

Part III: Variational Bayes and beyond

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MIT

Bayesian inference

- Analysis goals: Point estimates, coherent uncertainties



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

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]

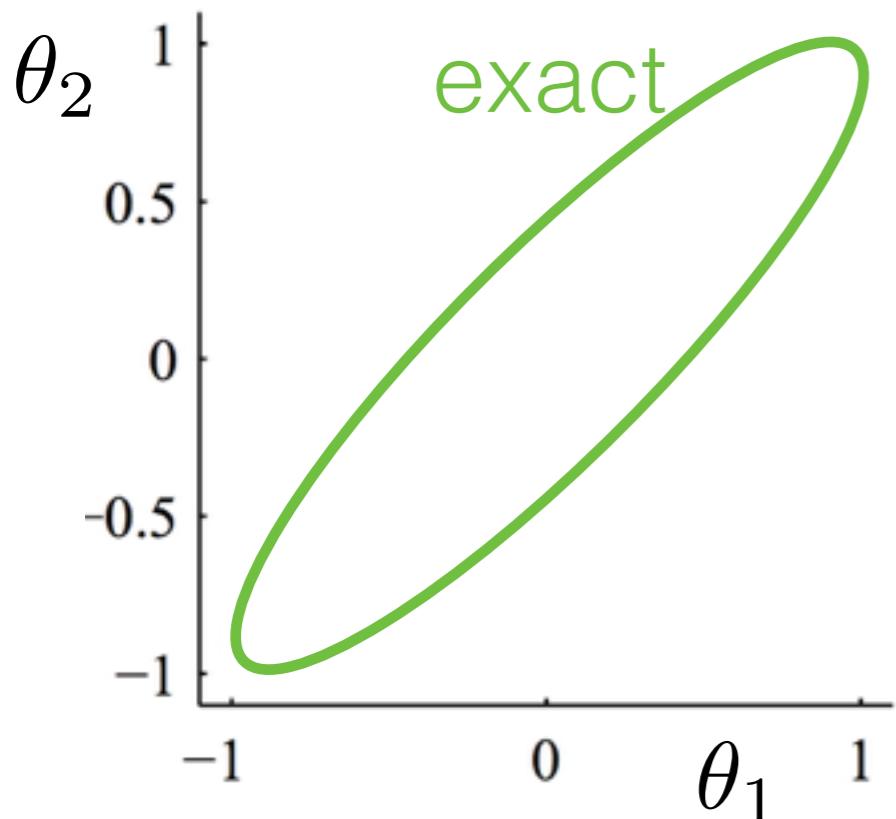
What about uncertainty?

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

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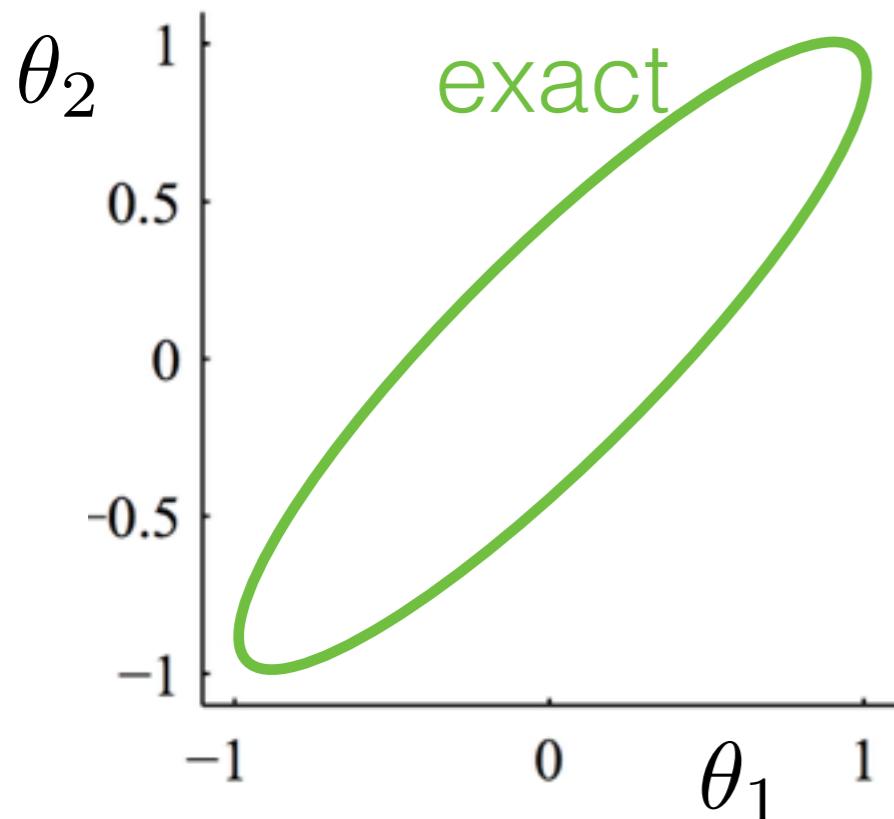


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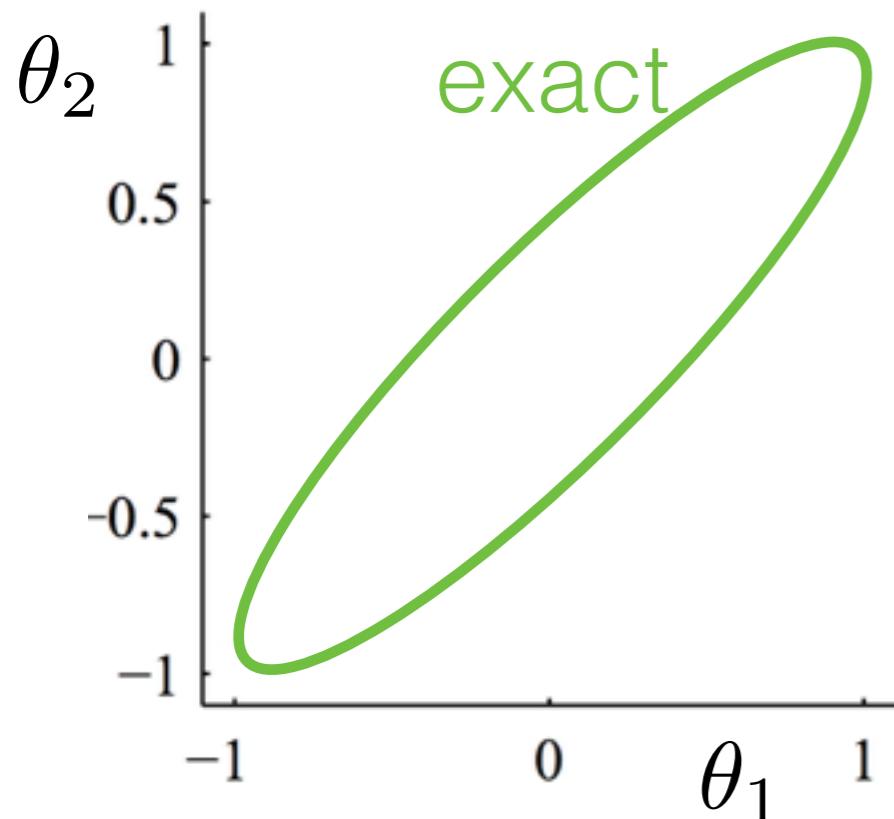
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- Conjugate linear regression

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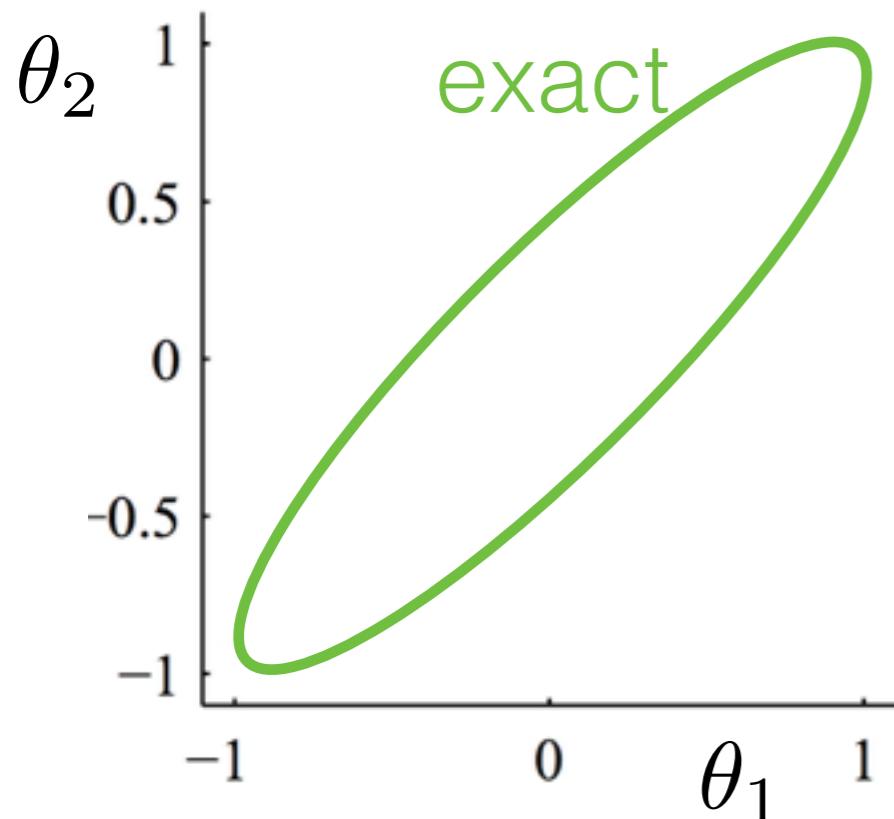
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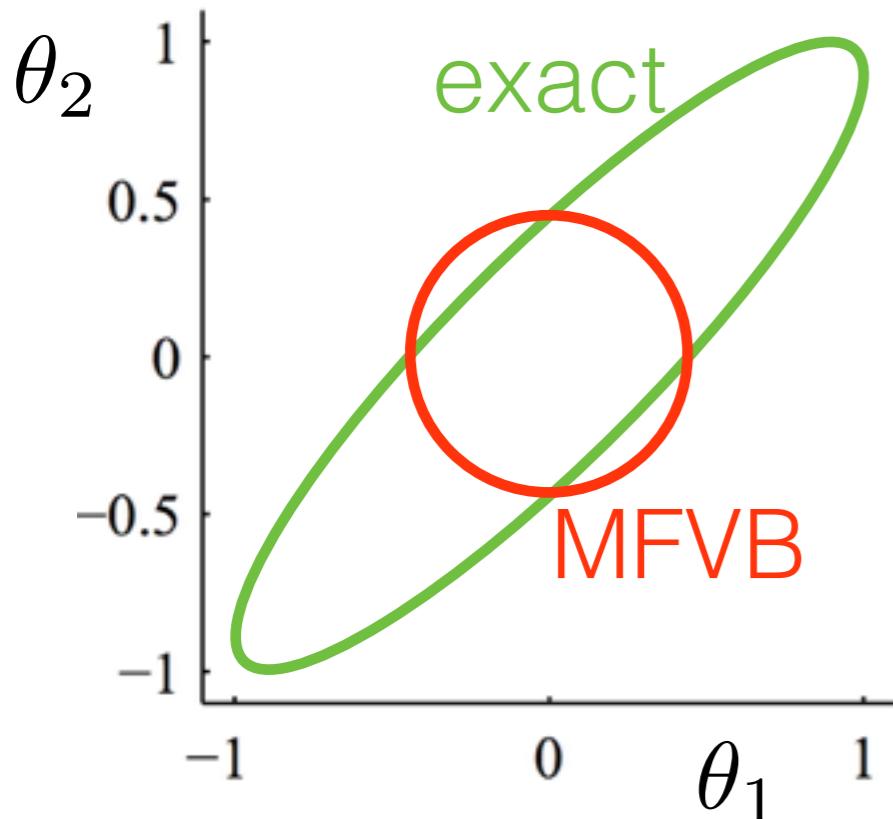
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[board]

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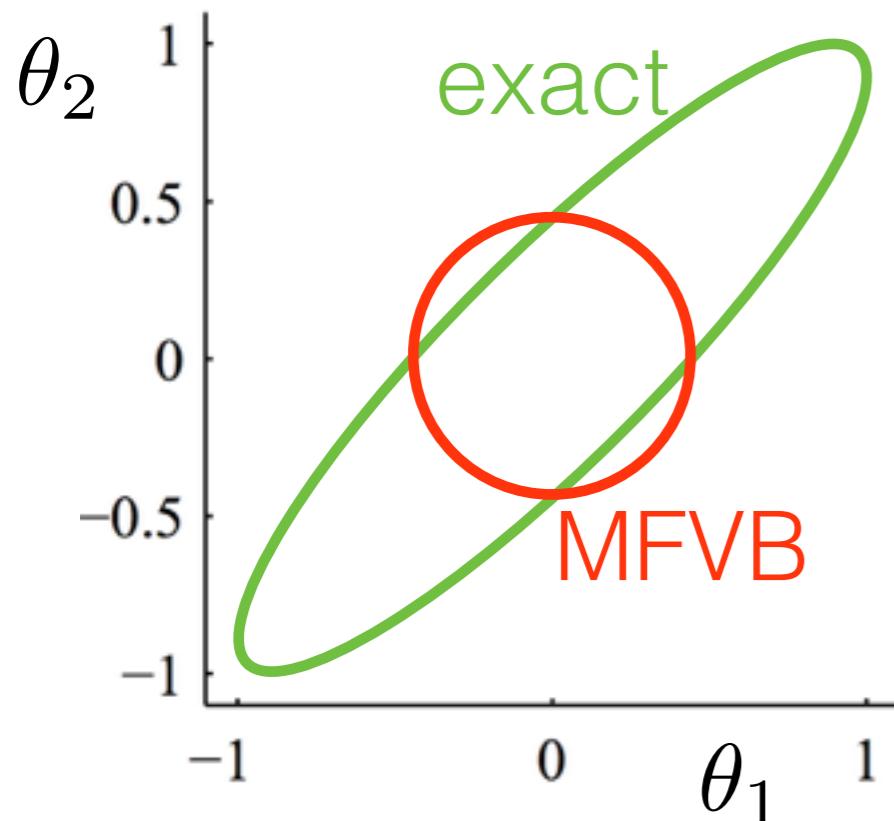
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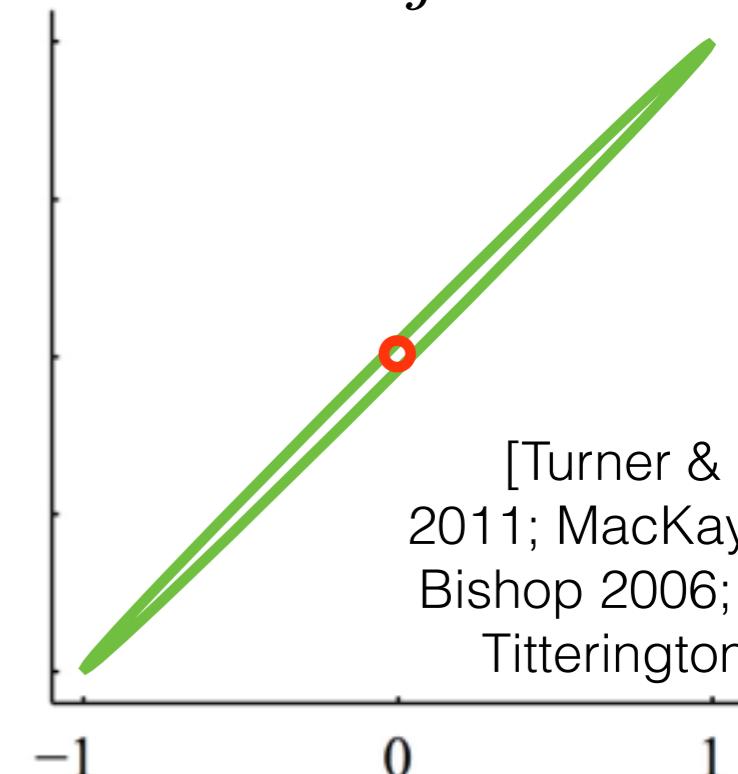
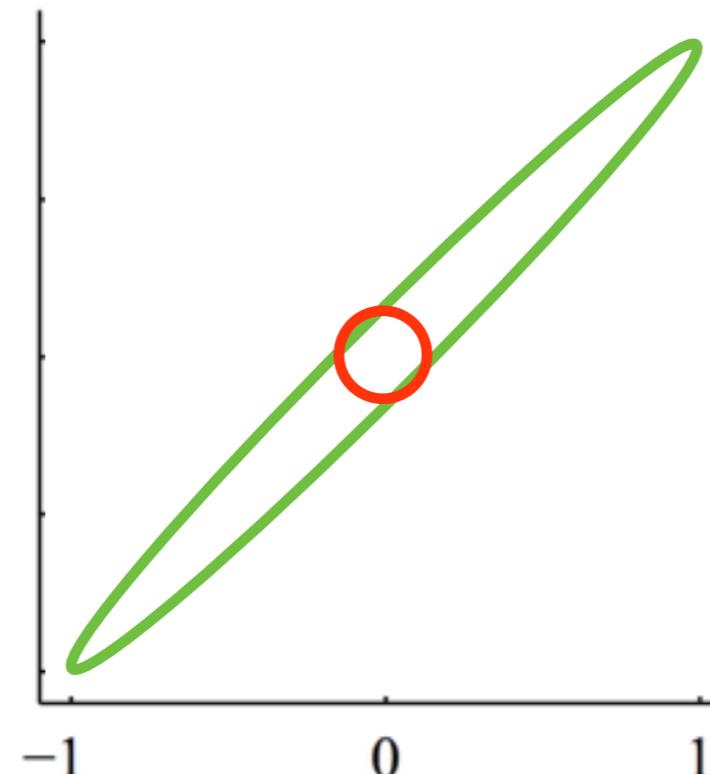
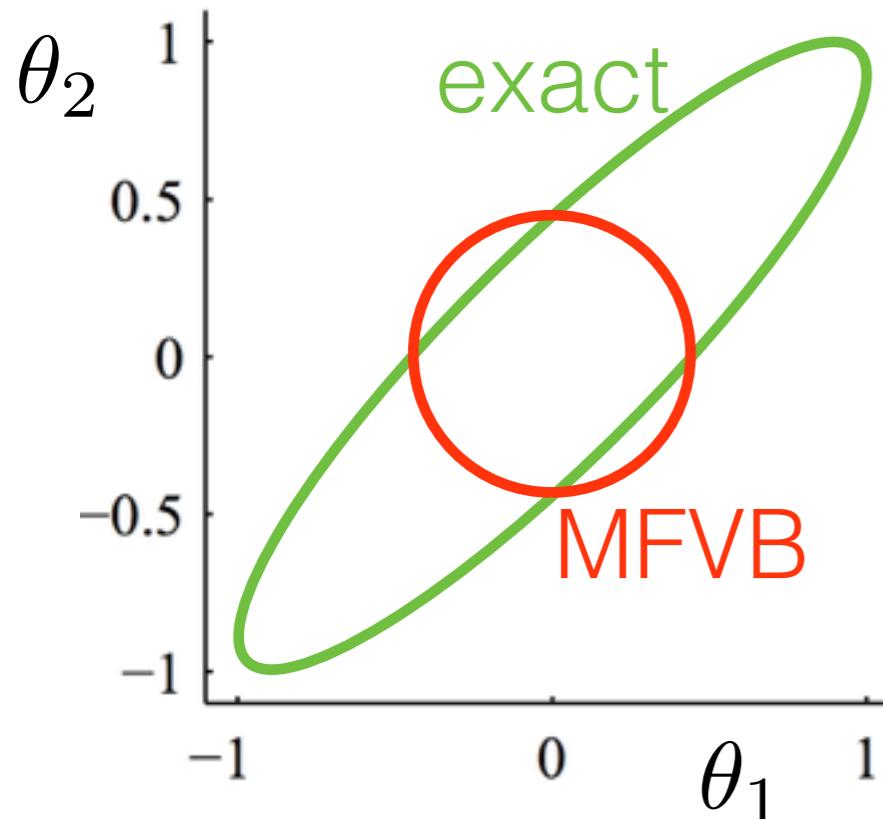
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- Underestimates variance (sometimes severely)
- Conjugate linear regression
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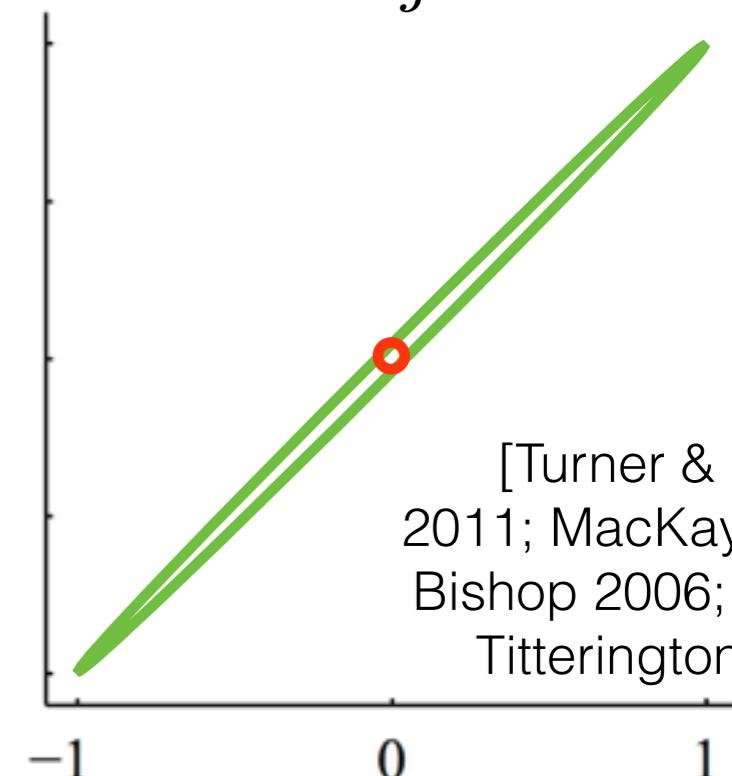
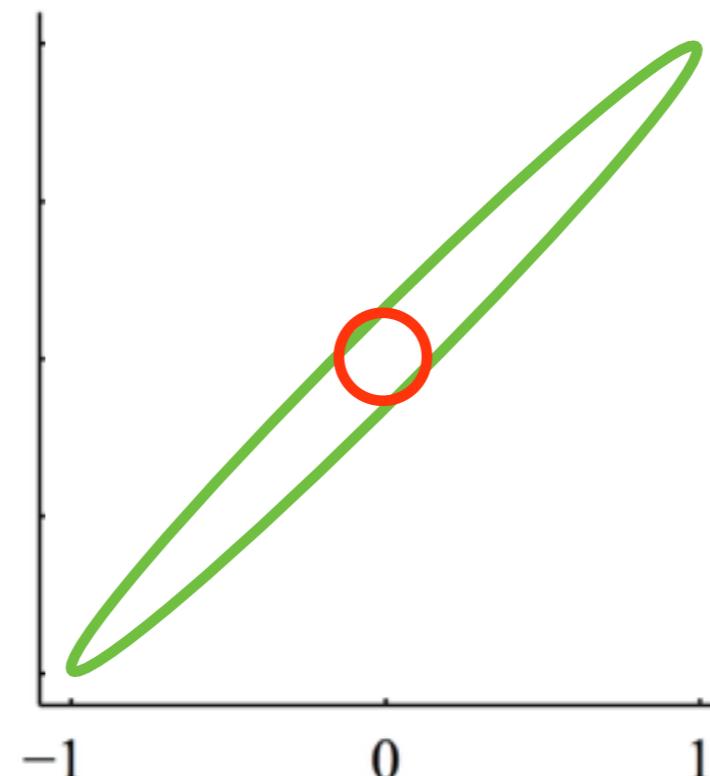
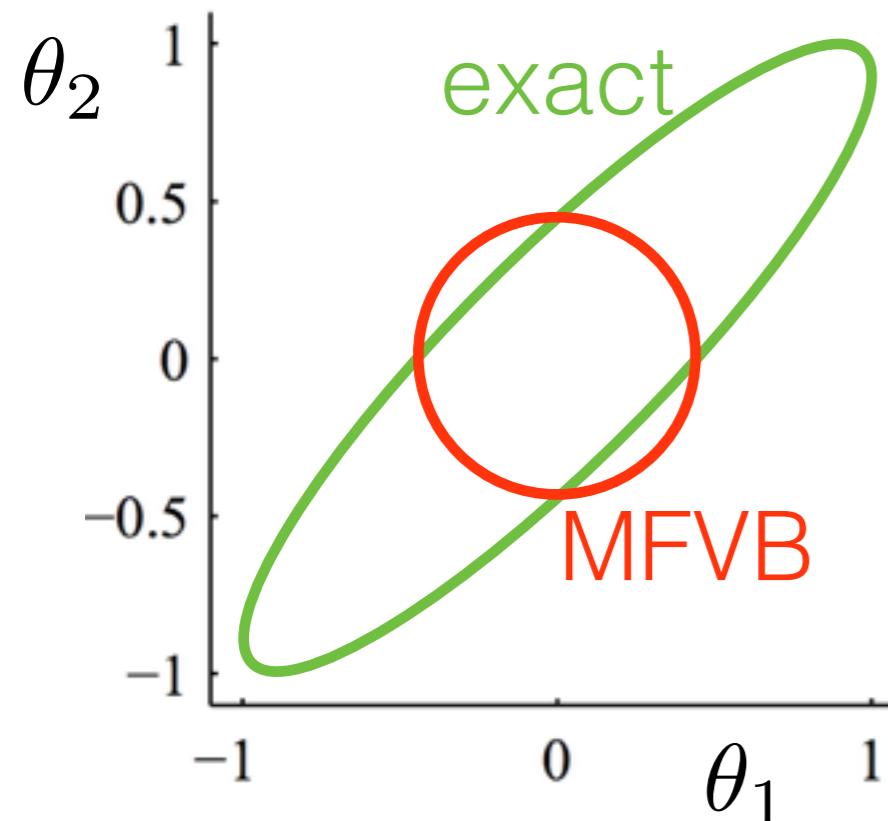


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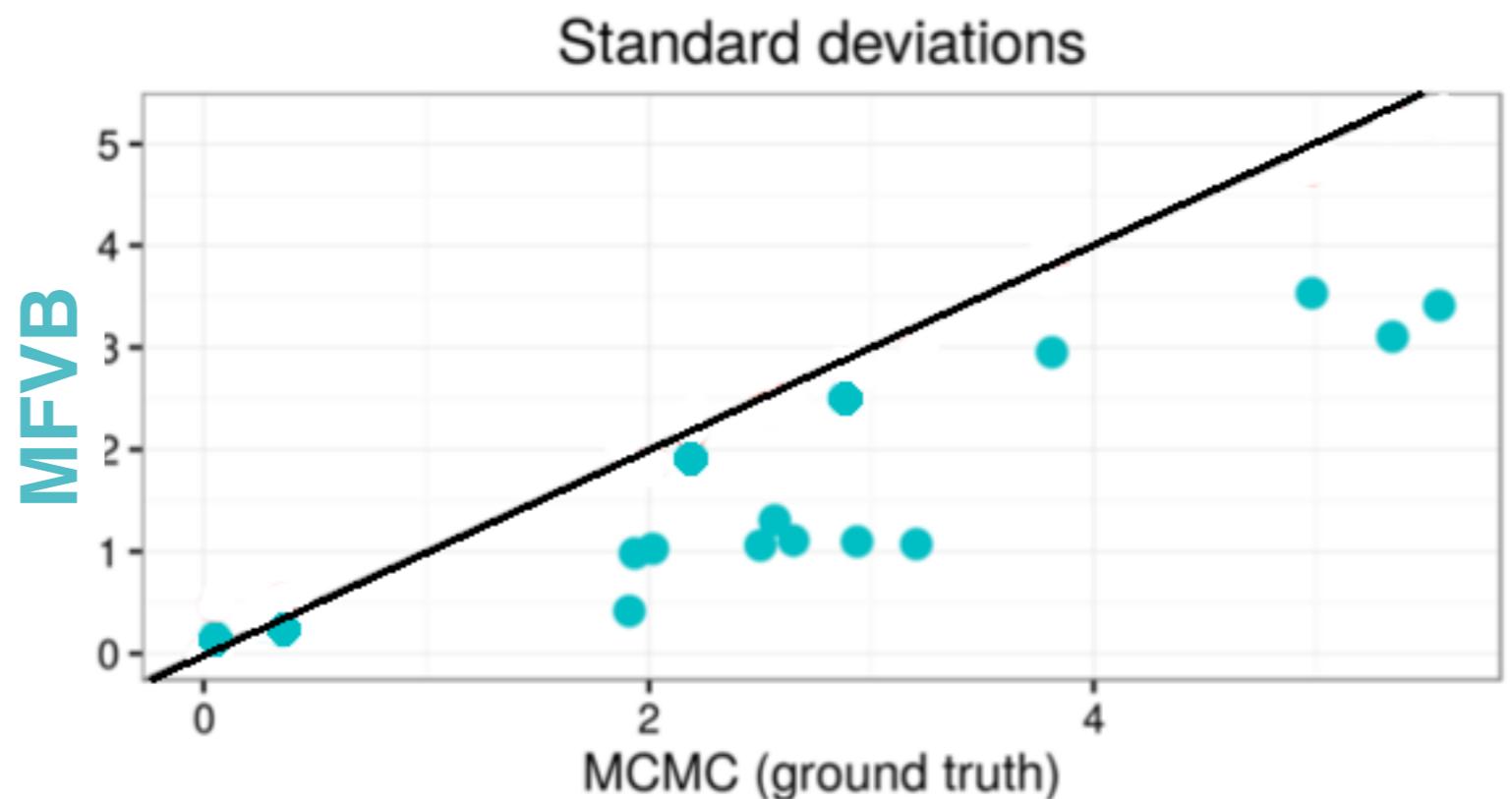
- Underestimates variance (sometimes severely)
- No covariance estimates
- Conjugate linear regression
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What about uncertainty?

- Microcredit

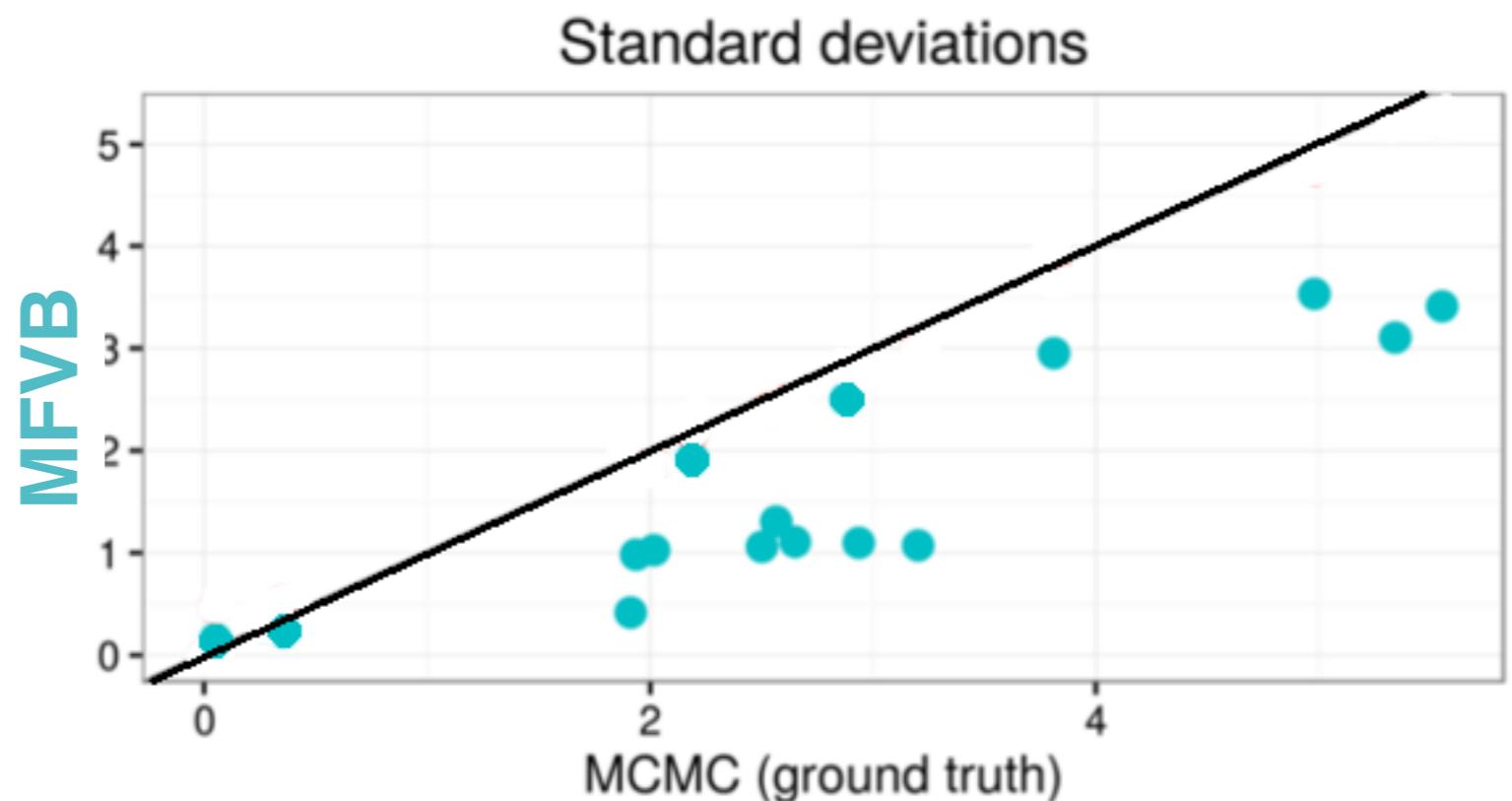
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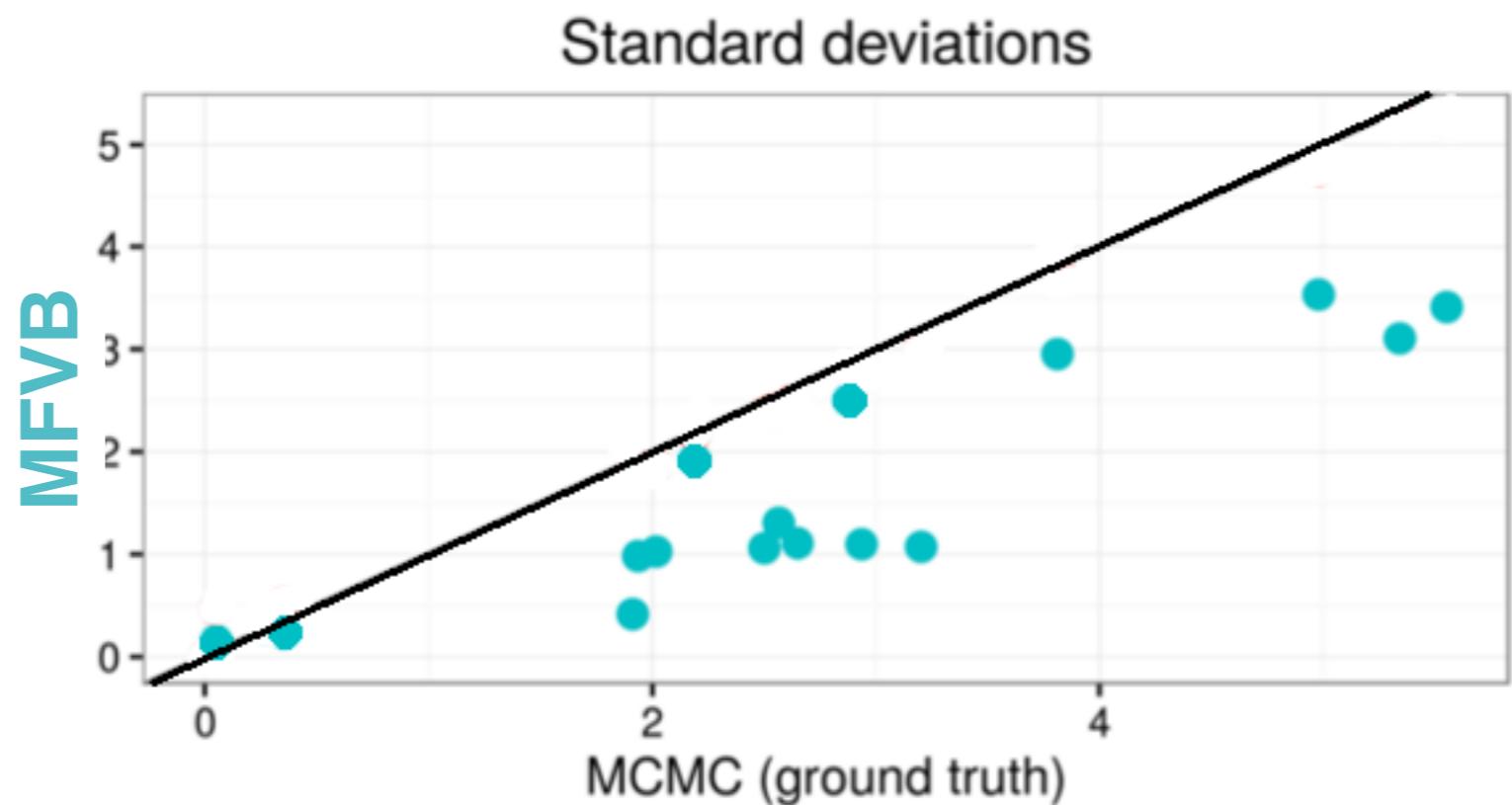
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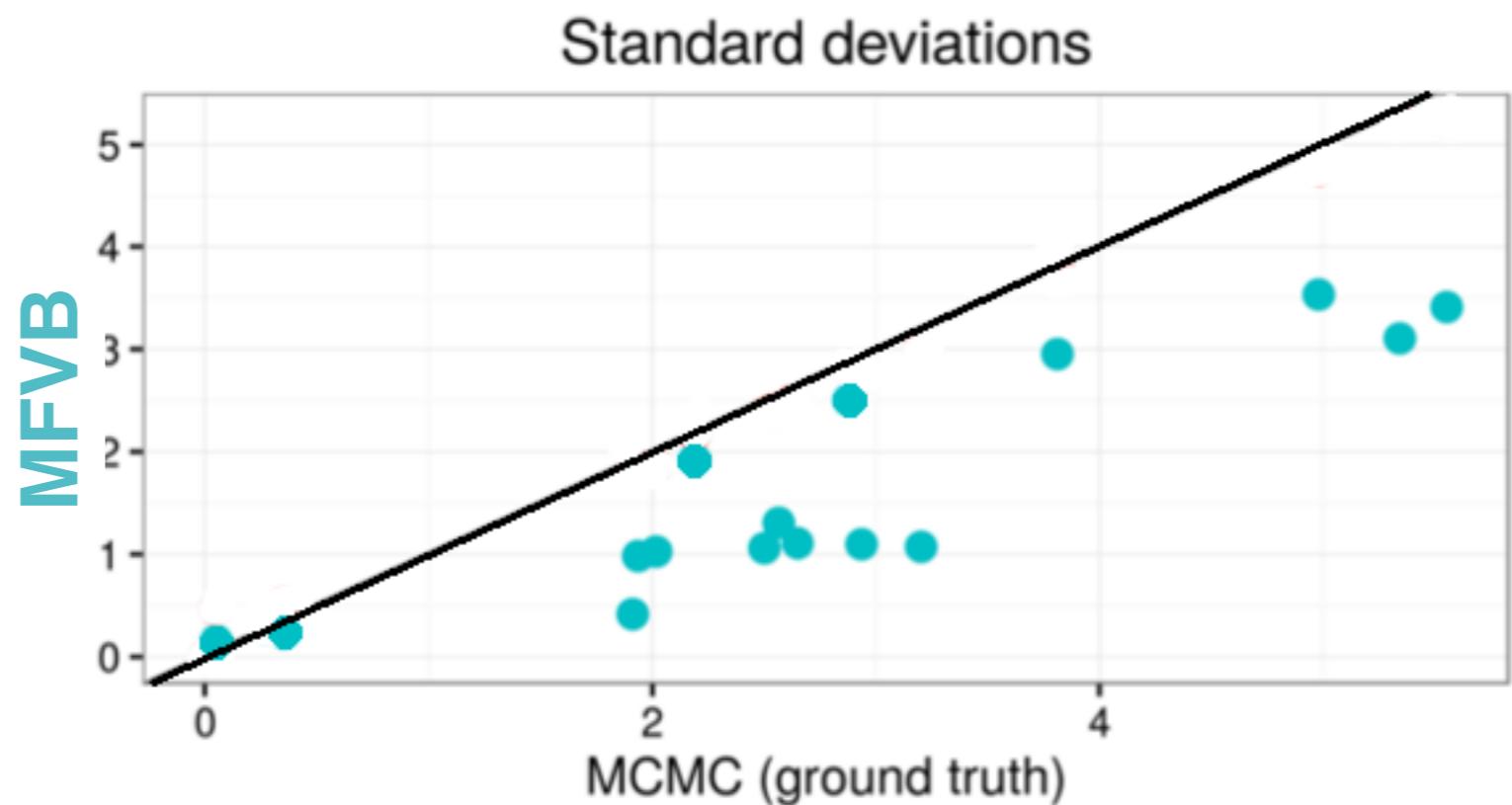
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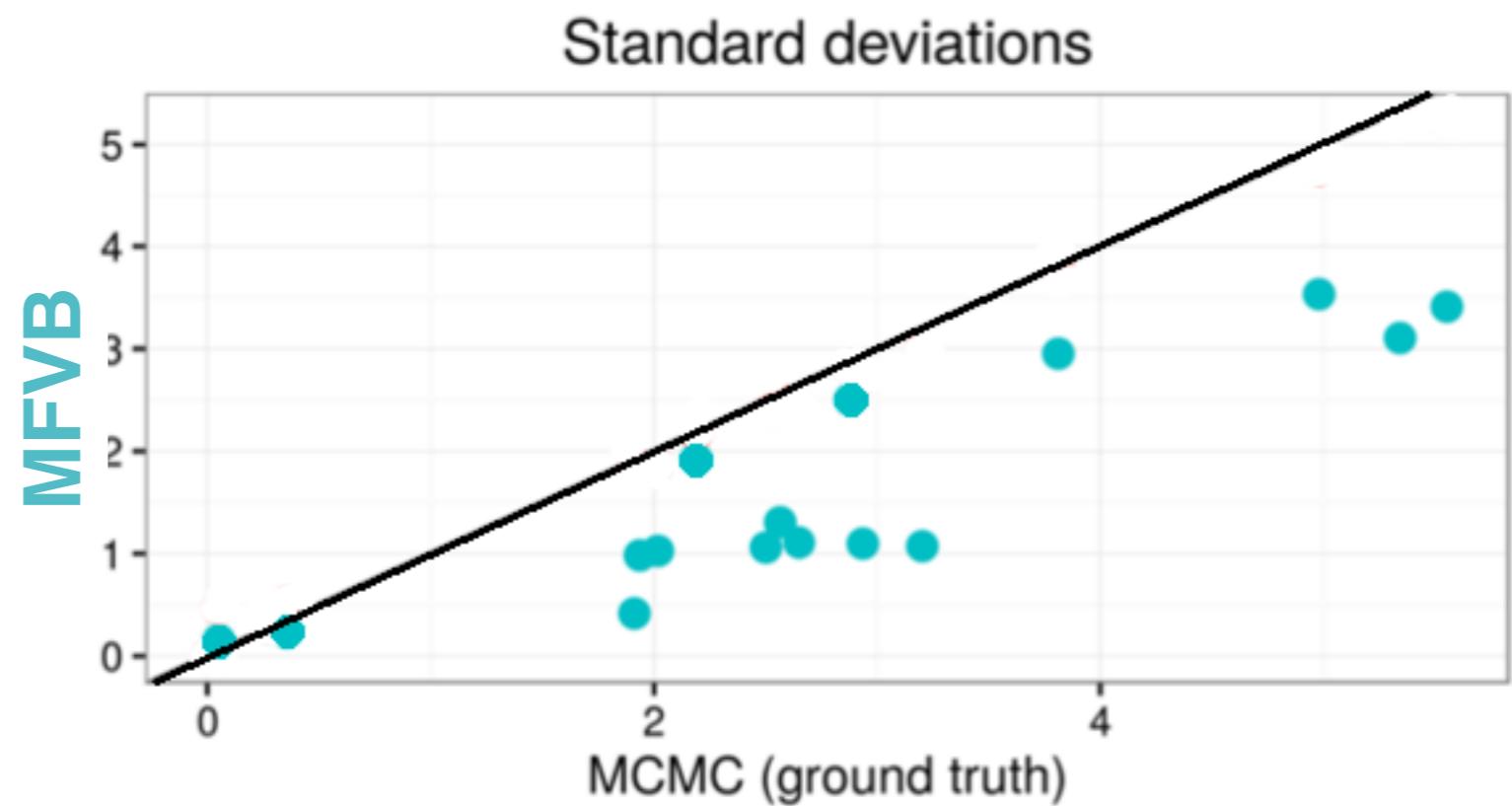
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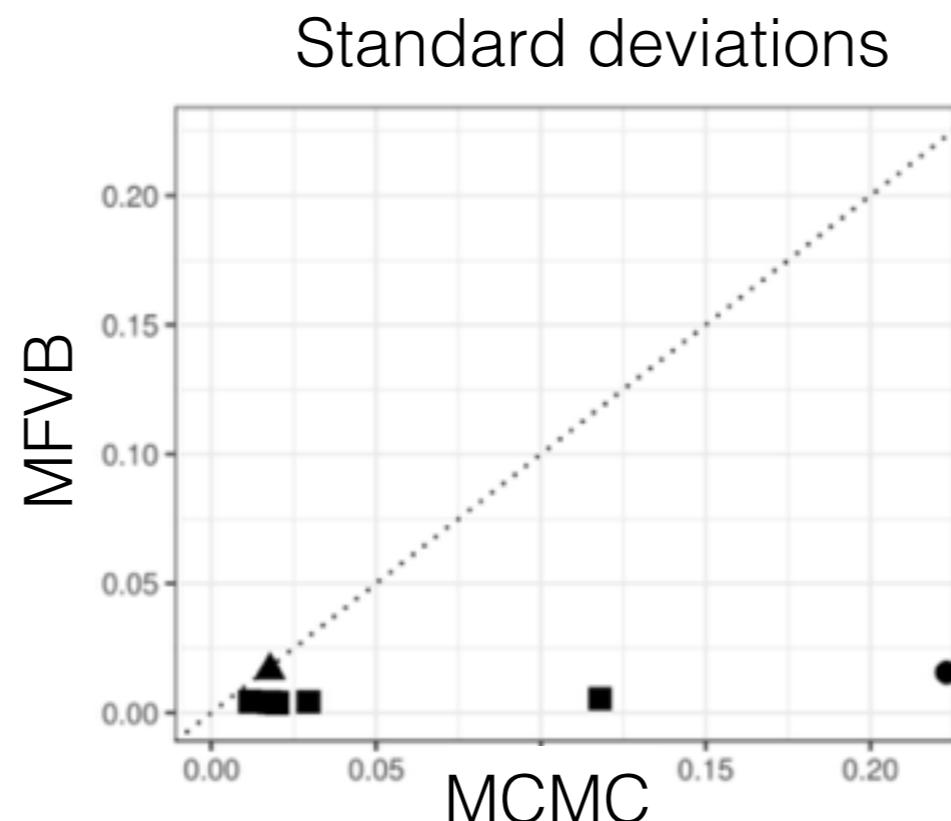


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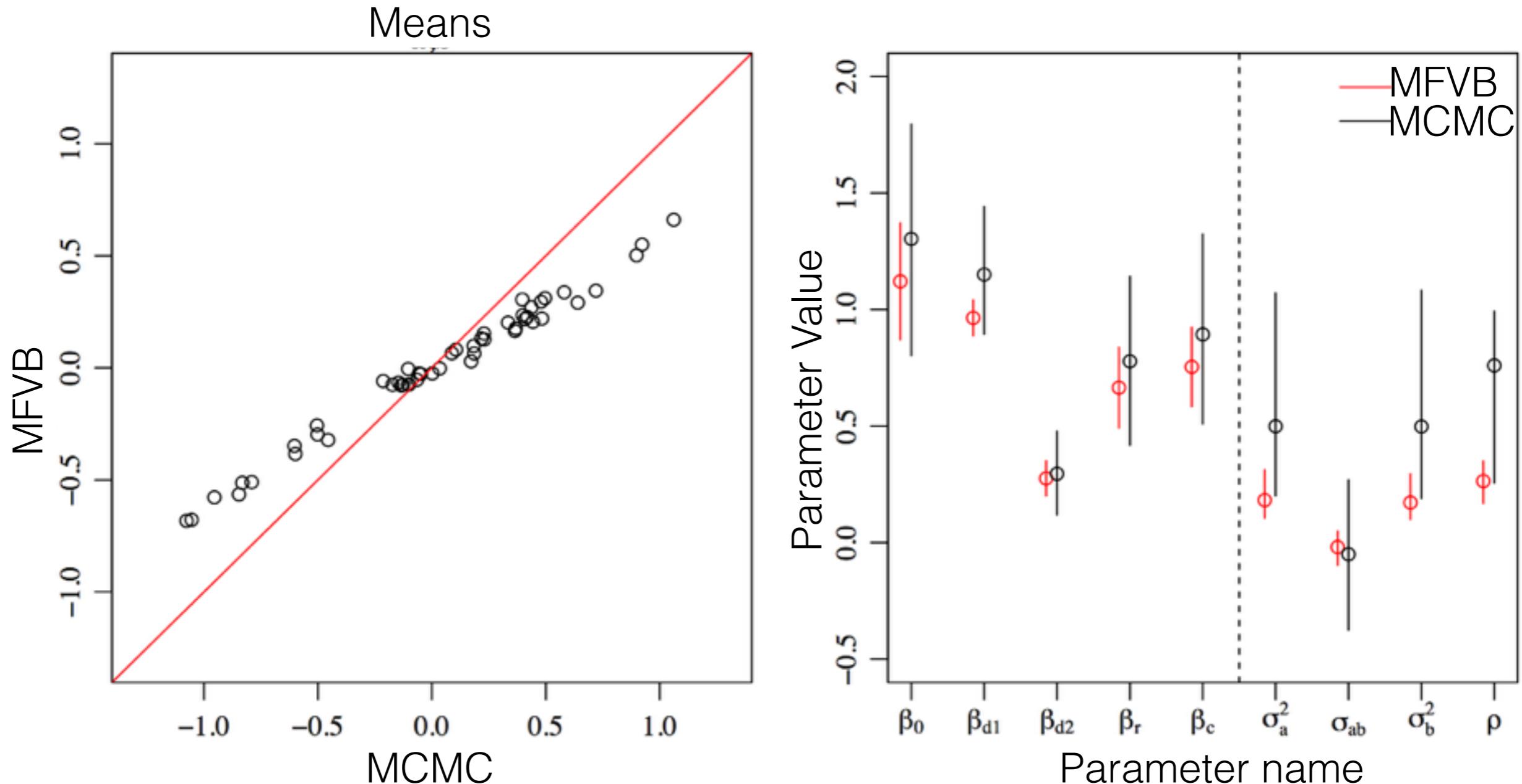


- Criteo
online ads
experiment



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

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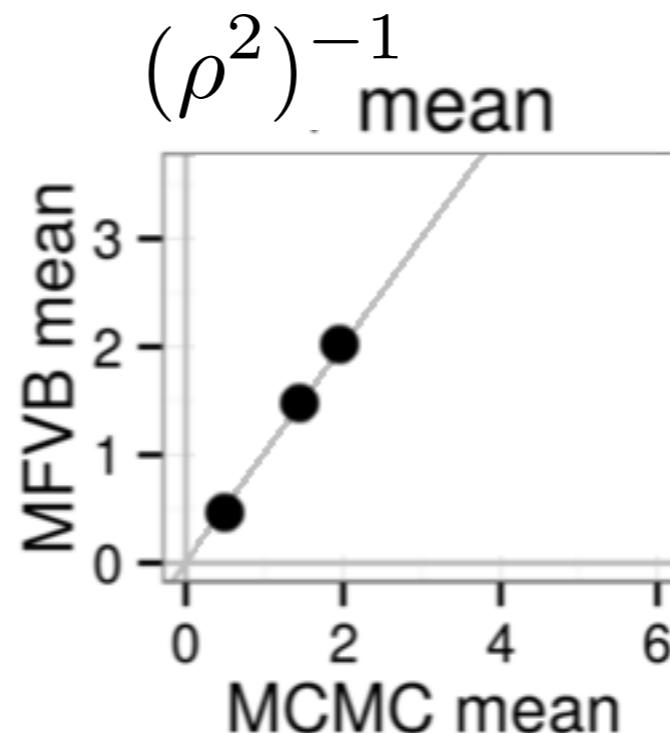
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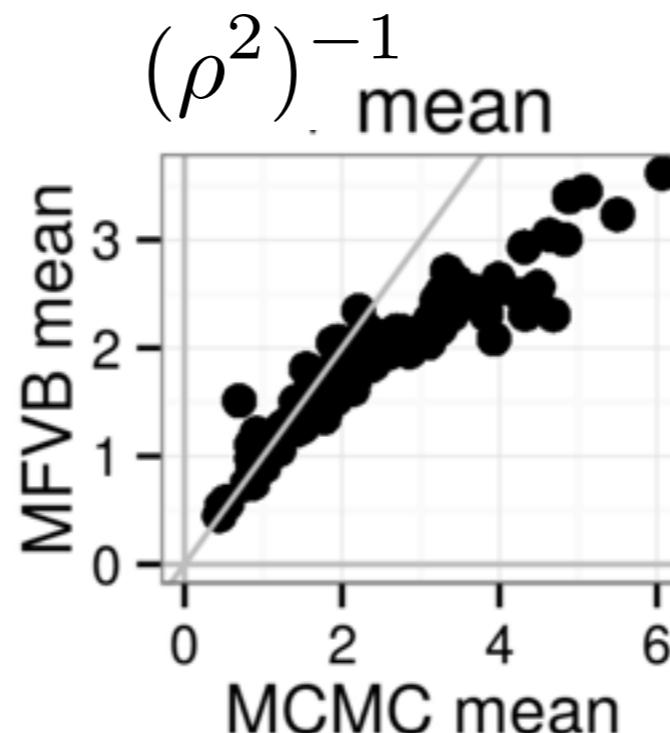
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- Data simulated from model (100 data sets, 300 data points):



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?

