

Fast Quantification of Uncertainty and Robustness with Variational Bayes

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MIT

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Uncertainty & robustness quantification

- Bayesian inference

Uncertainty & robustness quantification

- Bayesian inference
 - Complex, modular models

Uncertainty & robustness quantification

- Bayesian inference
 - Complex, modular models; posterior distribution

Uncertainty & robustness quantification

- Bayesian inference $p(\theta)$
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 - Time-consuming

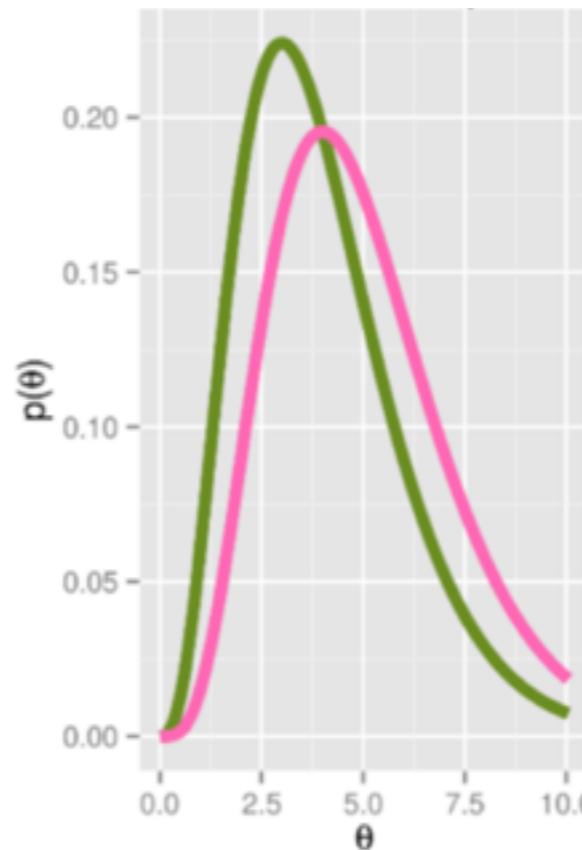
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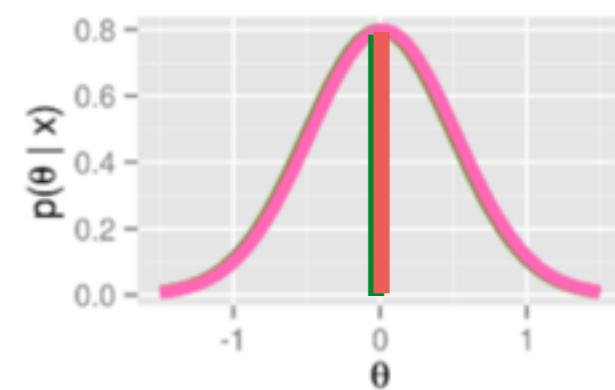
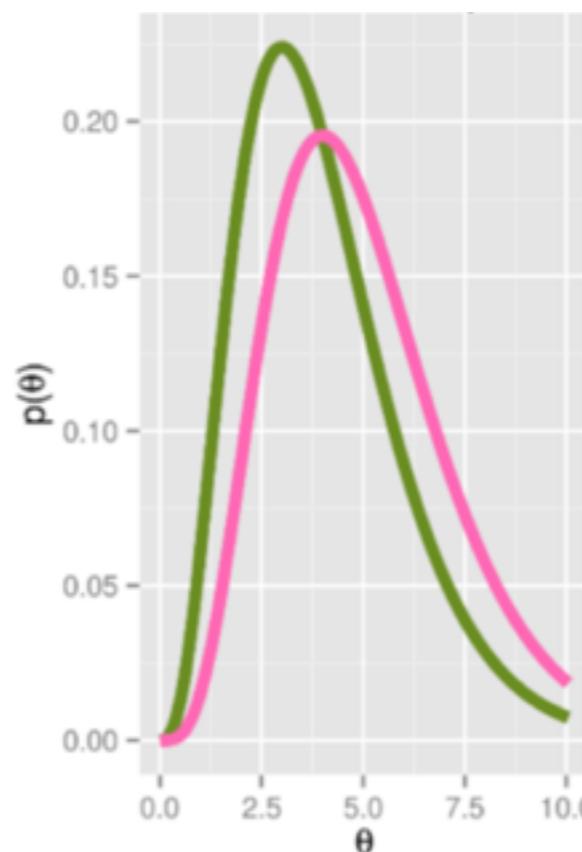
Some reasonable priors



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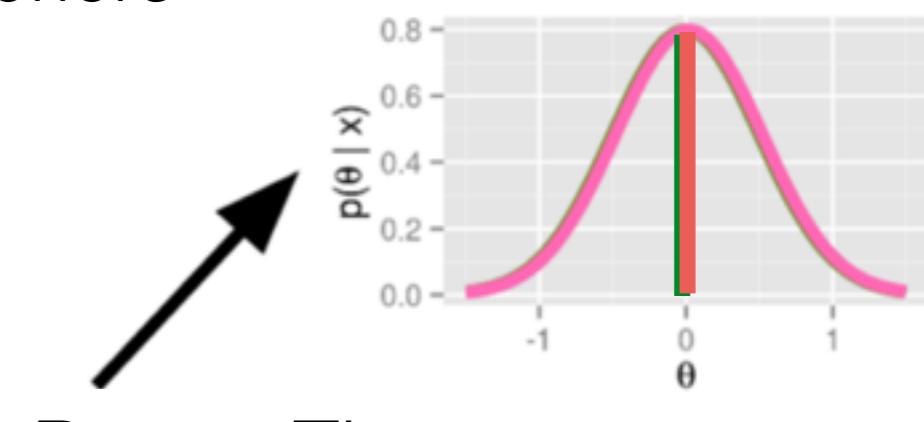
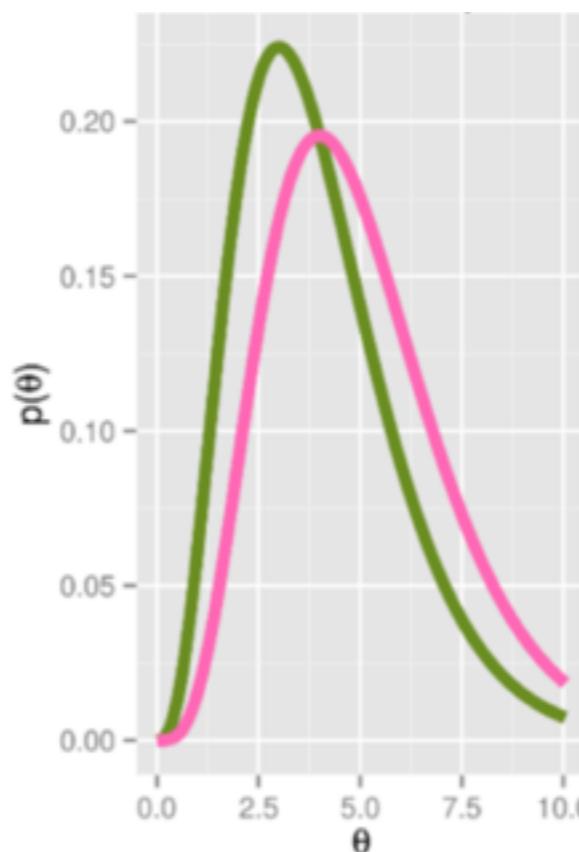


Bayes Theorem

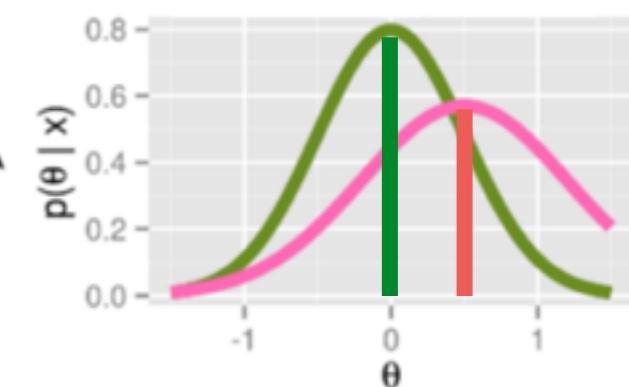
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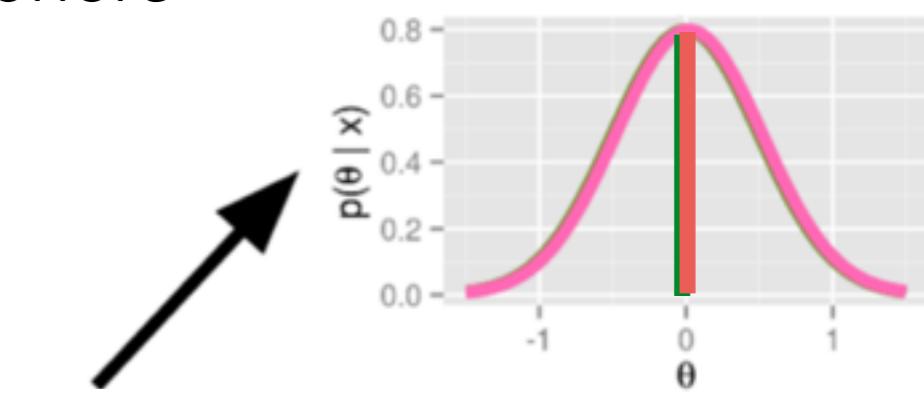
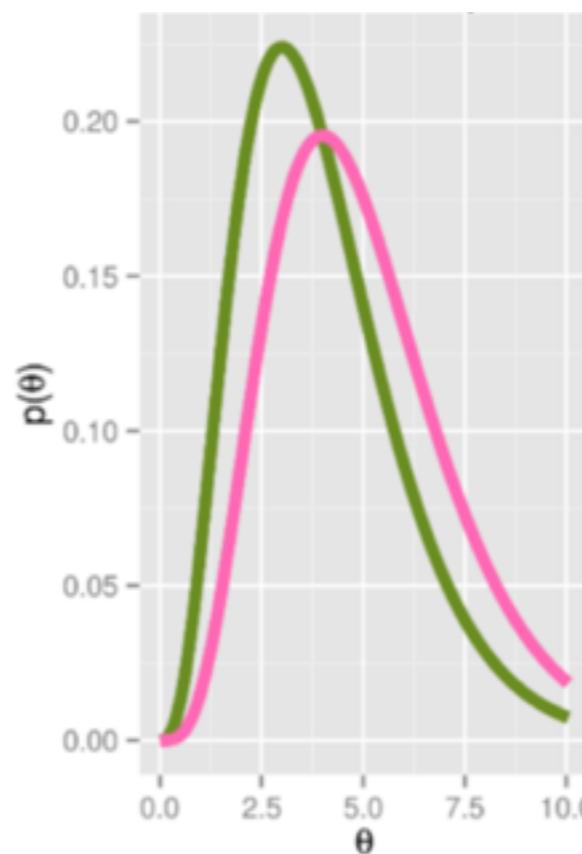
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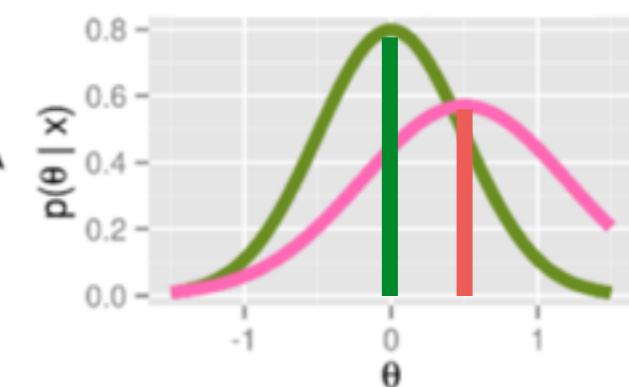
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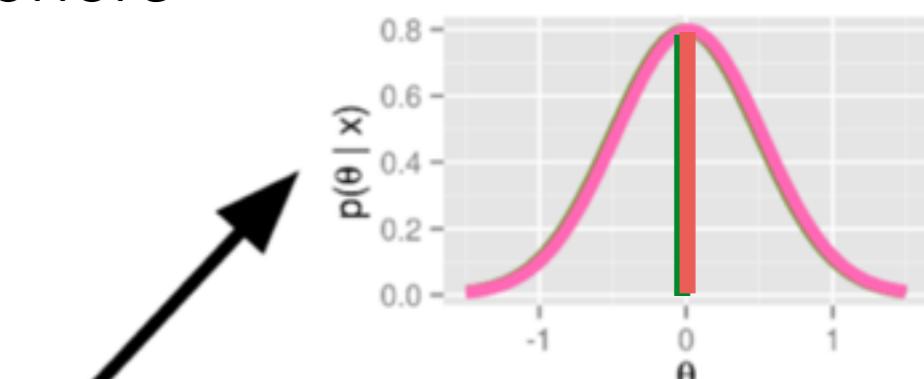
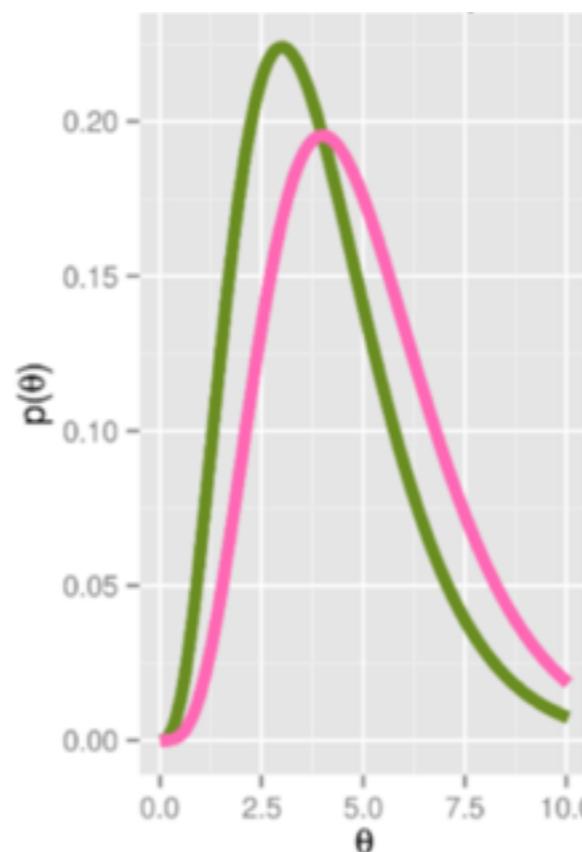
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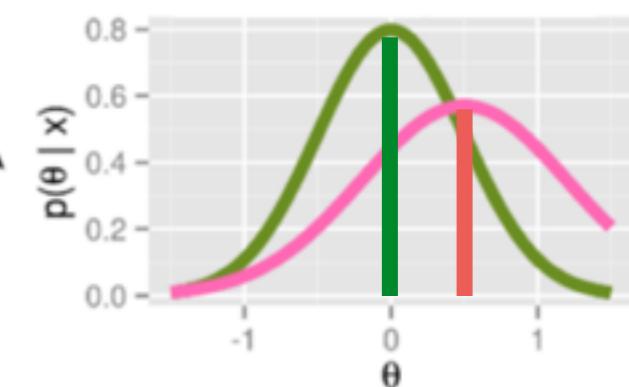
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Approximating the posterior can be computationally expensive

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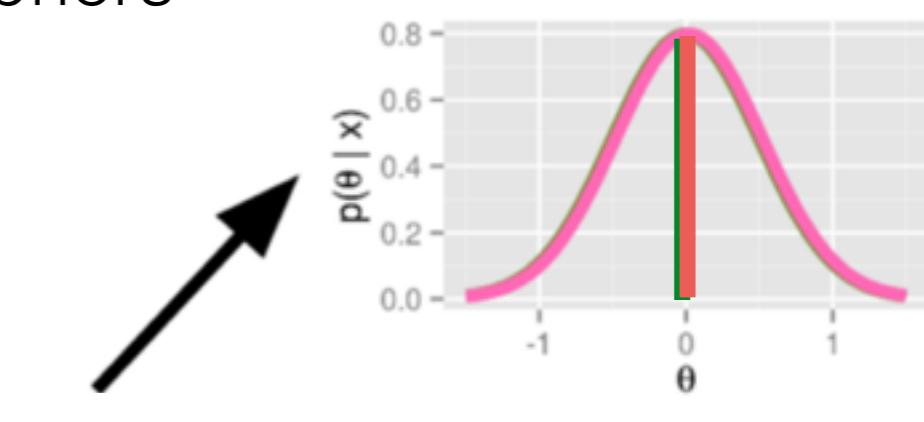
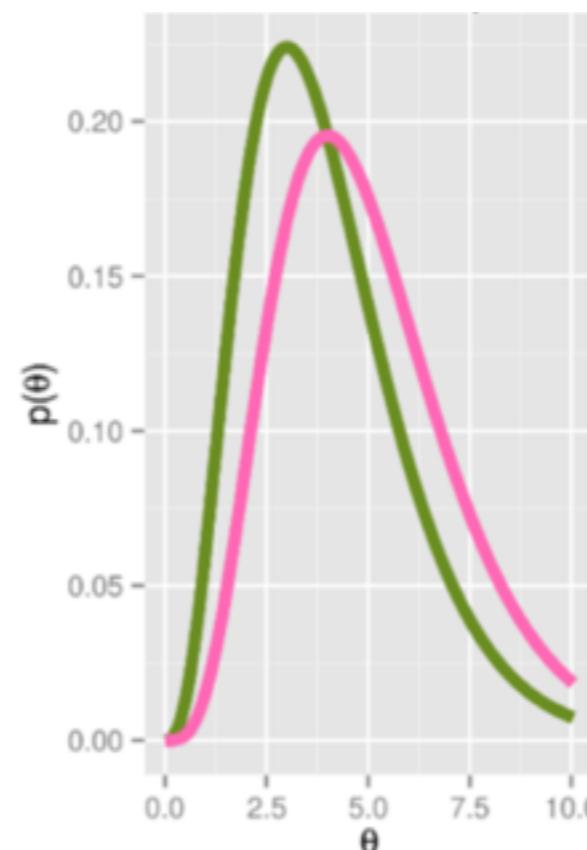
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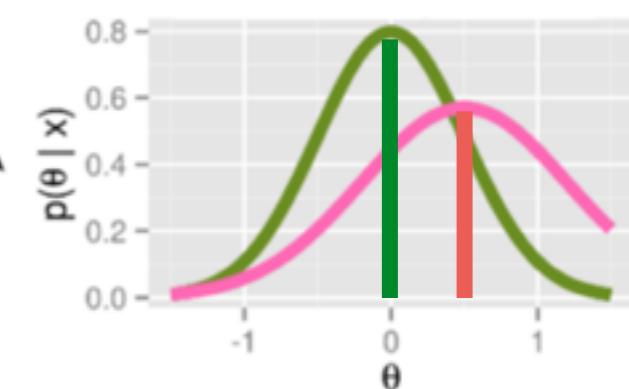
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Bayes Theorem



- We propose: *linear response variational Bayes*

Roadmap

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- Variational Bayes as an alternative to MCMC

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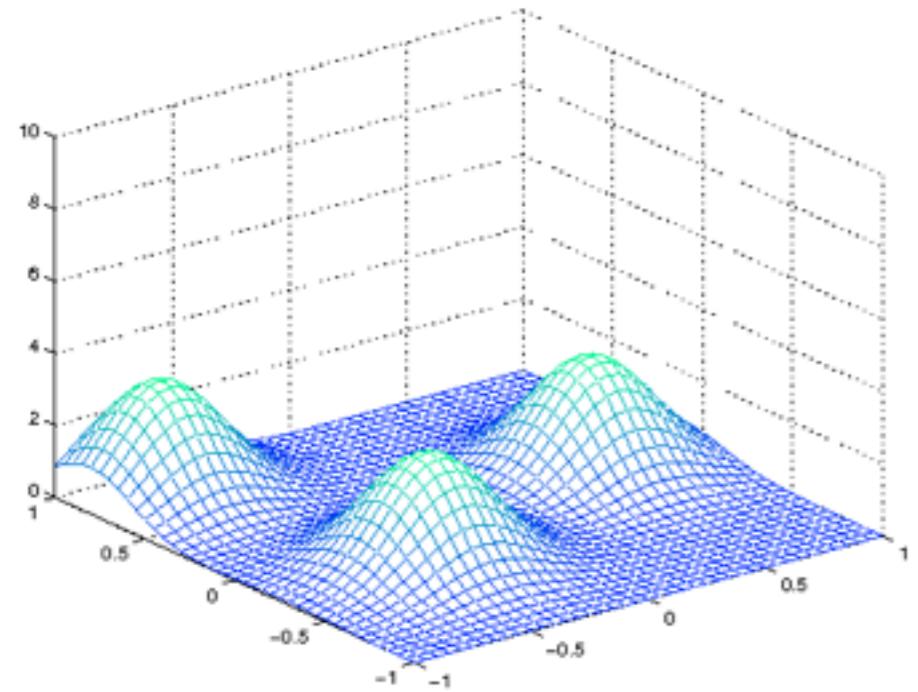
- Variational Bayes as an alternative to MCMC
- Challenges of VB
- Accurate uncertainties from VB
- Accurate robustness quantification from VB
- Big idea: derivatives/perturbations are relatively easy in VB

