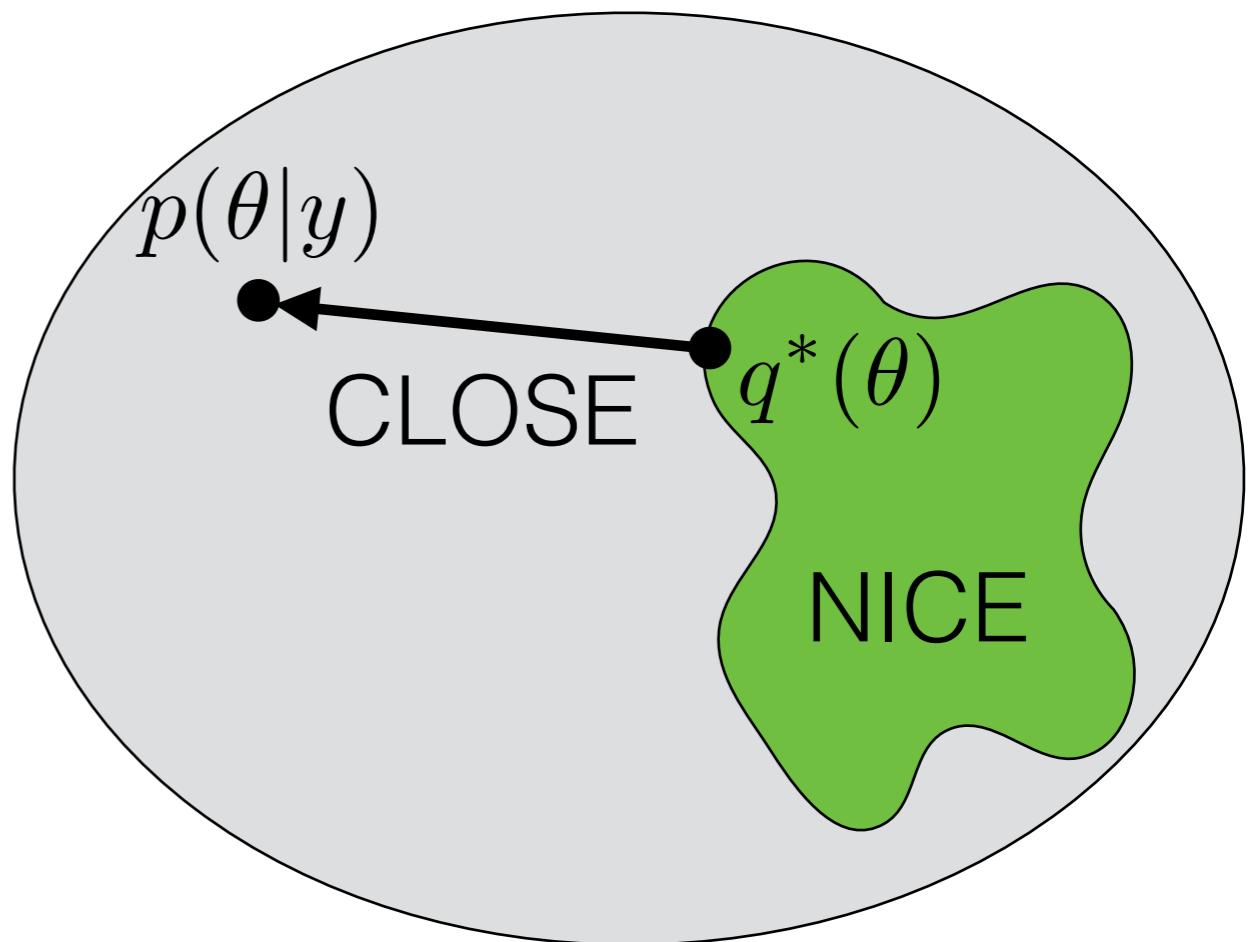
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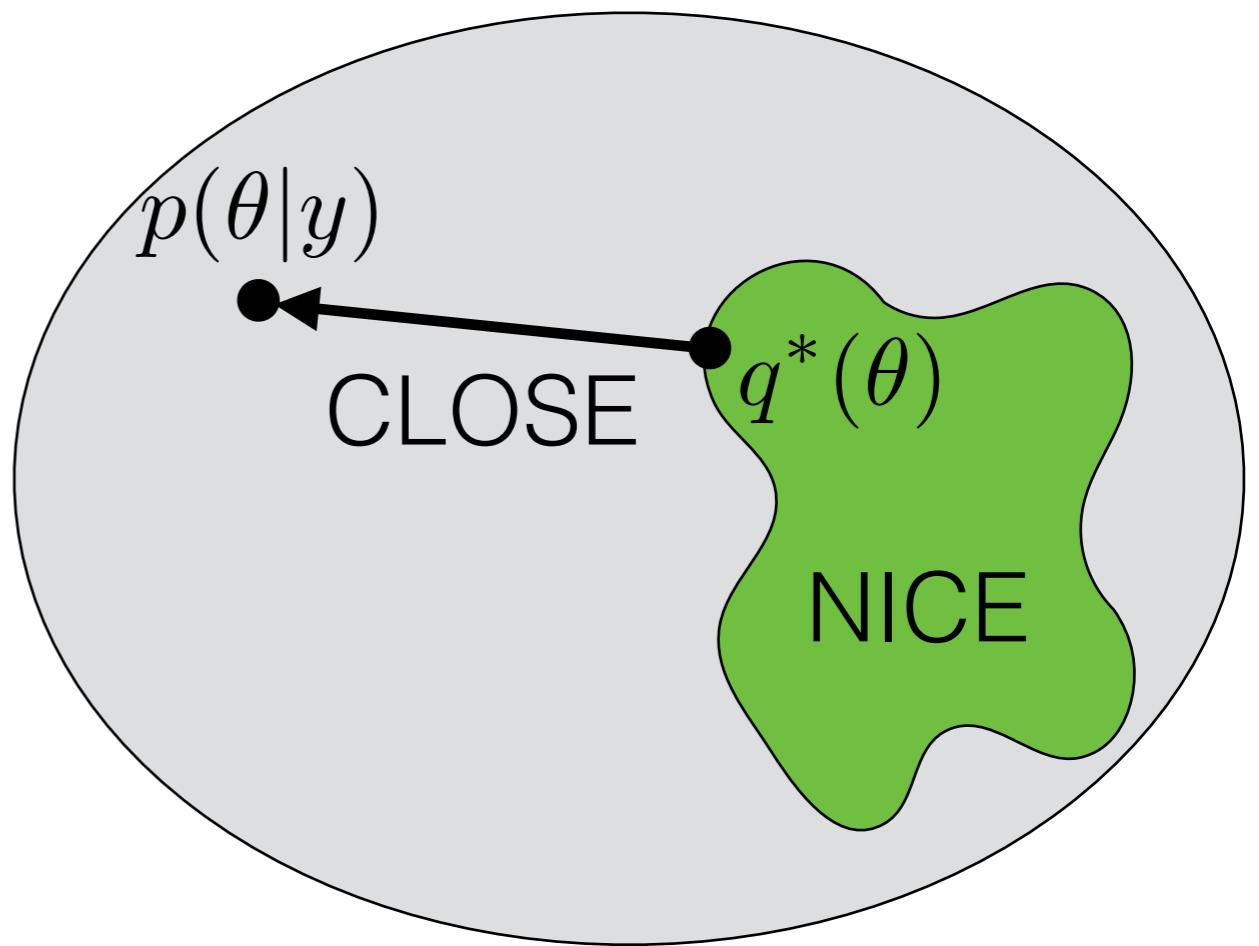
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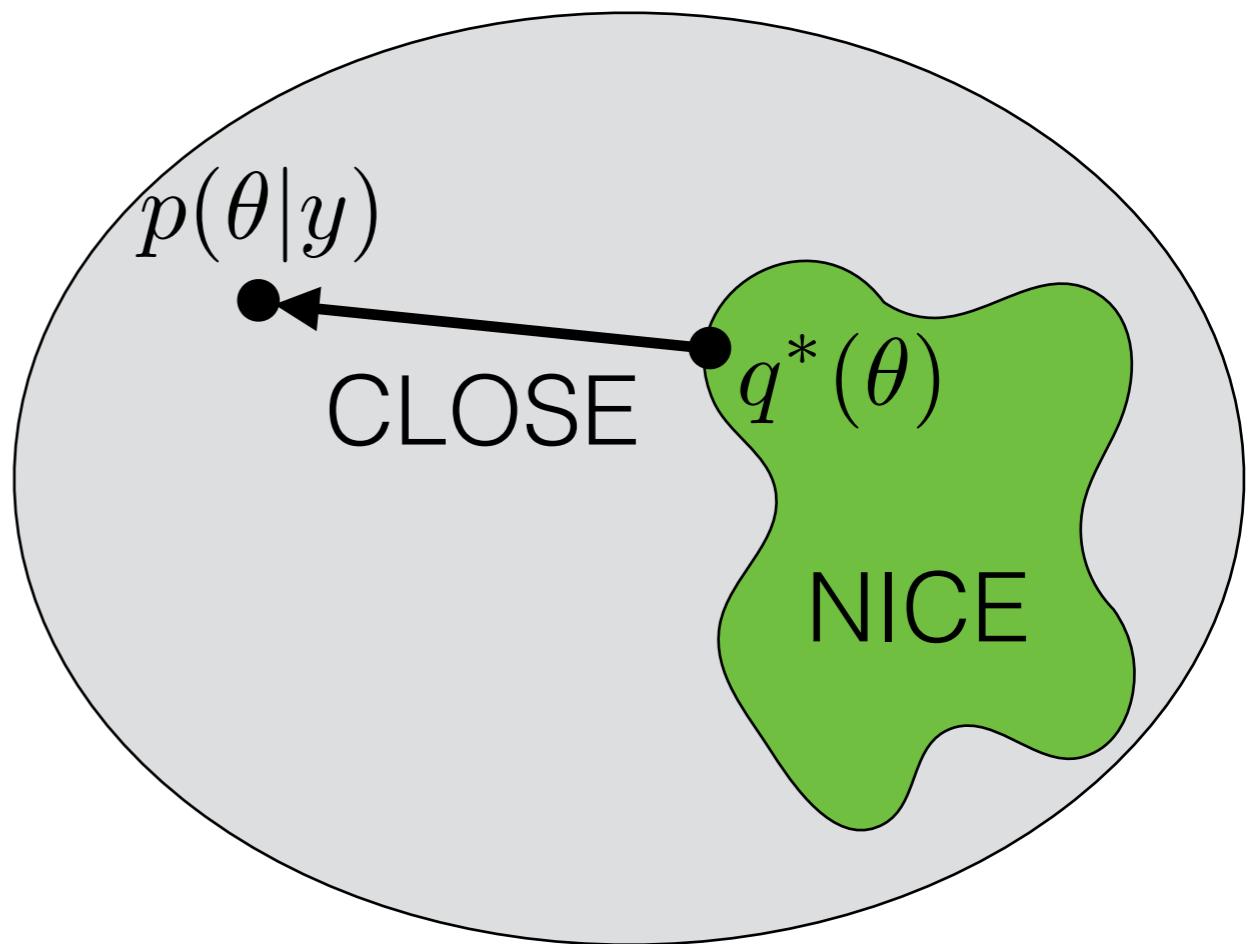
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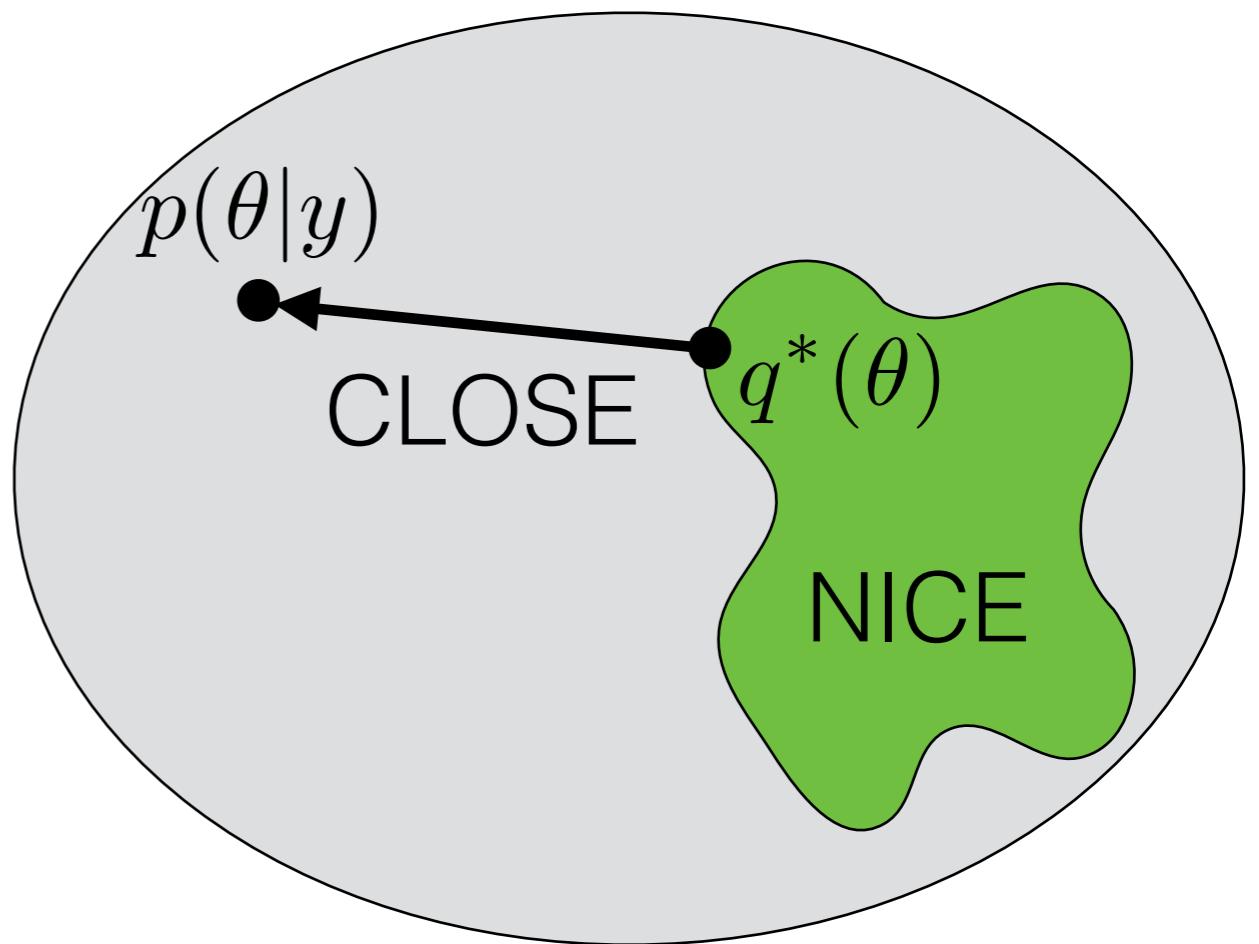
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“Evidence lower bound” (ELBO)

Why KL?

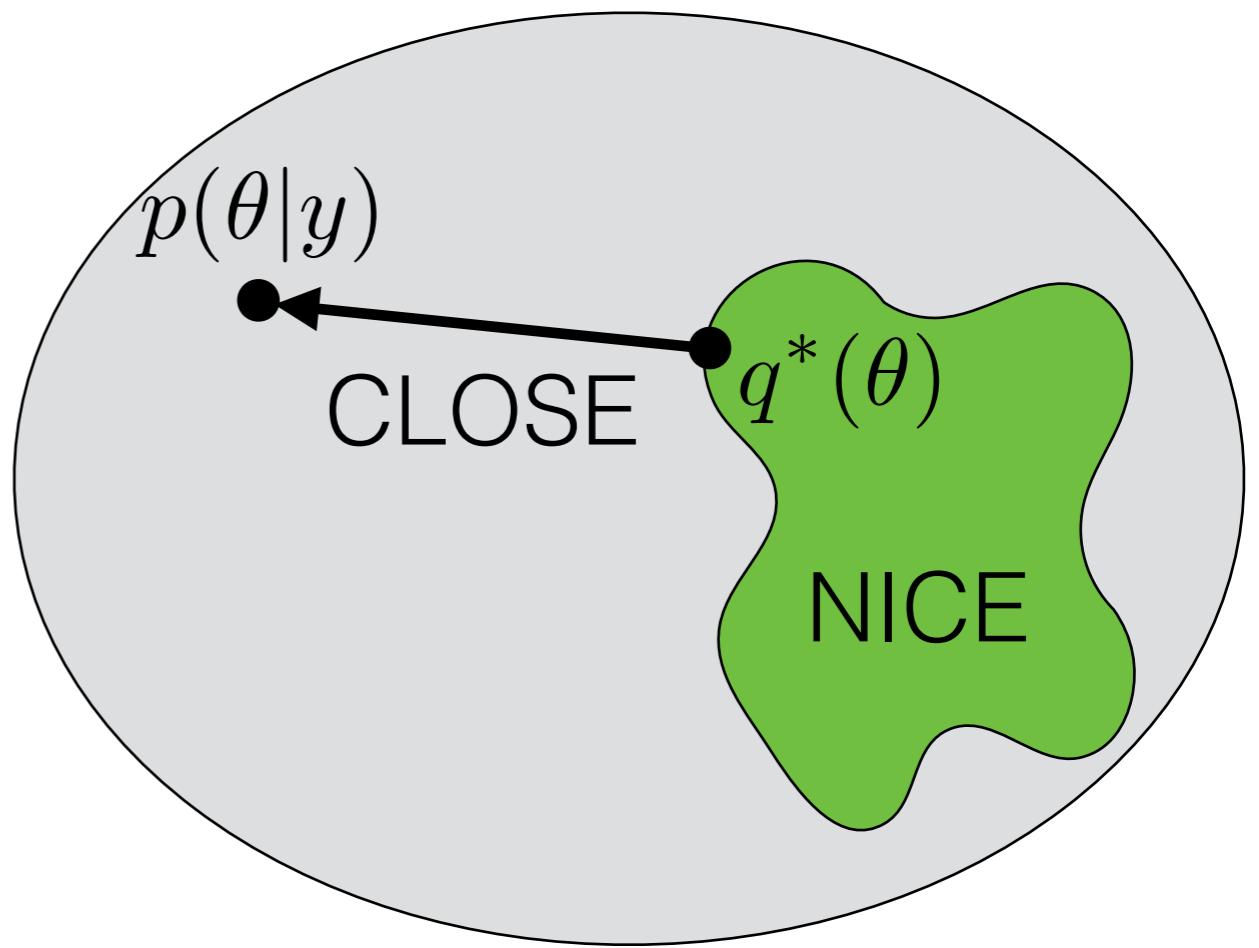
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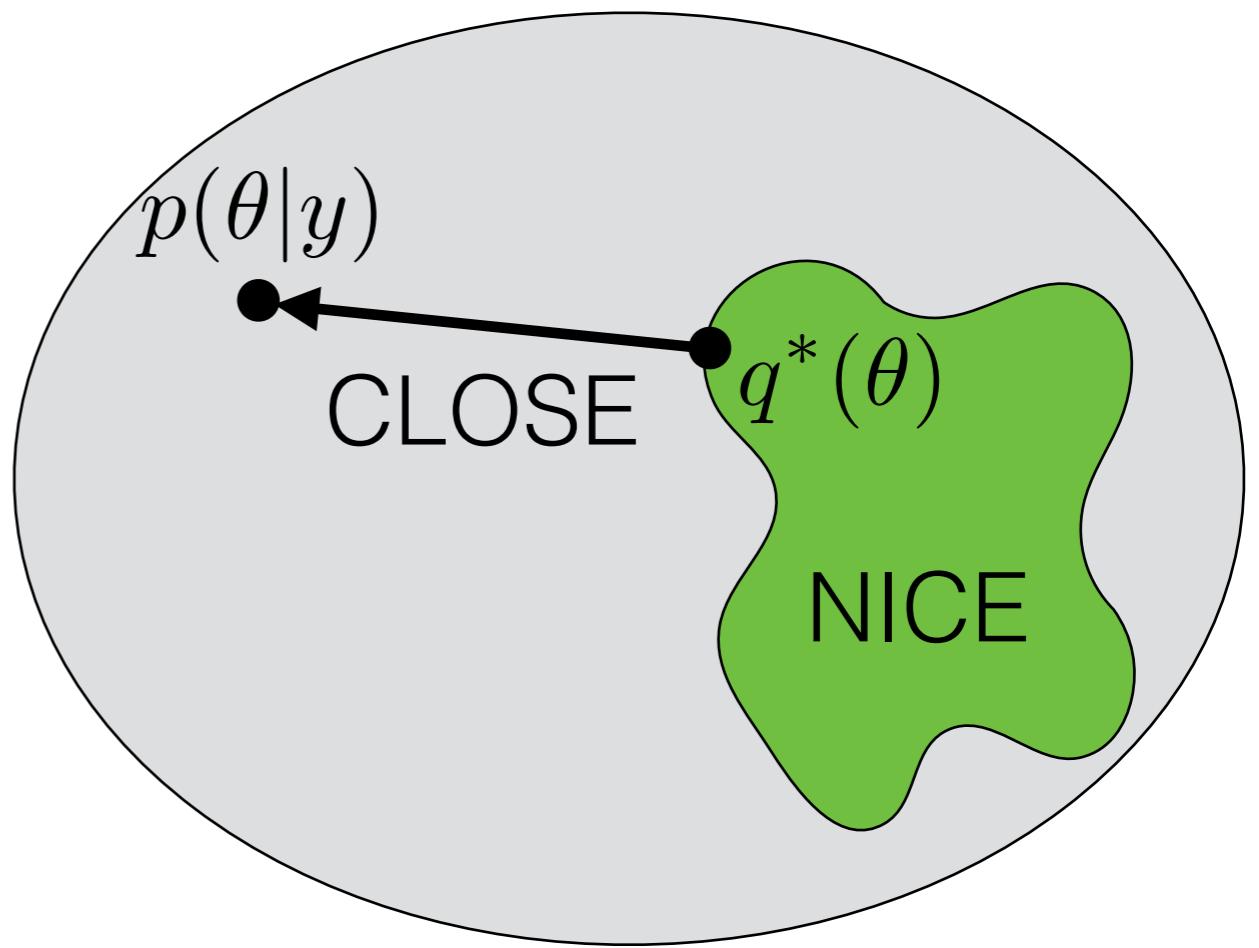
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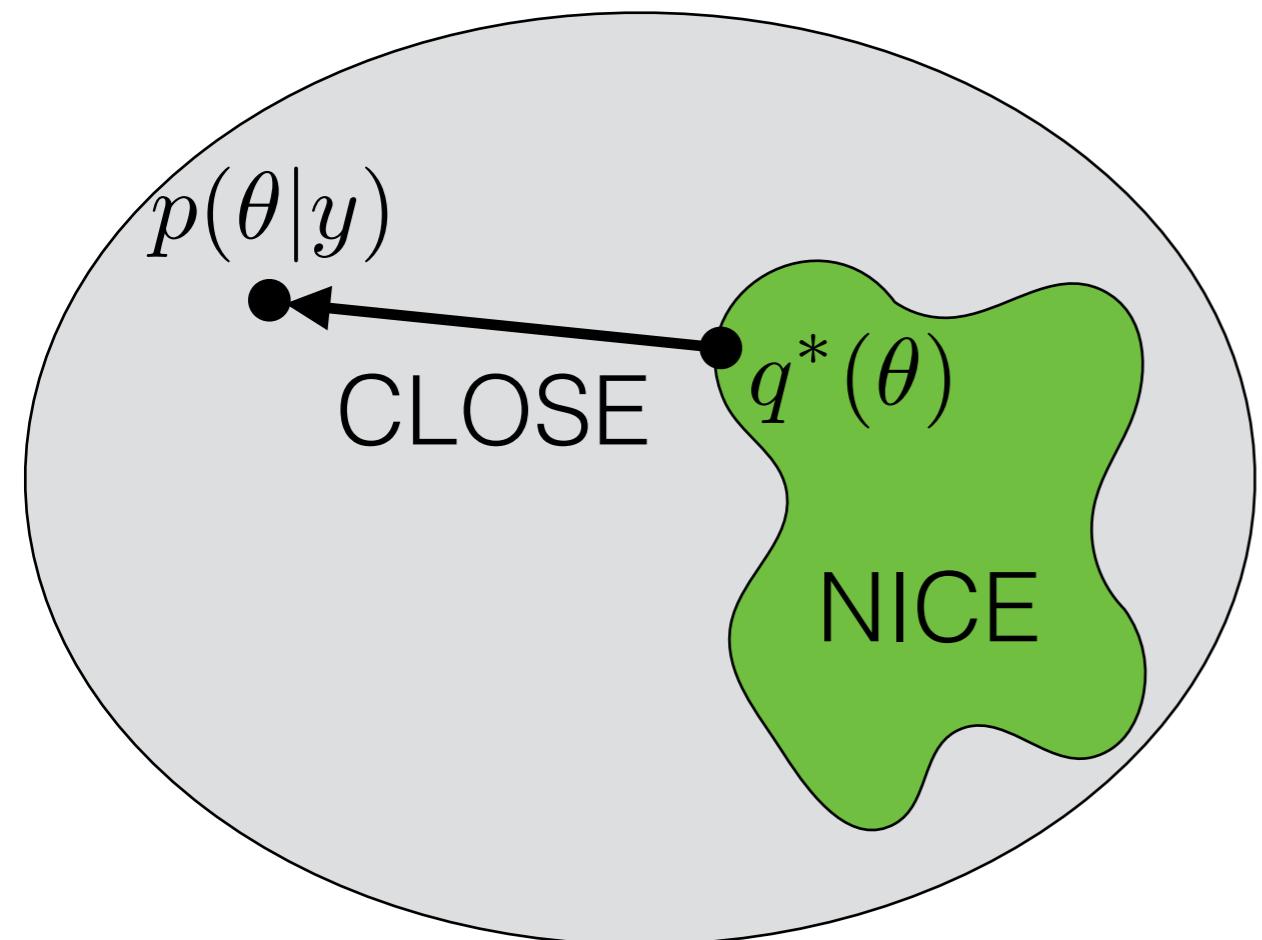


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- Why KL (in this direction)?

“Evidence lower bound” (ELBO)

Variational Bayes

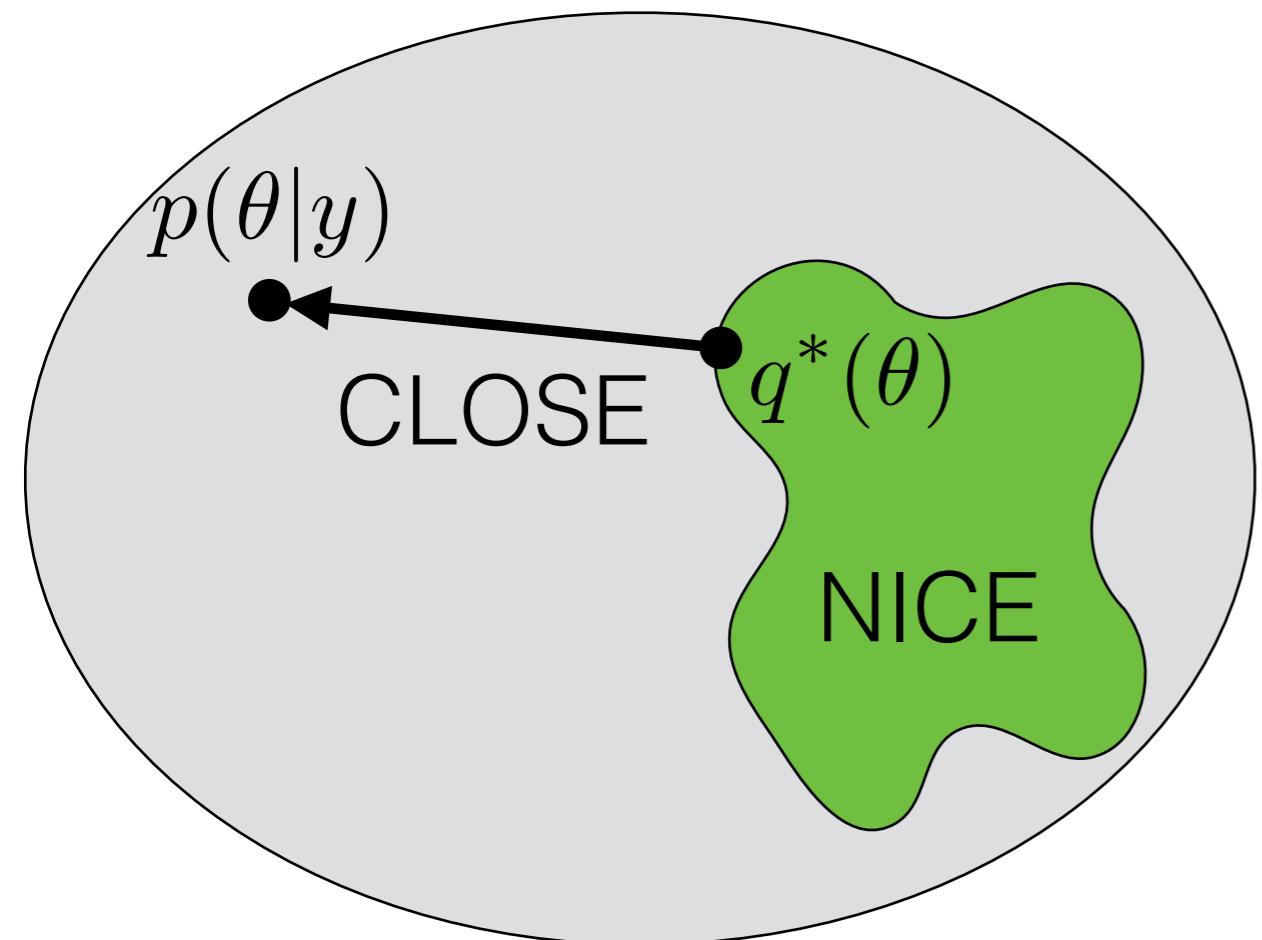
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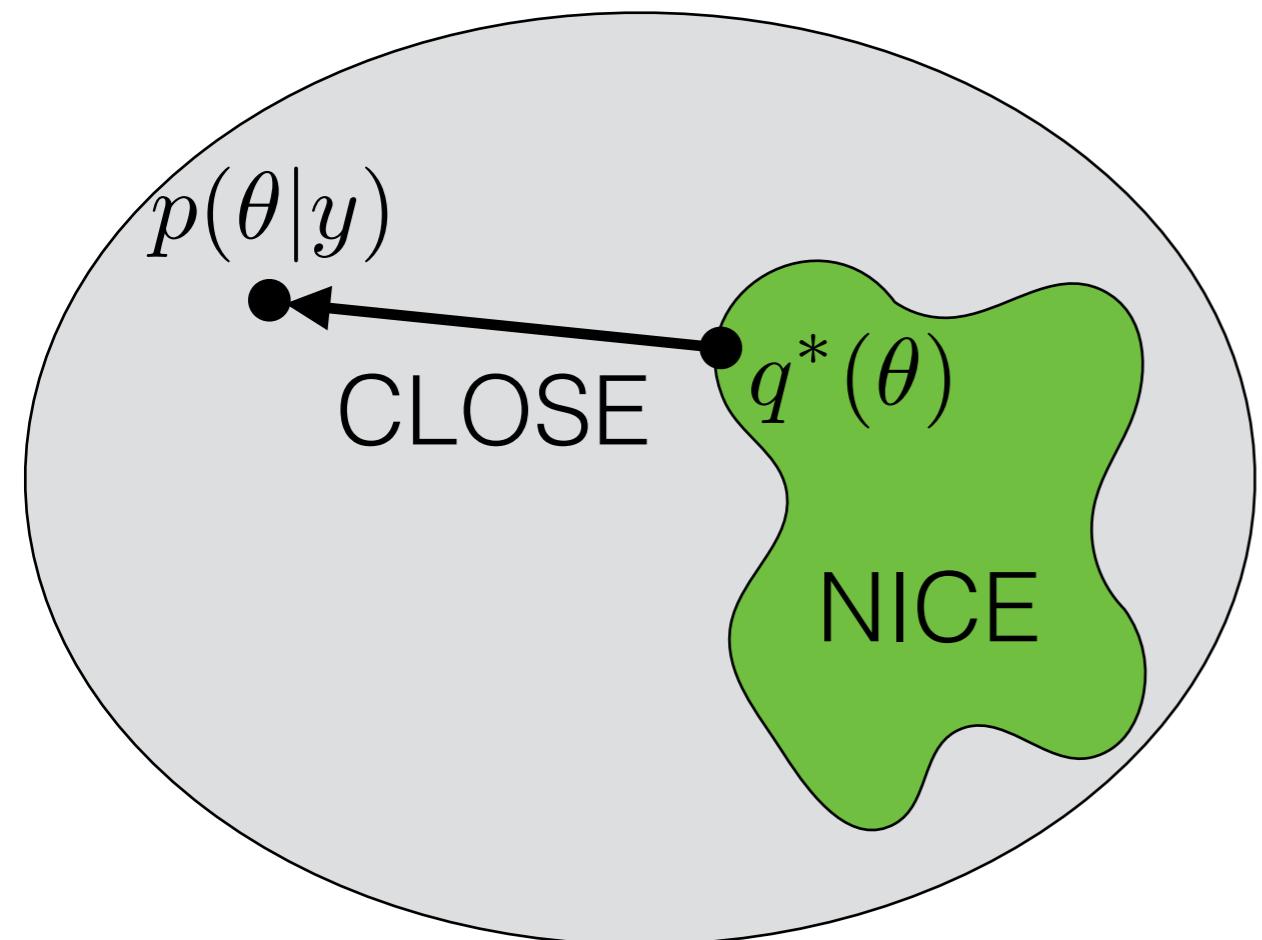
Choose “NICE” distributions