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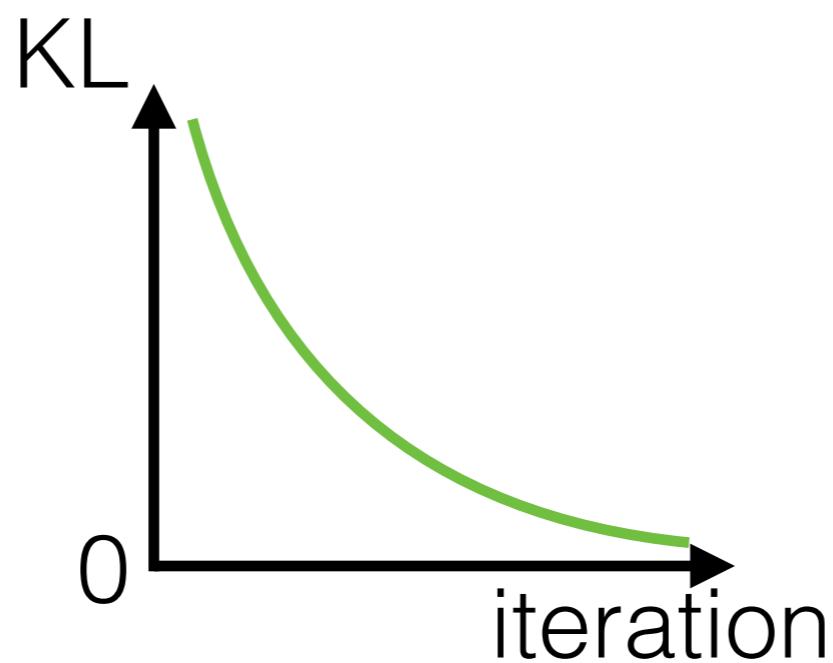
- Reliable diagnostics

What can we do?

- Reliable diagnostics
 - KL vs ELBO

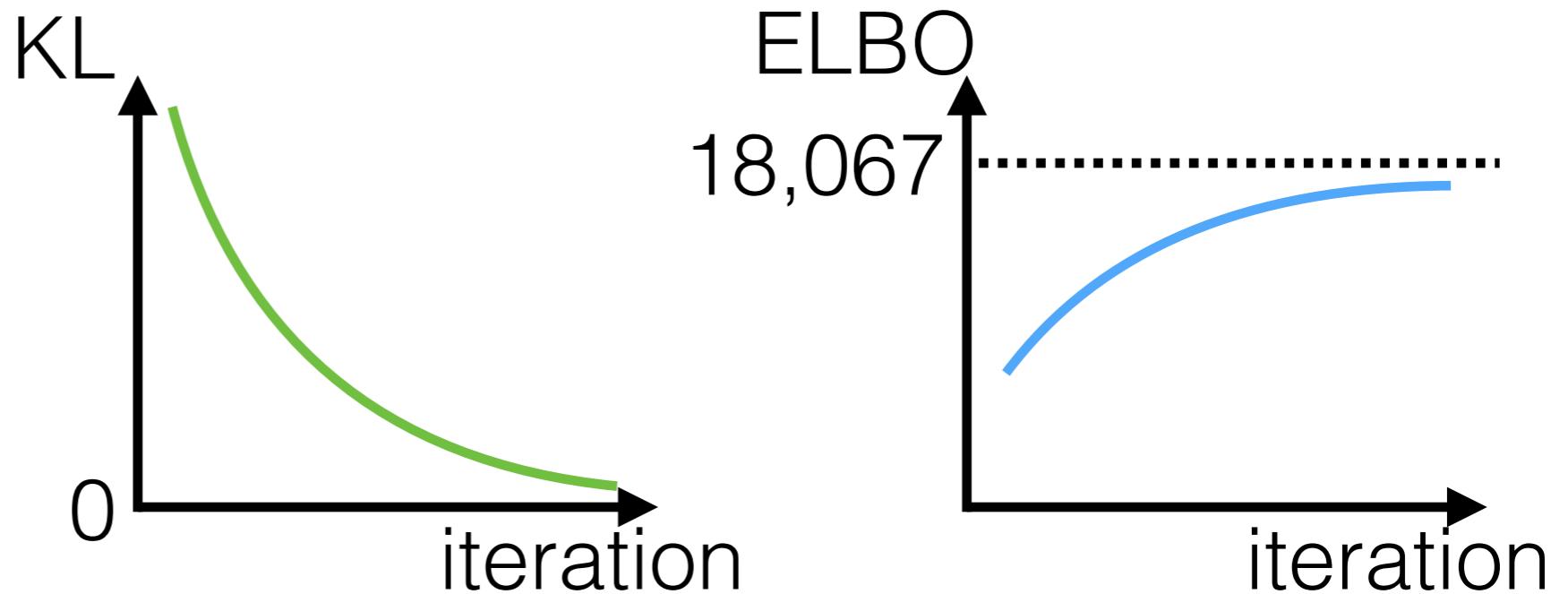
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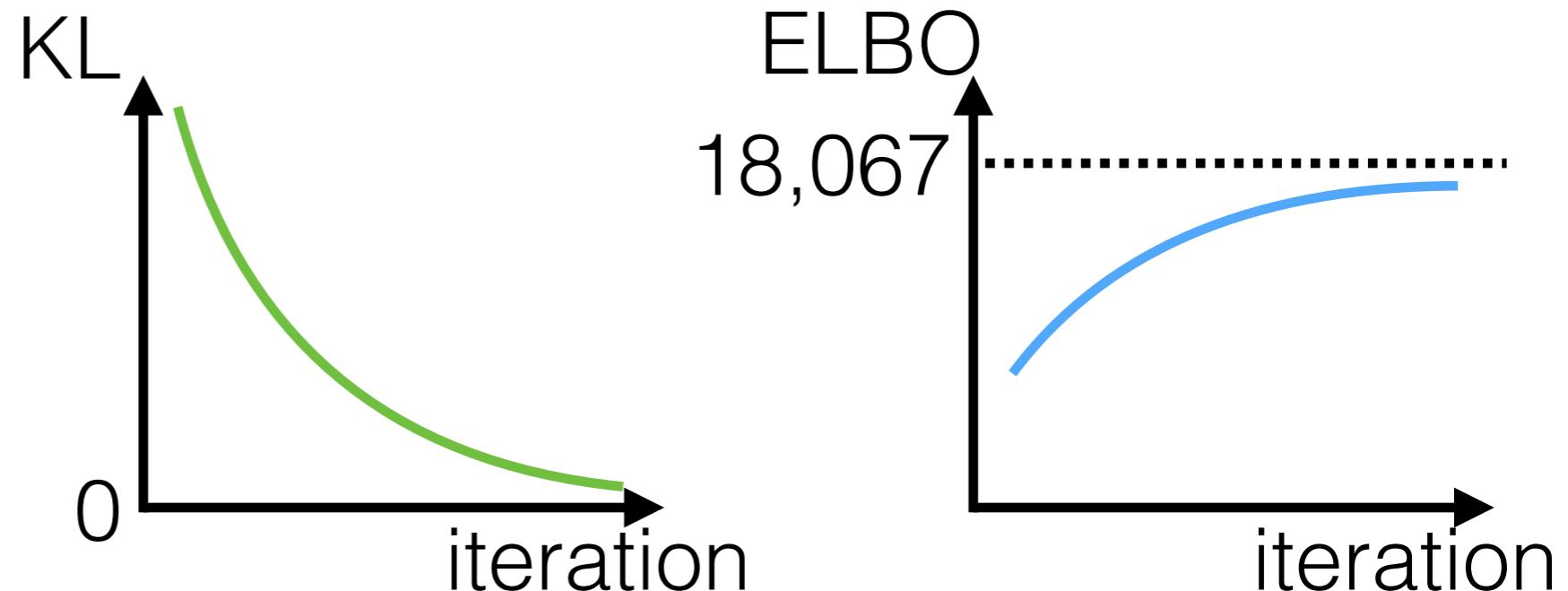
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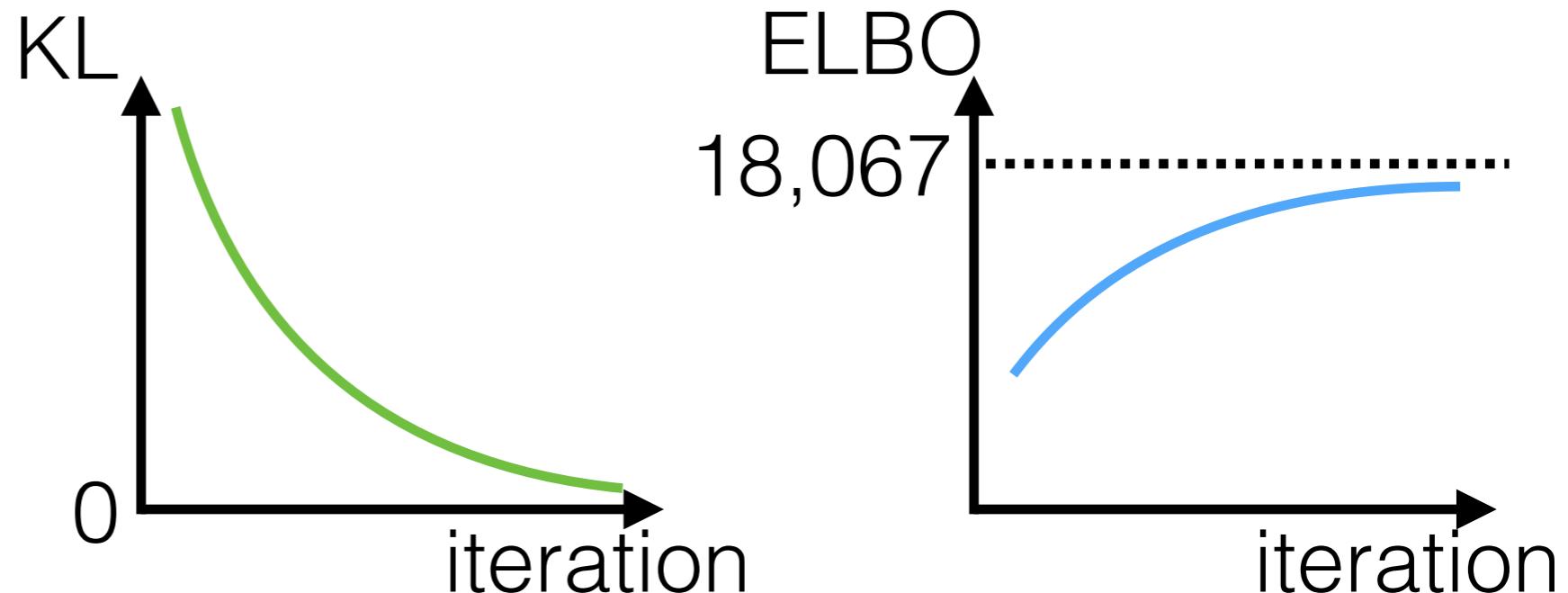


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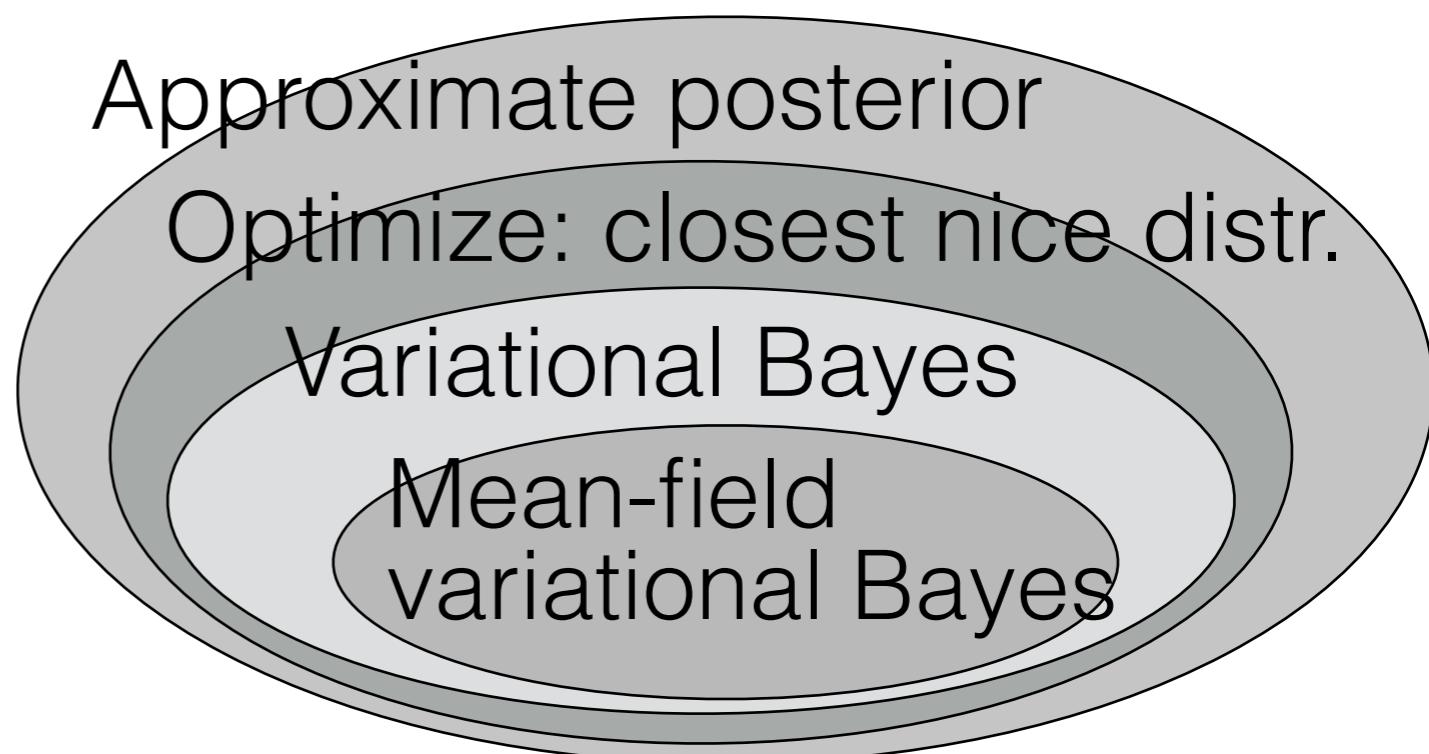
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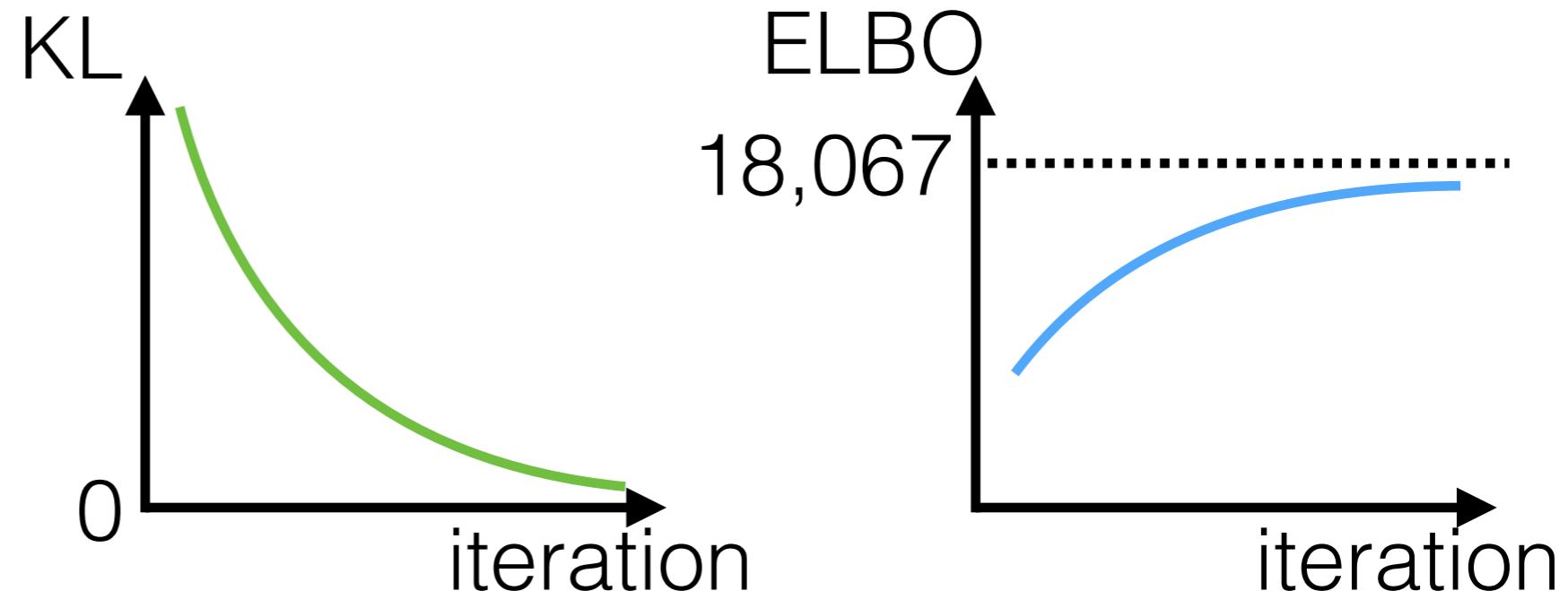
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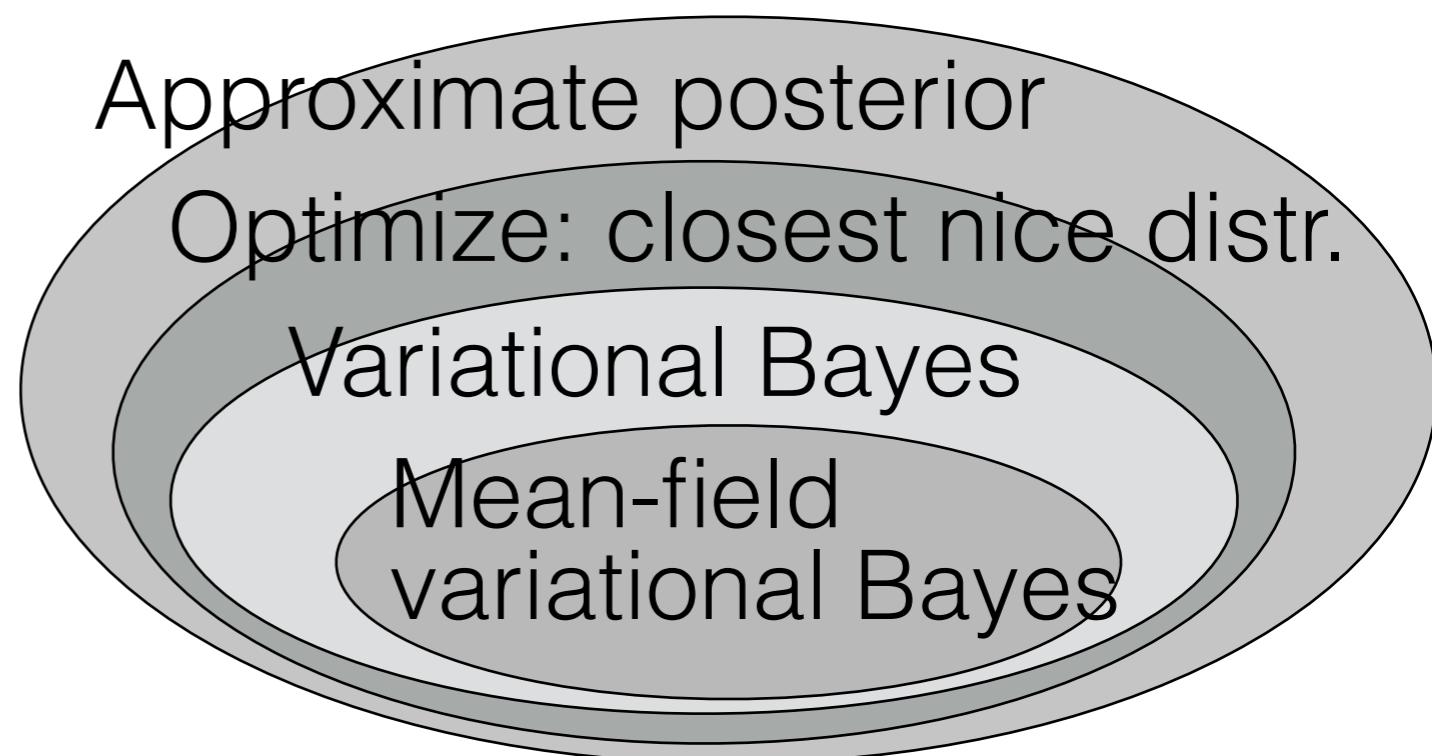
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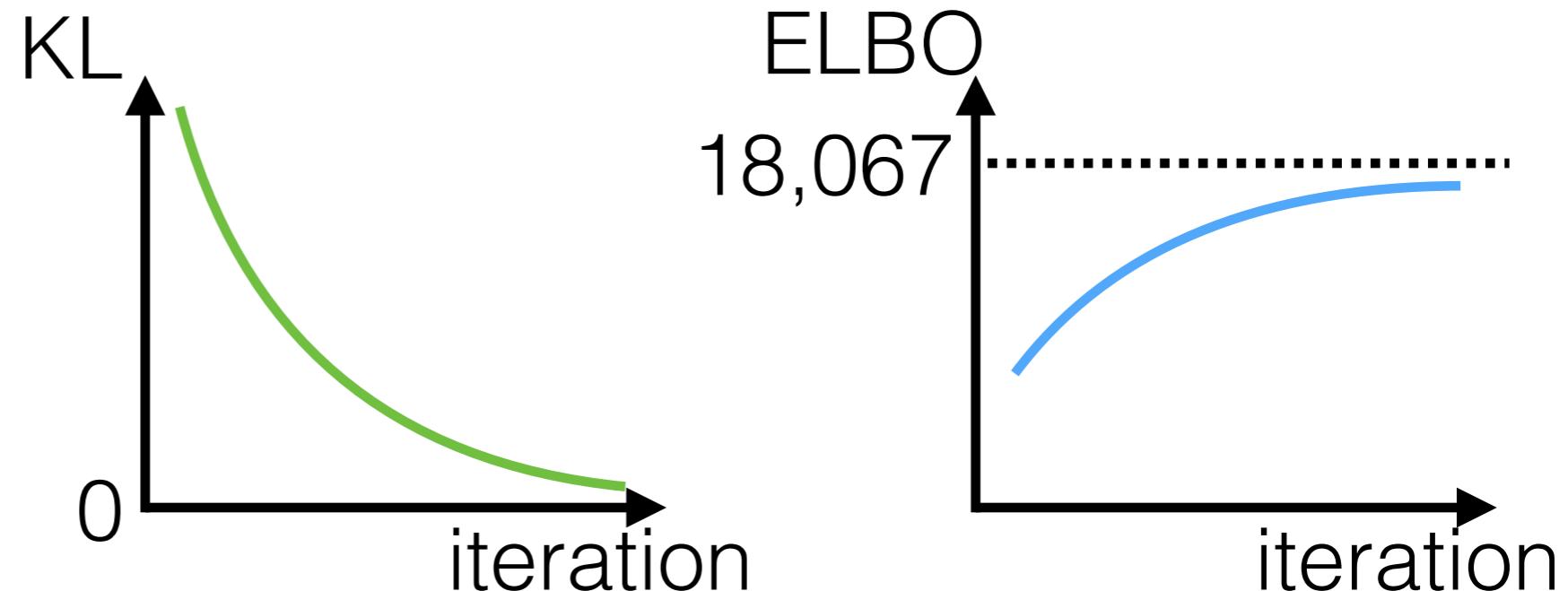
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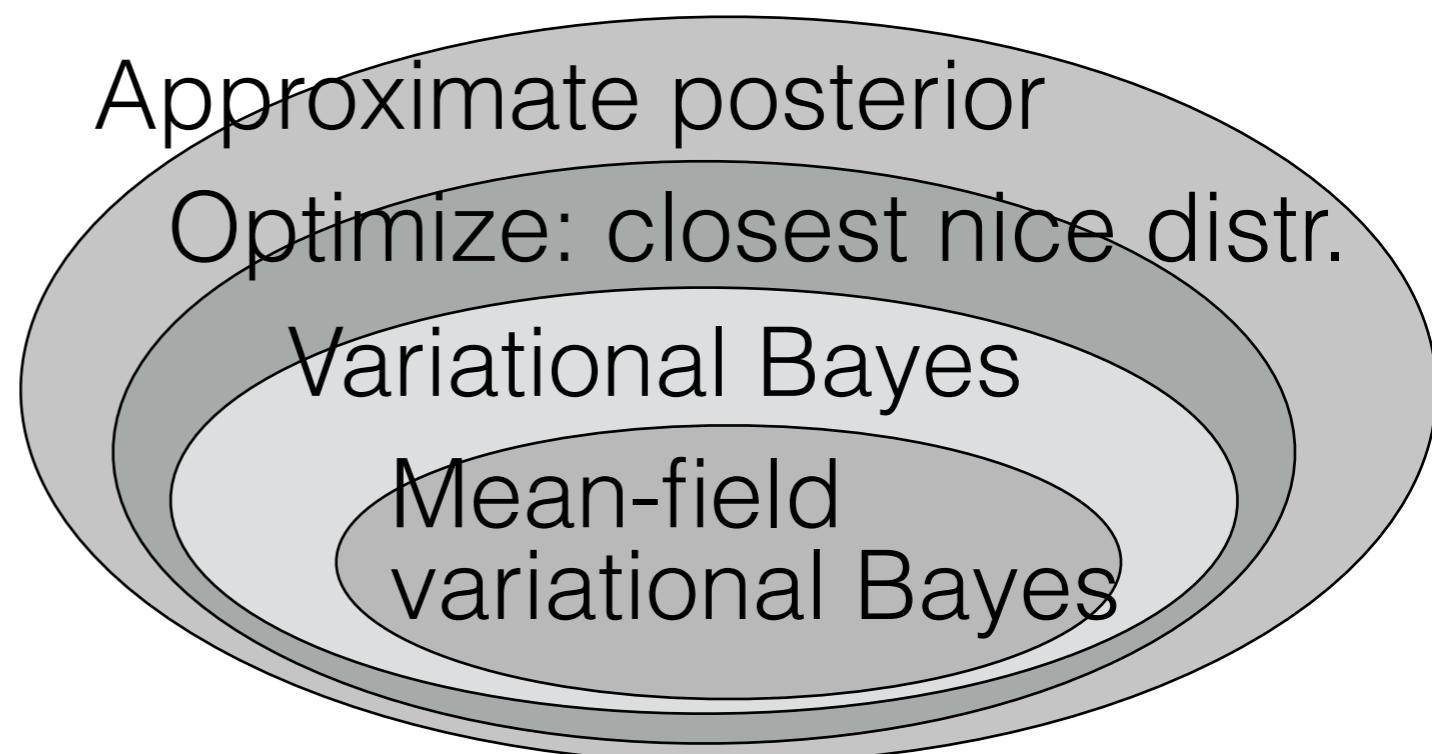
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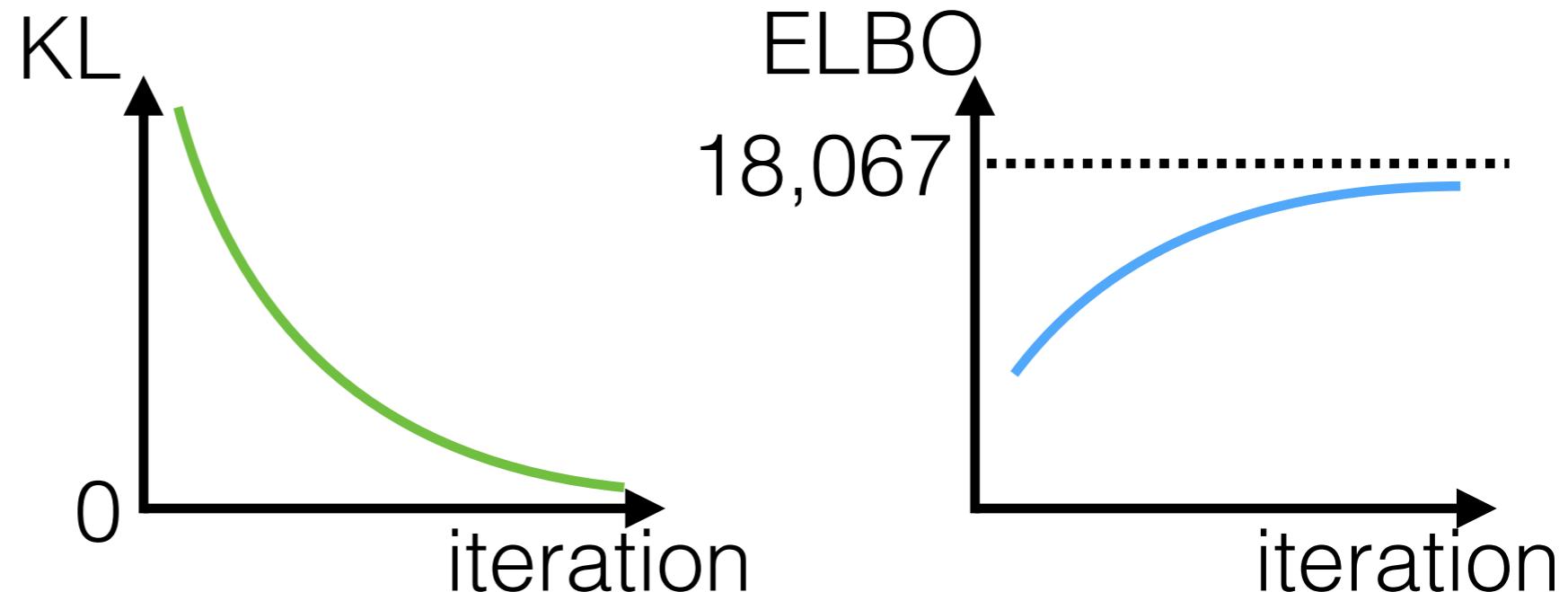
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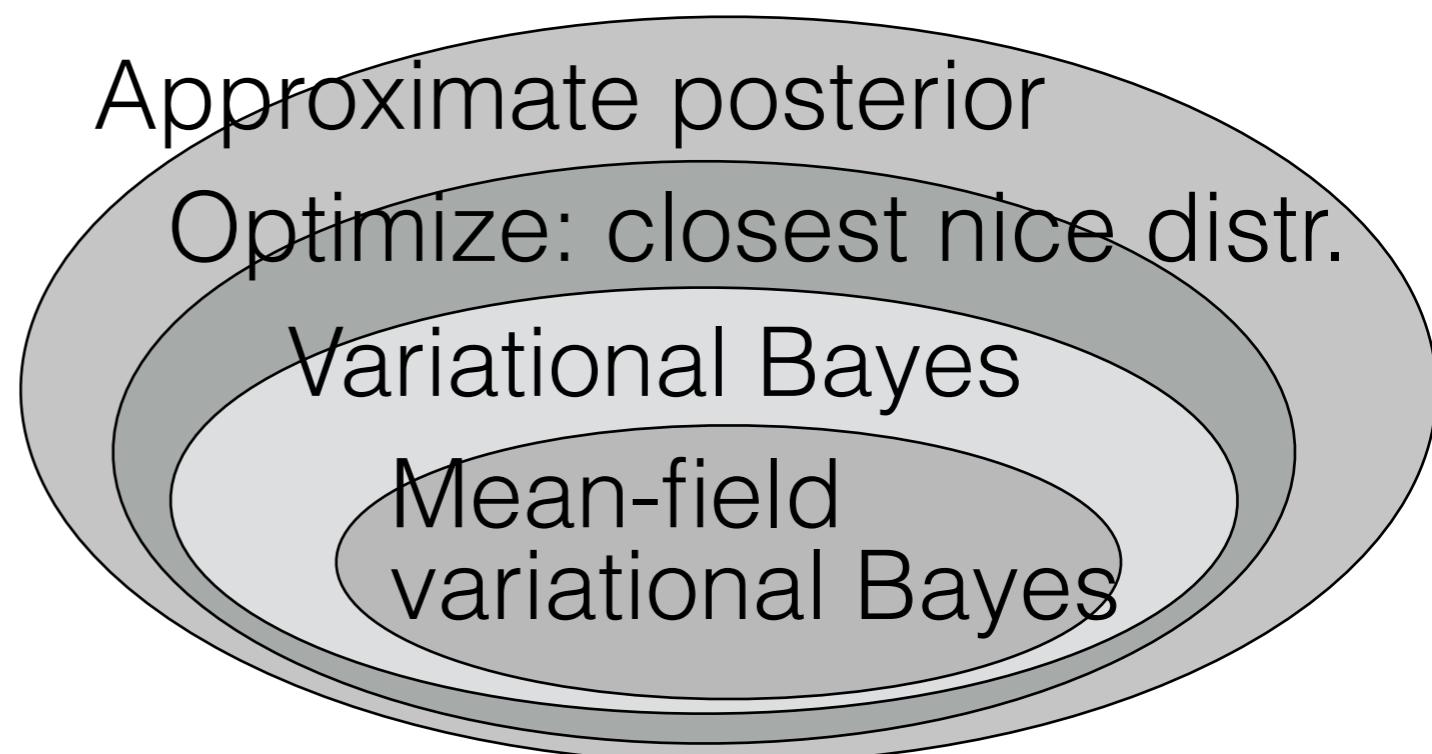
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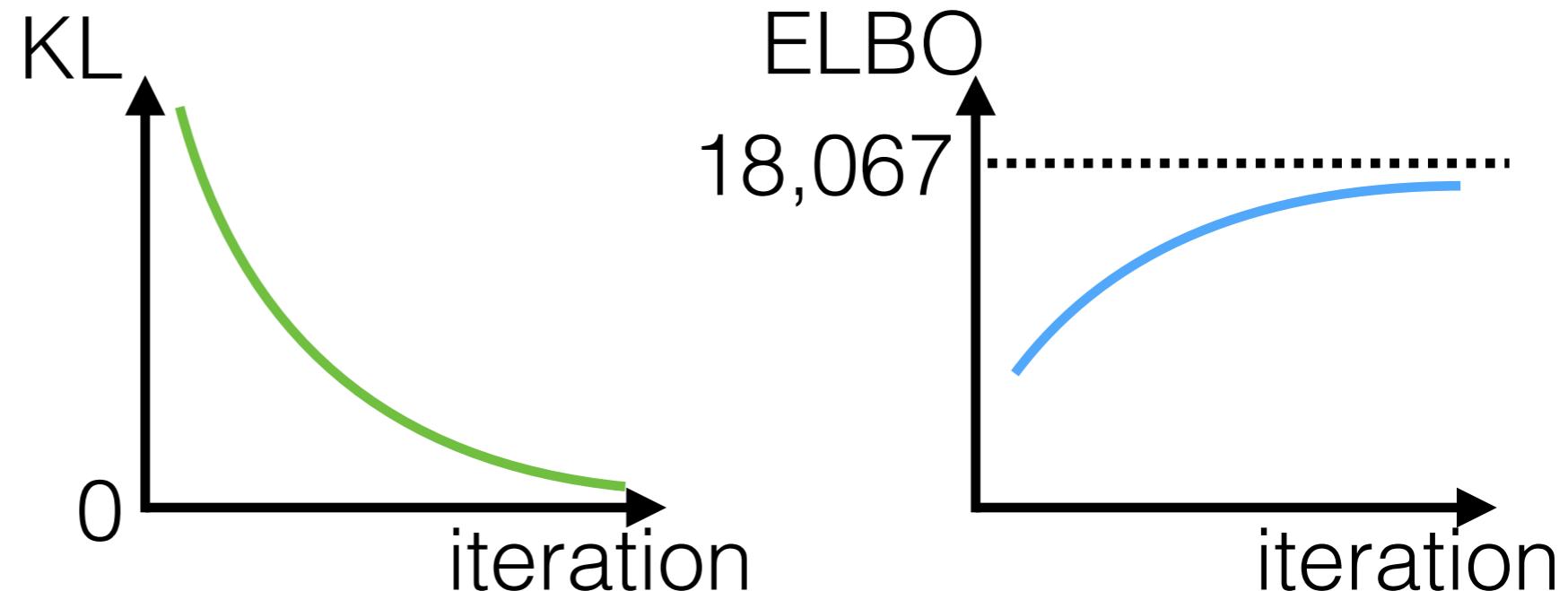
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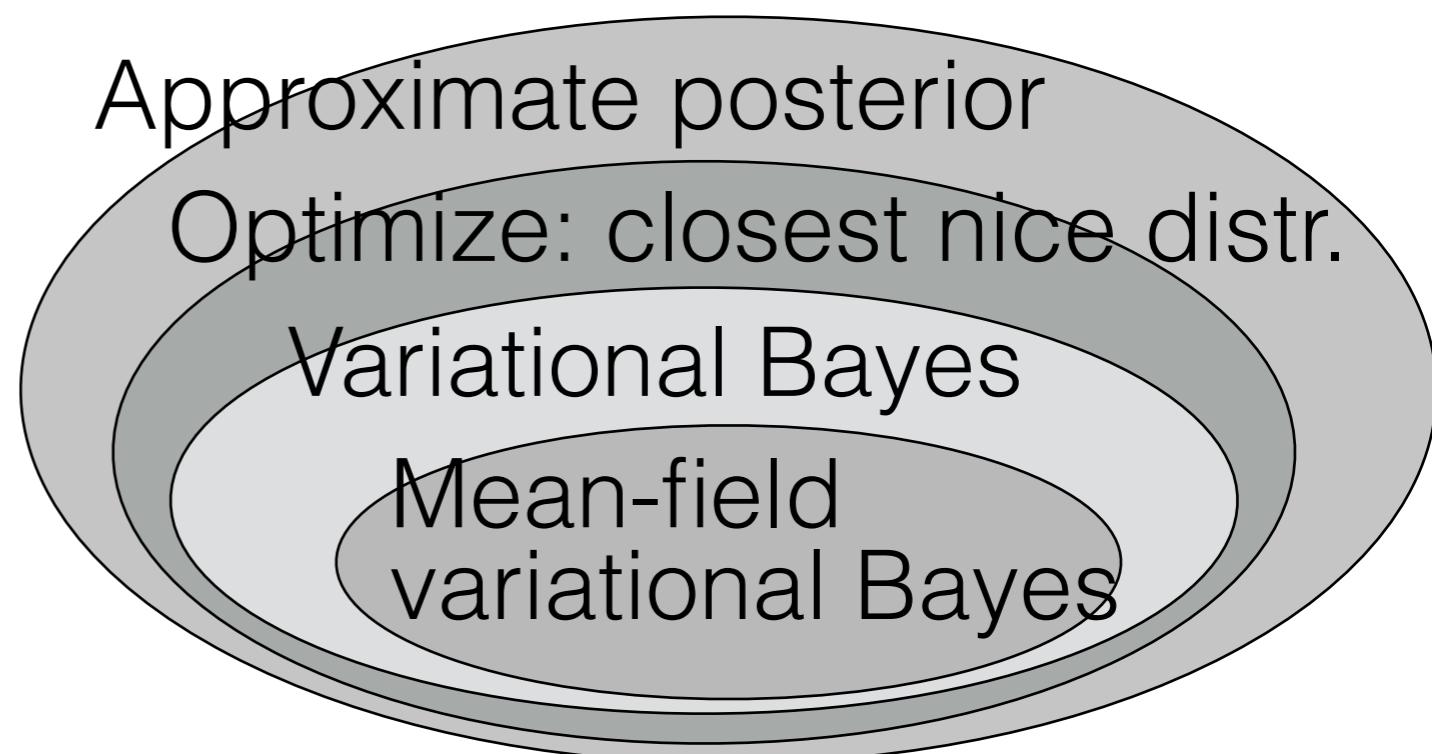
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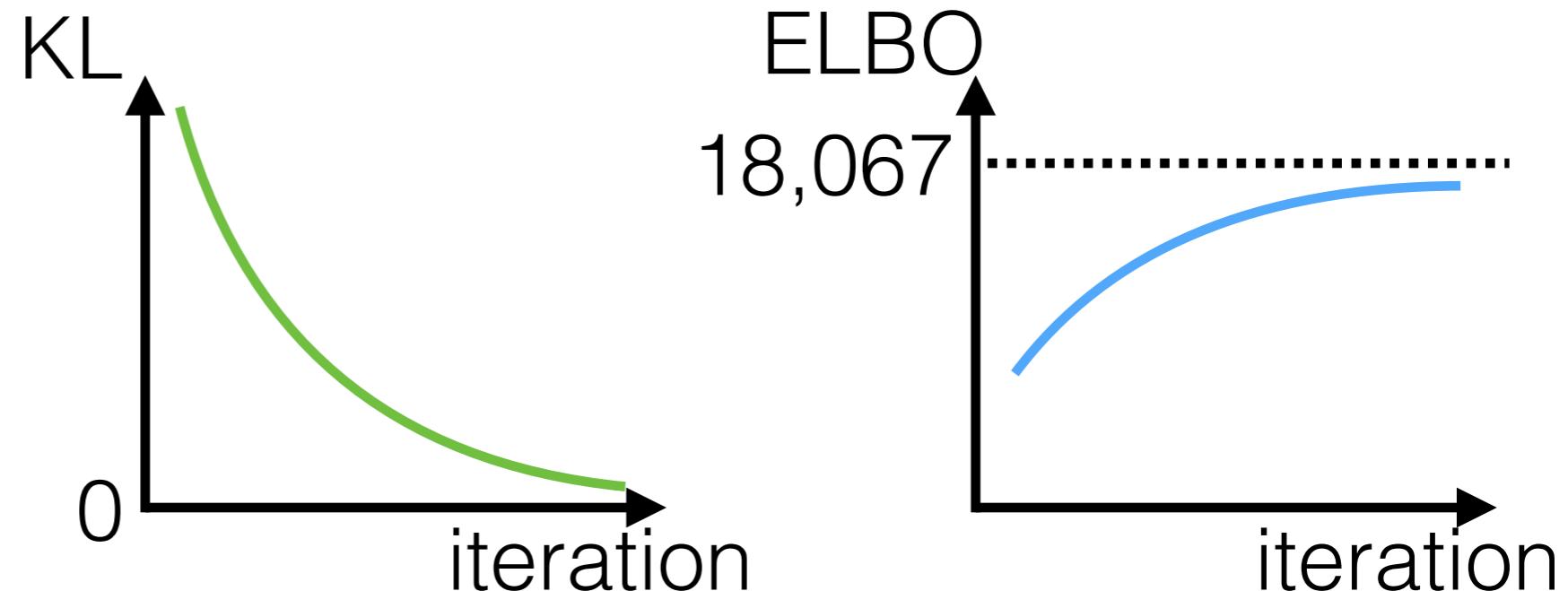
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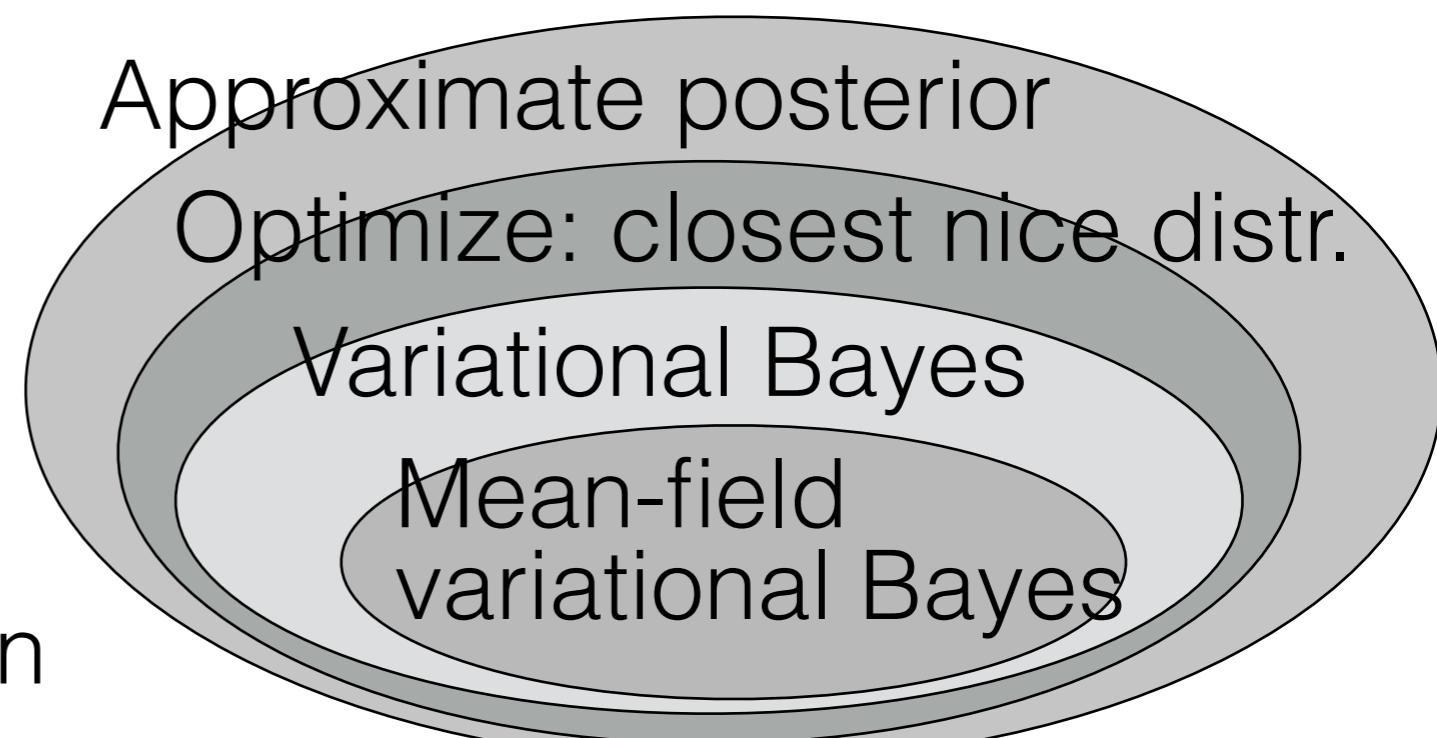
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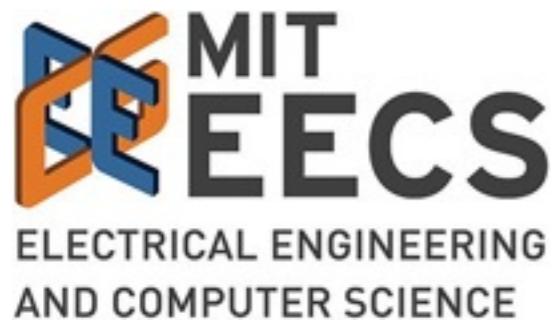


What to read next

- 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. *Journal of Machine Learning Research*, to appear. ArXiv:1709.02536.