Variational Bayes

Variational Bayes

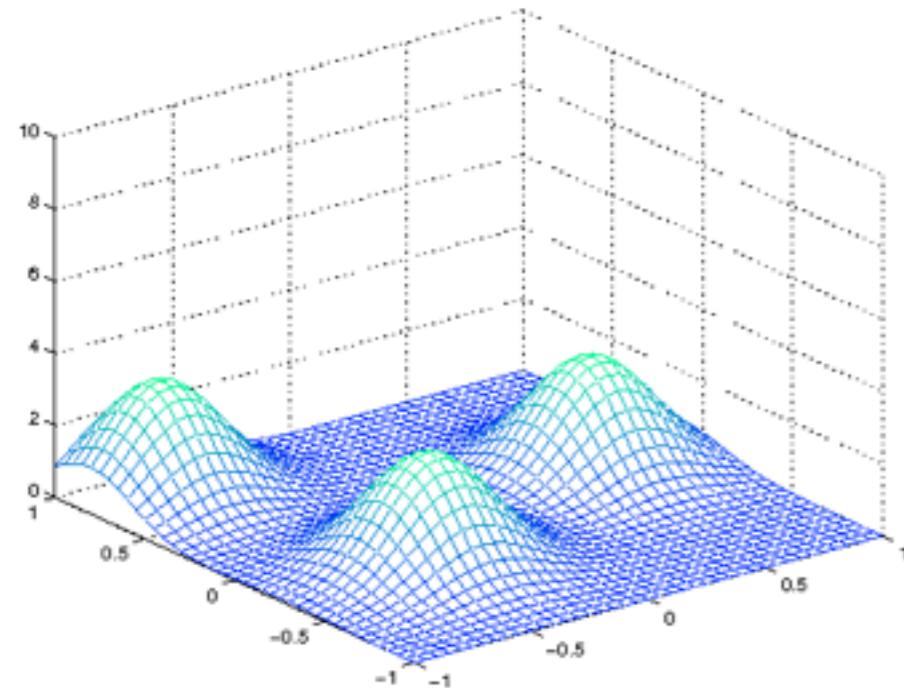
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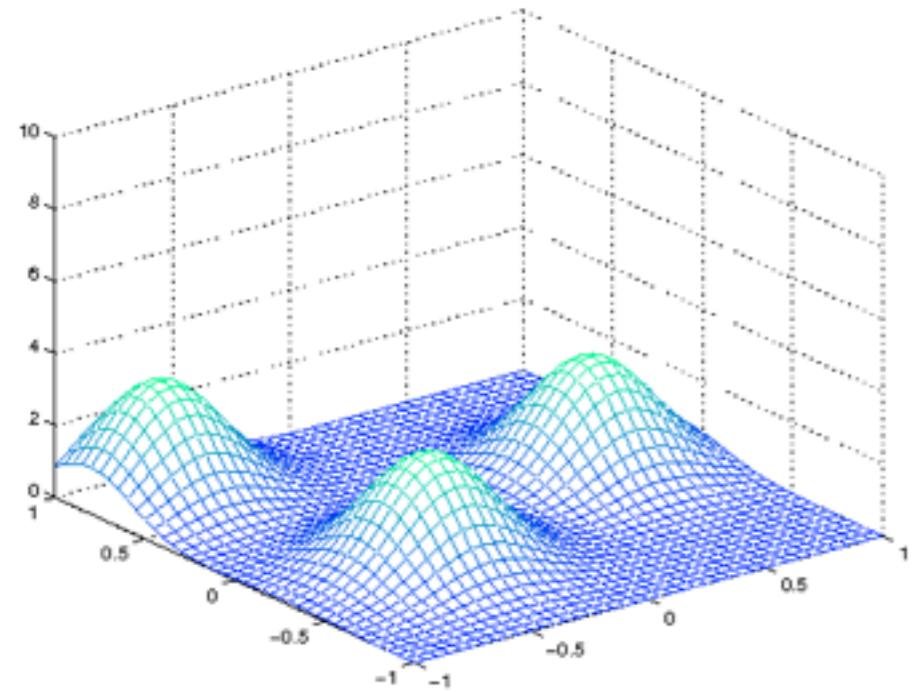
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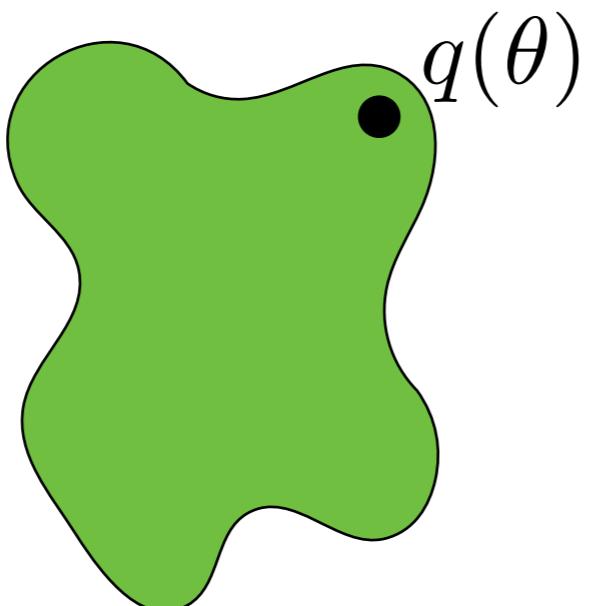


- Variational Bayes (VB)
 - Approximation $q^*(\theta)$ for posterior $p(\theta|x)$

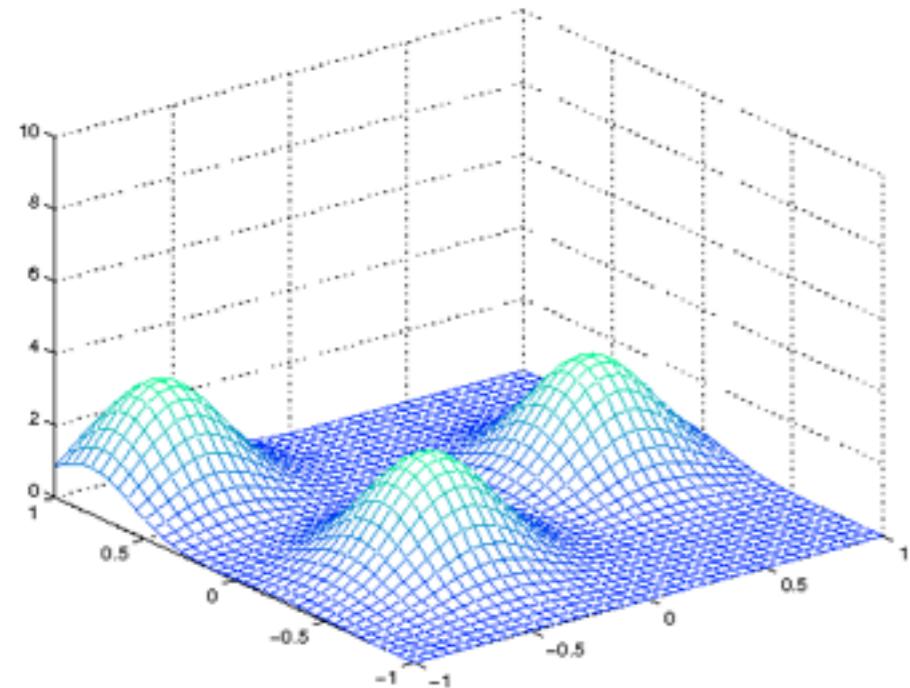
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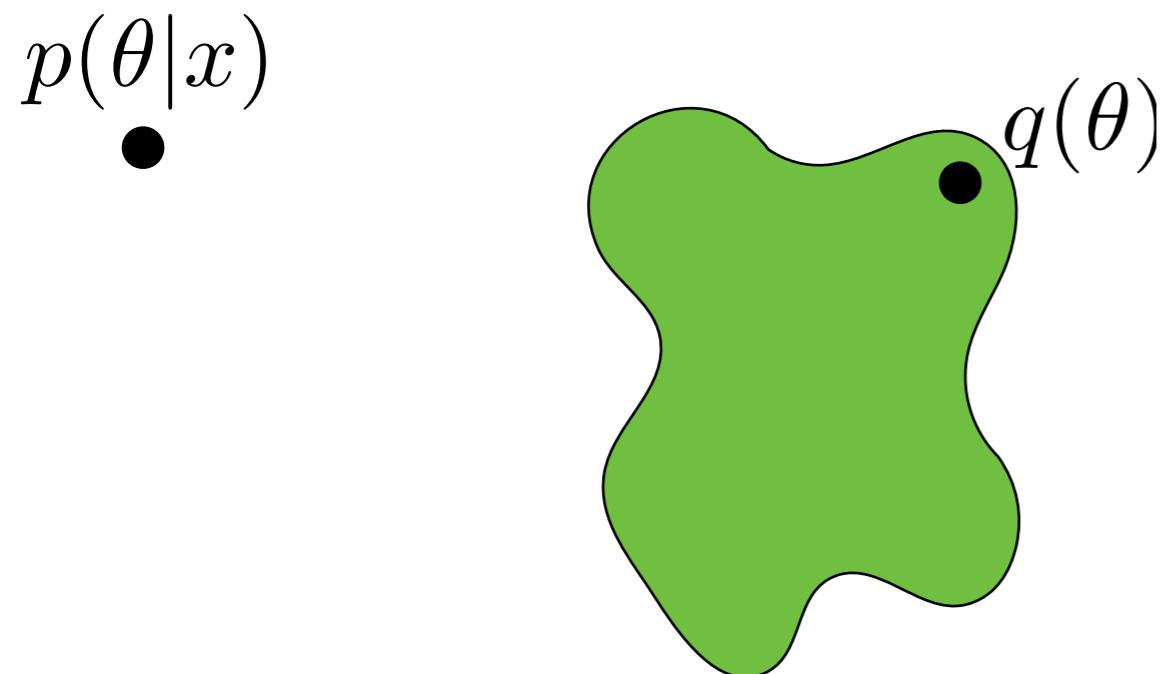
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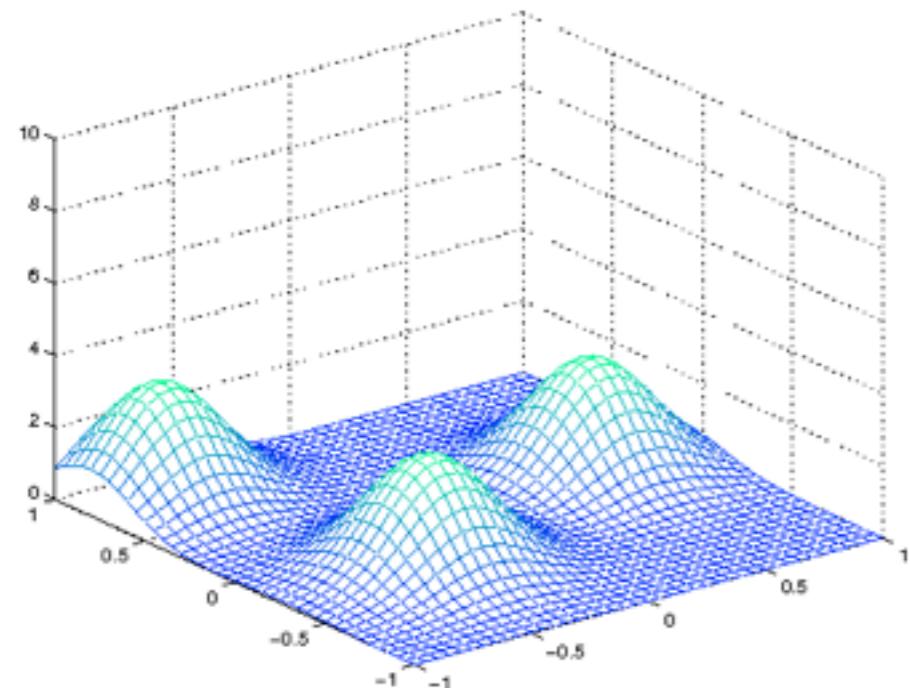
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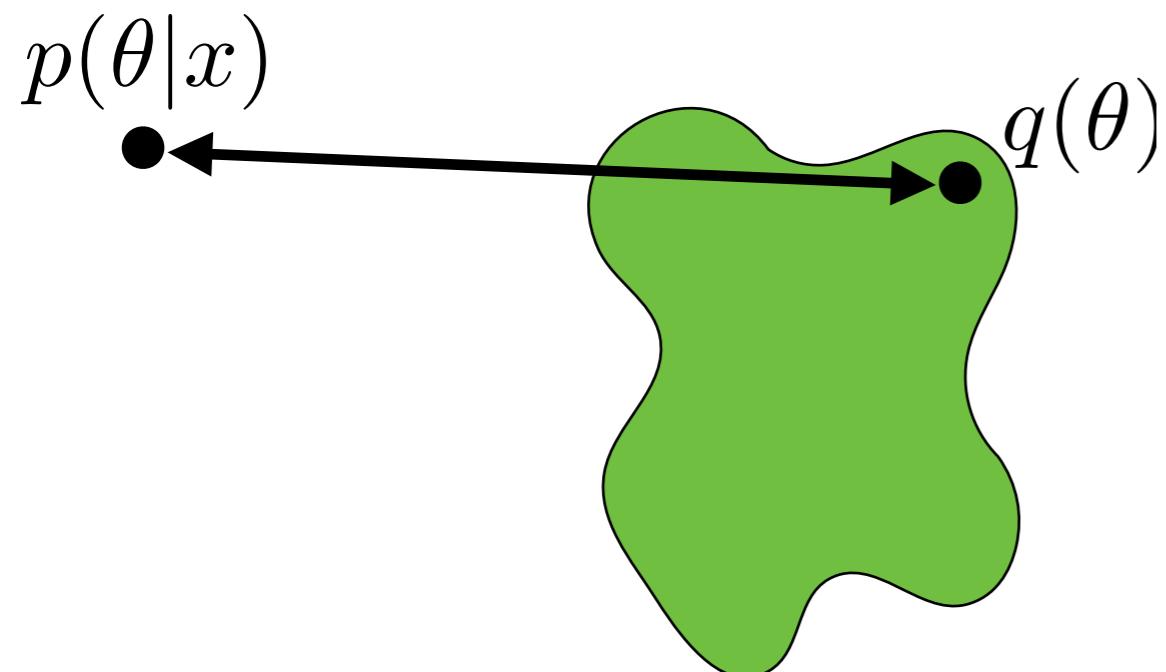
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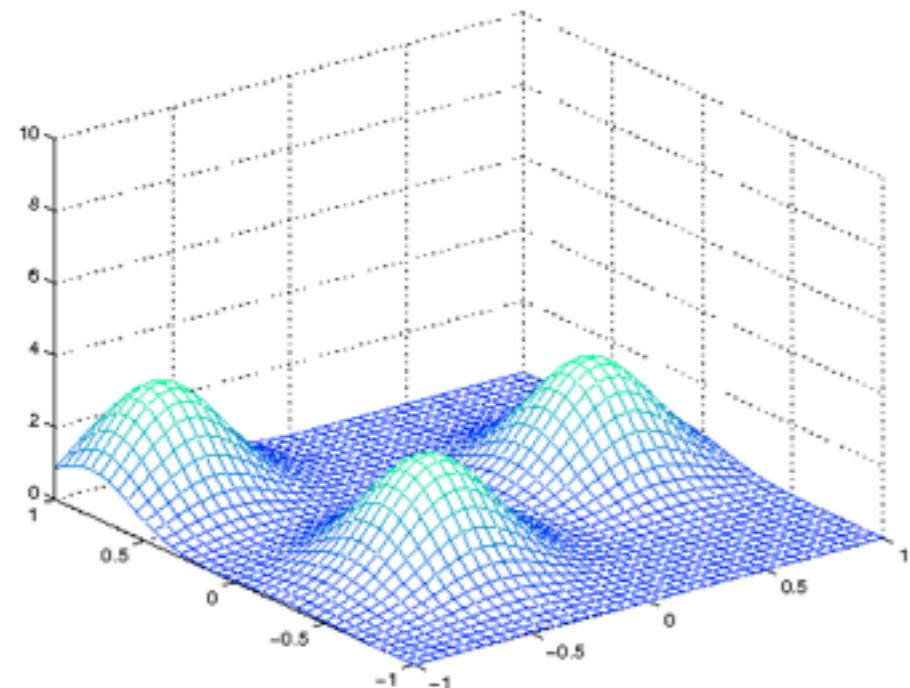
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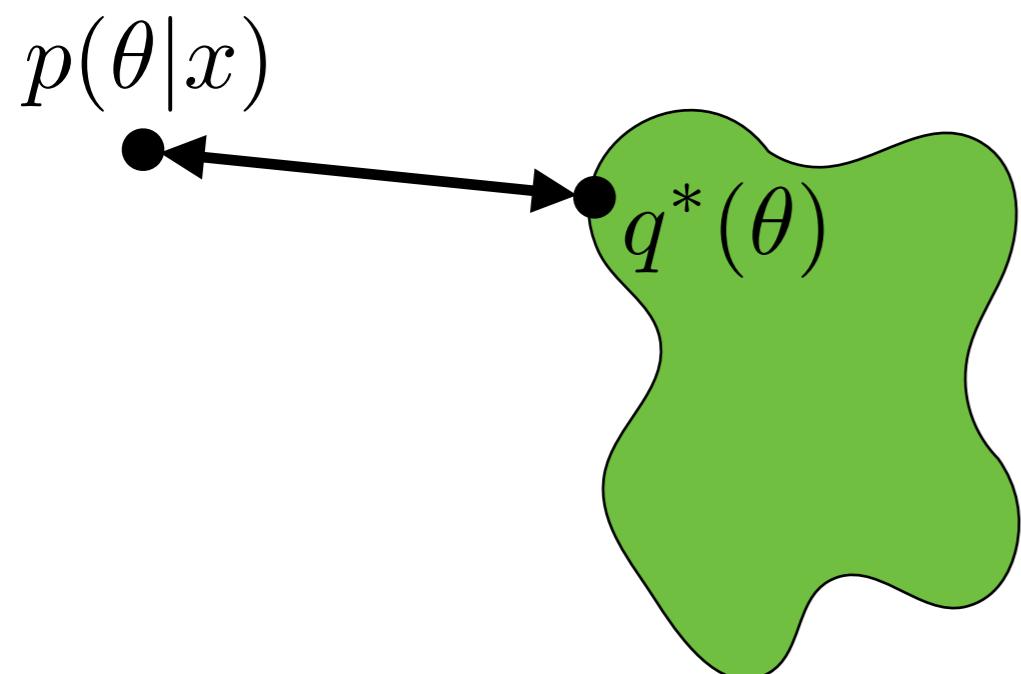
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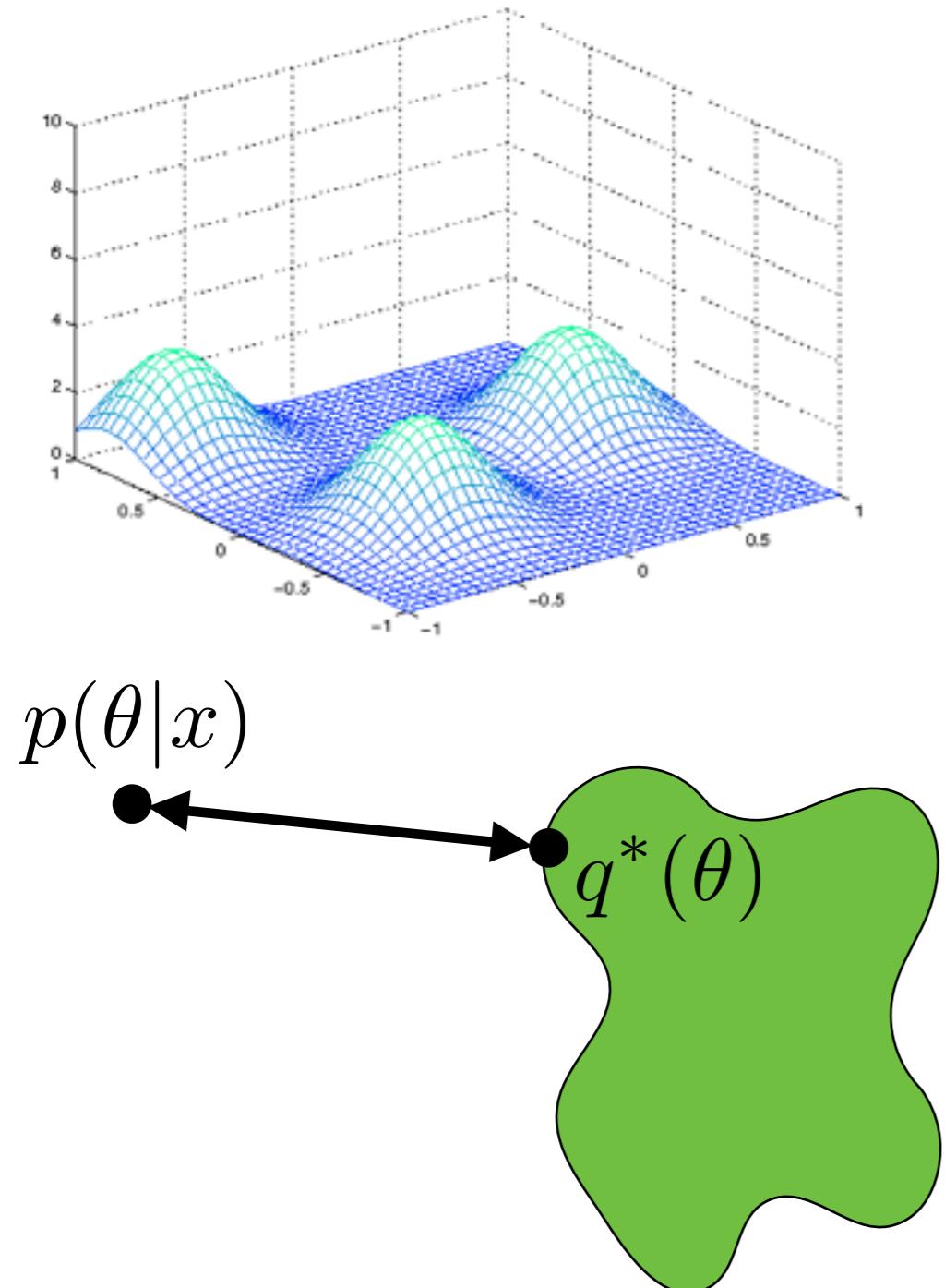
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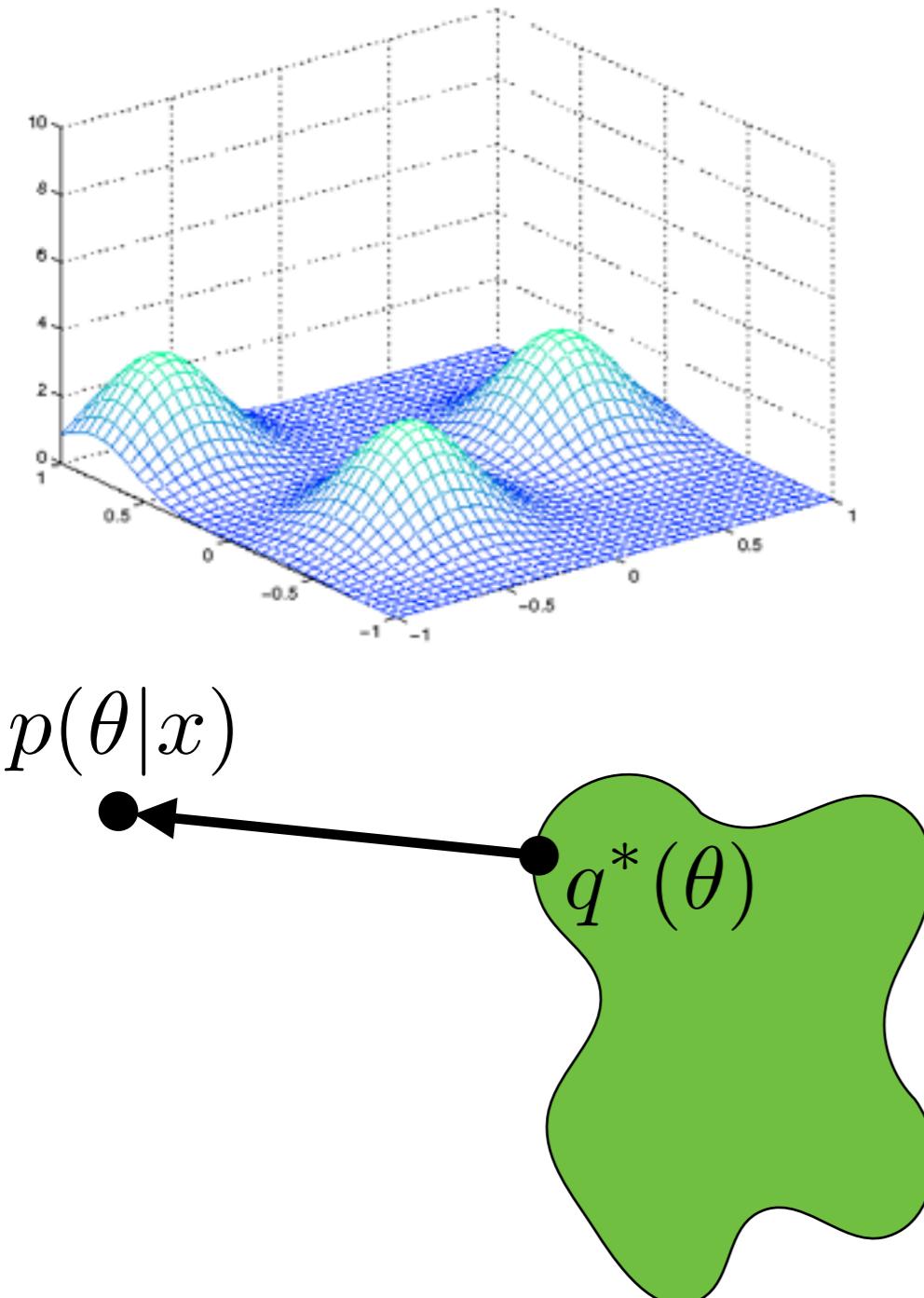
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- Variational Bayes (VB)
 - Approximation $q^*(\theta)$ for posterior $p(\theta|x)$
 - Minimize Kullback-Liebler (KL) divergence:

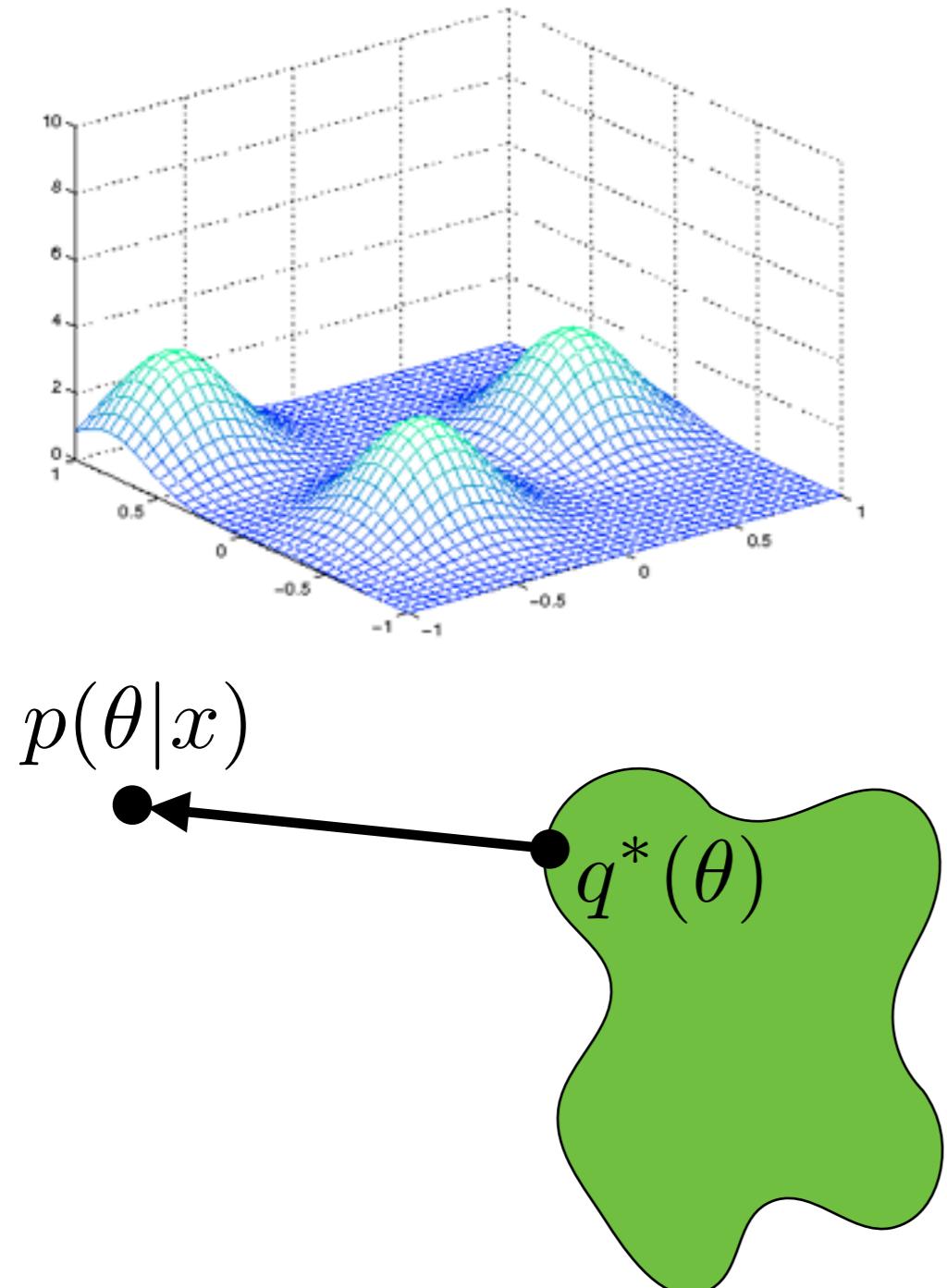
$$KL(q\|p(\cdot|x))$$

Variational Bayes



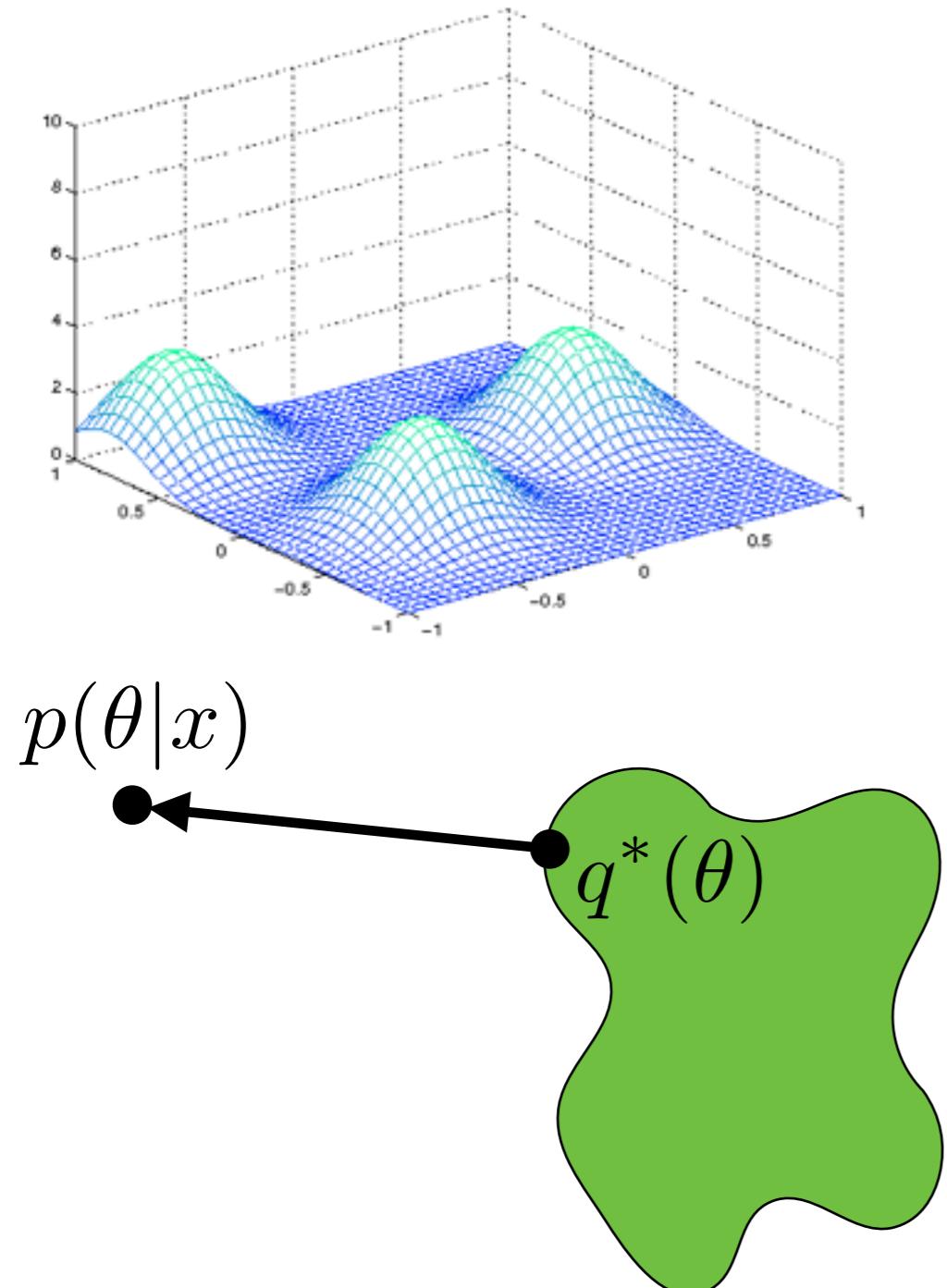
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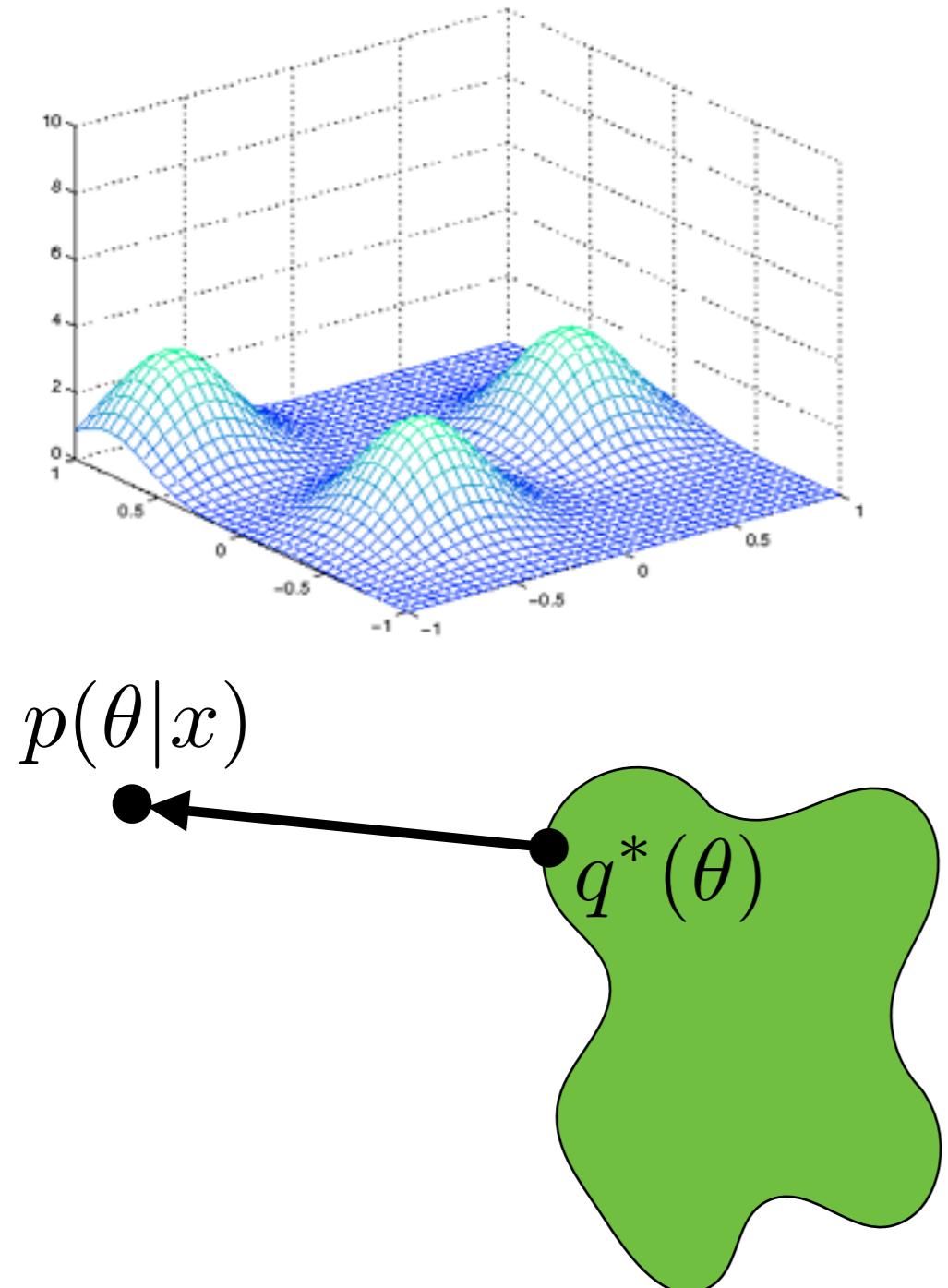
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Variational Bayes



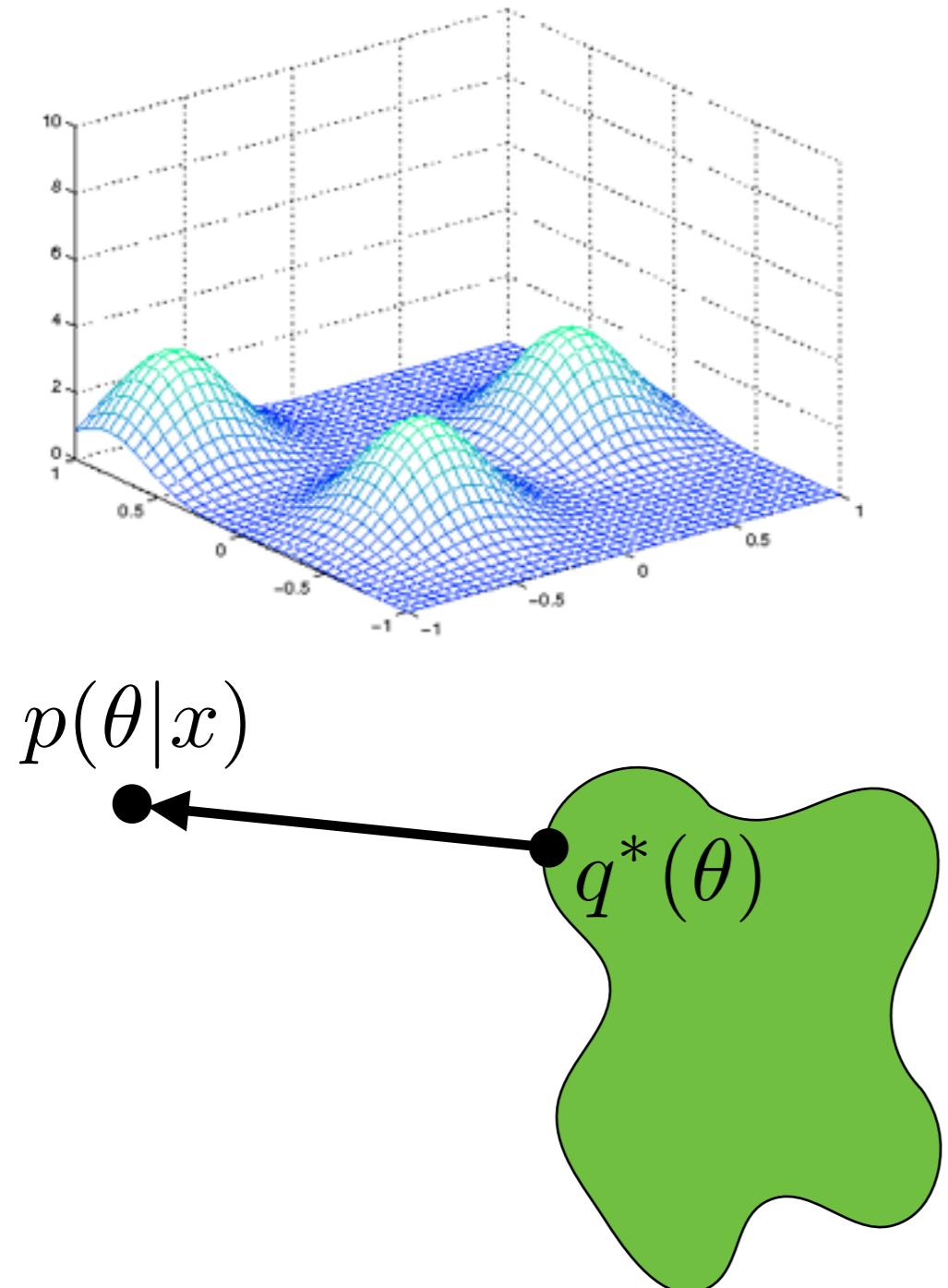
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 - point estimates and prediction

Variational Bayes



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Variational Bayes



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 - point estimates and prediction
 - fast, streaming, distributed