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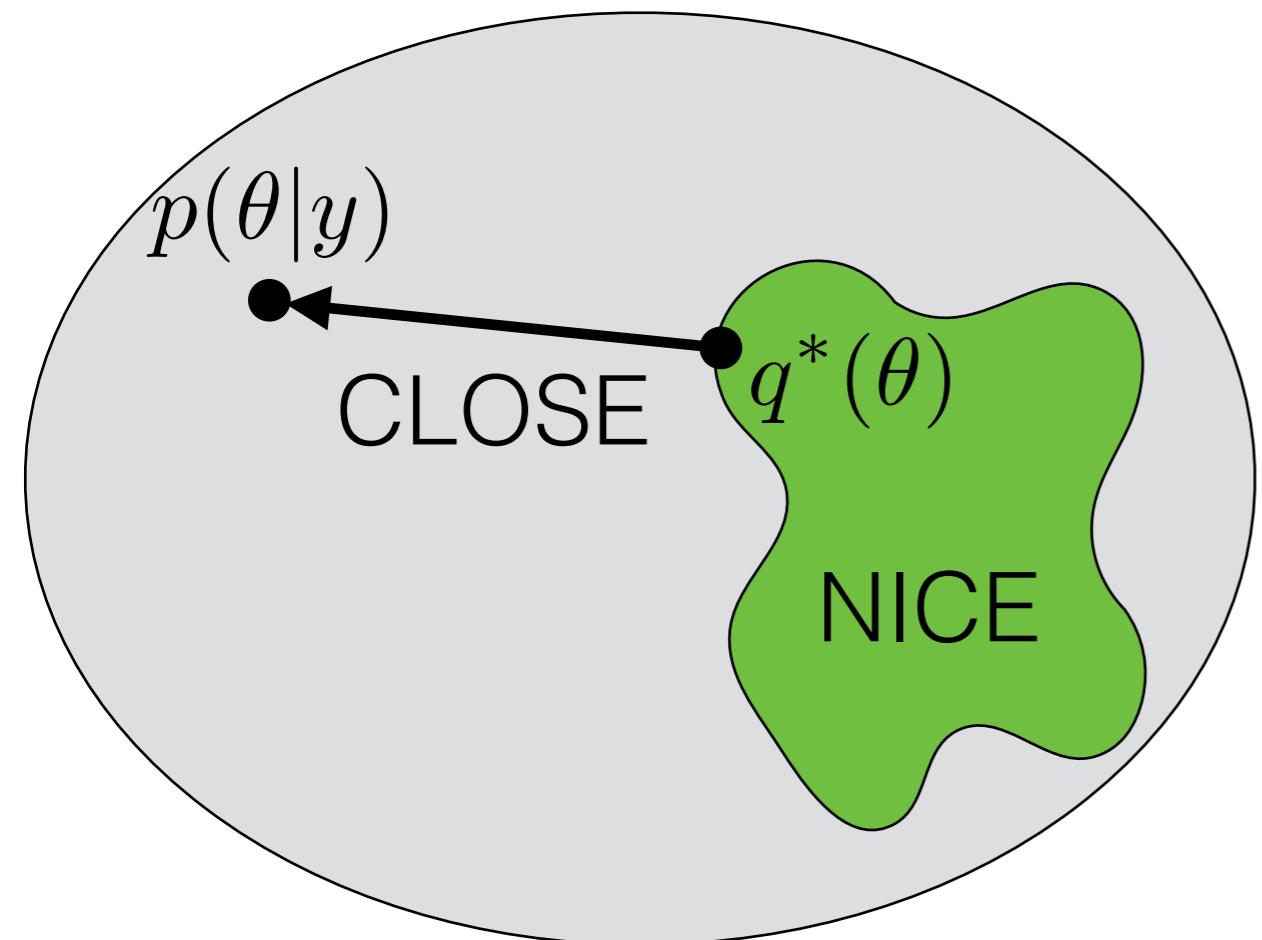
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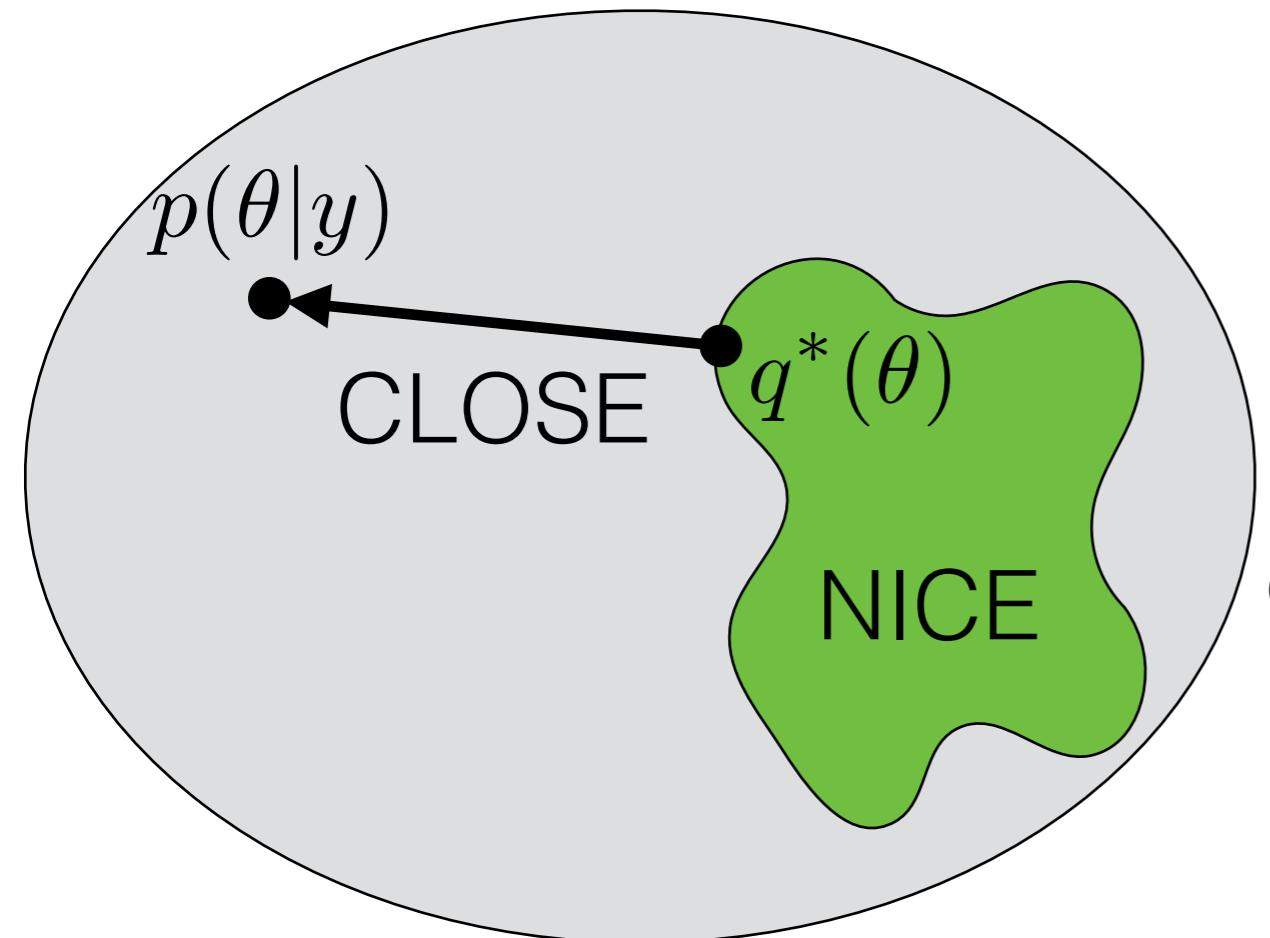
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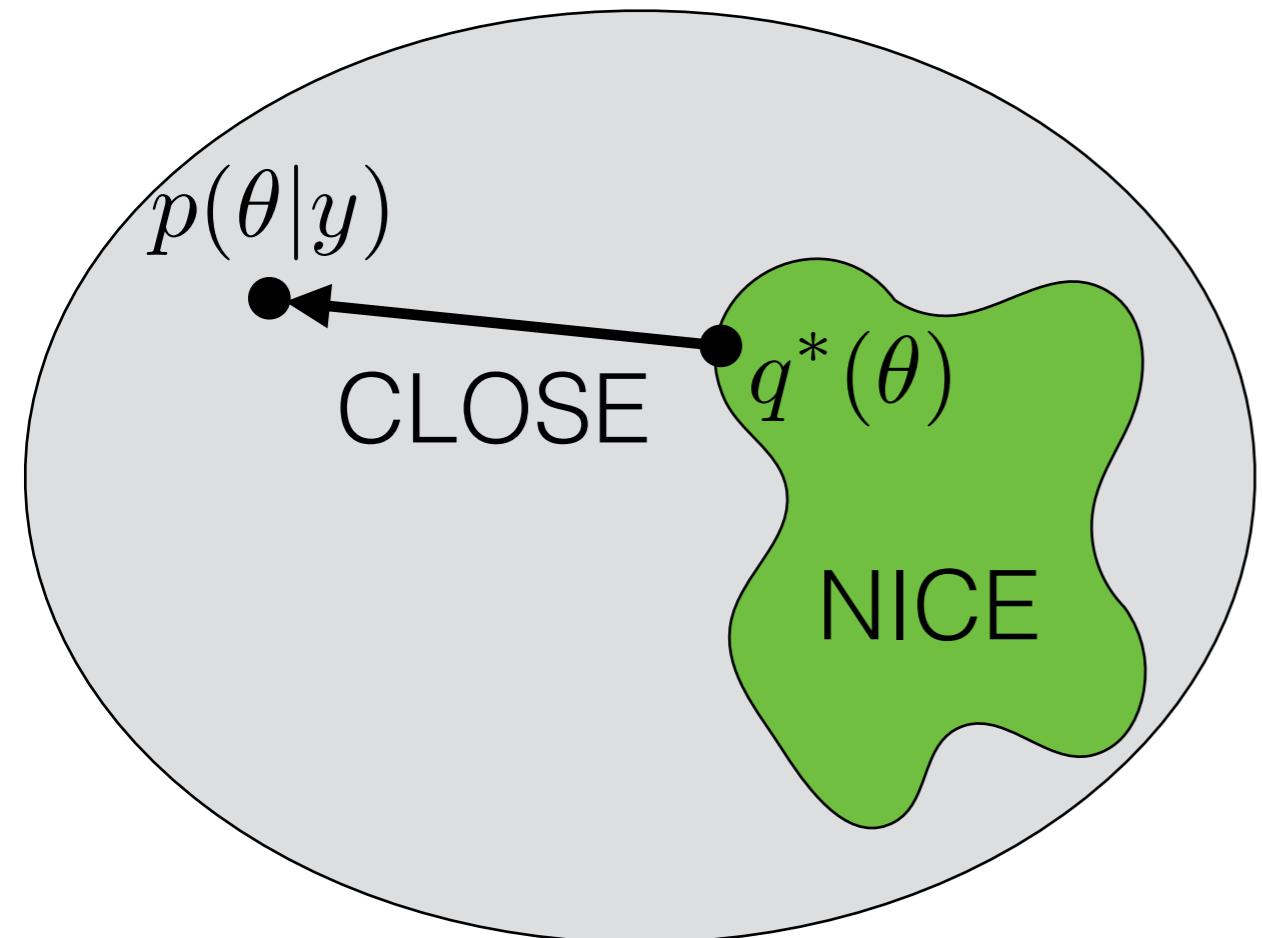
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$$Q_{MFVB} := \left\{ q : q(\theta) = \prod_{j=1}^J q_j(\theta_j) \right\}$$

Variational Bayes

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Choose “NICE” distributions

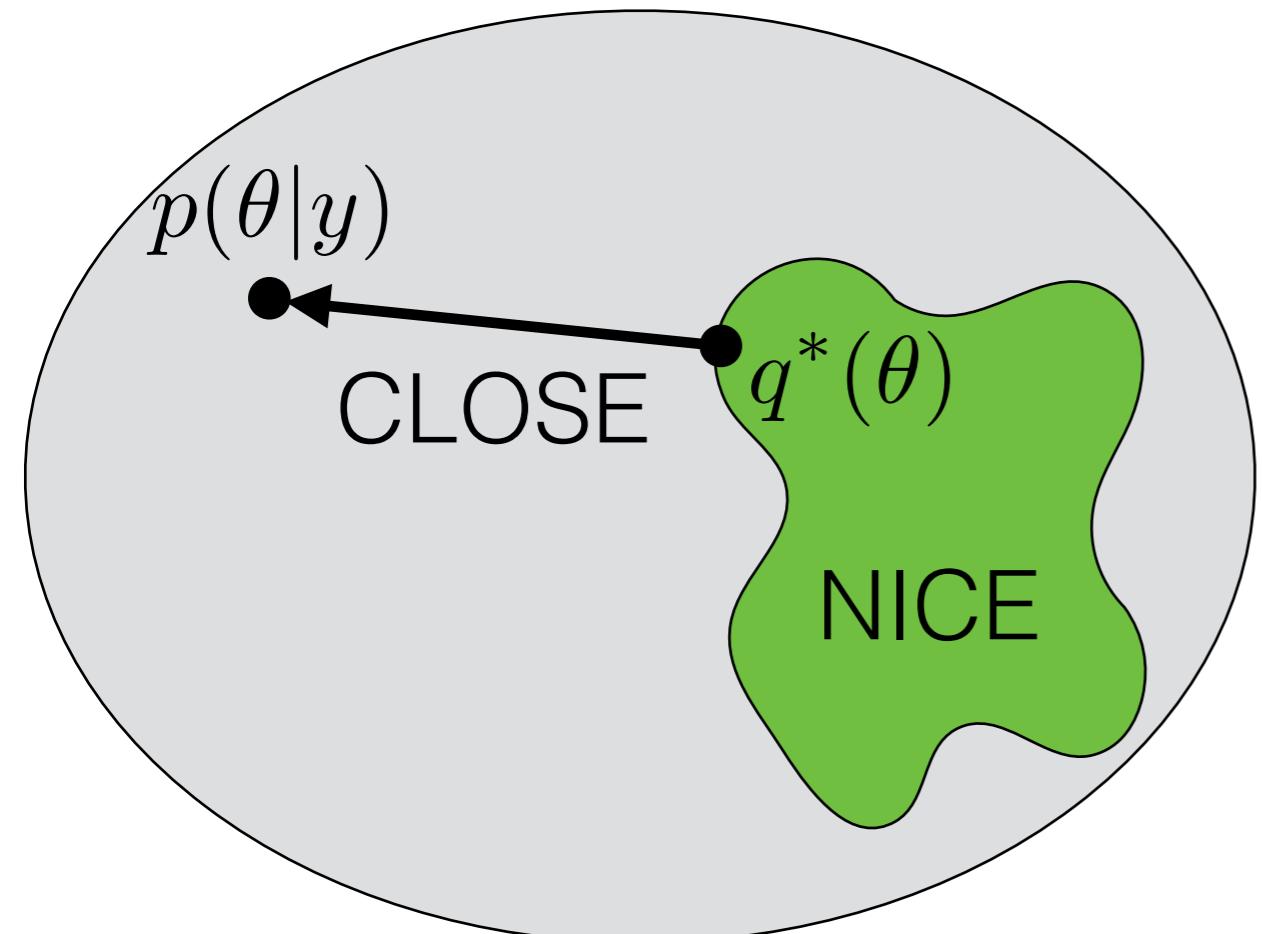
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- Often also exponential family

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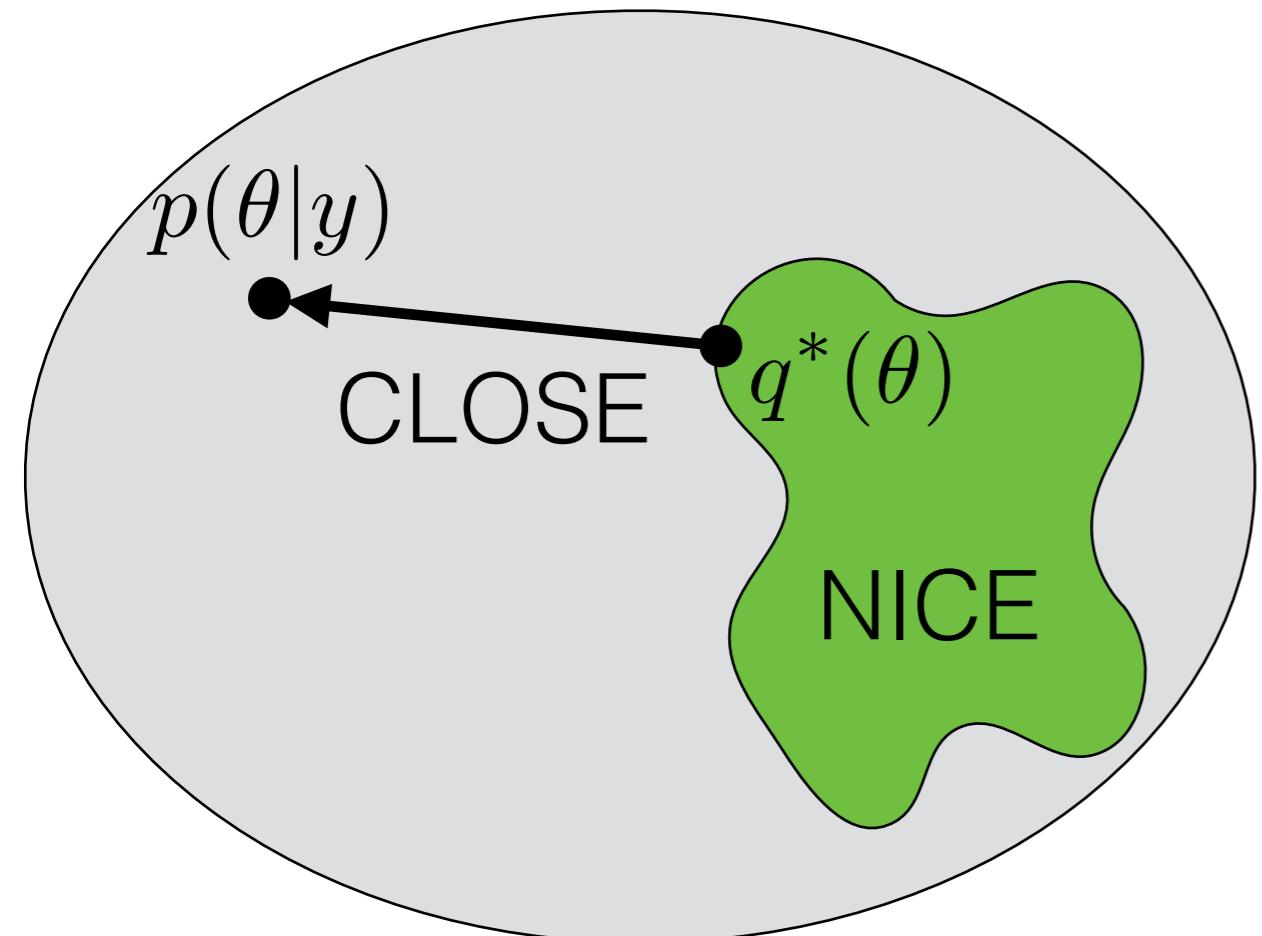
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- Not a modeling assumption

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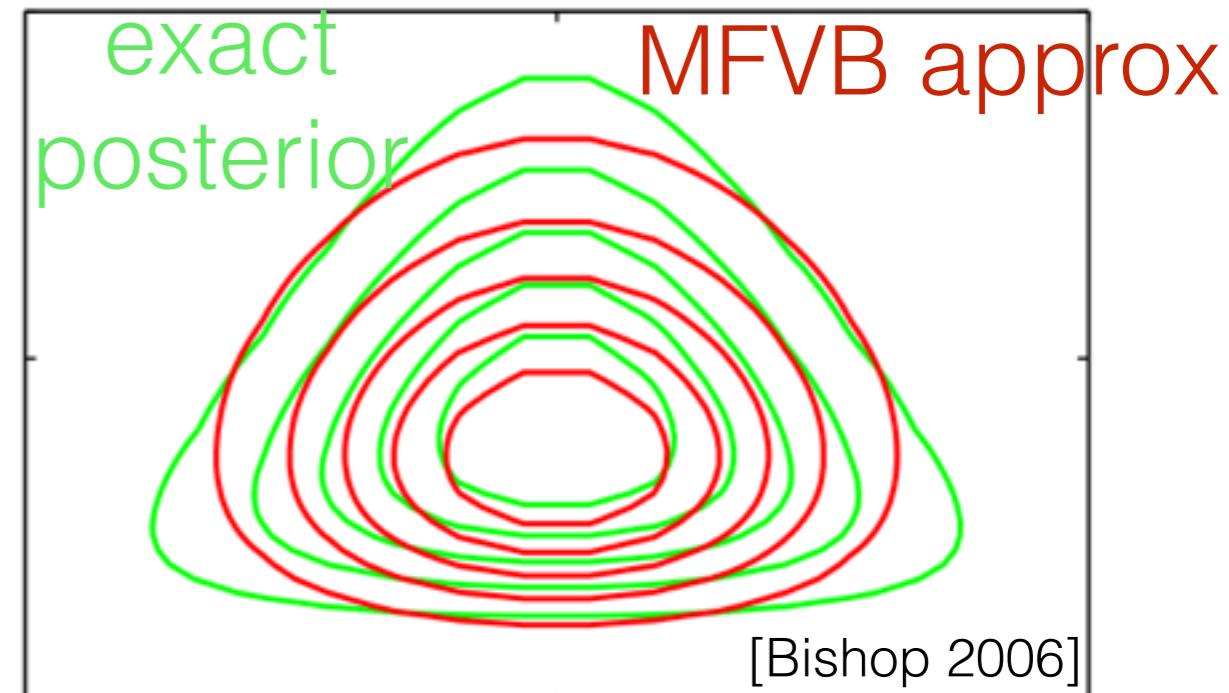


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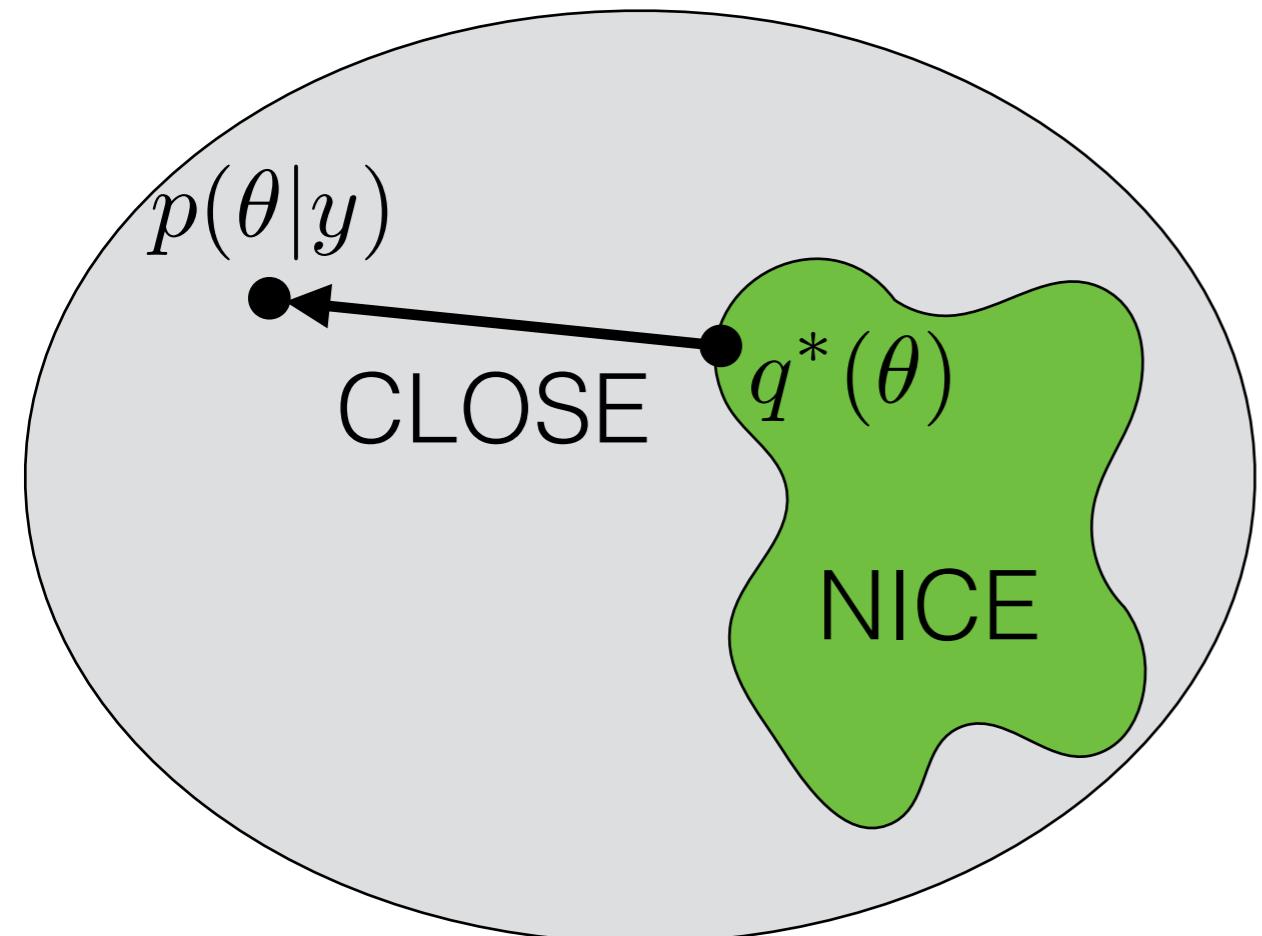
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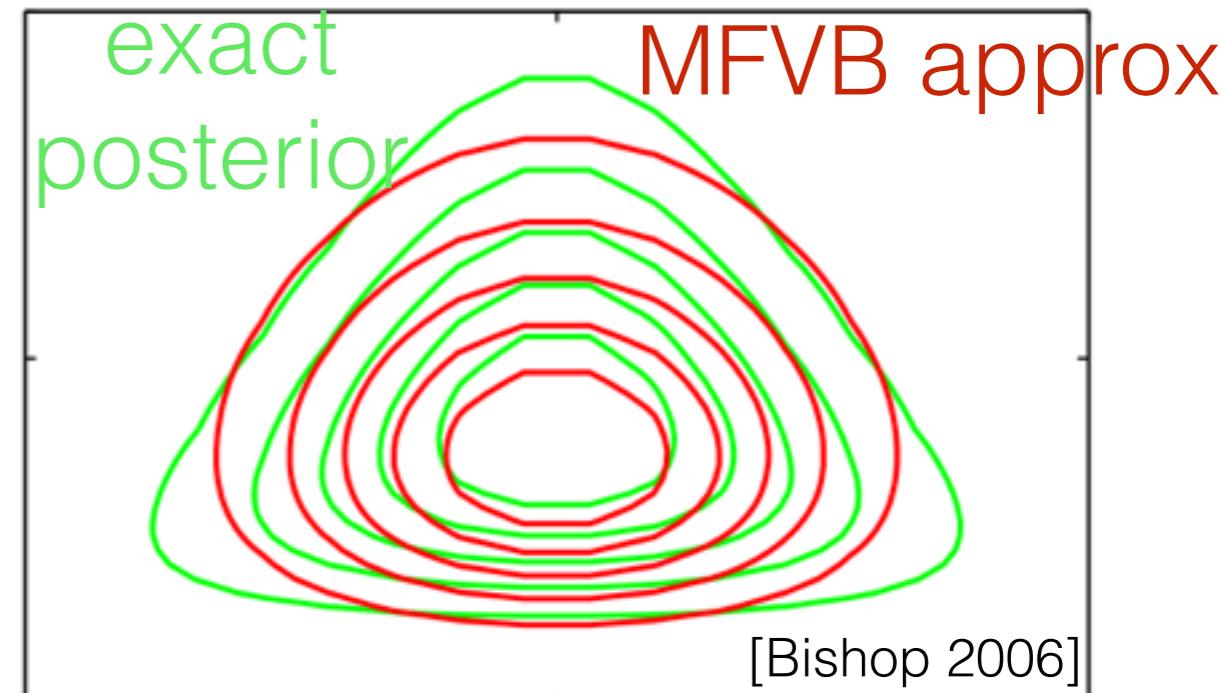
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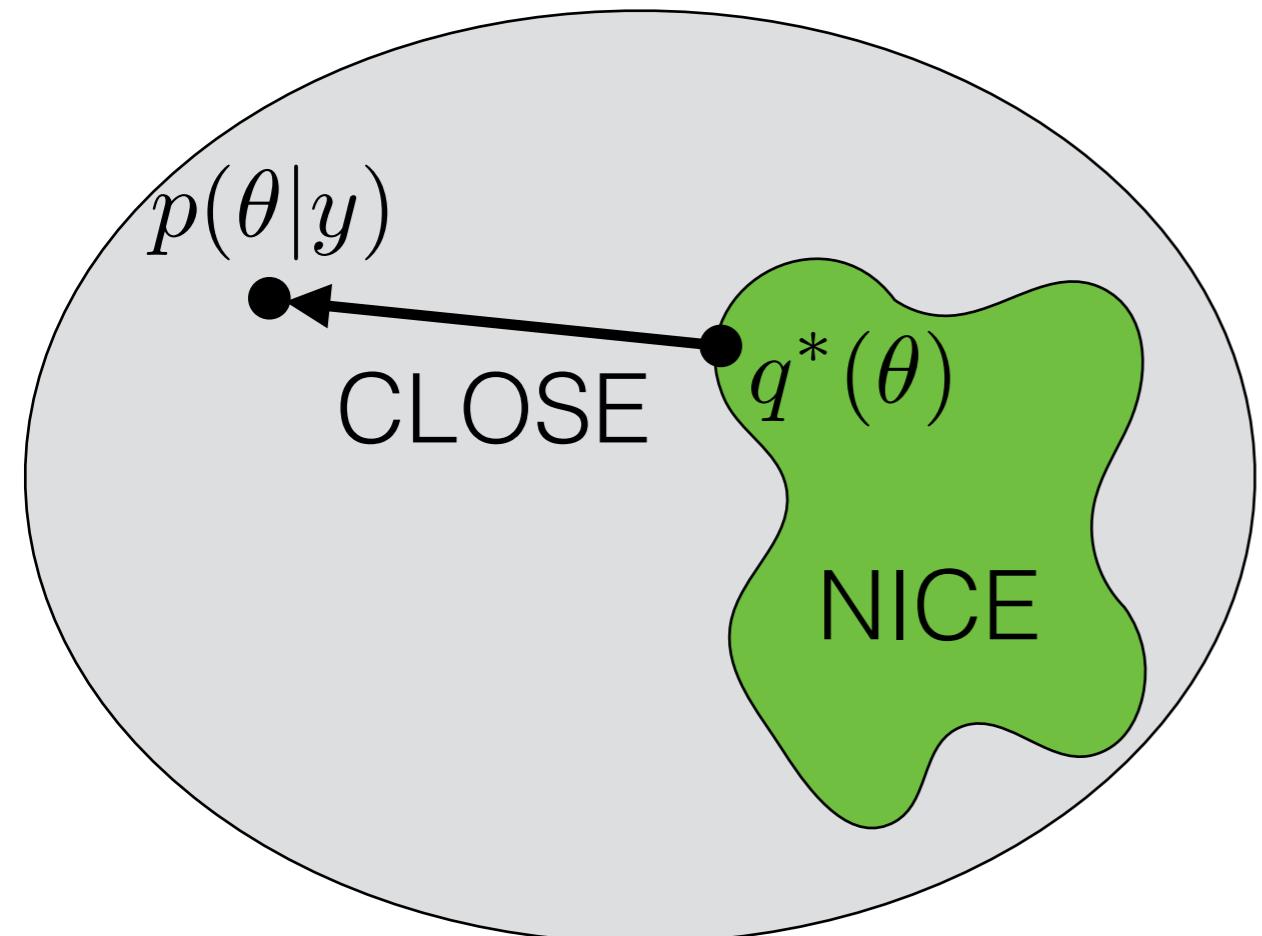
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[Bishop 2006]

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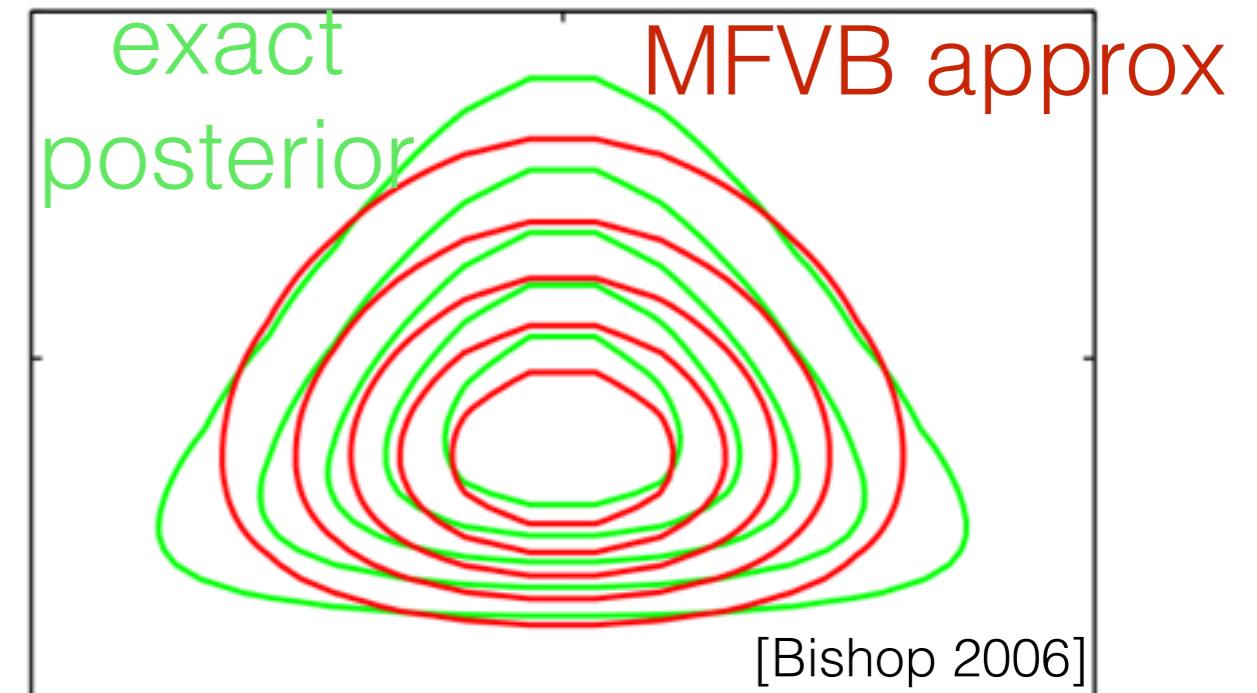
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Now we have an optimization problem; how to solve it?

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



Approximate Bayesian inference

Approximate Bayesian inference

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

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Optimization

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Approximate Bayesian inference

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- Bayes & Approximate Bayes review
- What is:
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- Why use MFVB?
- When can we trust MFVB?
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Midge wing length

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



[CSIRO 2004]