References

- See the end of Part II for reference list up to this point



Covariances, Robustness, and Variational Bayes

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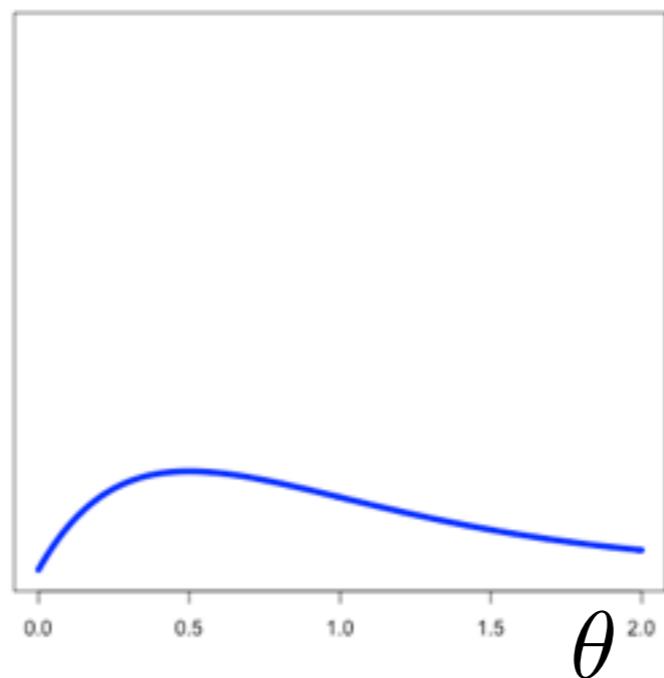
With: Ryan Giordano, Rachael Meager,
Jonathan H. Huggins, Michael I. Jordan

- Bayesian inference

- Bayesian inference $p(\theta)$

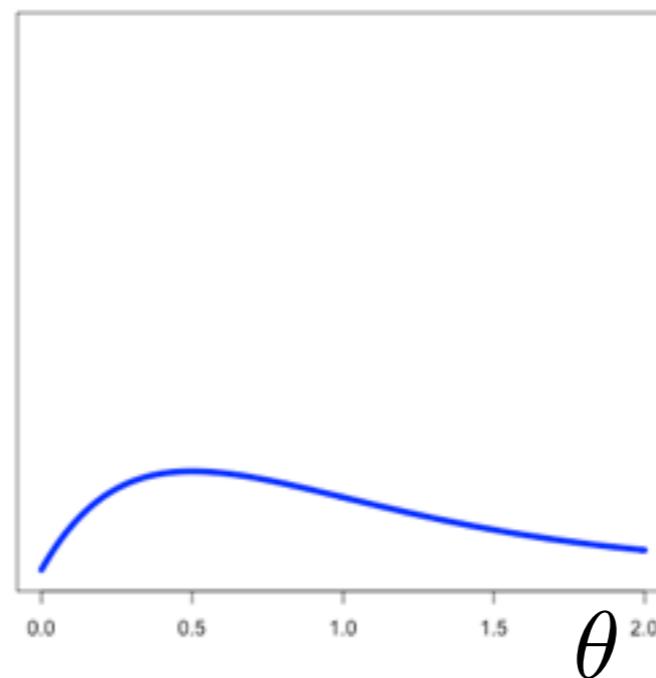
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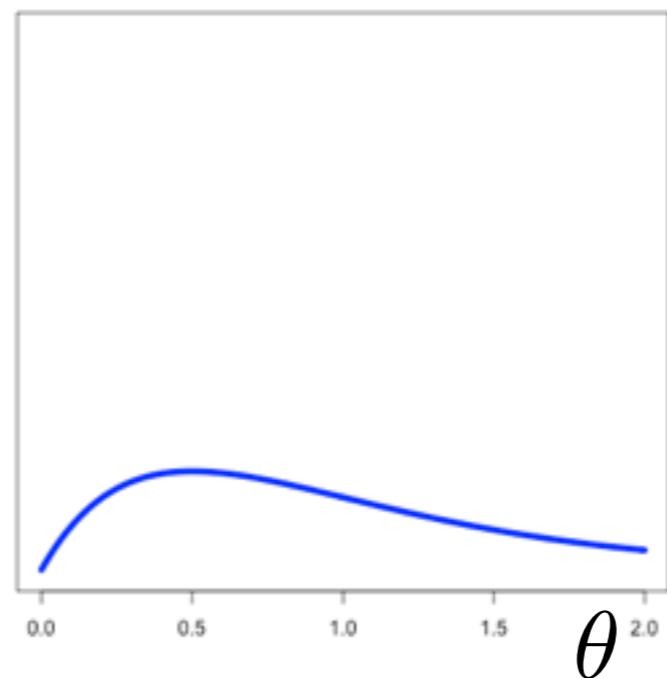


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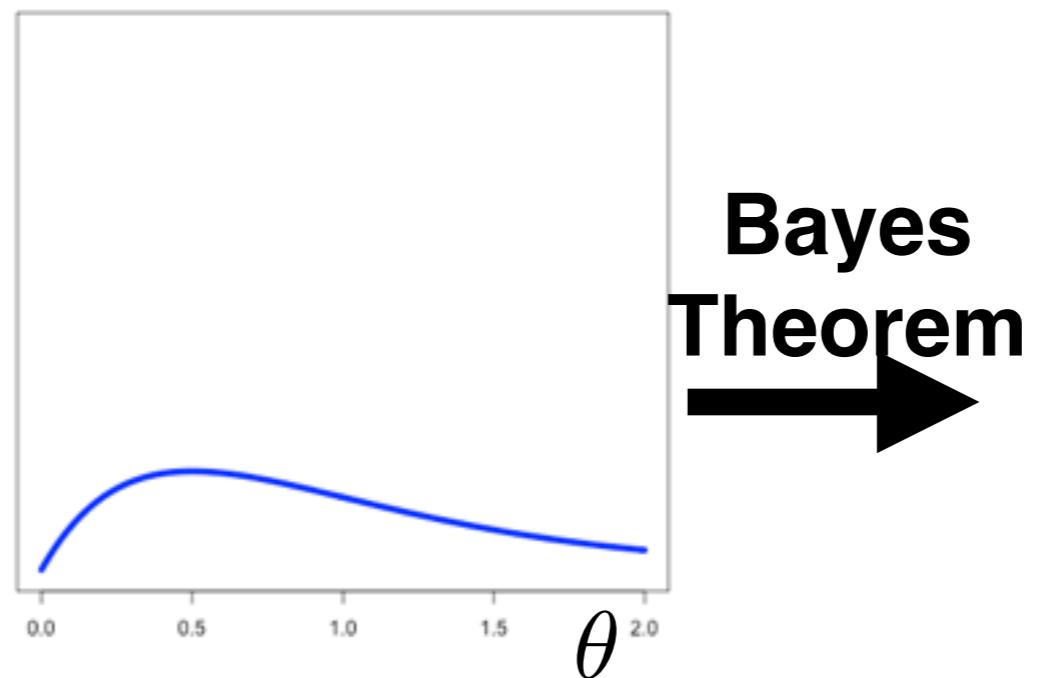
$$p(y|\theta)p(\theta)$$



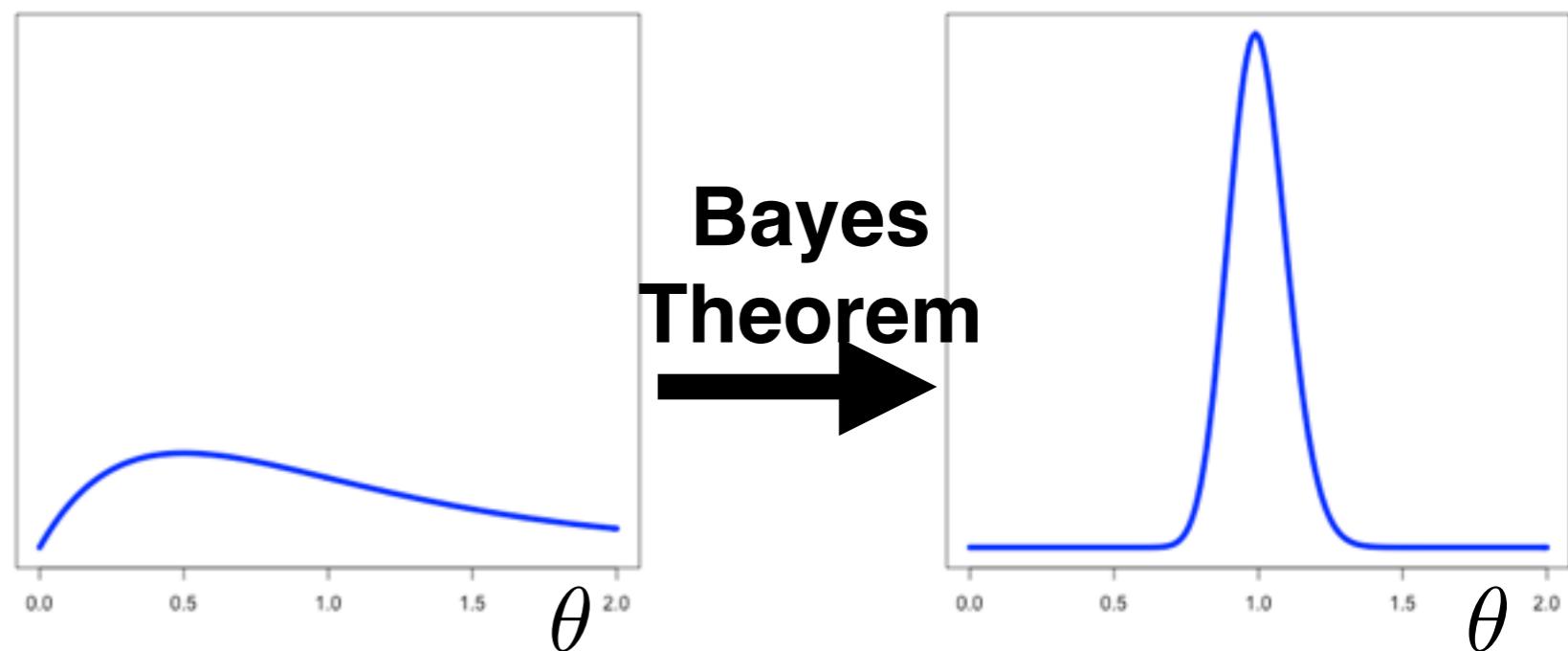
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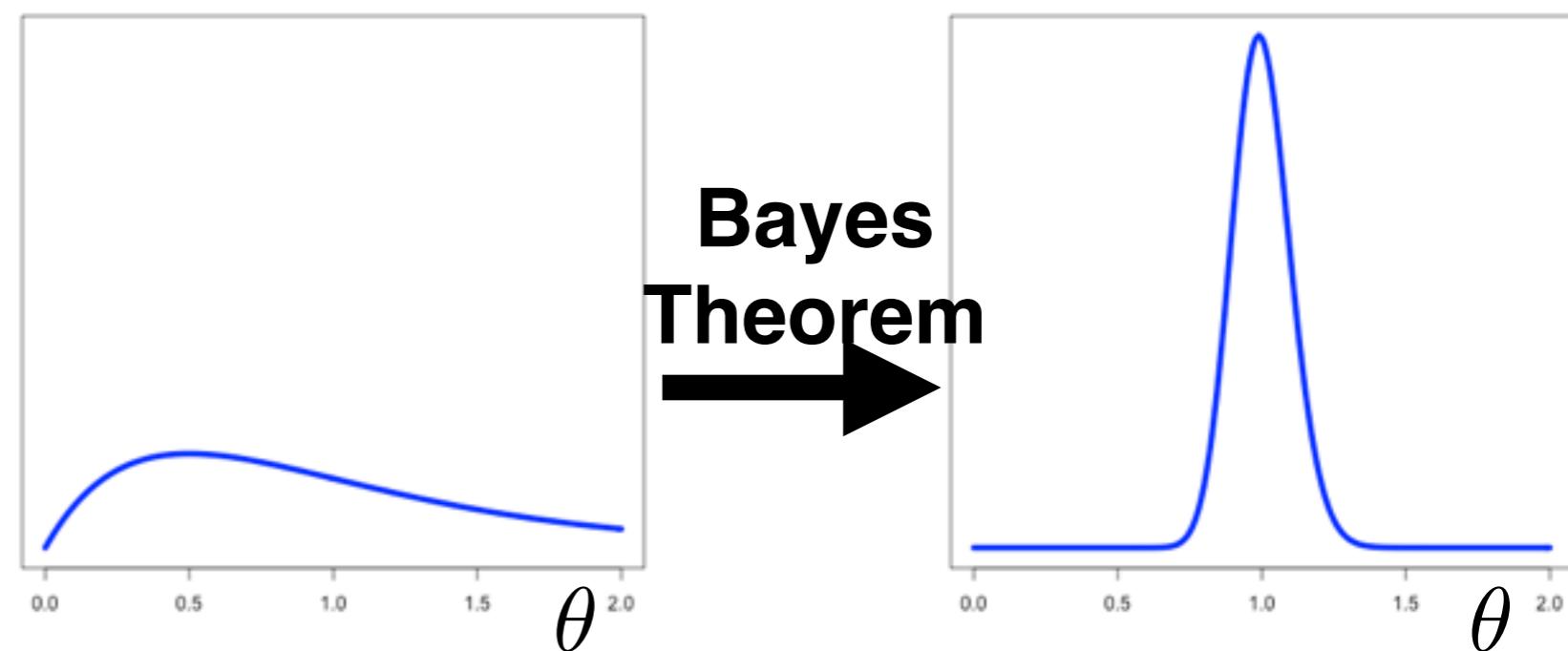


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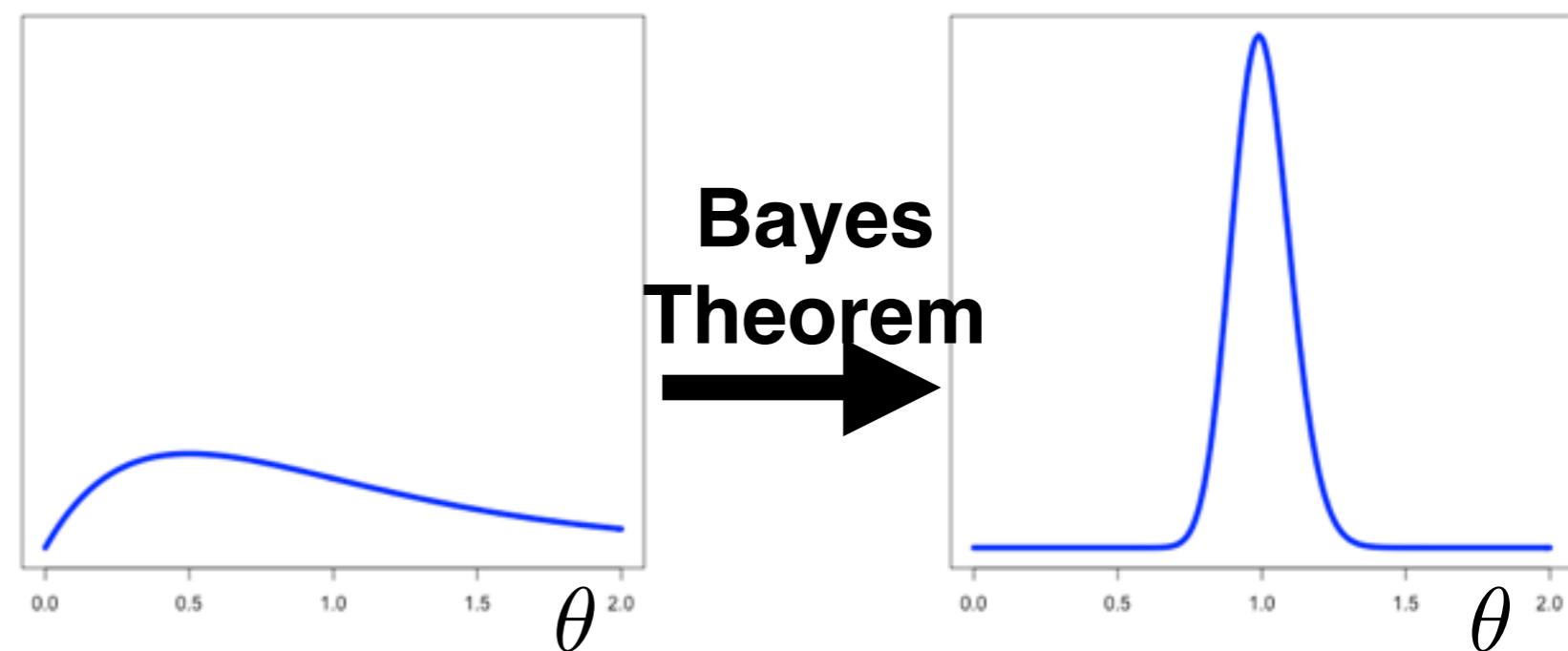
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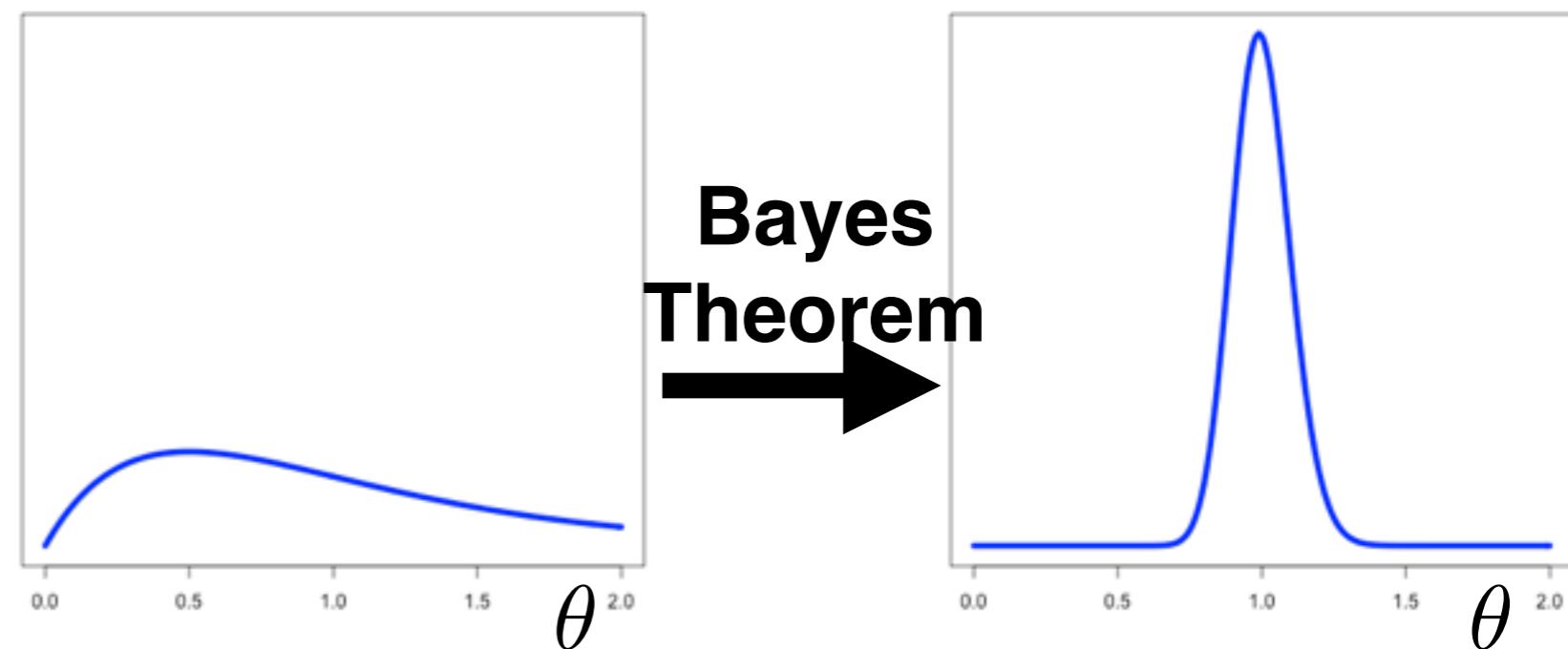
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- Time-consuming

$$p(\theta|y) \propto_{\theta} p(y|\theta)p(\theta)$$



- Bayesian inference
- Challenge: Express knowledge in a distribution (prior, likelihood)
- Time-consuming; subjective

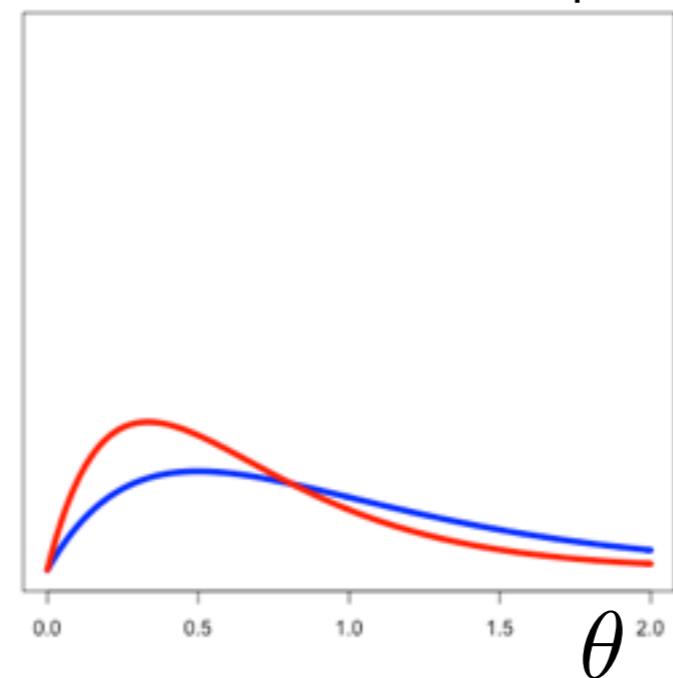
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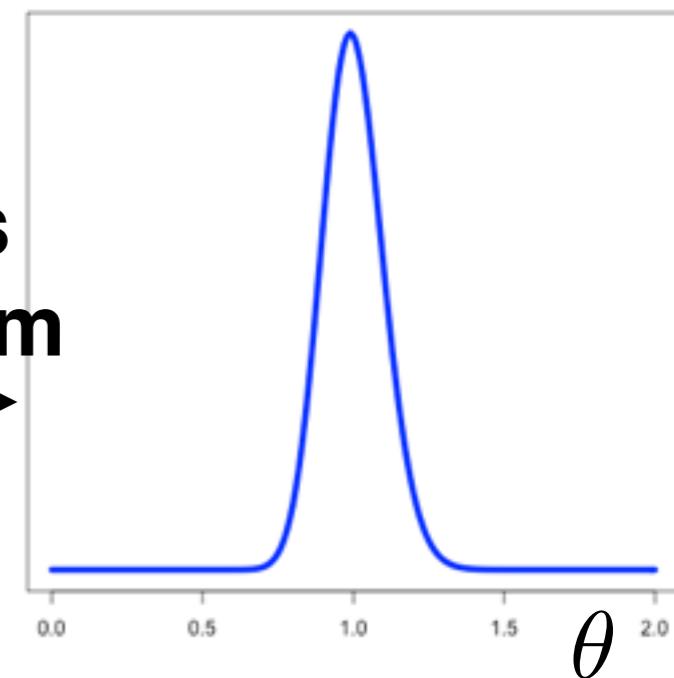
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Some reasonable priors



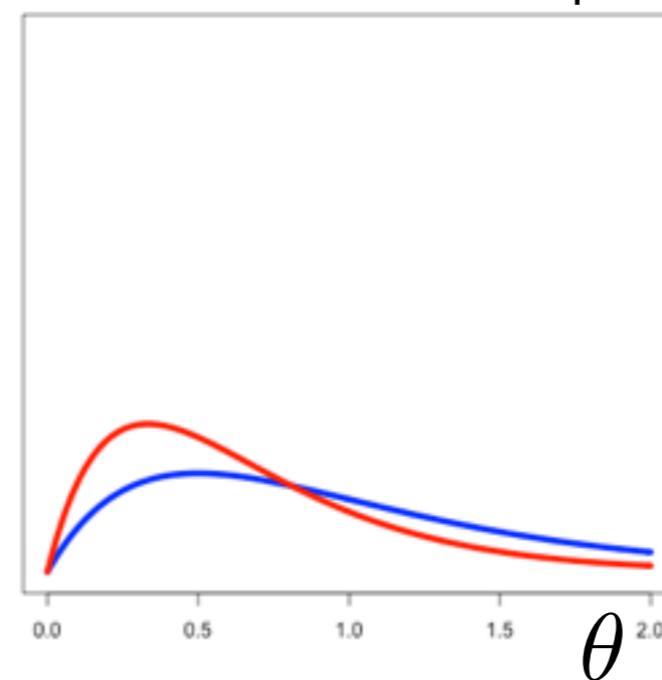
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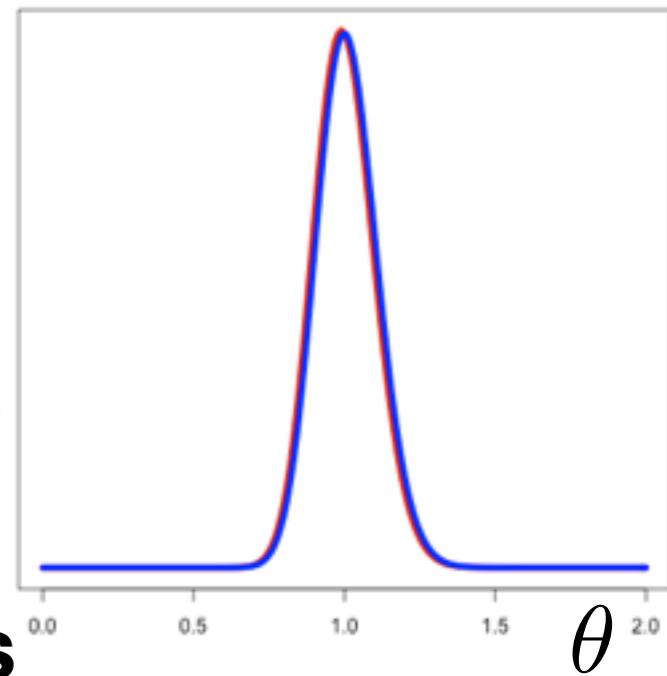
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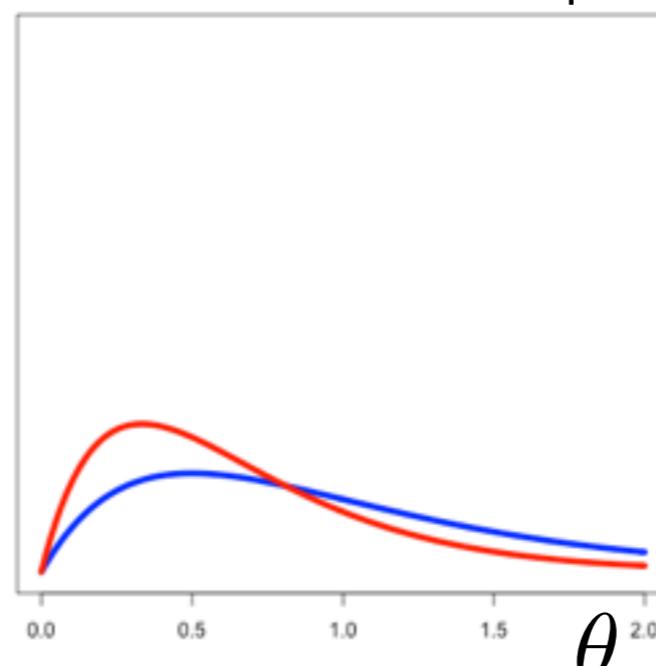
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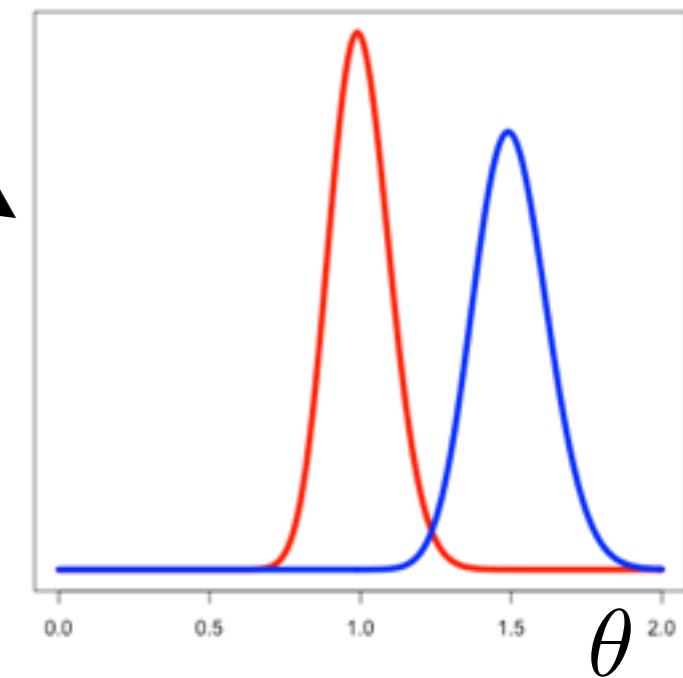
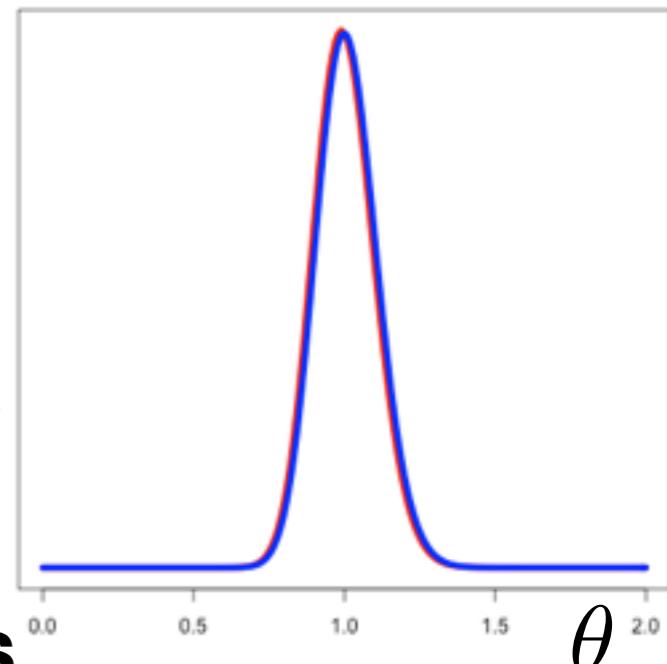
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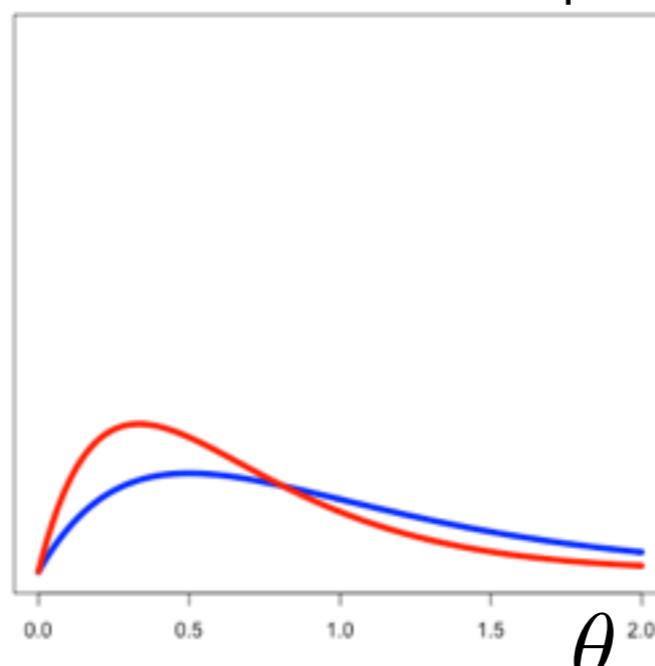
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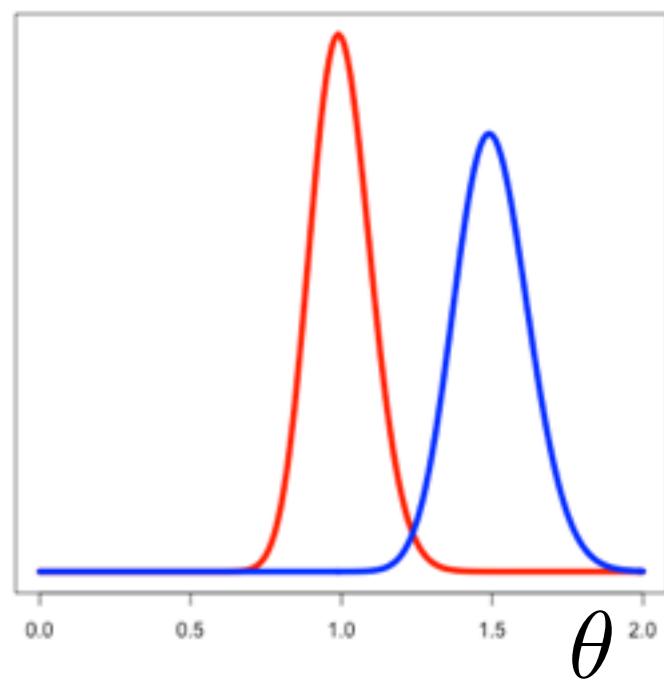
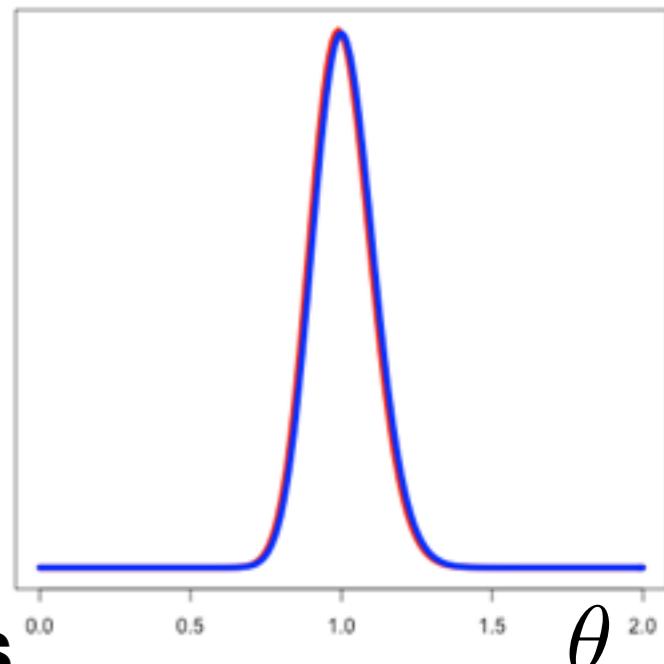
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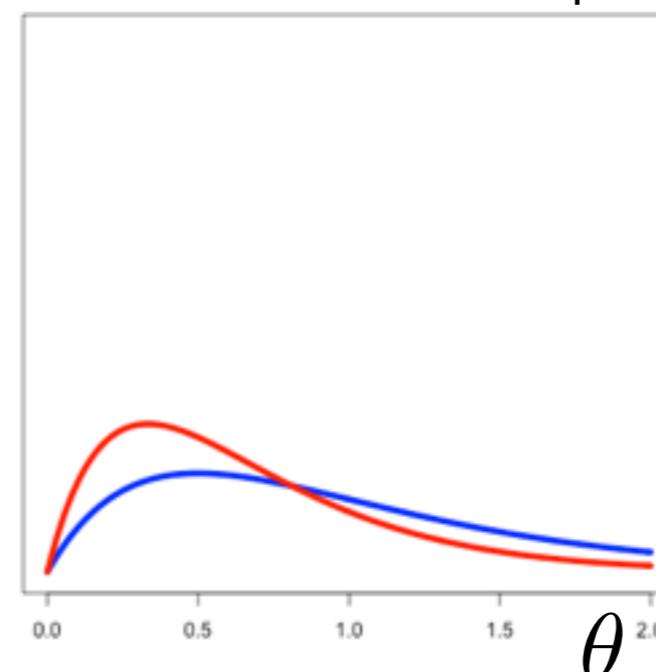


robustness quantification

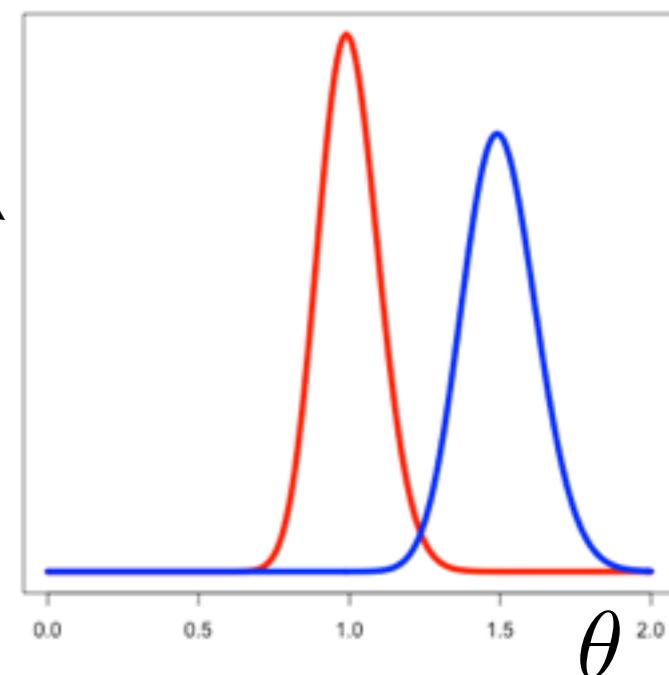
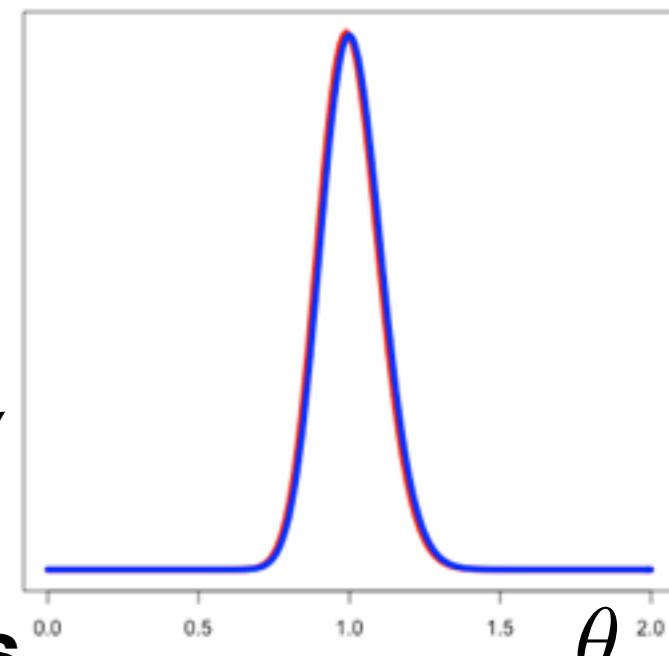
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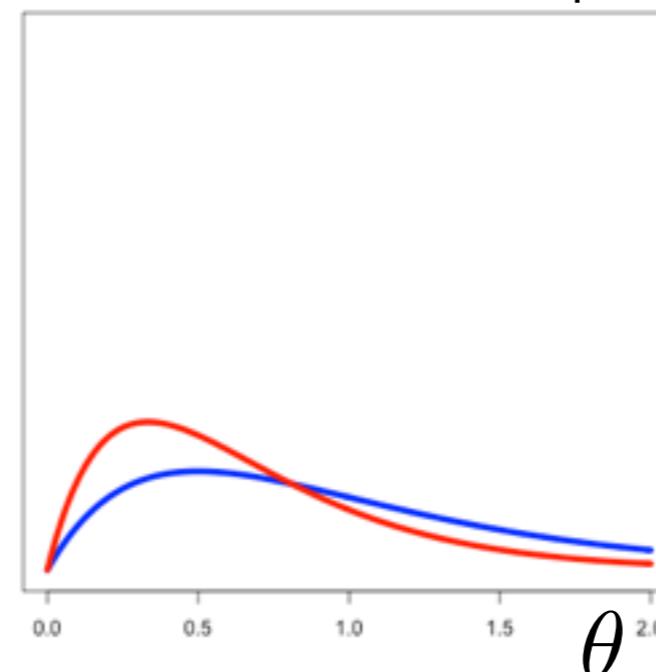


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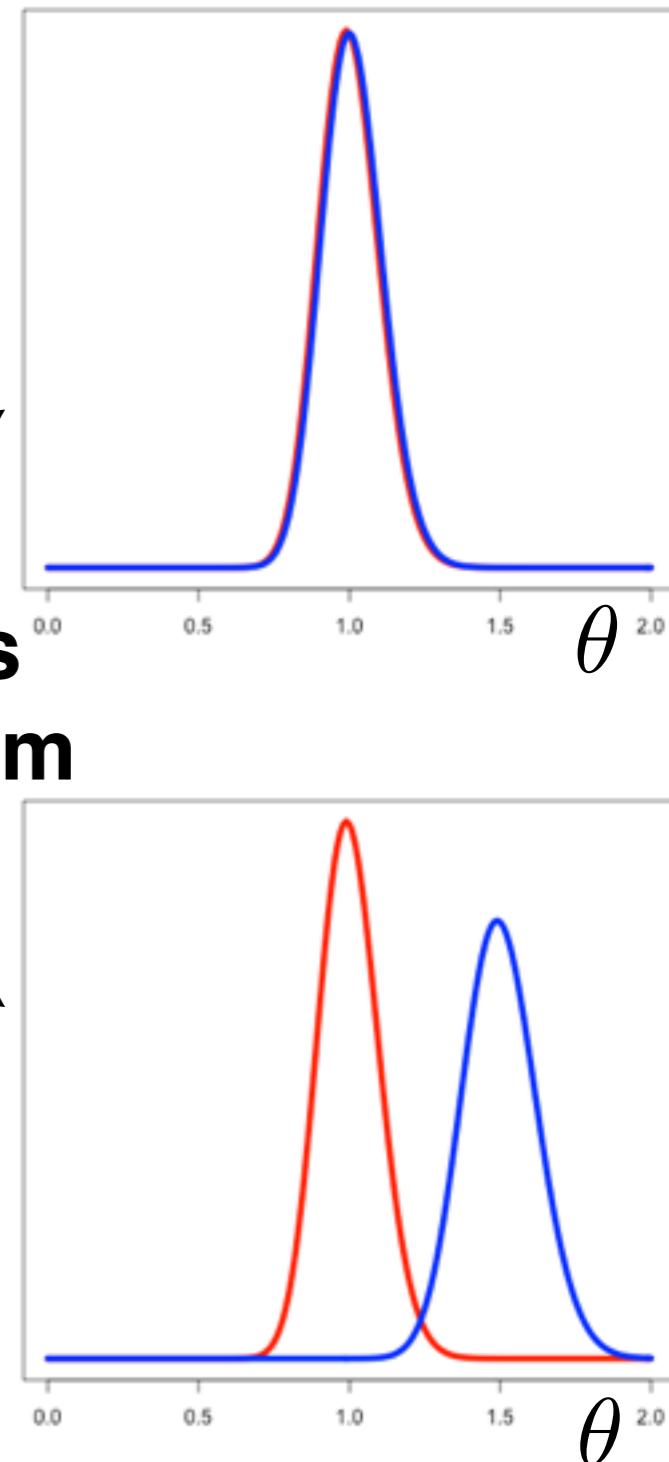
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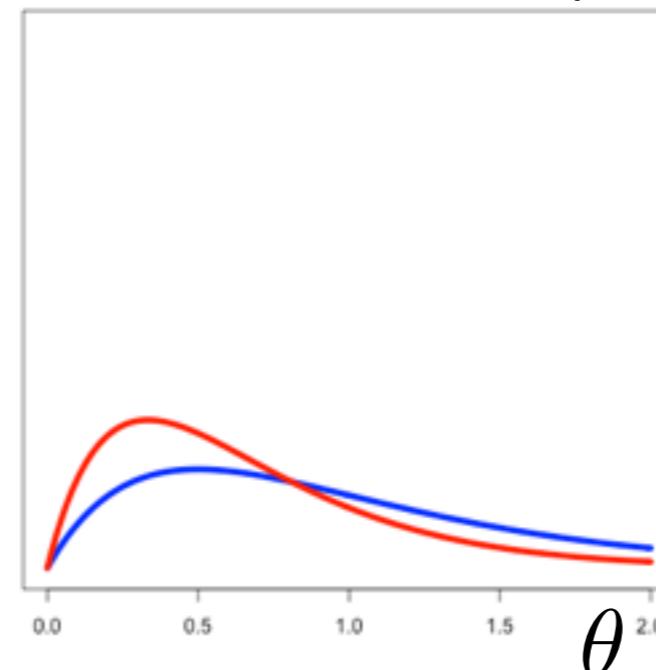


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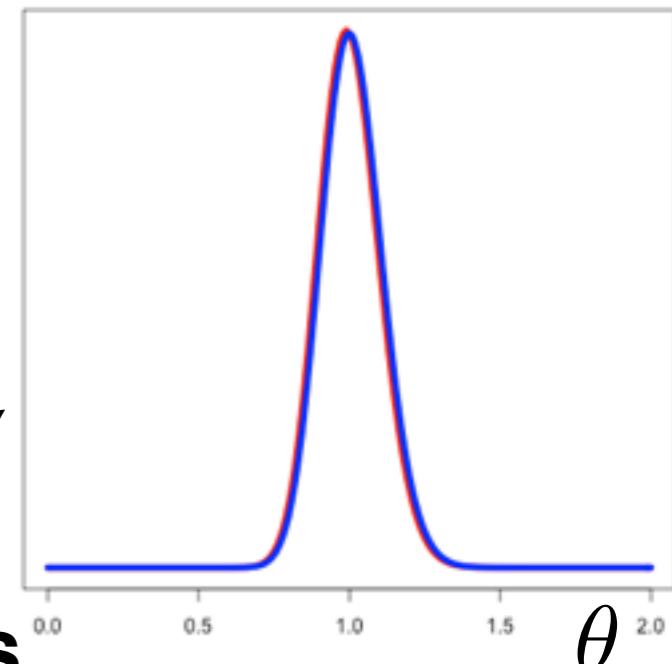
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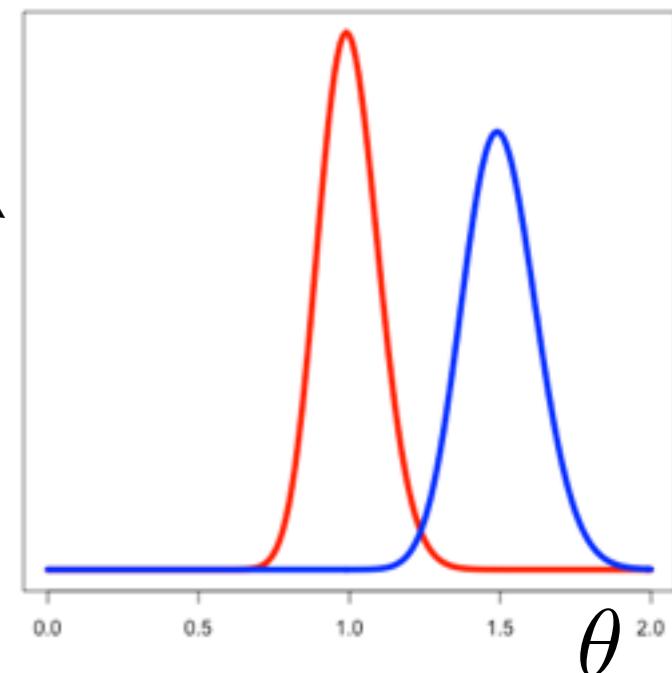
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- Challenge: Approximating the posterior can be computationally expensive
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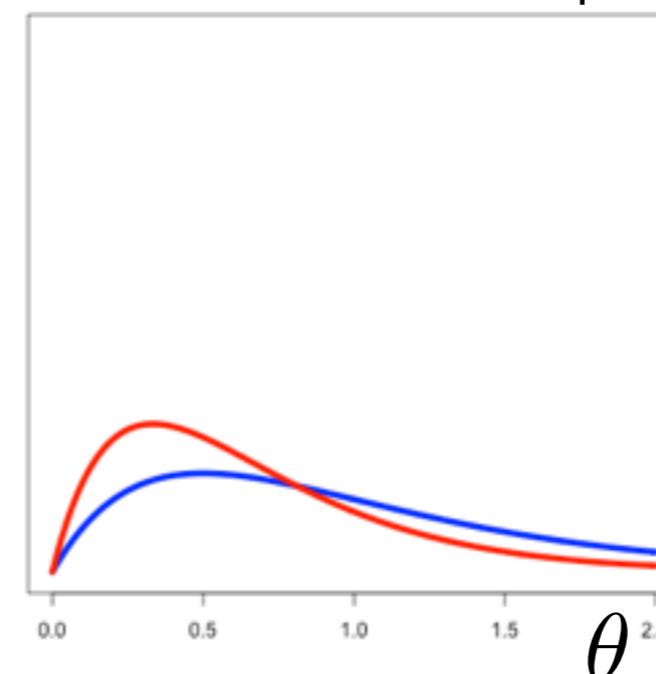


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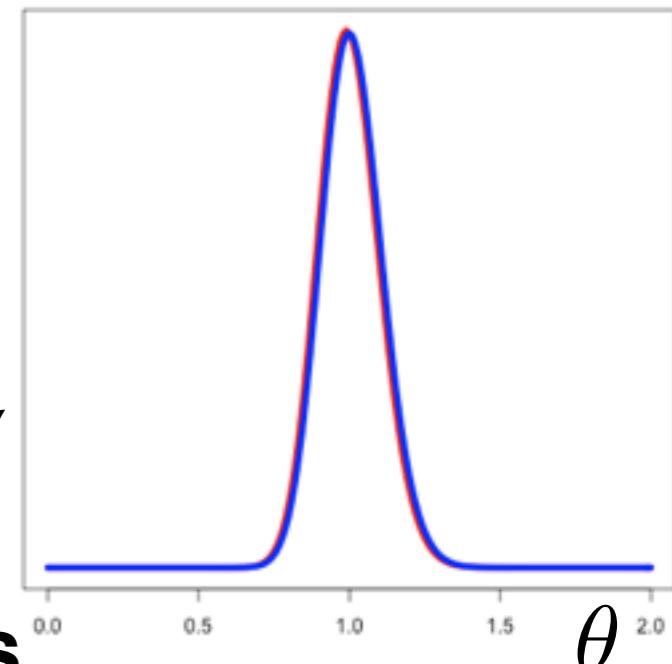
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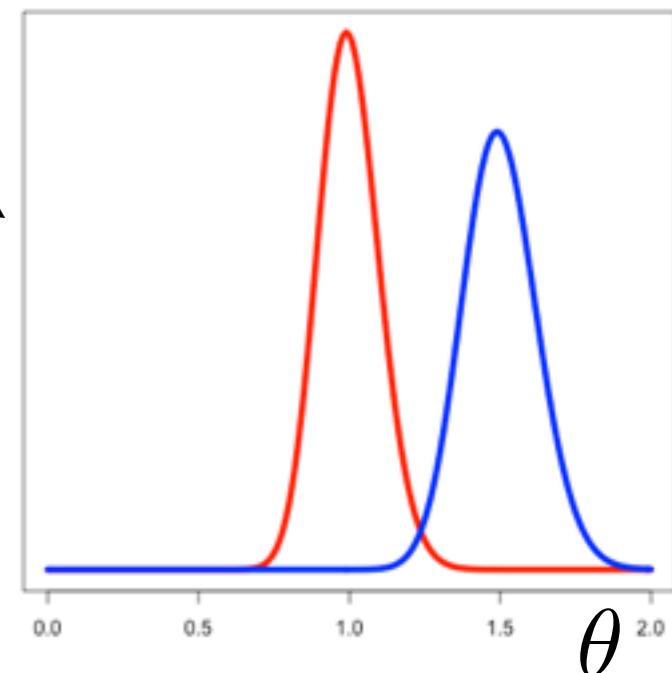
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variational Bayes

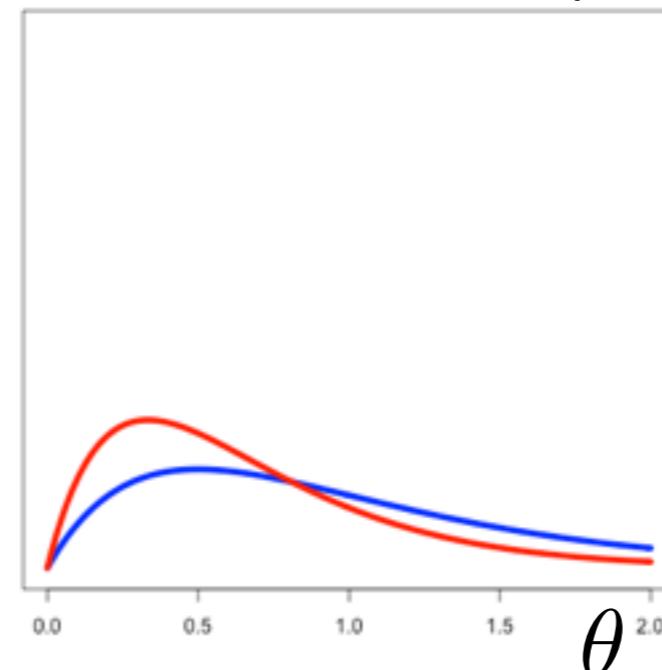


Uncertainty & robustness quantification

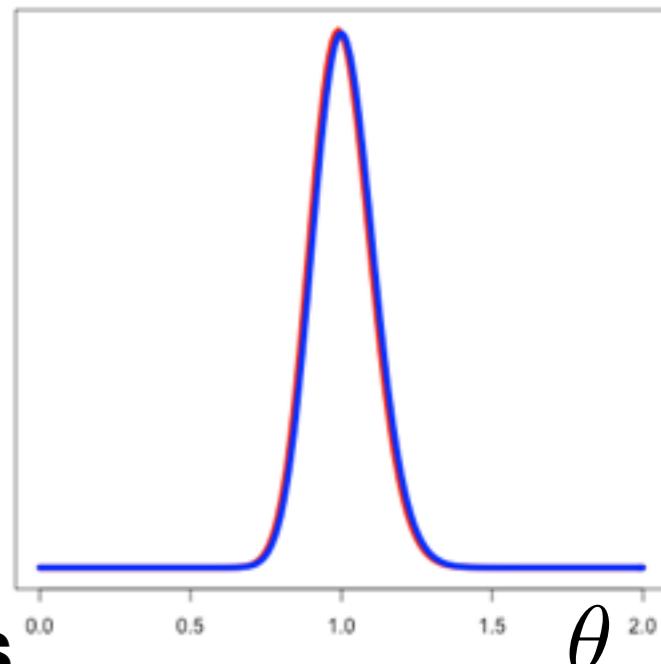
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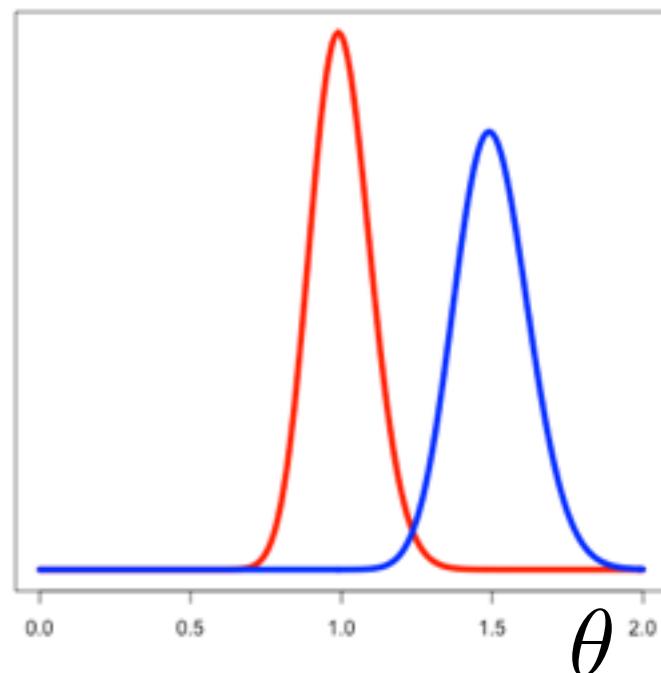