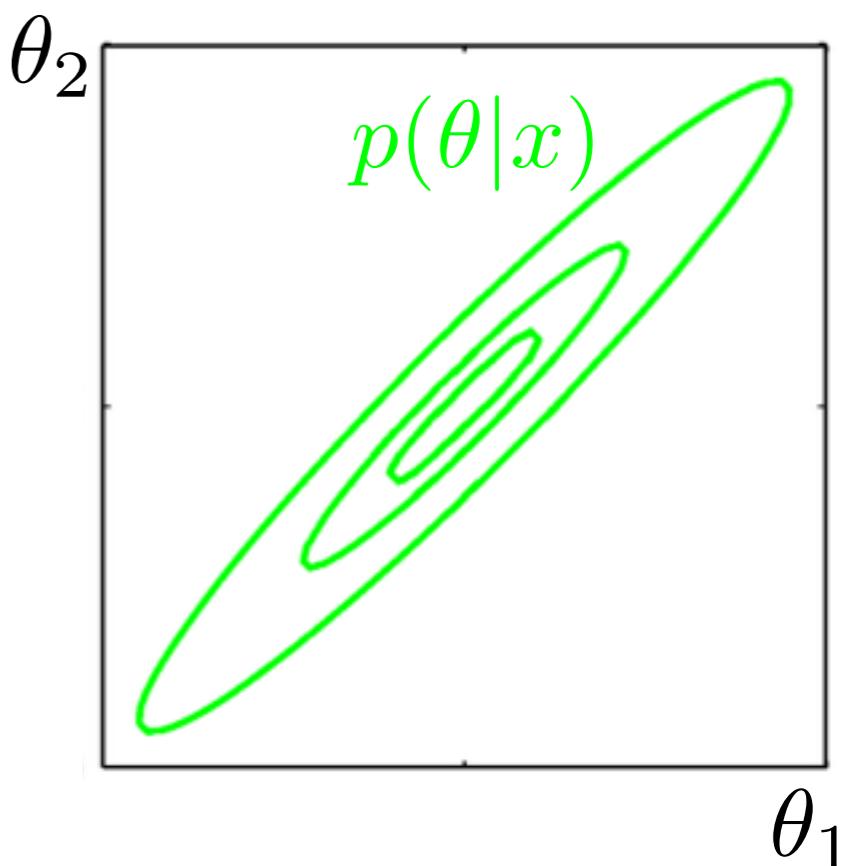
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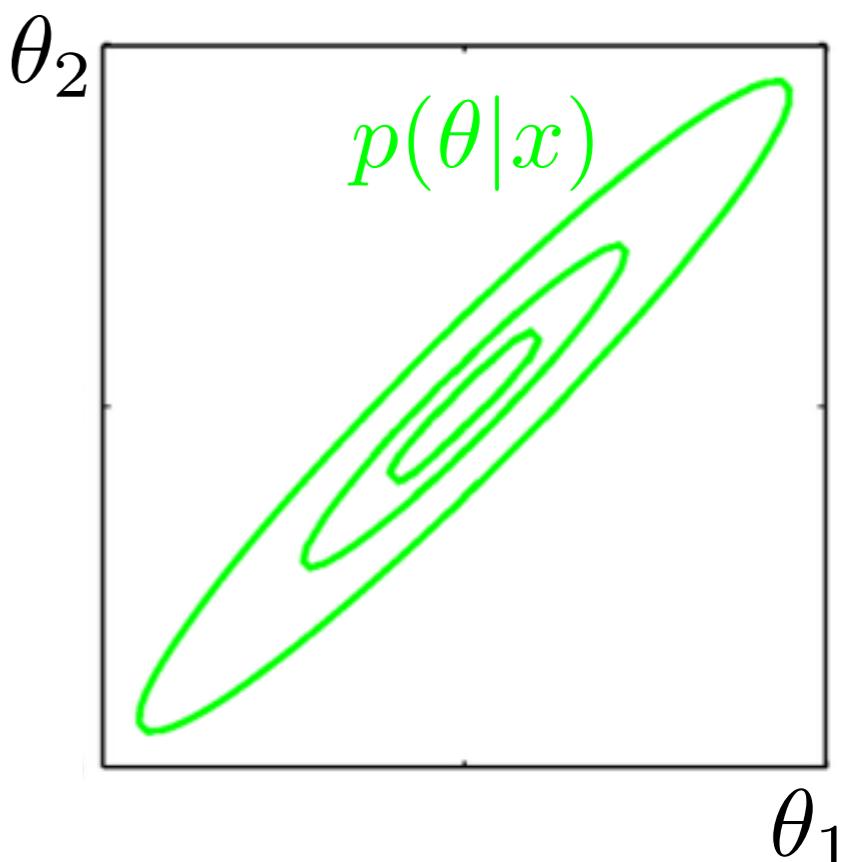
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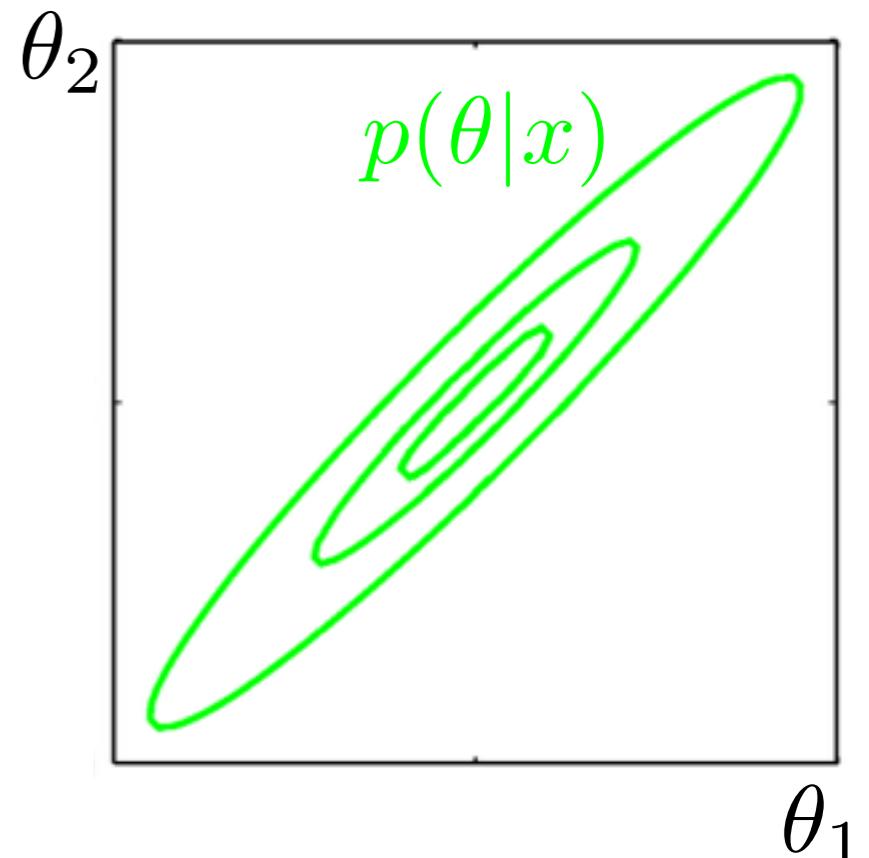
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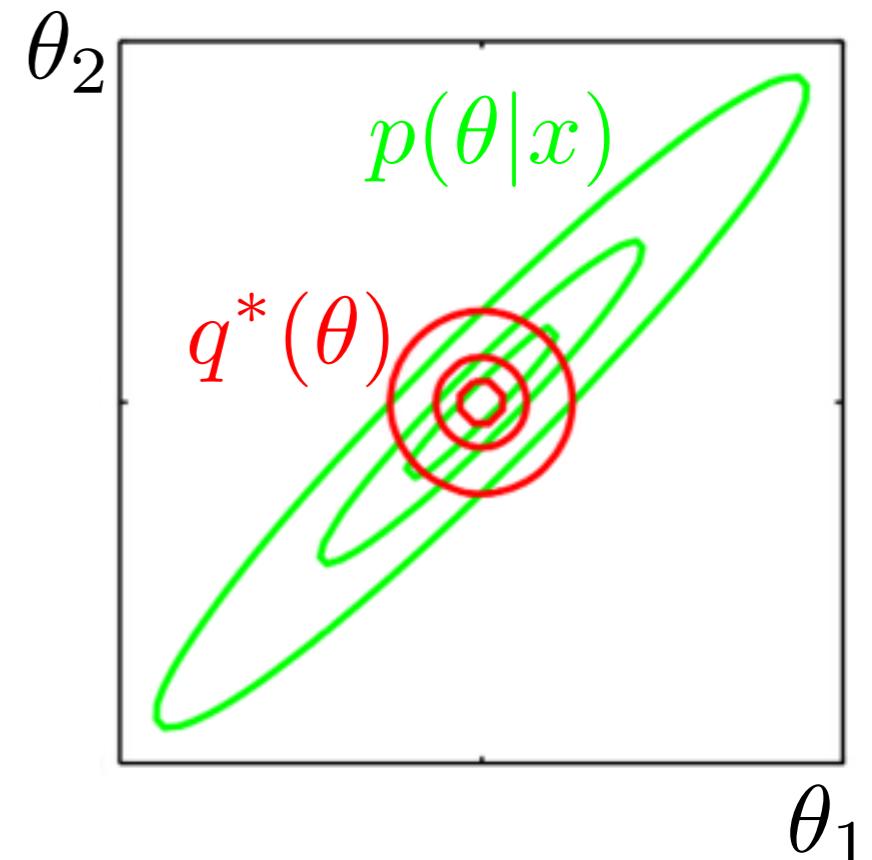
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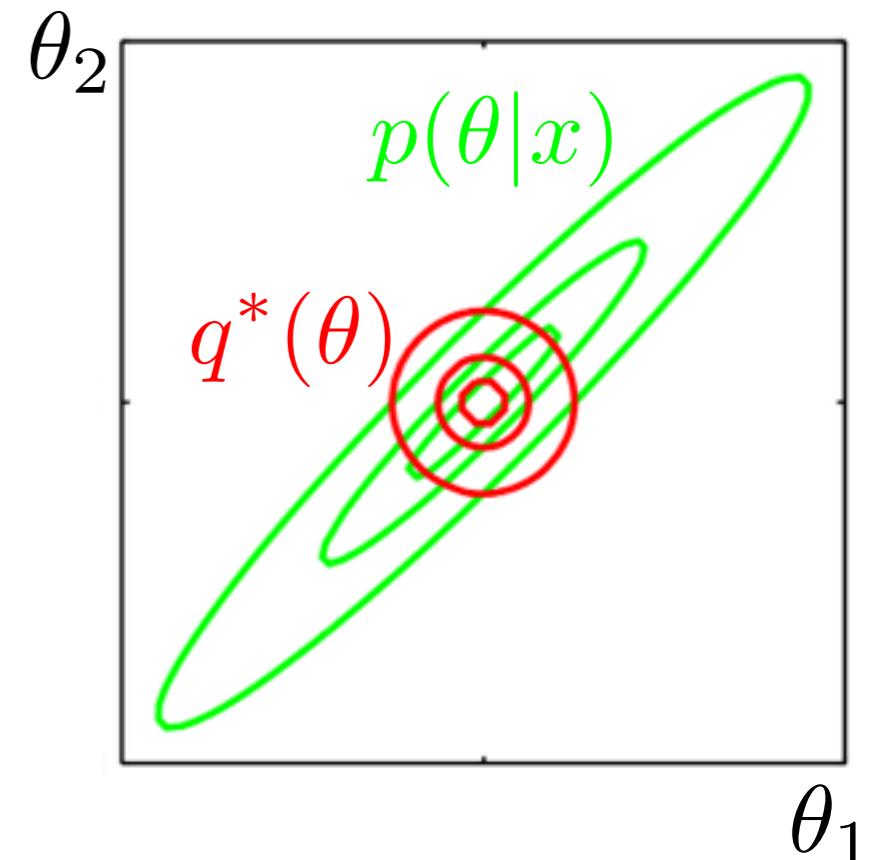
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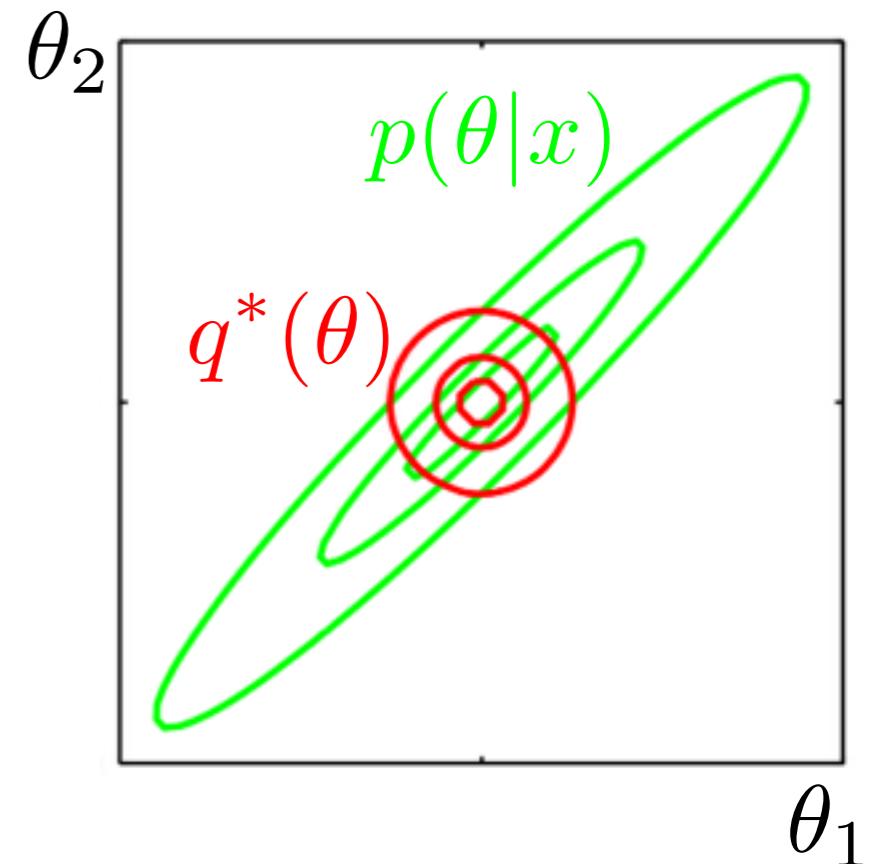
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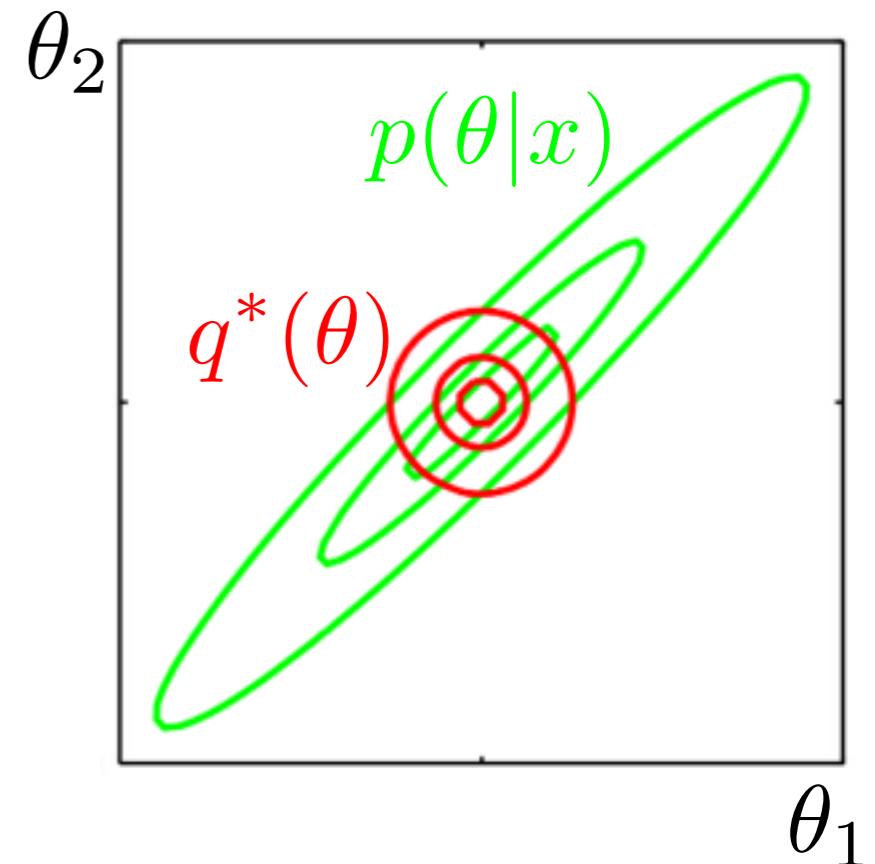
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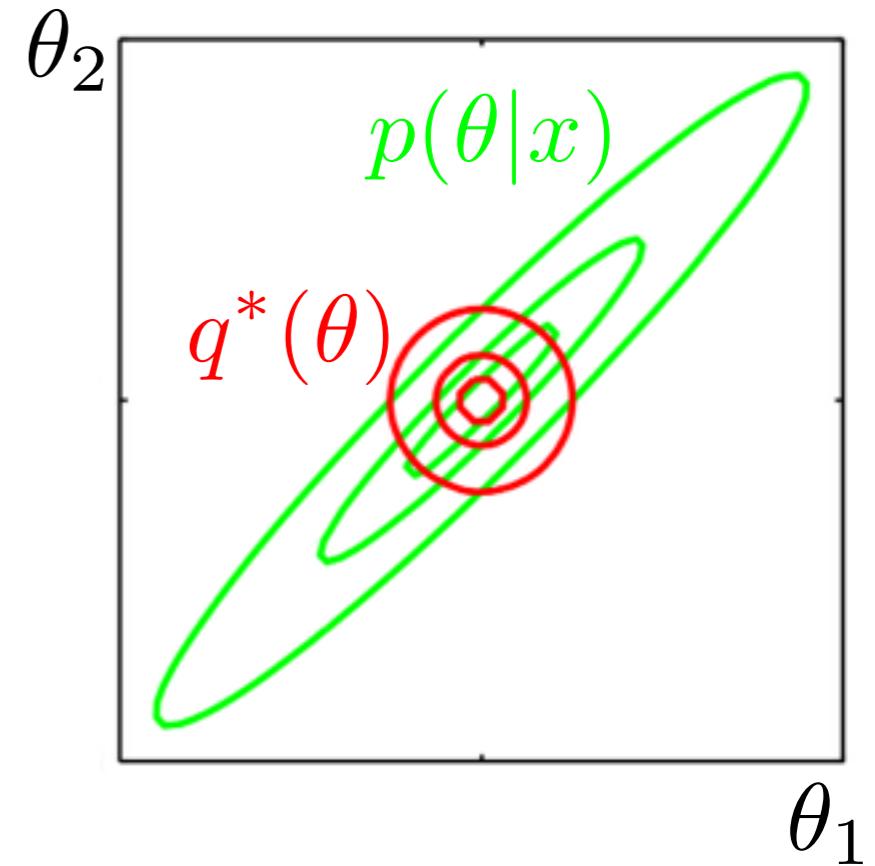
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[MacKay 2003; Bishop 2006; Wang, Titterington 2004; Turner, Sahani 2011]

[Fosdick 2013; Dunson 2014; Bardenet, Doucet, Holmes 2015]