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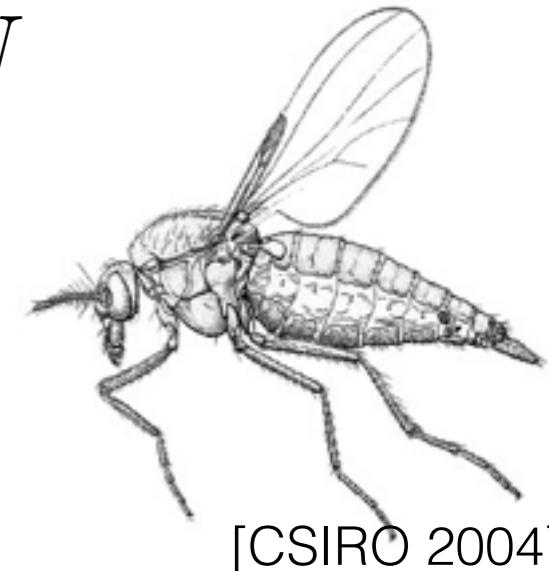
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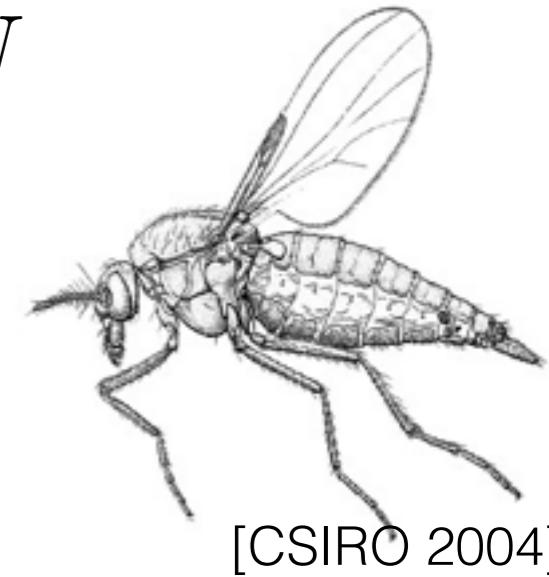
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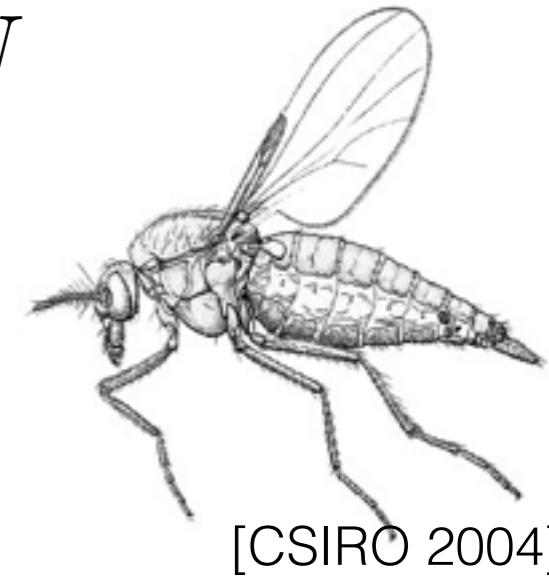
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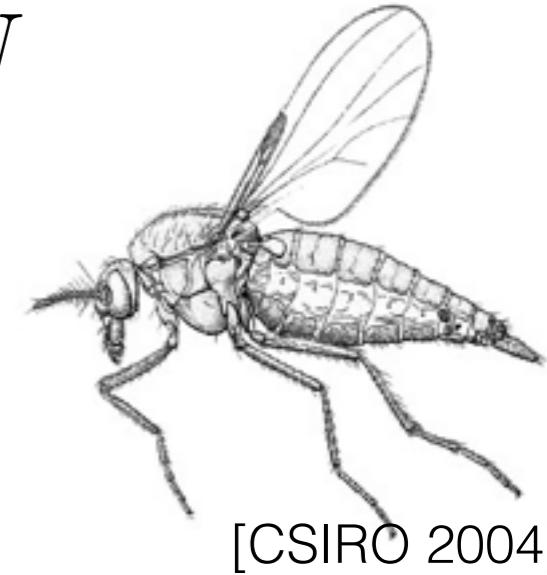
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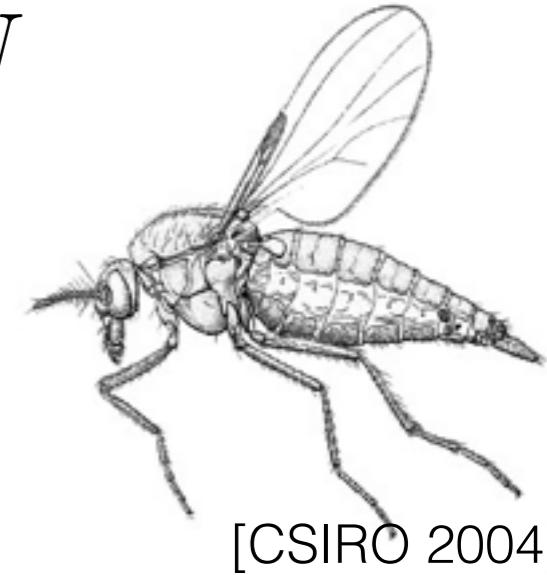
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“variational
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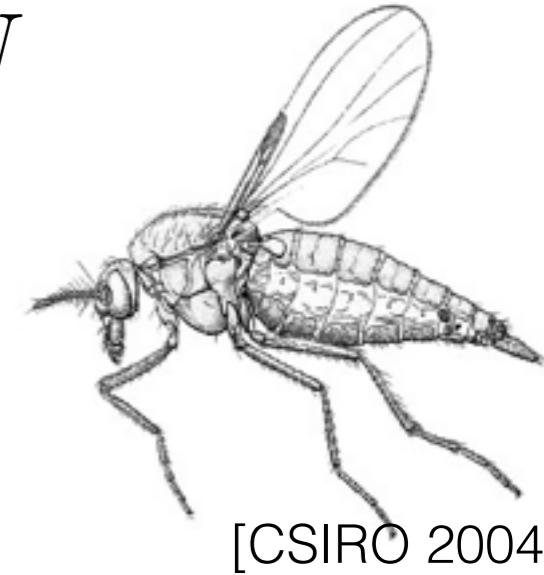
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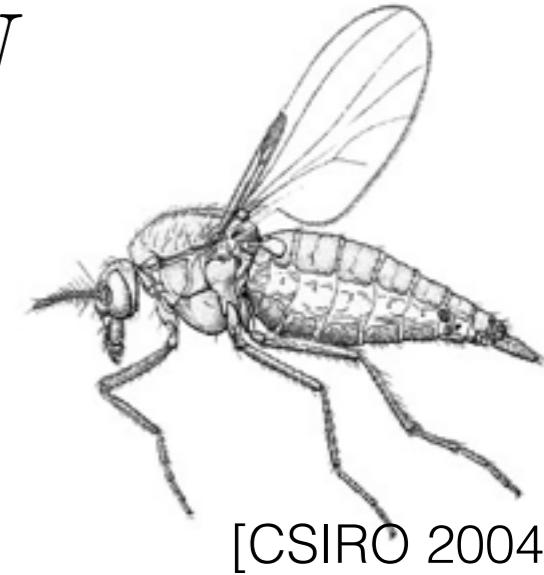
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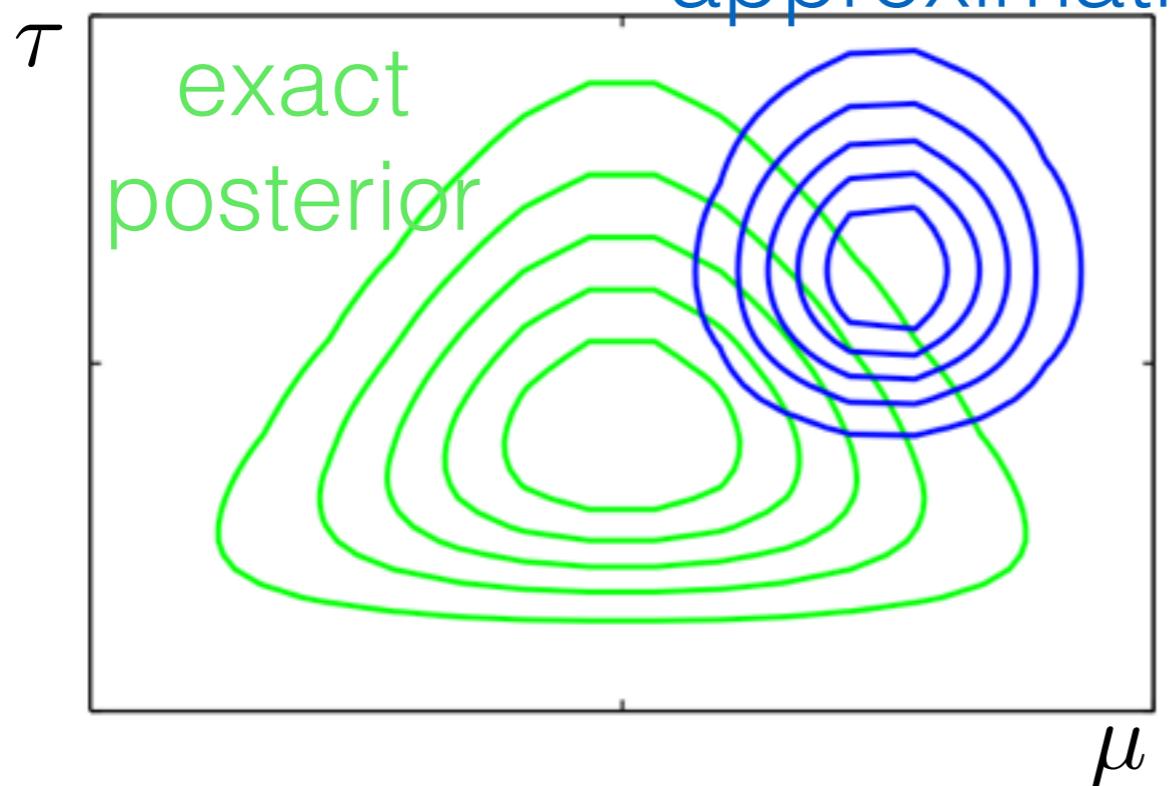
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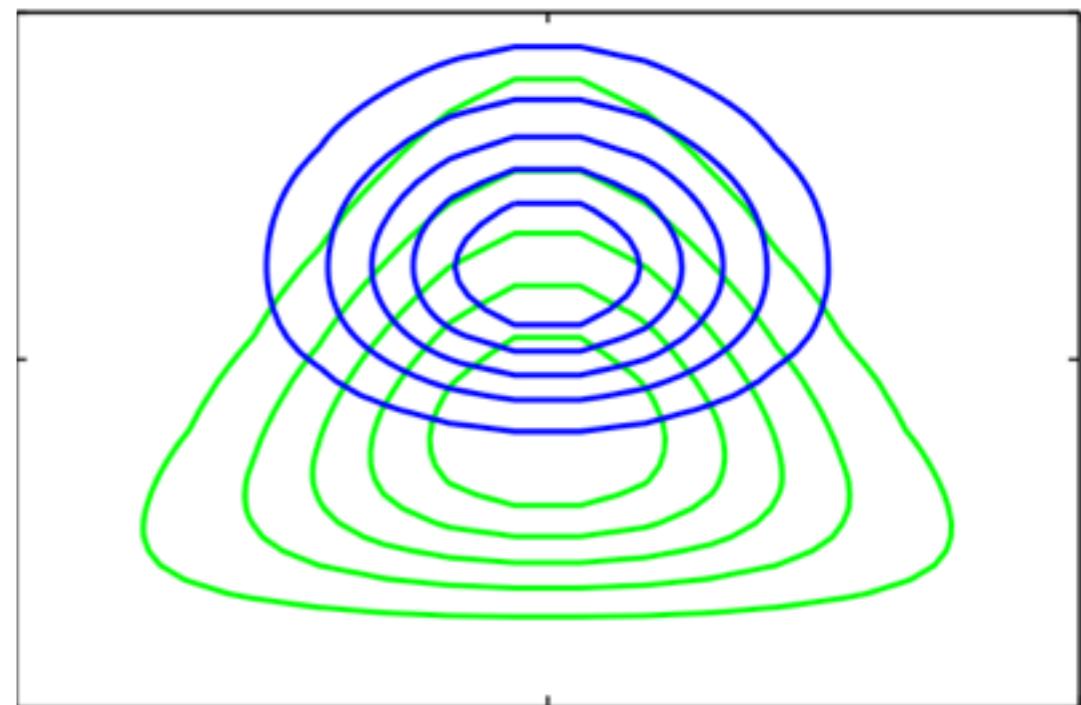
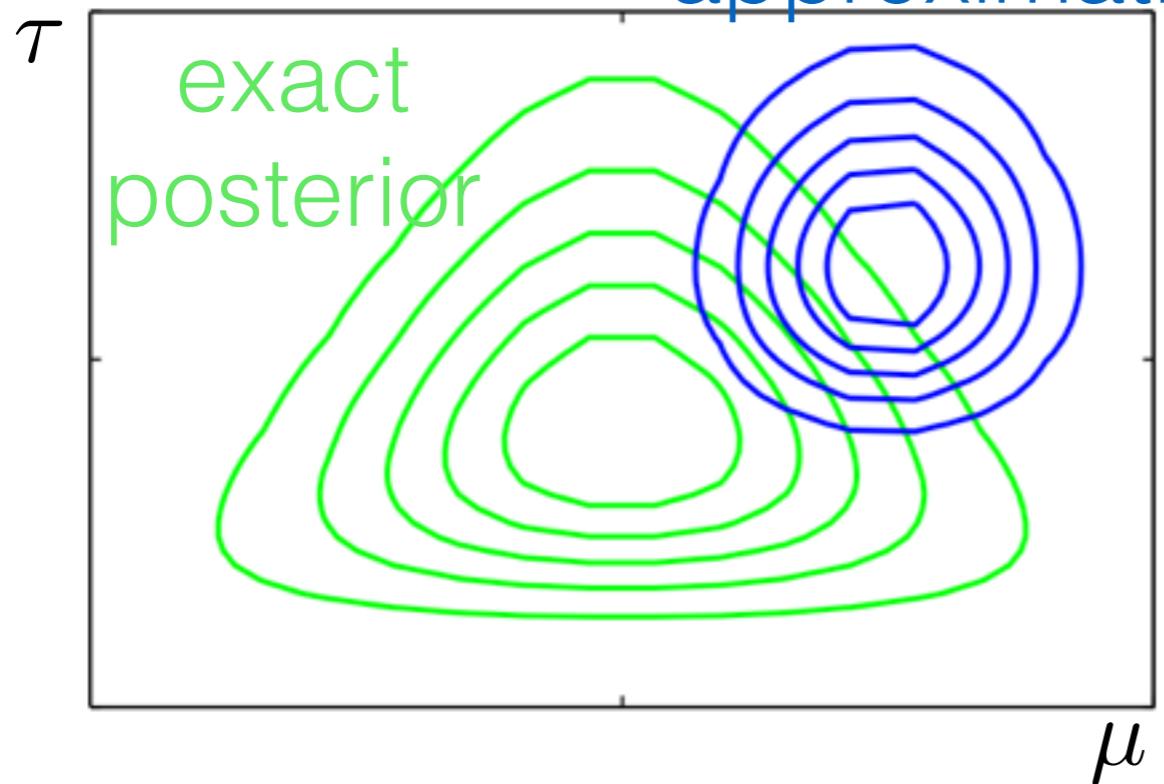
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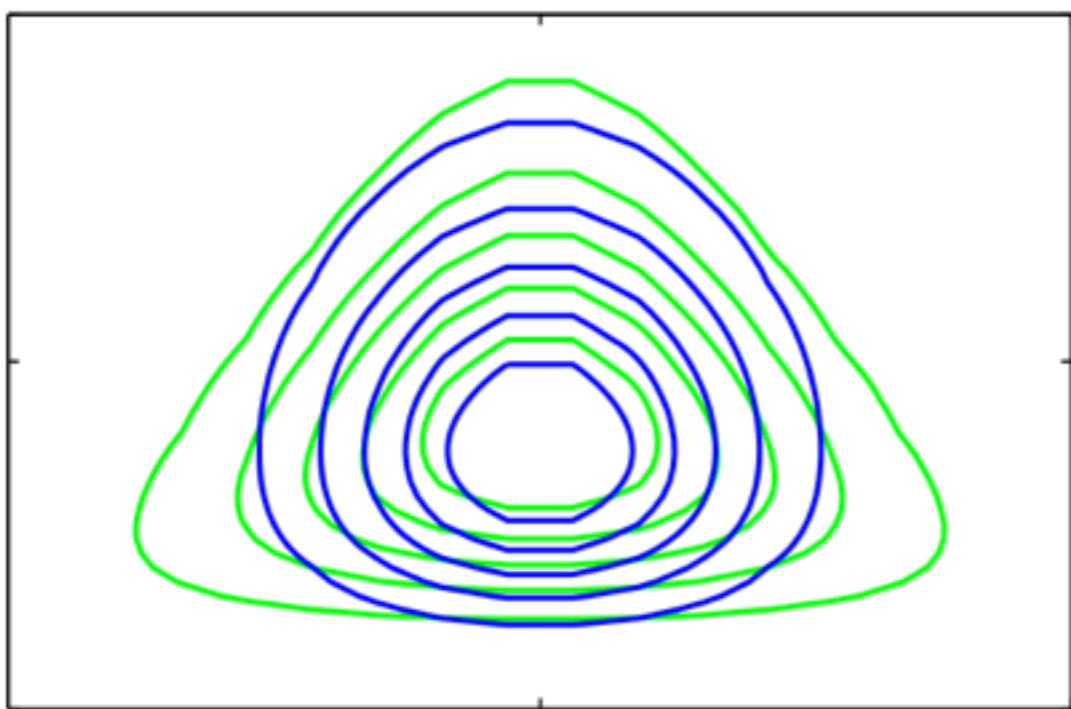
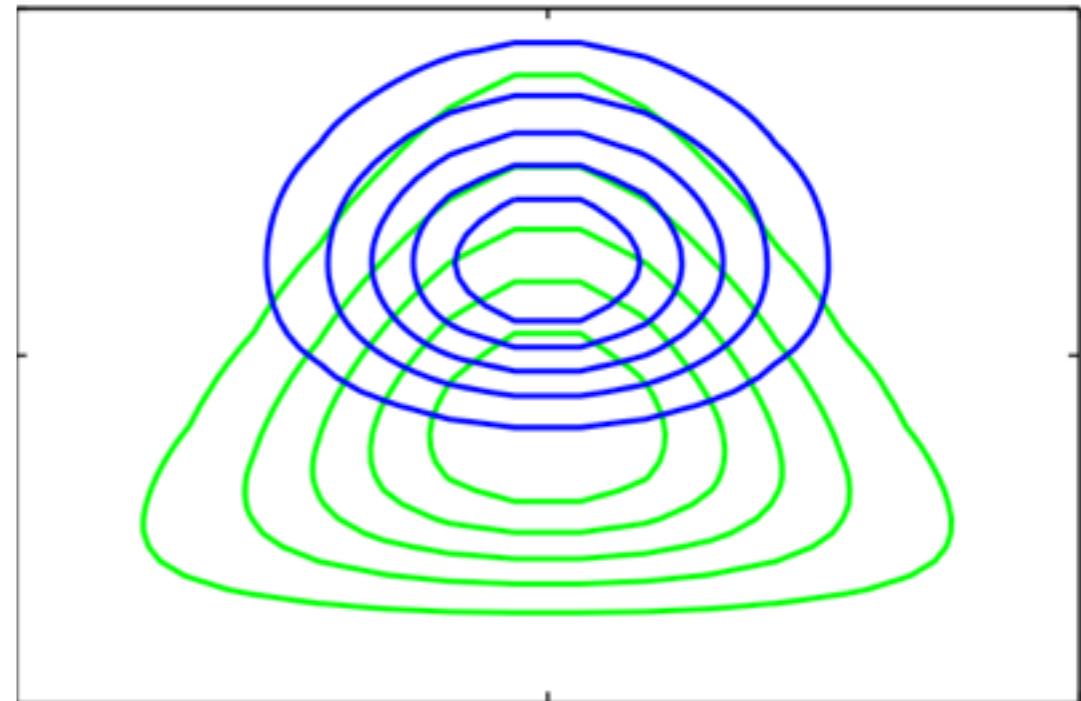
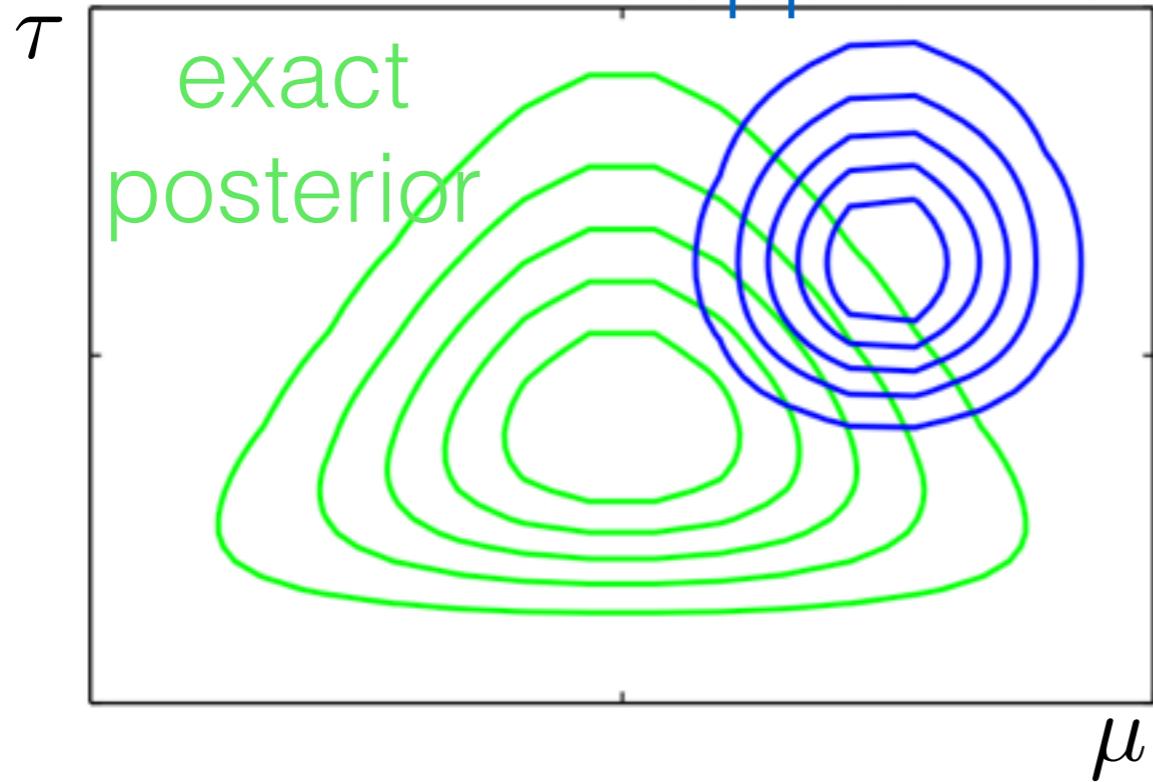
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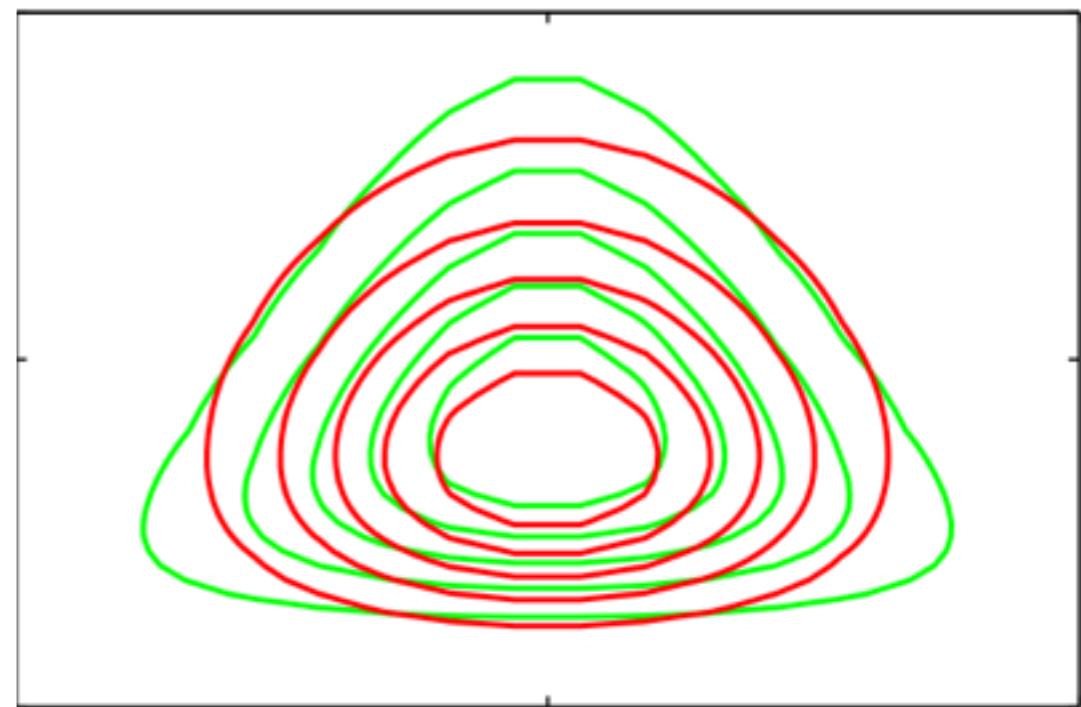
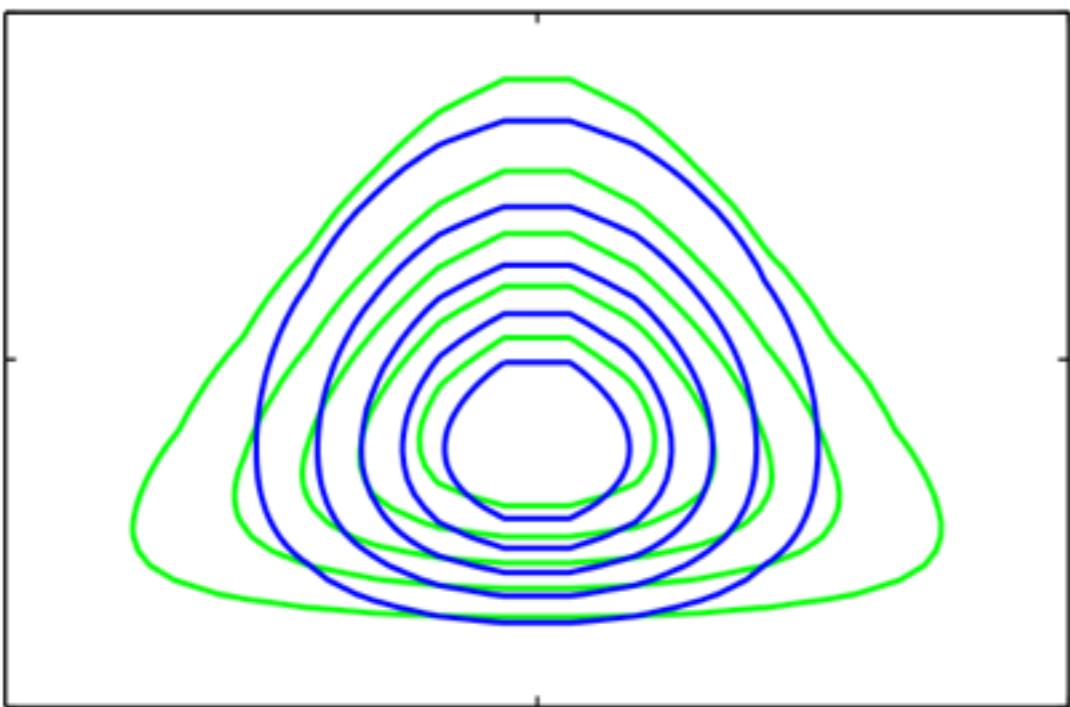
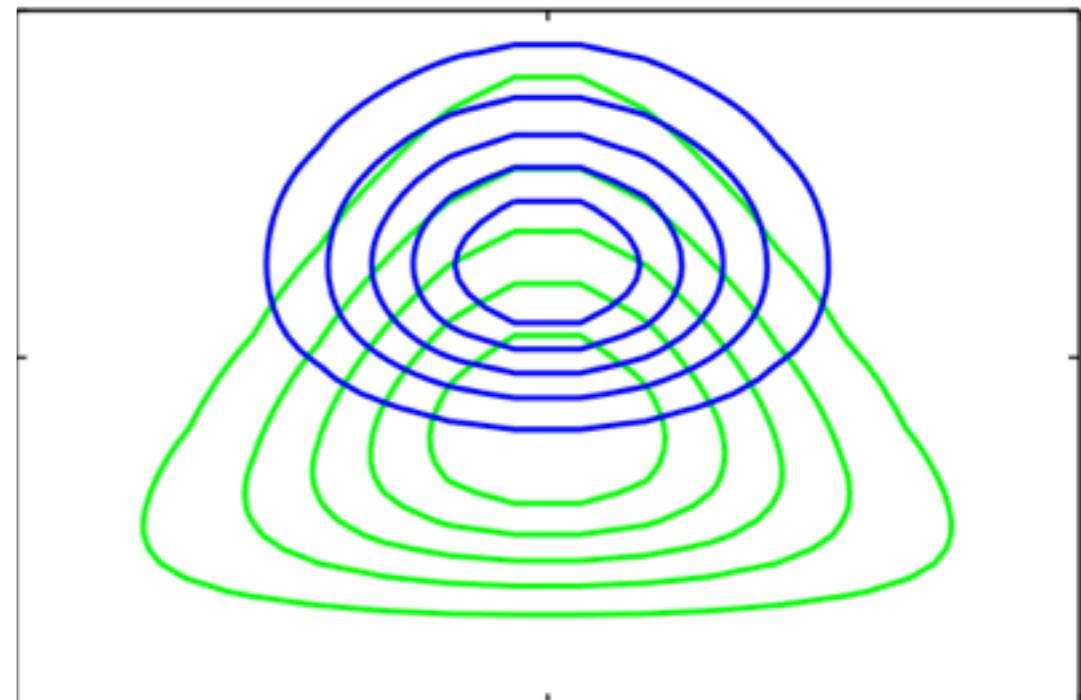
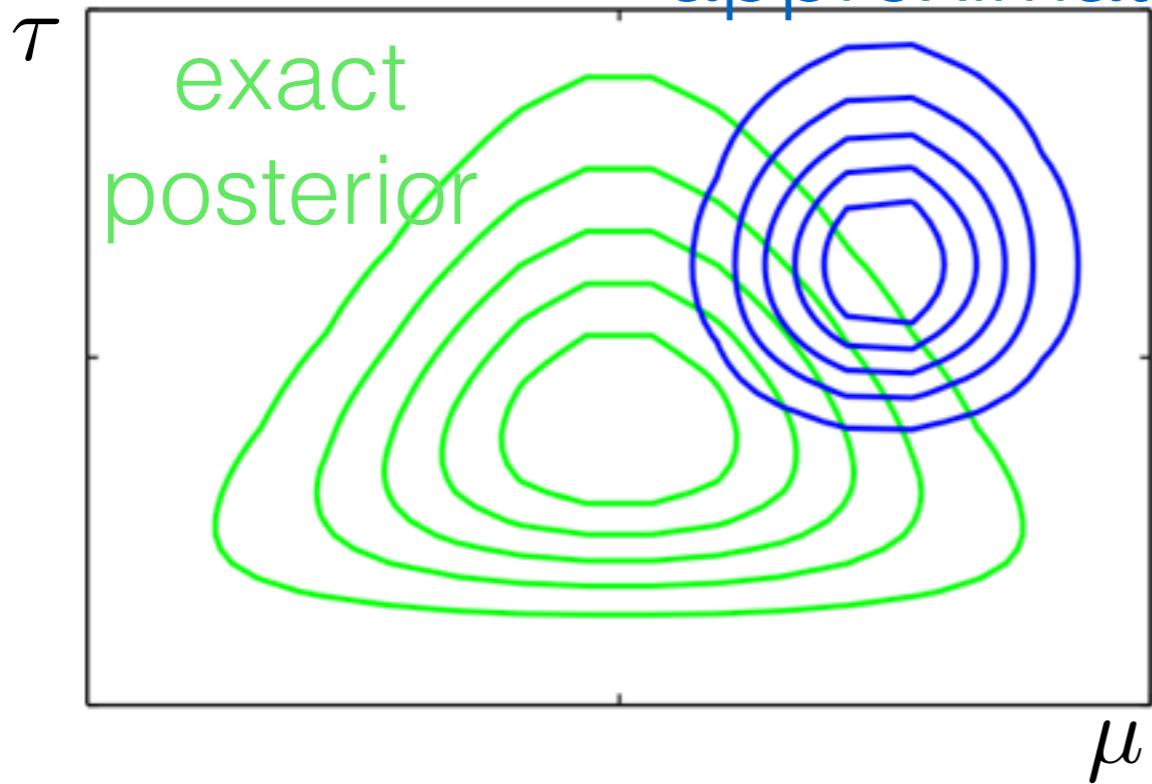
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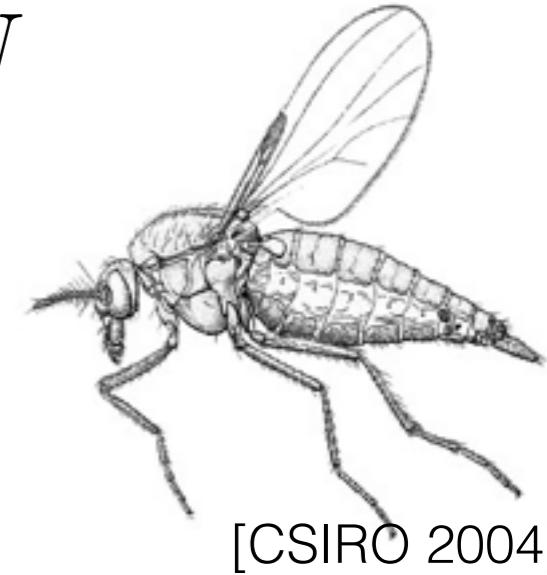
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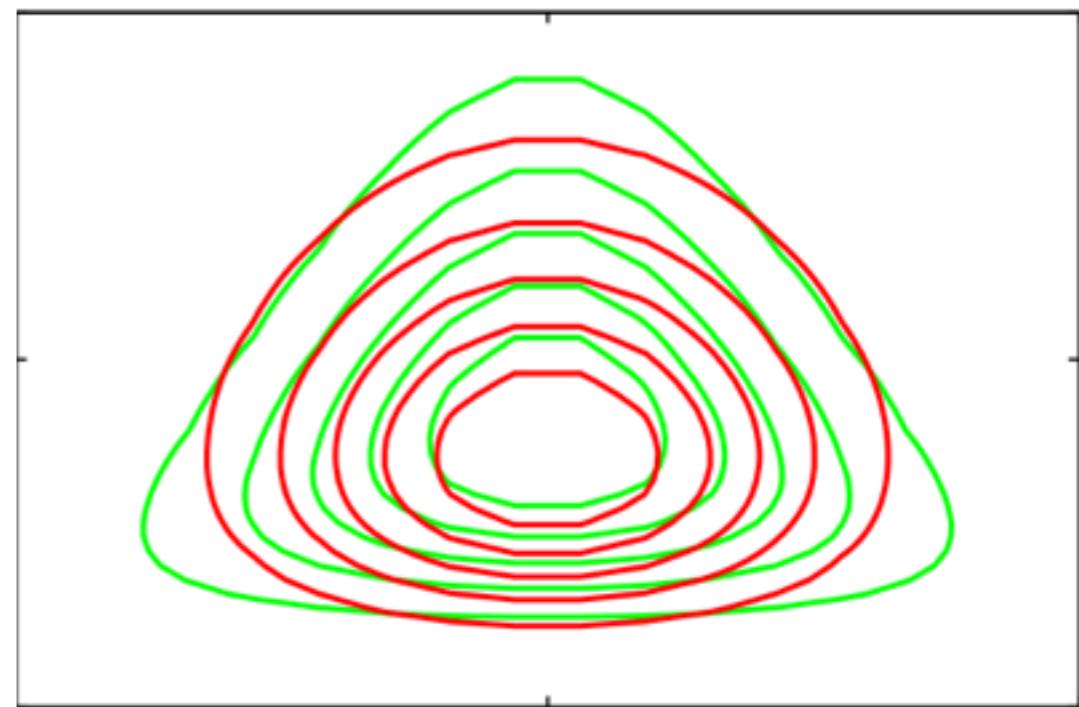
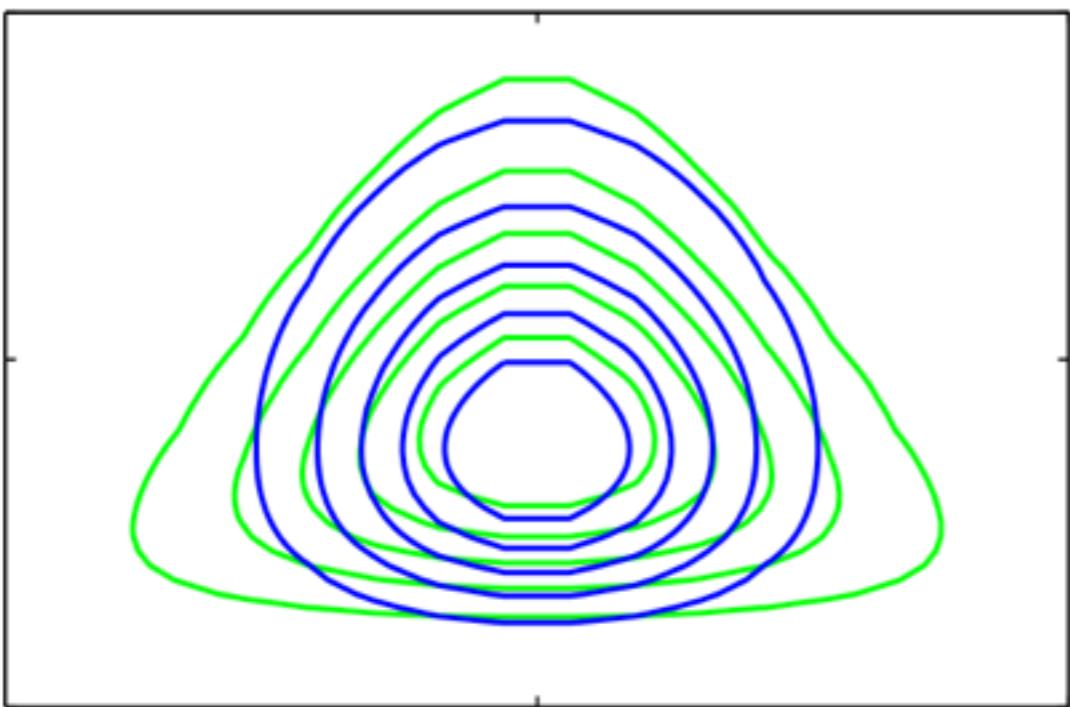
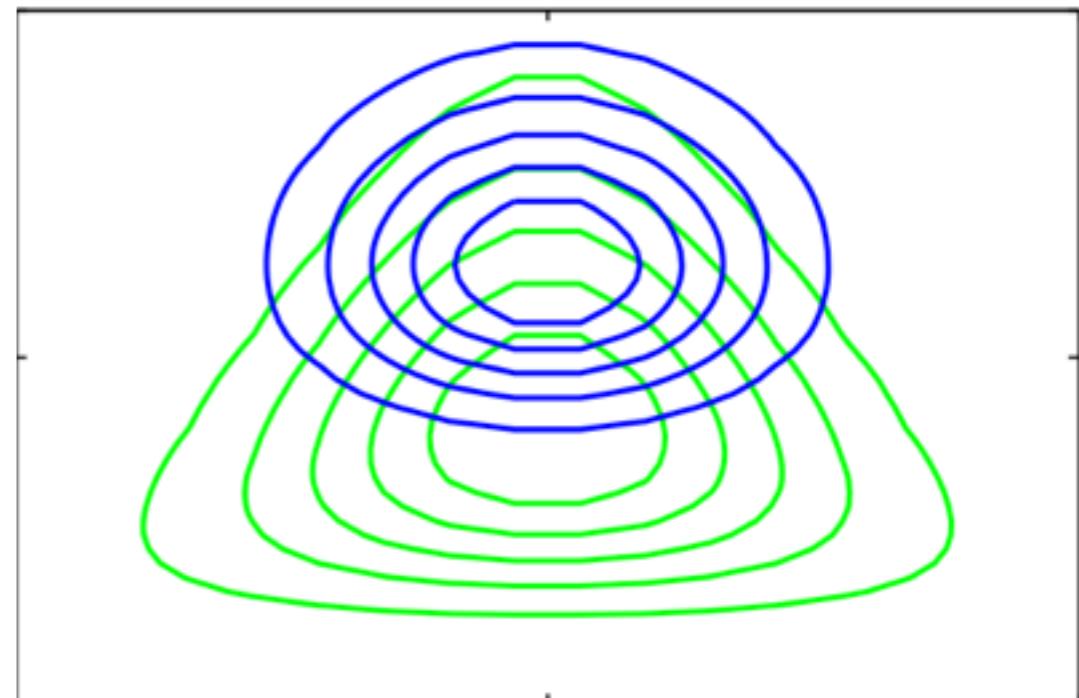
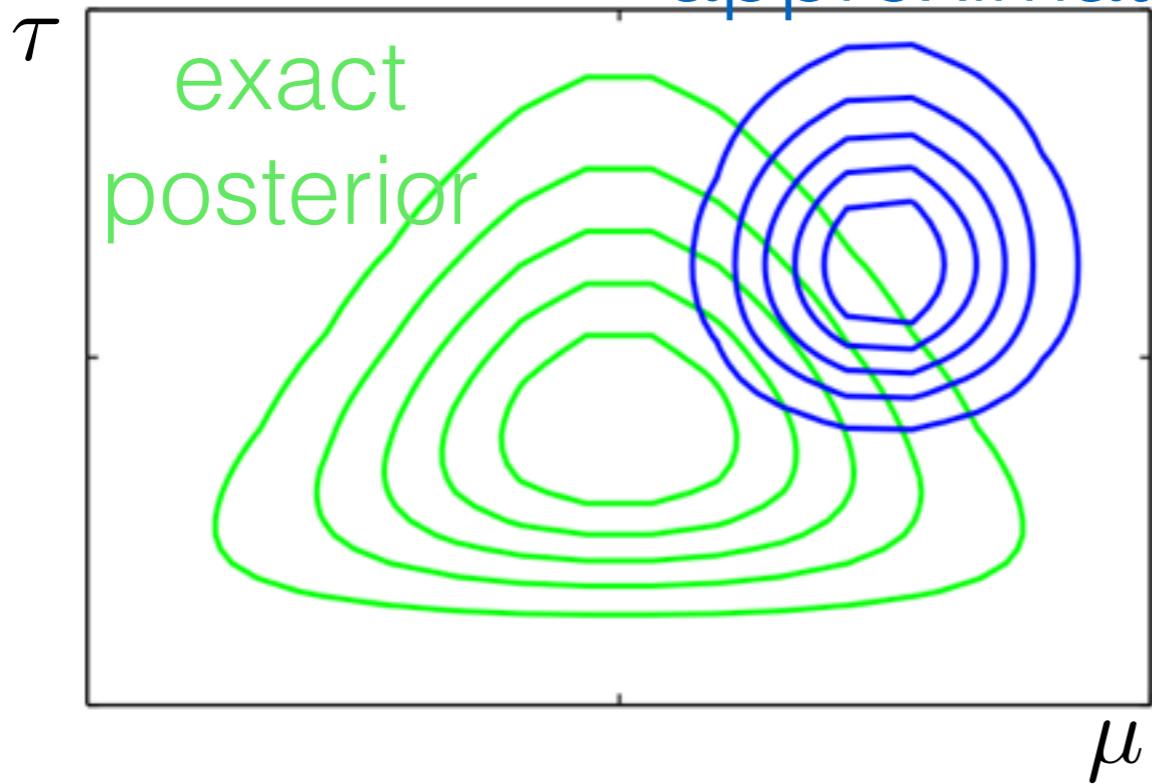
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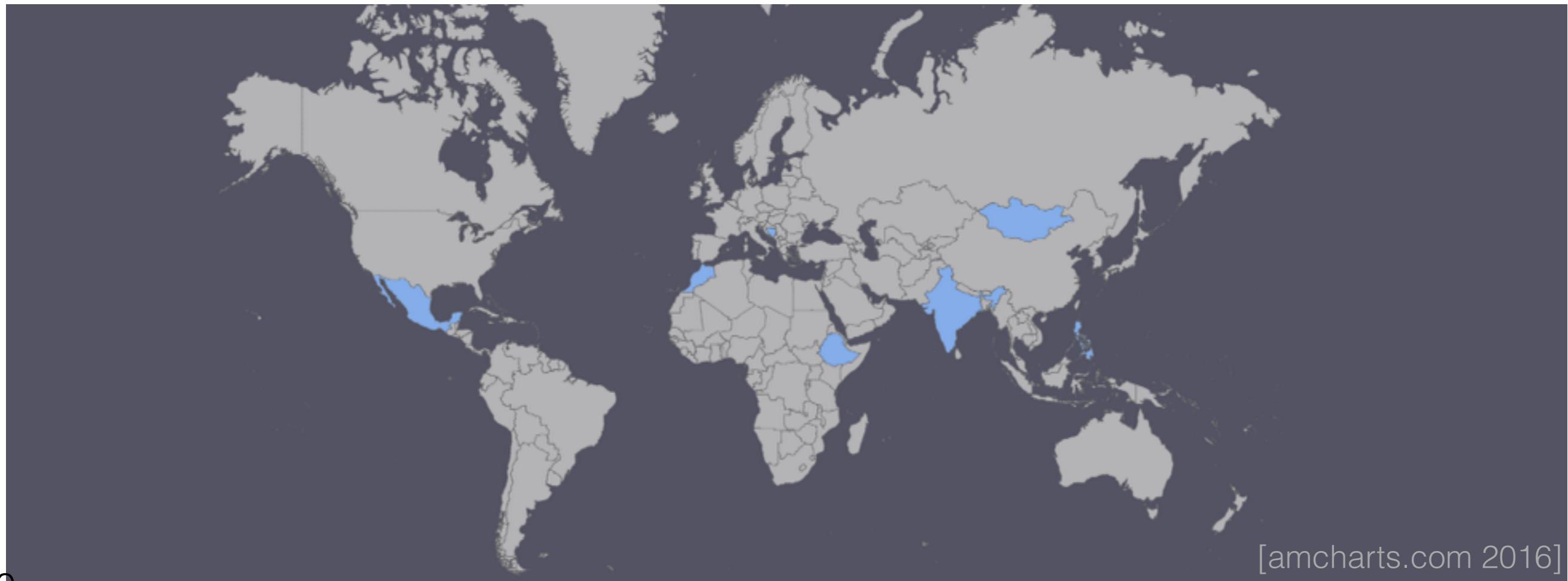
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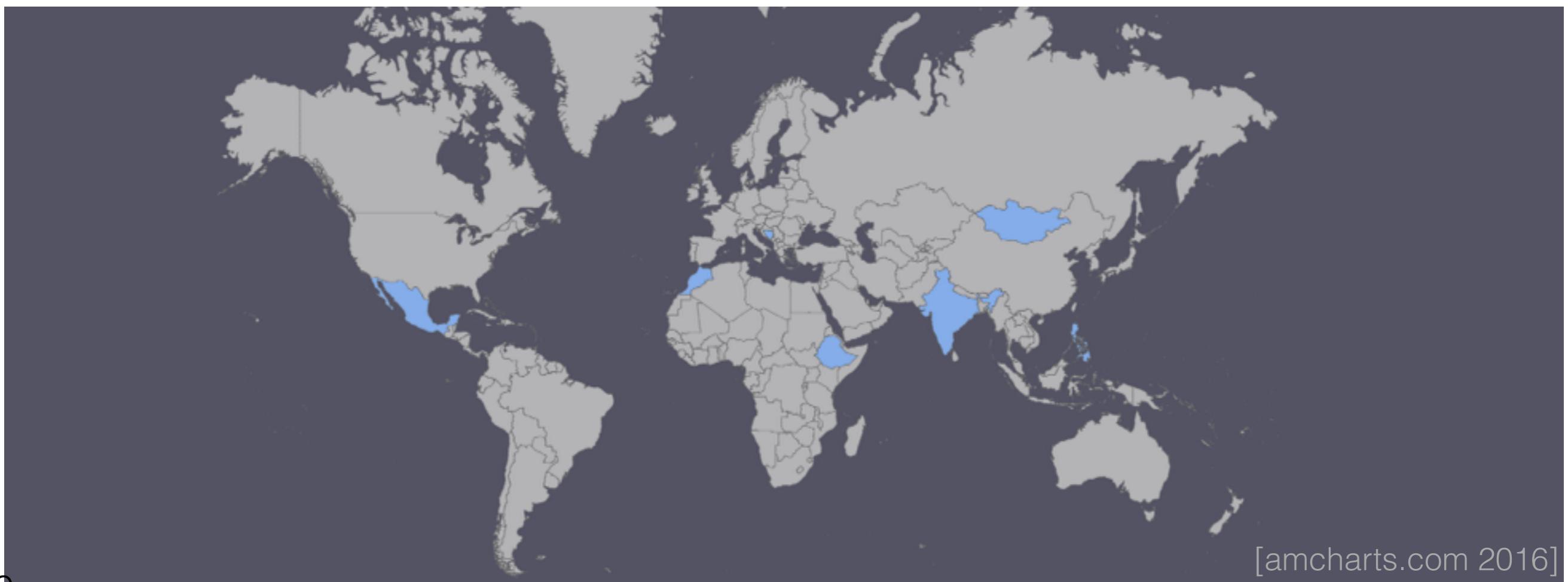