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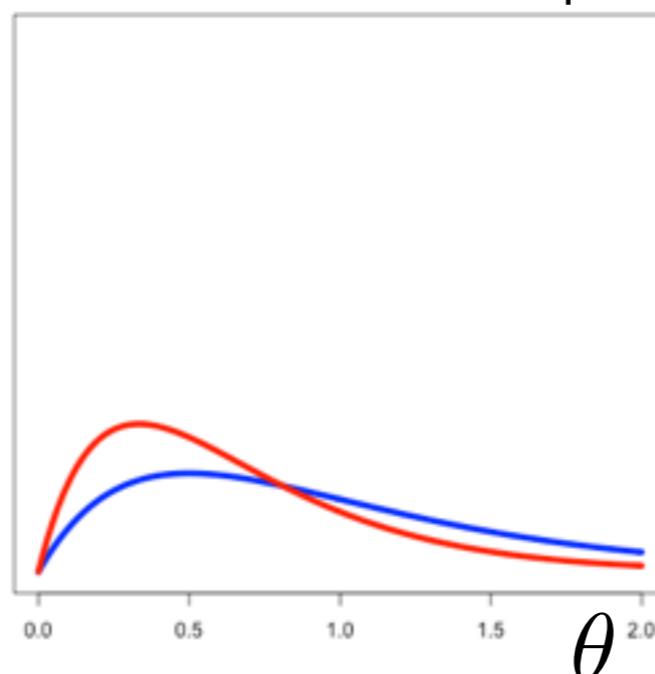


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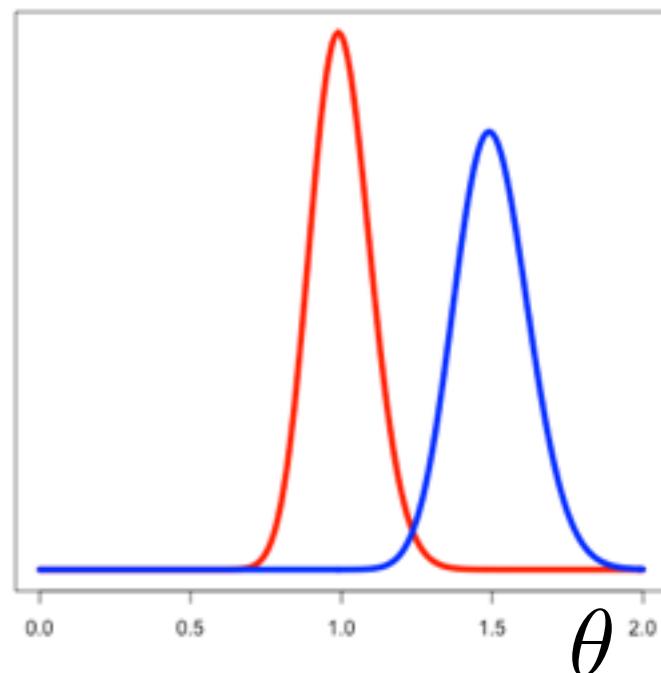
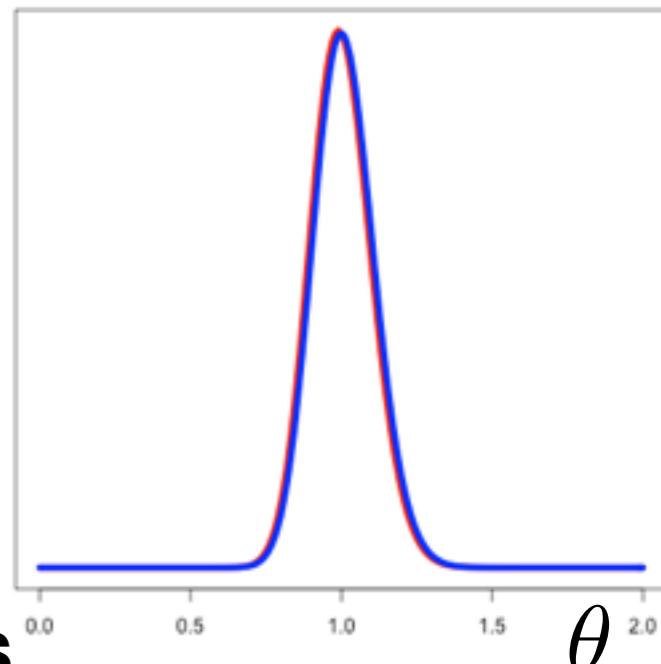
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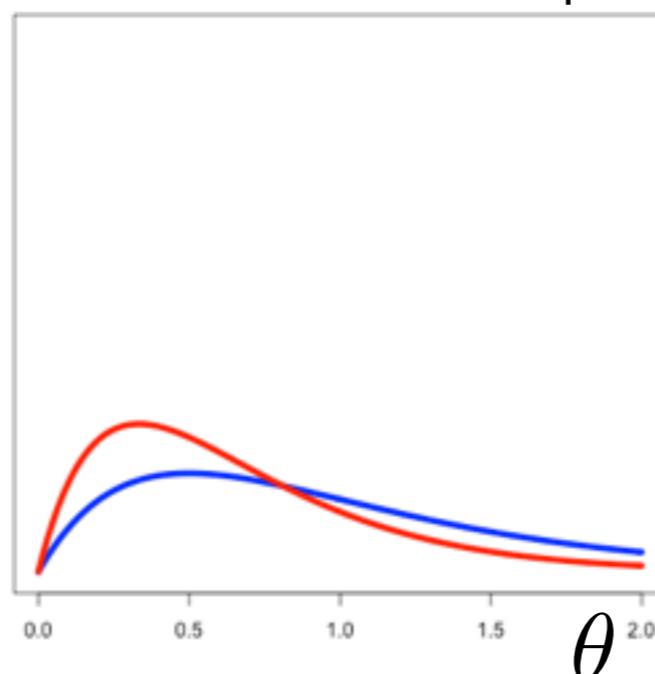
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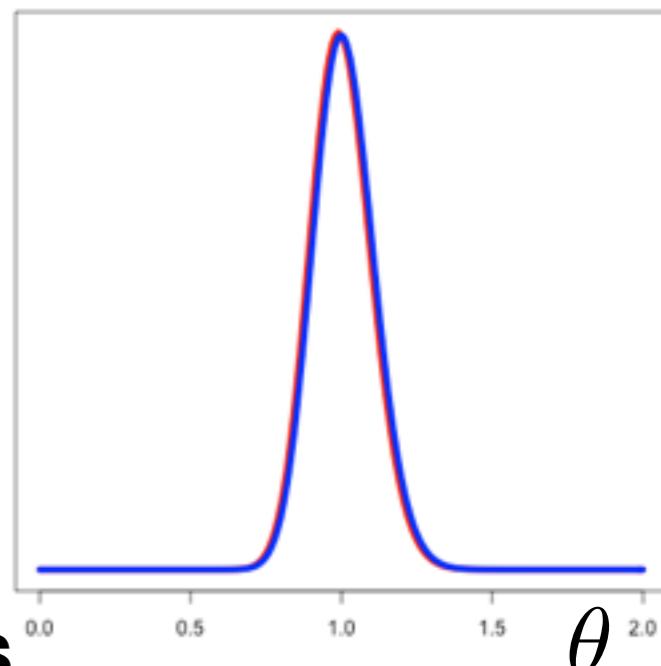
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[see also Opper, Winther 2003]

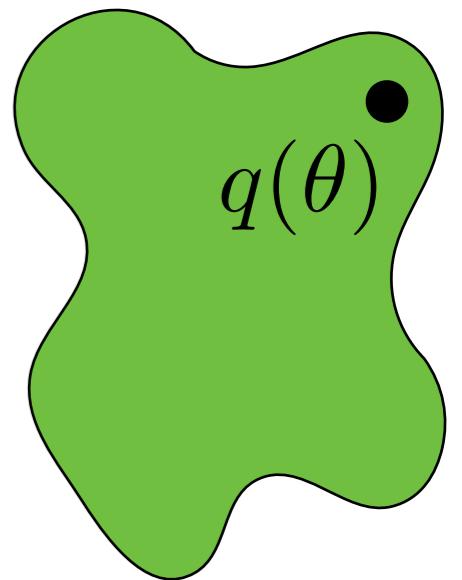
Roadmap

- Challenges of VB
- Accurate uncertainties from VB
- Accurate robustness quantification from VB
 - Big idea: derivatives/perturbations are relatively easy in VB

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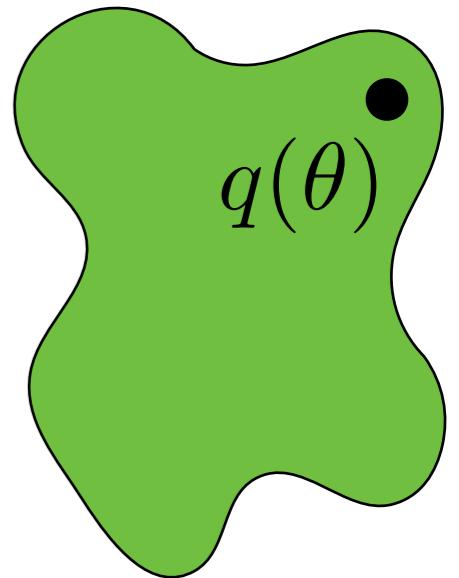
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What about uncertainty?



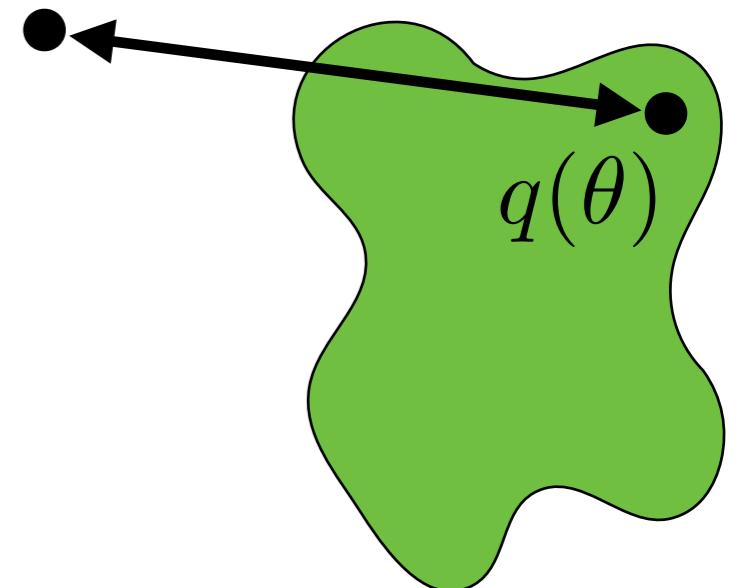
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$$p(\theta|y)$$



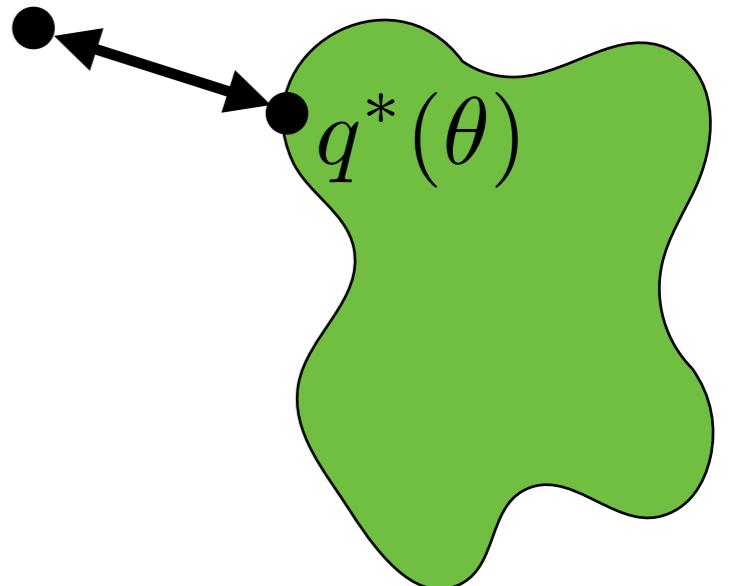
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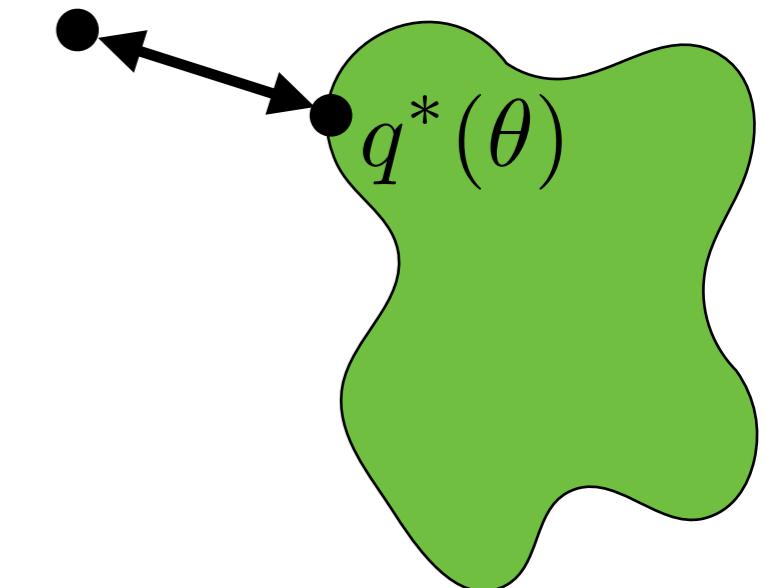


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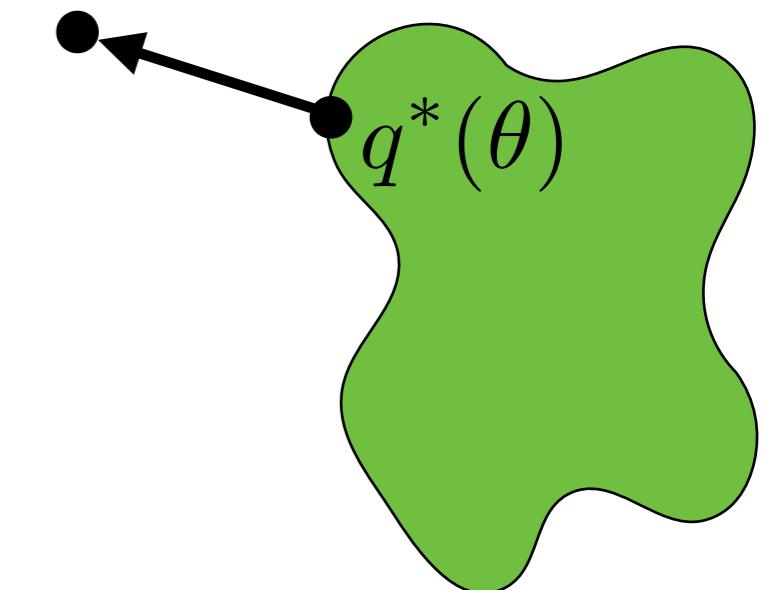


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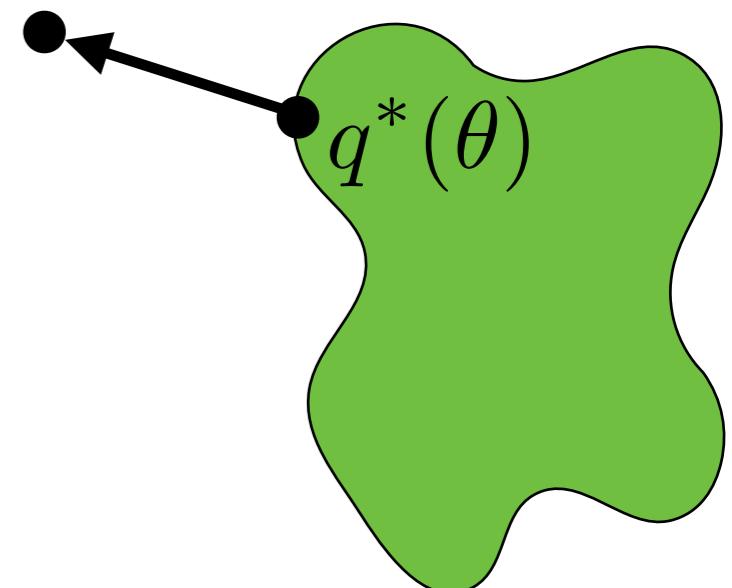
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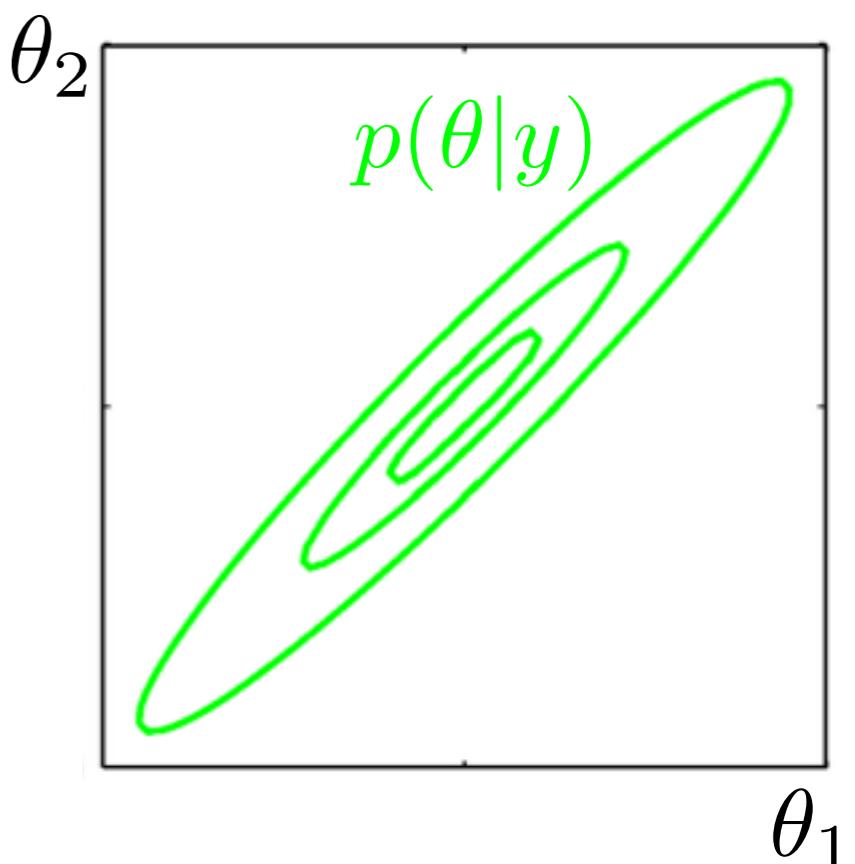
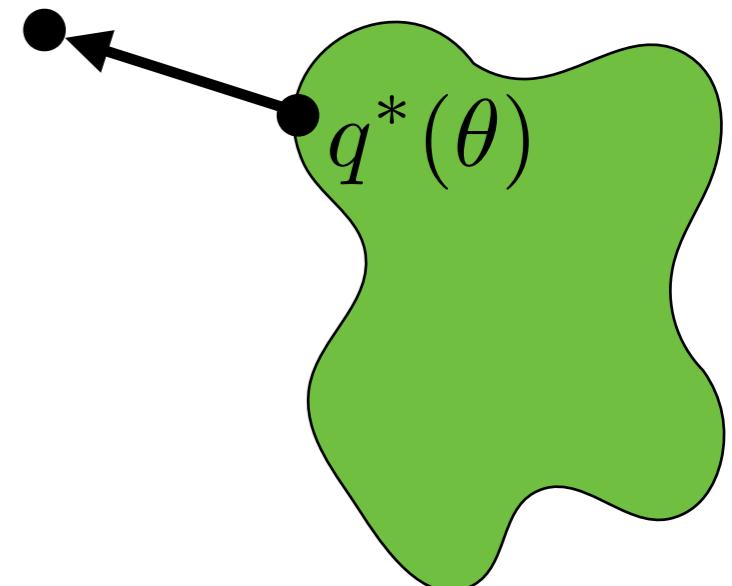
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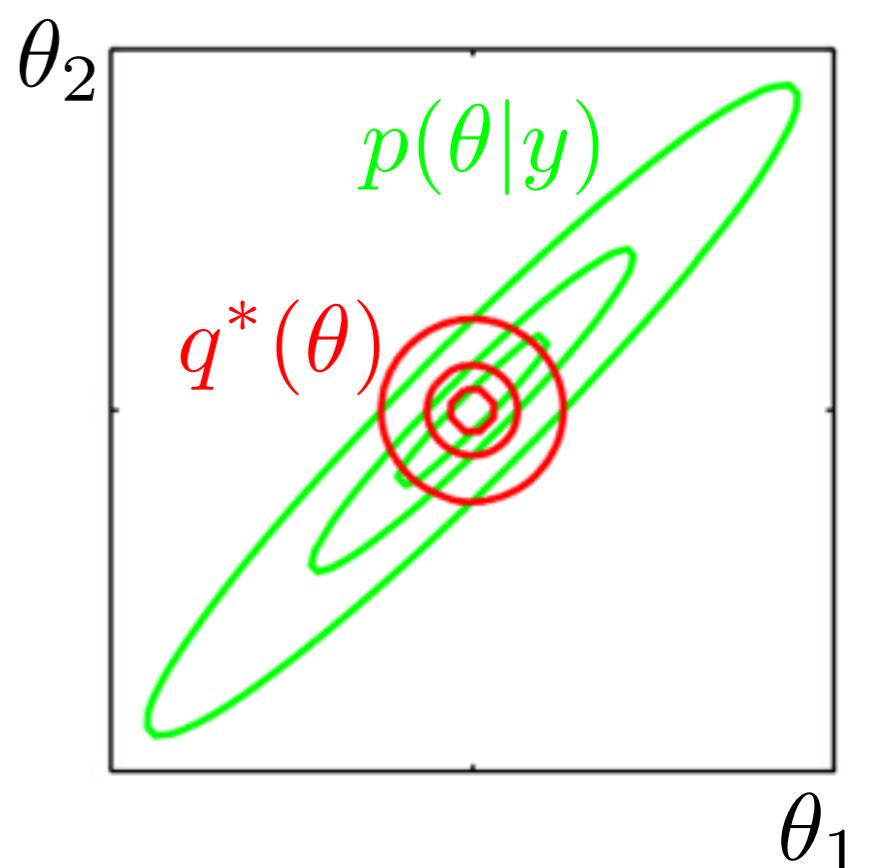
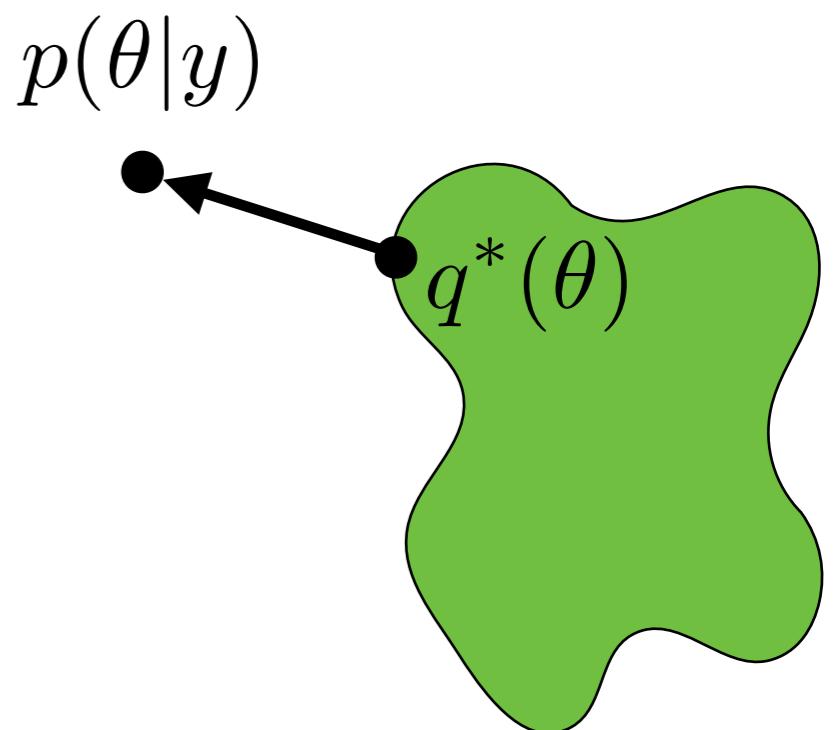
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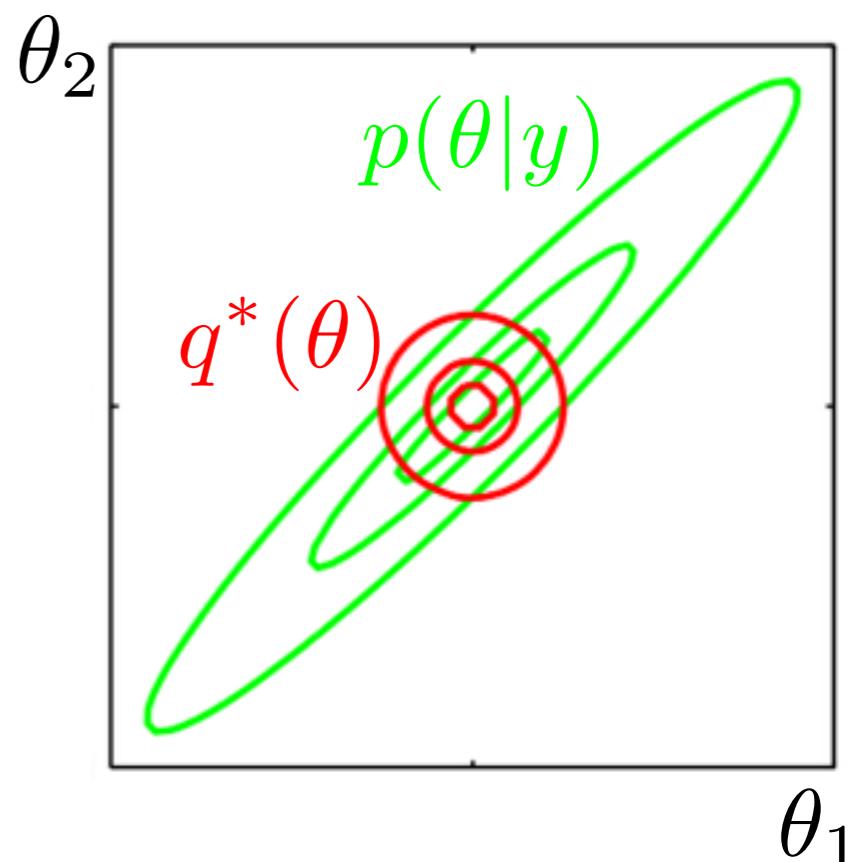
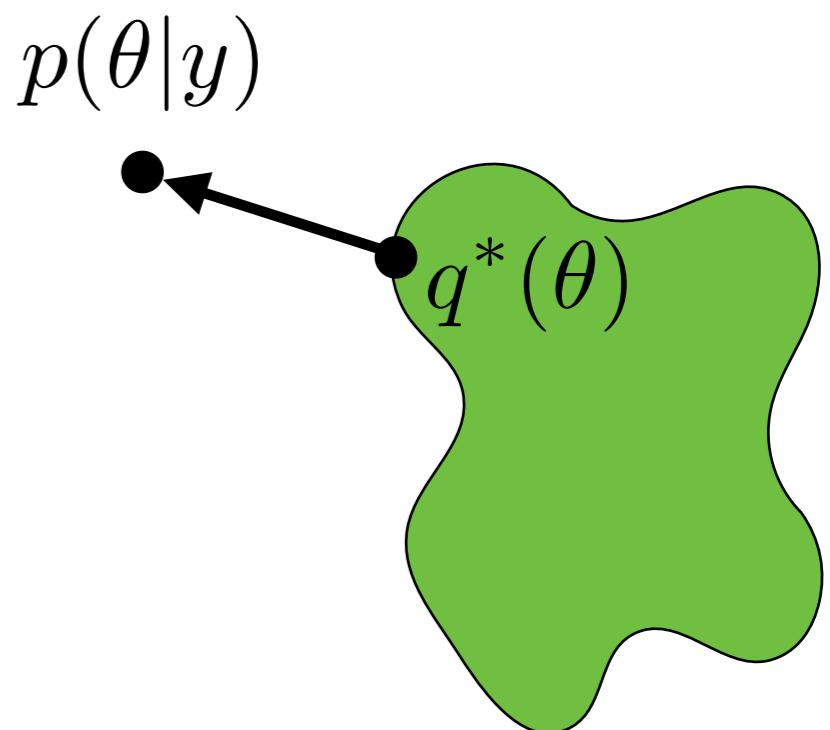
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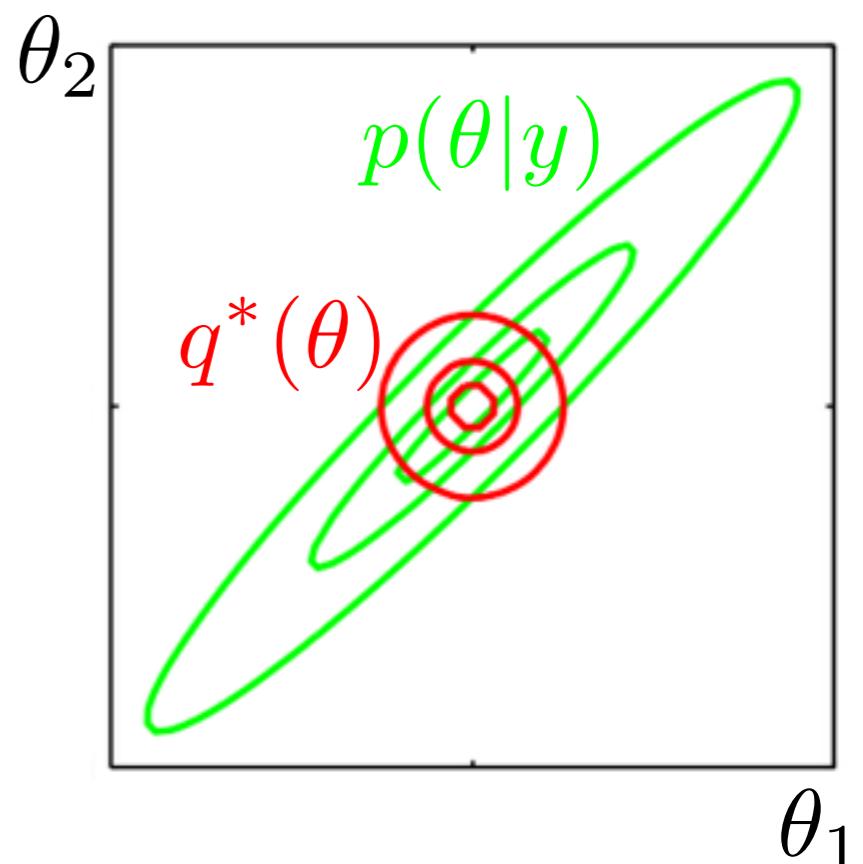
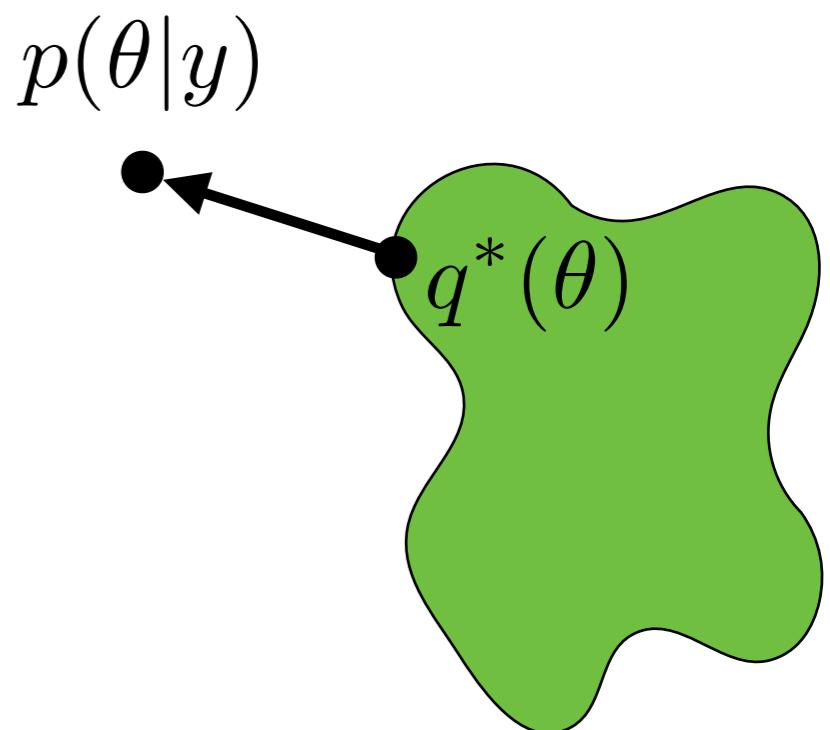
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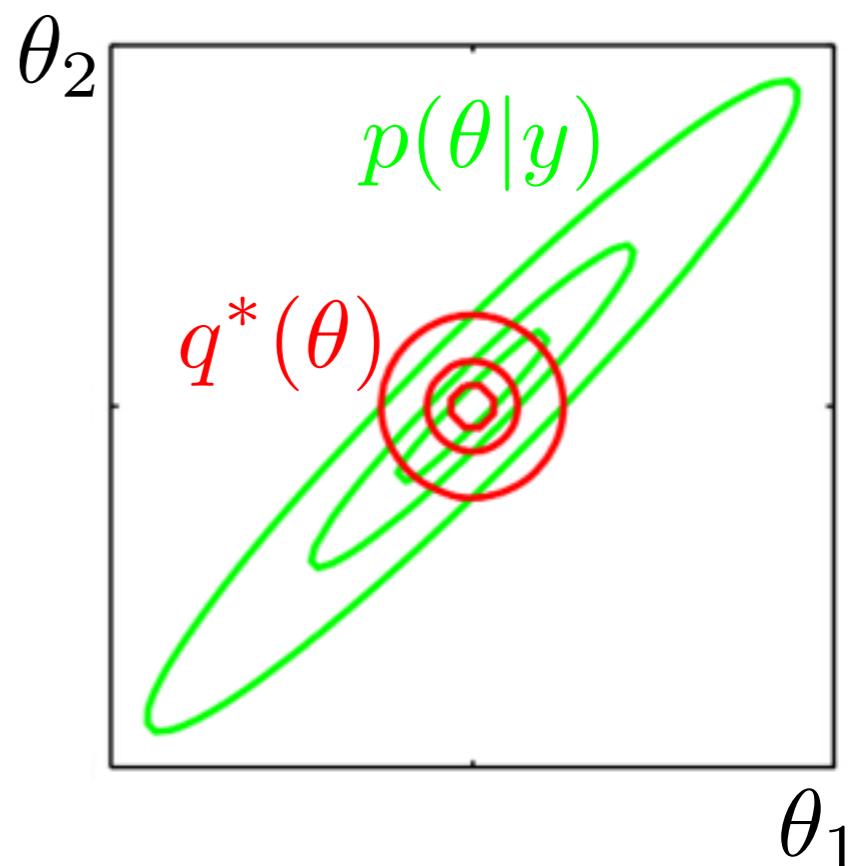
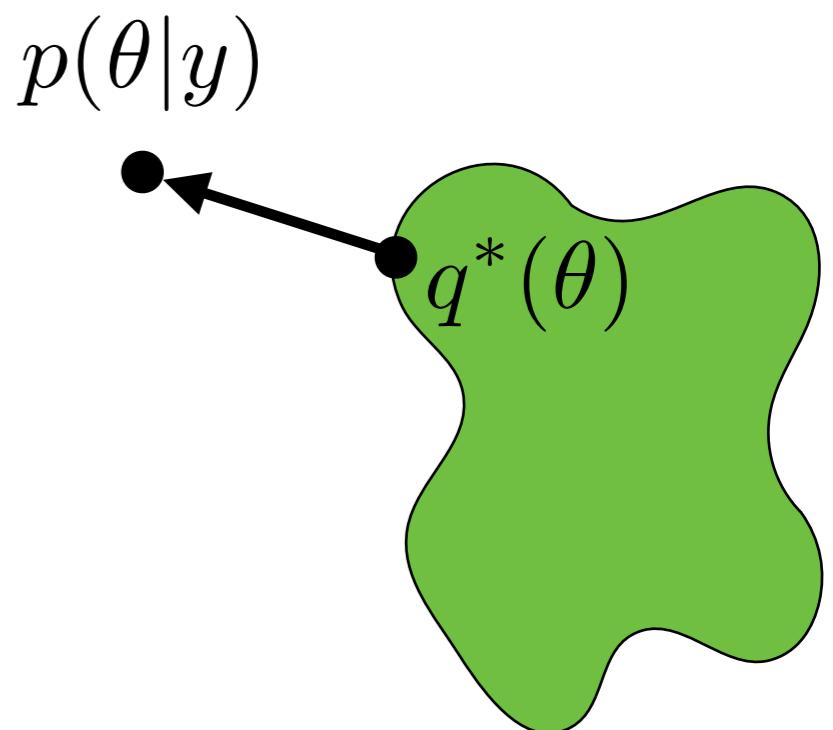
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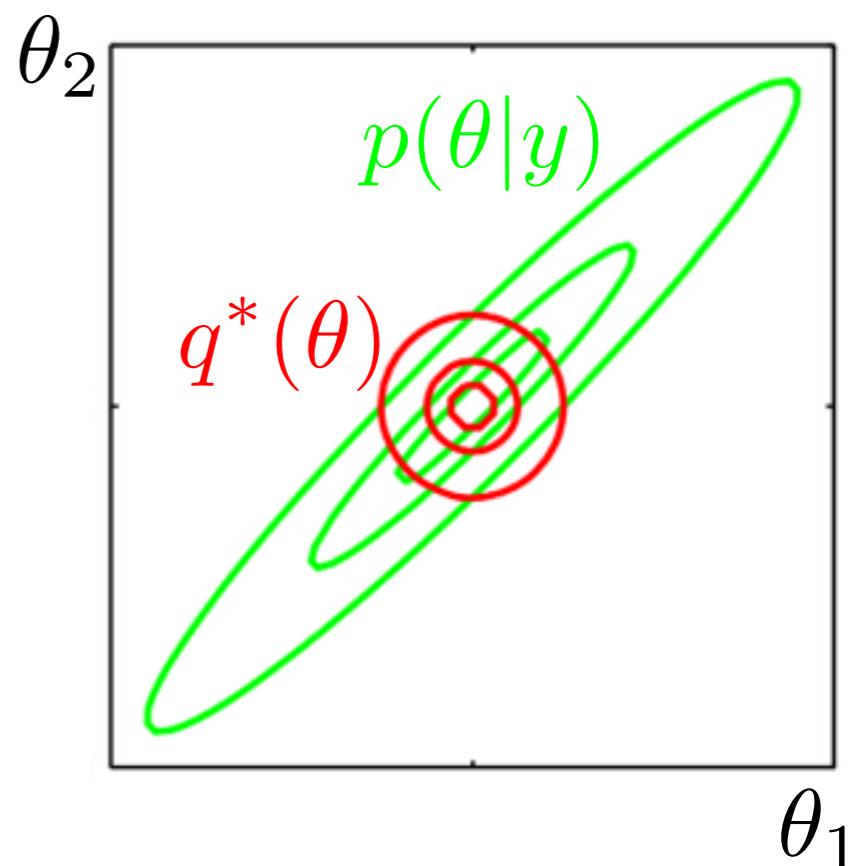
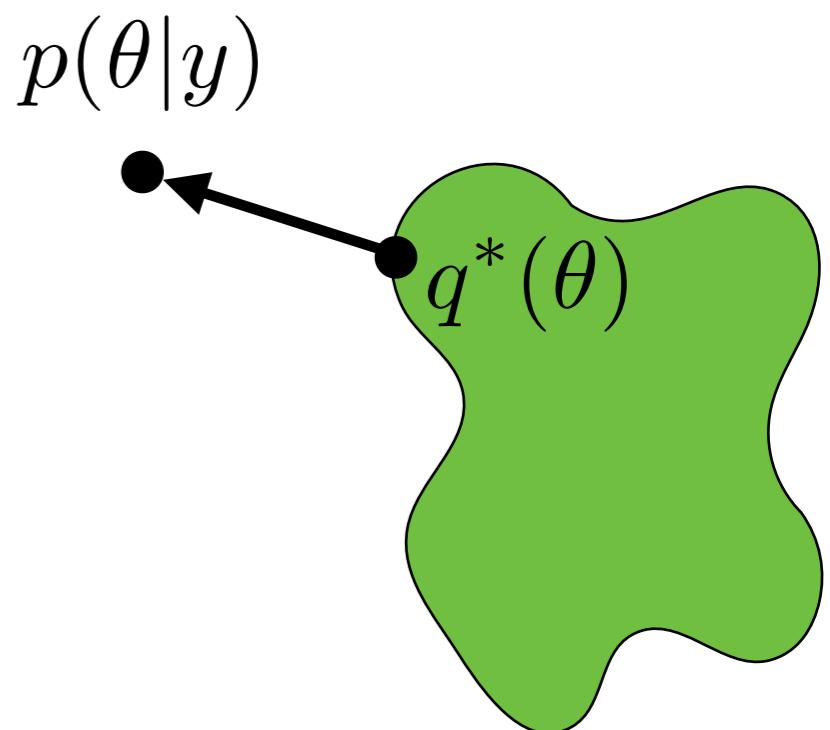
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[MacKay 2003; Bishop 2006; Wang, Titterington 2004; Turner, Sahani 2011]

[Fosdick 2013; Dunson 2014; Bardenet, Doucet, Holmes 2017]

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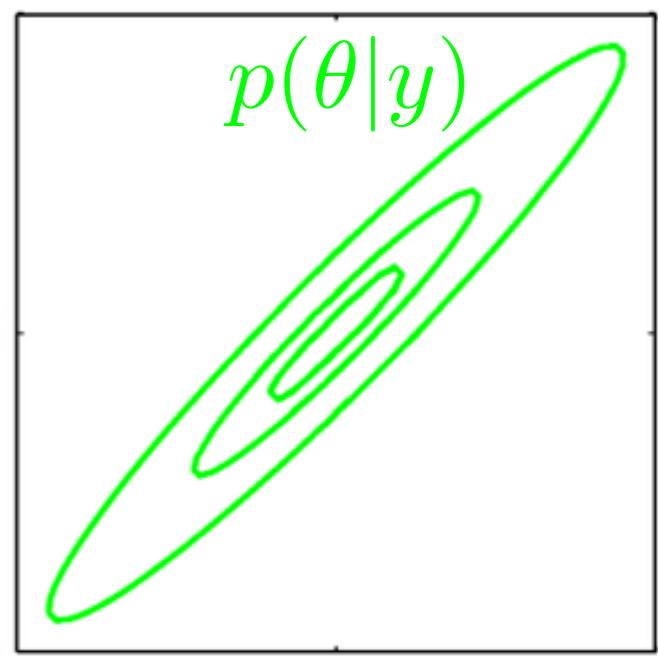
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[adapted from Bishop 2006]

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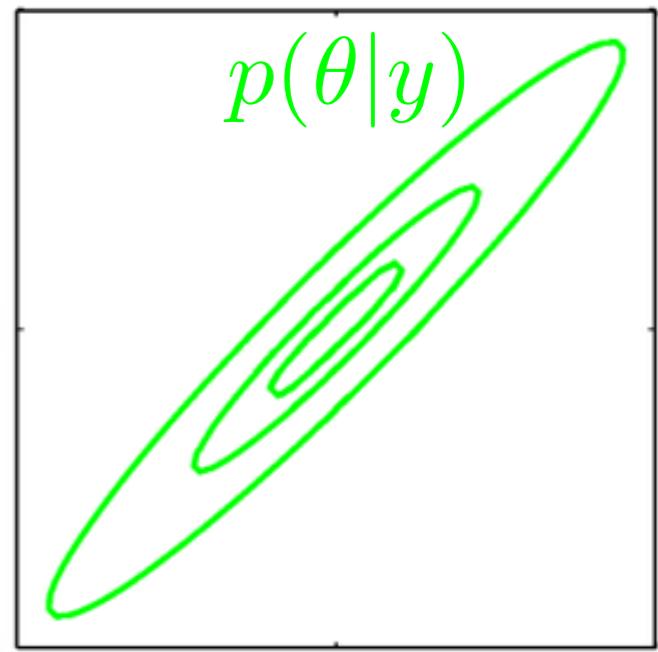
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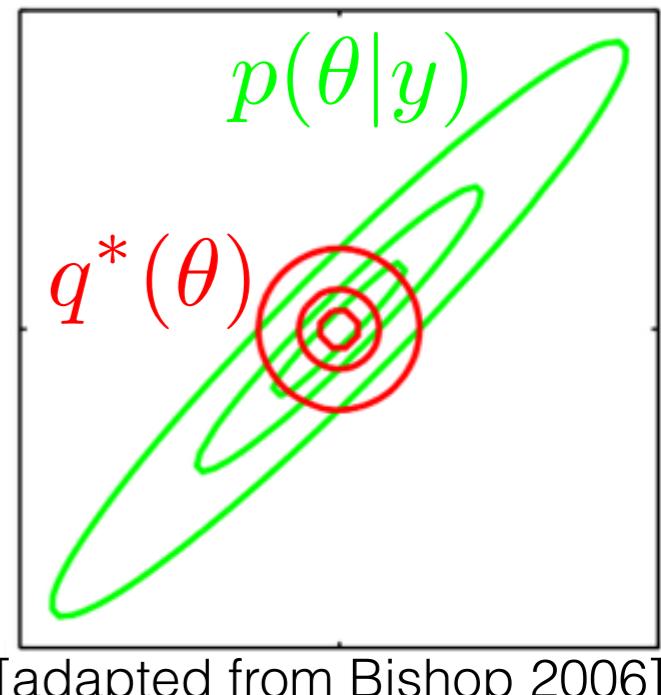
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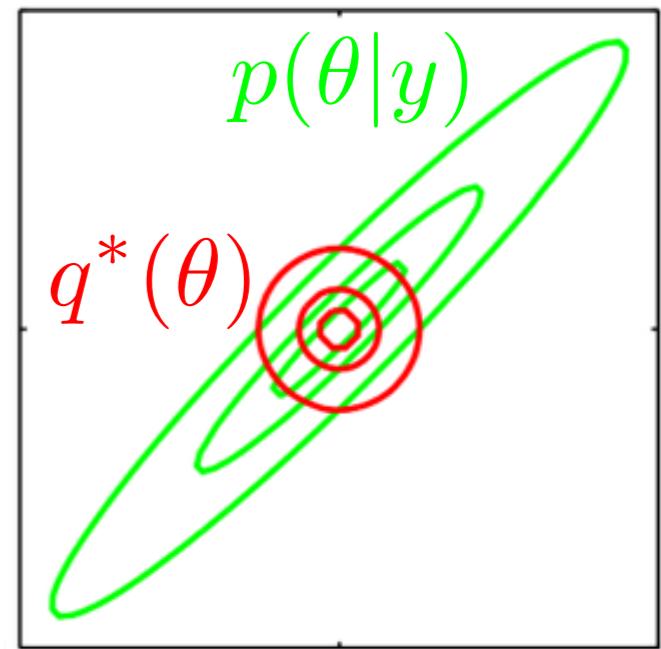
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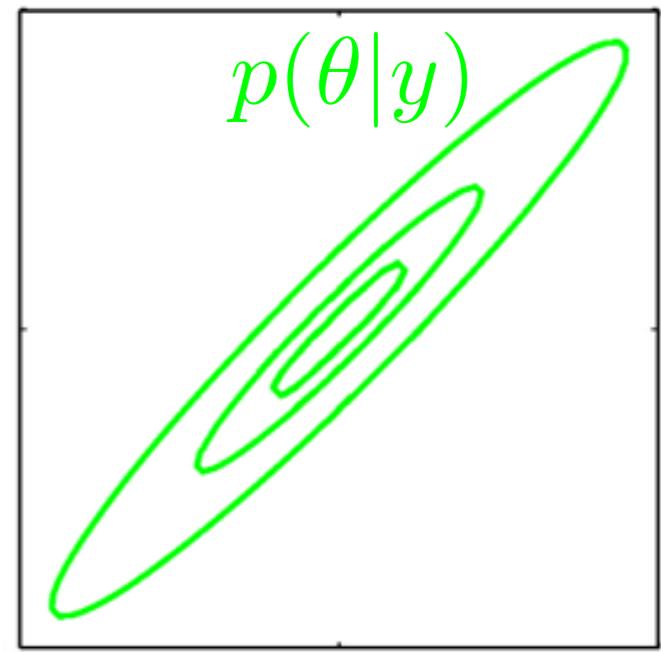
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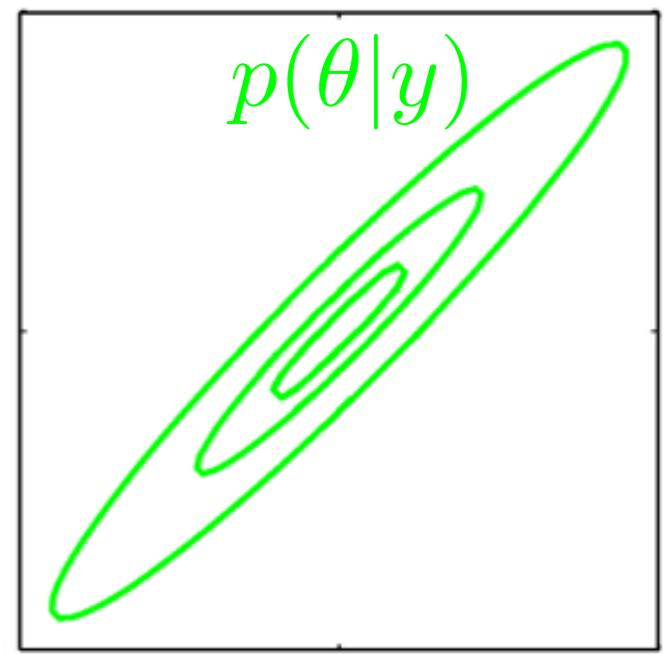
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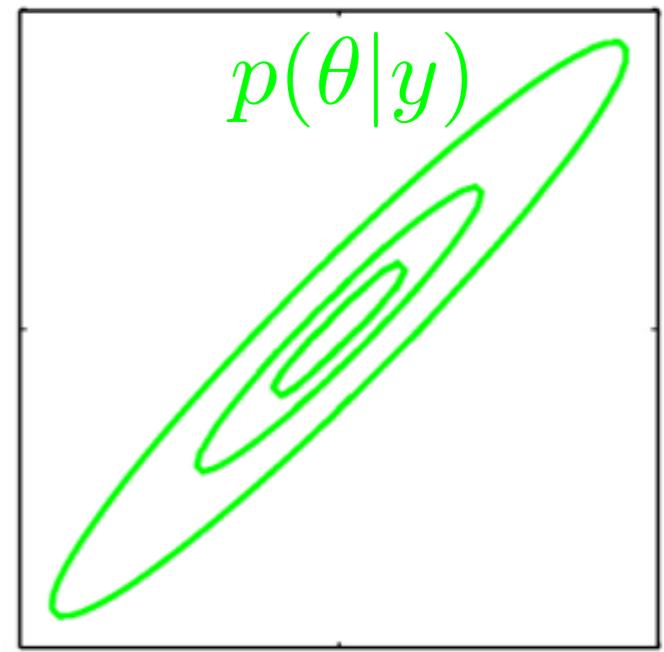
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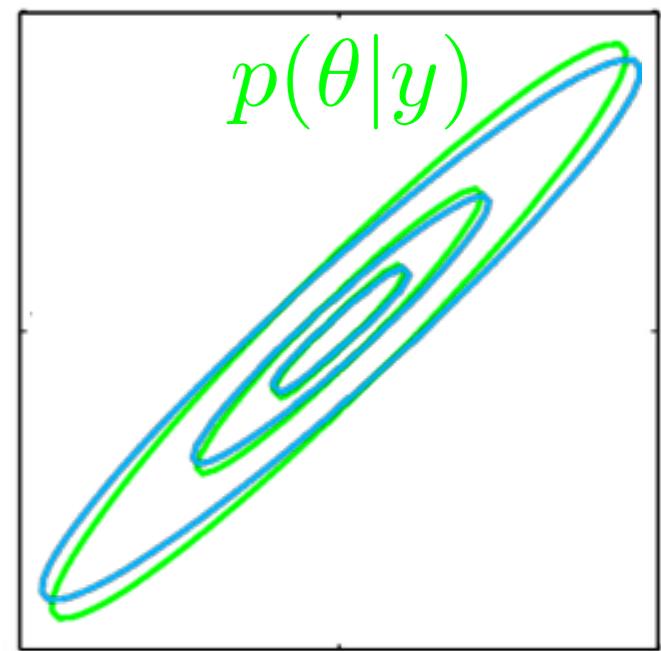
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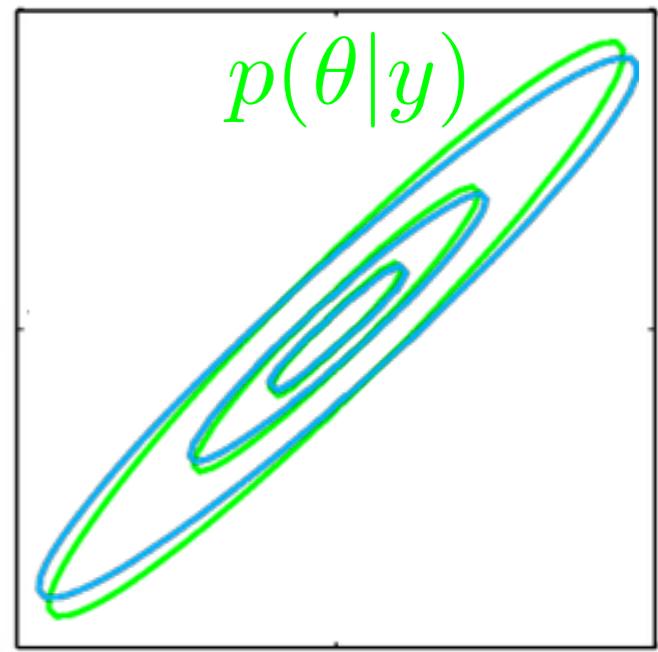
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$$C(t) := \log \mathbb{E} e^{t^T \theta}$$

$$\text{mean} = \left. \frac{d}{dt} C(t) \right|_{t=0}$$

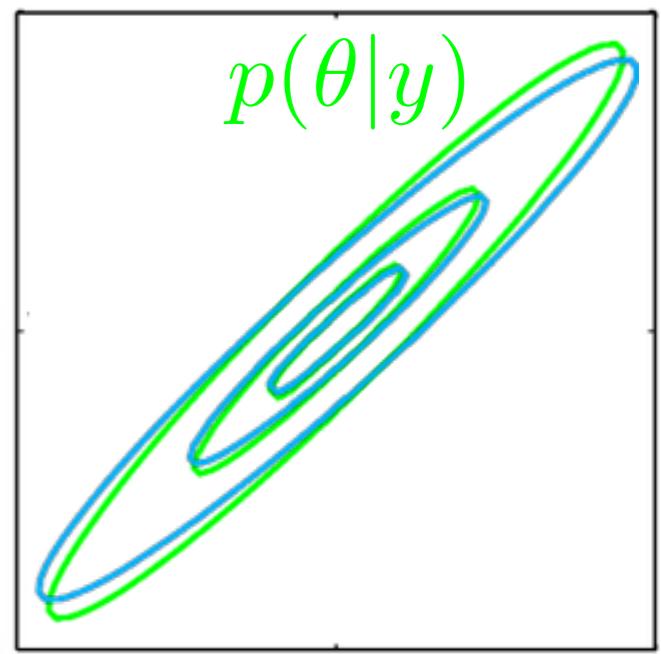
- Exact posterior covariance vs MFVB covariance