Linear response

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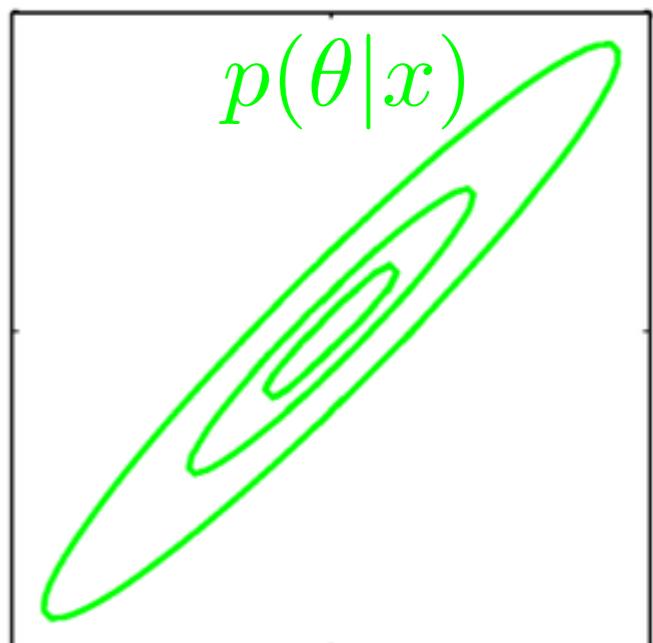
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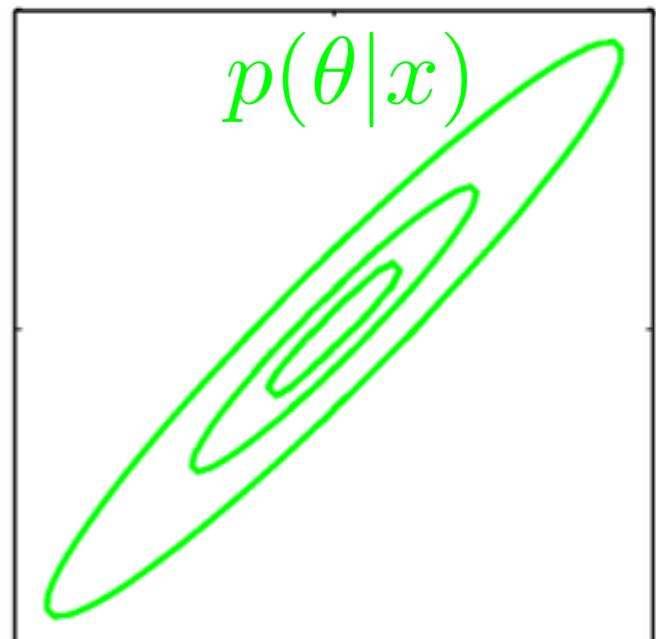
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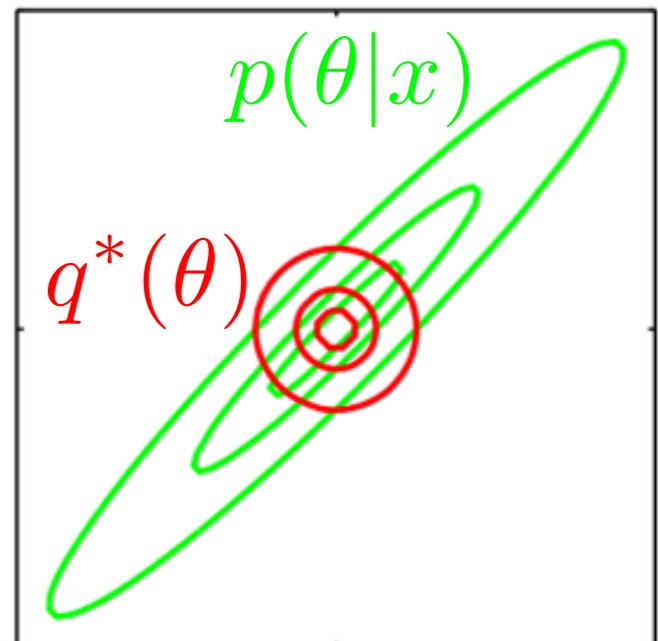
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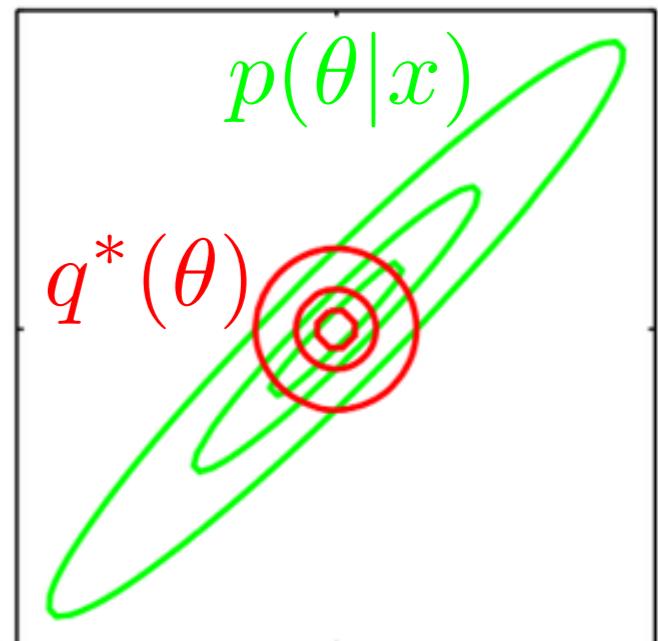
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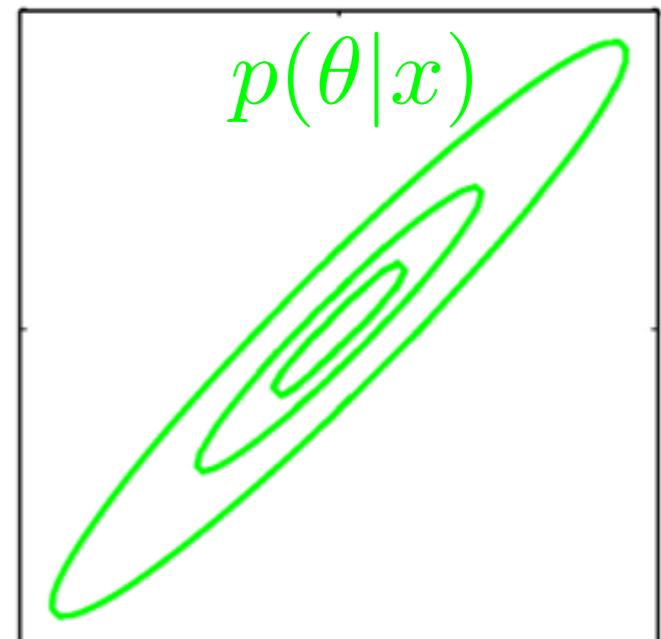
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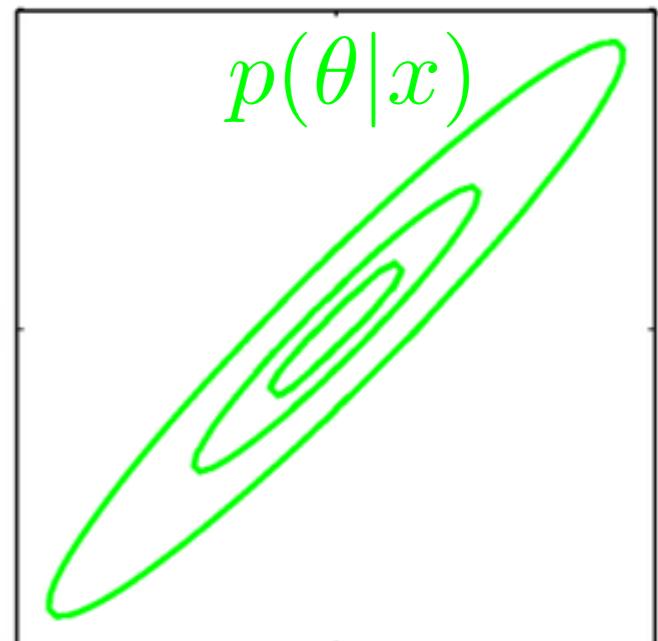
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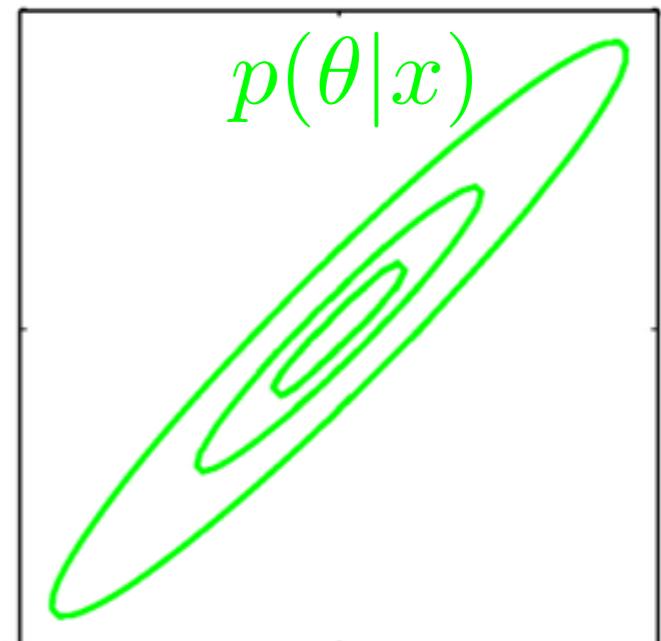
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- “Linear response”

$$\log p(\theta|x) + t^T \theta$$



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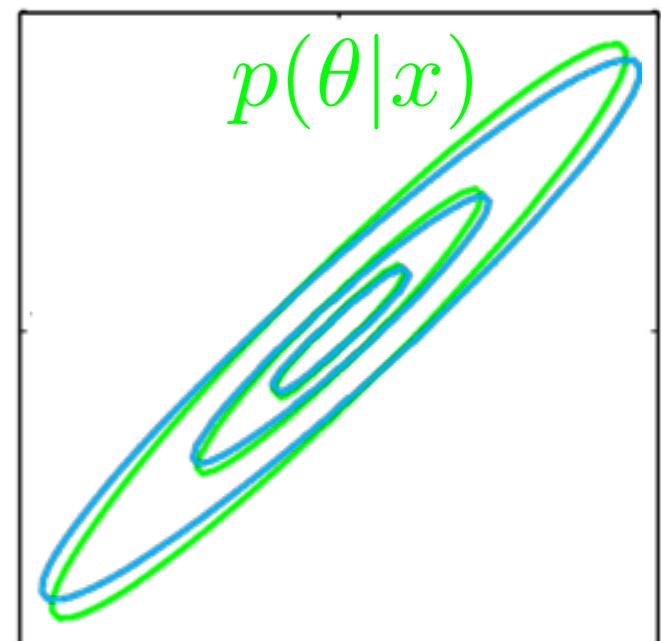
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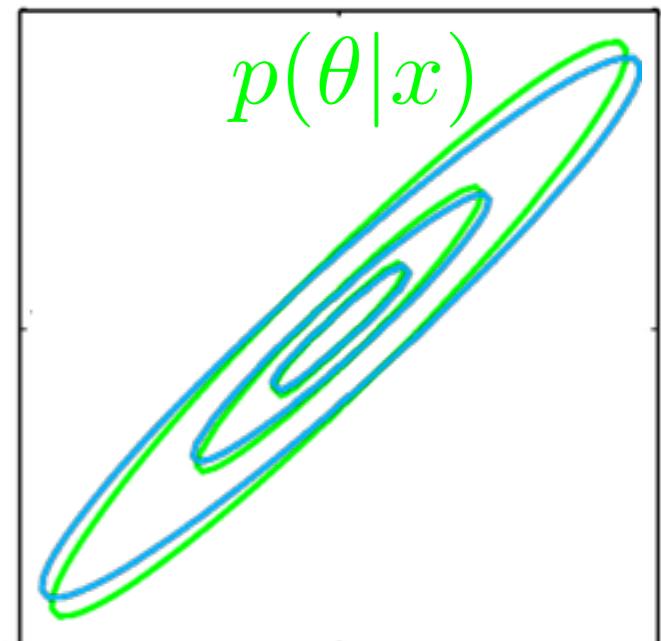
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$$\log p_t(\theta) := \log p(\theta|x) + t^T \theta$$



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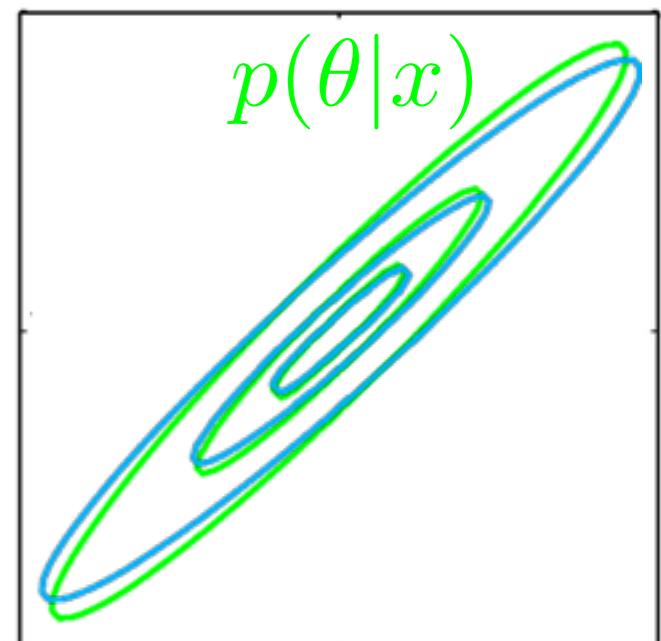
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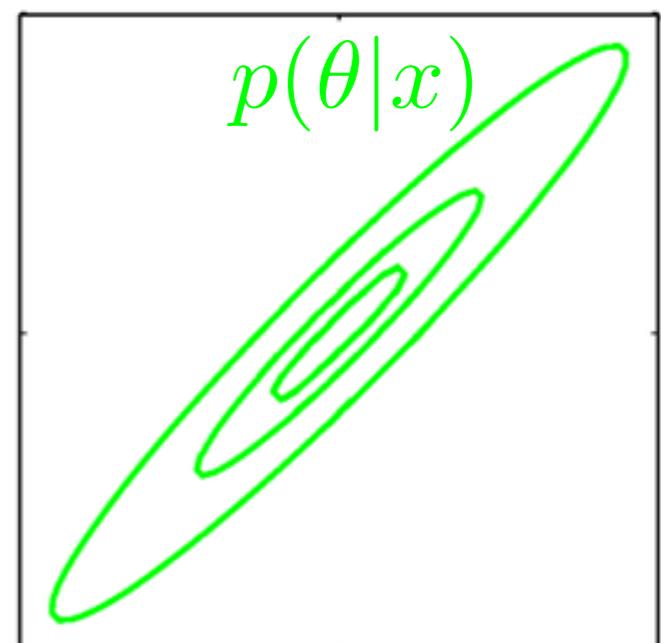
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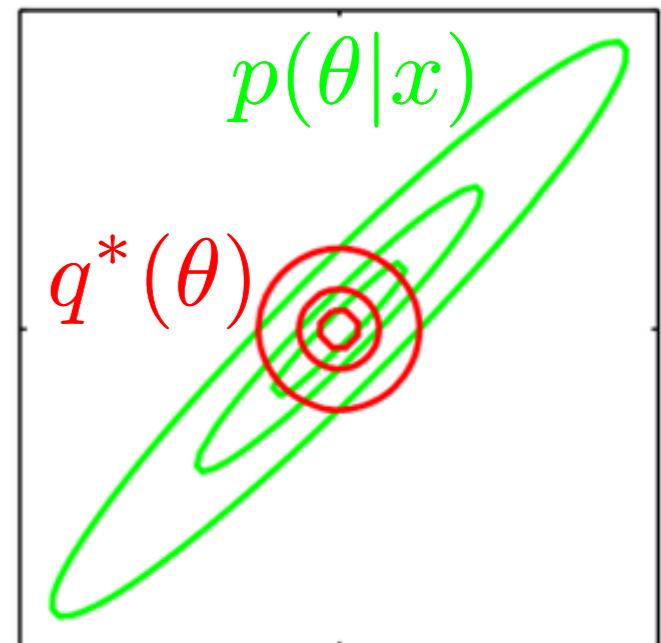
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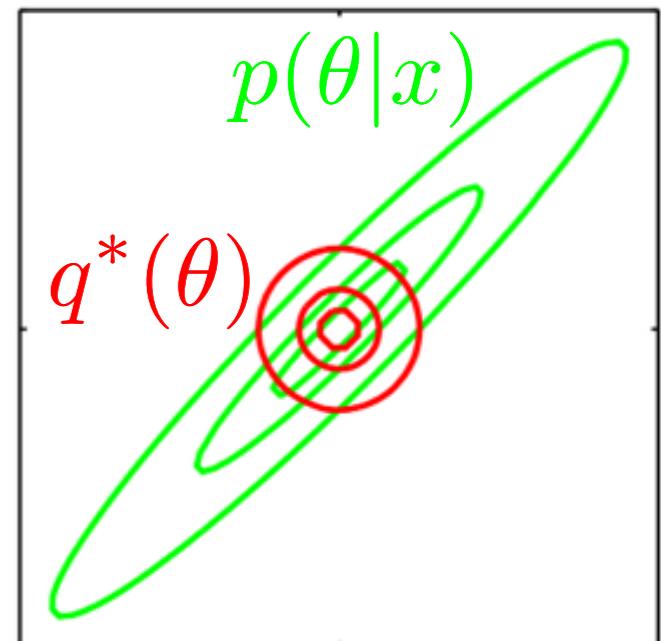
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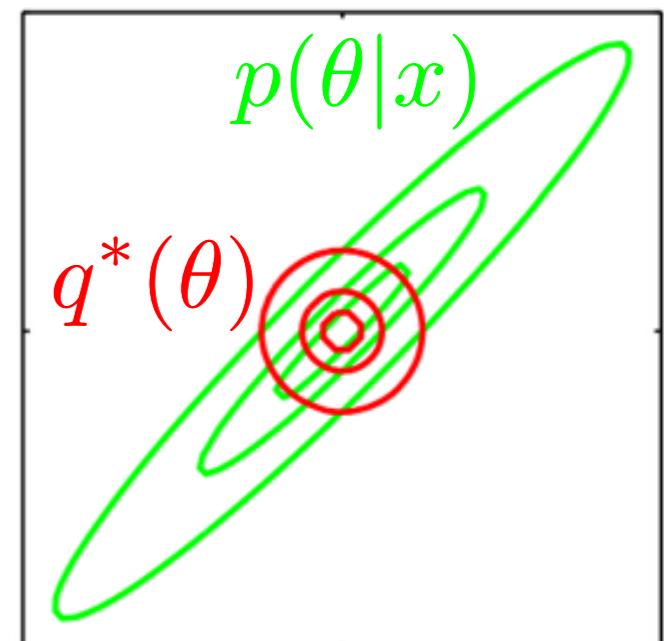
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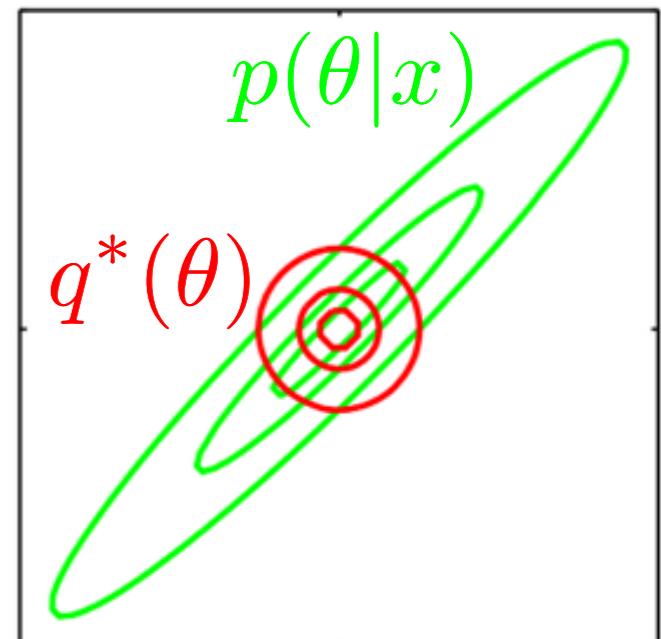
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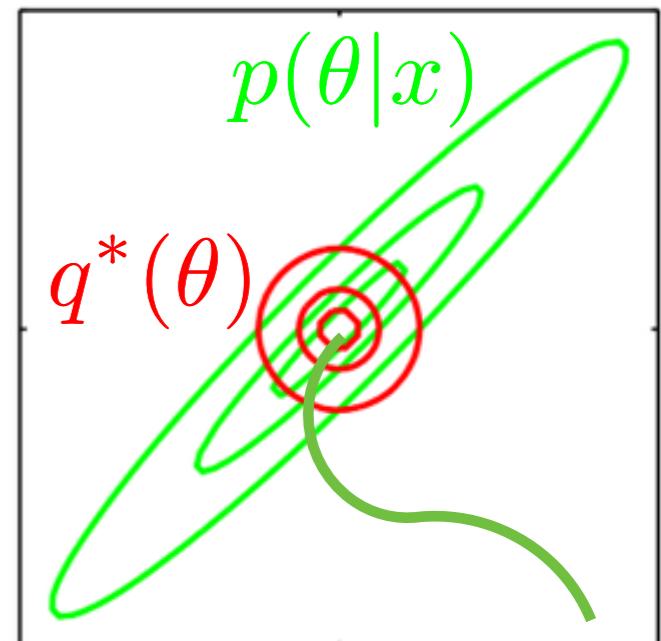
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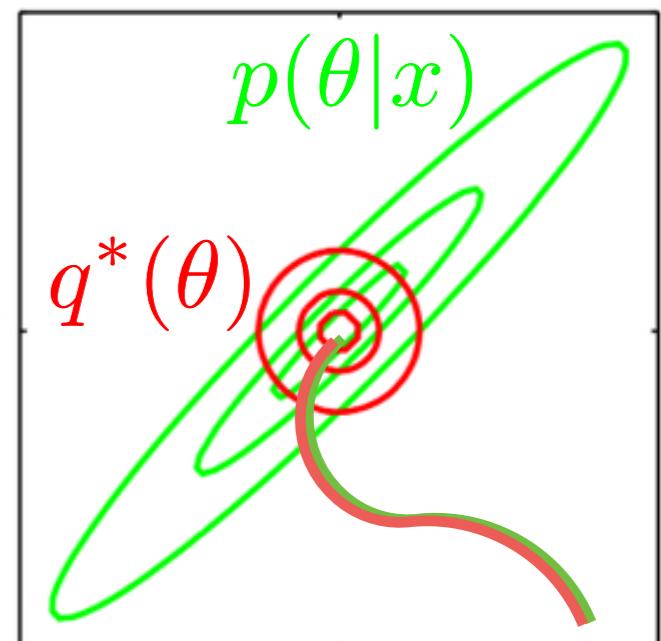
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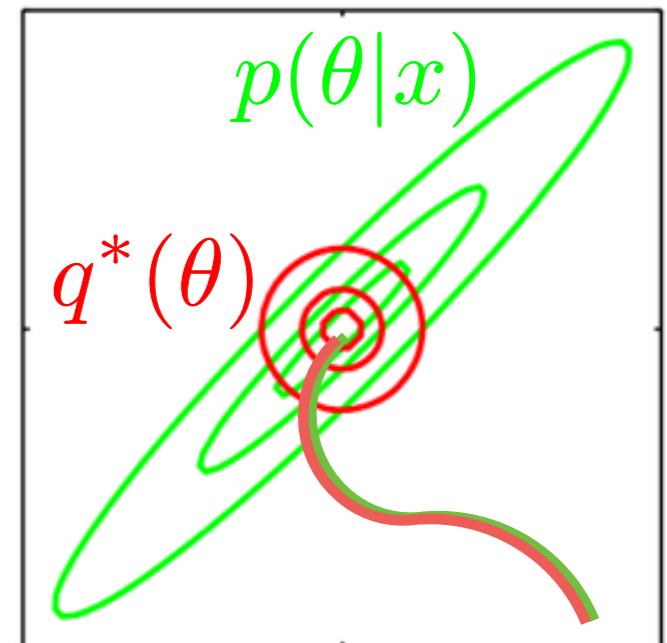
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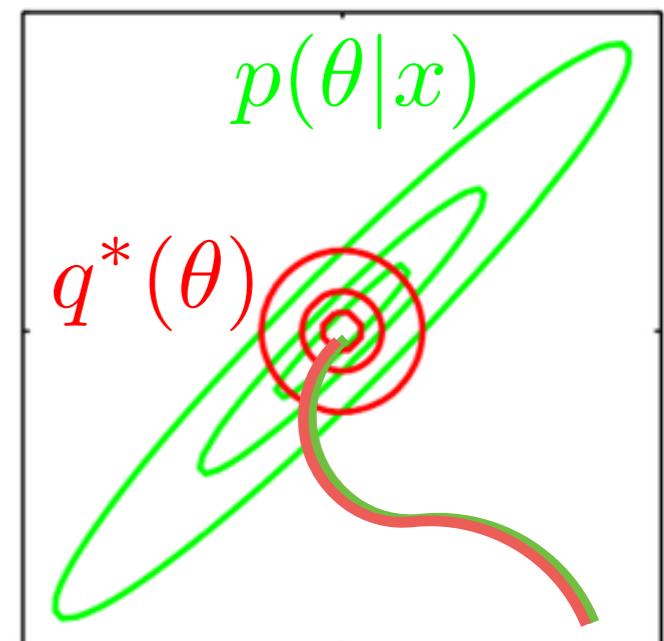
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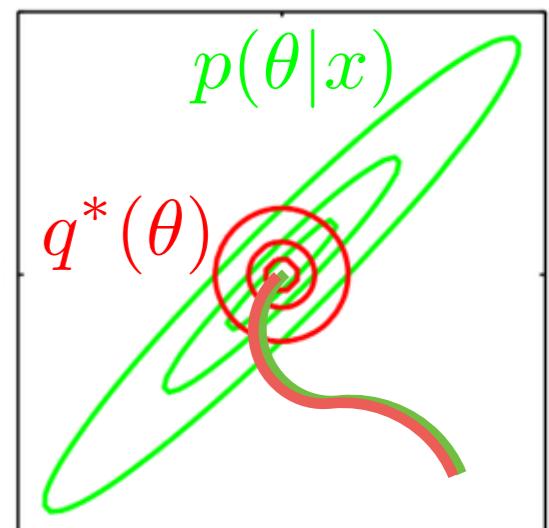
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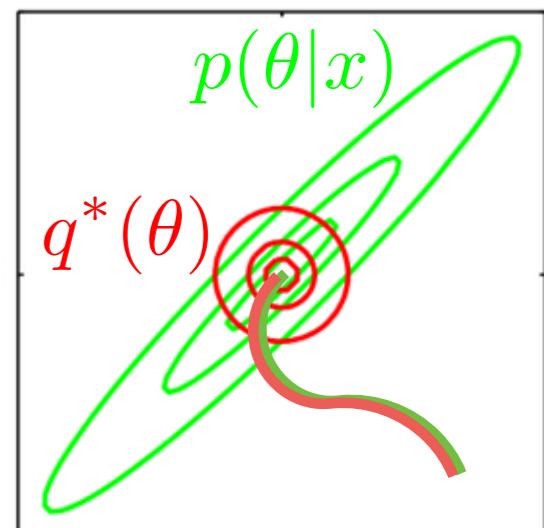
[Bishop 2006]