Microcredit Experiment



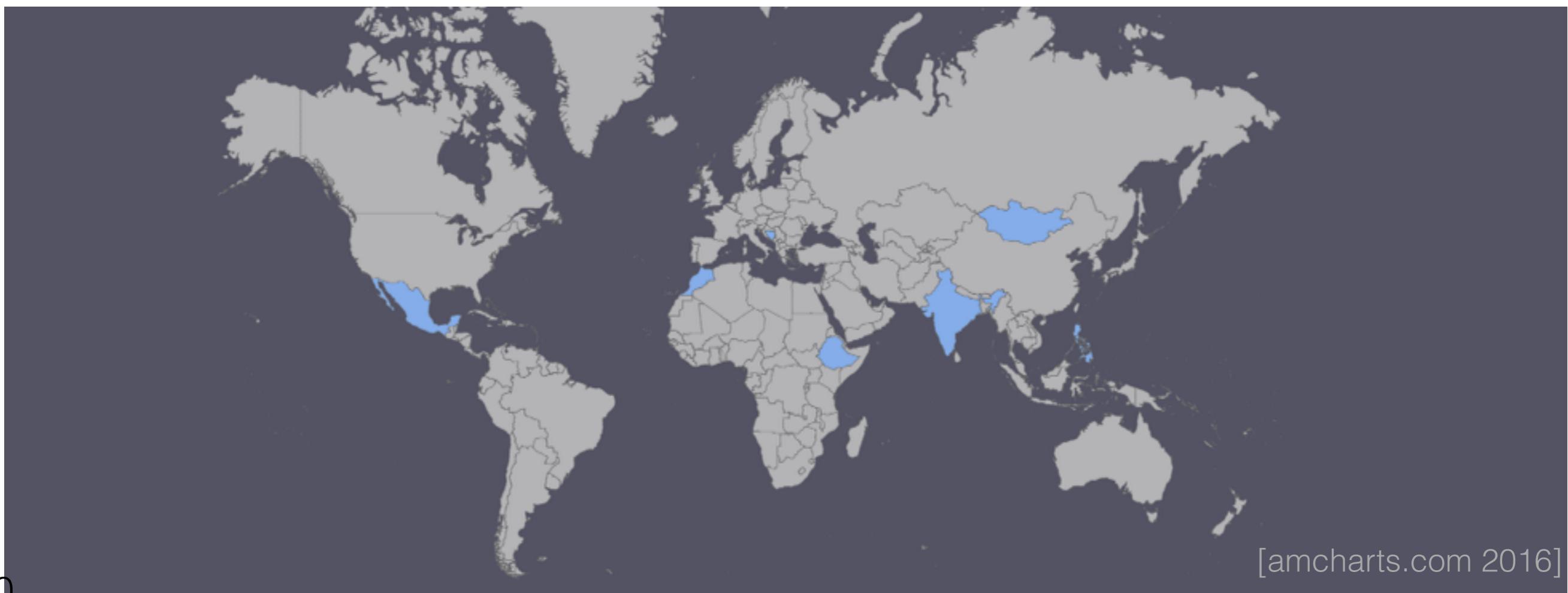
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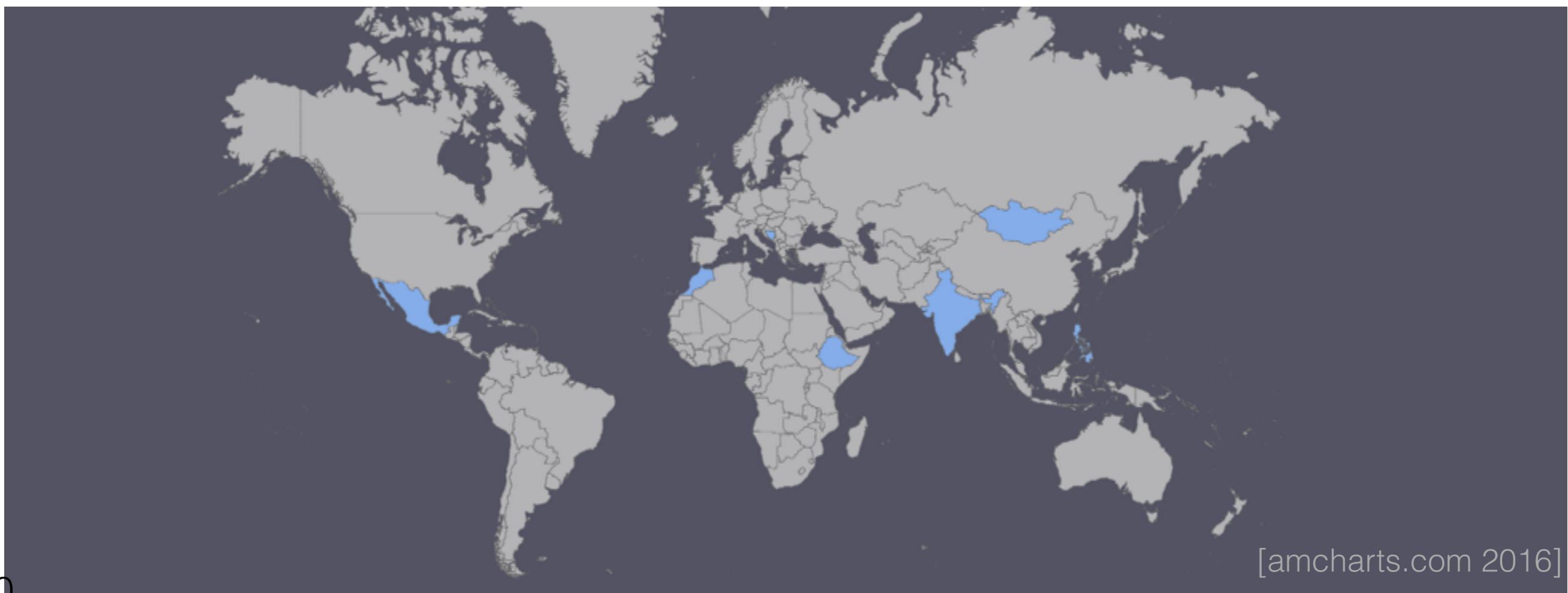
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1 if microcredit $\rightarrow \tau_k$

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profit 1 if microcredit

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- Simplified from Meager (2018a)
- $K = 7$ microcredit trials (Mexico, Mongolia, Bosnia, India, Morocco, Philippines, Ethiopia)
- N_k businesses in k th site (~ 900 to $\sim 17K$)
- Profit of n th business at k th site:

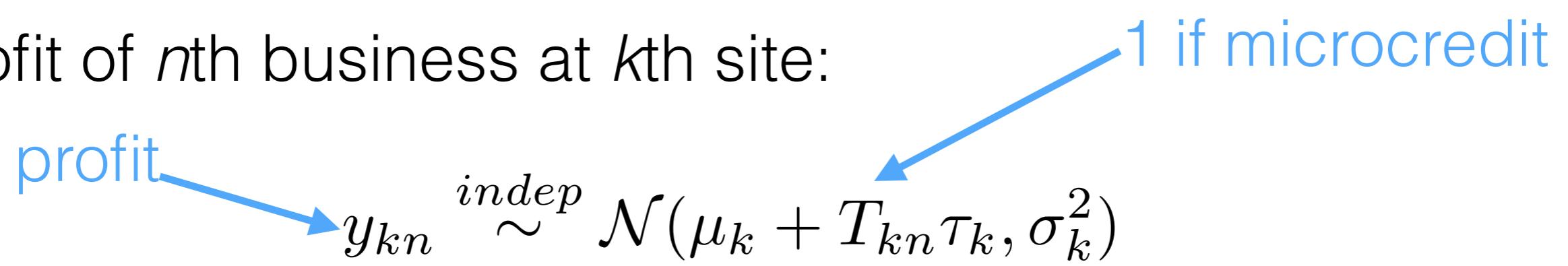
$$\text{profit} \rightarrow y_{kn} \stackrel{\text{indep}}{\sim} \mathcal{N}(\mu_k + T_{kn}\tau_k, \sigma_k^2)$$

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- Priors and hyperpriors:

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profit → y_{kn} ← **1 if microcredit**

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$$\begin{pmatrix} \mu_k \\ \tau_k \end{pmatrix} \stackrel{iid}{\sim} \mathcal{N}\left(\begin{pmatrix} \mu \\ \tau \end{pmatrix}, C\right)$$

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profit

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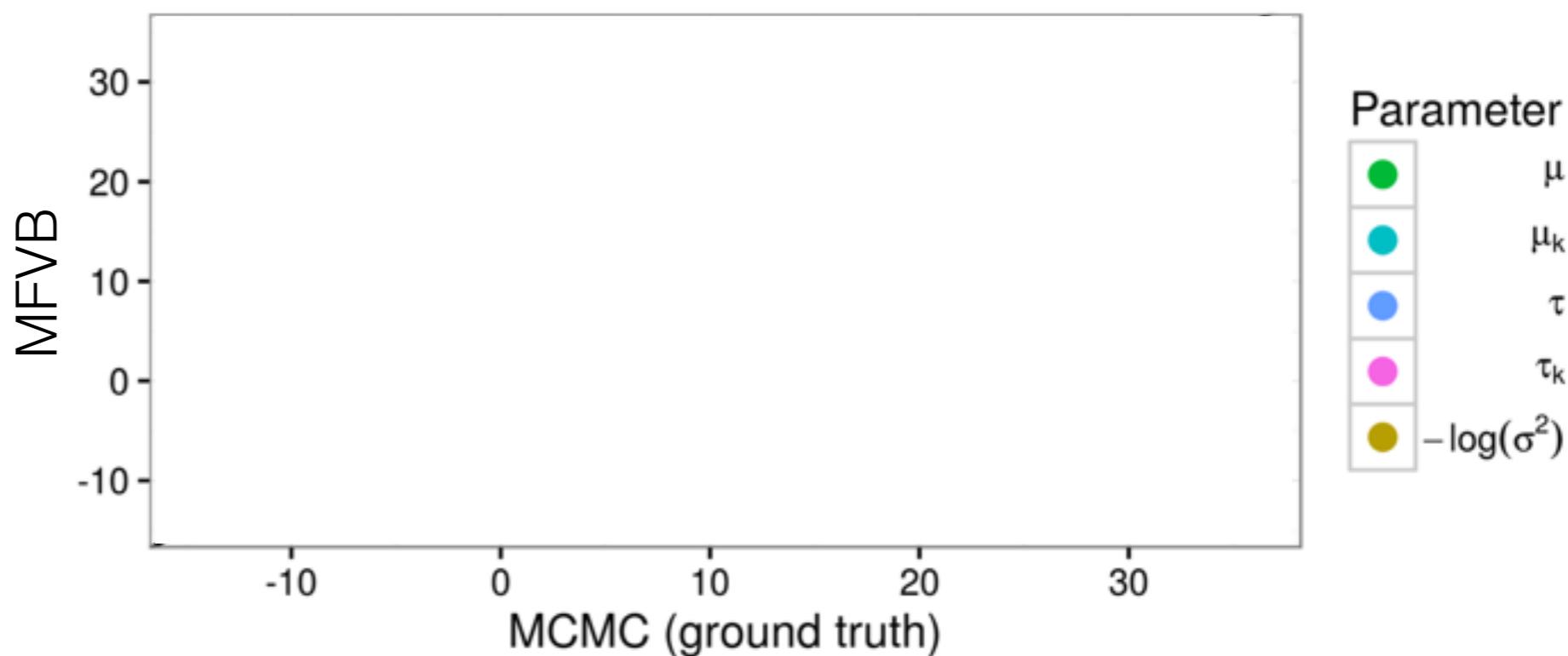
$$C \sim \text{Sep\&LKJ}(\eta, c, d)$$

Microcredit

MFVB: How will we know if it's working?

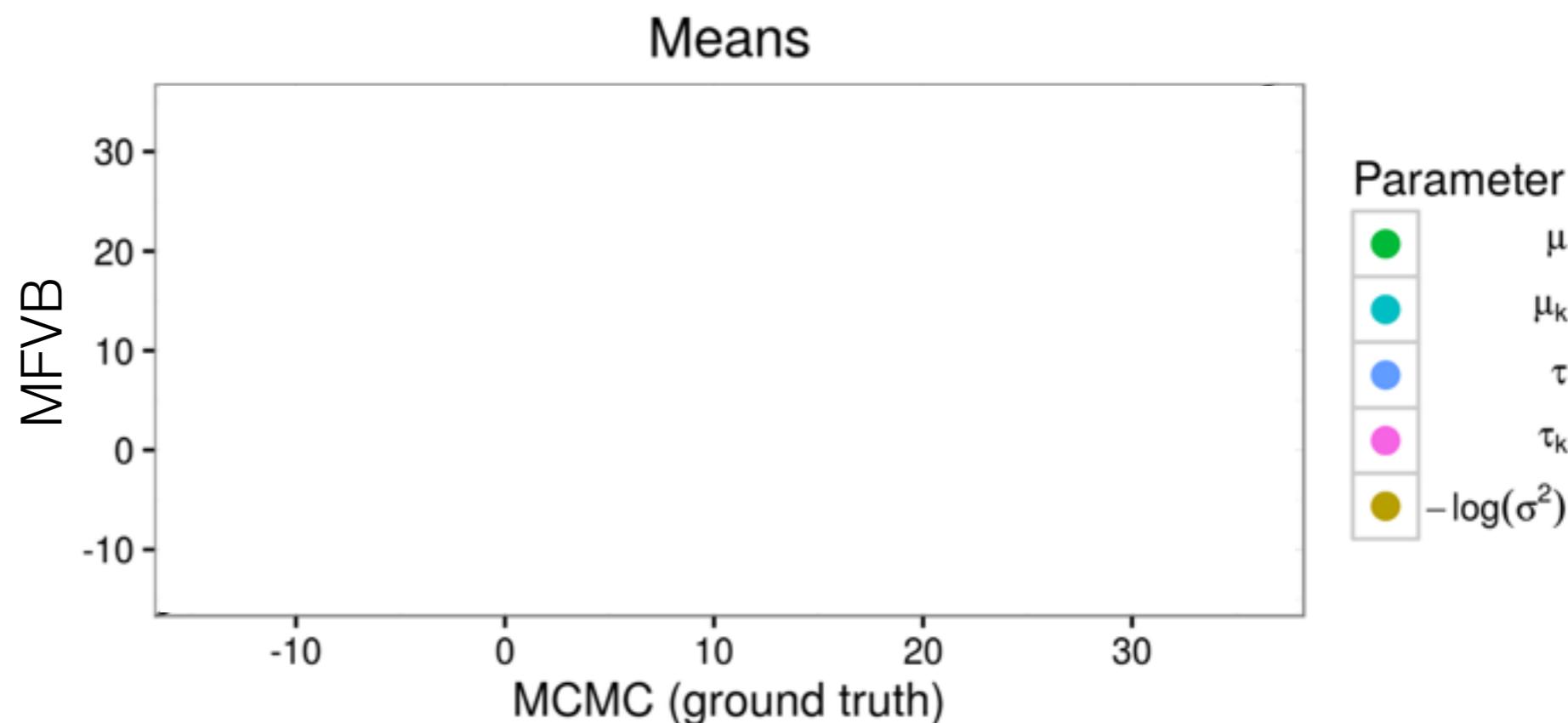
Microcredit

Means



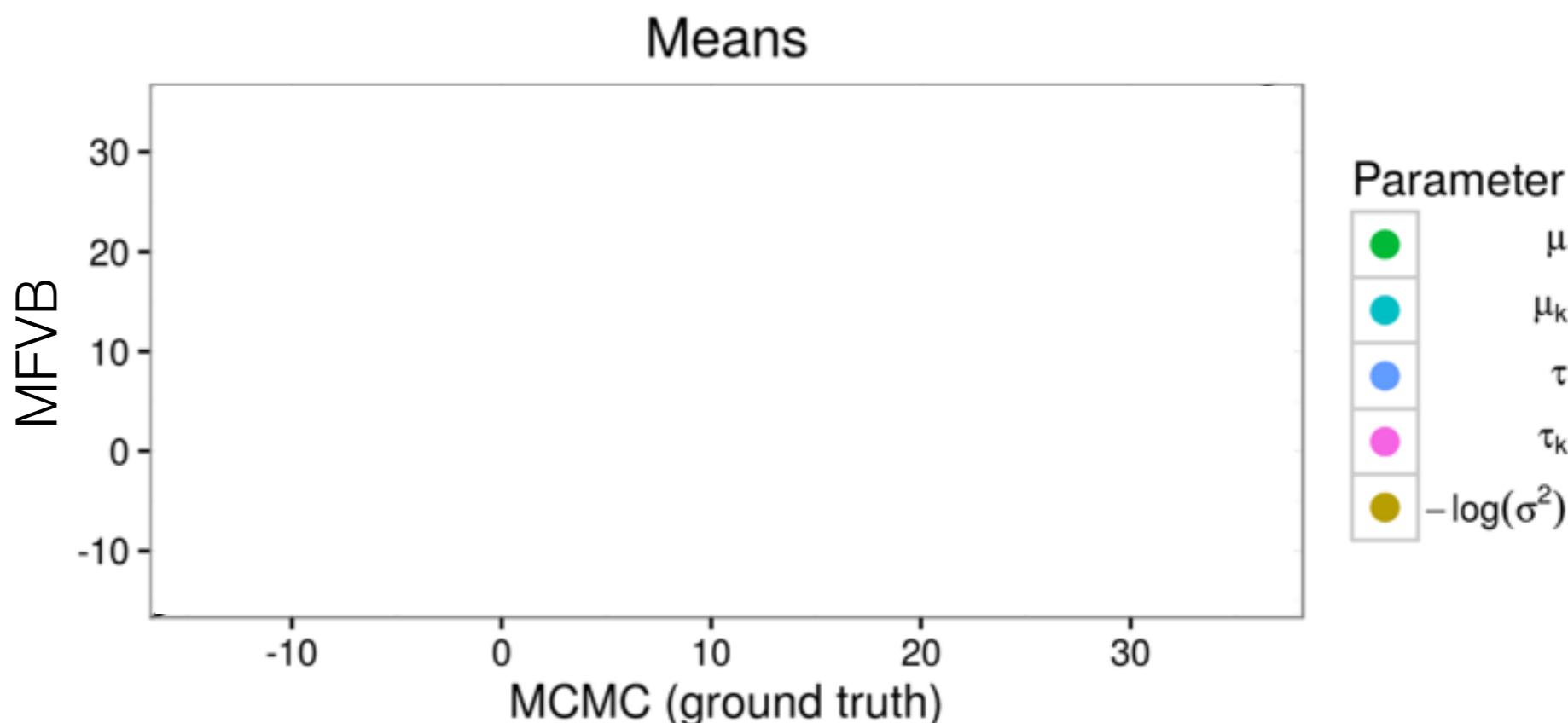
Microcredit

- One set of 2500 MCMC draws:
45 minutes



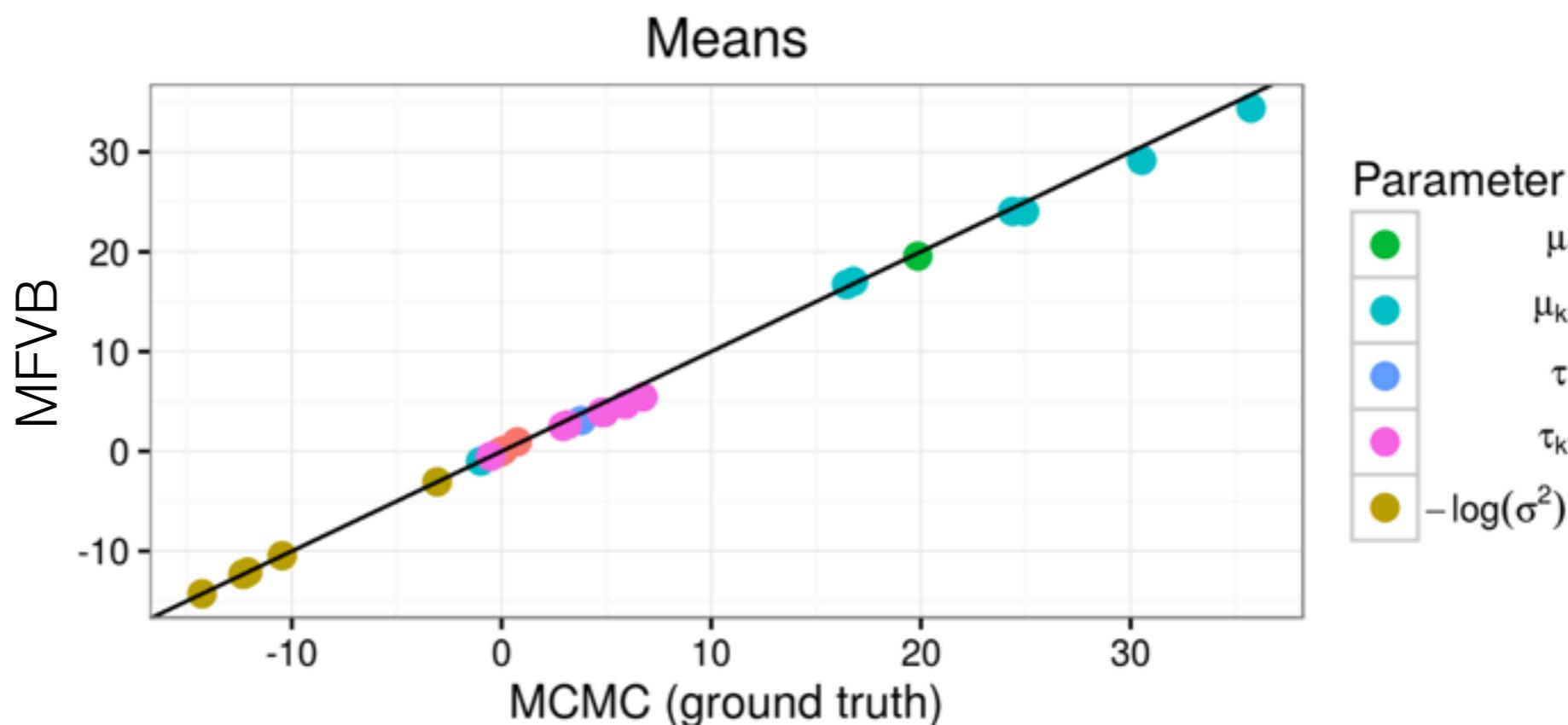
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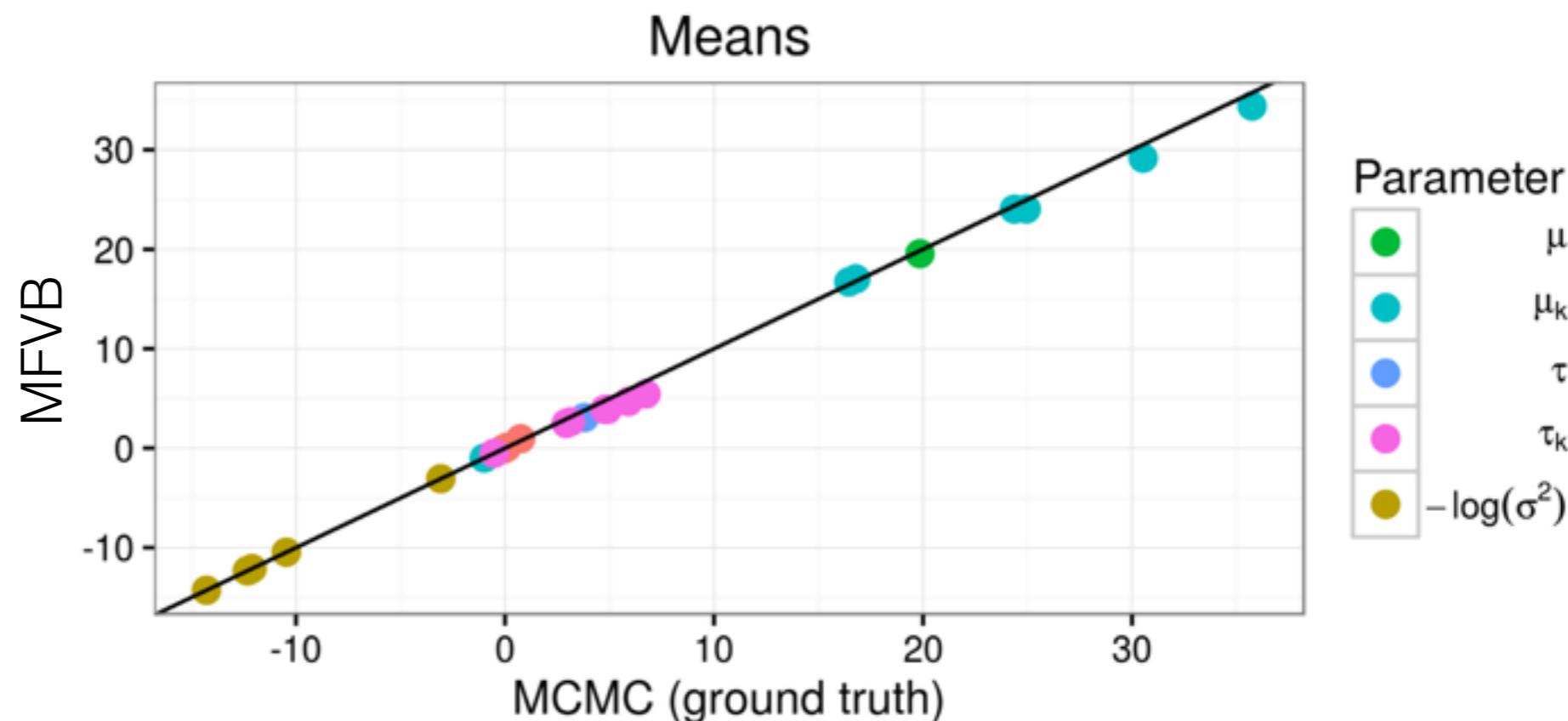
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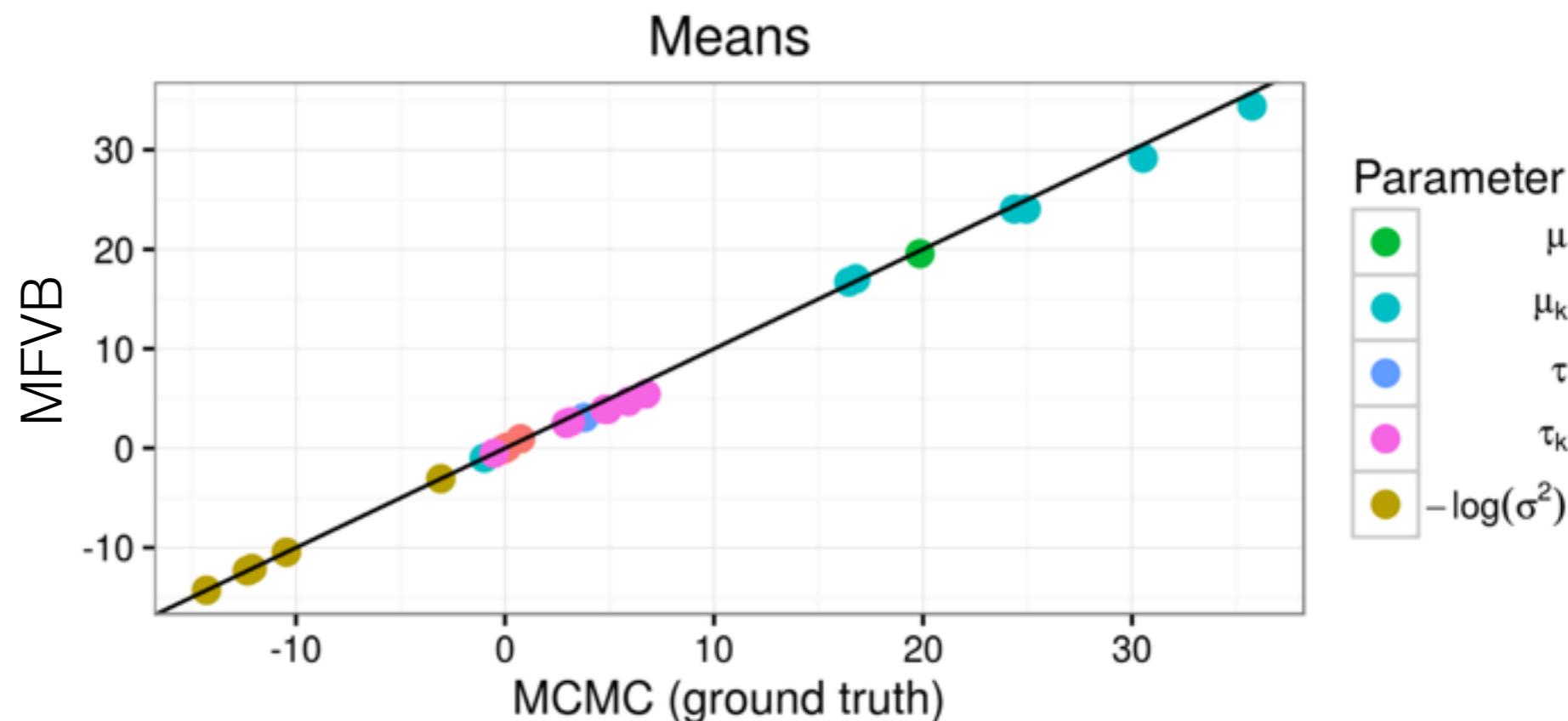


Criteo Online Ads Experiment

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

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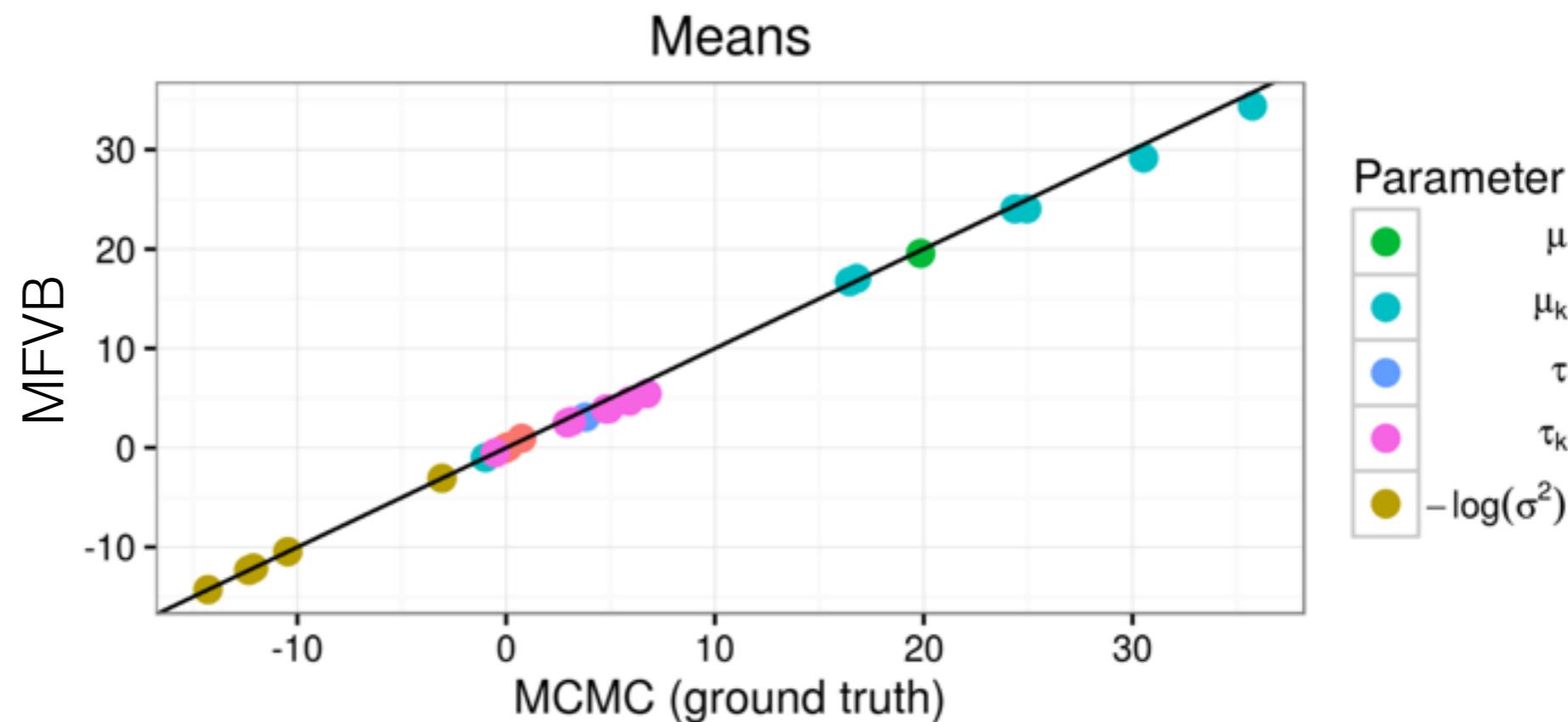