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[adapted from Bishop 2006]

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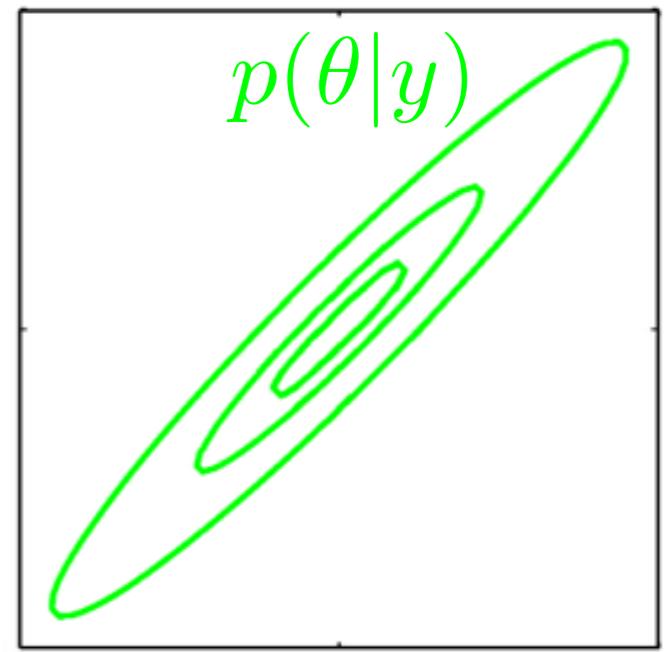
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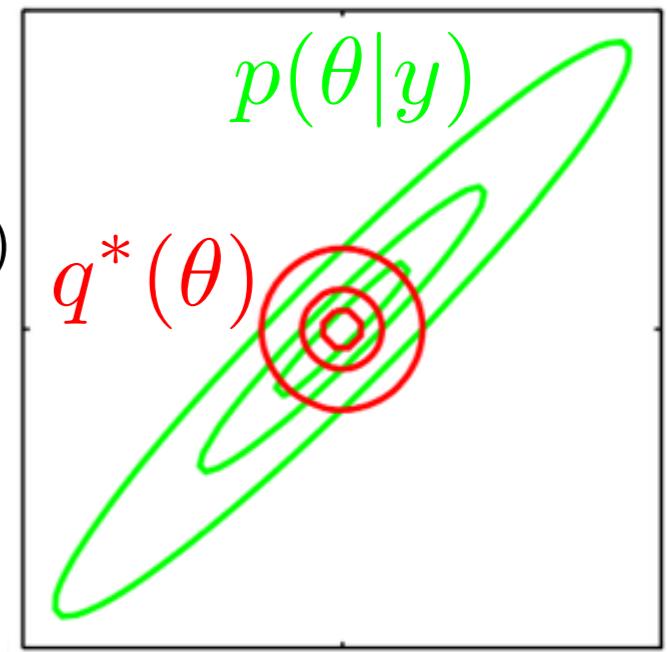
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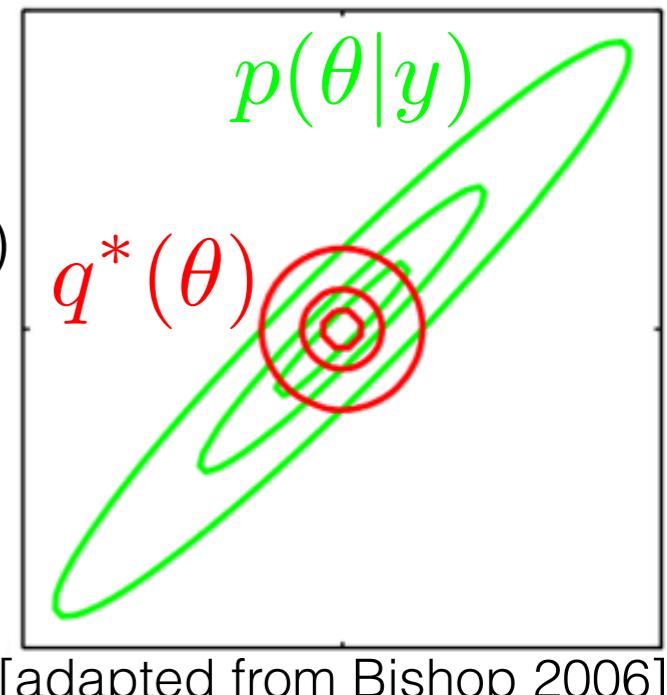
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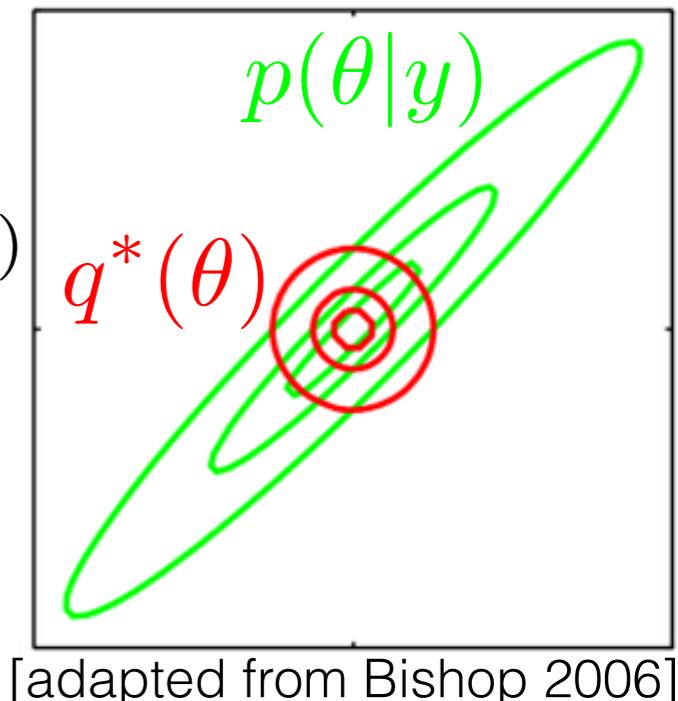
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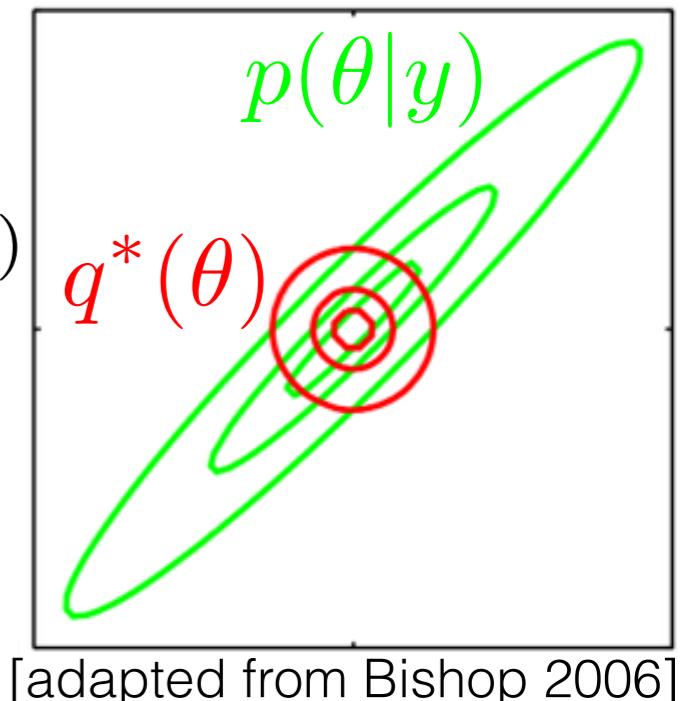
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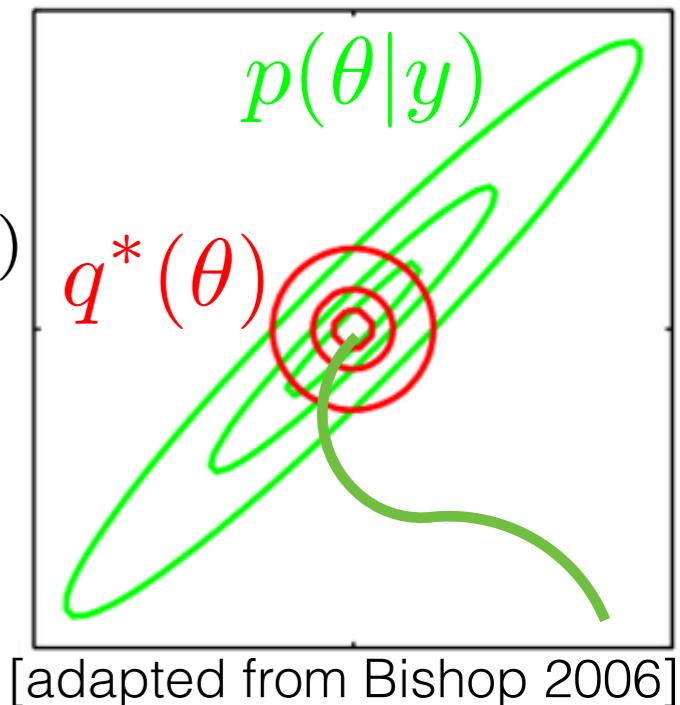
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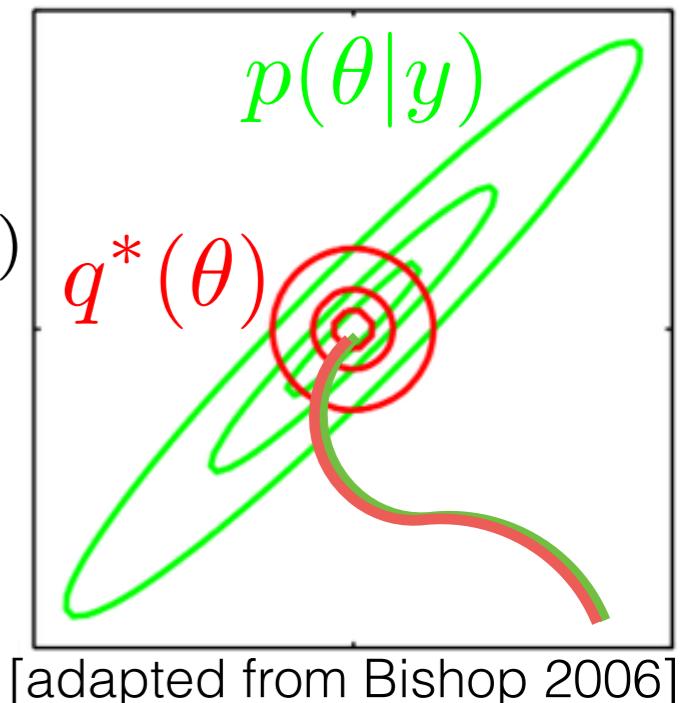
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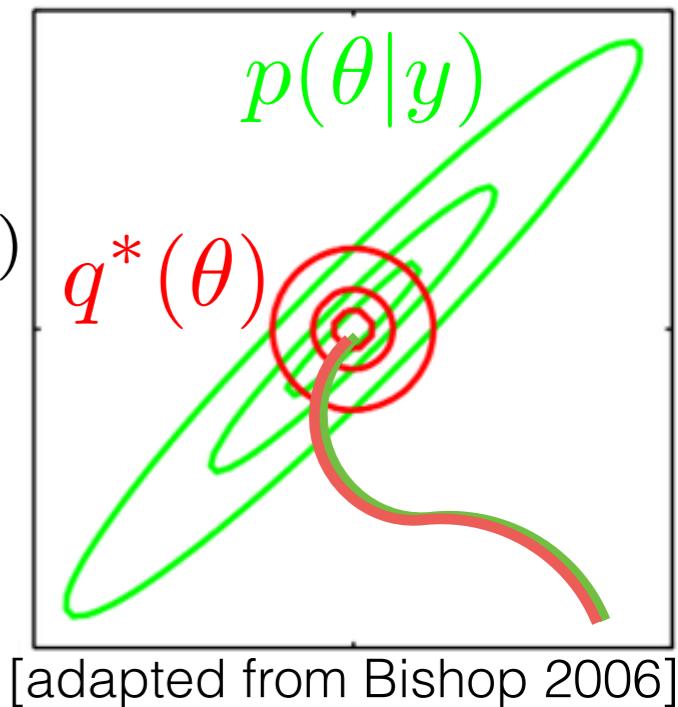
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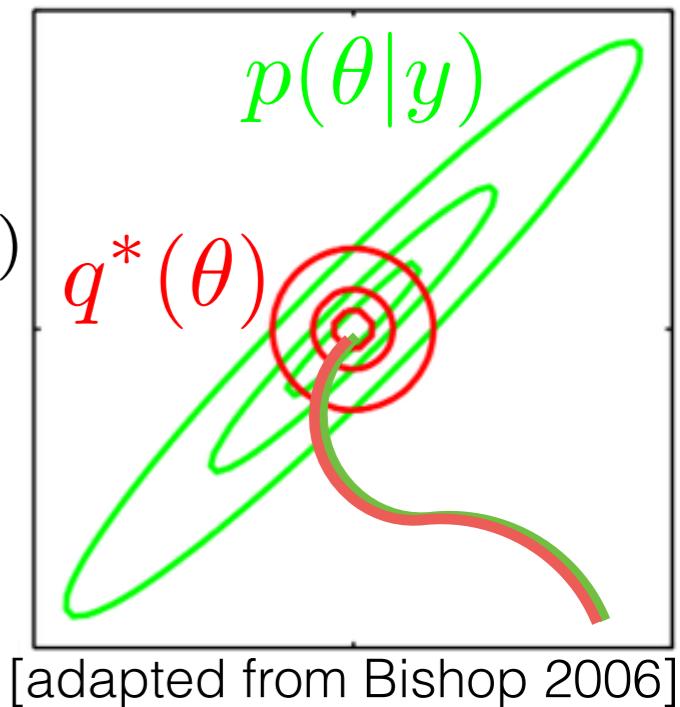
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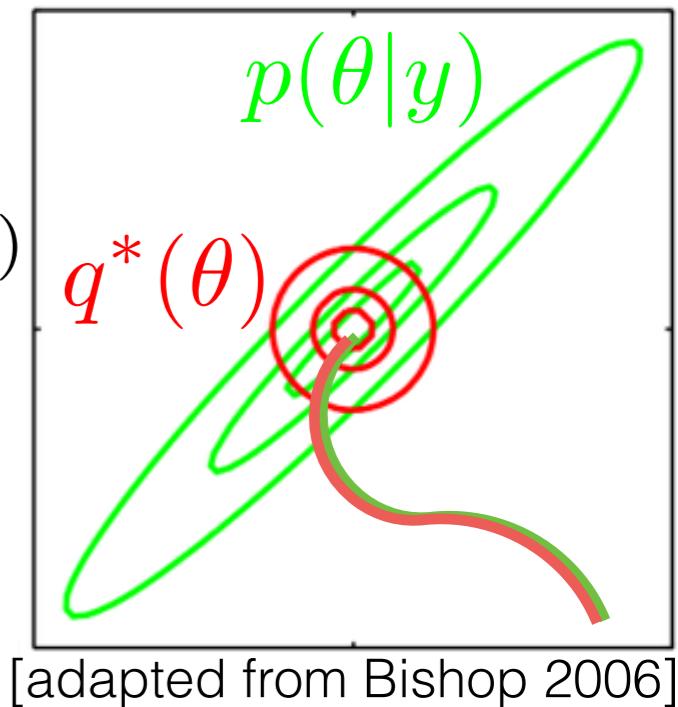
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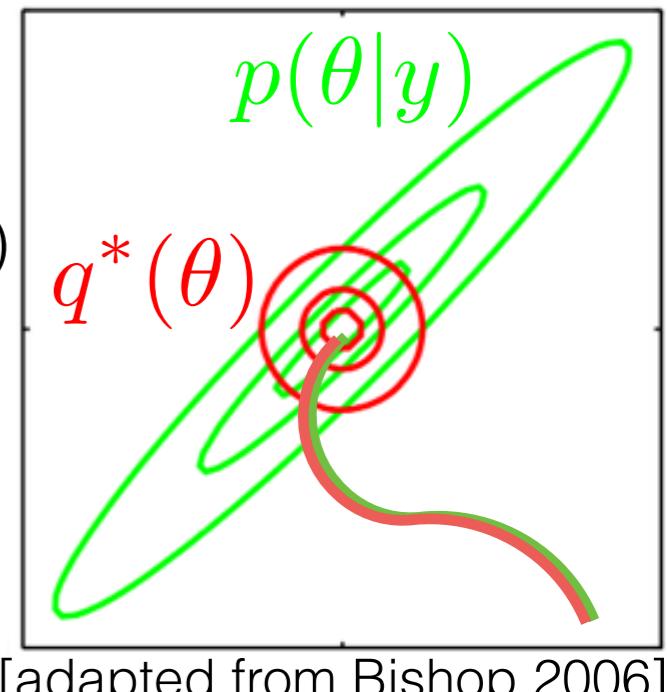
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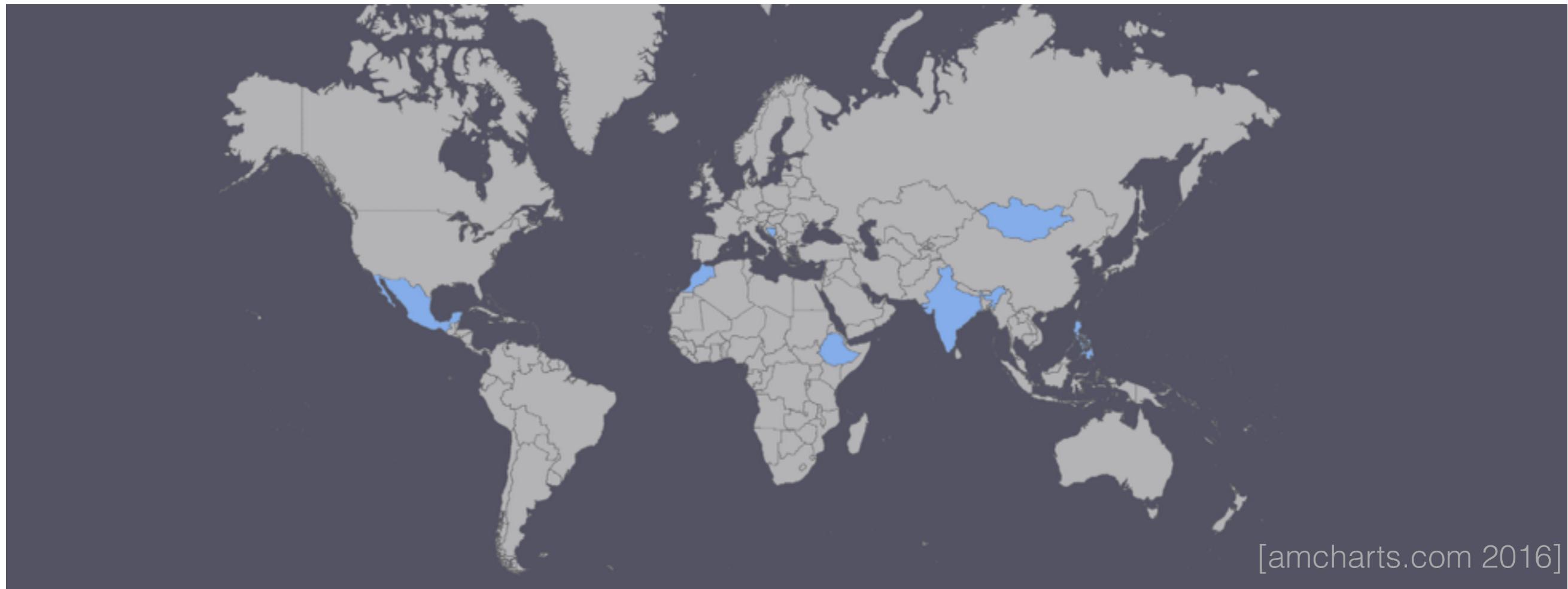
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Microcredit Experiment



[amcharts.com 2016]

Microcredit Experiment

- Simplified from Meager (2018a)
- K 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:
$$y_{kn} \stackrel{\text{indep}}{\sim} \mathcal{N}(\mu_k + T_{kn}\tau_k, \sigma_k^2)$$

profit

1 if microcredit

- Priors and hyperpriors:

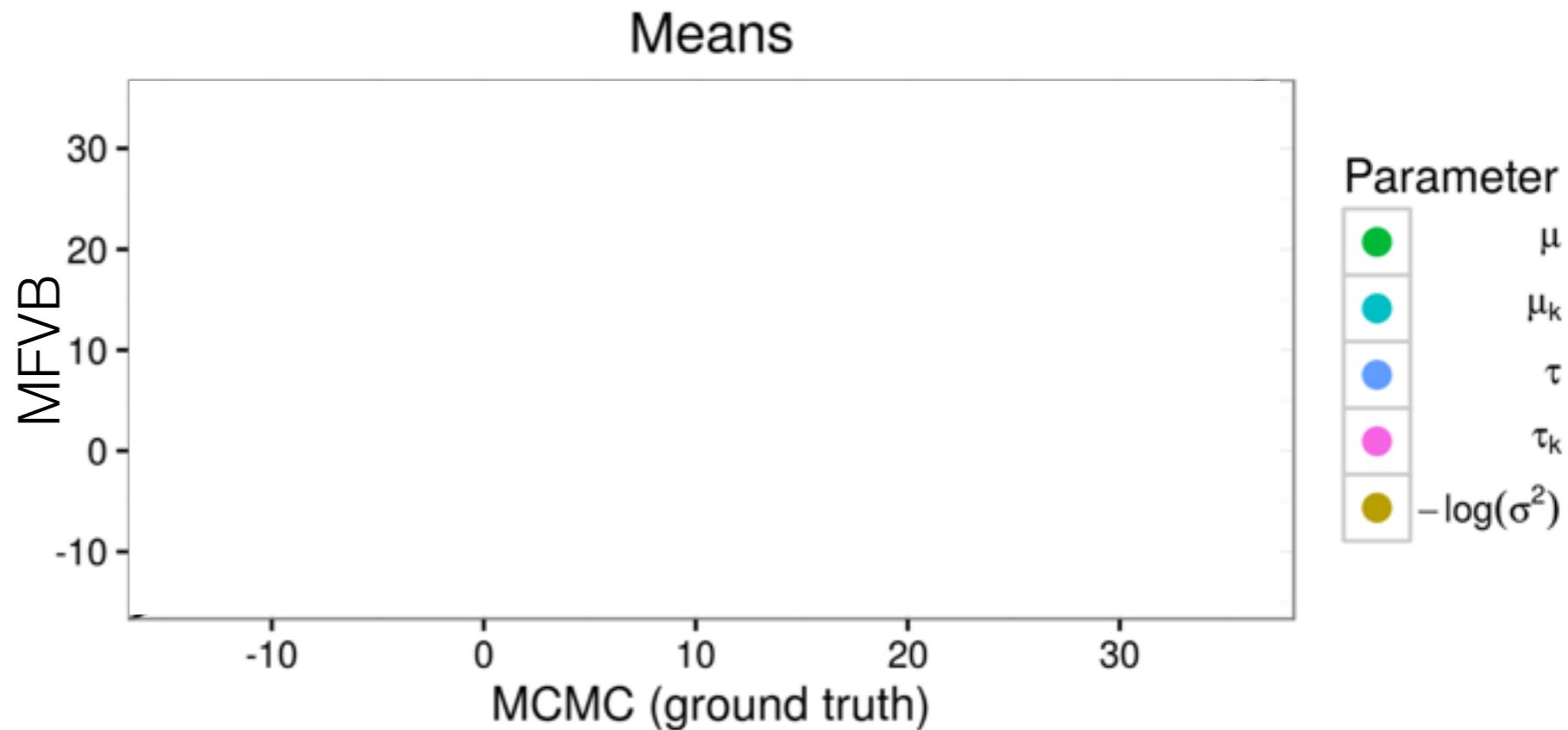
$$\begin{pmatrix} \mu_k \\ \tau_k \end{pmatrix} \stackrel{iid}{\sim} \mathcal{N}\left(\begin{pmatrix} \mu \\ \tau \end{pmatrix}, C\right)$$

$$\begin{pmatrix} \mu \\ \tau \end{pmatrix} \stackrel{iid}{\sim} \mathcal{N}\left(\begin{pmatrix} \mu_0 \\ \tau_0 \end{pmatrix}, \Lambda^{-1}\right)$$

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

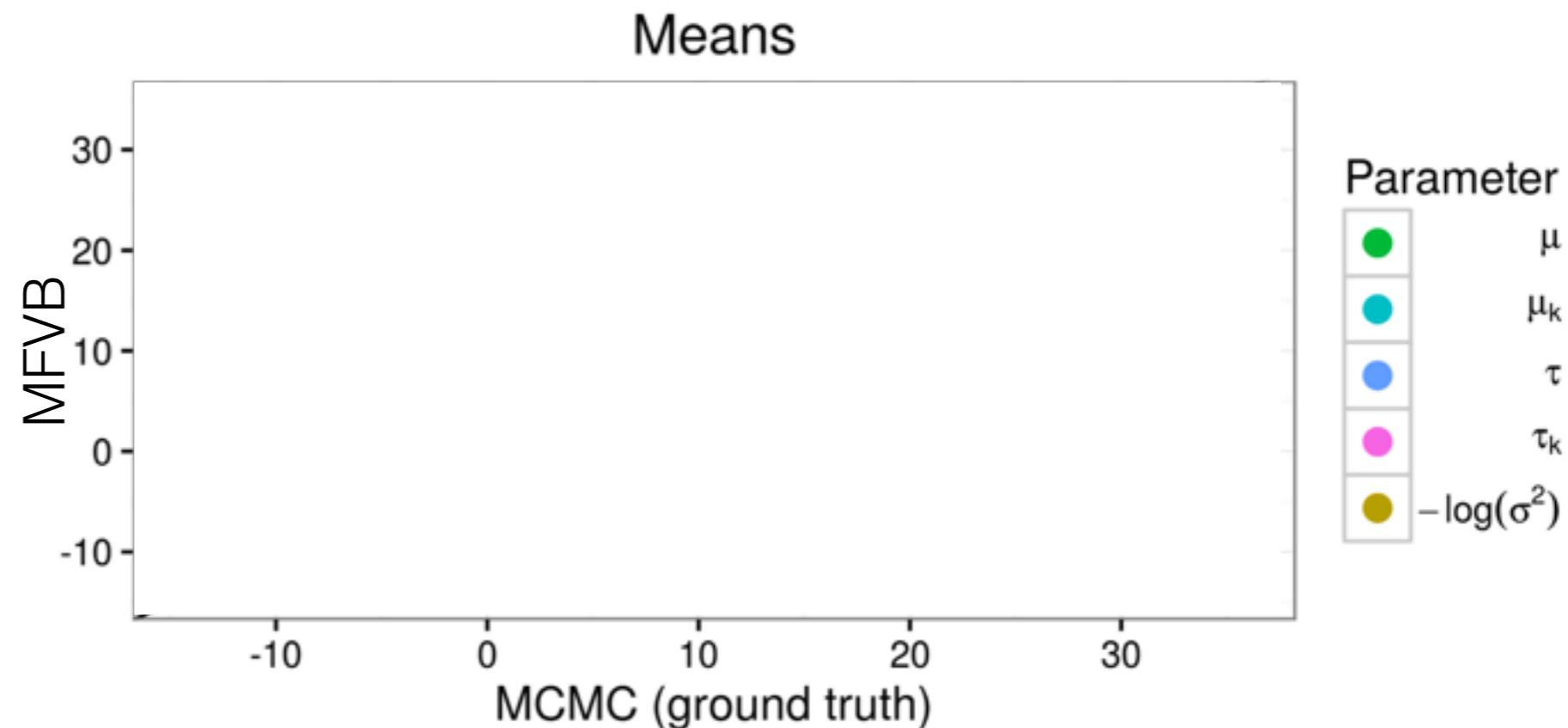
$$C \sim \text{Sep\&LKJ}(\eta, c, d)$$

Microcredit Experiment



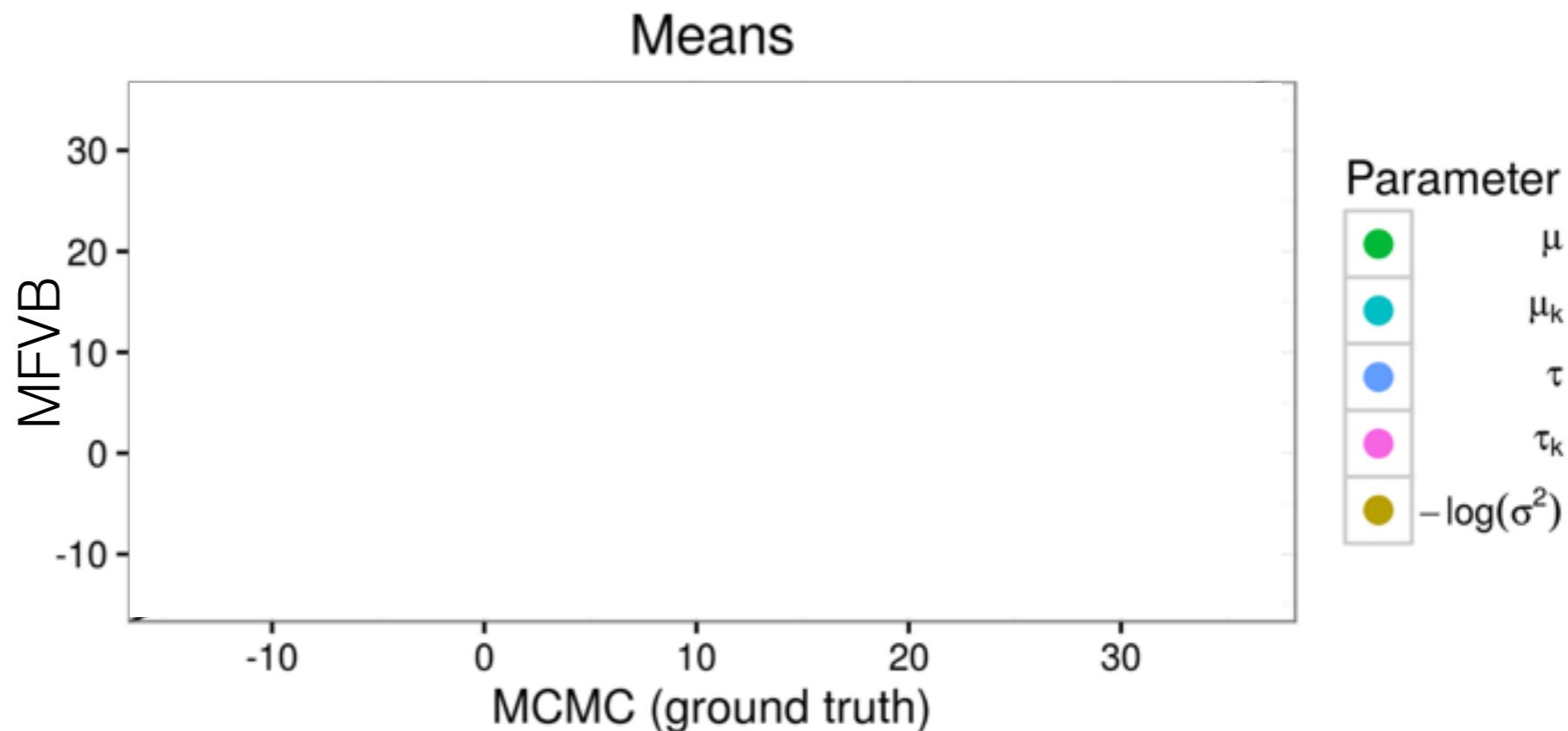
Microcredit Experiment

- One set of 2500 MCMC draws:
45 minutes



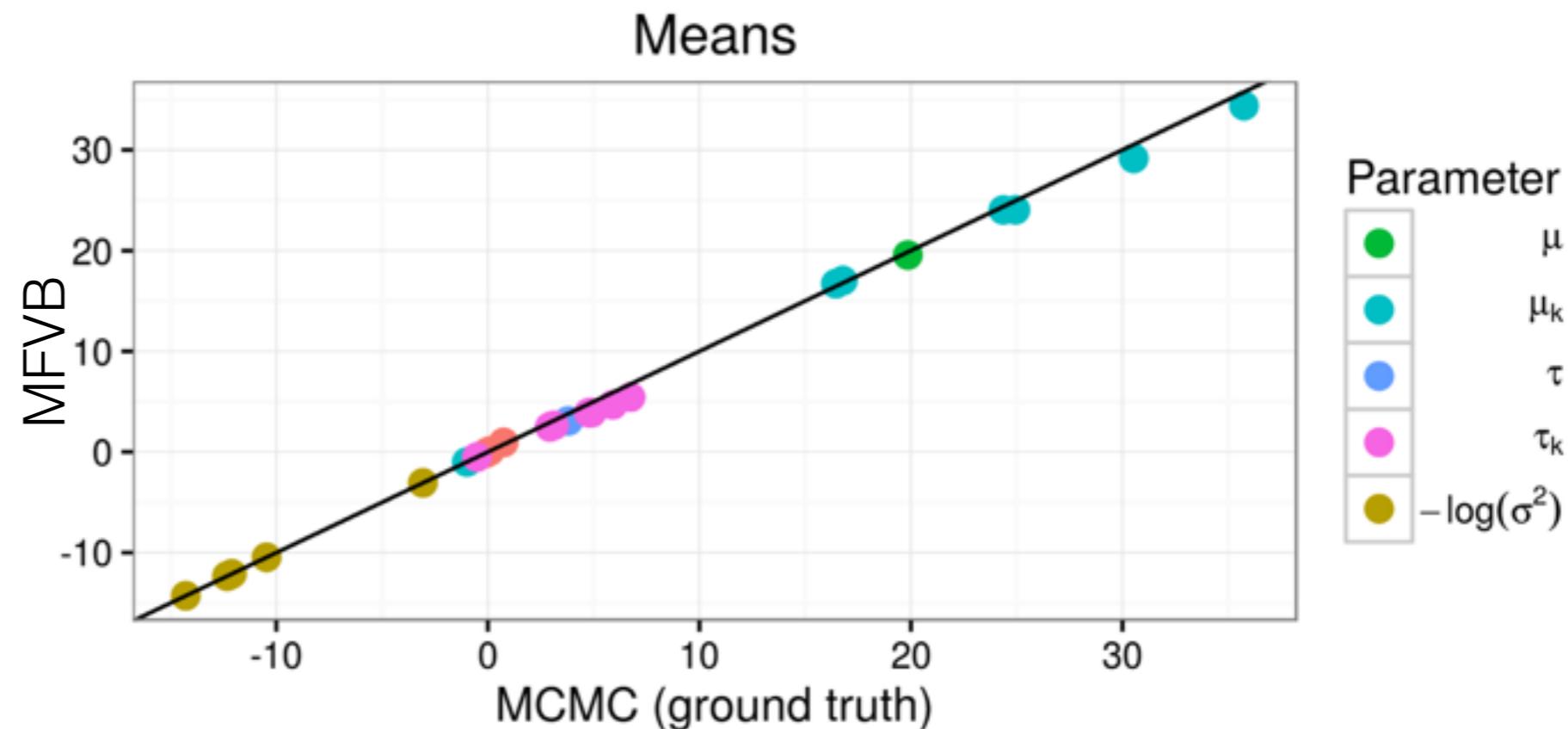
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- All of MFVB optimization, LRVB uncertainties, all sensitivity measures:
58 seconds



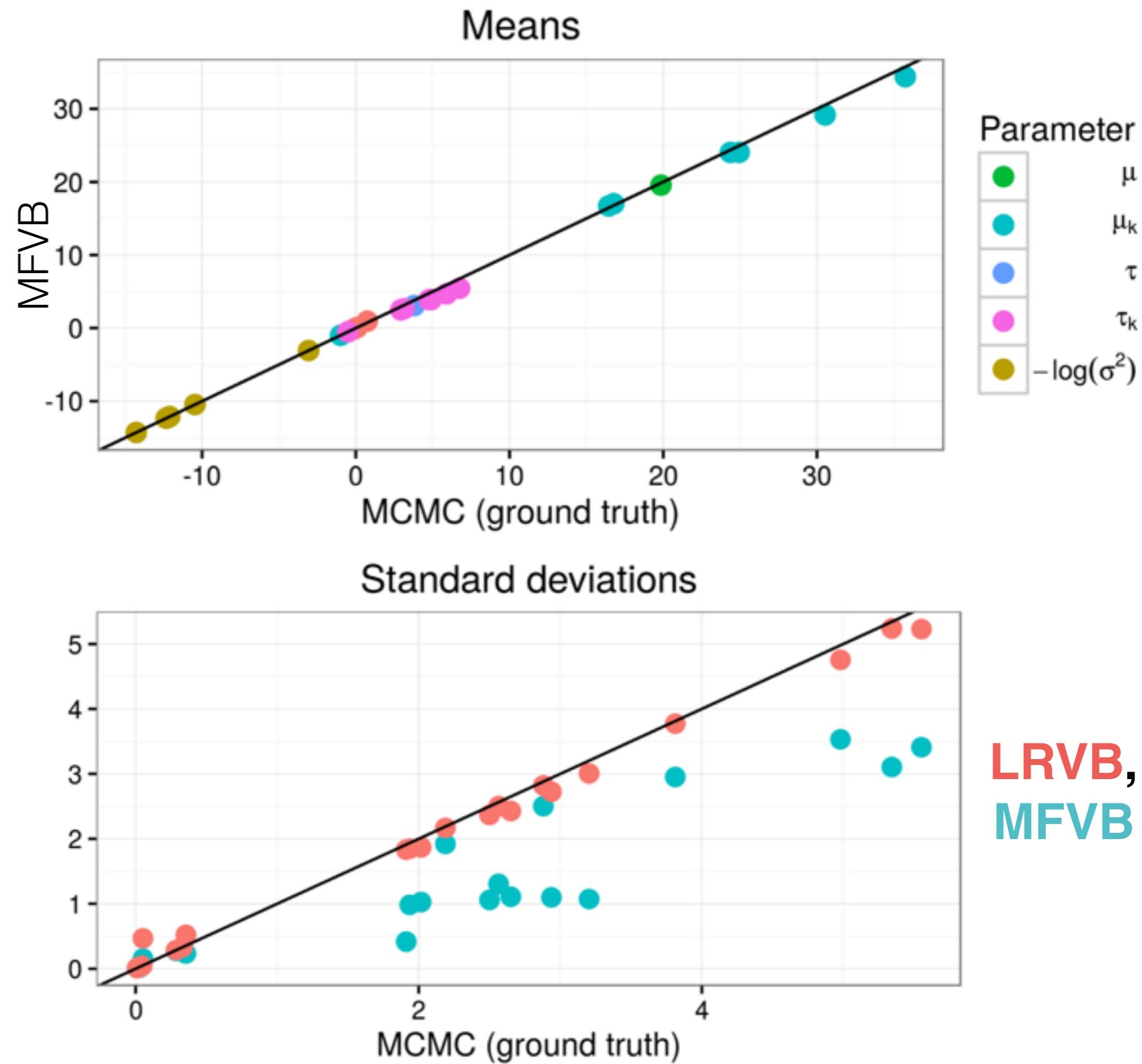
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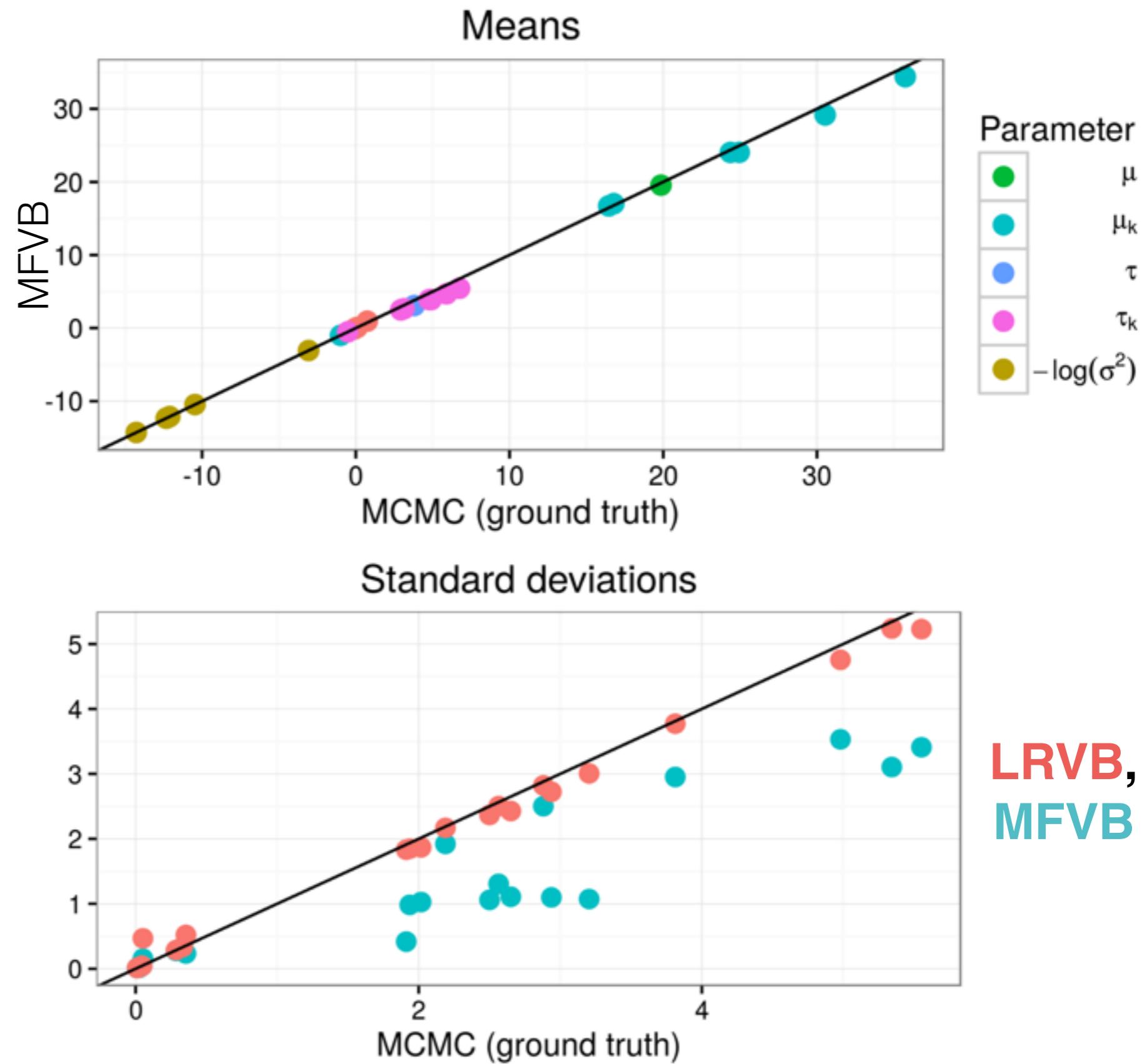
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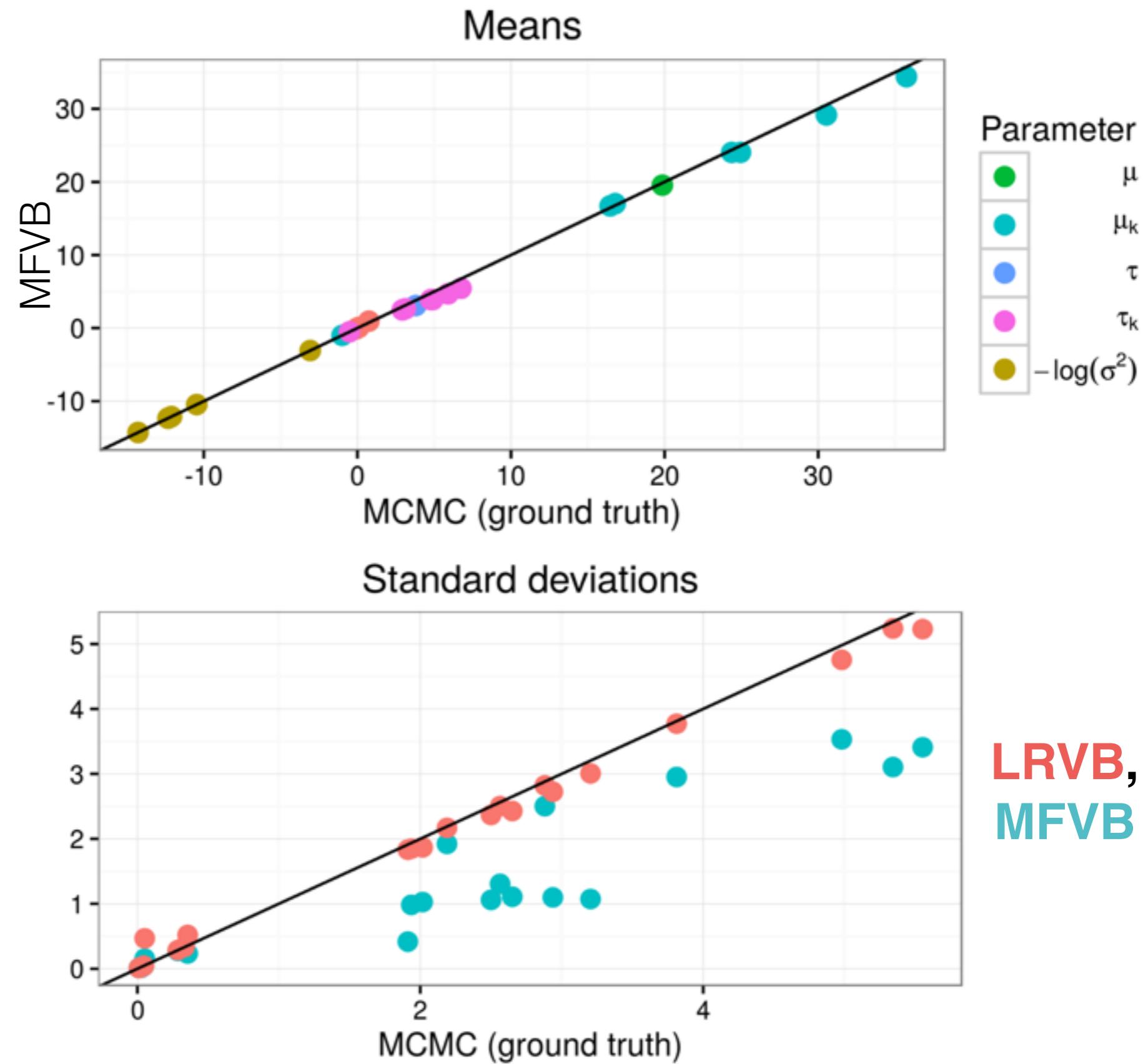
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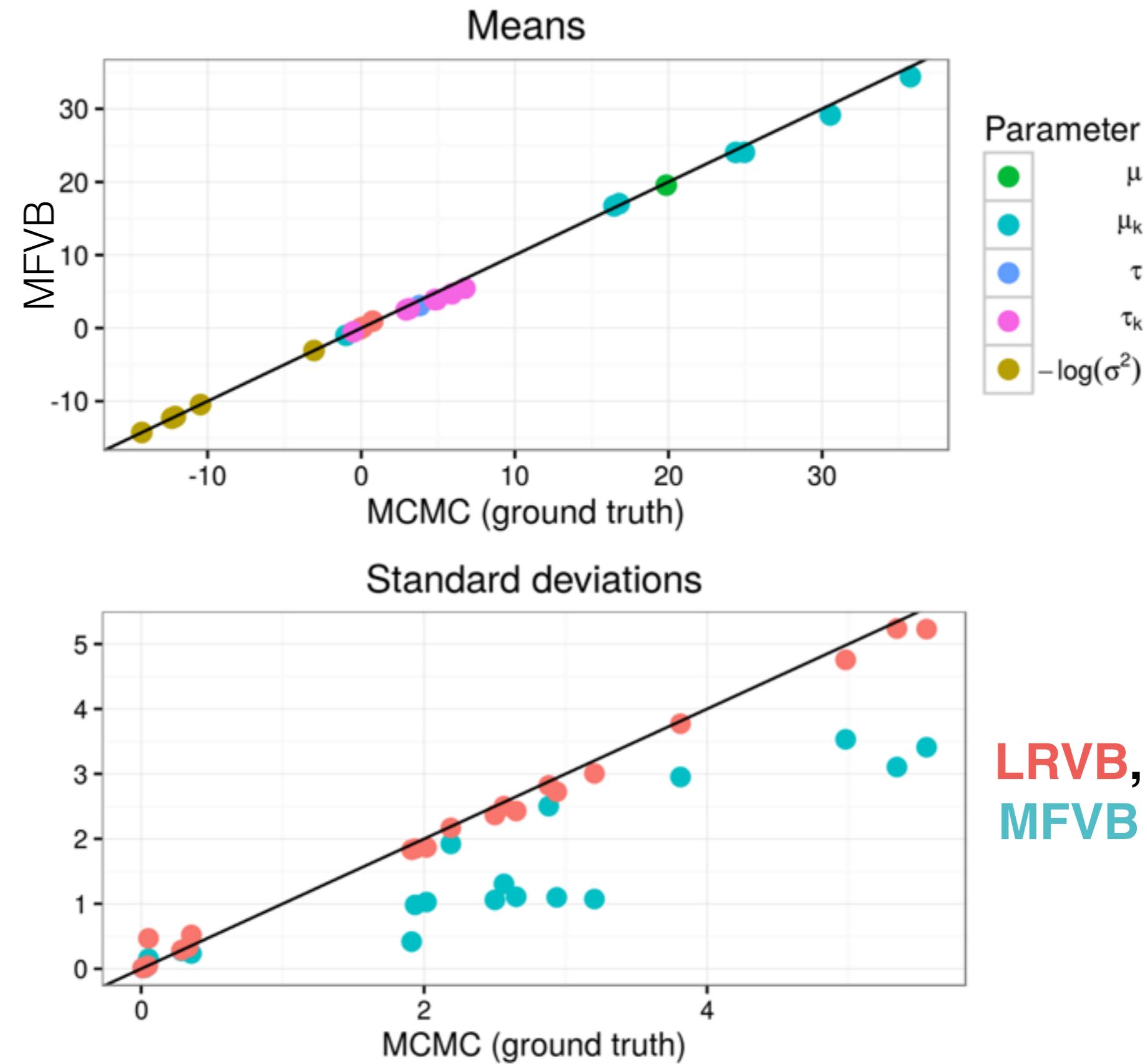
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- Mean is 1.68 std dev from 0