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[Bishop 2006]

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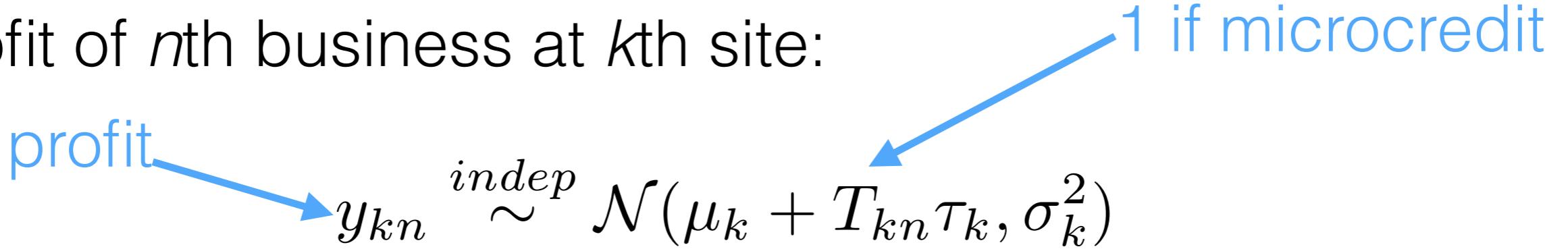
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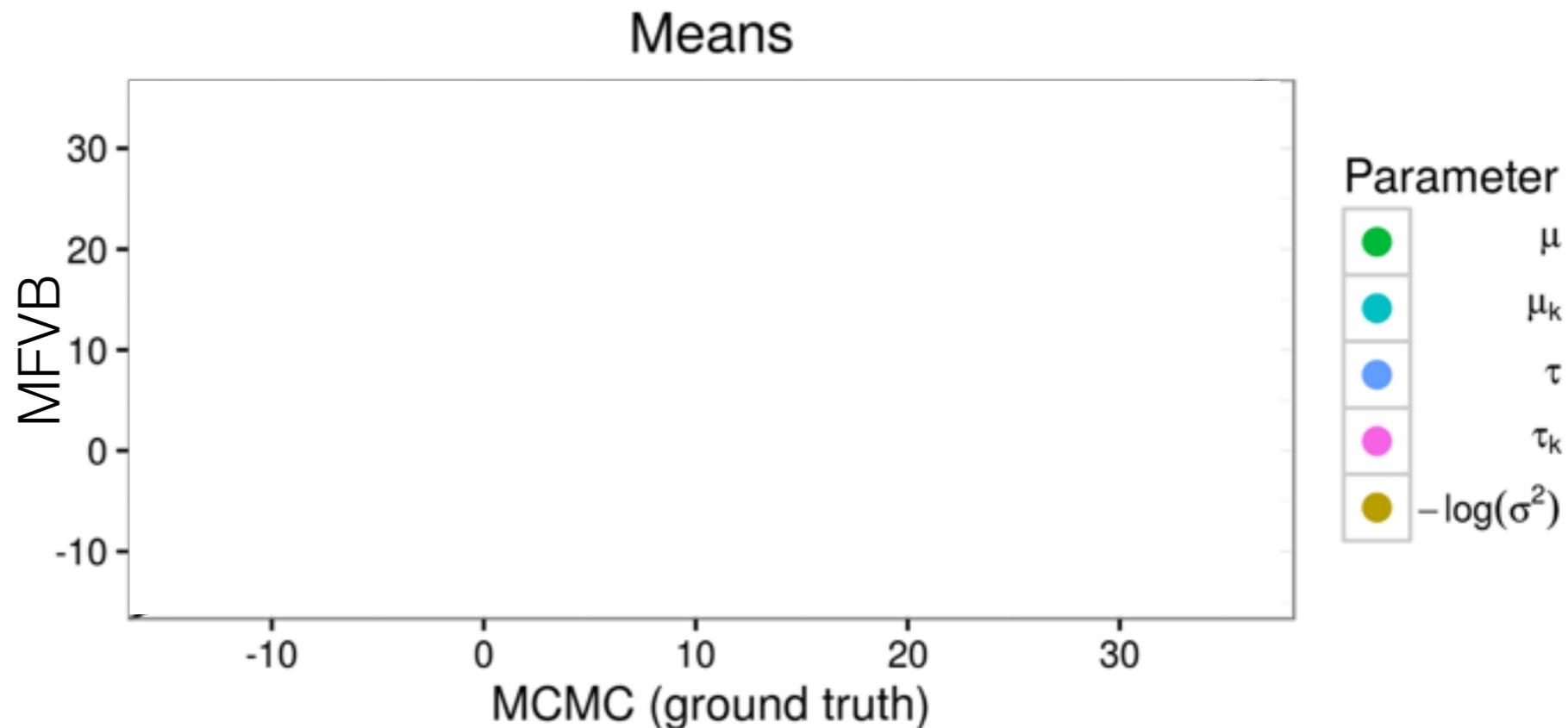
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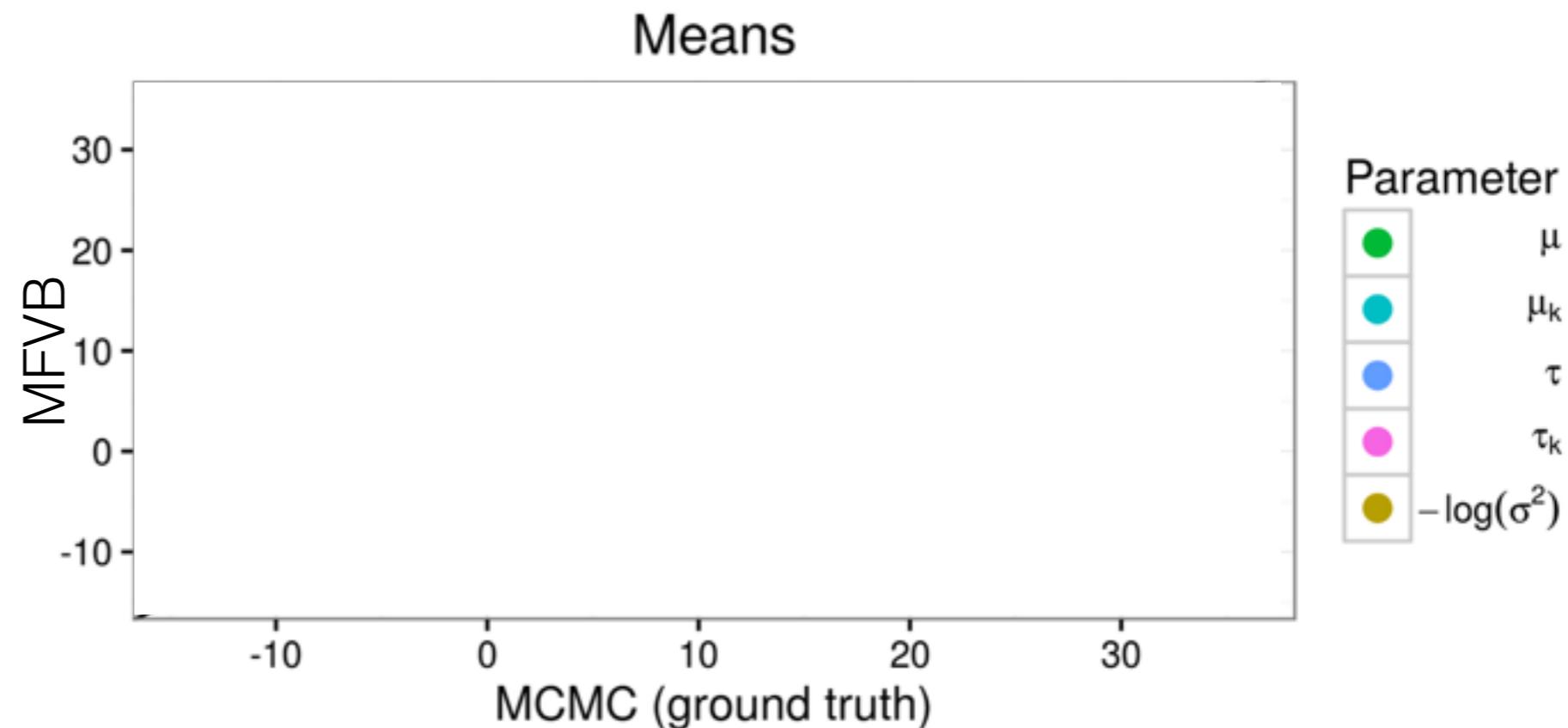
$$C \sim \text{Sep\&LKJ}(\eta, c, d)$$

Microcredit Experiment



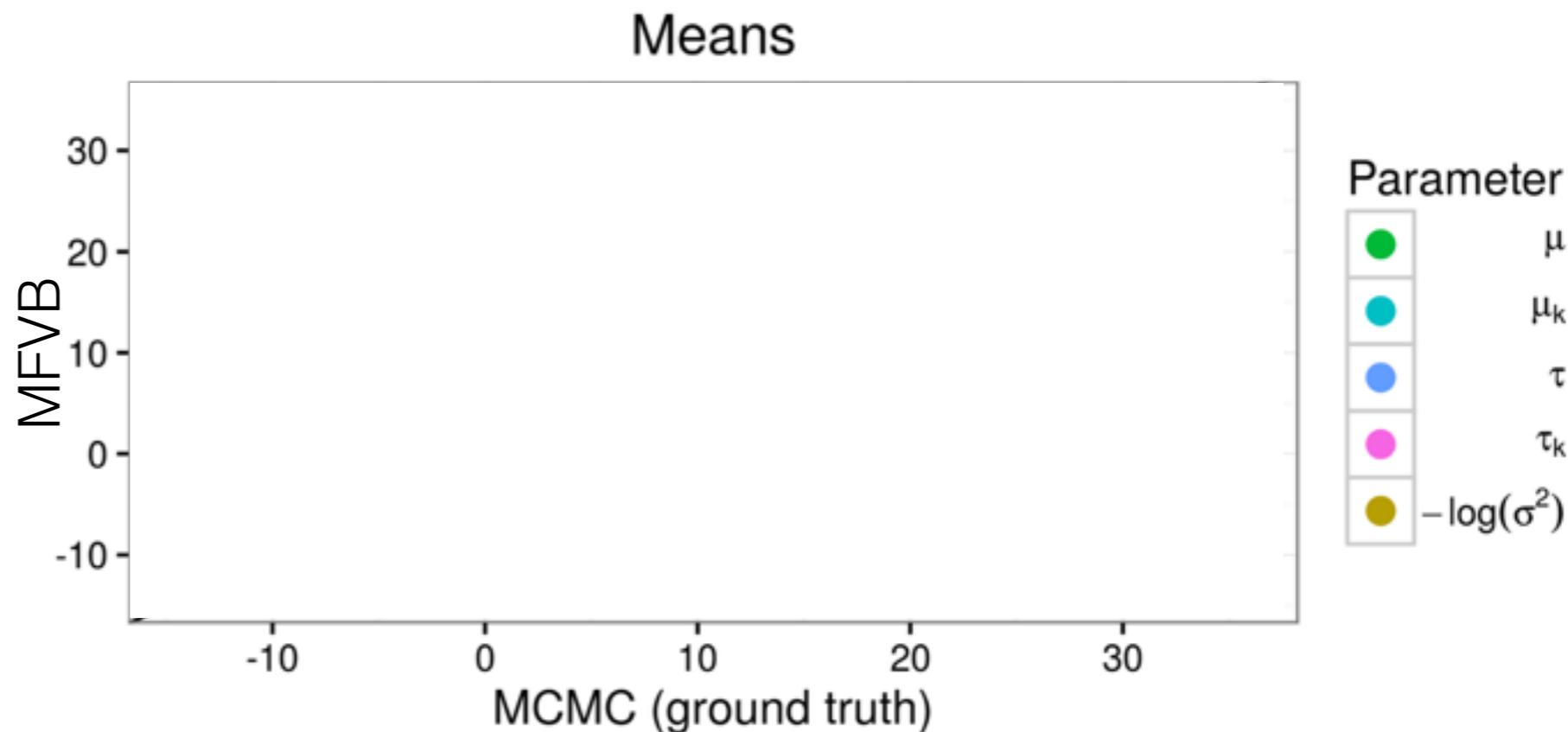
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- One set of 2500 MCMC draws:
45 minutes