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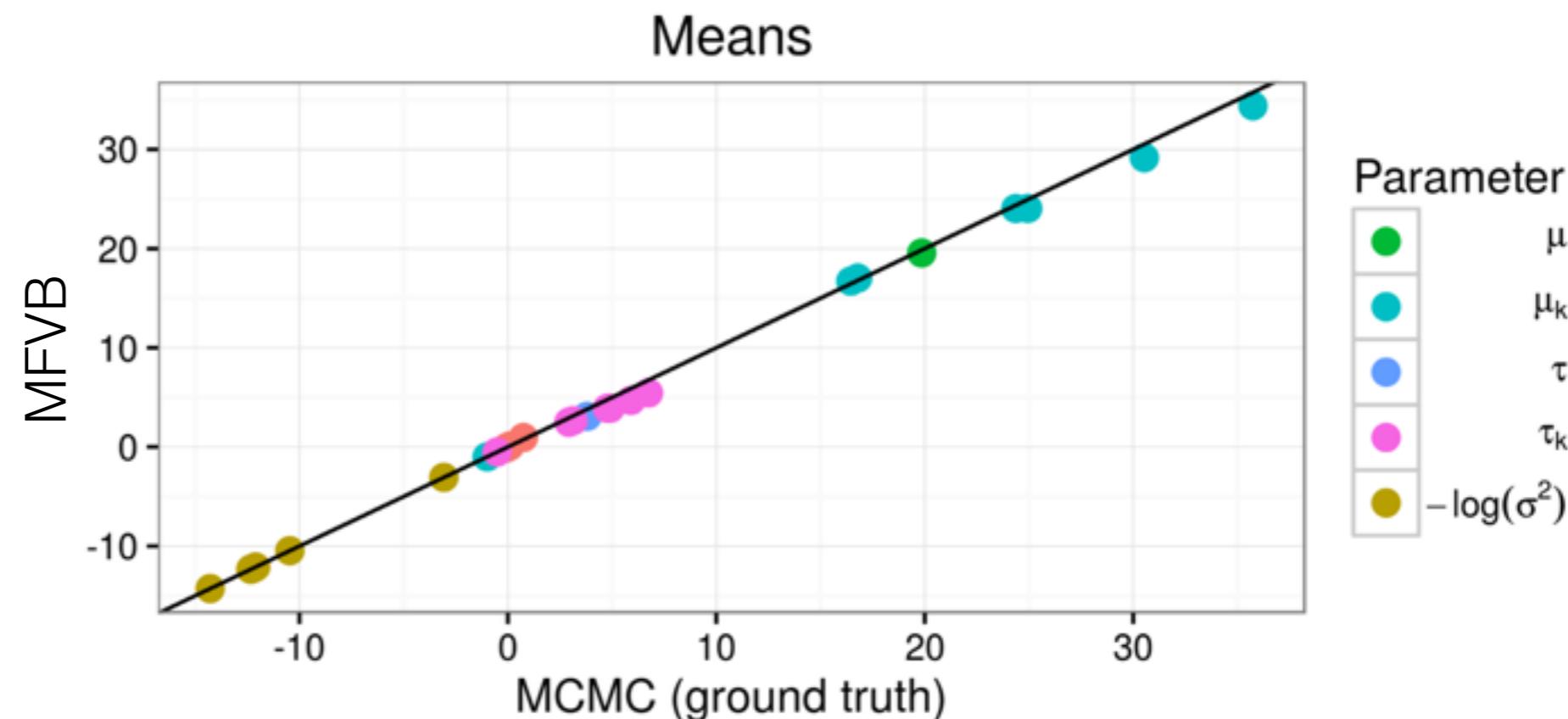


Criteo Online Ads Experiment

- Click-through conversion prediction
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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

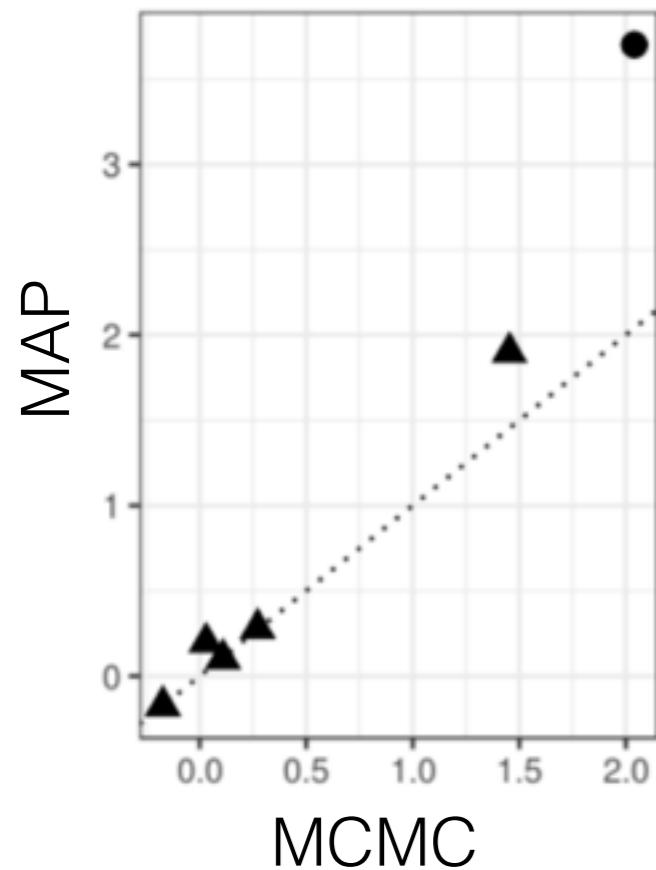
Criteo Online Ads Experiment

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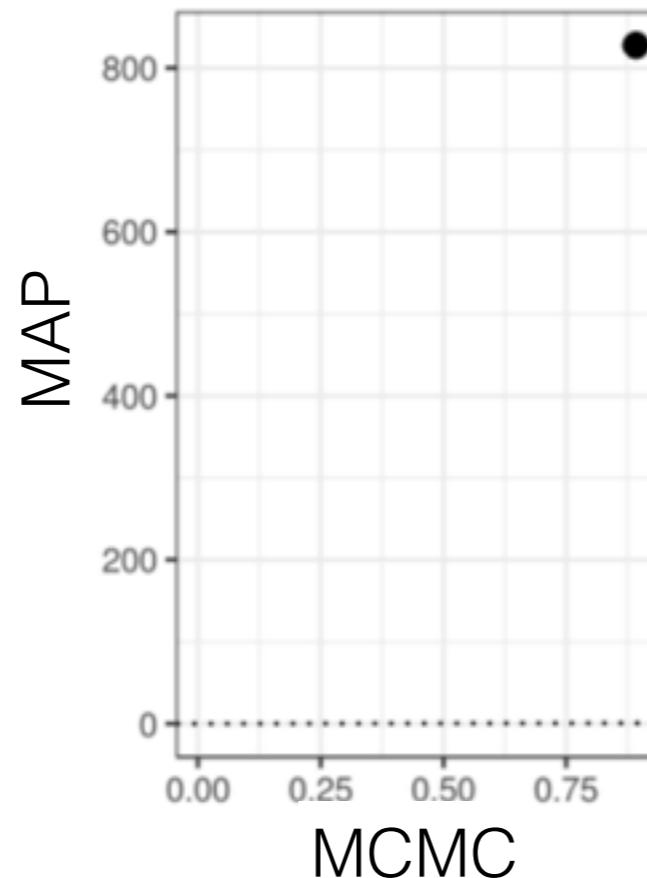
- MAP: **12 s**

Criteo Online Ads Experiment

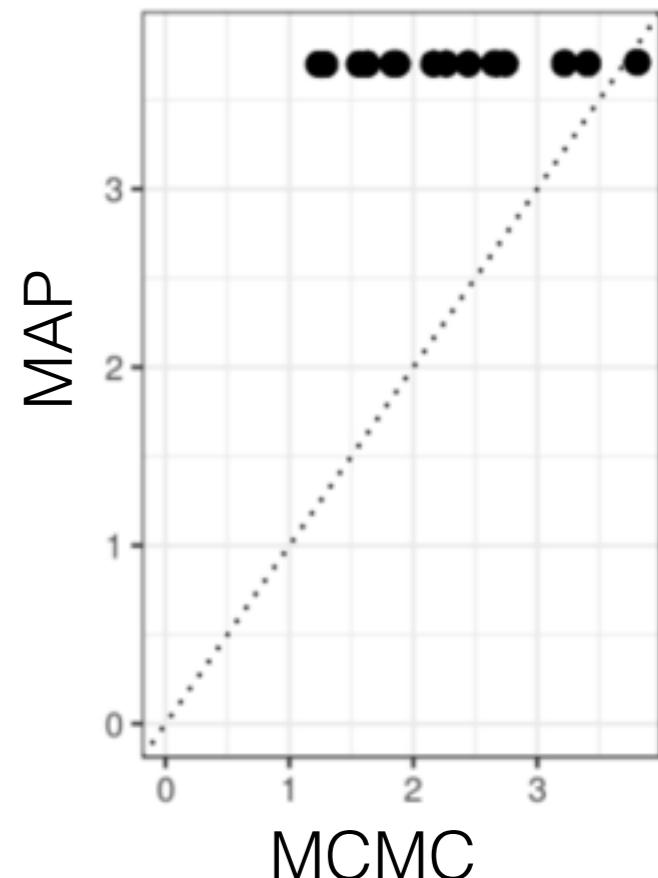
Global parameters ($-\tau$)



Global parameter τ



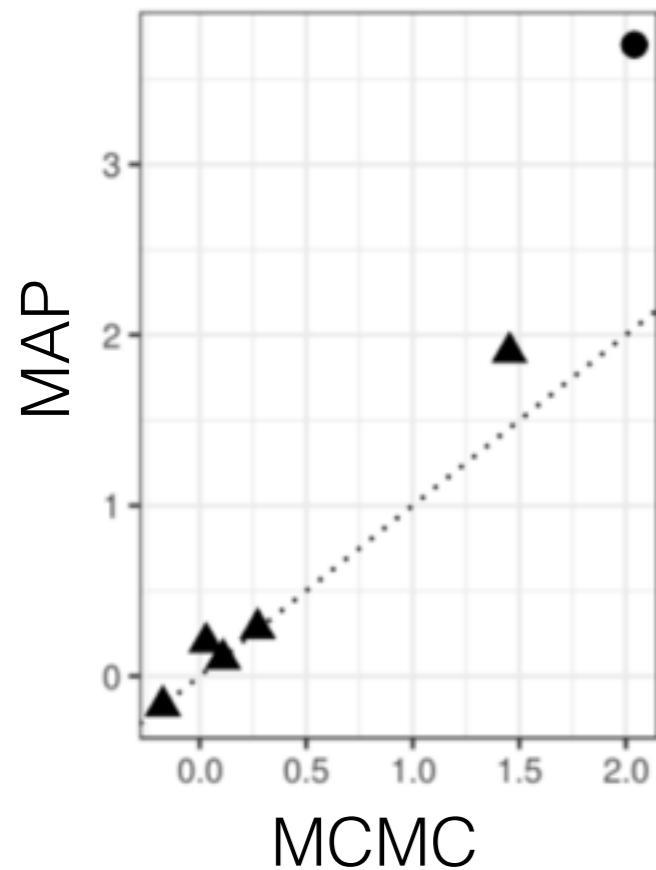
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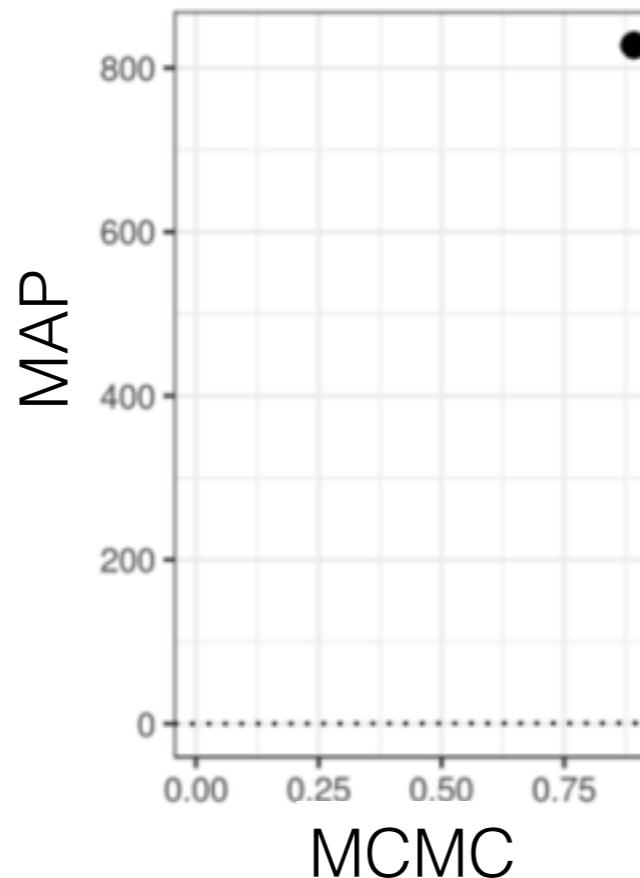
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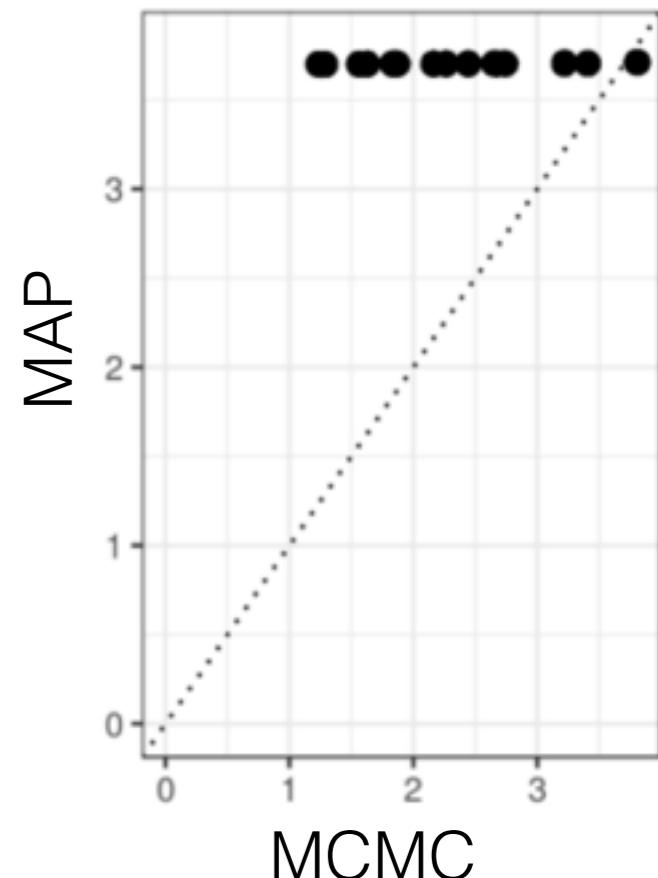
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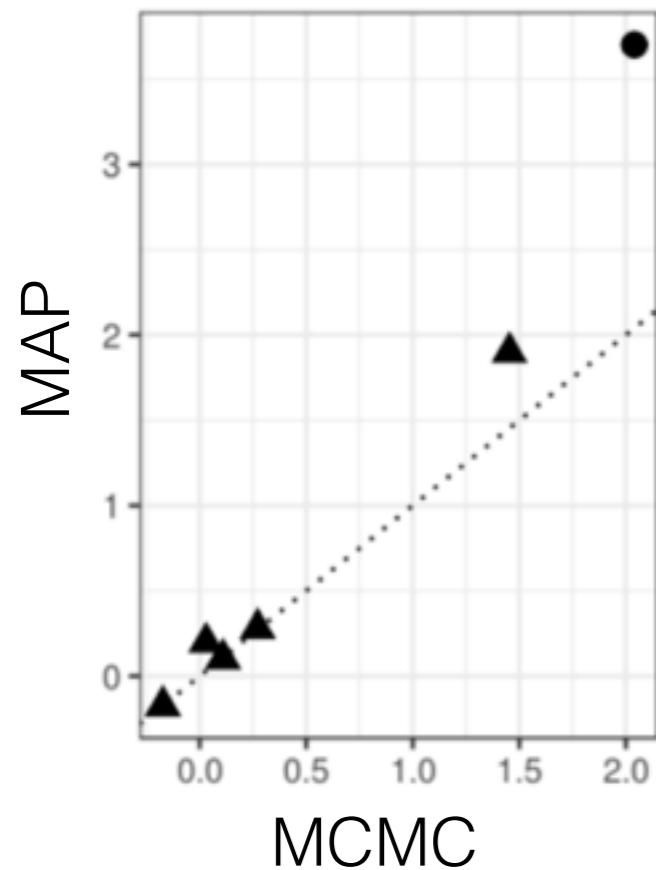
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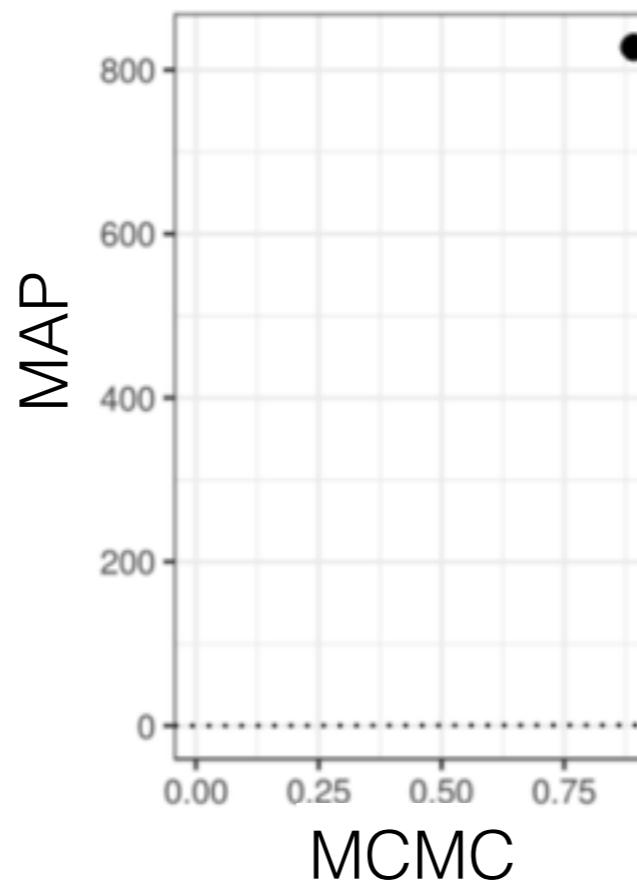
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- MFVB: **57 s**

Criteo Online Ads Experiment

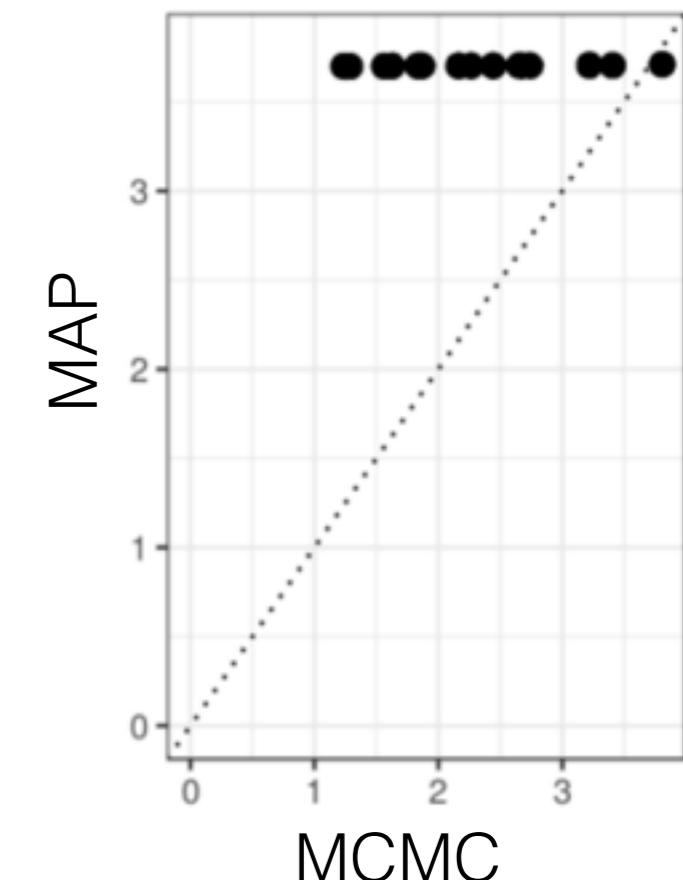
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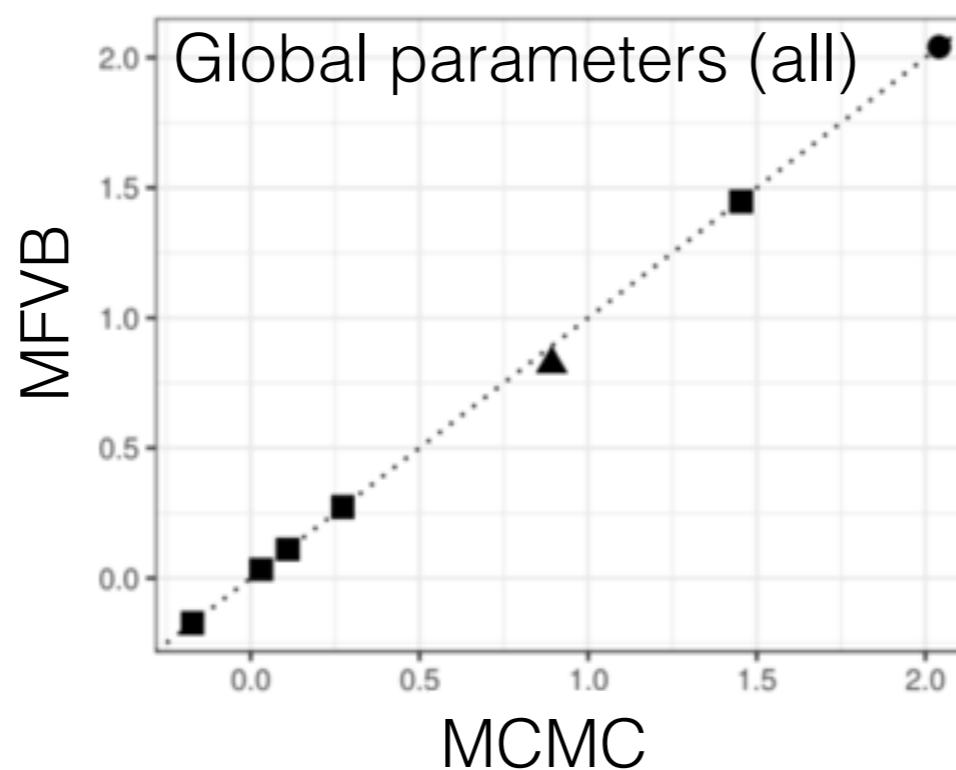
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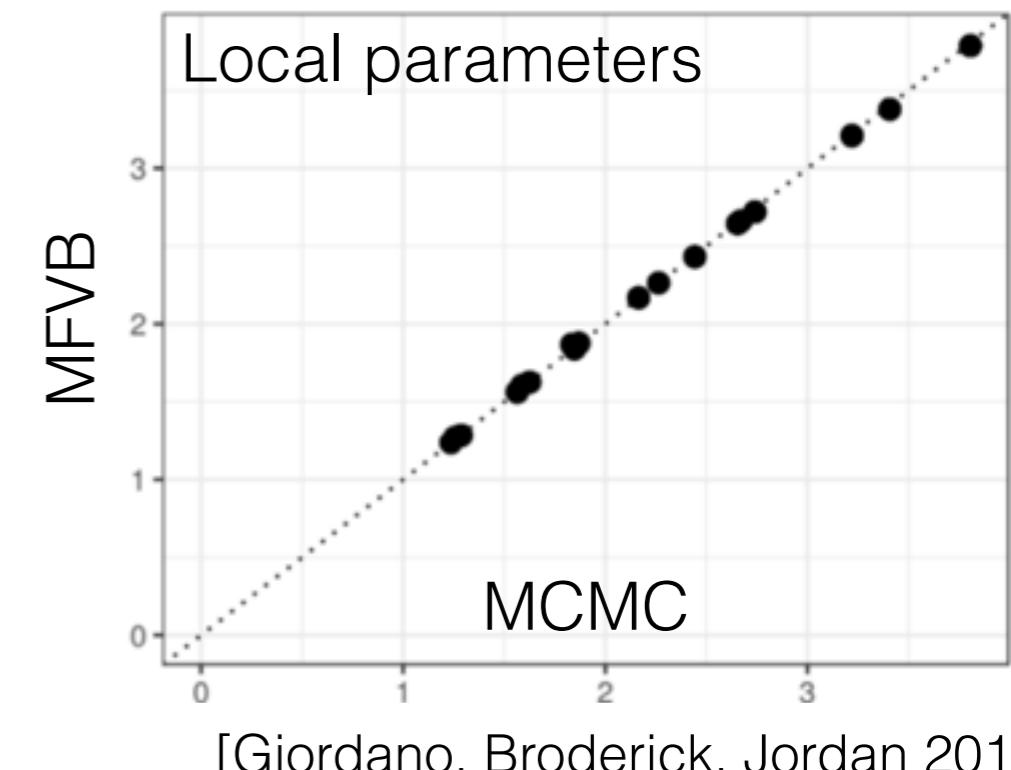
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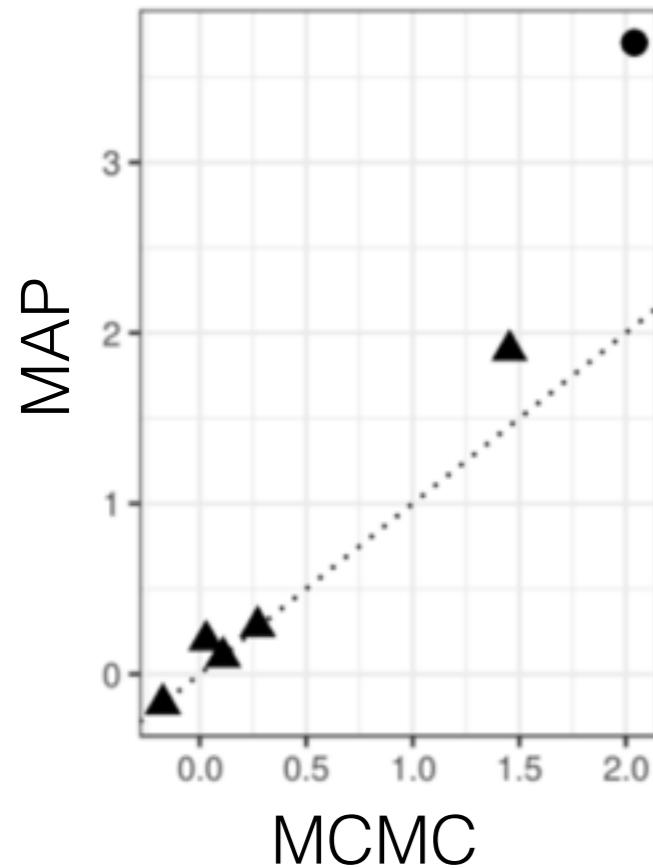
Global parameters (all)



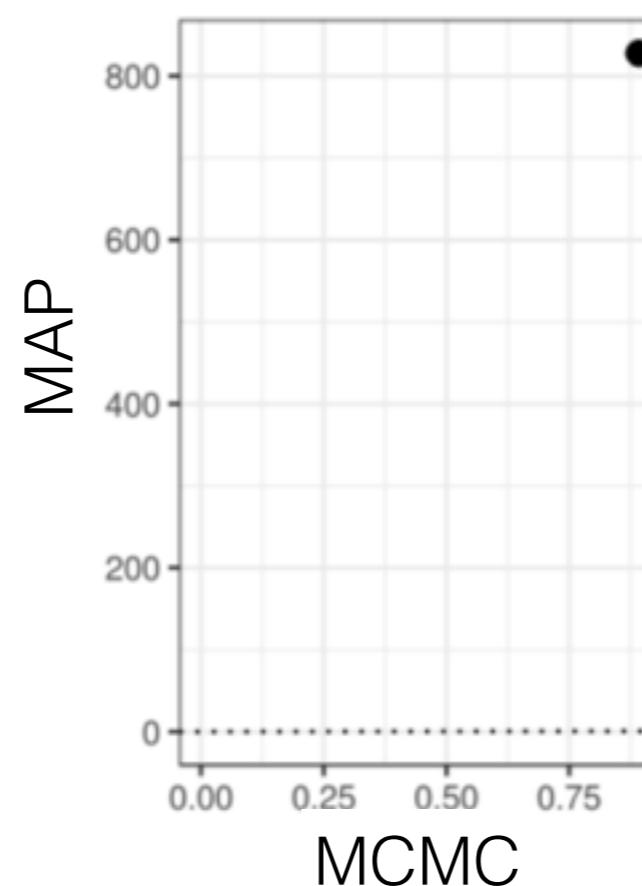
MCMC

Criteo Online Ads Experiment

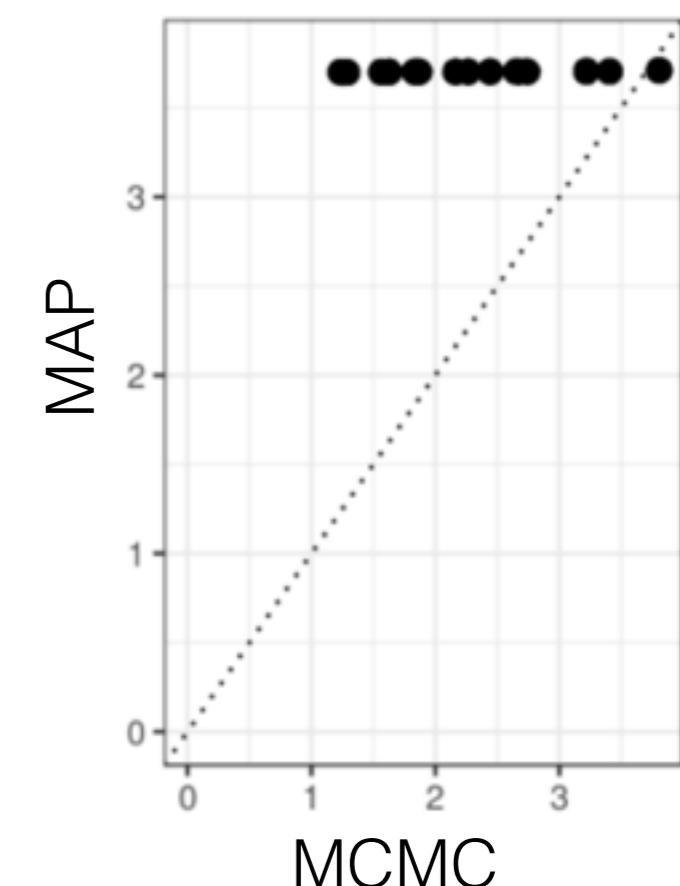
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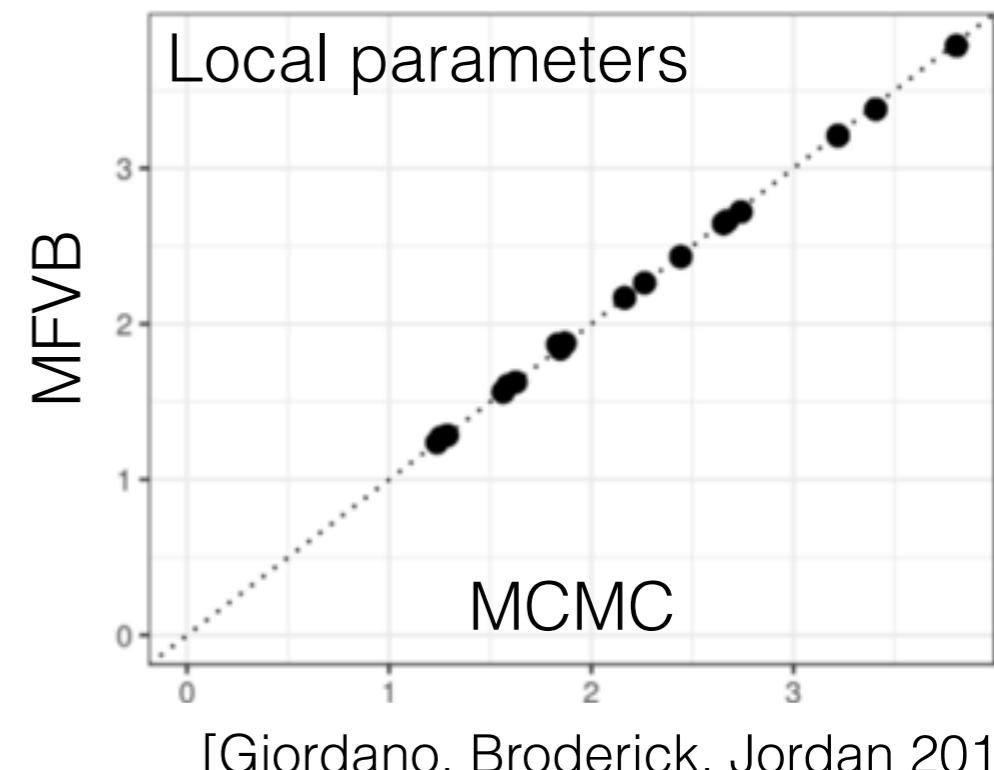
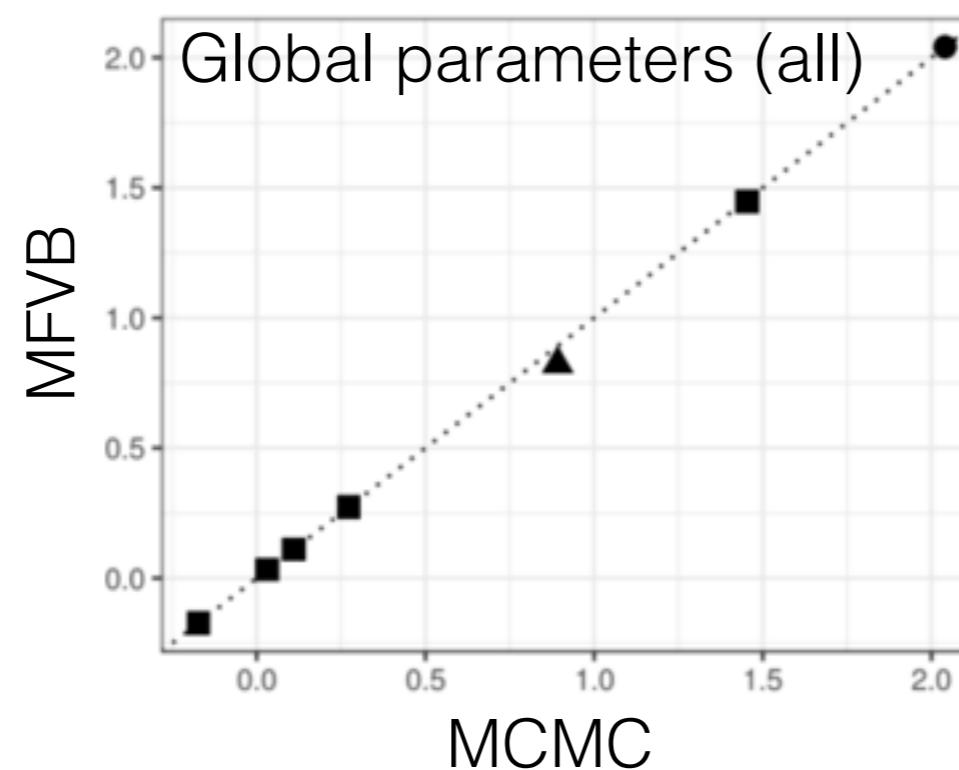
Global parameter τ



Local parameters



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

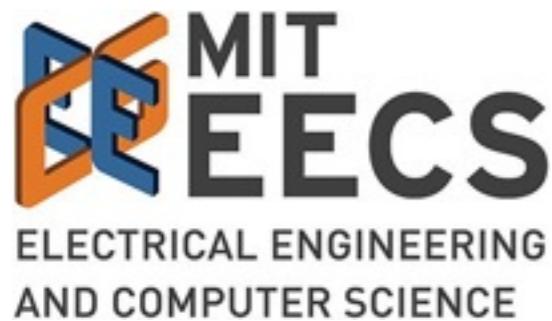


Roadmap

- 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?