Roadmap

- Challenges of VB
- Accurate uncertainties from VB
- Accurate robustness quantification from VB

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Robustness quantification

- Bayes Theorem

$$p(\theta|y)$$

$$\propto_{\theta} p(y|\theta)p(\theta)$$

Robustness quantification

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$$p(\theta|y, \alpha)$$

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Robustness quantification

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$$p_\alpha(\theta) := p(\theta|y, \alpha)$$
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Robustness quantification

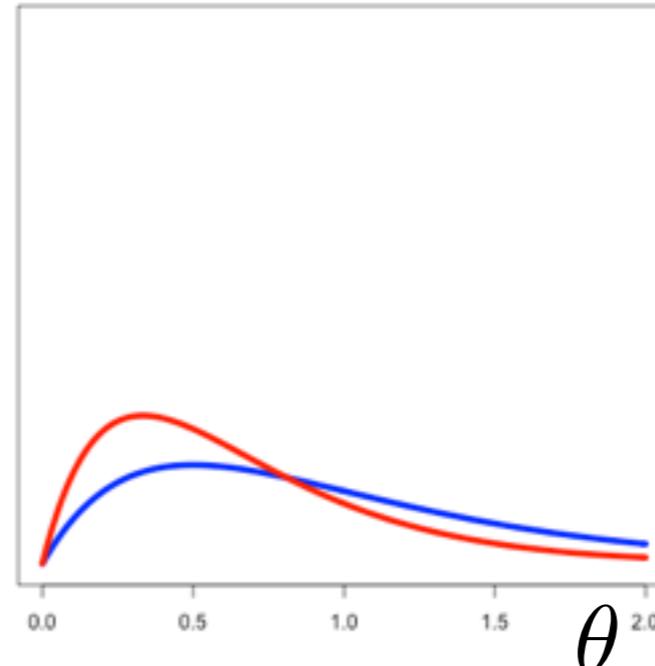
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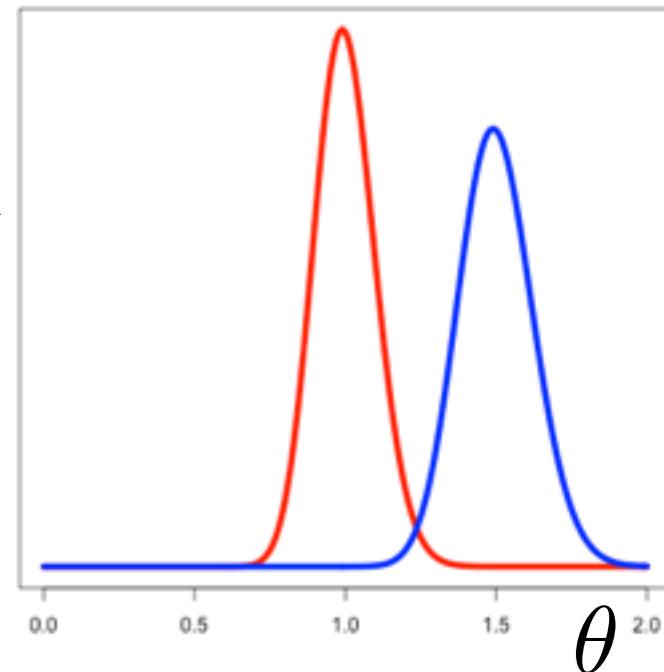
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- Sensitivity

Some reasonable priors



**Bayes
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Robustness quantification

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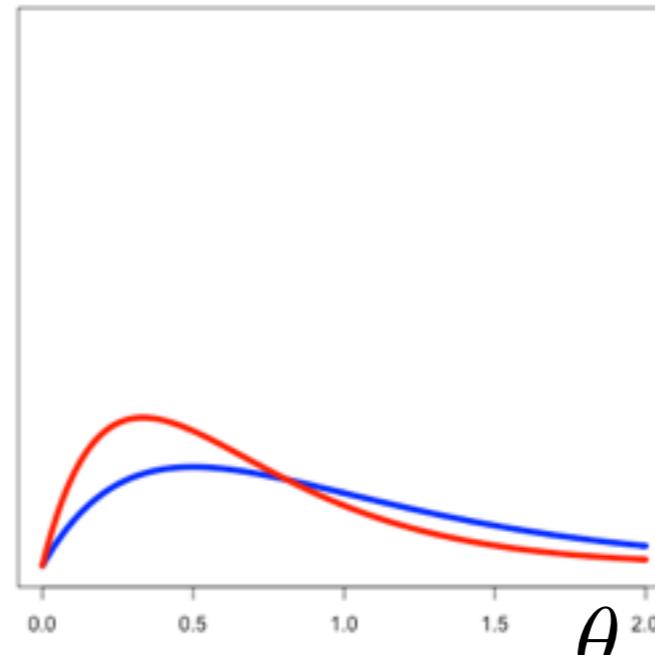
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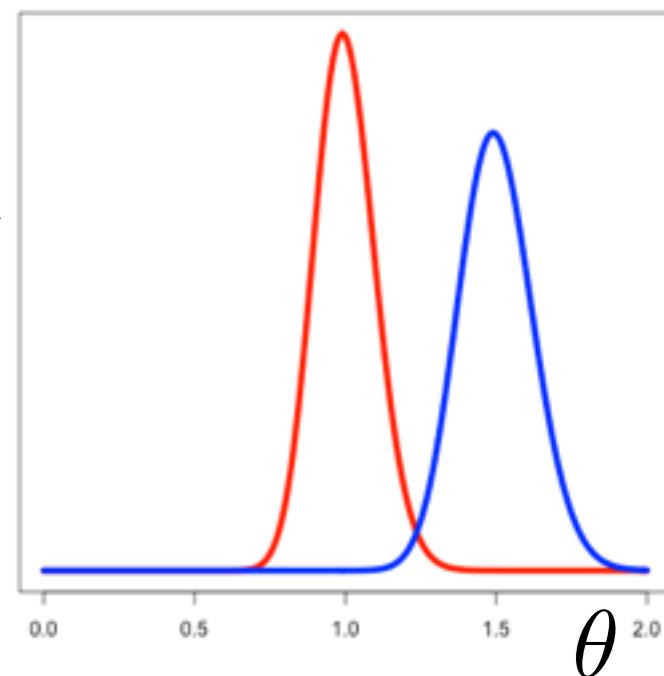
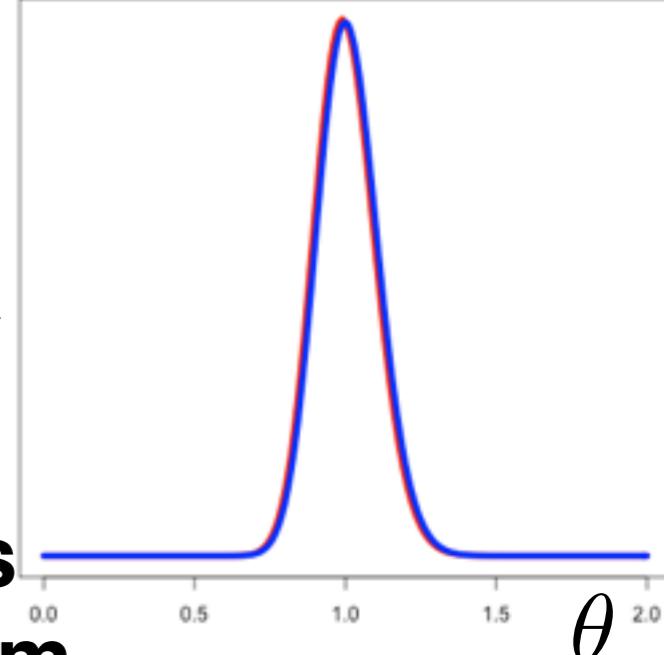
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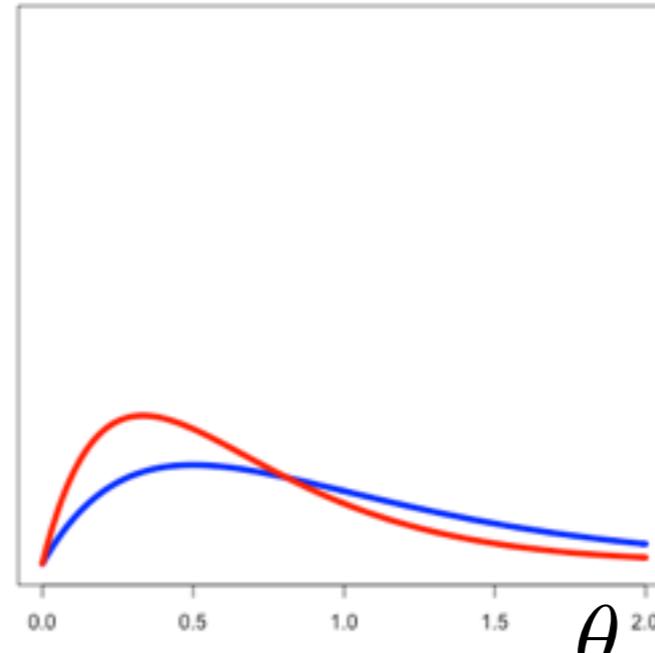
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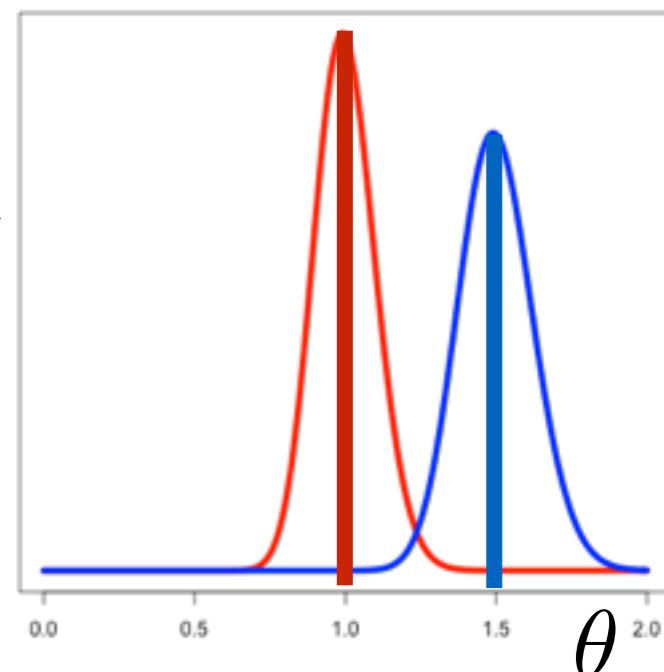
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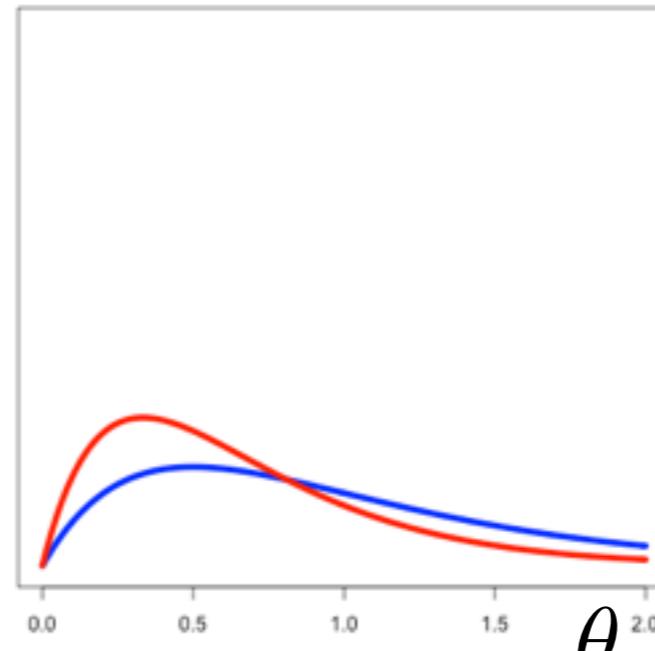
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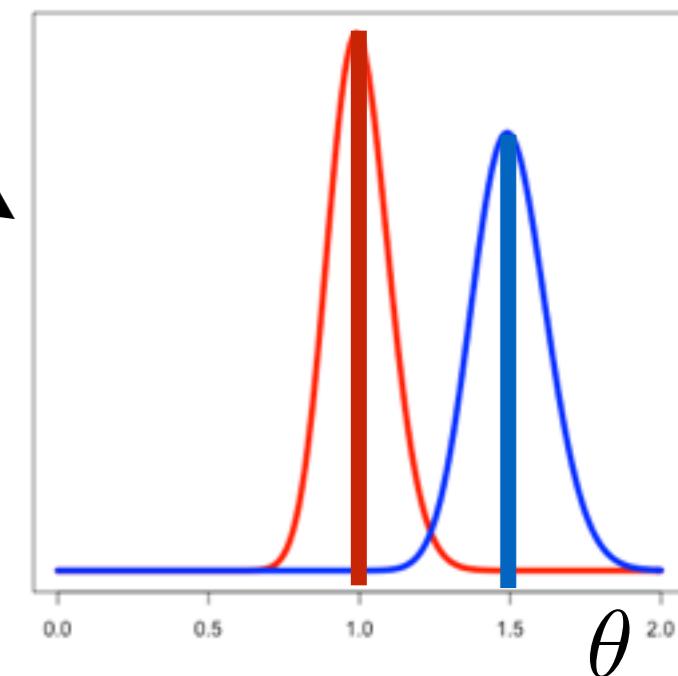
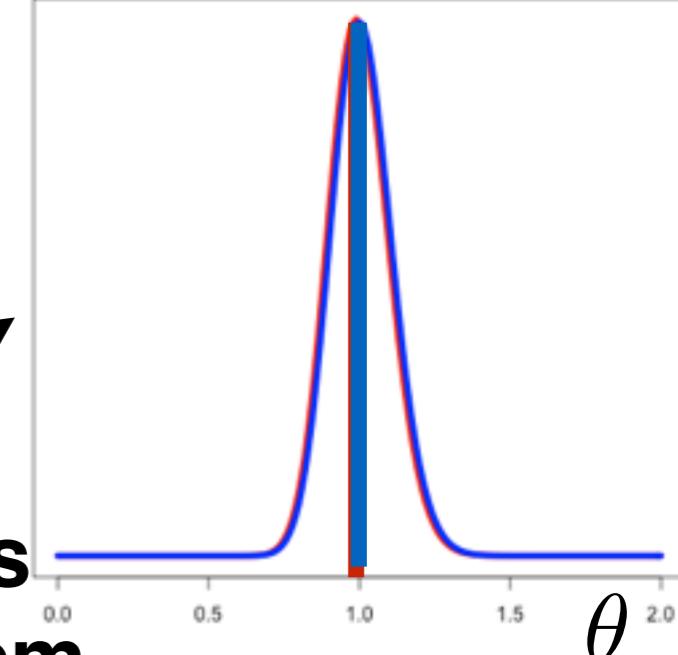
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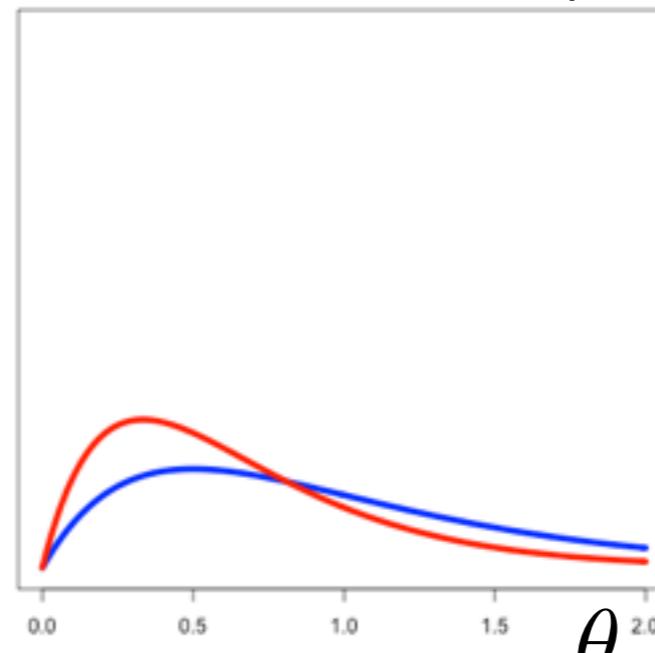
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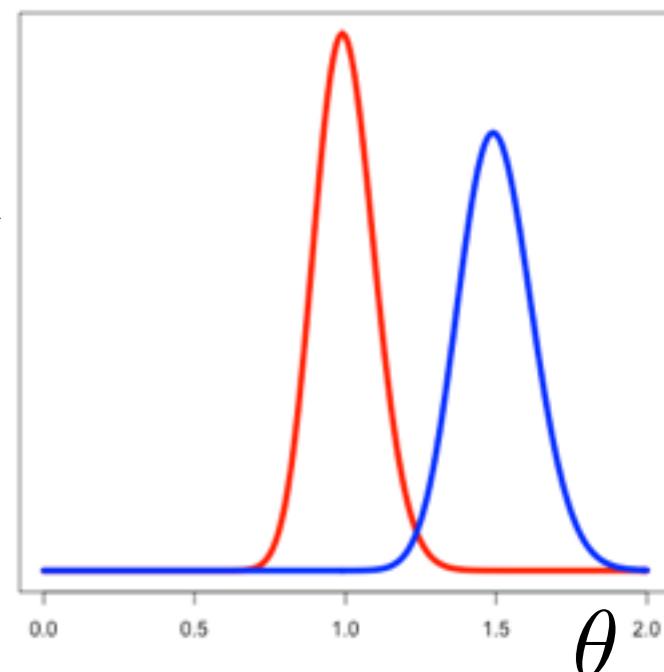
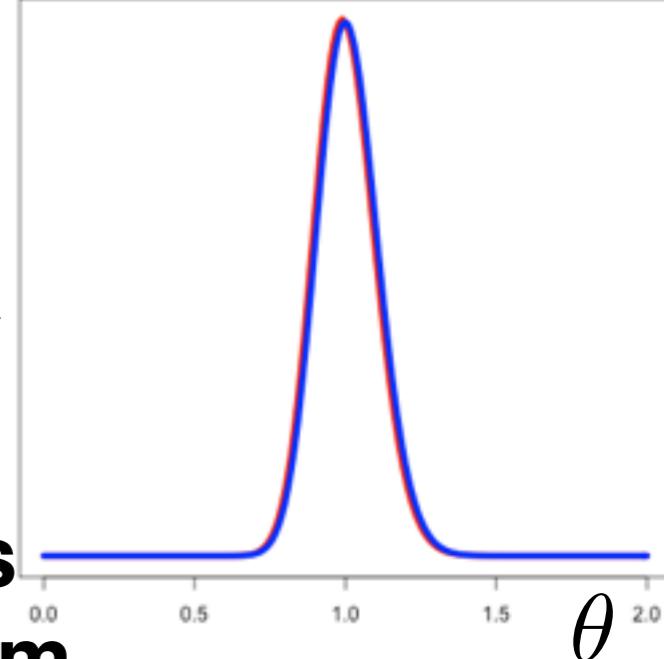
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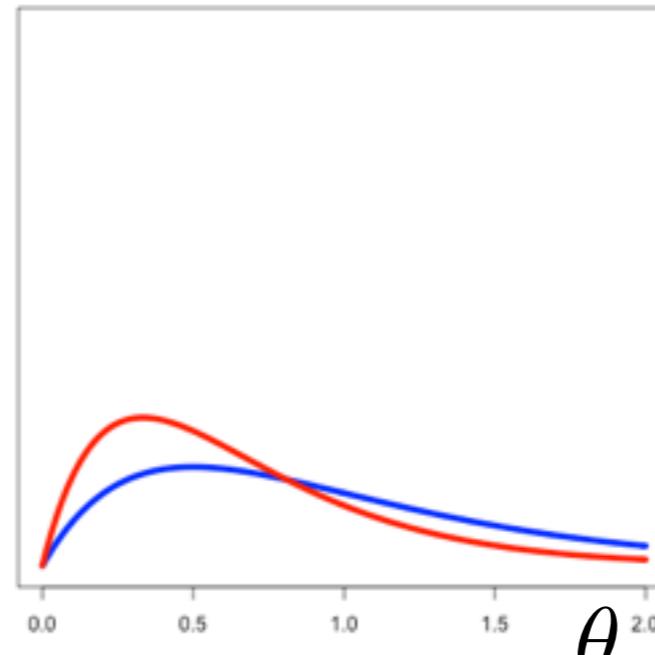
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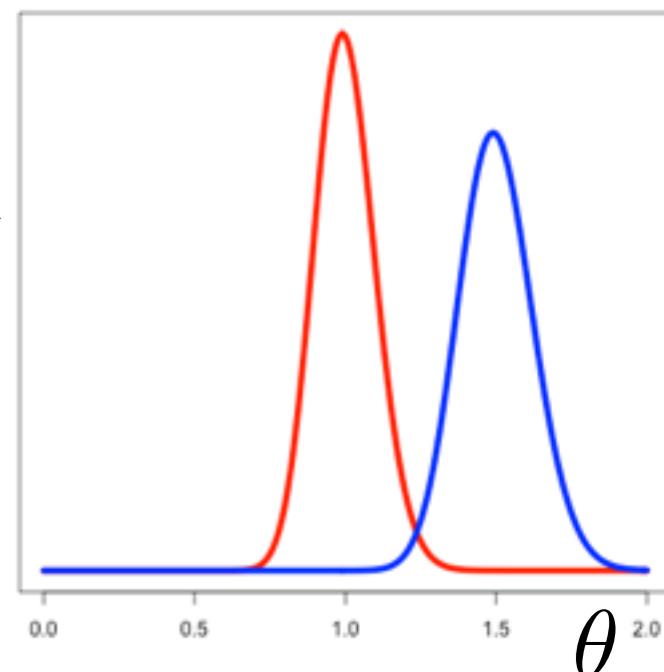
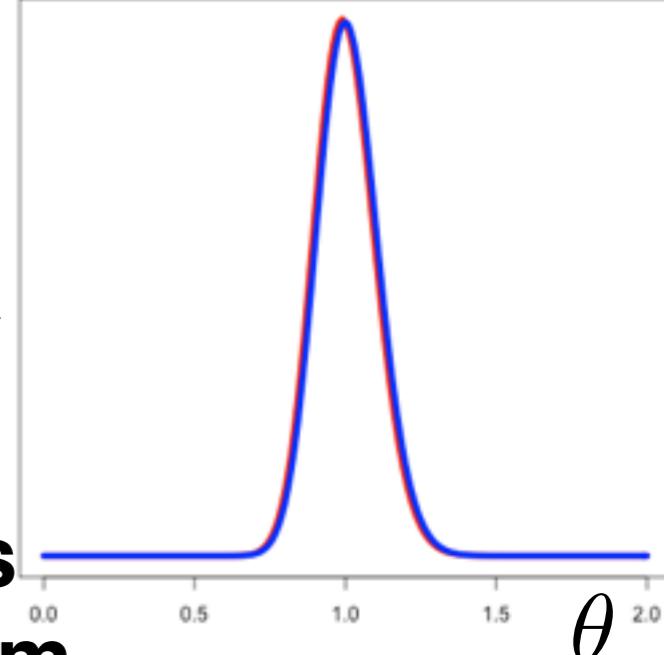
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$$S := \left. \frac{d\mathbb{E}_{p_\alpha}[g(\theta)]}{d\alpha} \right|_{\alpha}$$

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Theorem**



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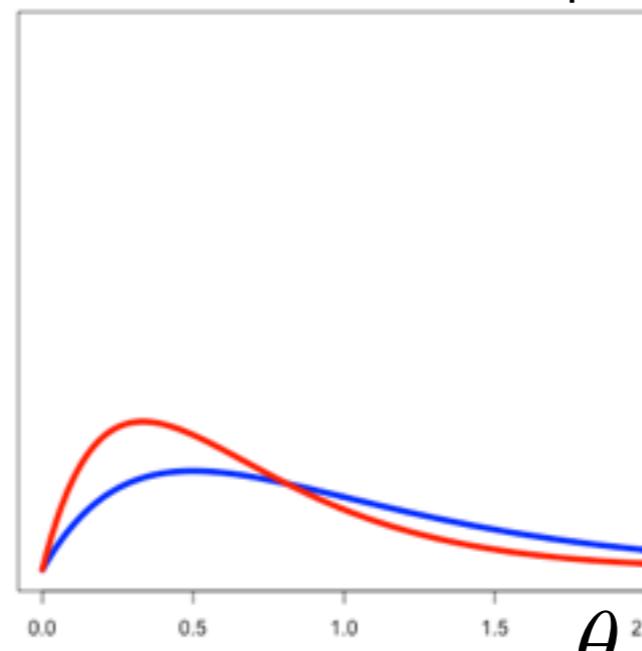
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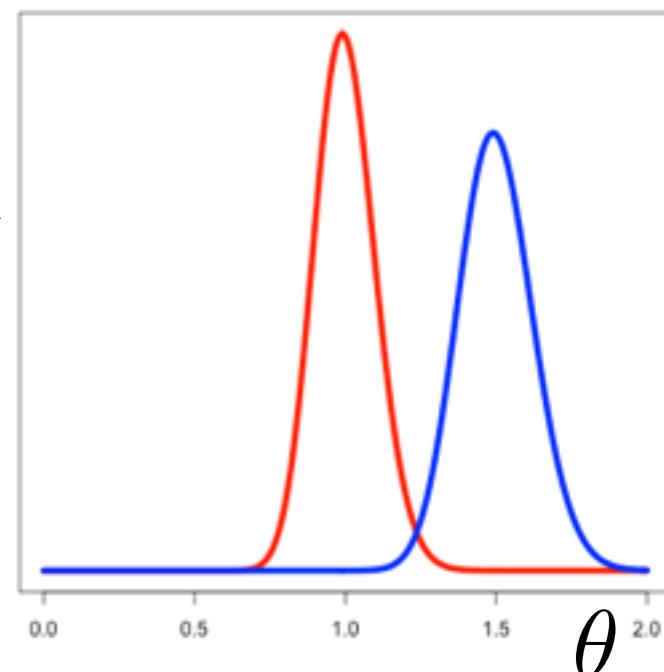
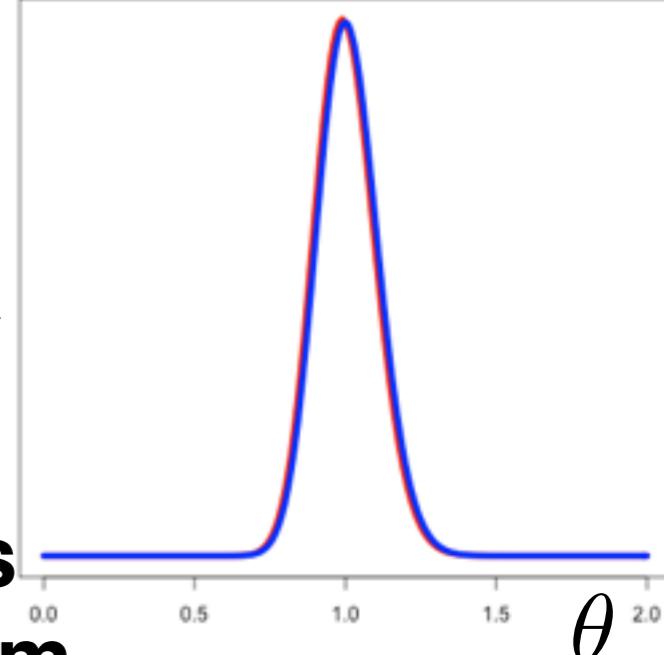
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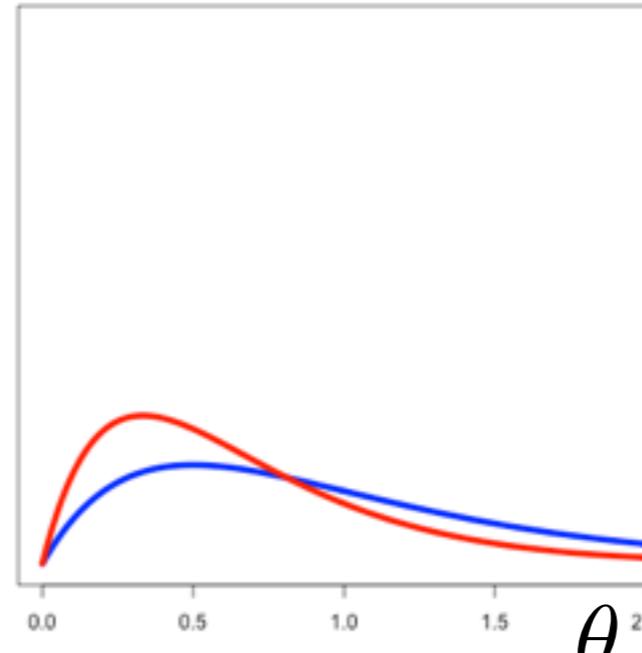
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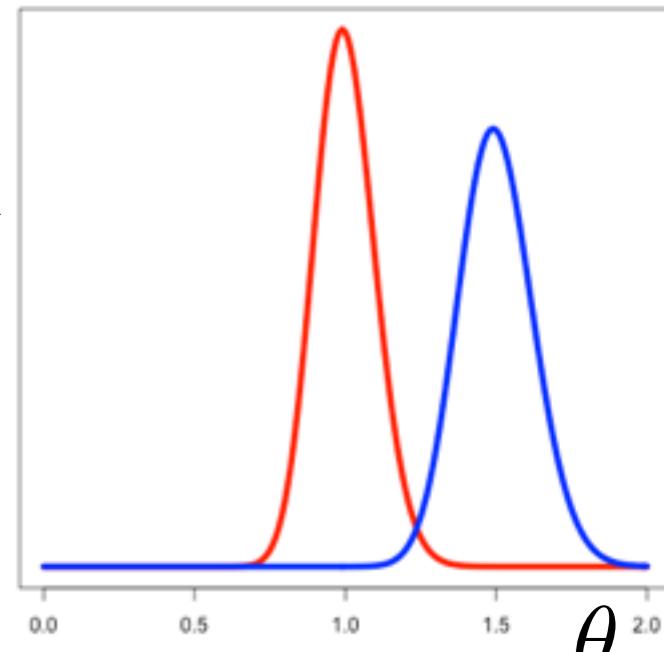
$$S := \left. \frac{d\mathbb{E}_{p_\alpha}[g(\theta)]}{d\alpha} \right|_{\alpha} \Delta\alpha$$

$$\approx \left. \frac{d\mathbb{E}_{q_\alpha^*}[g(\theta)]}{d\alpha} \right|_{\alpha} \Delta\alpha =: \hat{S}$$

Some reasonable priors



**Bayes
Theorem**



Robustness quantification

- Bayes Theorem

$$p_\alpha(\theta) := p(\theta|y, \alpha)$$

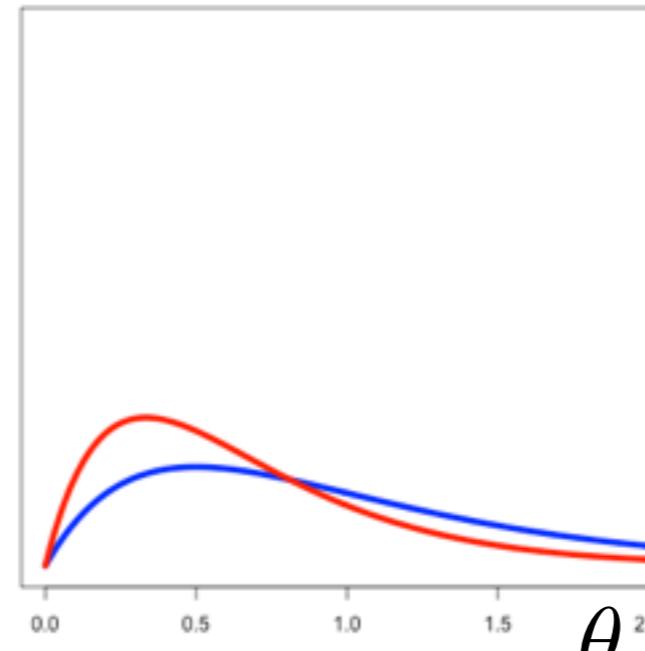
$$\propto_\theta p(y|\theta)p(\theta|\alpha)$$

- Sensitivity (local)

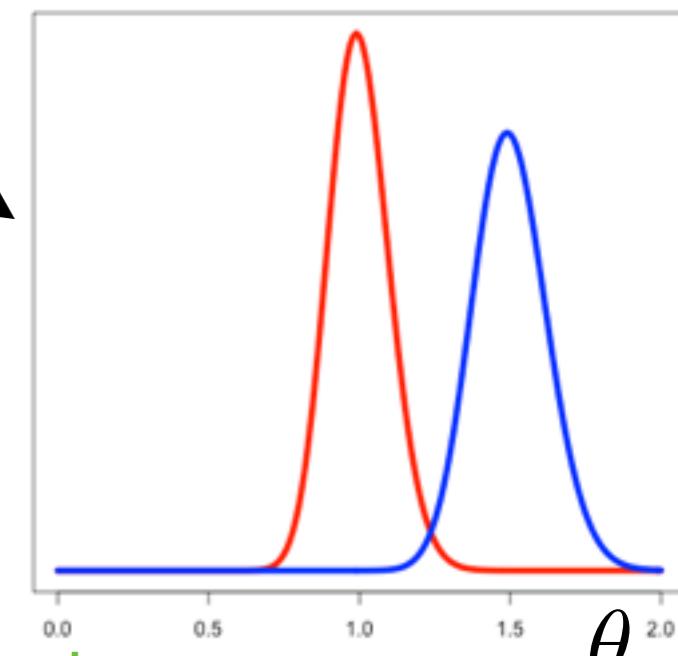
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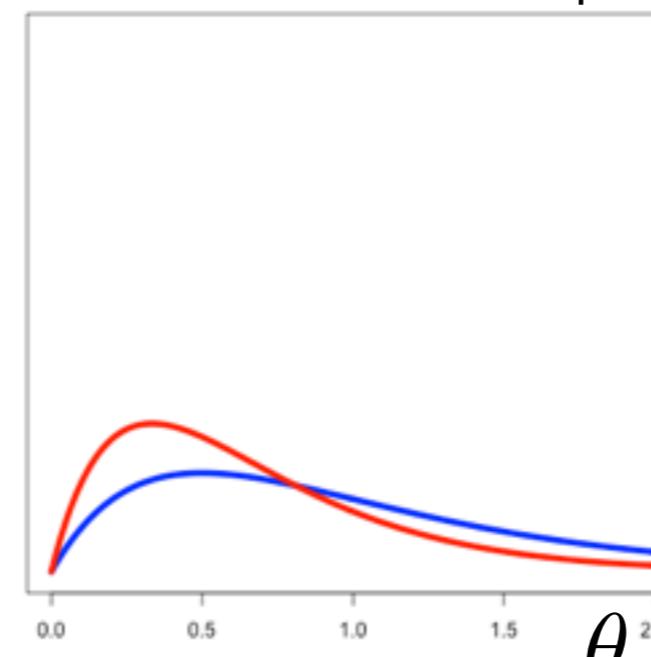
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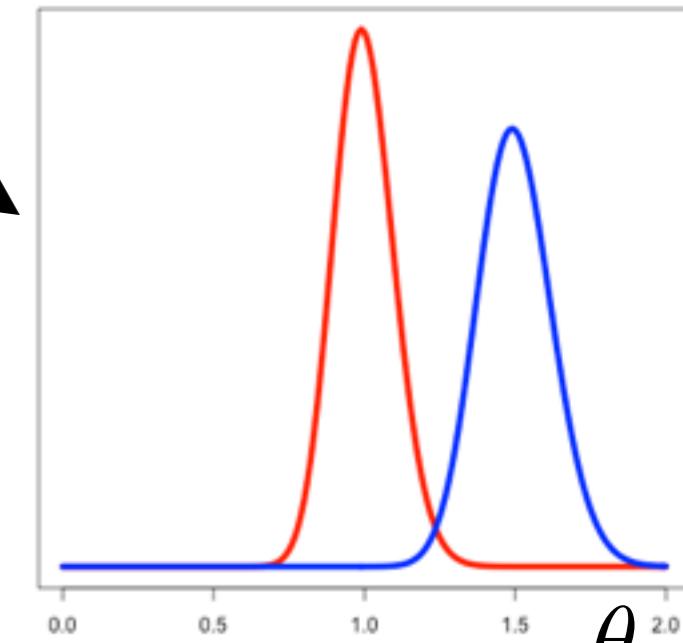
- Recall: our general LRVB formula applies for:

$$\log p_t(\theta) = \log p(\theta|y) + f(\theta, t) - \text{Const}(t)$$

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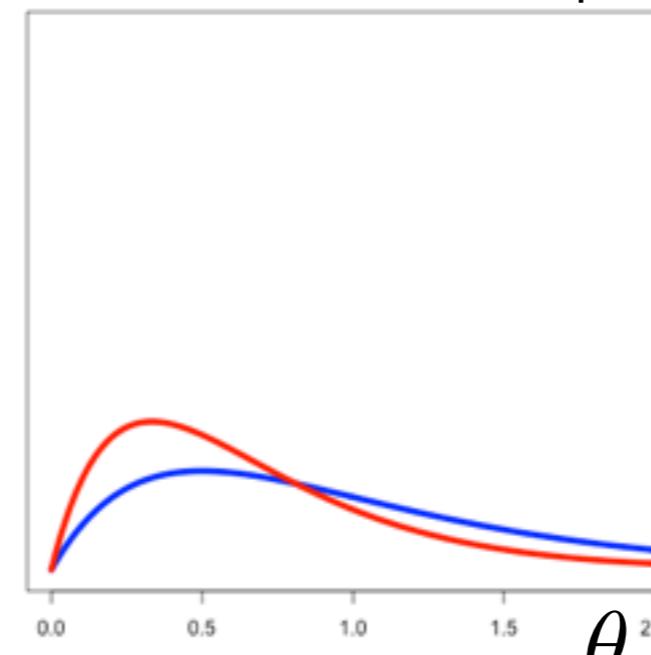
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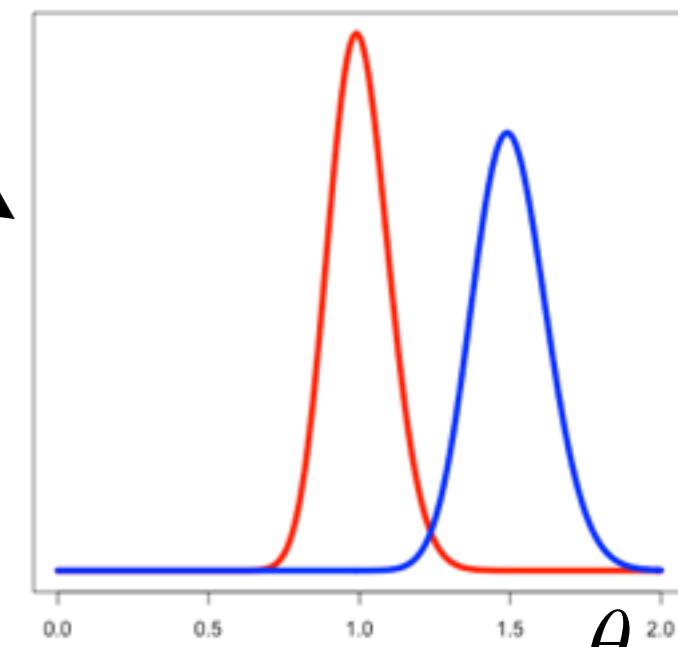
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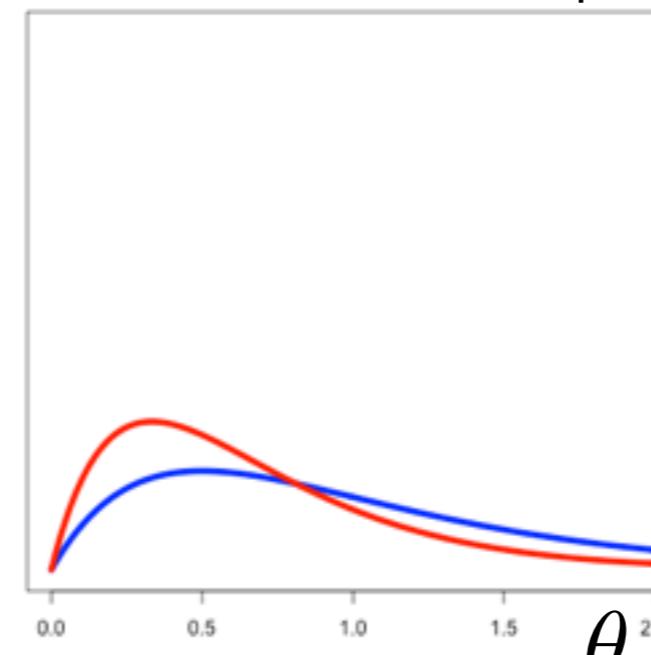
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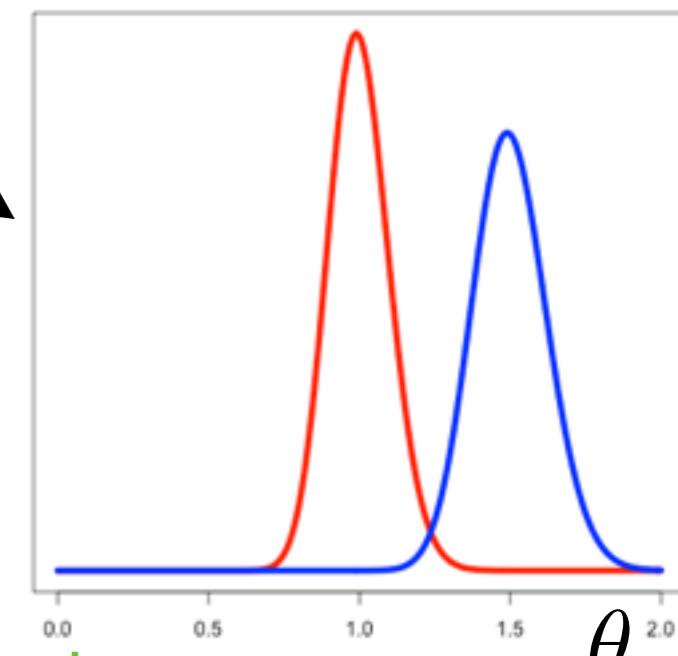
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- Here: $f(\theta, \alpha) = \log p(\theta|\alpha) - \log p(\theta|\alpha_0)$

Some reasonable priors



**Bayes
Theorem**



Microcredit Experiment

- Simplified from Meager (2015)
- K 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:
$$y_{kn} \stackrel{\text{indep}}{\sim} \mathcal{N}(\mu_k + T_{kn}\tau_k, \sigma_k^2)$$

profit

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

1 if microcredit

- Priors and hyperpriors:

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

$$\begin{pmatrix} \mu \\ \tau \end{pmatrix} \stackrel{iid}{\sim} \mathcal{N}\left(\begin{pmatrix} \mu_0 \\ \tau_0 \end{pmatrix}, \Lambda^{-1}\right)$$

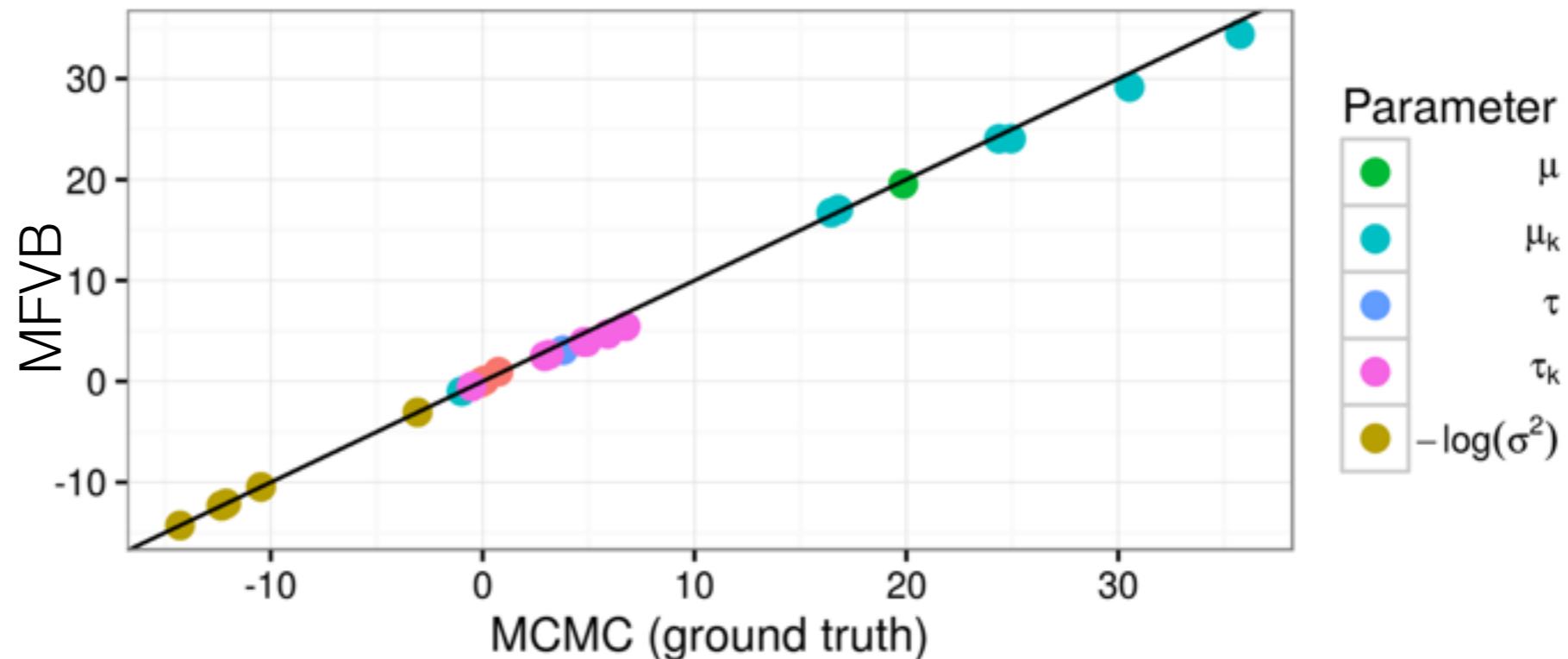
$$\sigma_k^{-2} \stackrel{iid}{\sim} \Gamma(a, b)$$