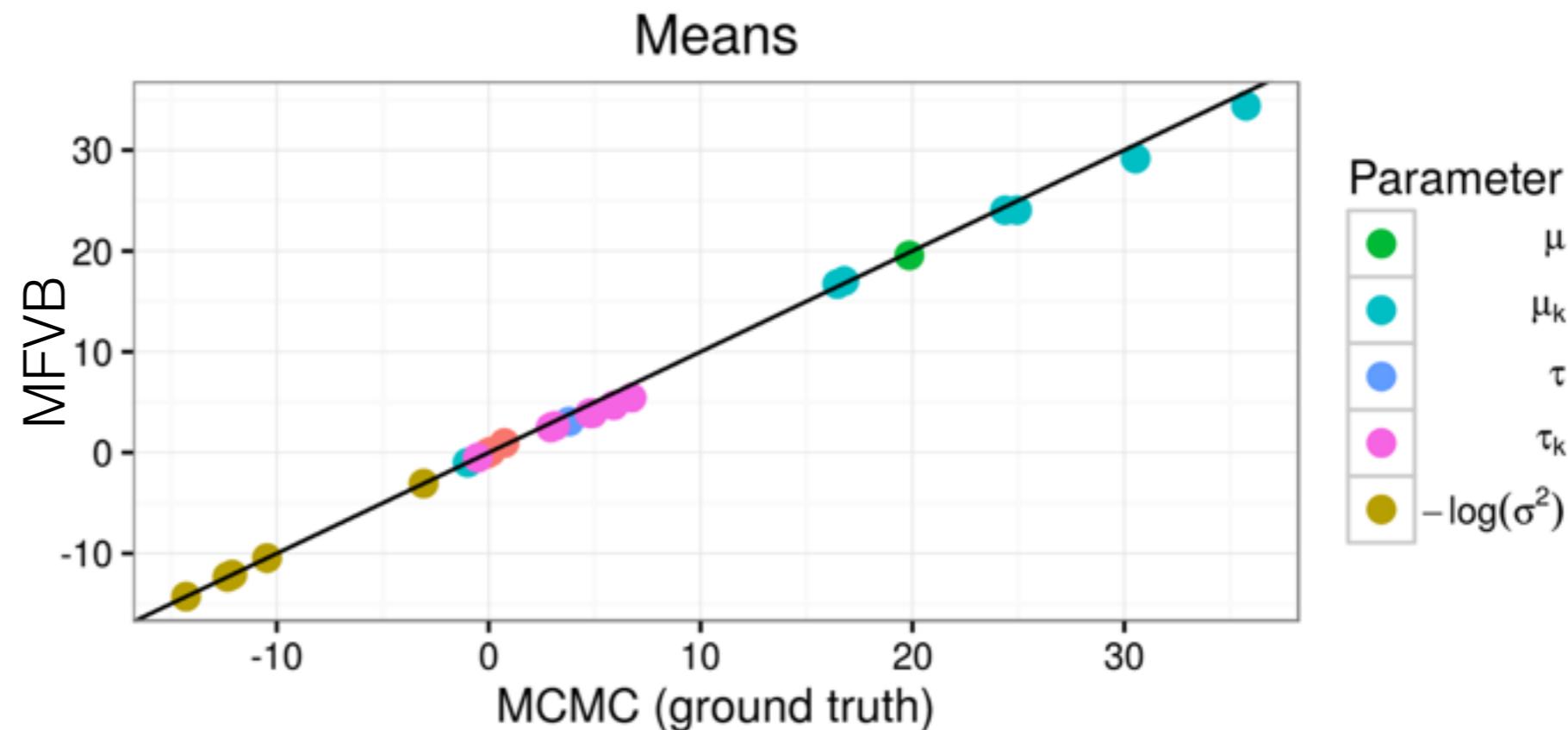
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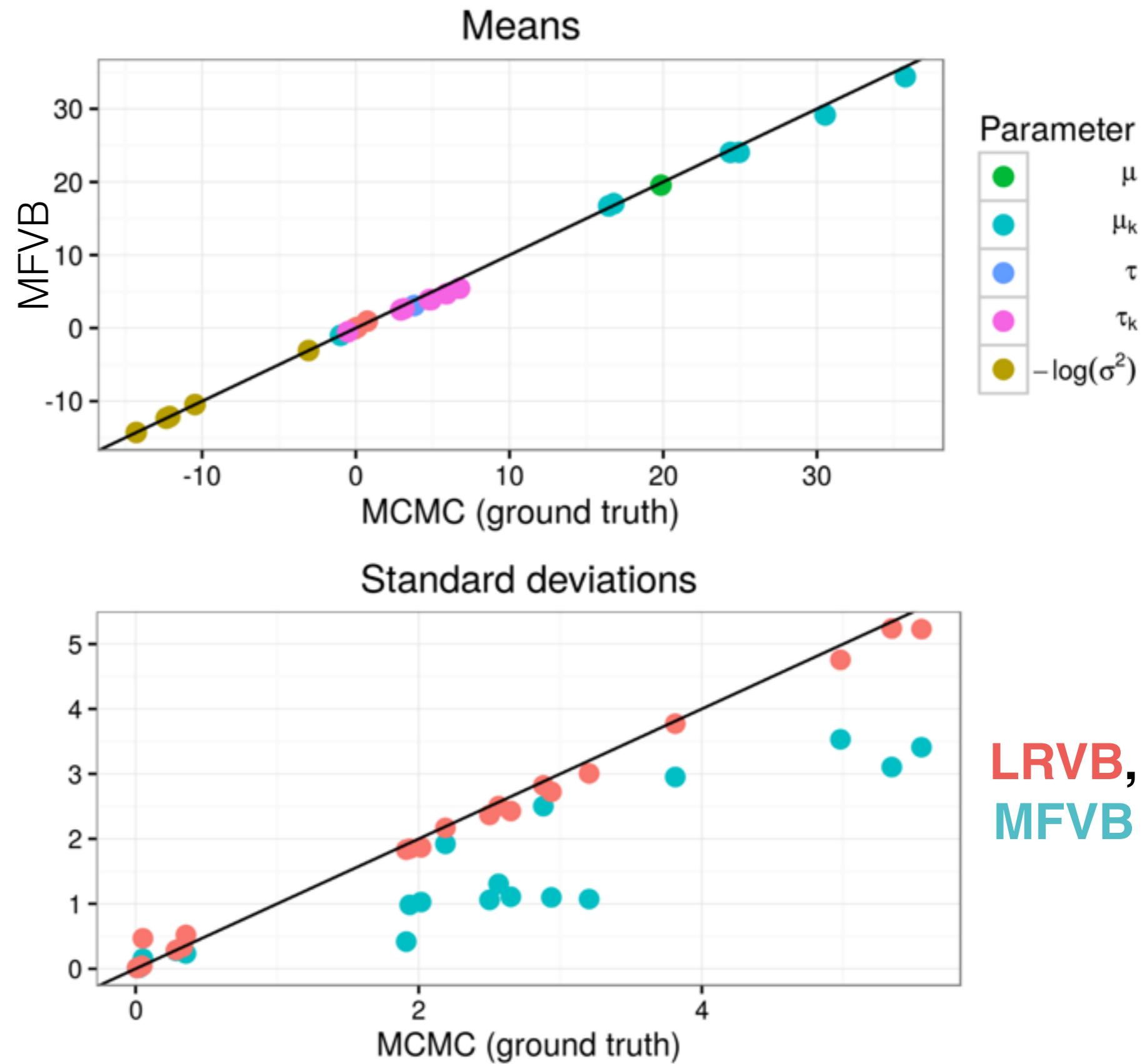
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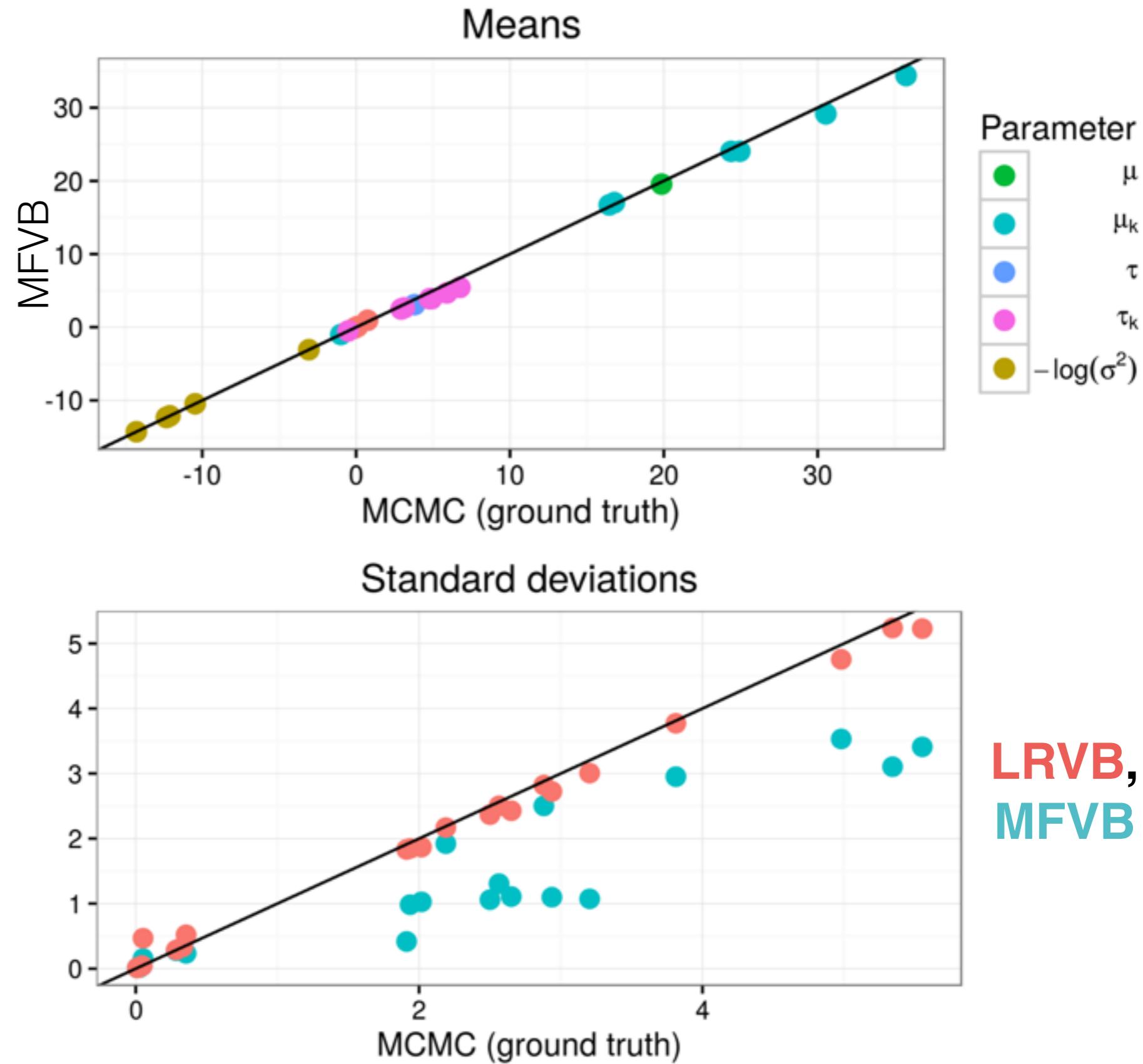
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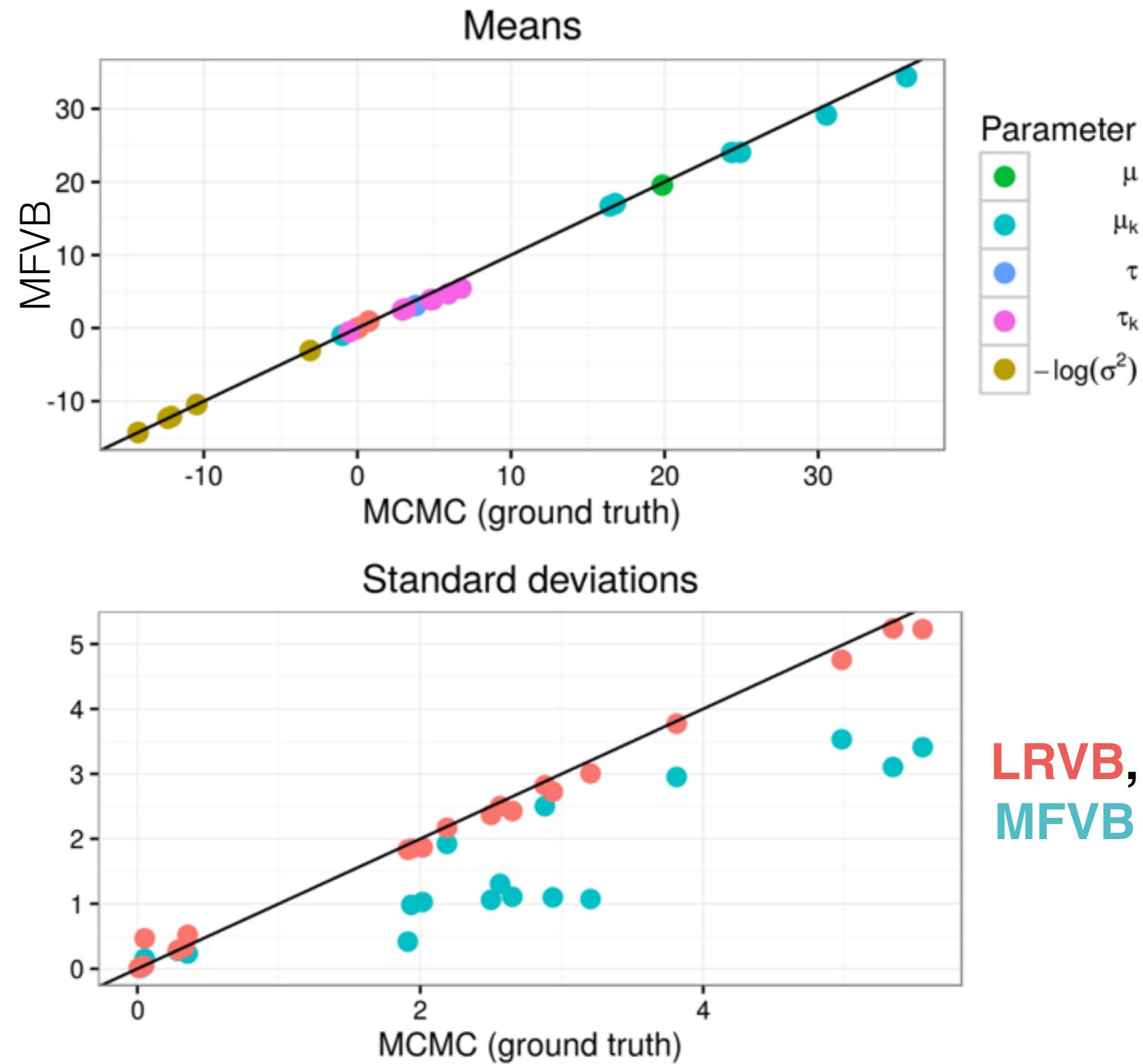
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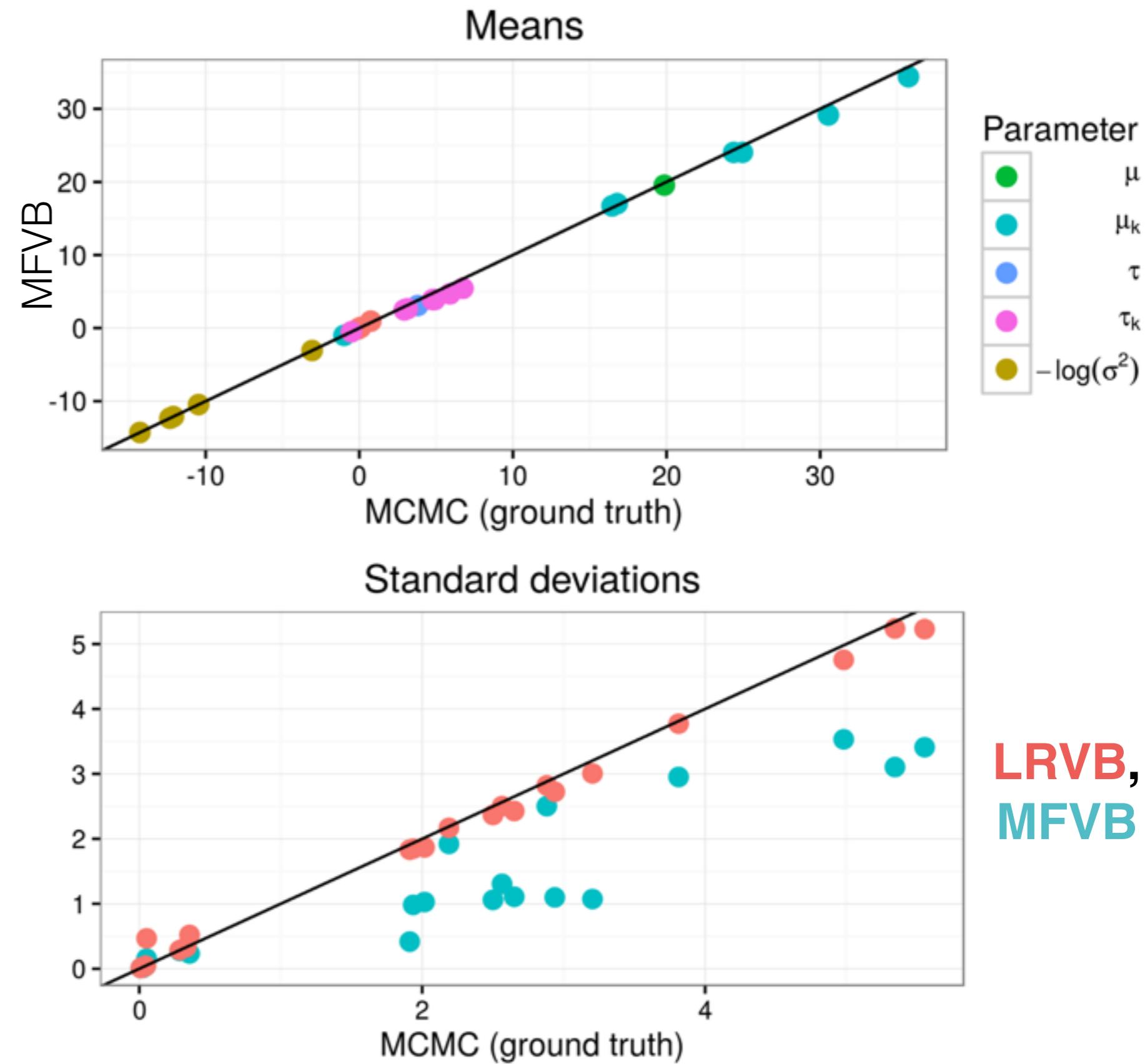
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- Mean is 1.68 std dev from 0



Experiments

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- Gaussian mixture model

$$P(z_{nk} = 1) = \pi_k, \quad p(x|\pi, \mu, \Lambda, z) = \prod_{n=1:N} \prod_{k=1:K} \mathcal{N}(x_n | \mu_k, \Lambda_k^{-1})^{z_{nk}}$$

with conjugate priors on π, μ, Λ

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10,000 data points each, R bayesm package

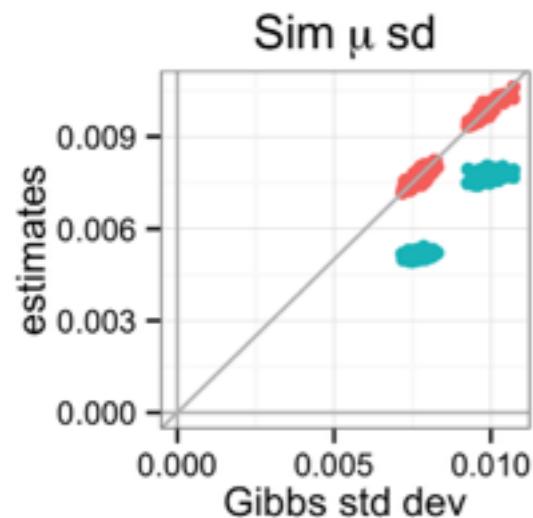
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LRVB,
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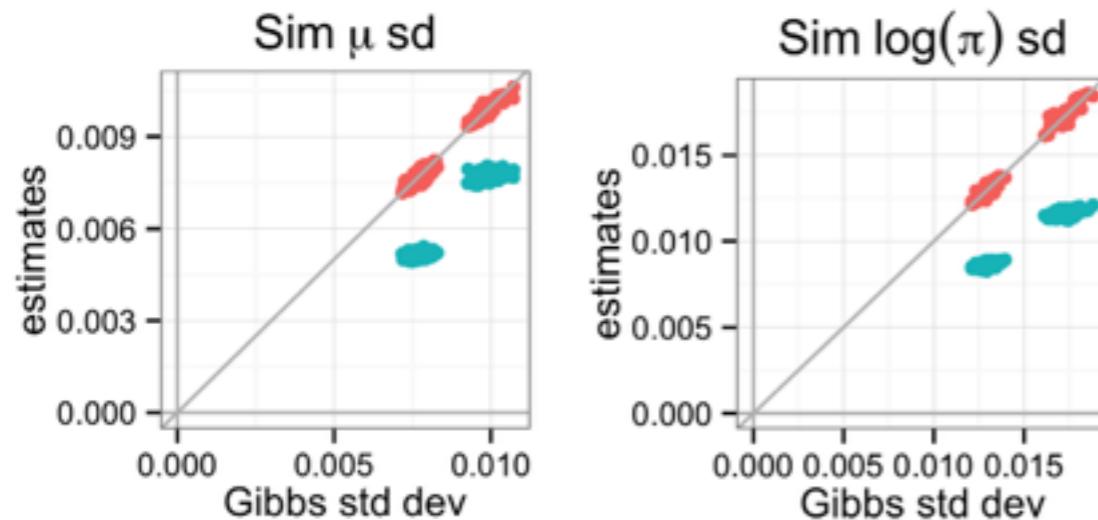
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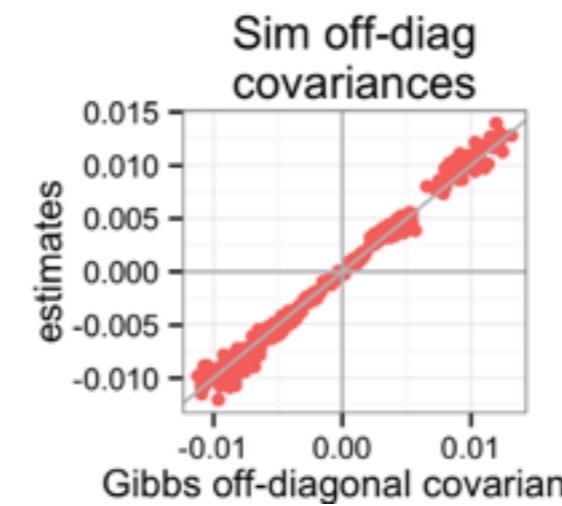
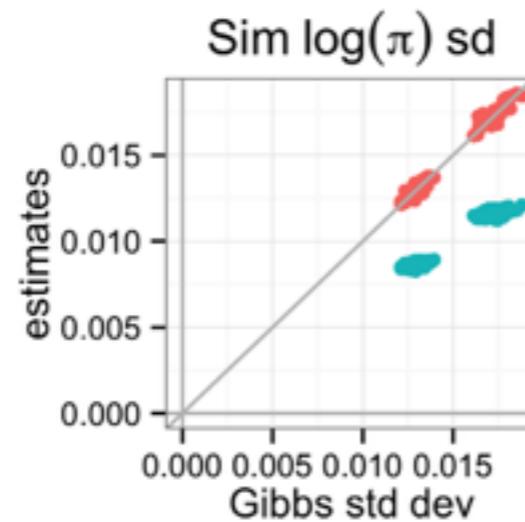
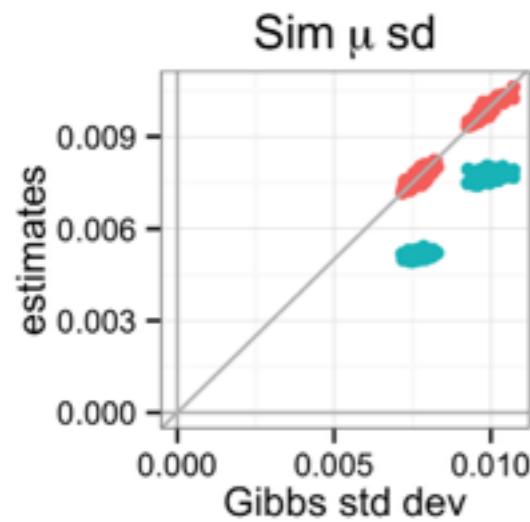
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with conjugate priors on π, μ, Λ