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Variational Bayes and beyond: Bayesian inference for big data

Tamara Broderick
ITT Career Development
Assistant Professor,
MIT

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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

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

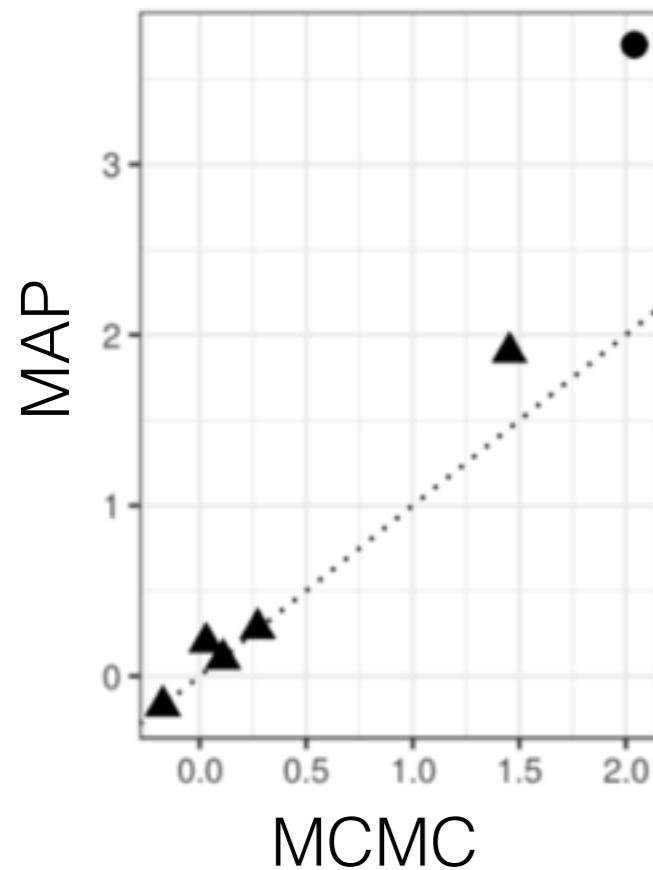
Mean-field variational Bayes

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

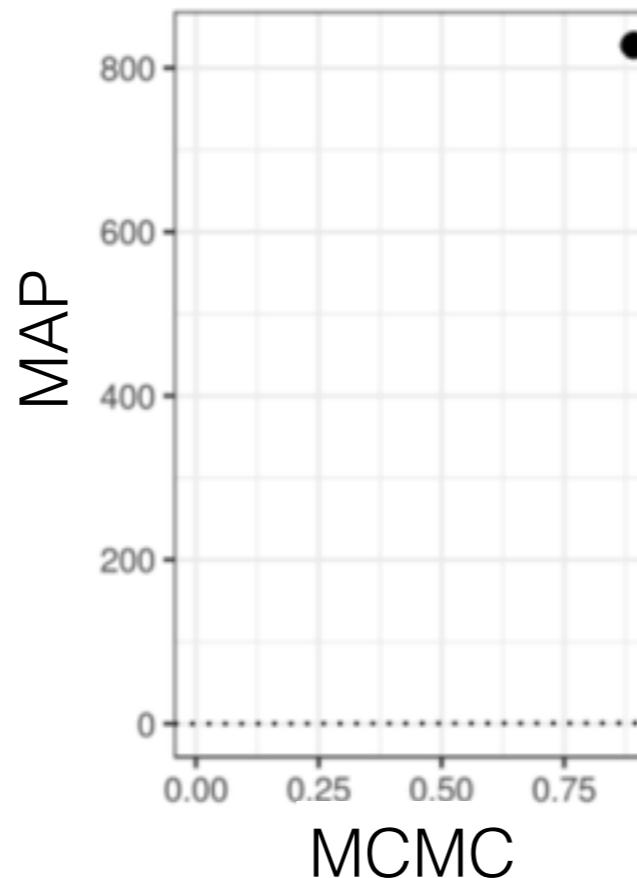
- Coordinate descent
- Stochastic variational inference (SVI) [Hoffman et al 2013]
- Automatic differentiation variational inference (ADVI) [Kucukelbir et al 2015, 2017]

Criteo Online Ads Experiment

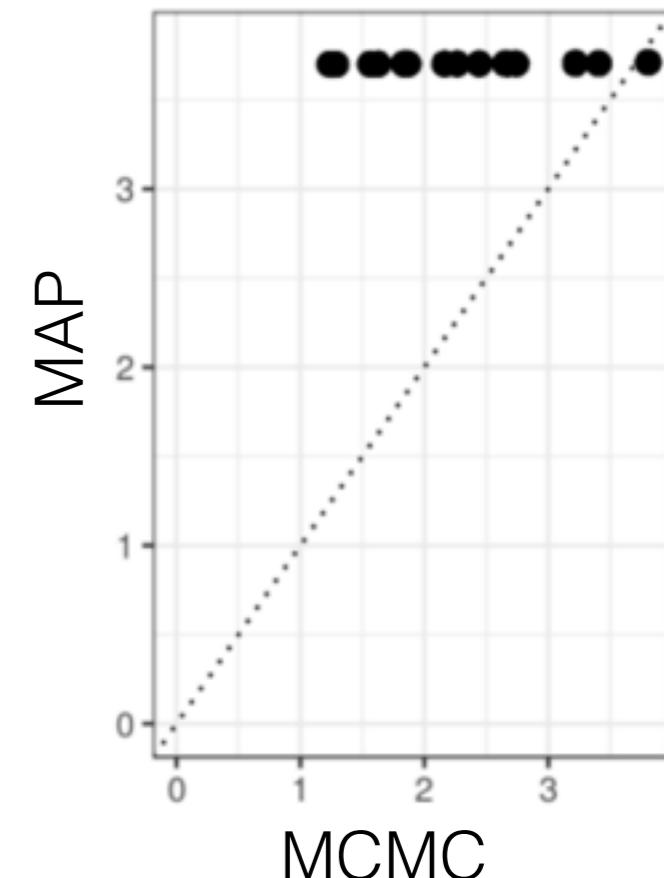
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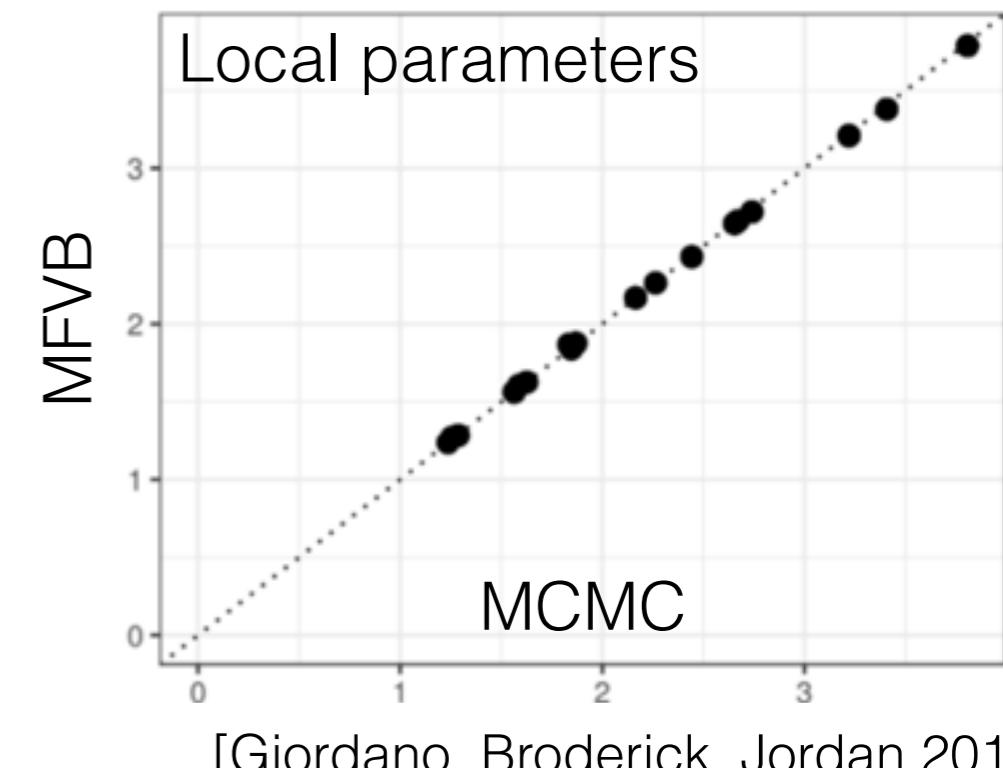
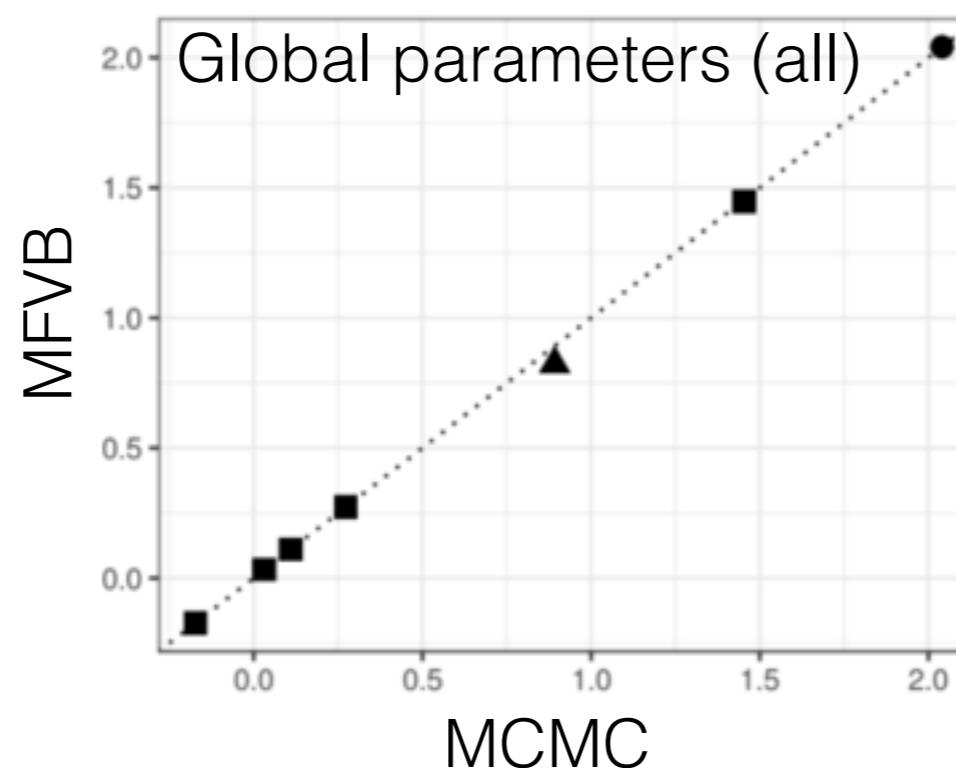
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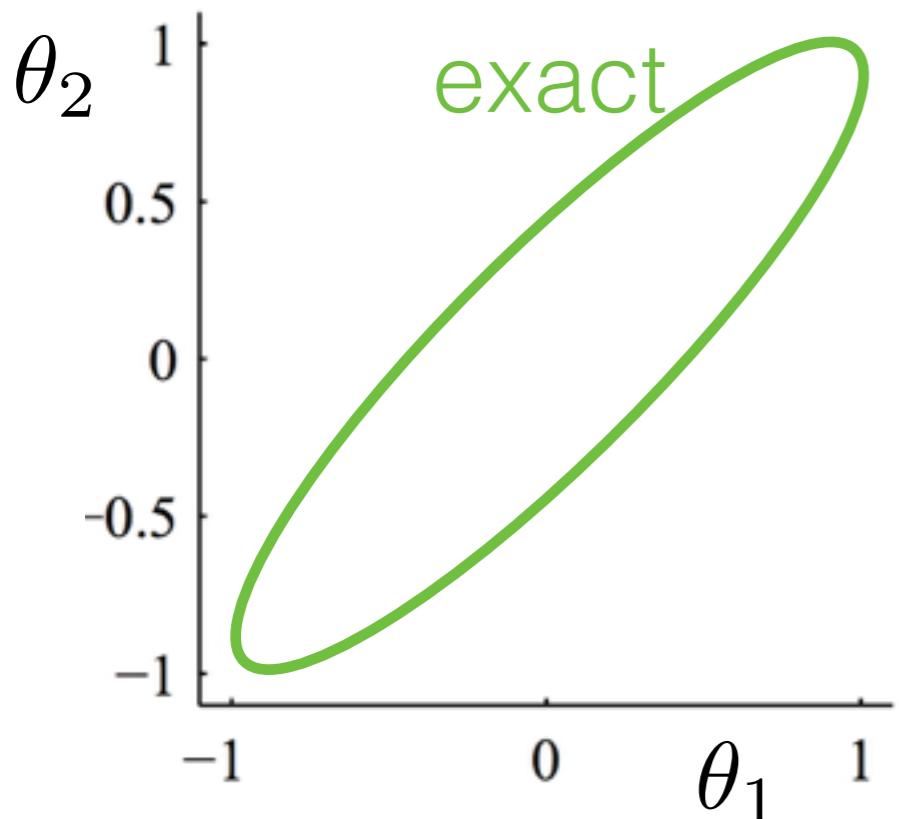
What about uncertainty?

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

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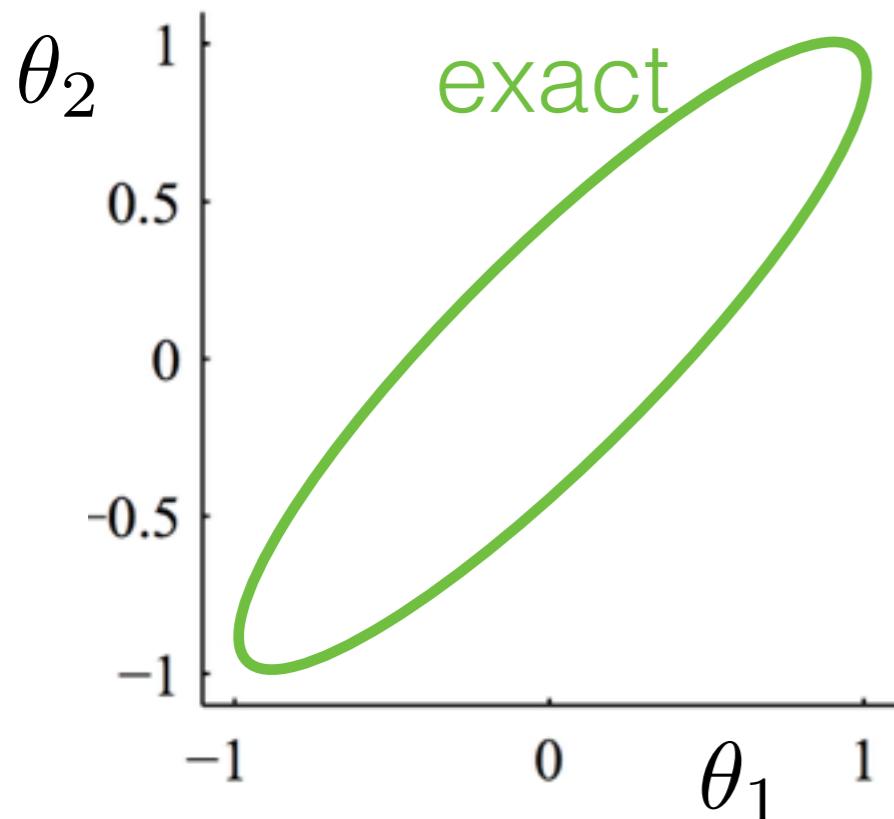


[Turner & Sahani
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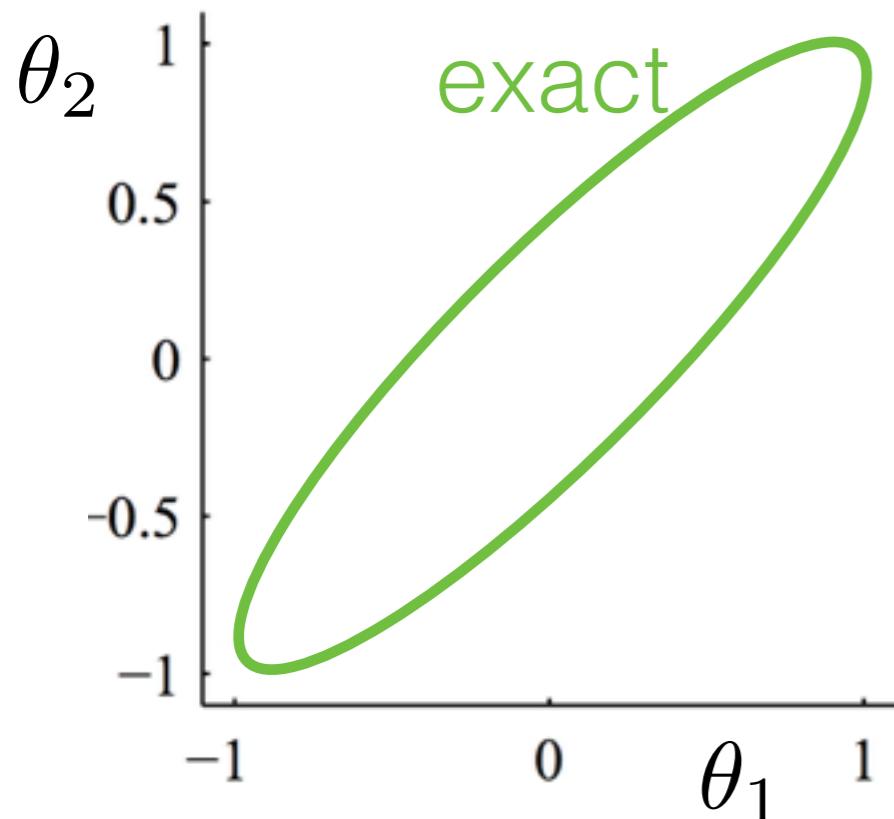
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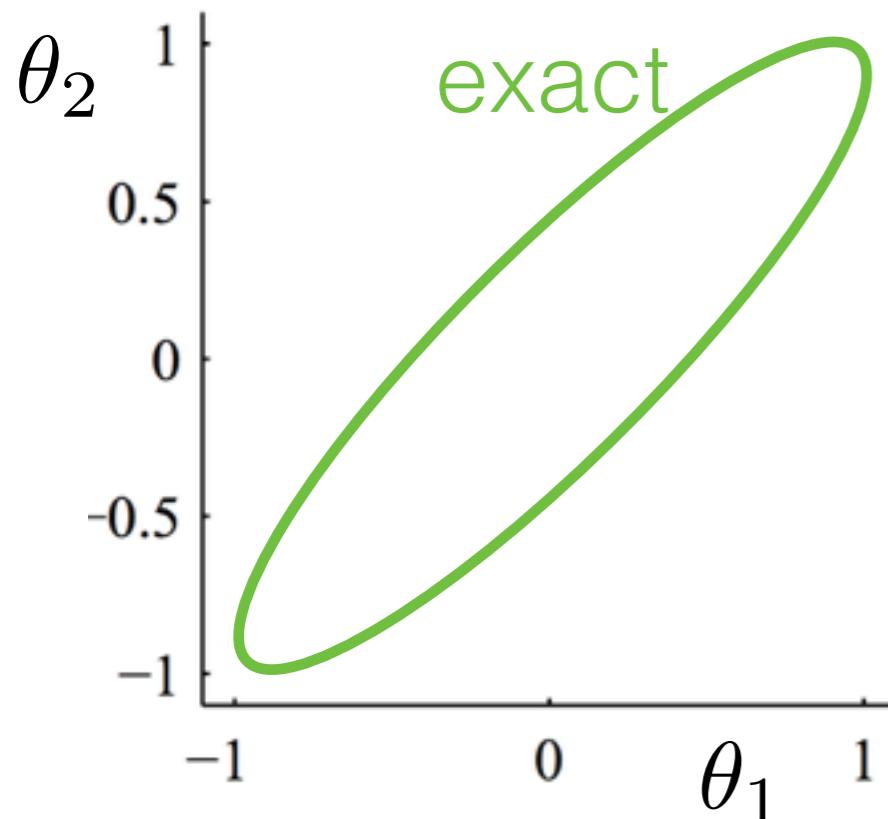
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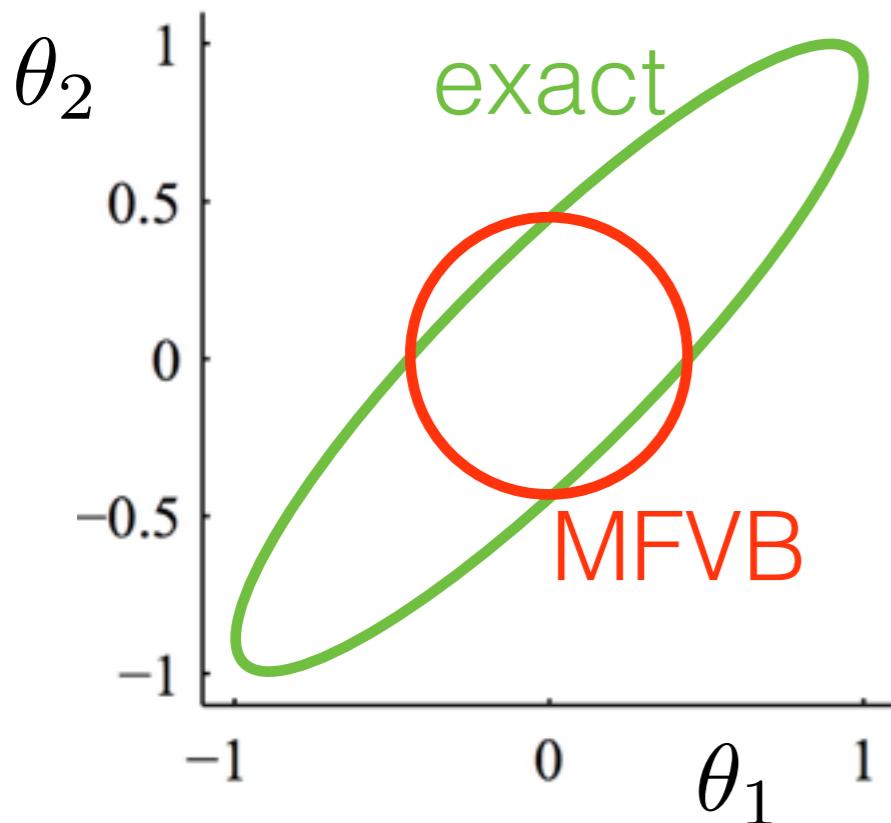
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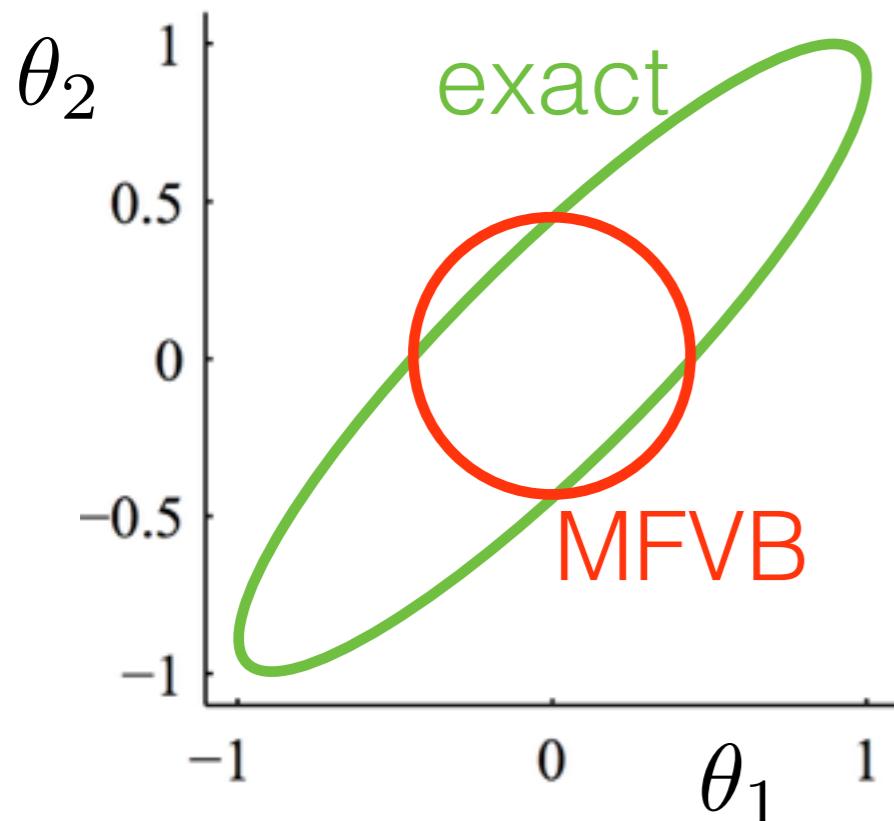
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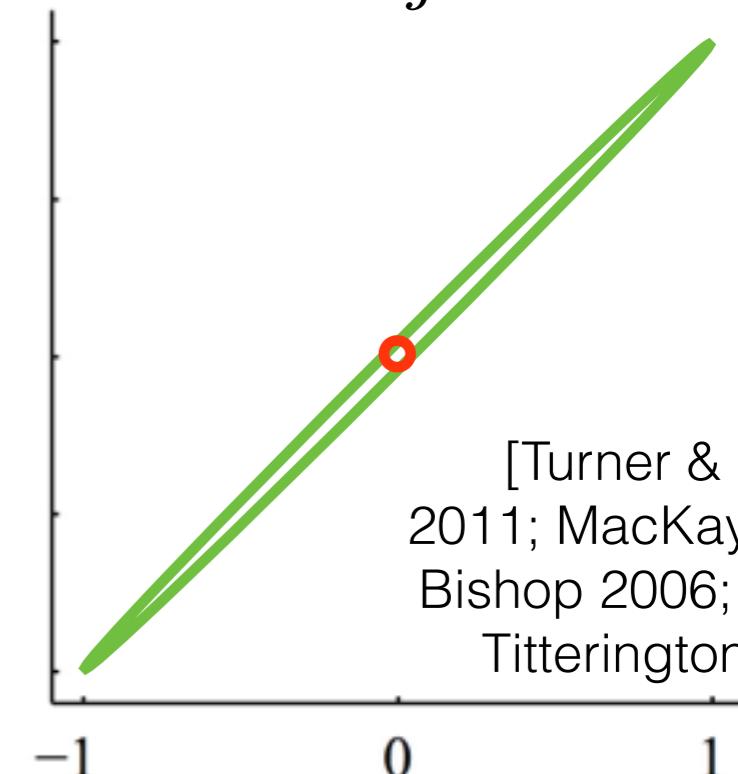
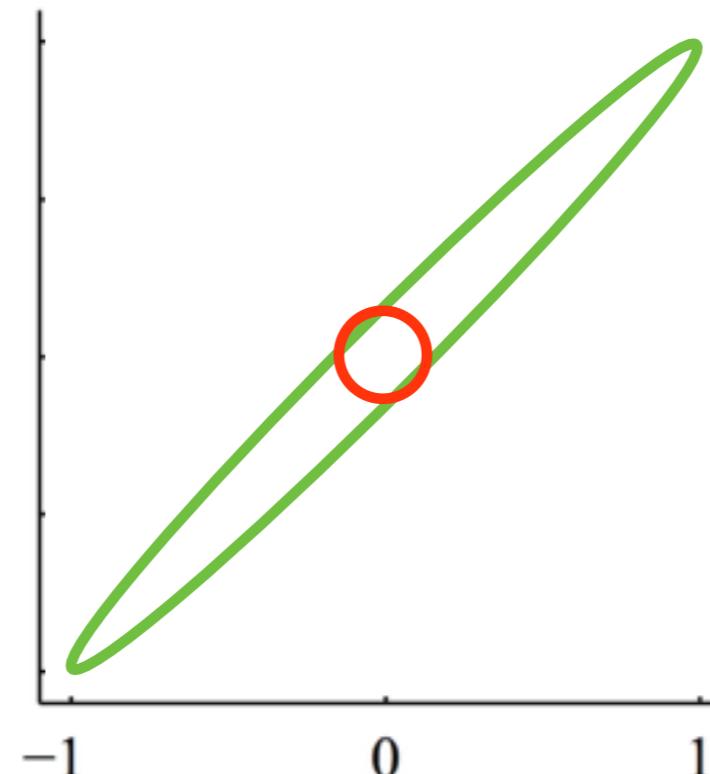
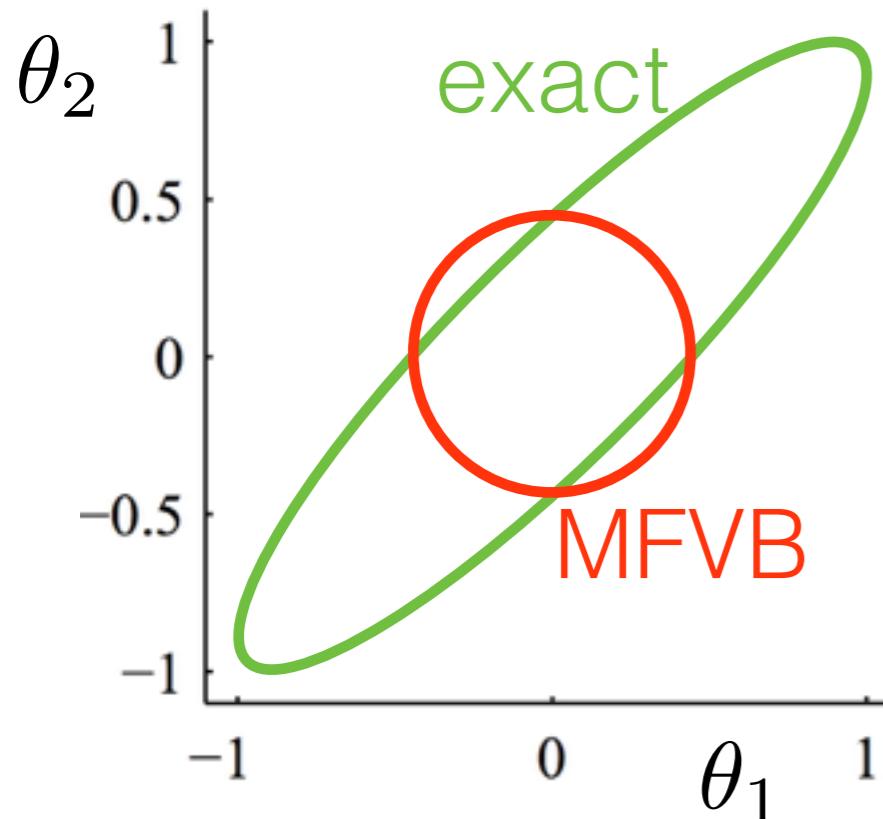
- Underestimates variance (sometimes severely)
- Conjugate linear regression
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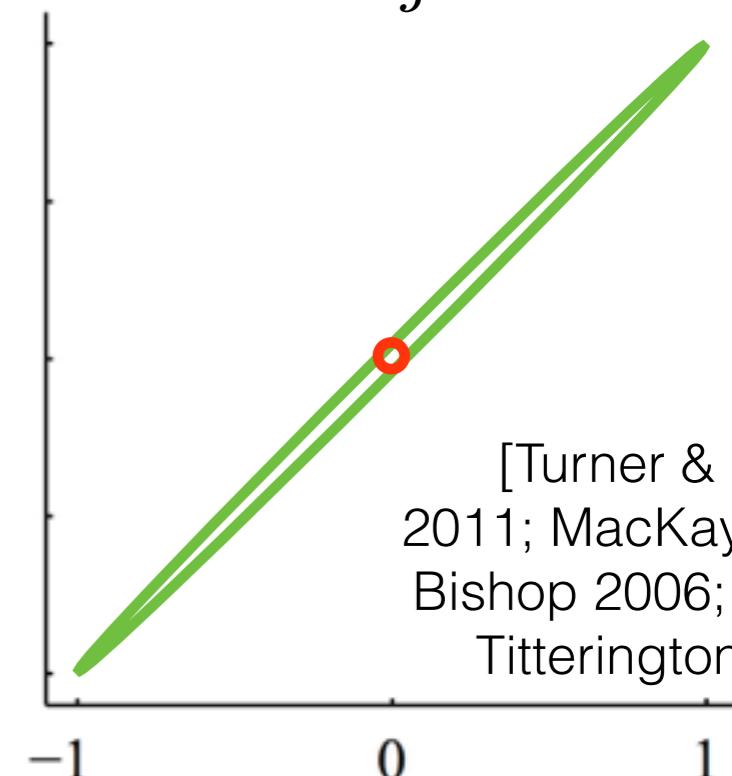
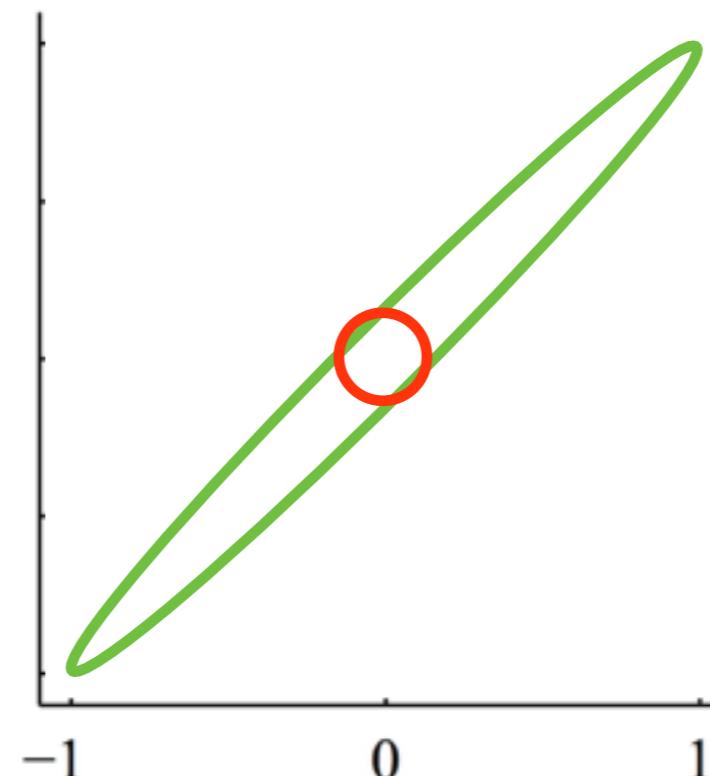
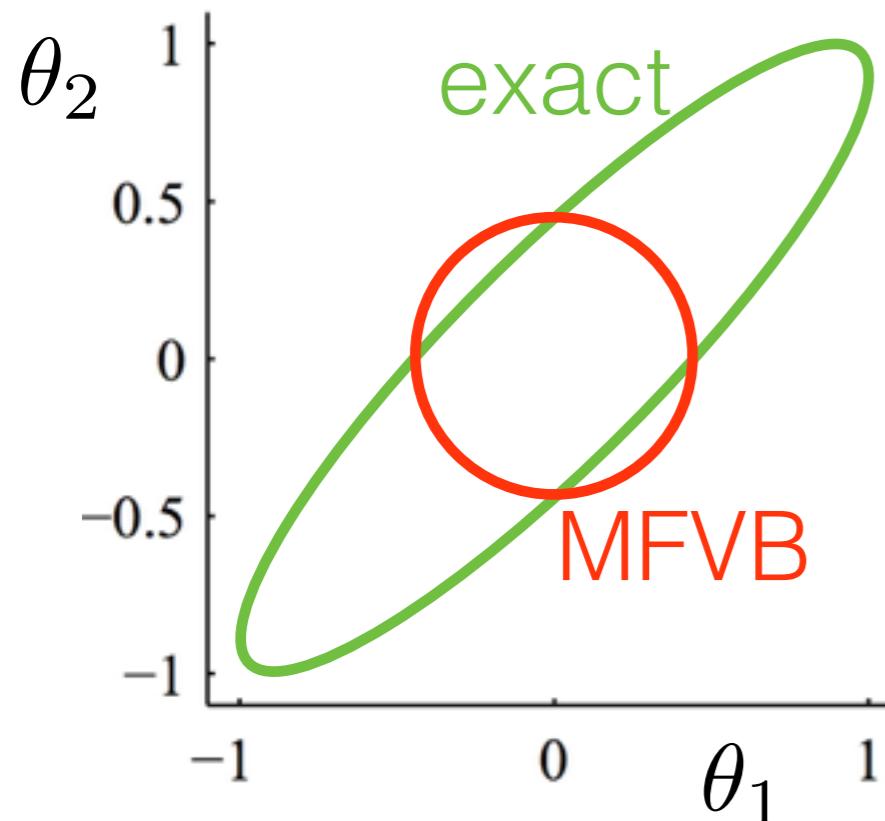
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- Underestimates variance (sometimes severely)
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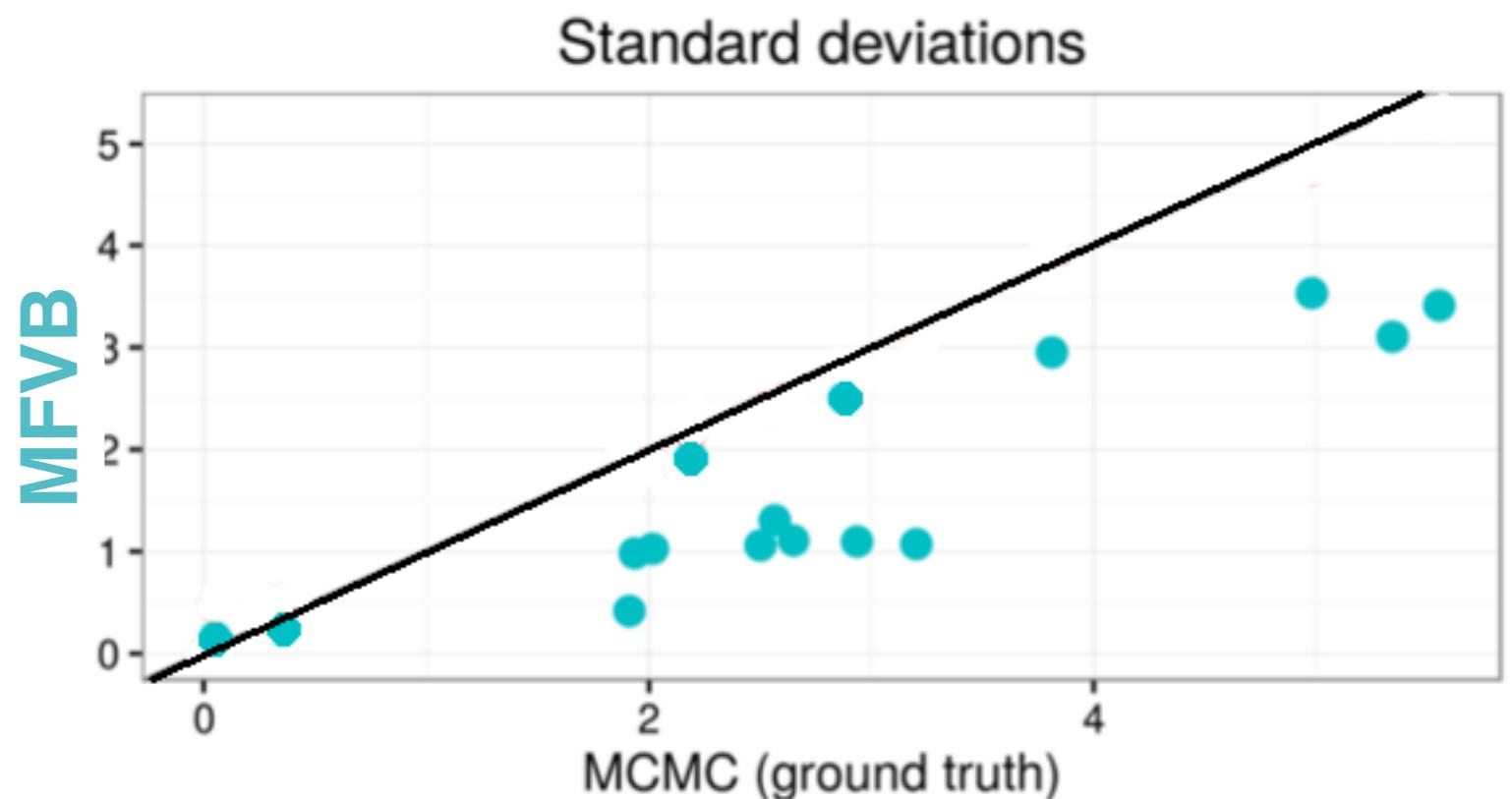
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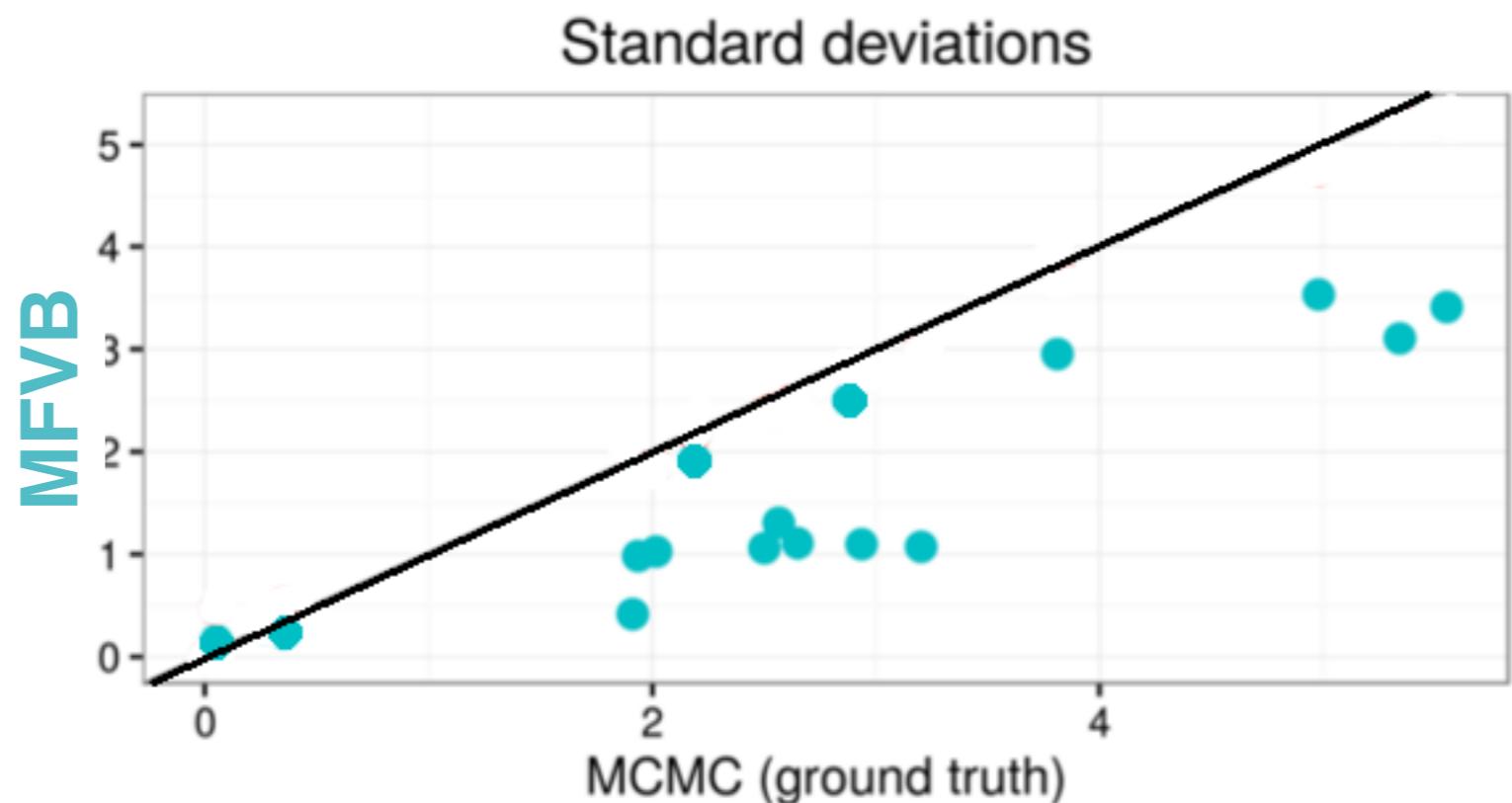
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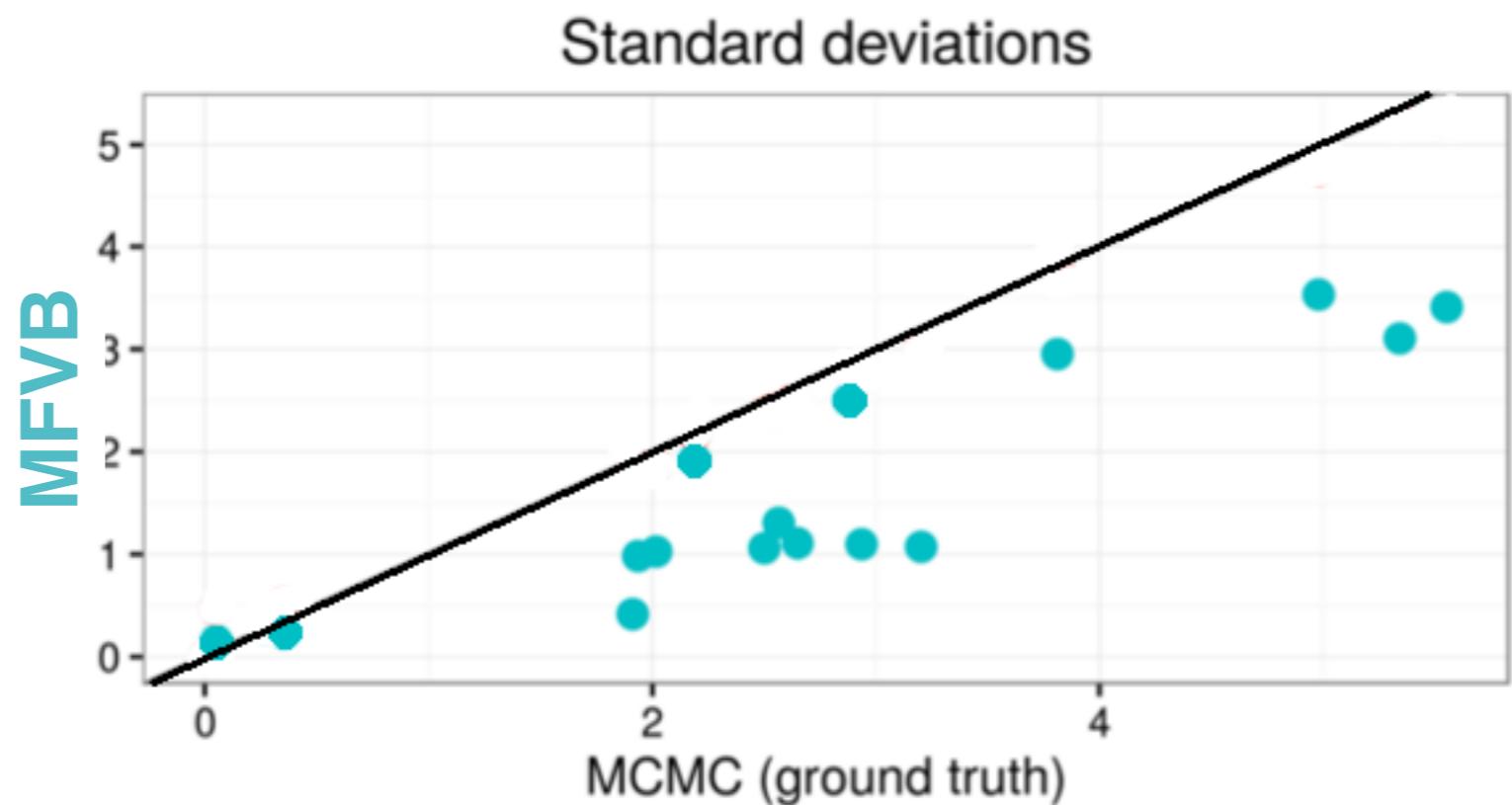
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- τ mean:
3.08 USD PPP