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

Microcredit Experiment

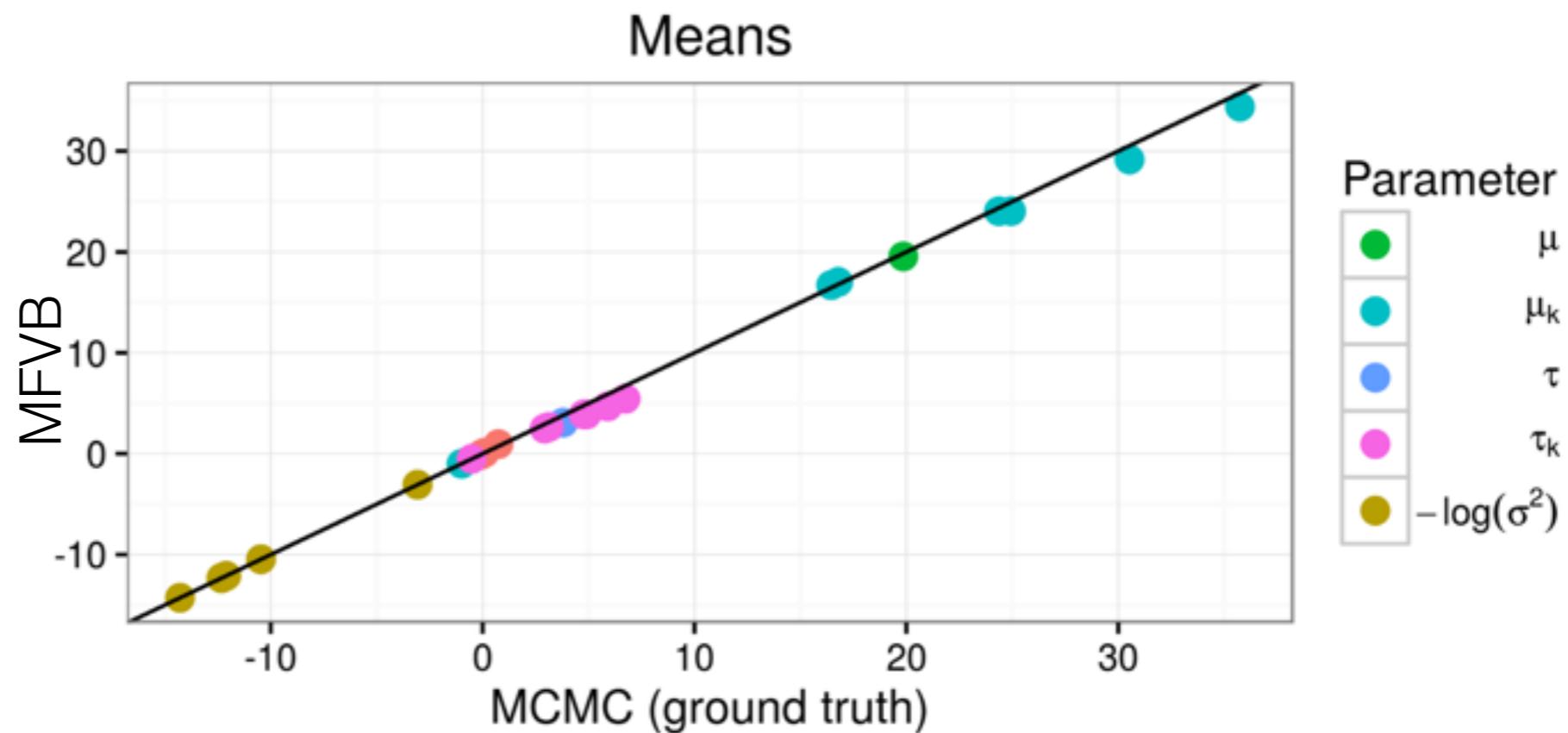
Microcredit Experiment

Means



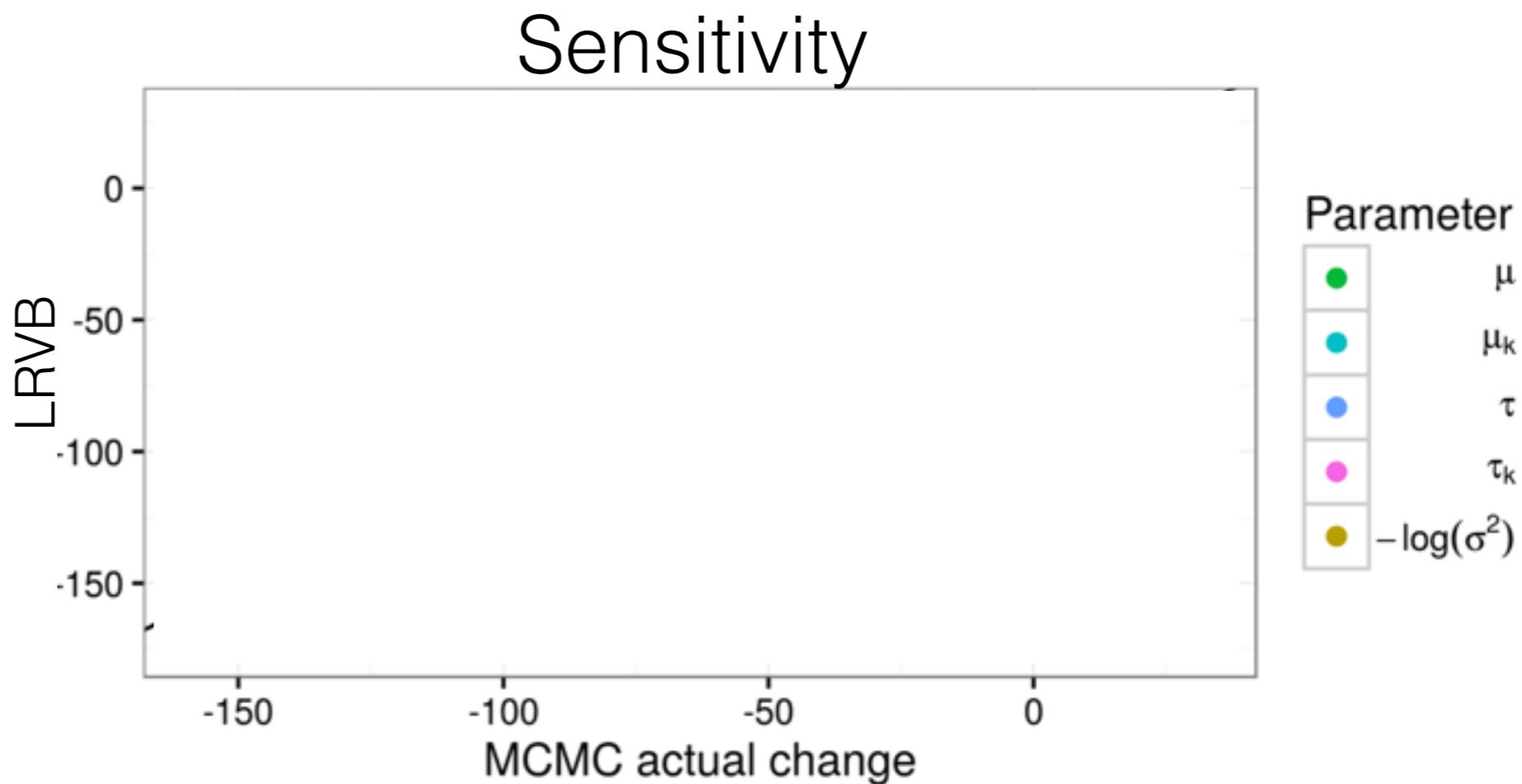
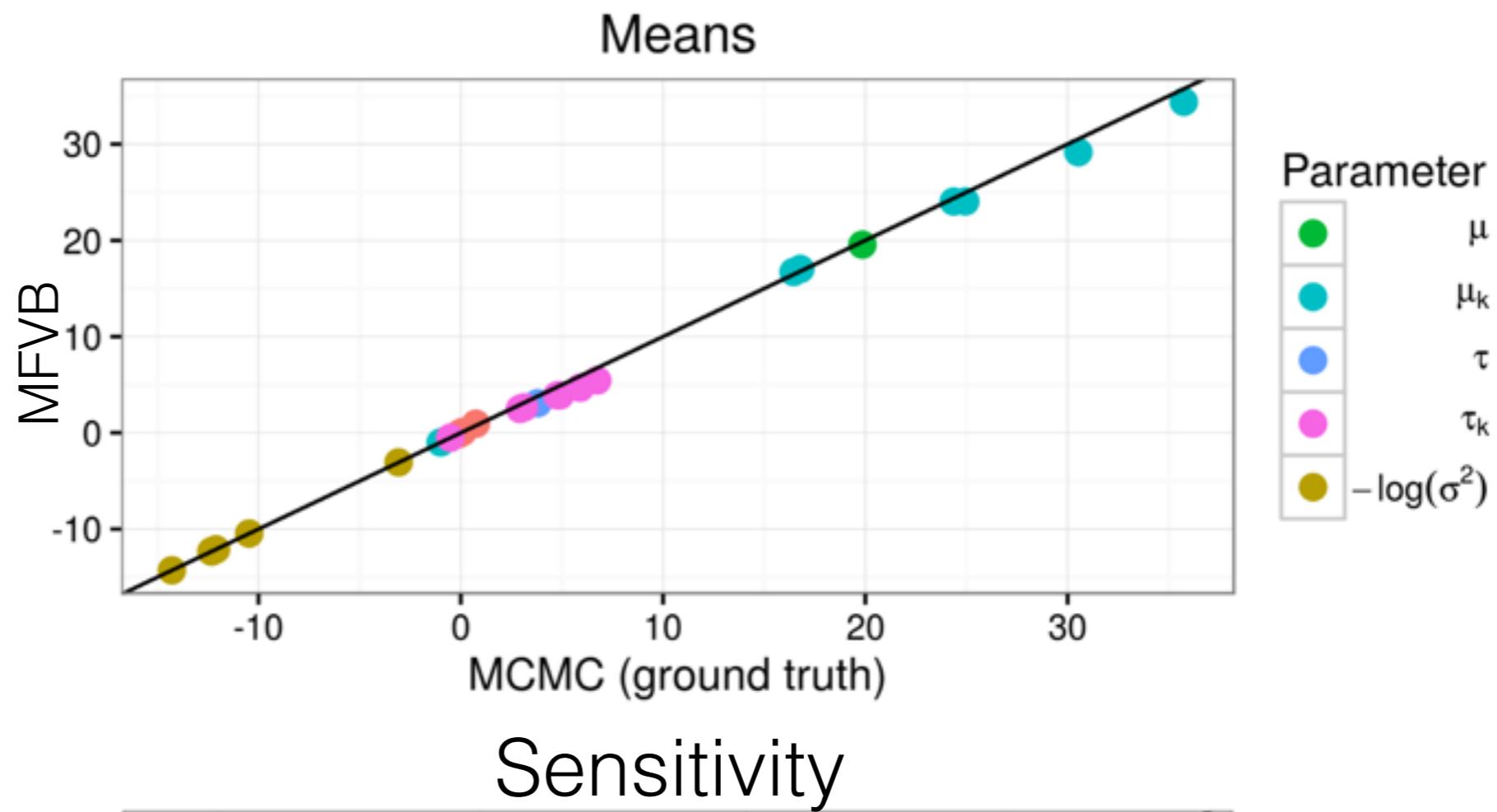
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- Perturb Λ_{11} :
 $0.03 \rightarrow 0.04$



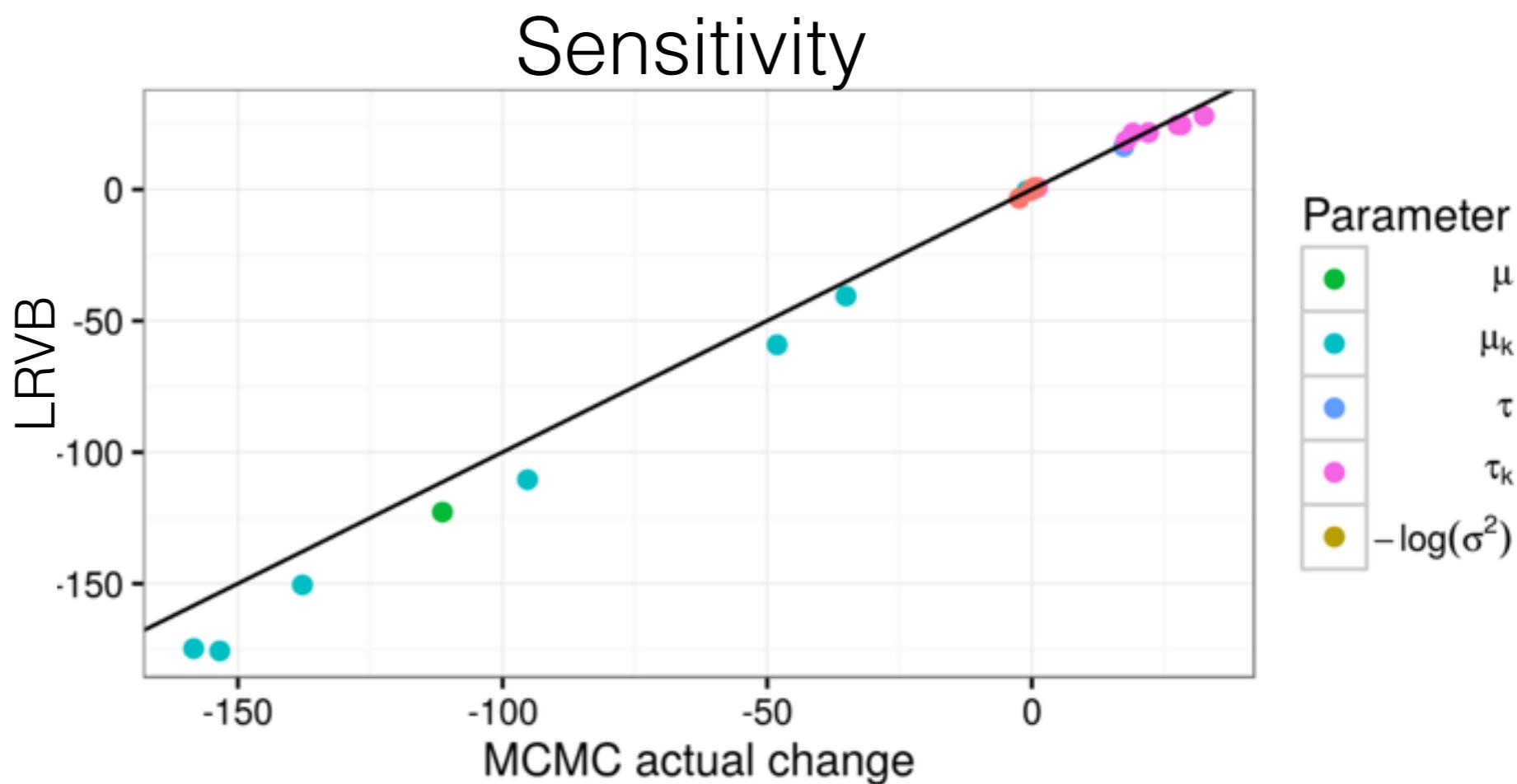
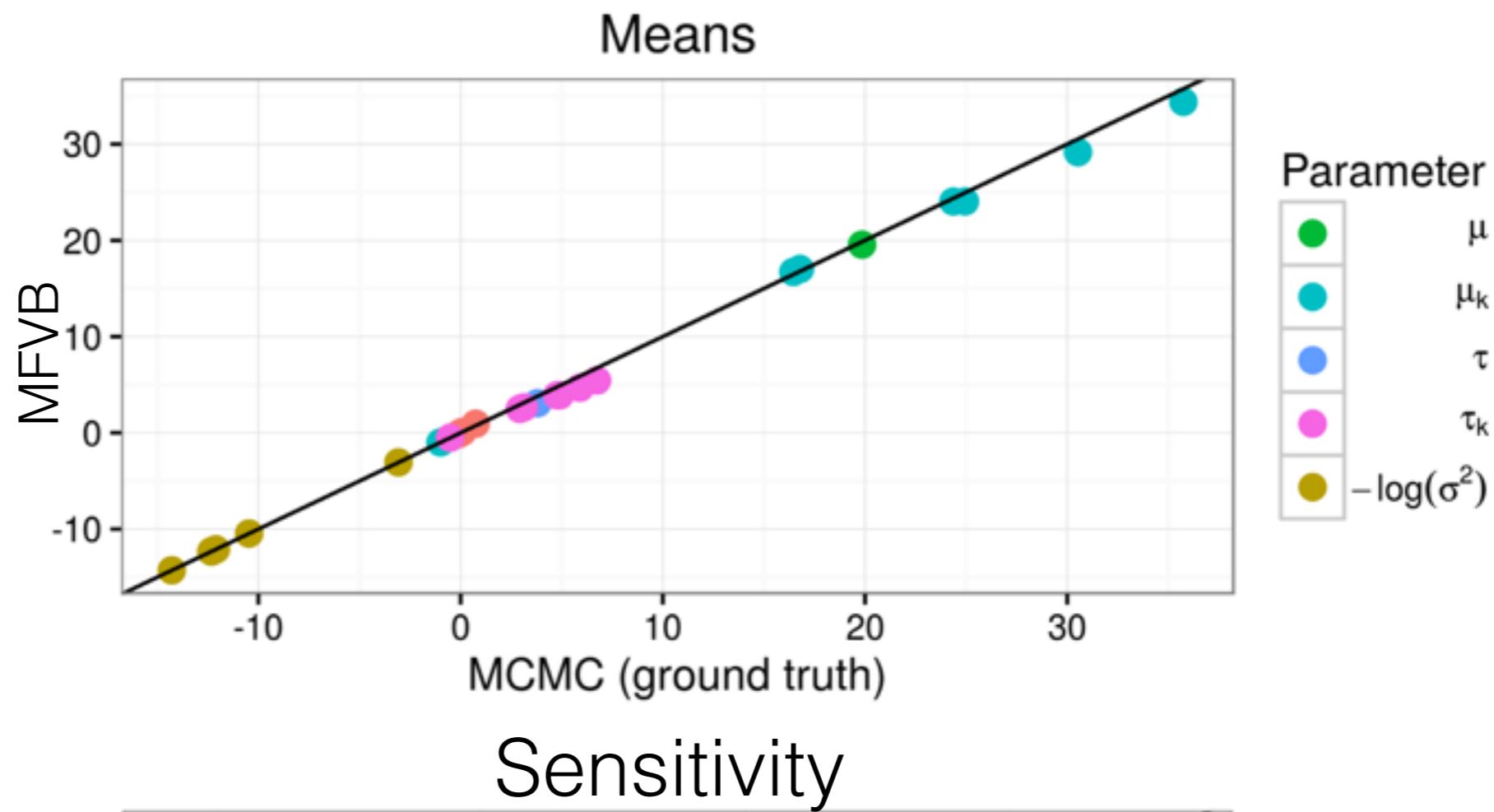
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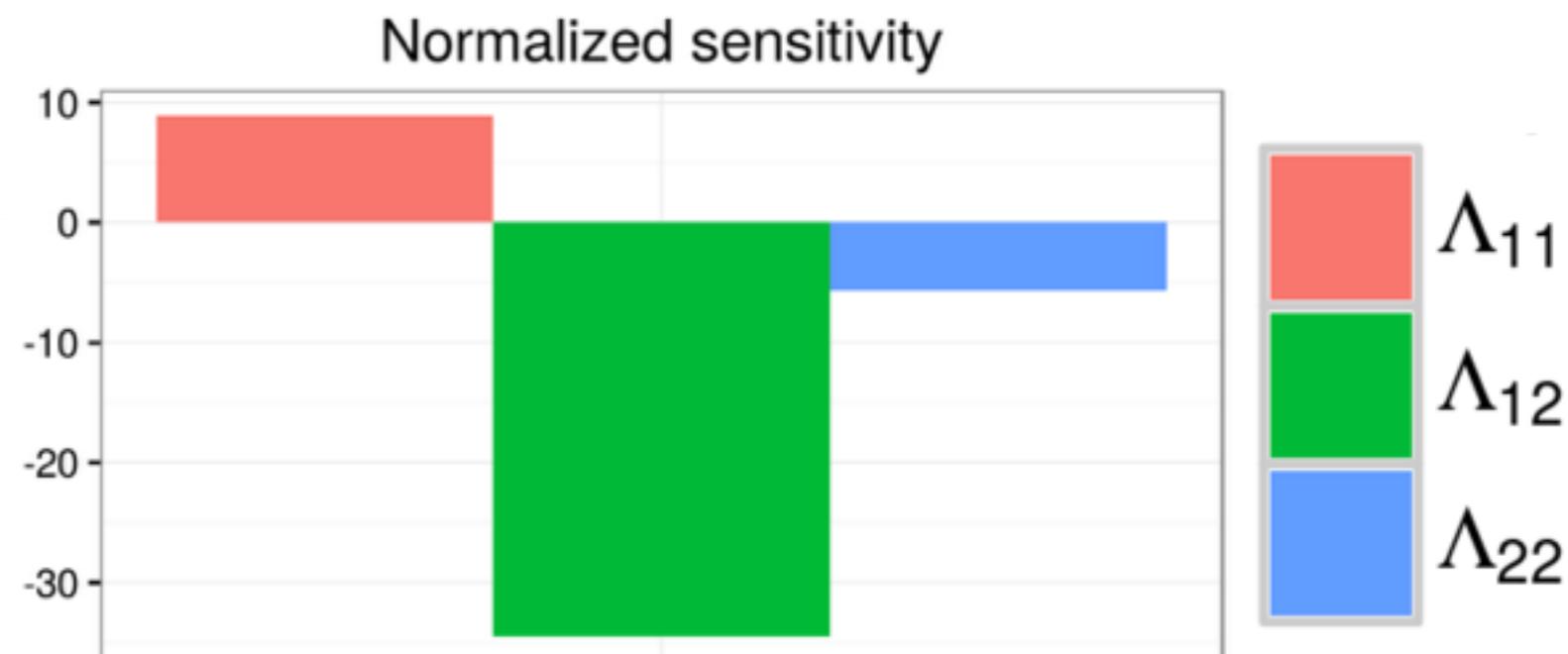
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Microcredit Experiment

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- Normalized to be on scale of τ std devs

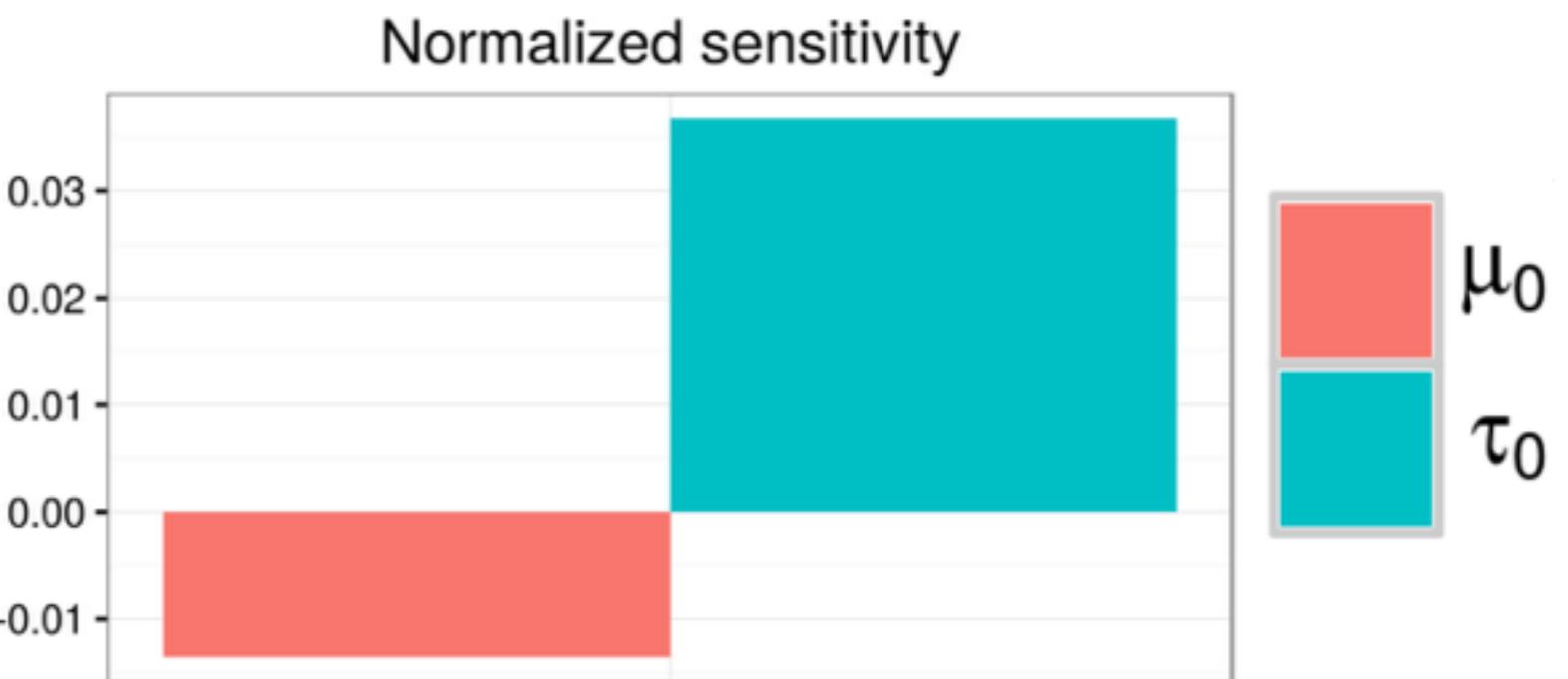
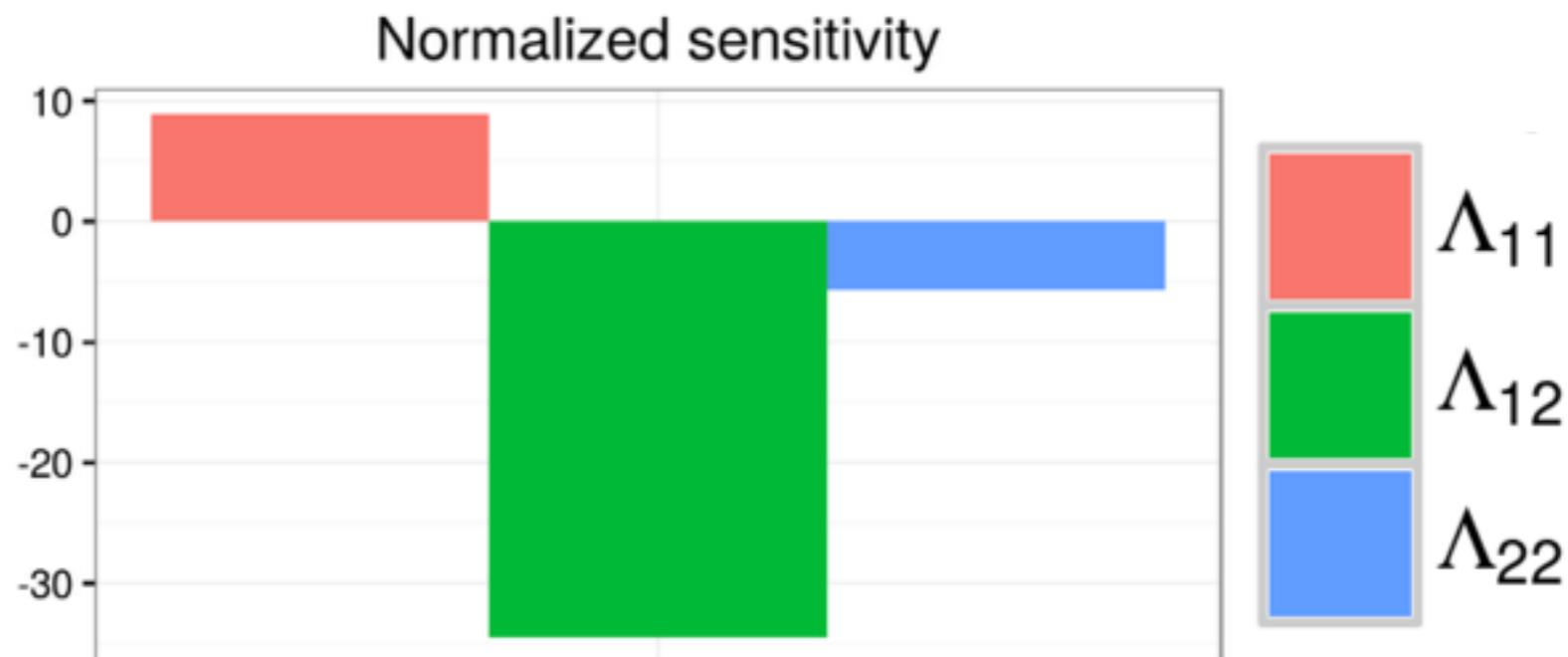
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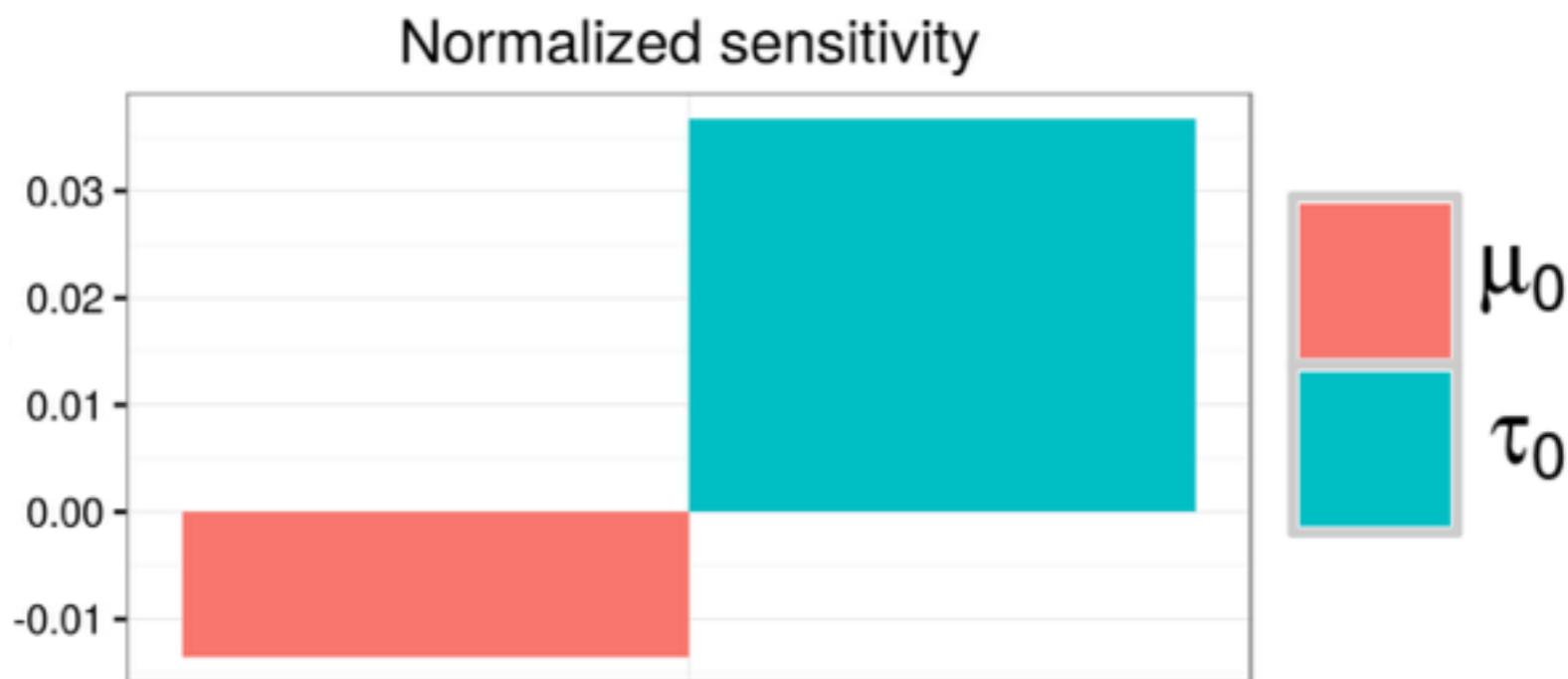
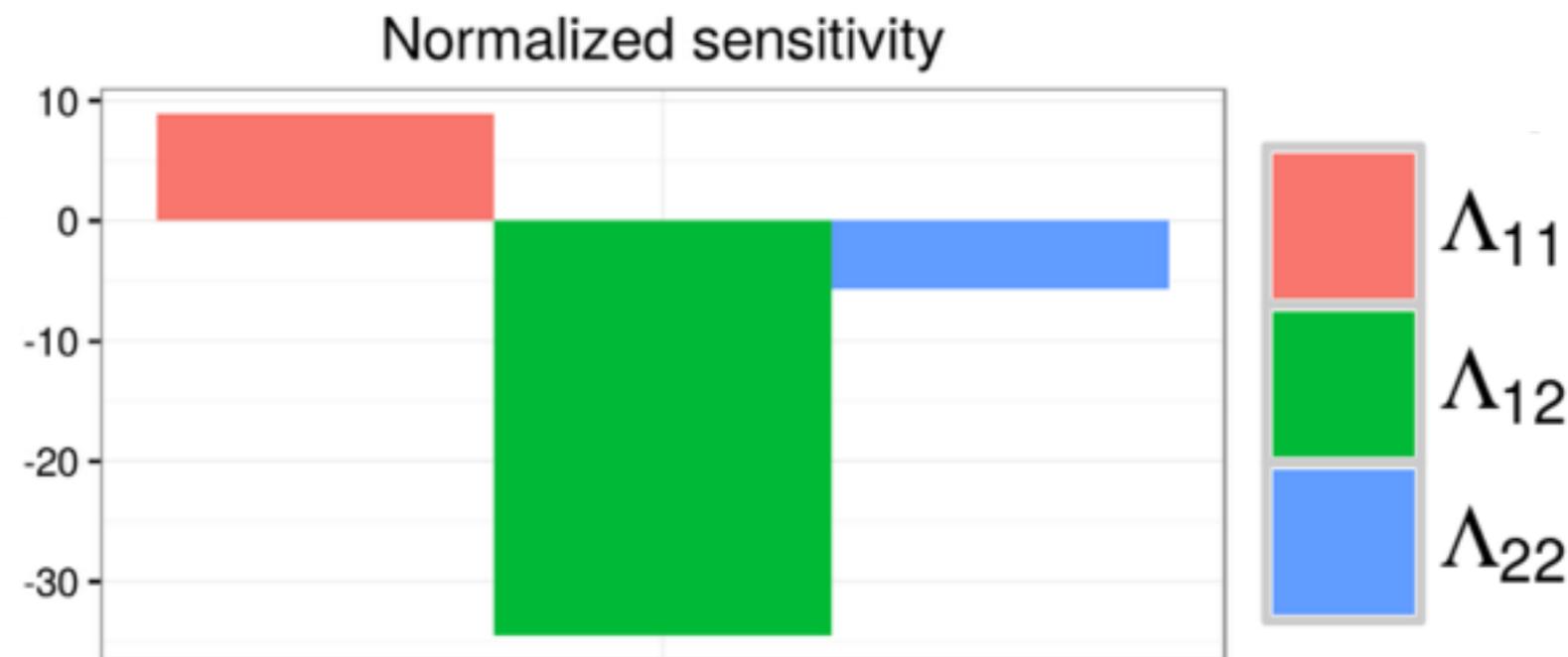
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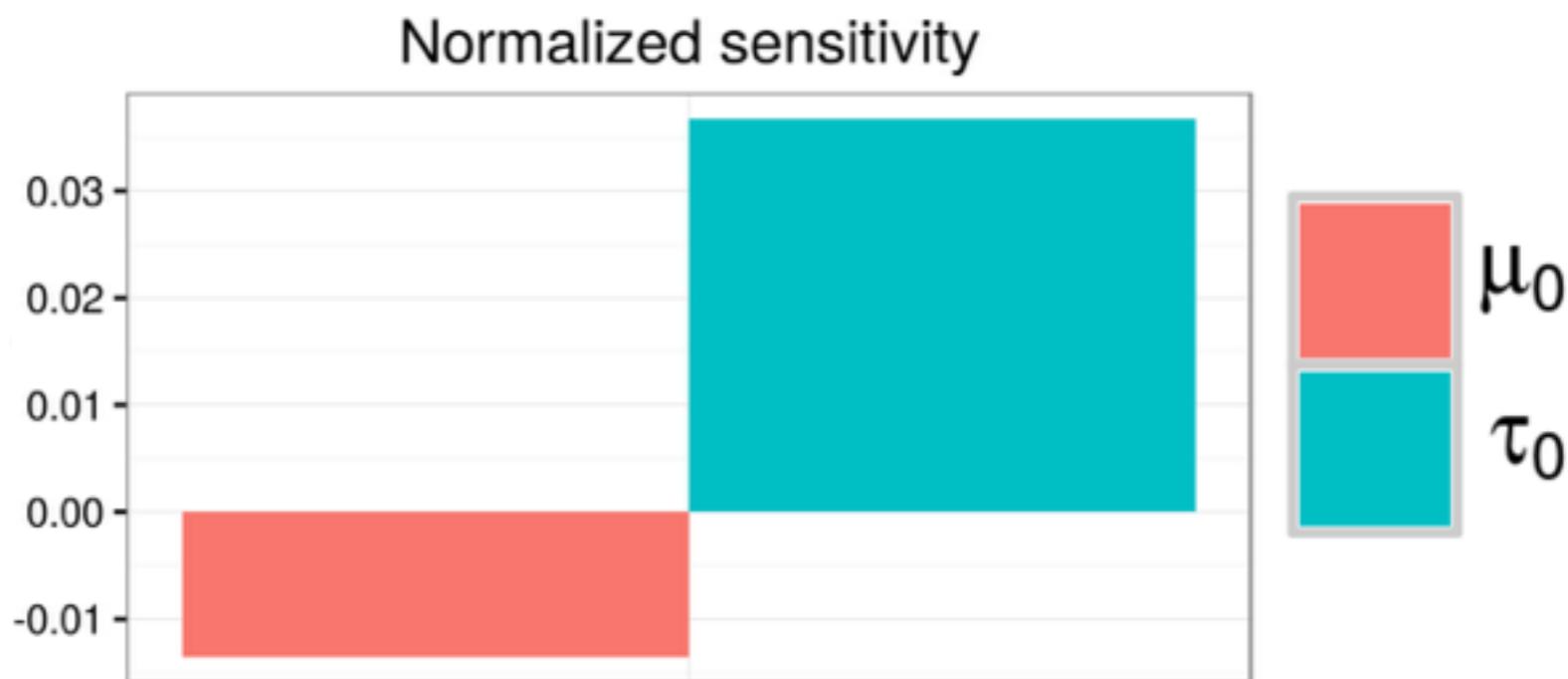
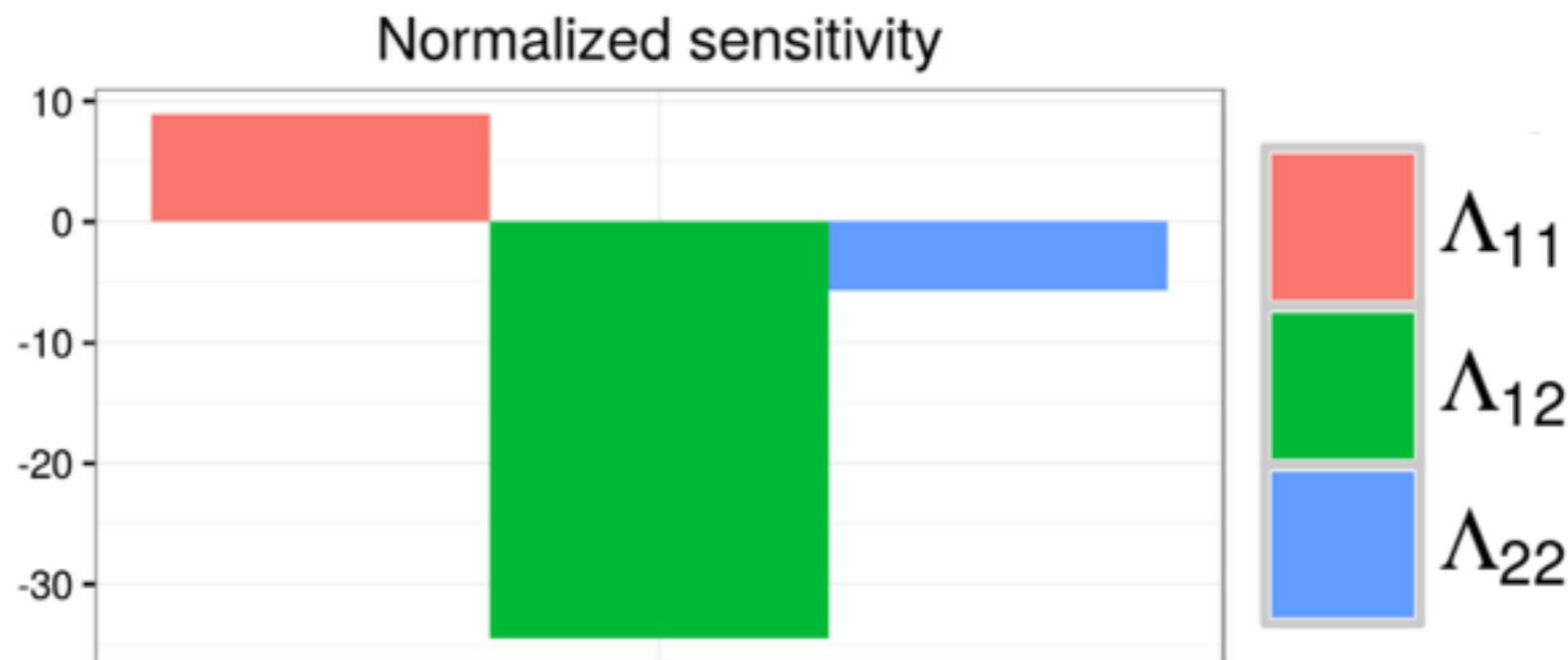
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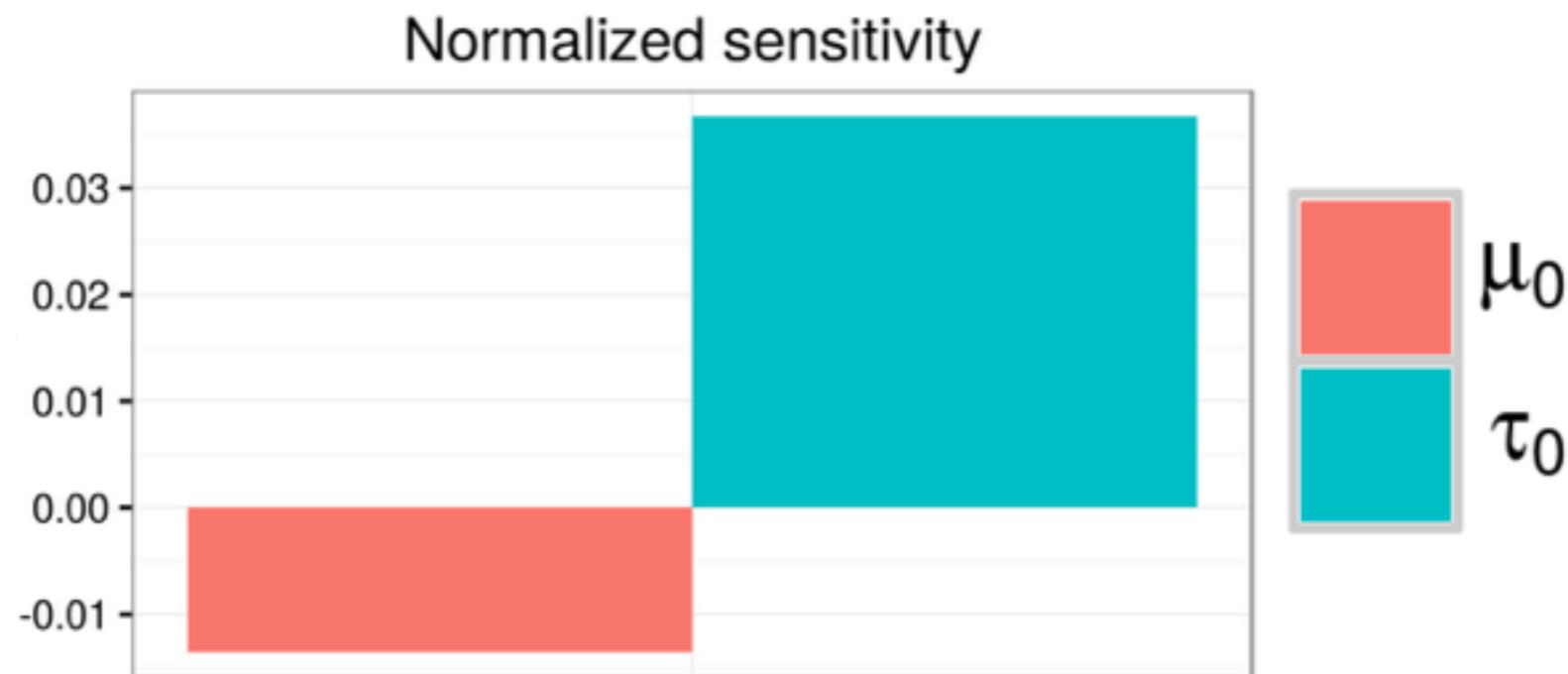
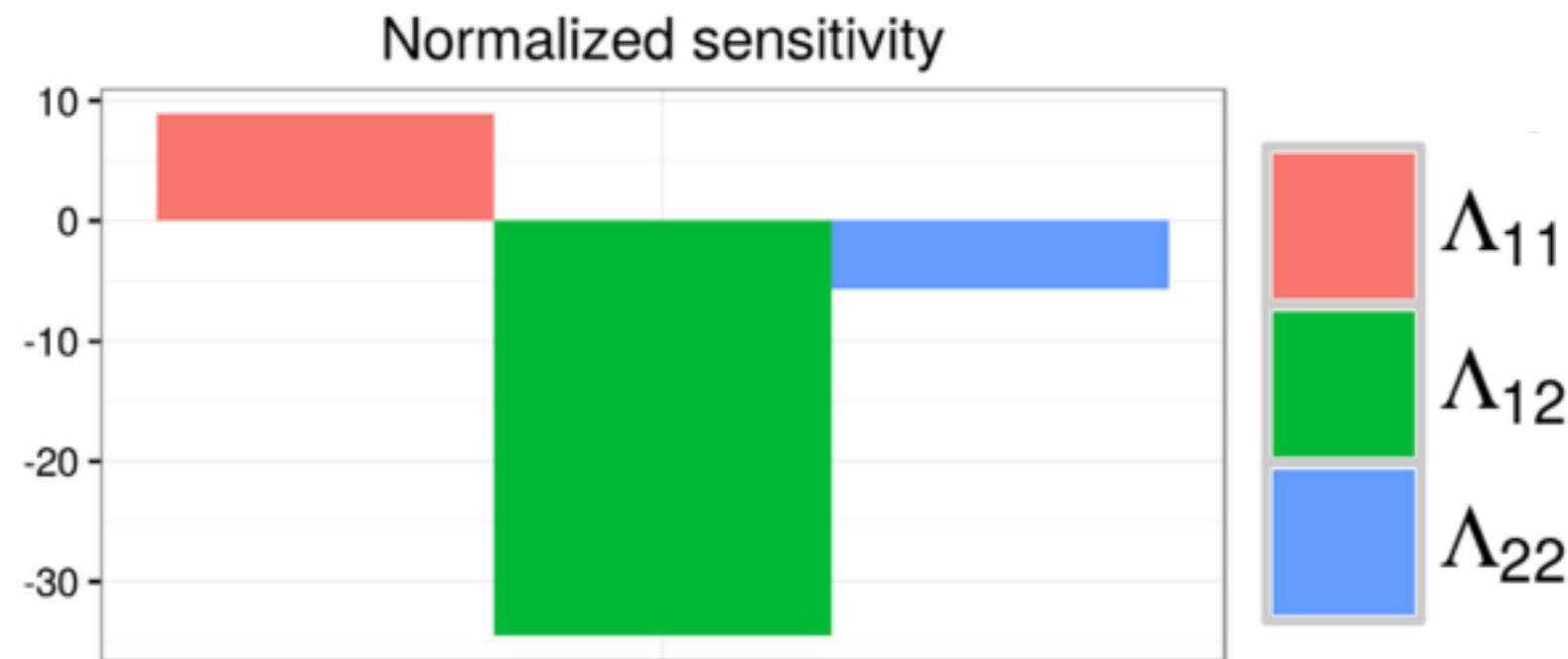
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⇒ Mean > 2 std dev



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
- Model:

$$y_{kn} \sim \text{Bernoulli}(p_{kn}) \quad p_{kn} = \frac{\exp(\rho_{kn})}{1 + \exp(\rho_{kn})}$$

$$\rho_{kn} = x_{kn}^T \beta + u_k$$

- Priors and hyperpriors:

$$u_k \sim \mathcal{N}(\mu, \sigma^2) \quad \beta \sim \mathcal{N}(\beta_0, \text{diag}(\gamma))$$

$$\mu \sim \mathcal{N}(\mu_0, \sigma_0^2)$$

$$(\sigma^2)^{-1} \sim \text{Gamma}(a, b)$$

Criteo Online Ads Experiment

Criteo Online Ads Experiment

- VB: 57 sec

Criteo Online Ads Experiment

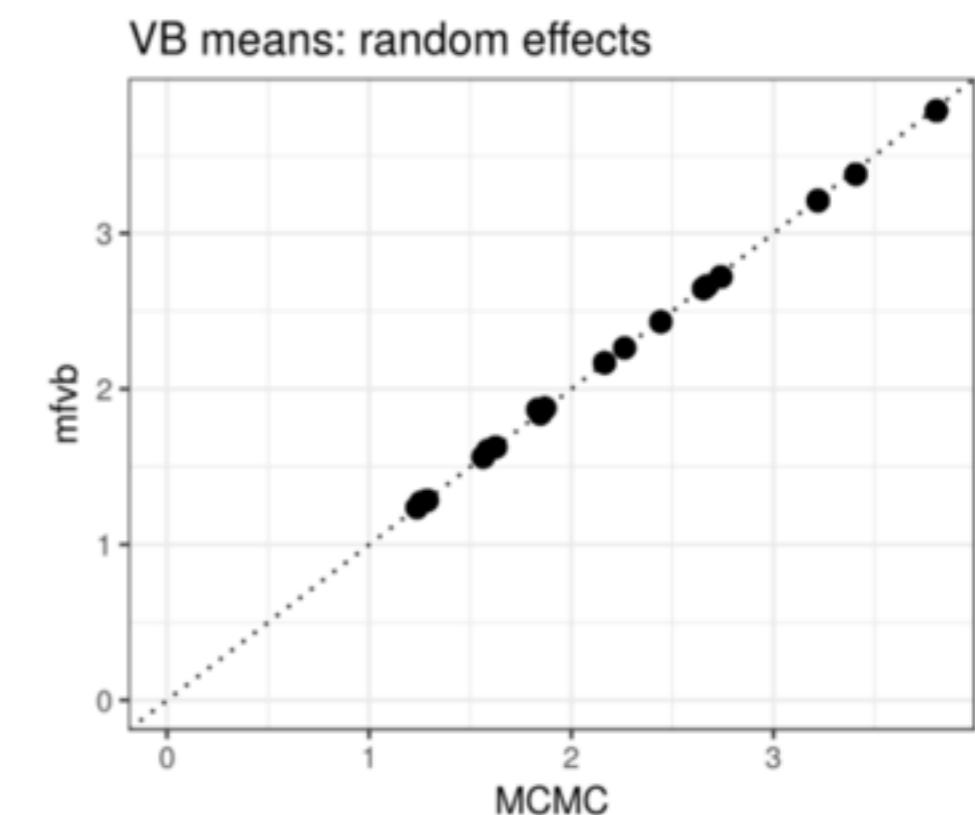
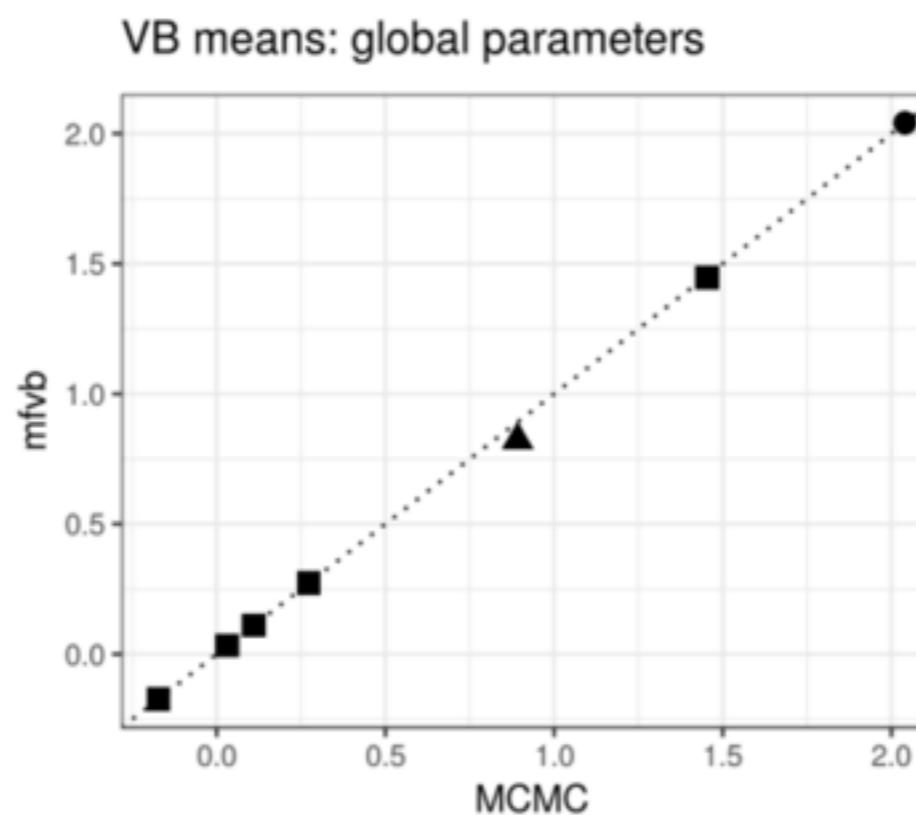
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553 sec
(9.2 min)