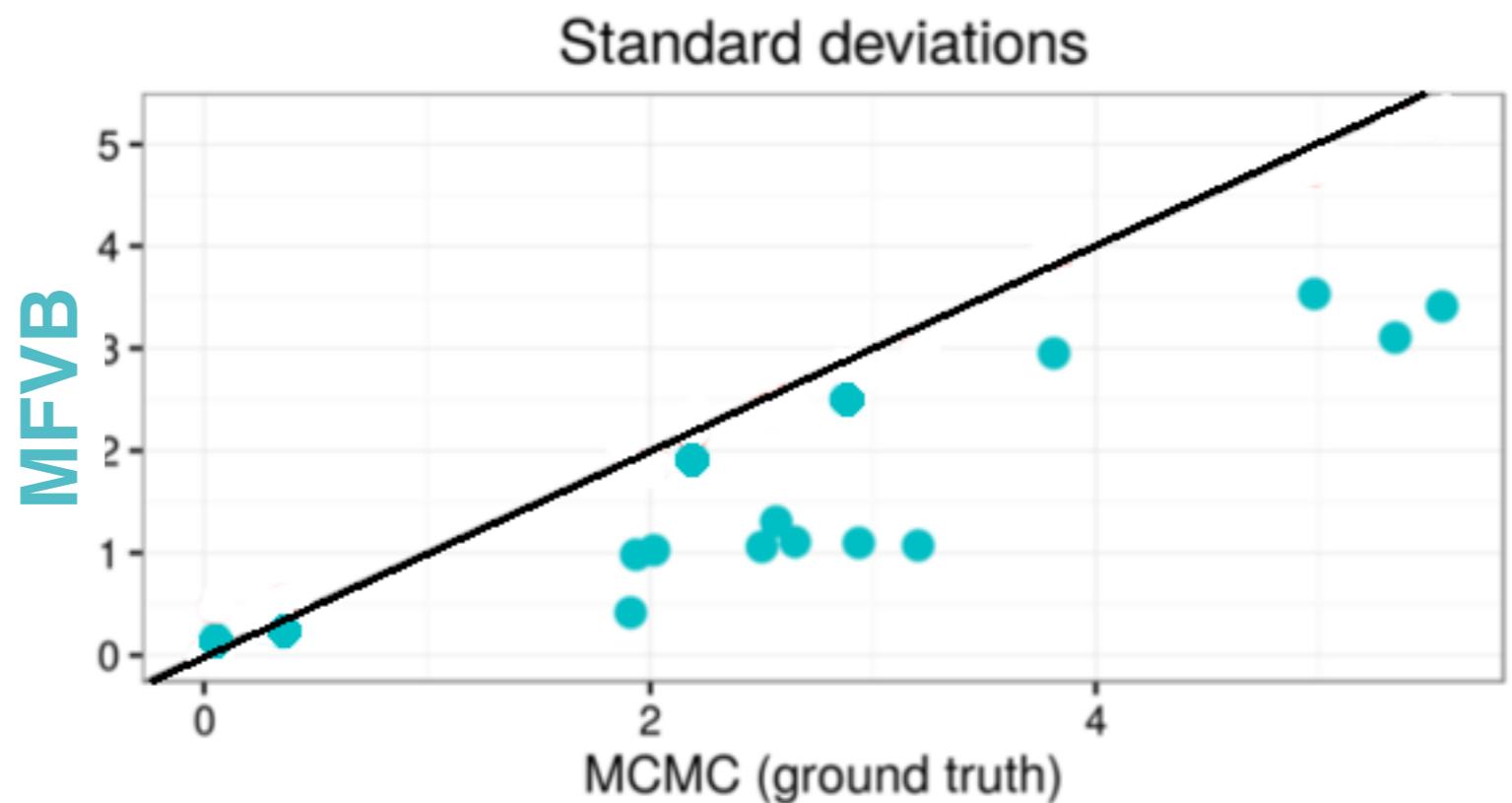
What about uncertainty?

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- τ std dev:
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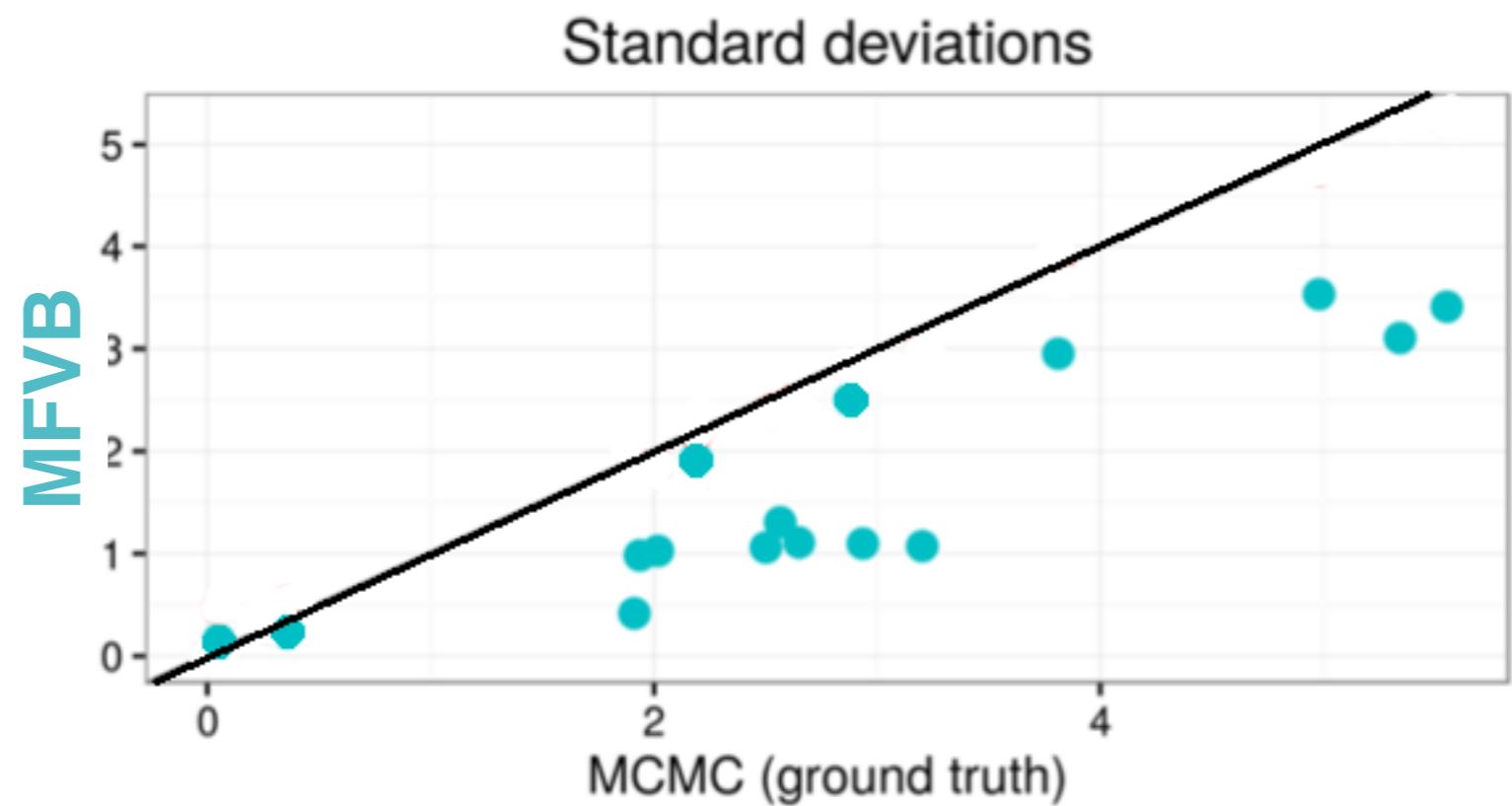
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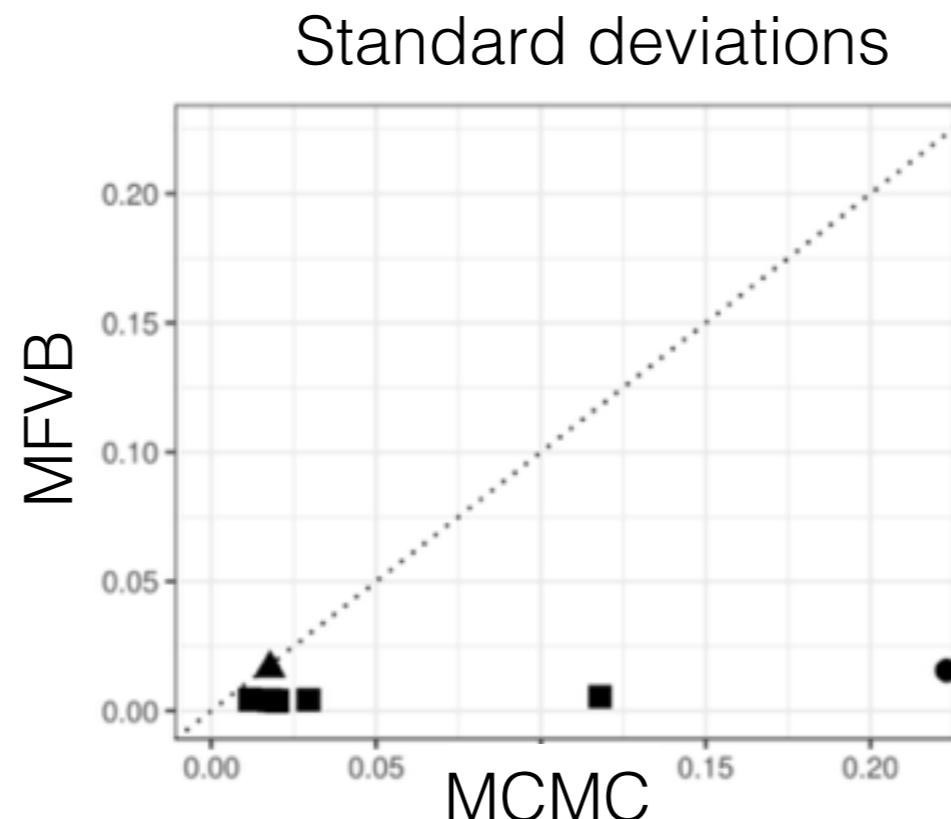


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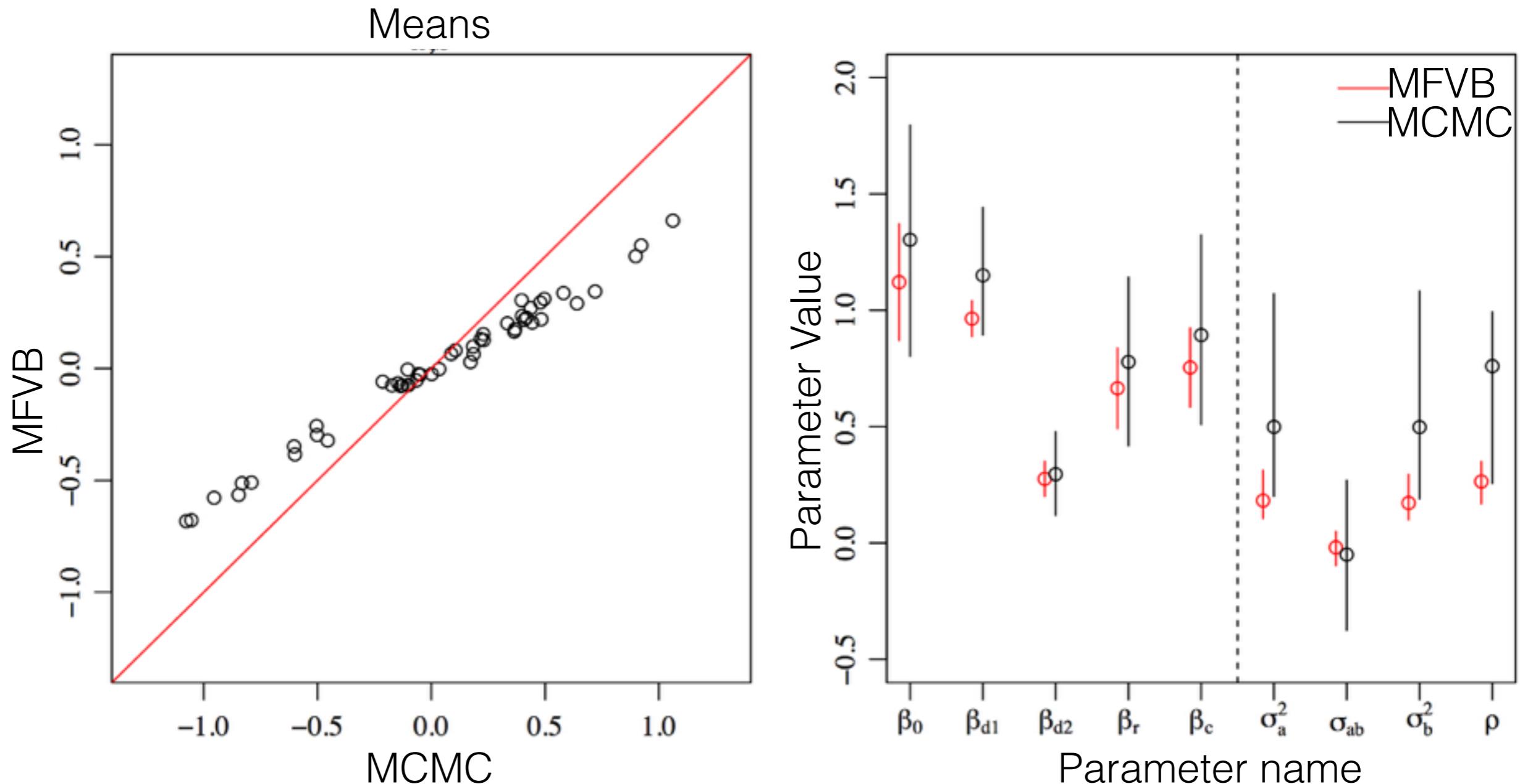


- Criteo
online ads
experiment



What about means?

- Model for relational data with covariates
- When 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

Posterior means: revisited

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

Posterior means: revisited

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Posterior means: revisited

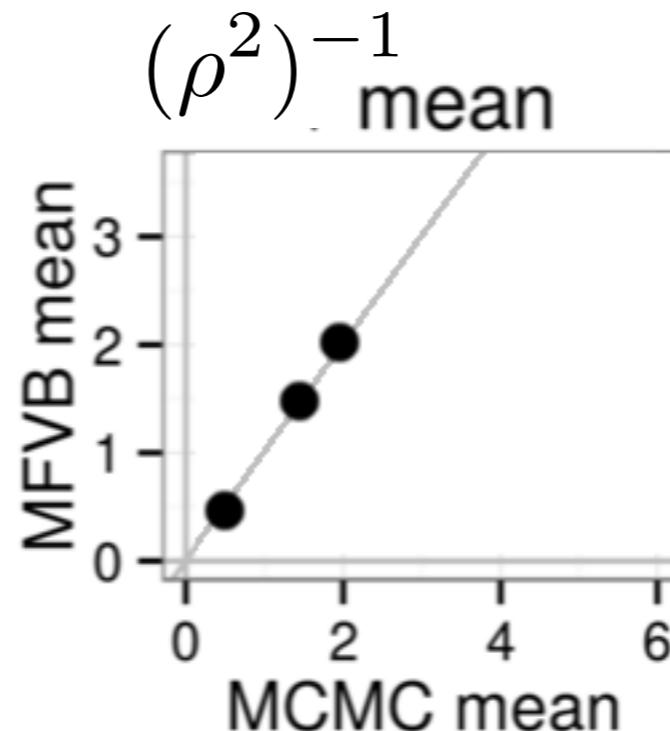
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- Model: $y_n | \beta, z, \sigma^2 \stackrel{\text{indep}}{\sim} \mathcal{N}(\beta^T x_n + z_{k(n)} r_n, \sigma^2)$

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- Collect: regional test scores r_n
- Model:
 $y_n | \beta, z, \sigma^2 \stackrel{\text{indep}}{\sim} \mathcal{N}(\beta^T x_n + z_{k(n)} r_n, \sigma^2)$
 $z_k | \rho^2 \stackrel{iid}{\sim} \mathcal{N}(0, \rho^2) \quad (\sigma^2)^{-1} \sim \text{Gamma}(a_{\sigma^2}, b_{\sigma^2})$
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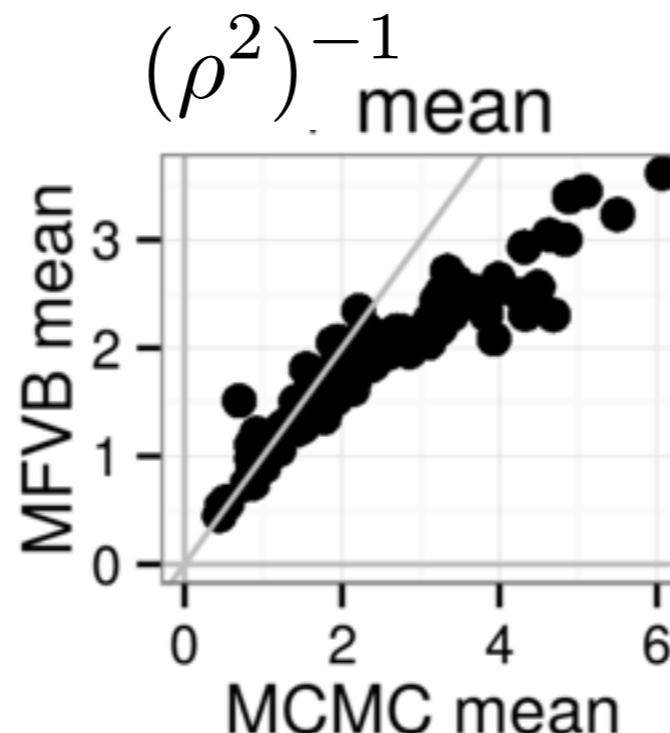
Posterior means: revisited

- Want to predict college GPA y_n
- Collect: standardized test scores (e.g., SAT, ACT) x_n
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- Data simulated from model (3 data sets, 300 data points):



Posterior means: revisited

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 $\beta \sim \mathcal{N}(0, \Sigma)$ $(\rho^2)^{-1} \sim \text{Gamma}(a_{\rho^2}, b_{\rho^2})$
- Data simulated from model (100 data sets, 300 data points):



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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What can we do?

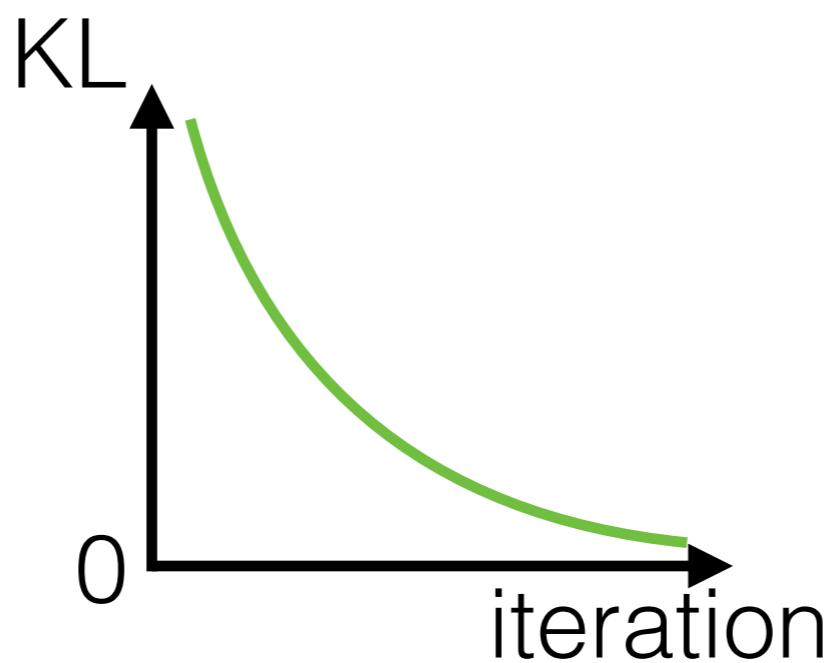
- Reliable diagnostics

What can we do?

- Reliable diagnostics
 - KL vs ELBO

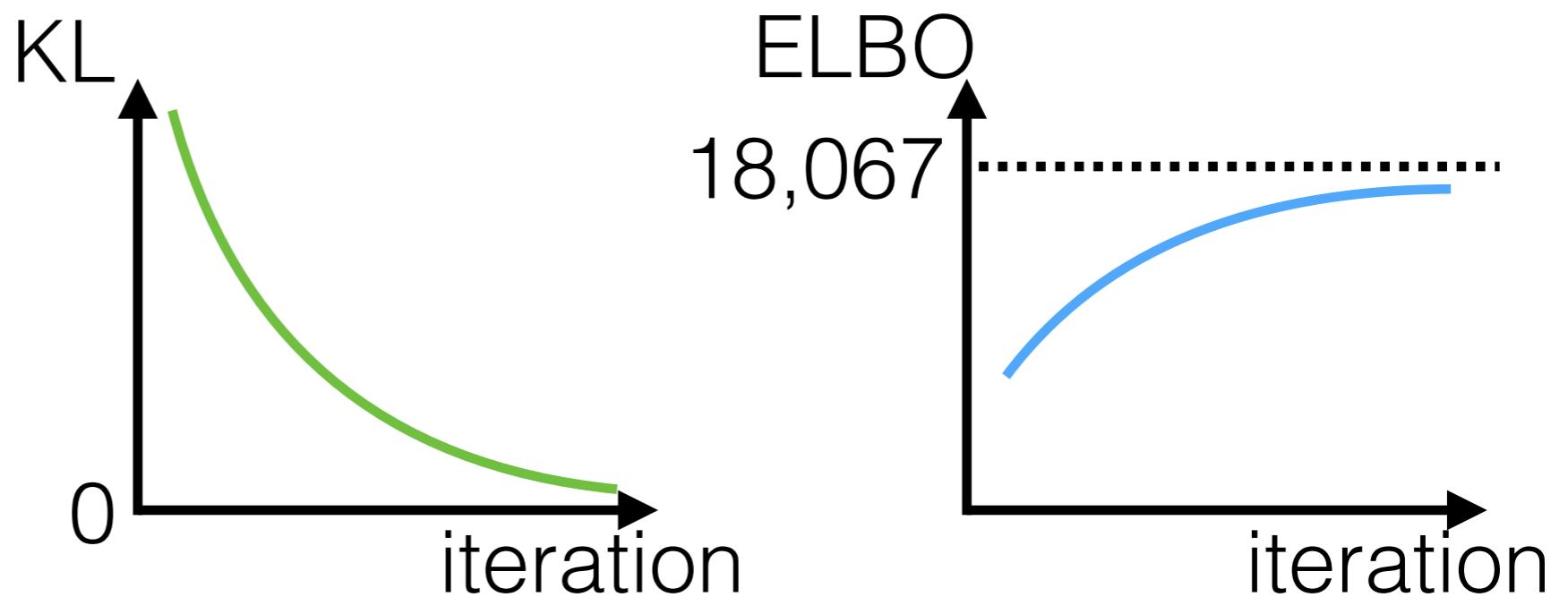
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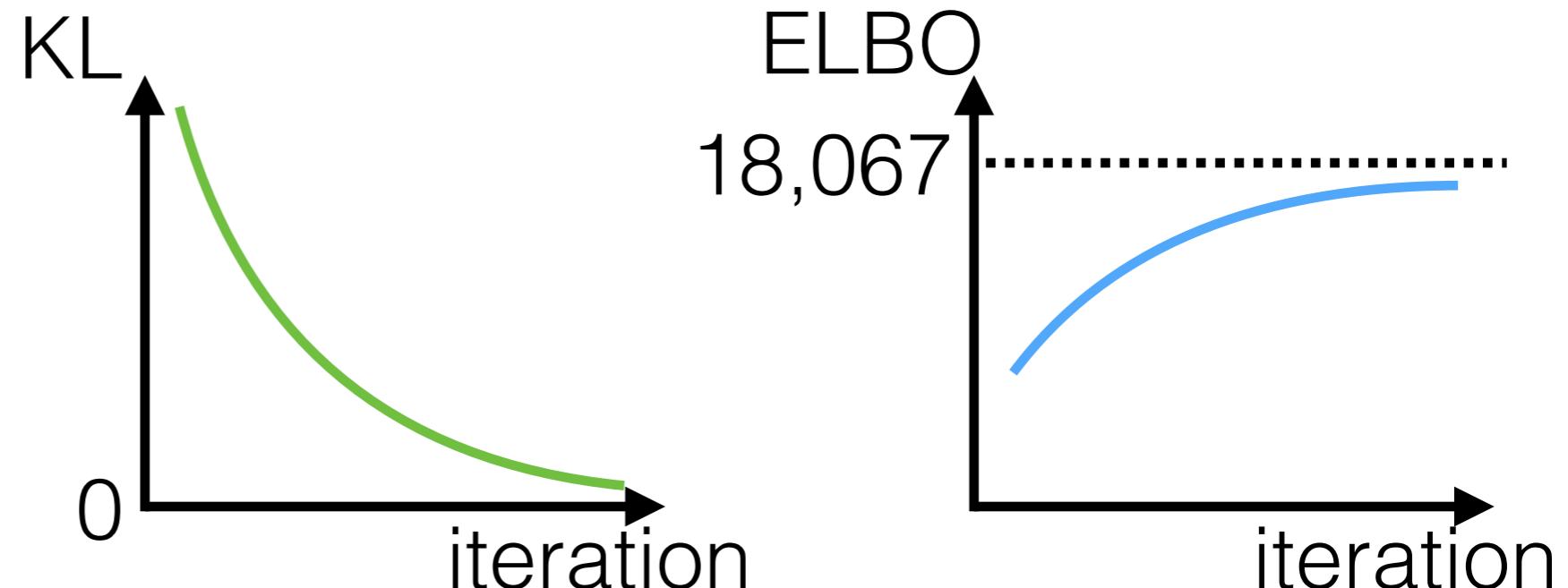
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[Gorham, Mackey 2015, 2017; Chwialkowski, Strathmann, Gretton 2016; Jitkrittum et al 2017; Talts et al 2018; Yao et al 2018, etc.]

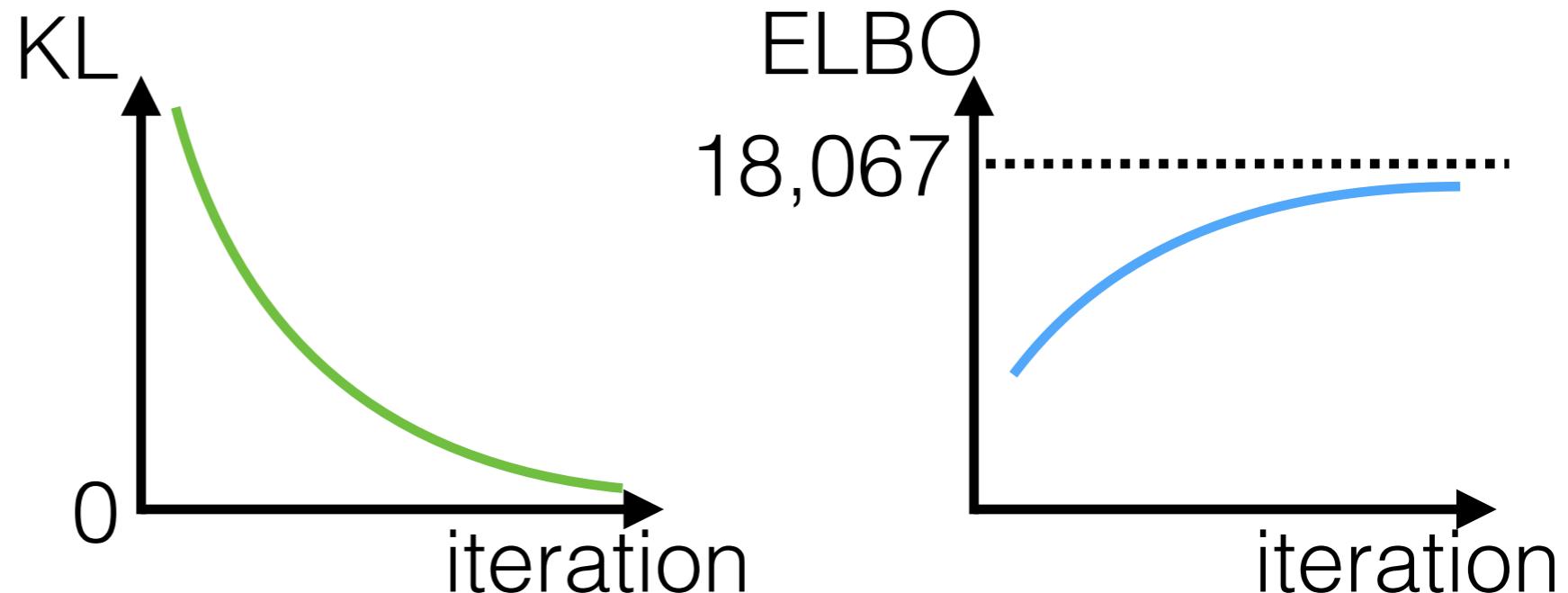


→ “Yes, but did it work? Evaluating variational inference” ICML 2018

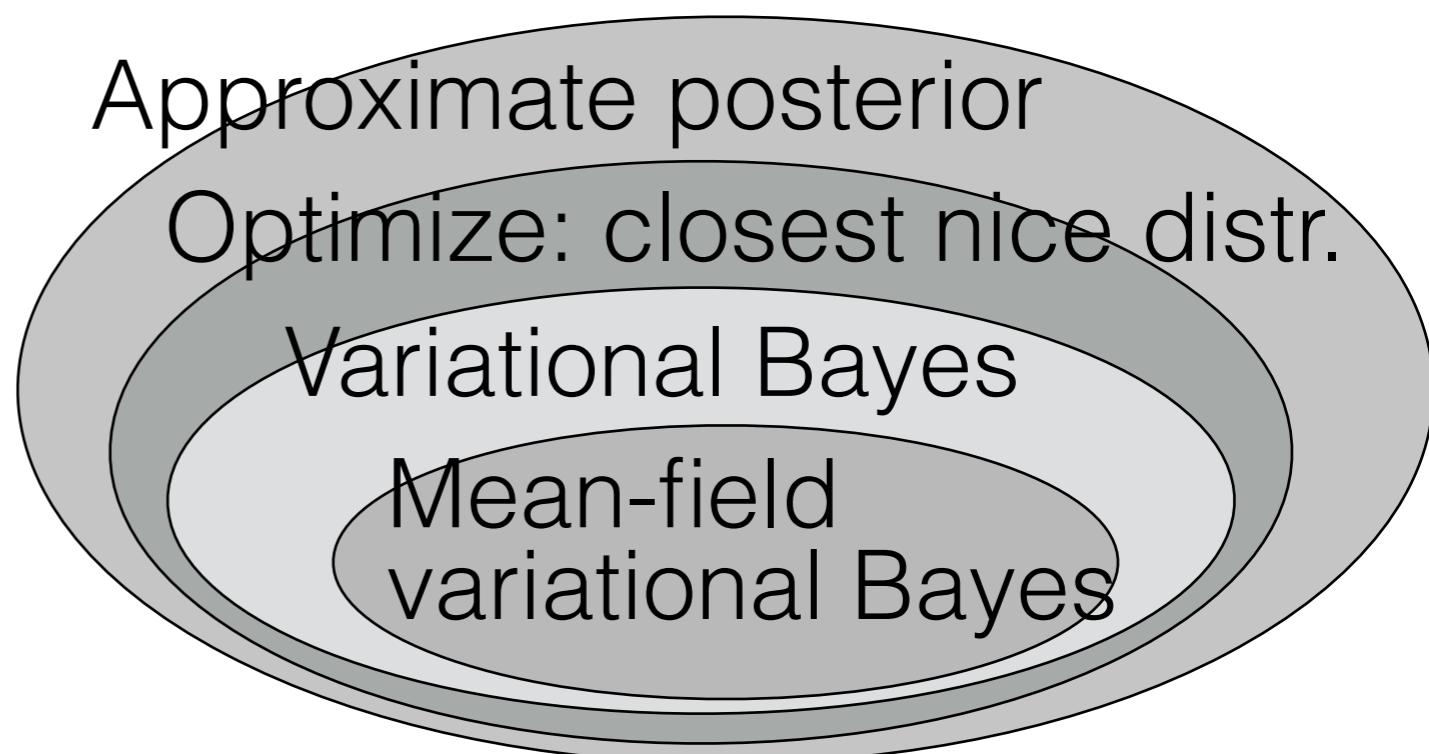
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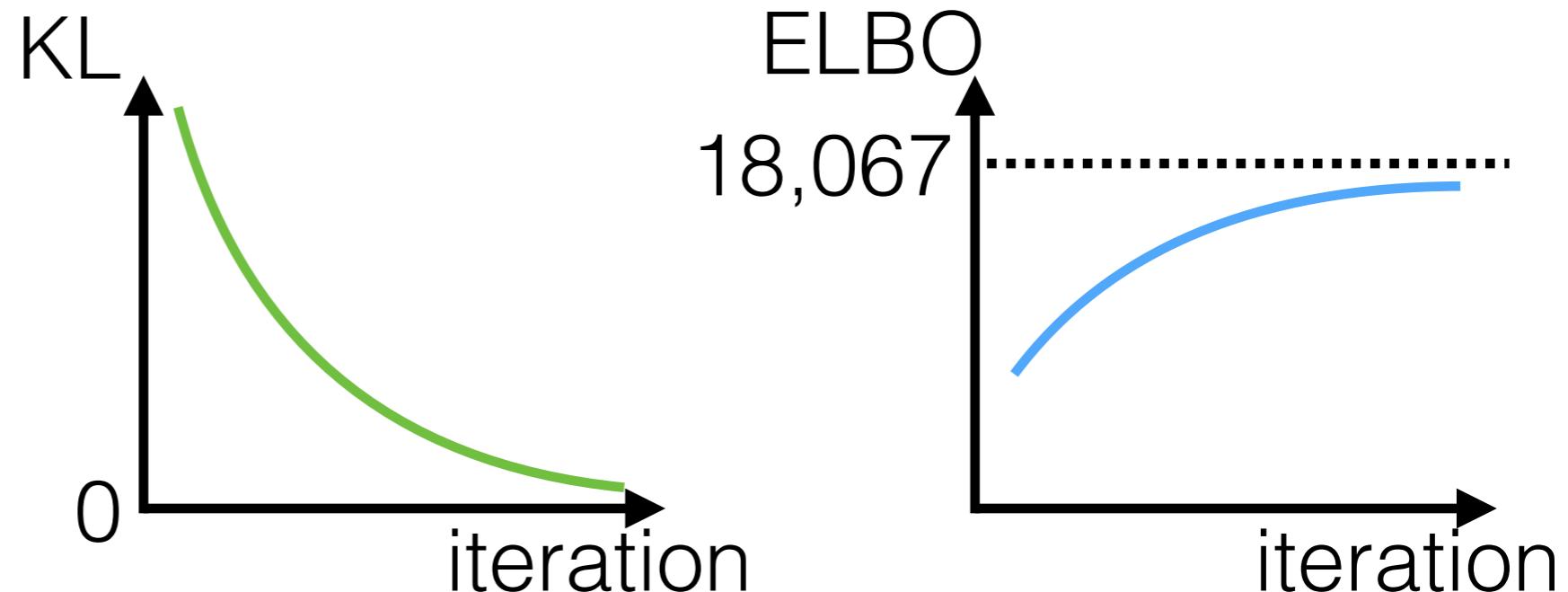
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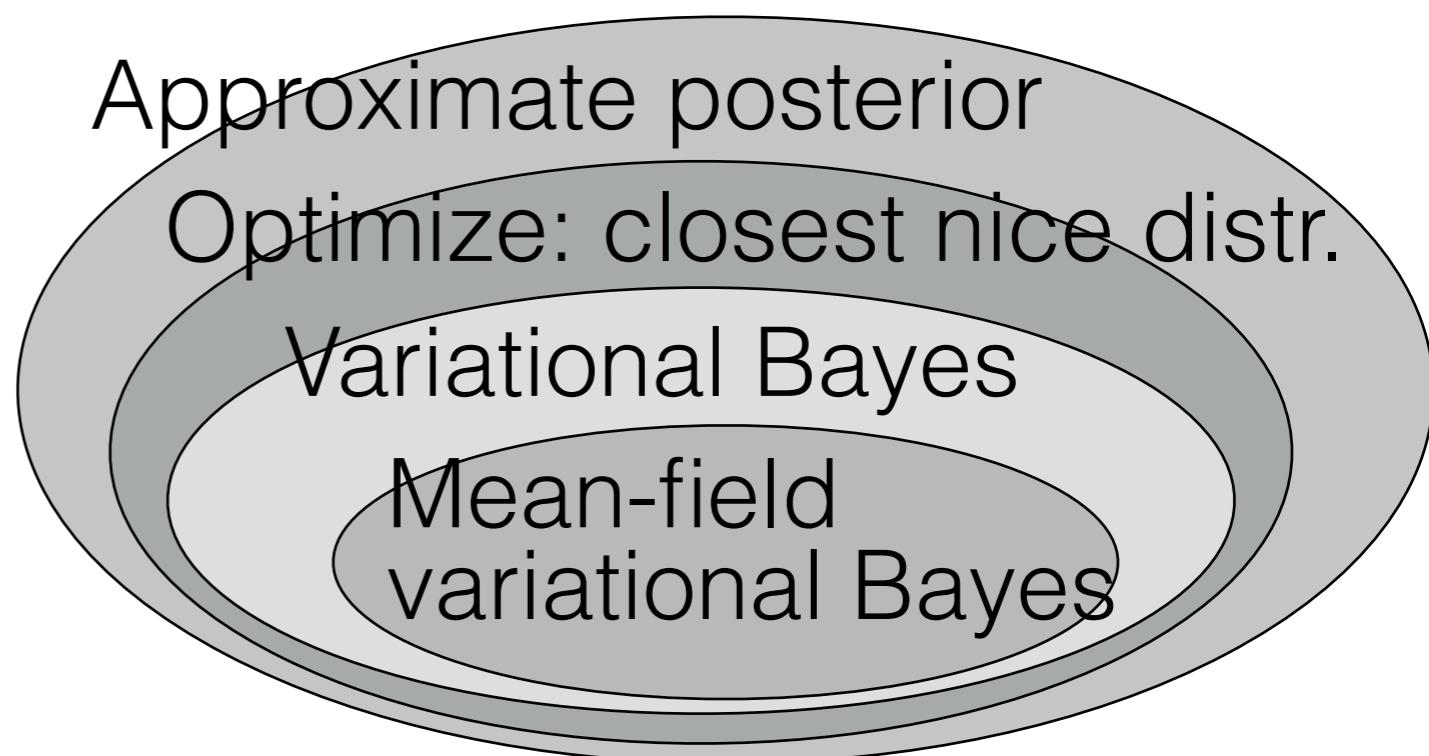
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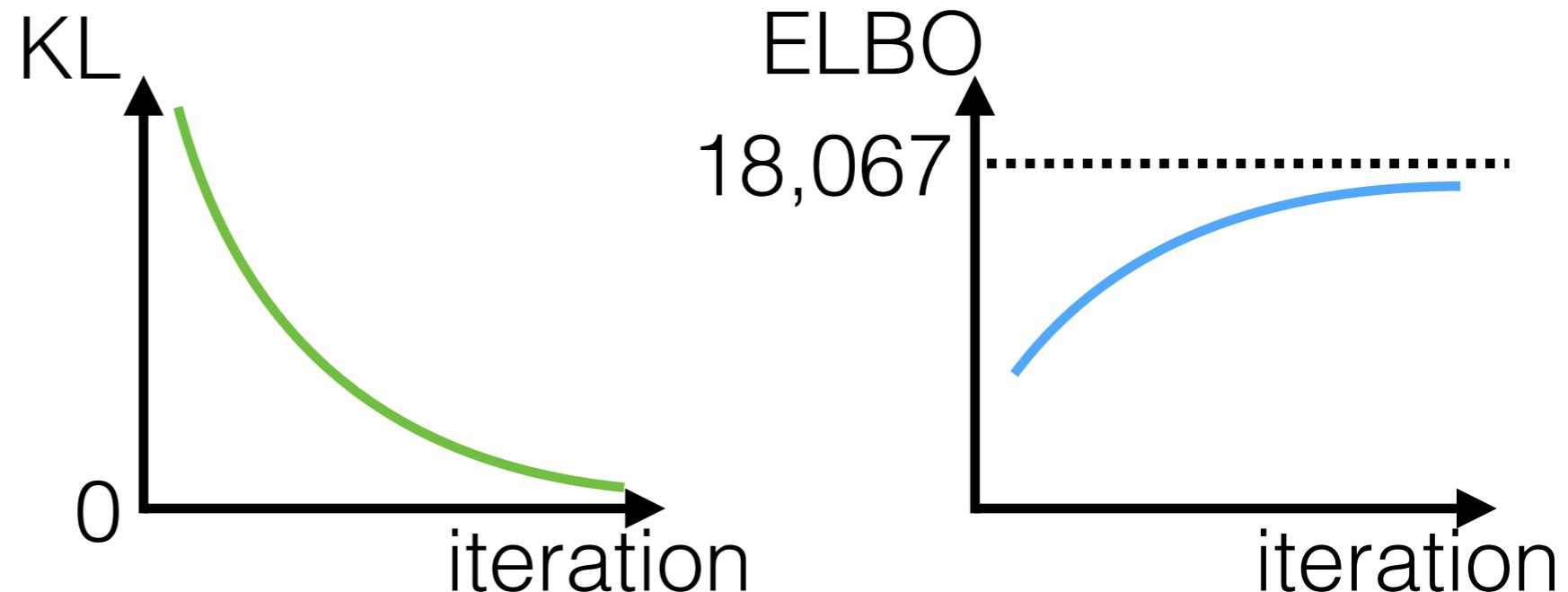
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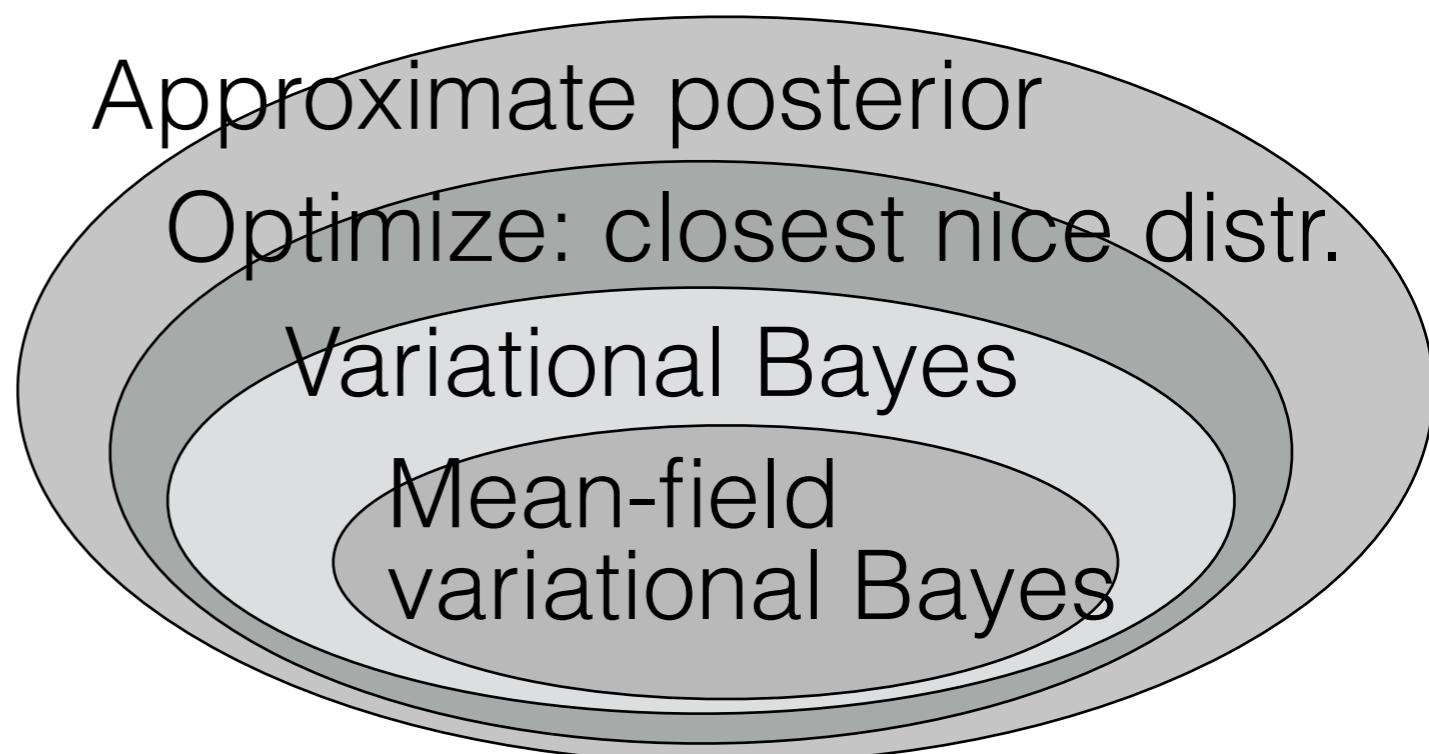
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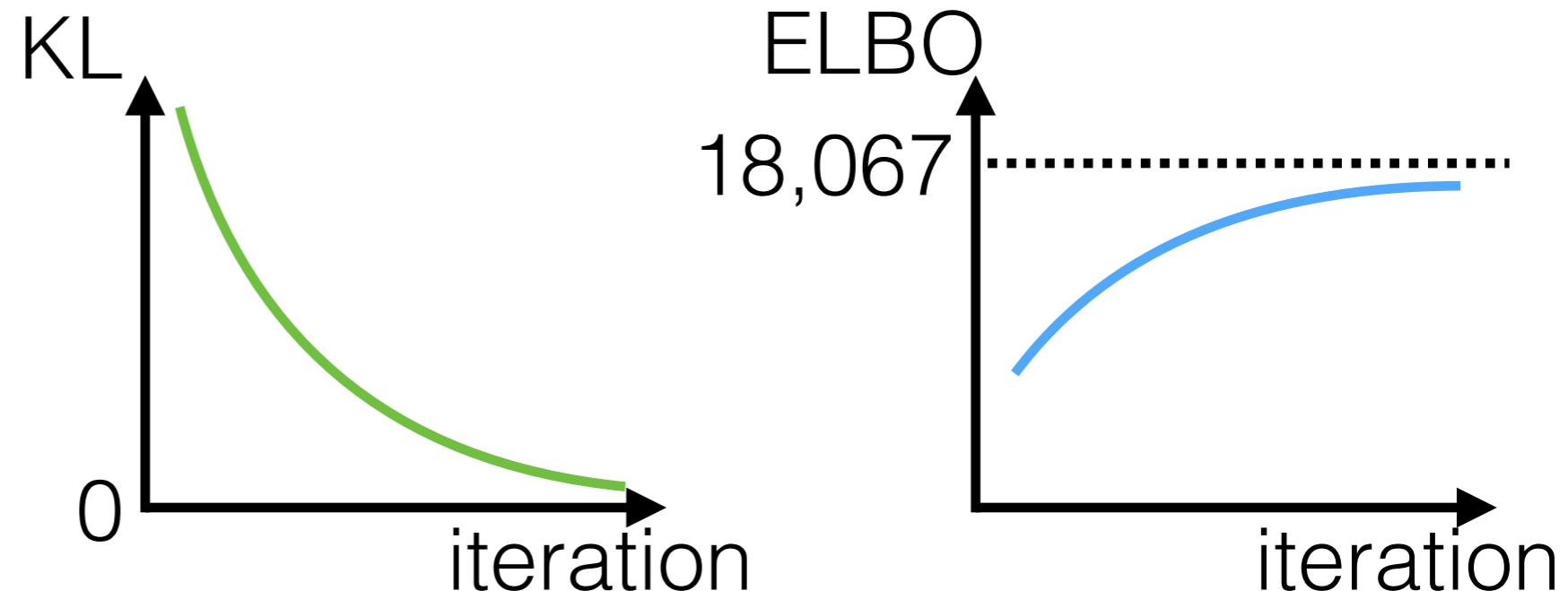
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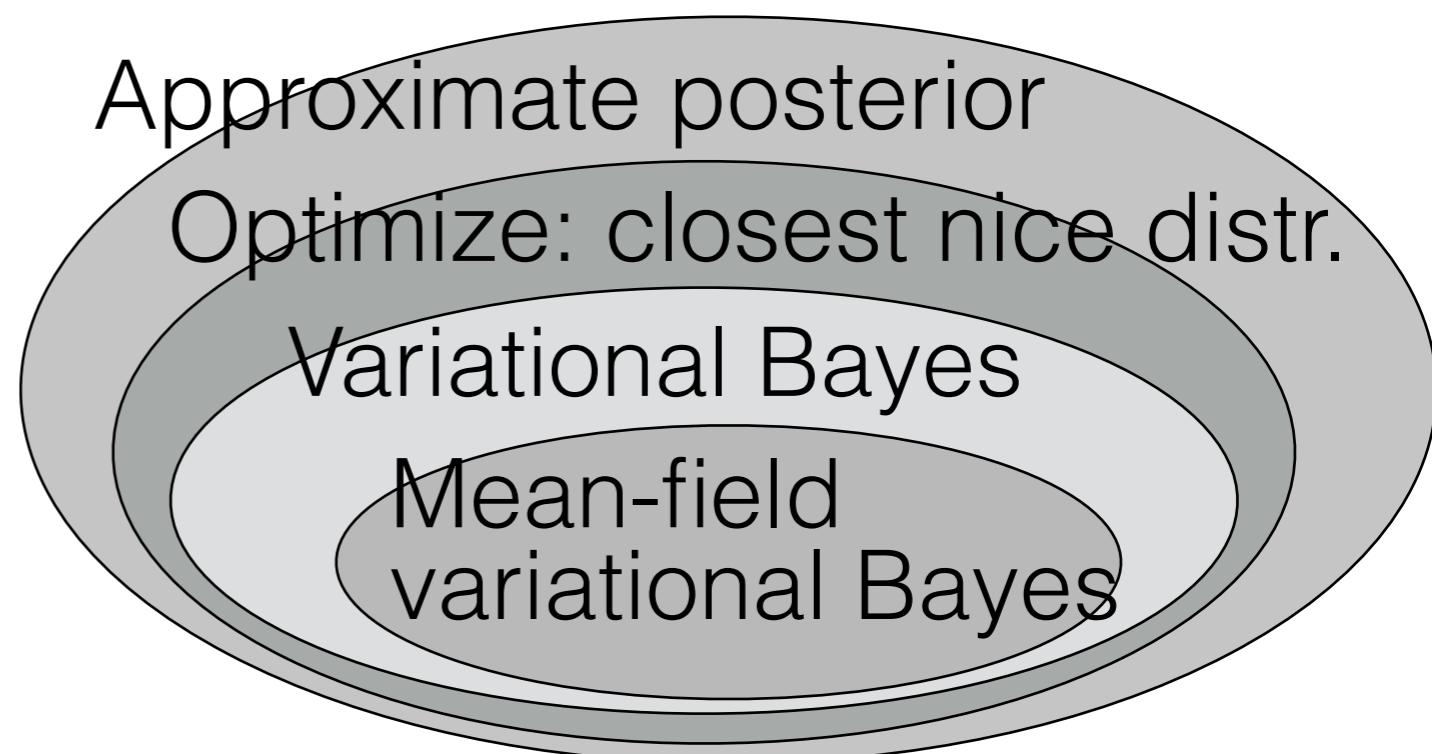
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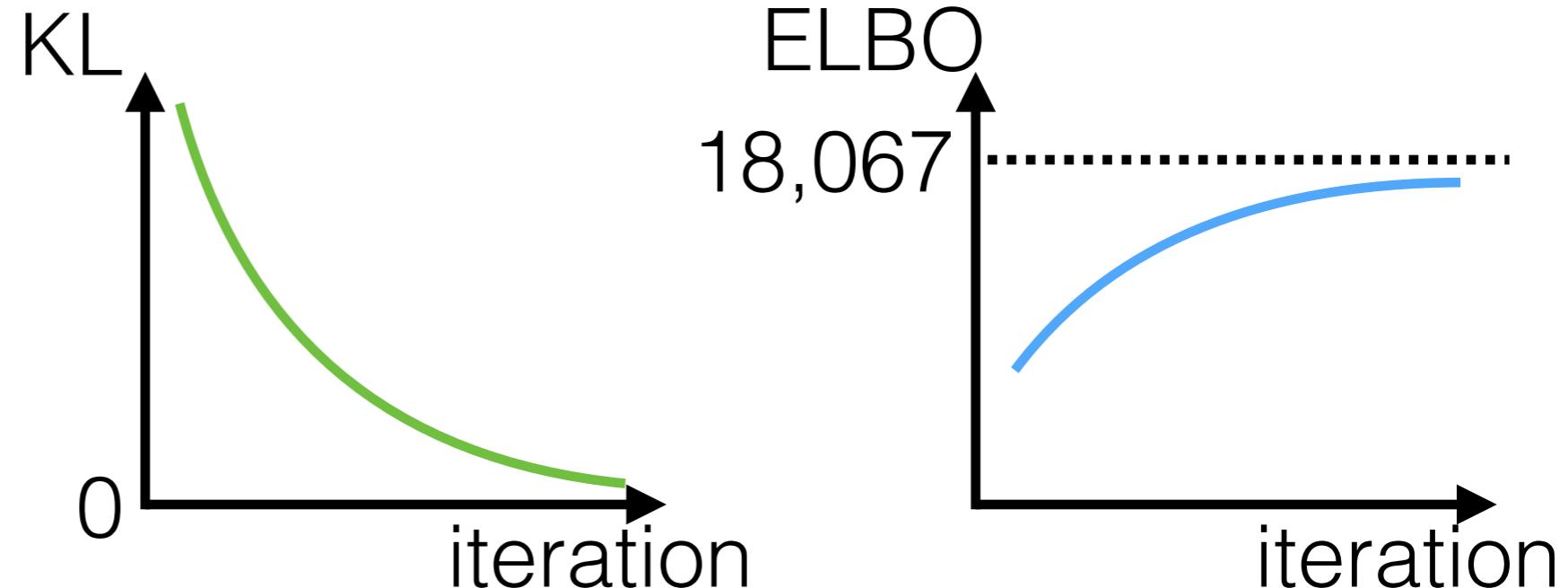
[Huggins, Kasprzak, Campbell, Broderick, 2018]



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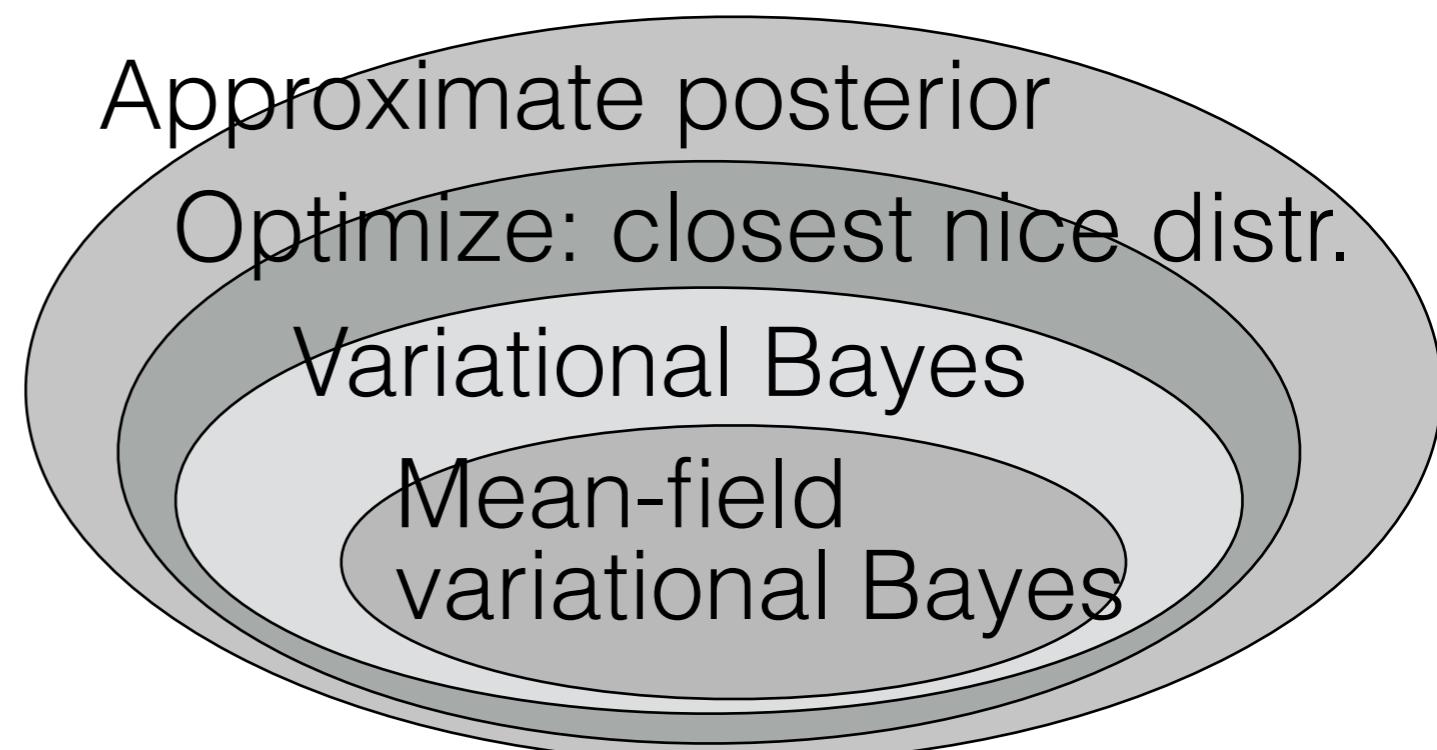
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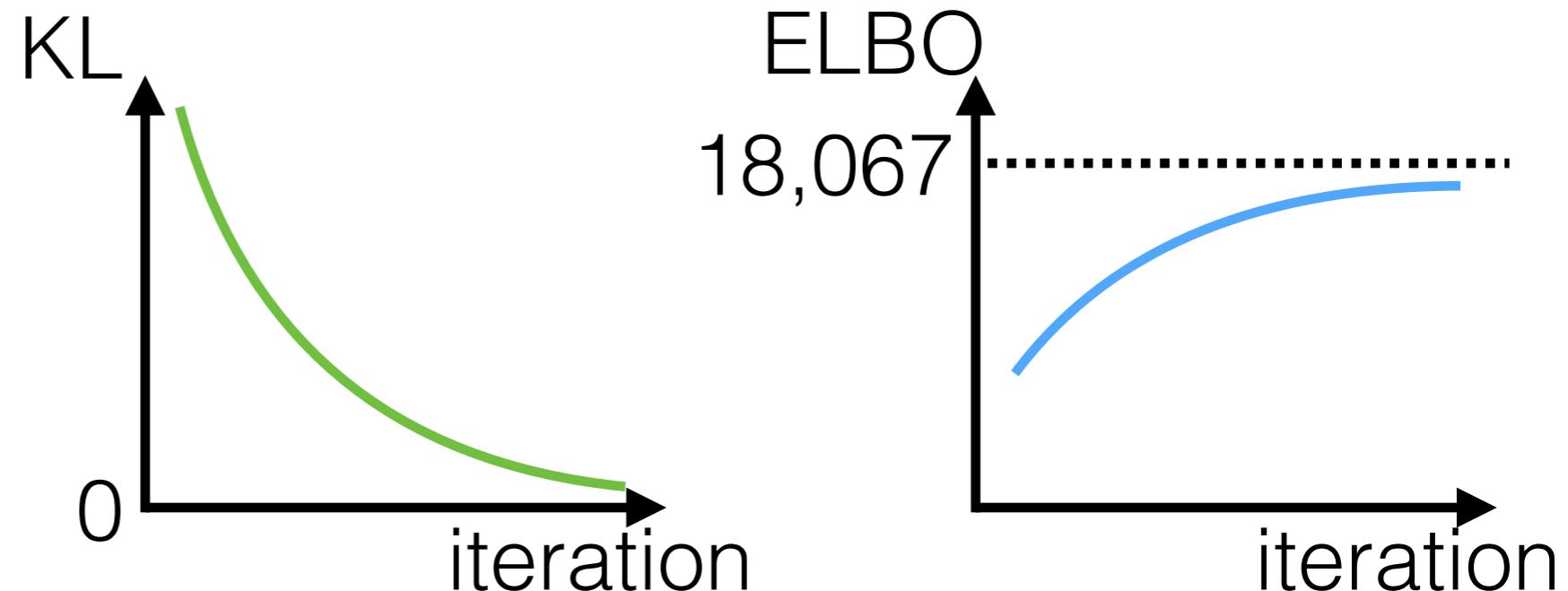
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 - Corrections [next]



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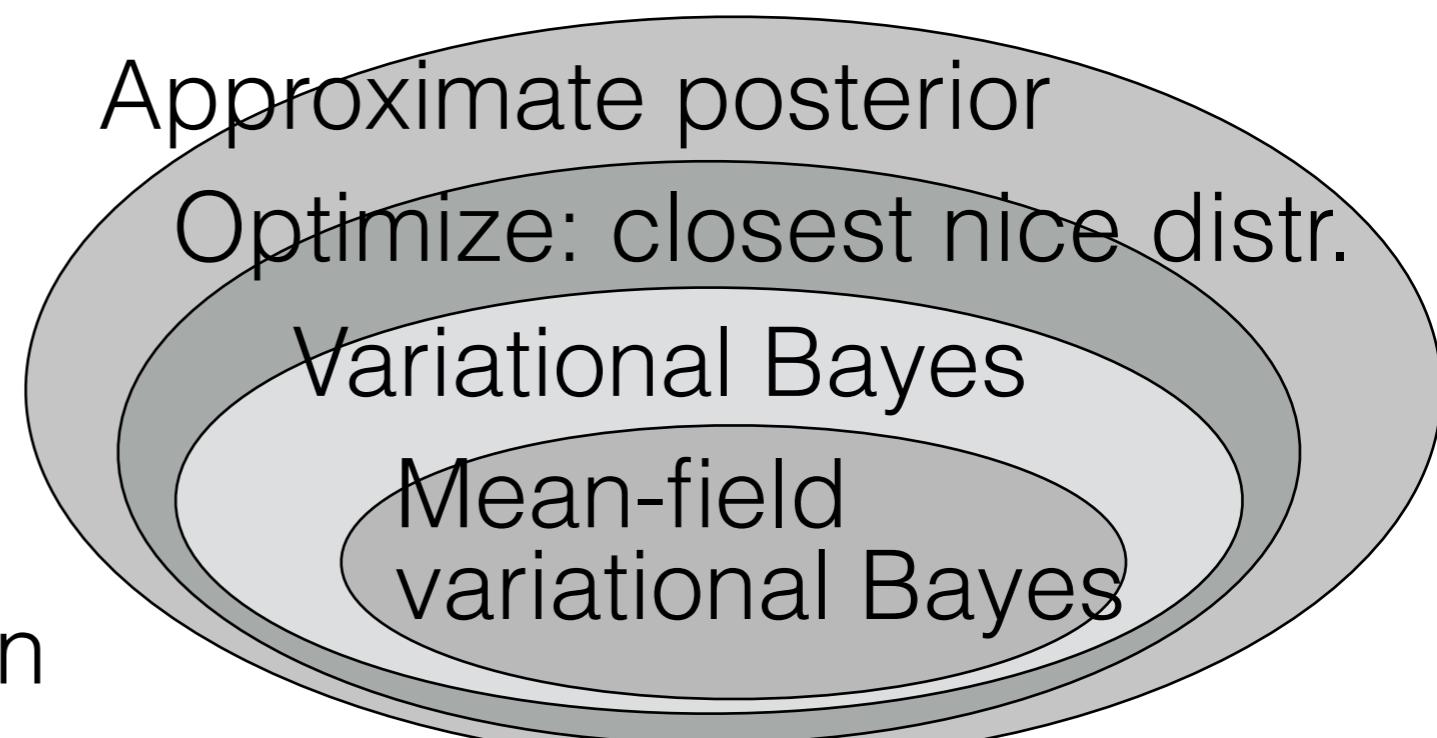
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[Turner, Sahani 2011]
[Huggins, Kasprzak, Campbell, Broderick, 2018]
 - Corrections [next]
 - Theoretical guarantees on finite-data quality [next]



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.
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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. *Journal of Machine Learning Research*, to appear. ArXiv:1709.02536.
- J Huggins, T Campbell, M Kasprzak, T Broderick. Practical bounds on the error of Bayesian posterior approximations: A nonasymptotic approach, 2018. ArXiv: 1809.09505.

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- MD Hoffman, DM Blei, C Wang, and J Paisley. "Stochastic variational inference." *The Journal of Machine Learning Research* 14.1 (2013): 1303-1347.
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- JH Huggins, RP Adams, and T Broderick. PASS-GLM: Polynomial approximate sufficient statistics for scalable Bayesian GLM inference. *NIPS* 2017.
- J Huggins, T Campbell, M Kasprzak, T Broderick. Practical bounds on the error of Bayesian posterior approximations: A nonasymptotic approach, 2018. ArXiv:1809.09505.
- A Kucukelbir, R Ranganath, A Gelman, and D Blei. "Automatic variational inference in Stan." *NIPS* 2015.
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