Criteo Online Ads Experiment

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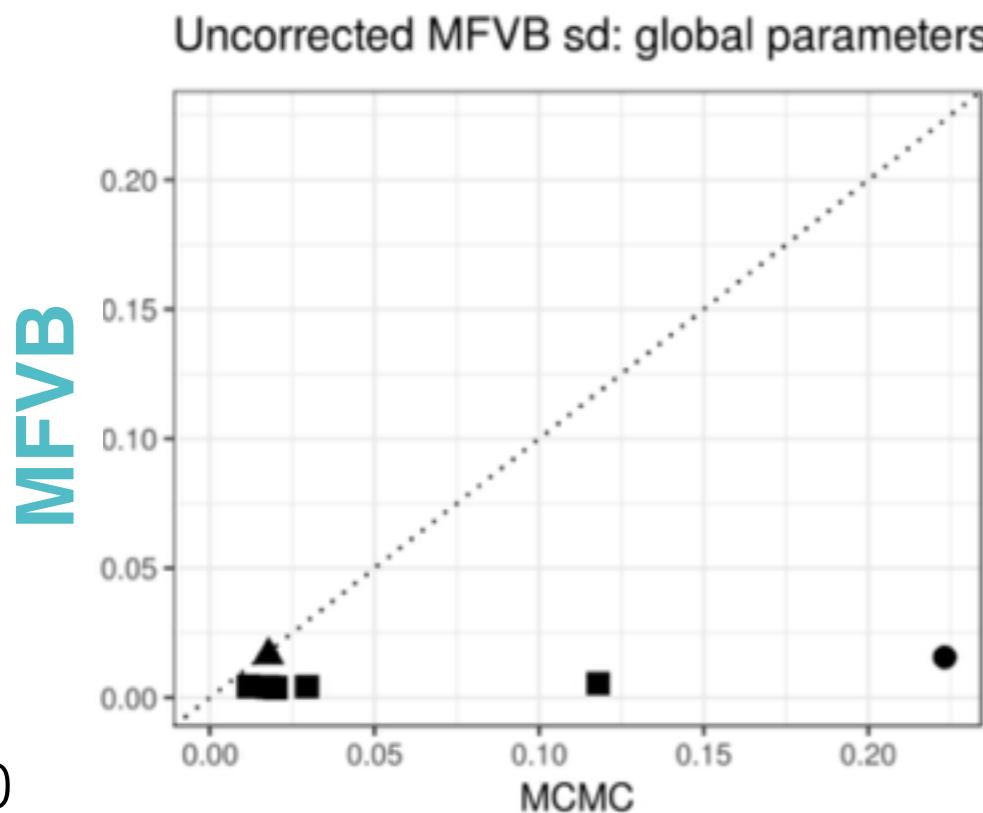
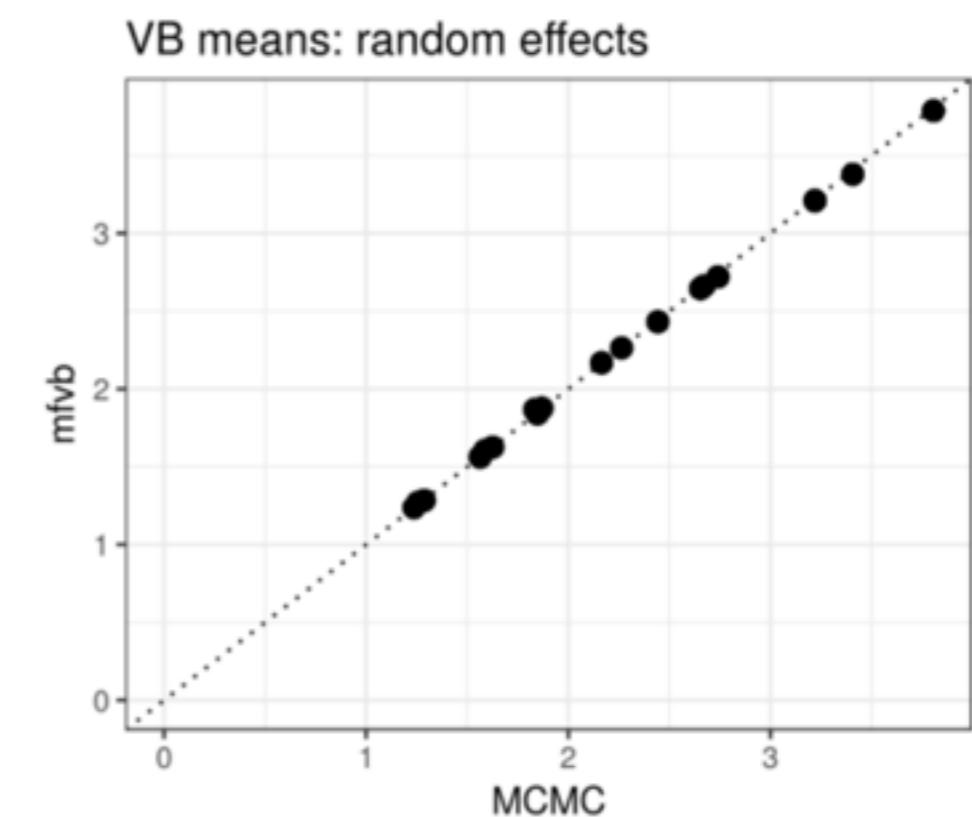
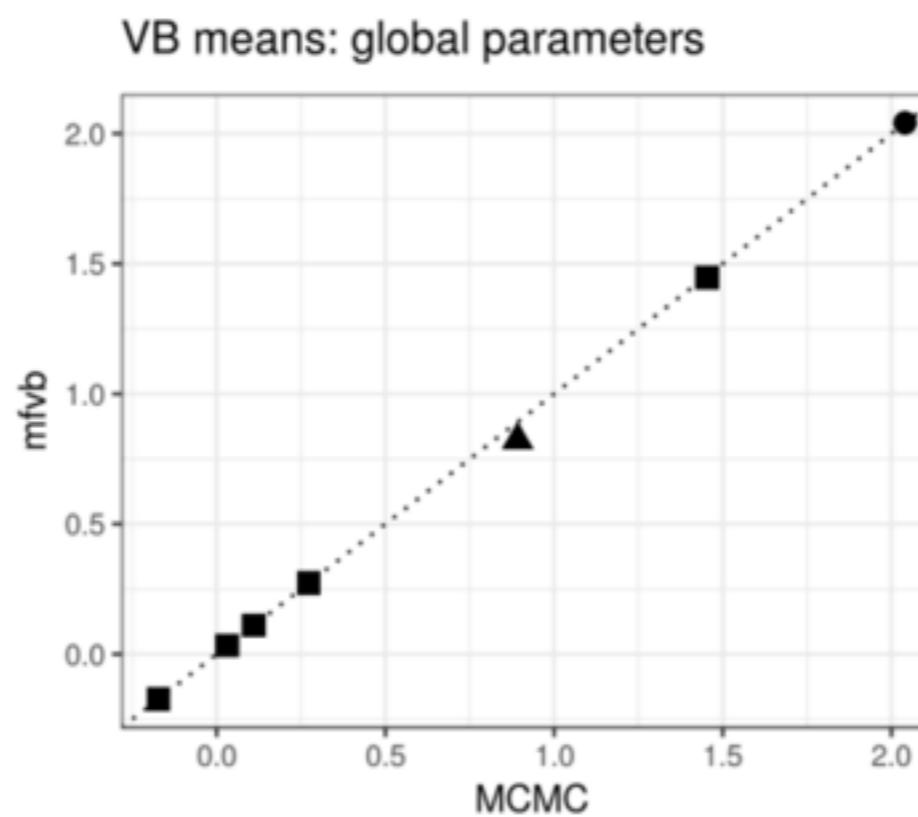
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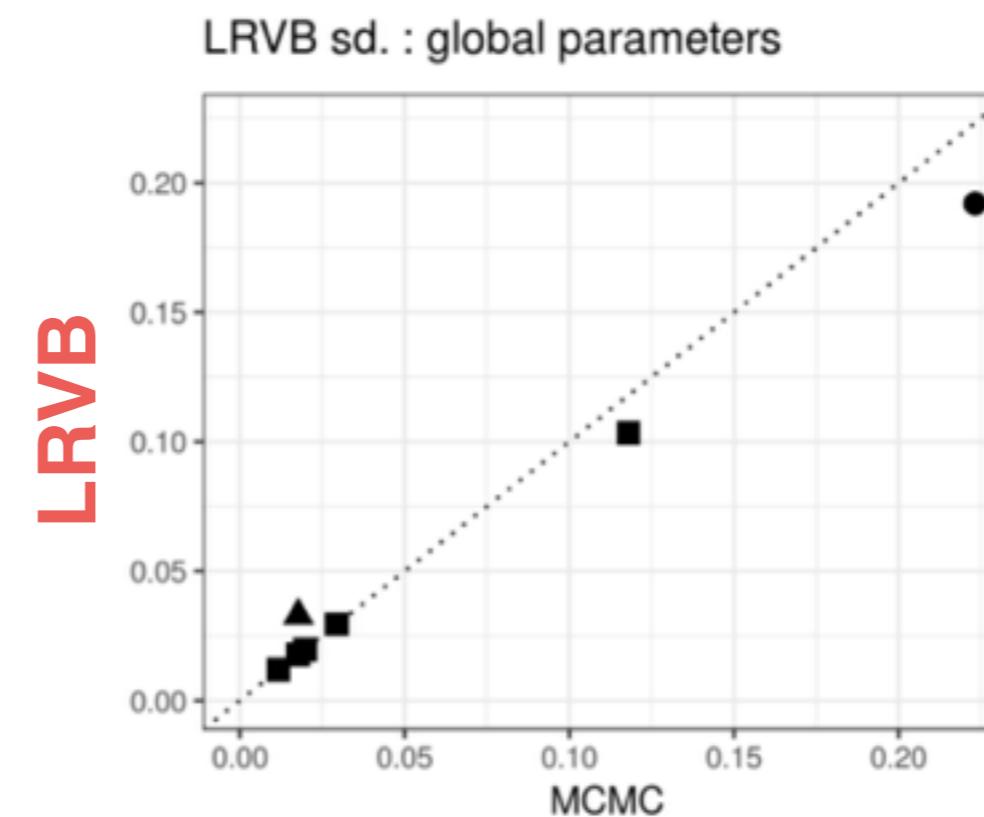
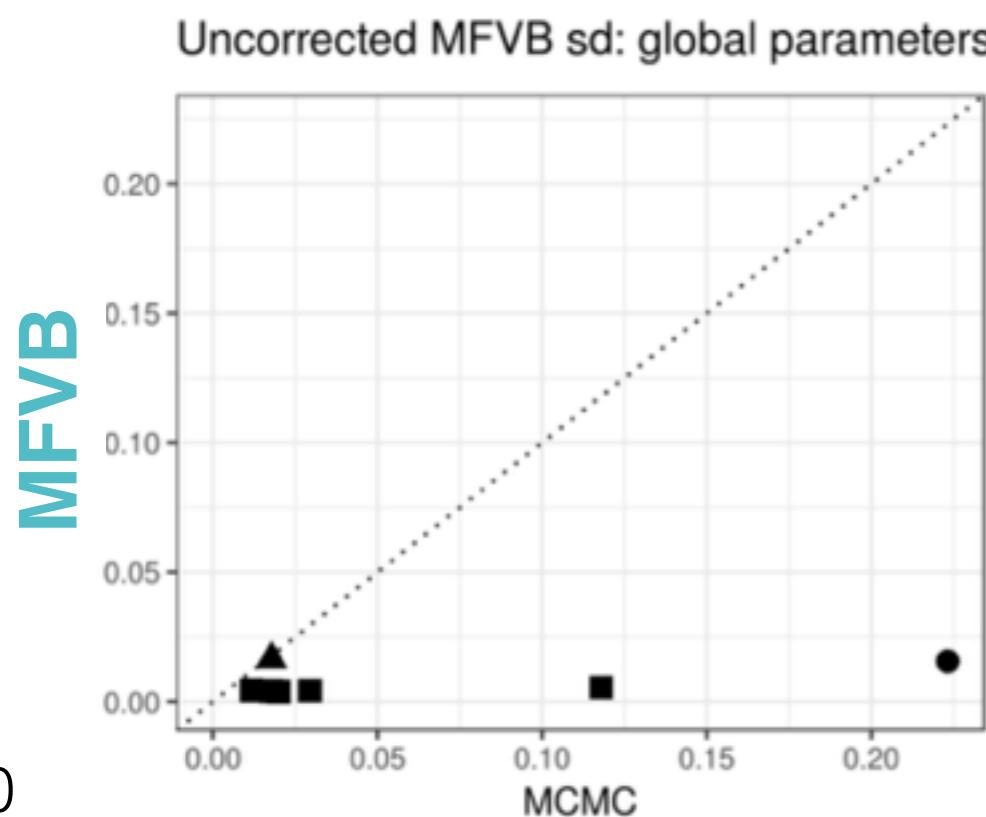
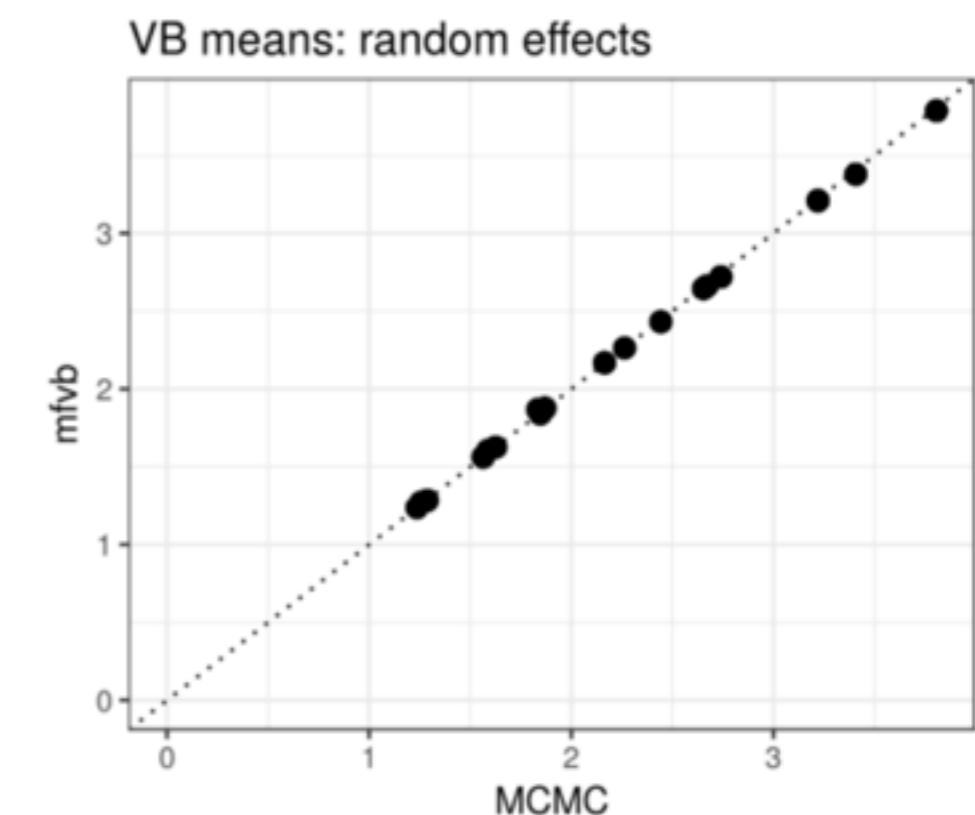
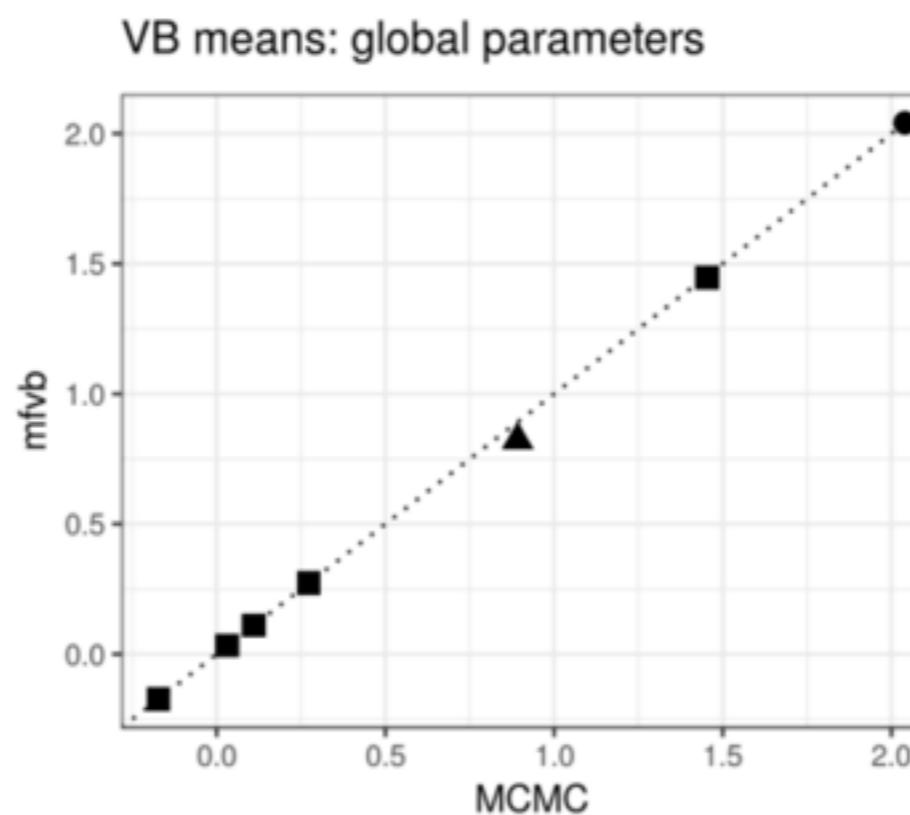
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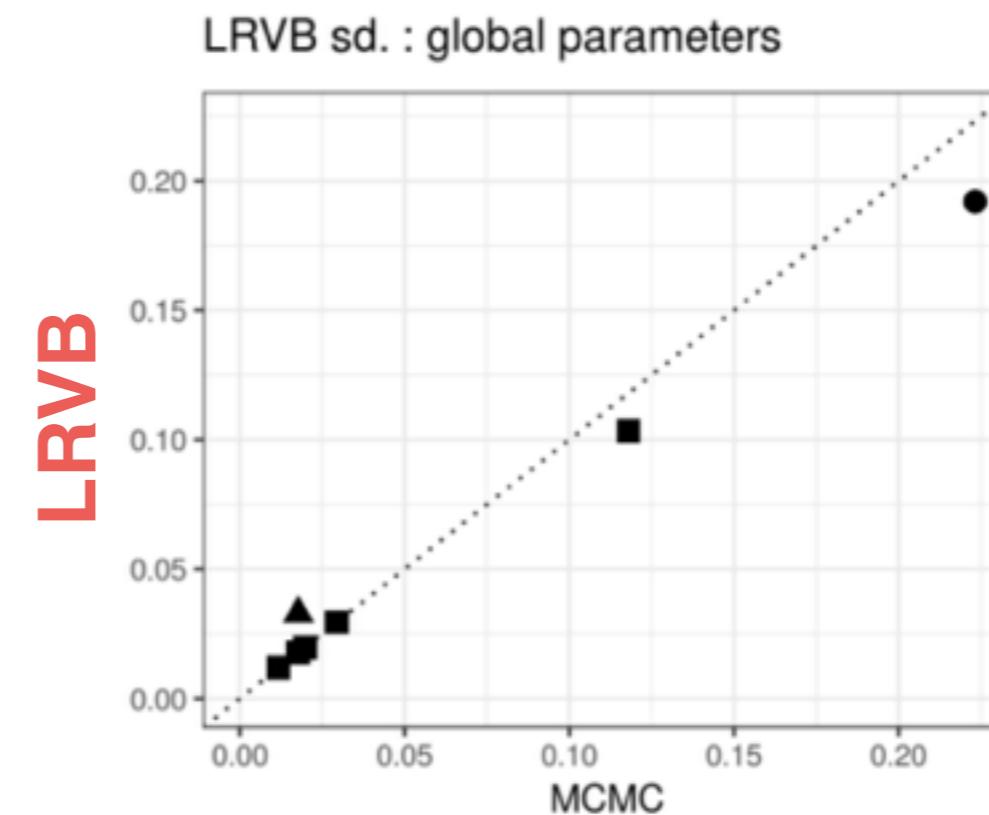
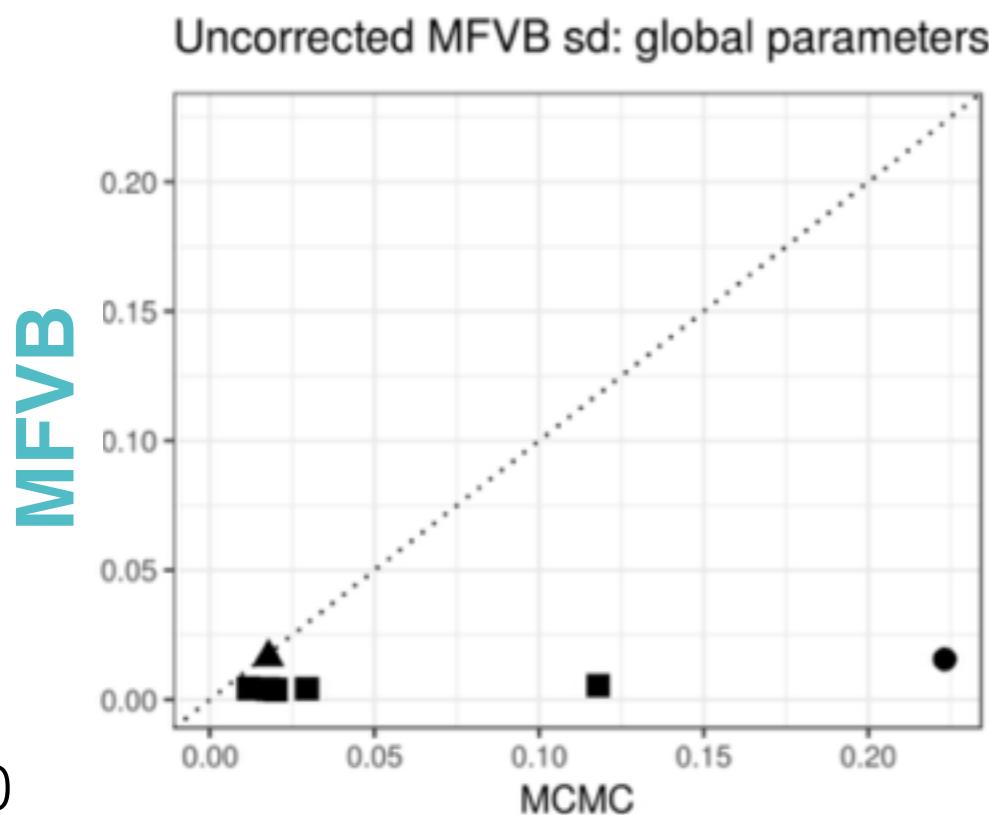
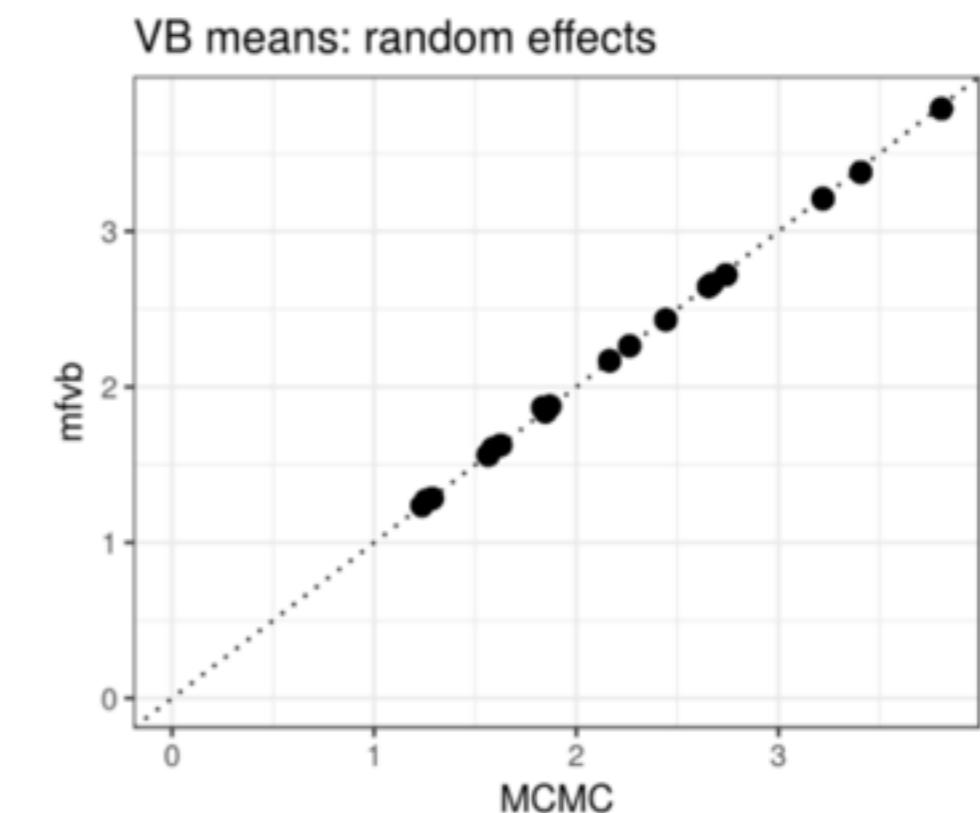
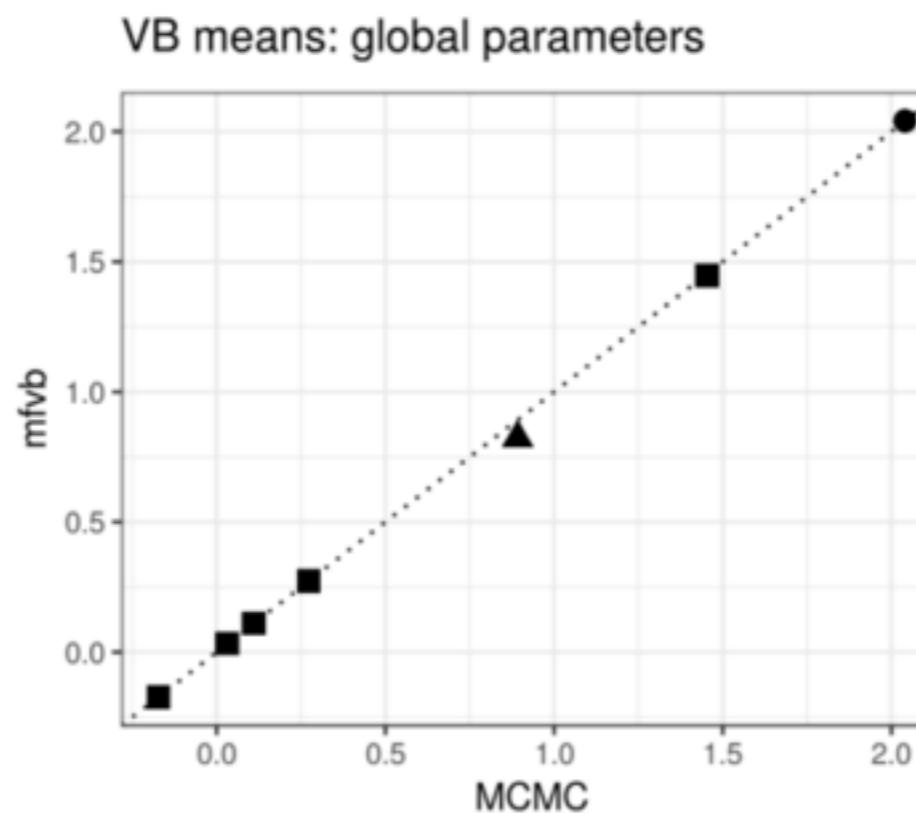
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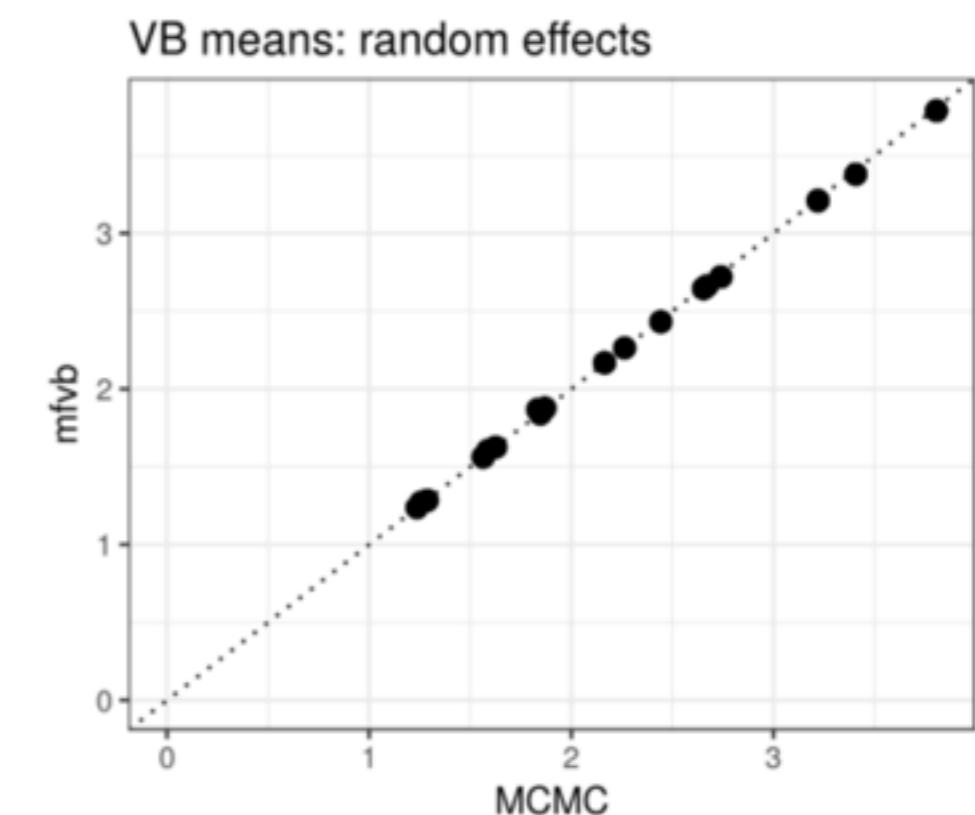
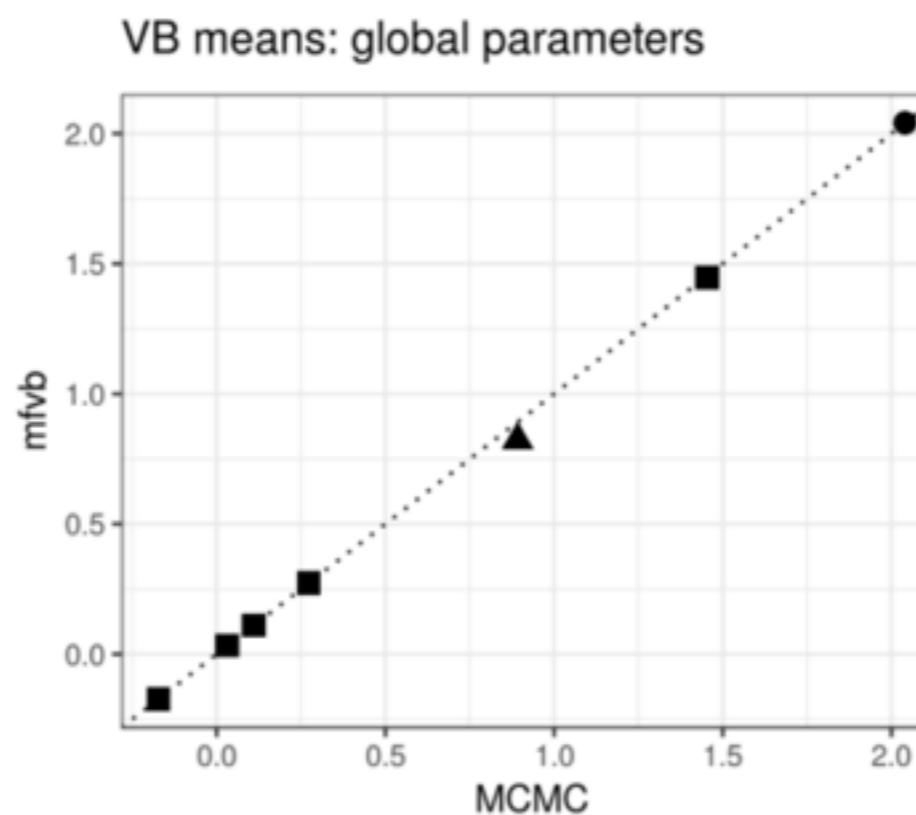
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Also good random effects sd and covariances

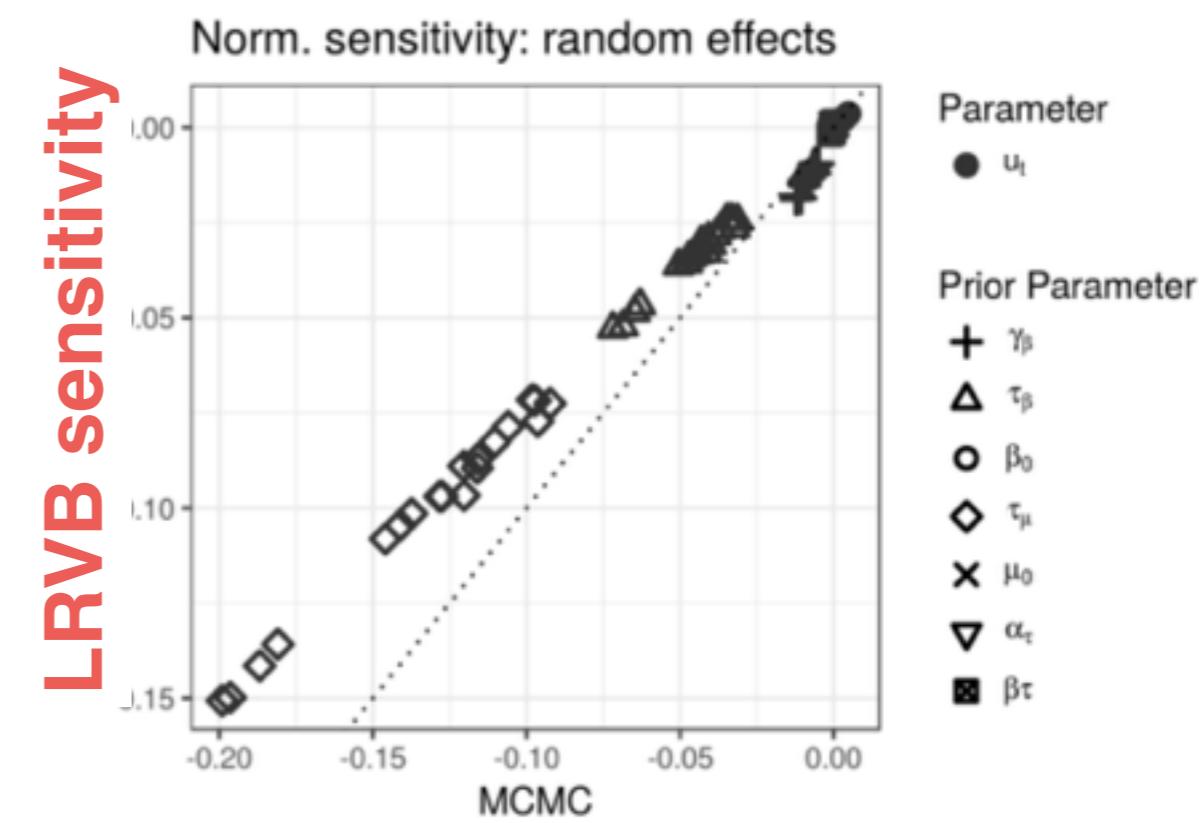
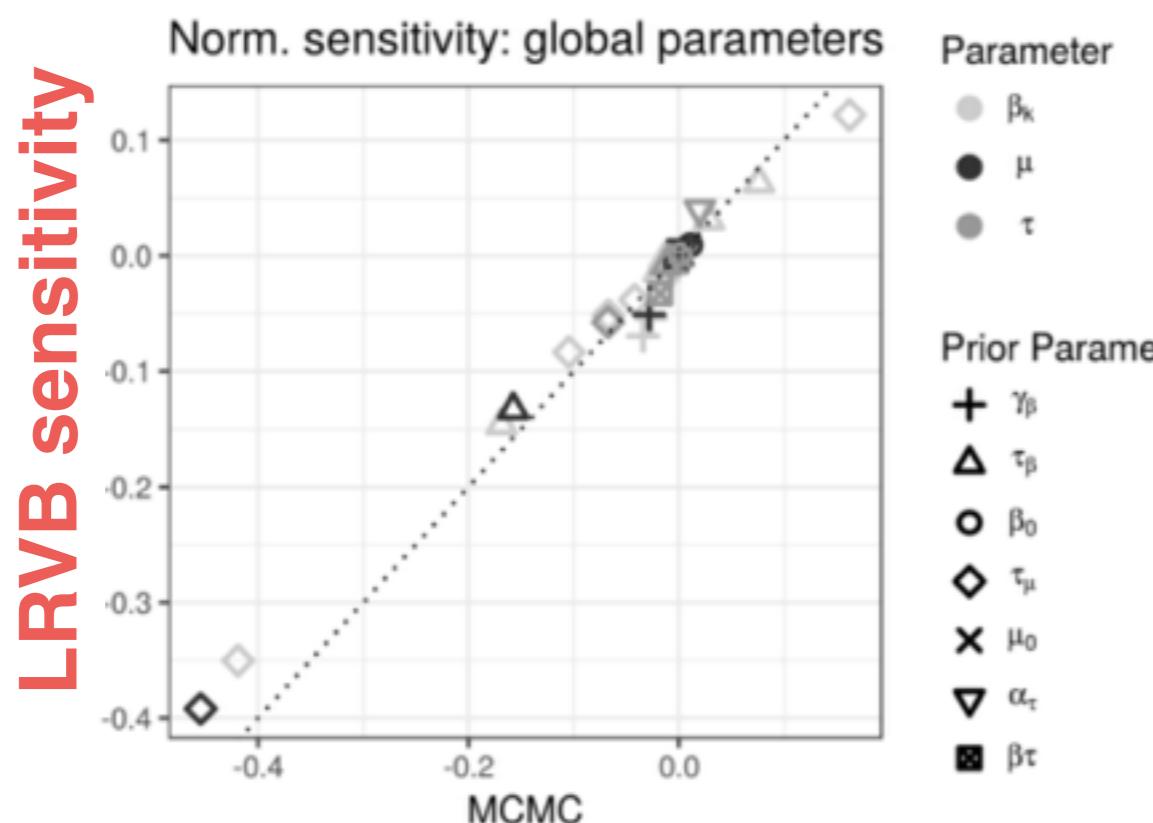
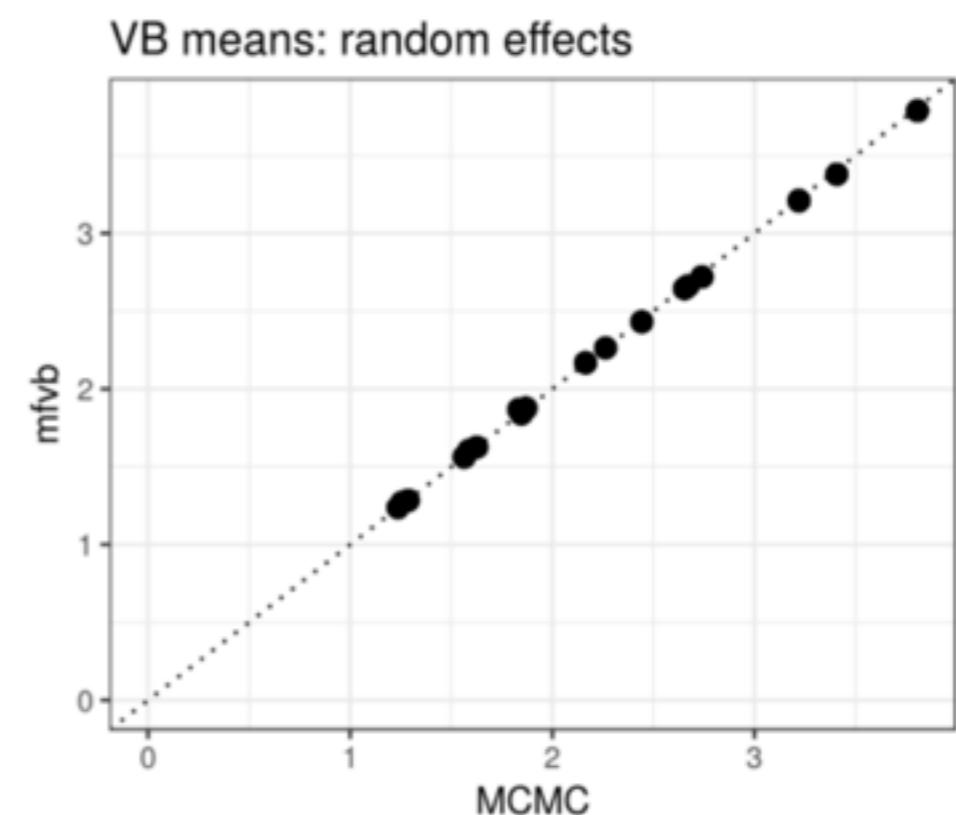
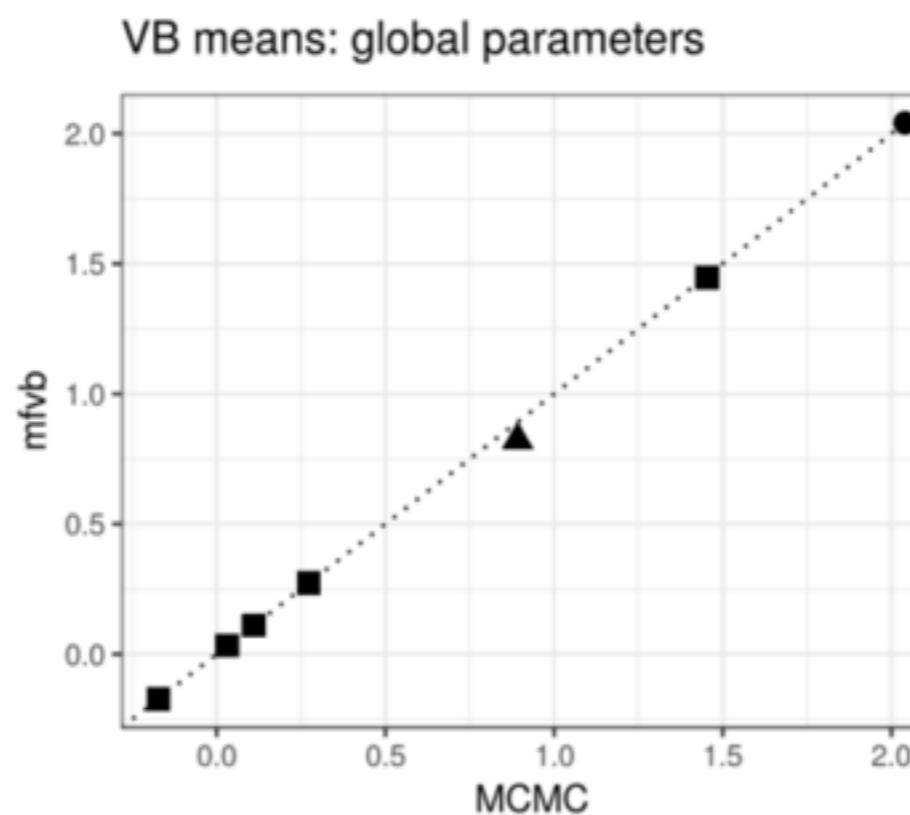
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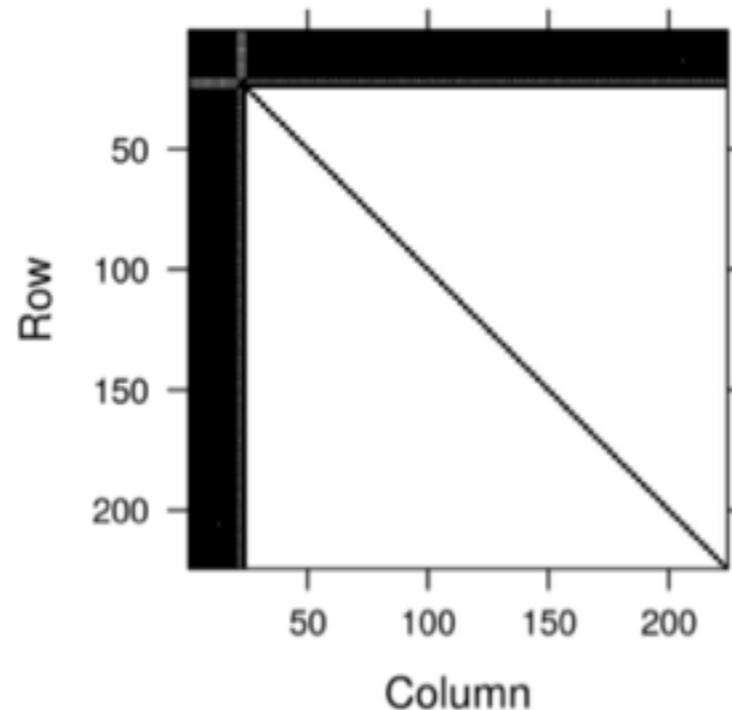
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Computational complexity

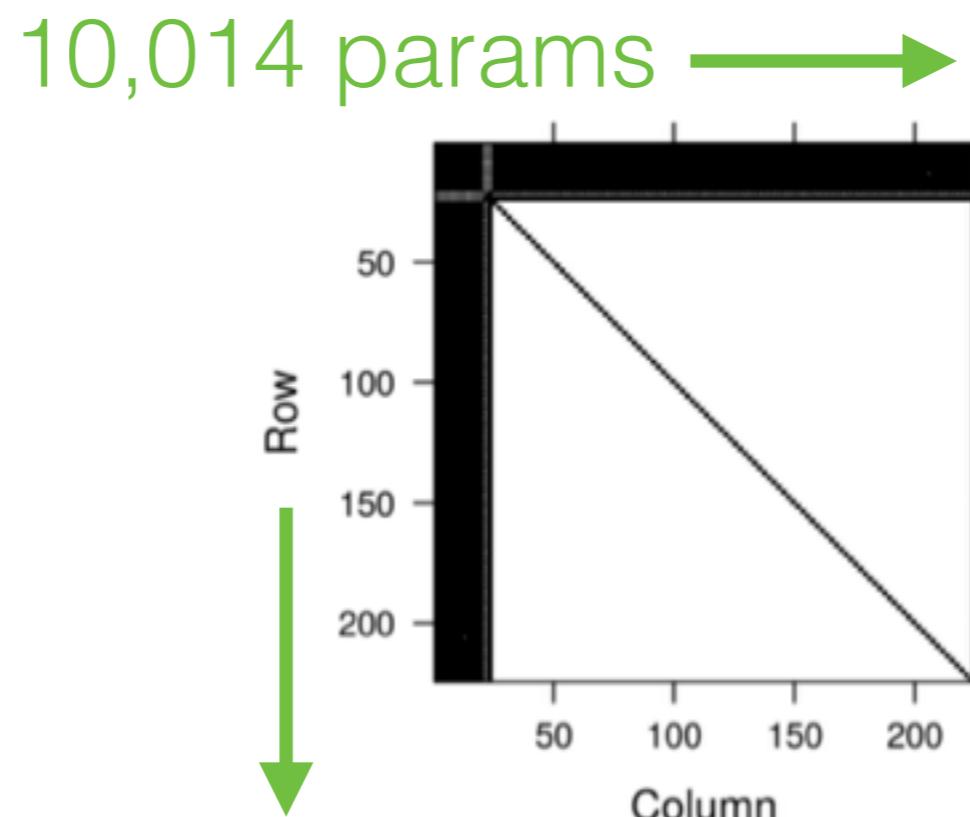
Computational complexity

- Top left submatrix for Criteo analysis



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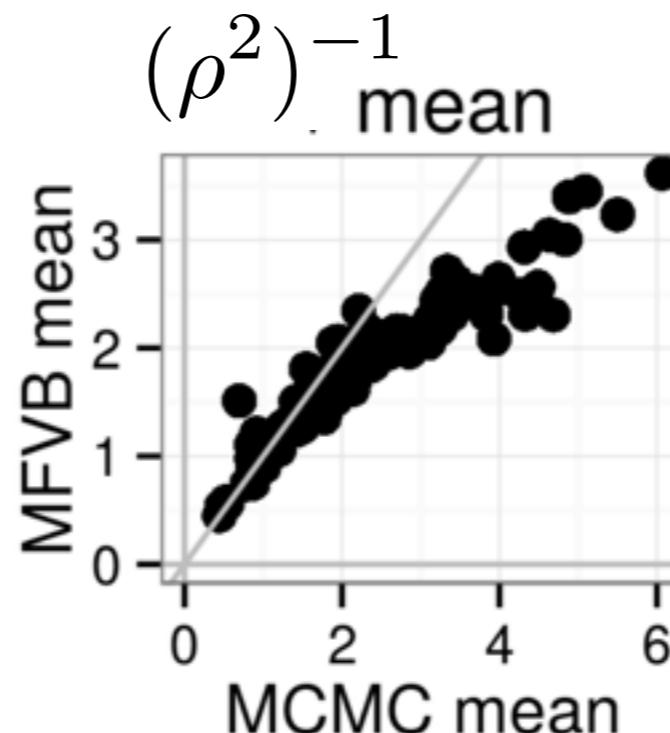
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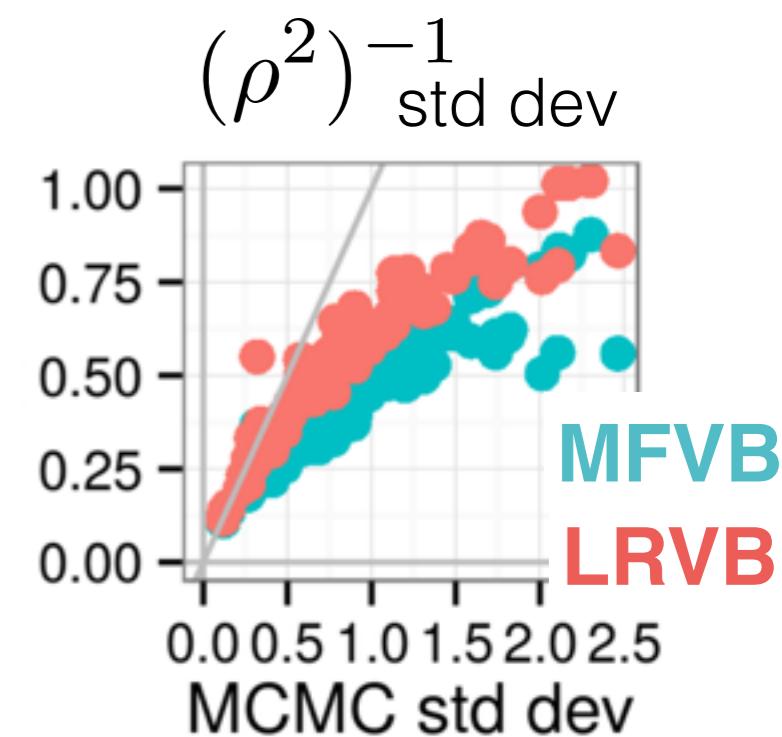
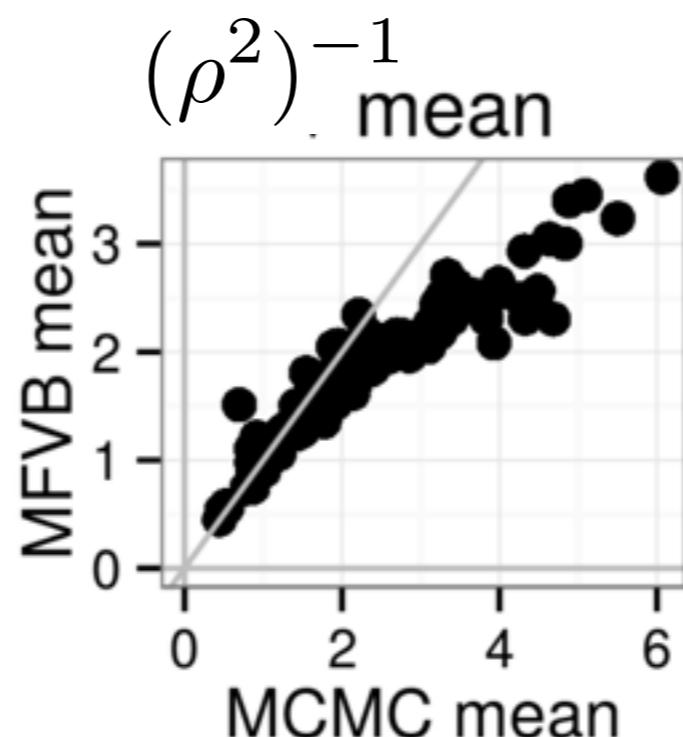
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 - Fast **robustness** quantification
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- Data summarization for scalability (Part IV)

References (1/2)

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