- 68 simulated data sets (2 components, 2 dimensions),
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LRVB,
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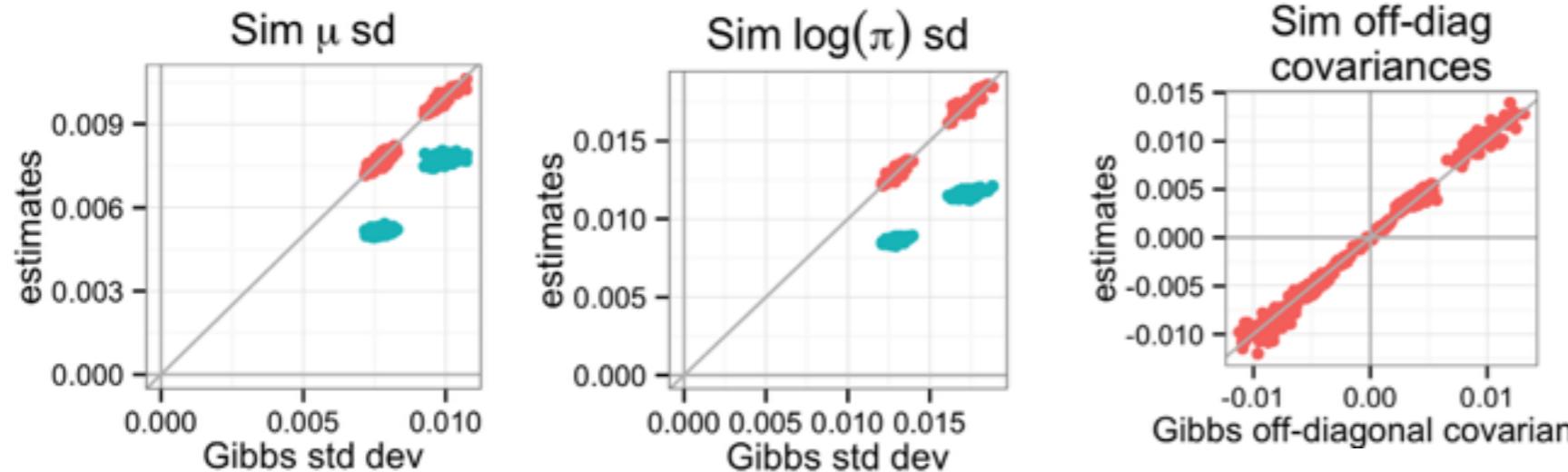
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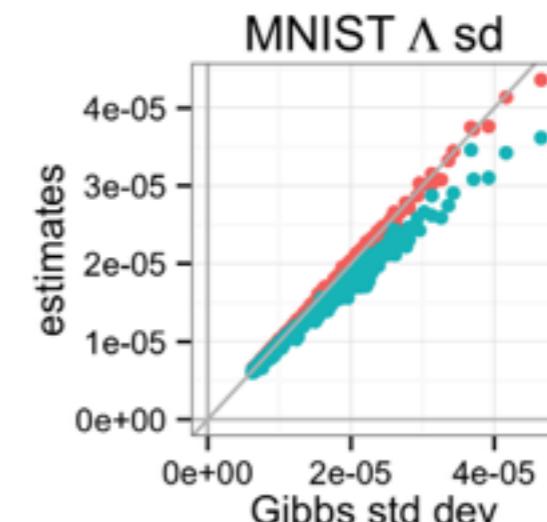
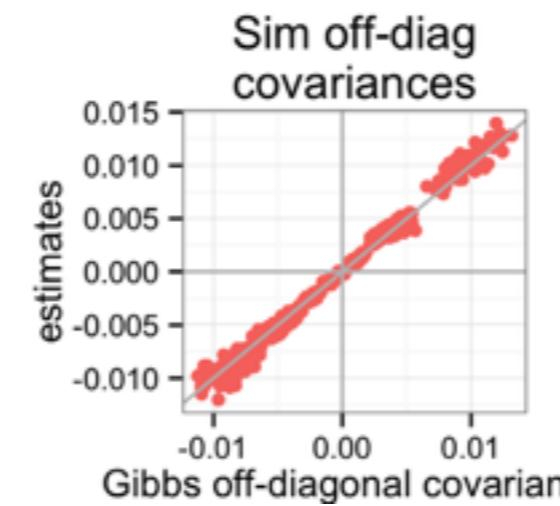
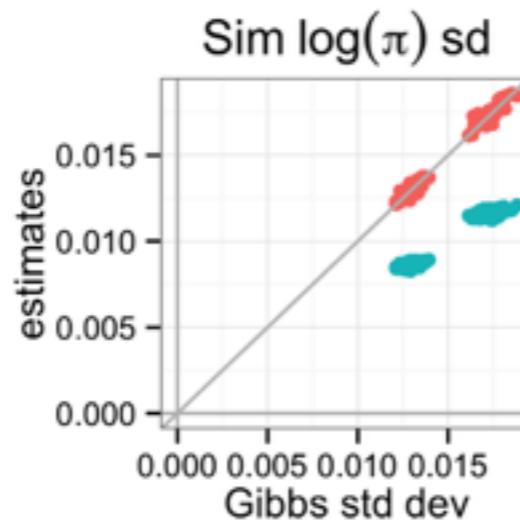
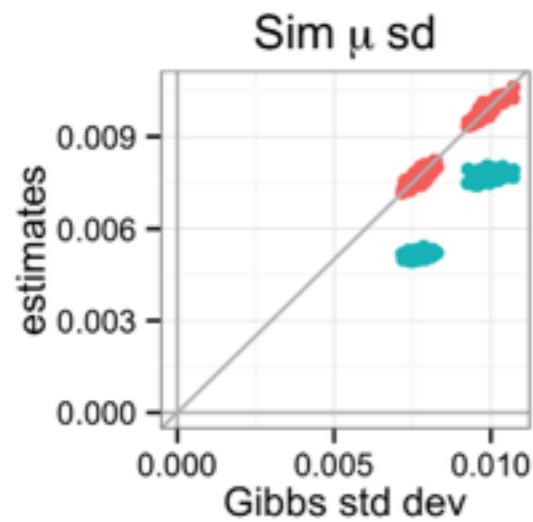
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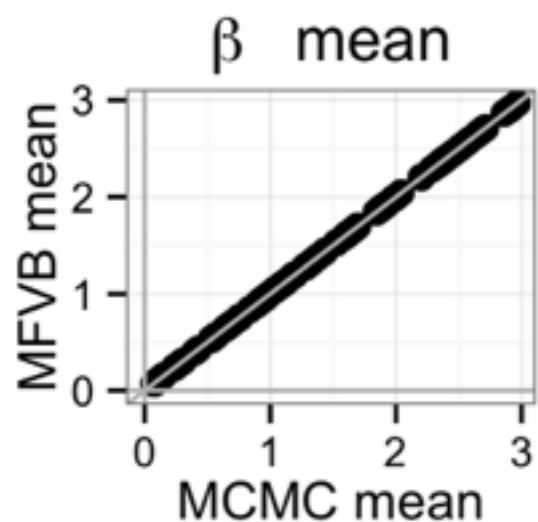
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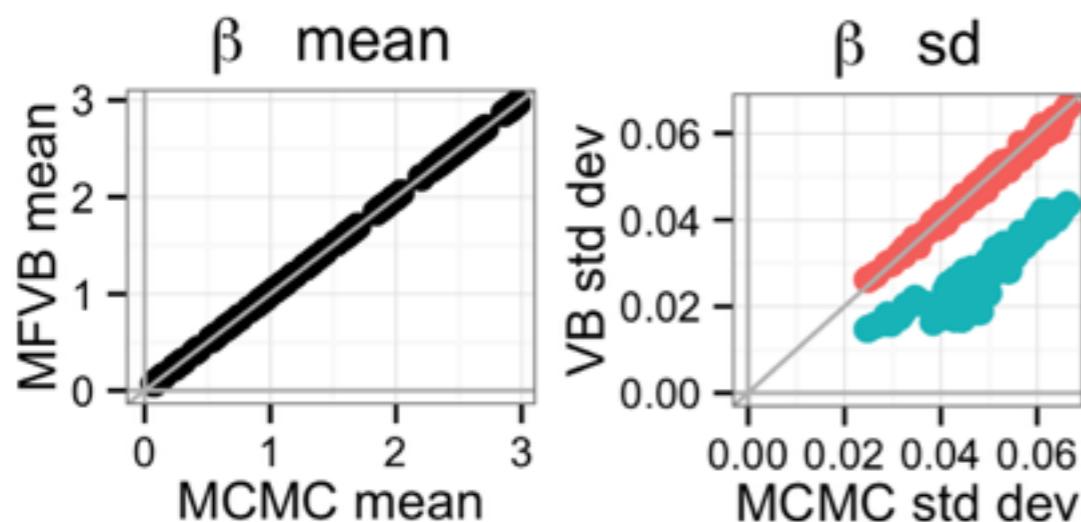
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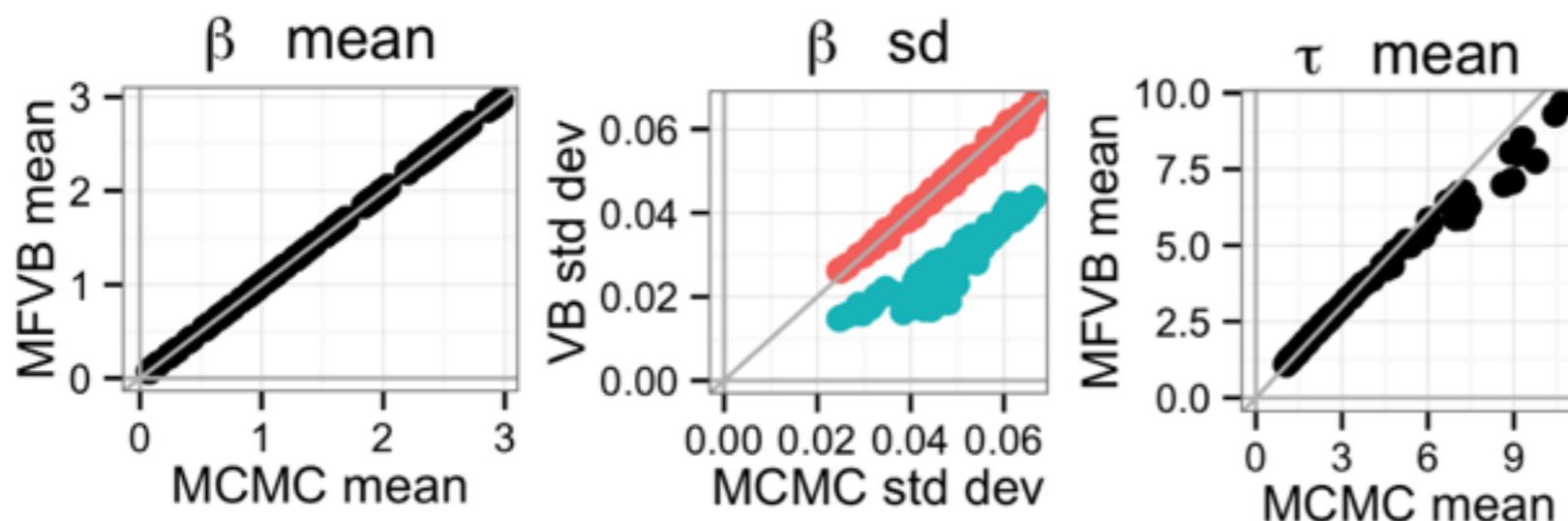
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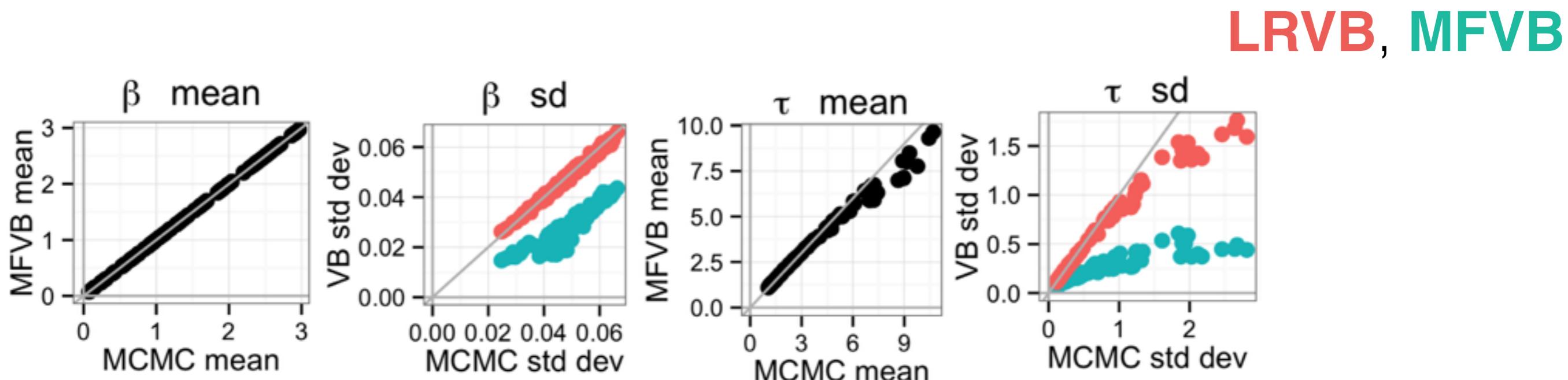
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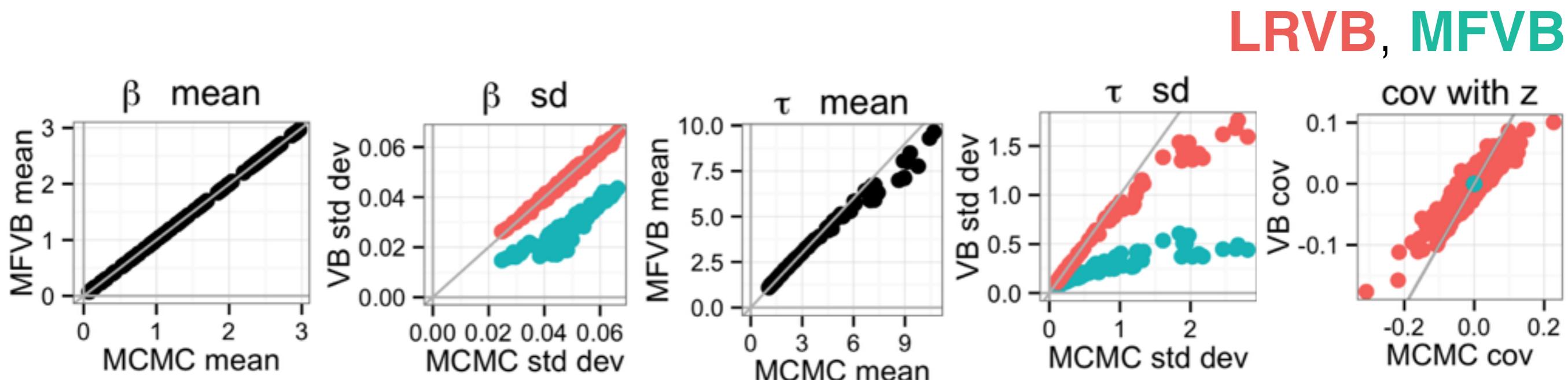
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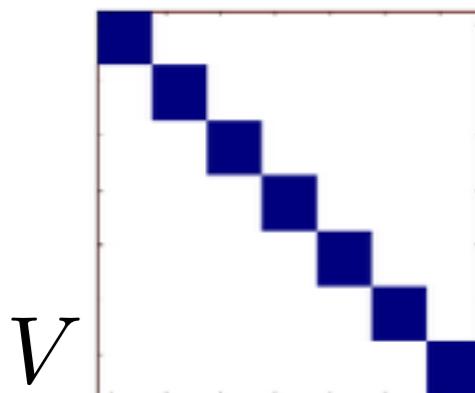
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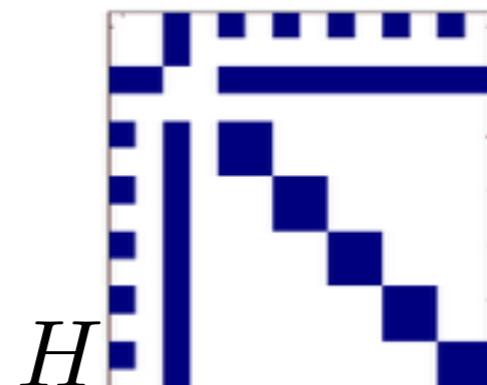
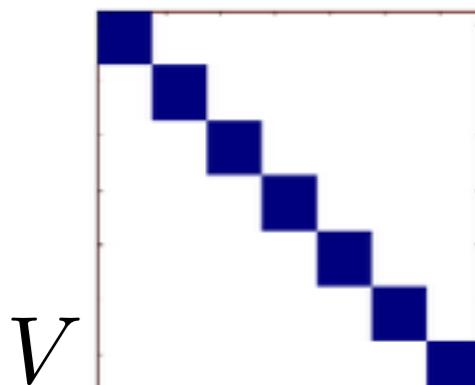
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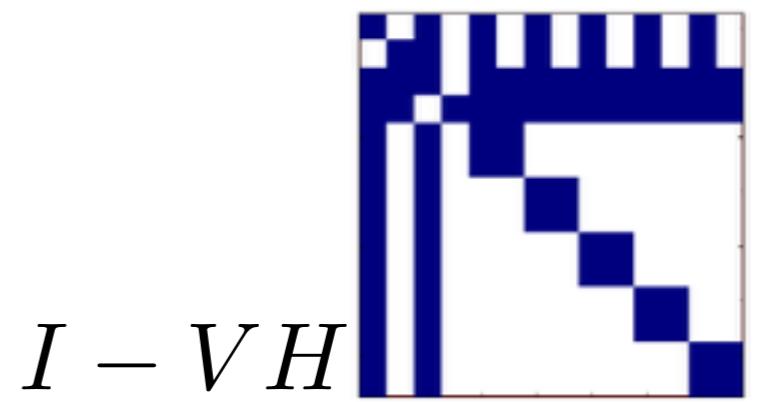
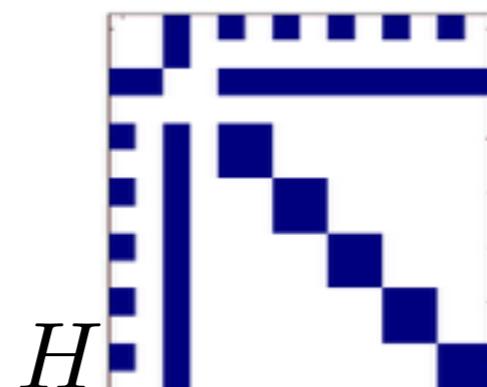
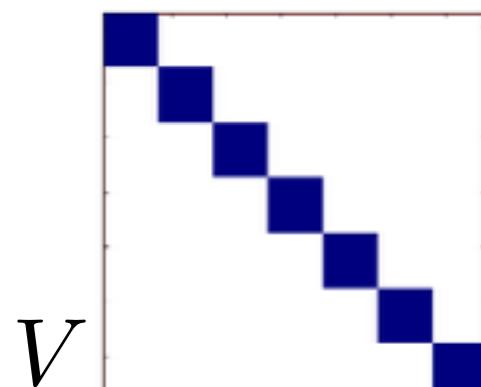
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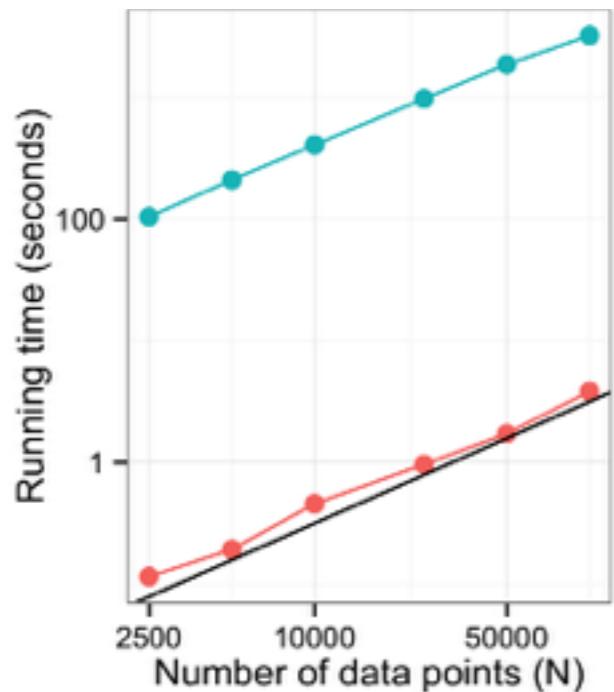
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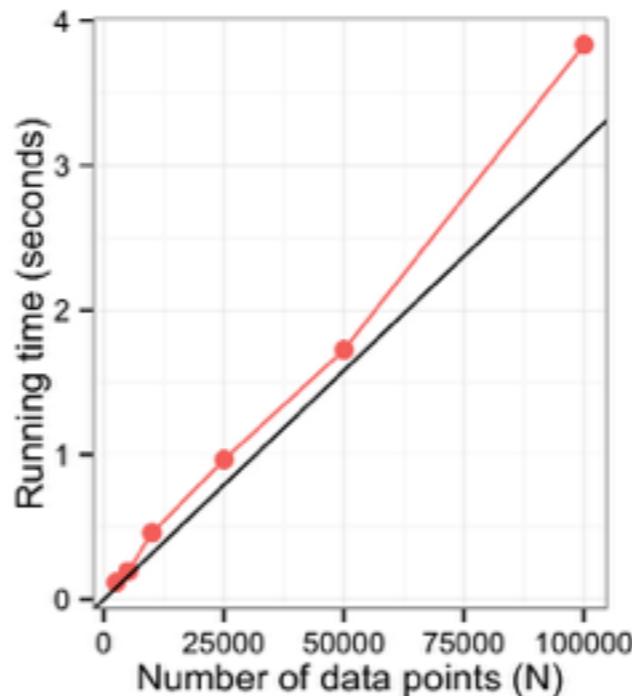
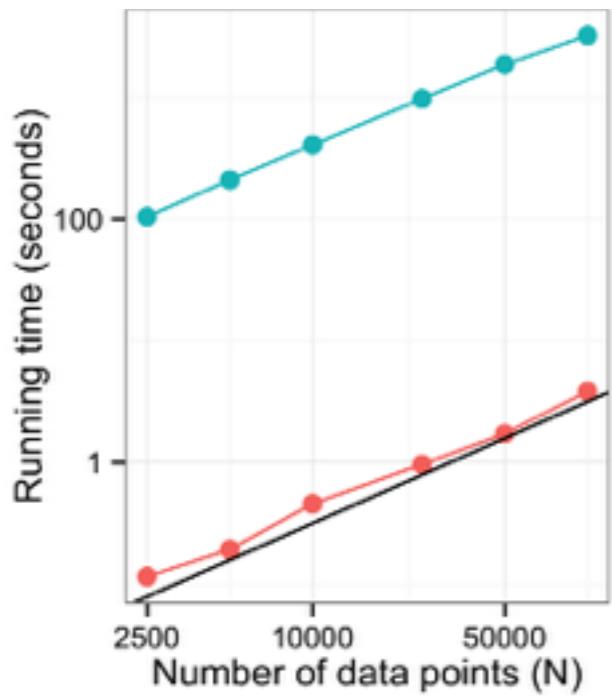
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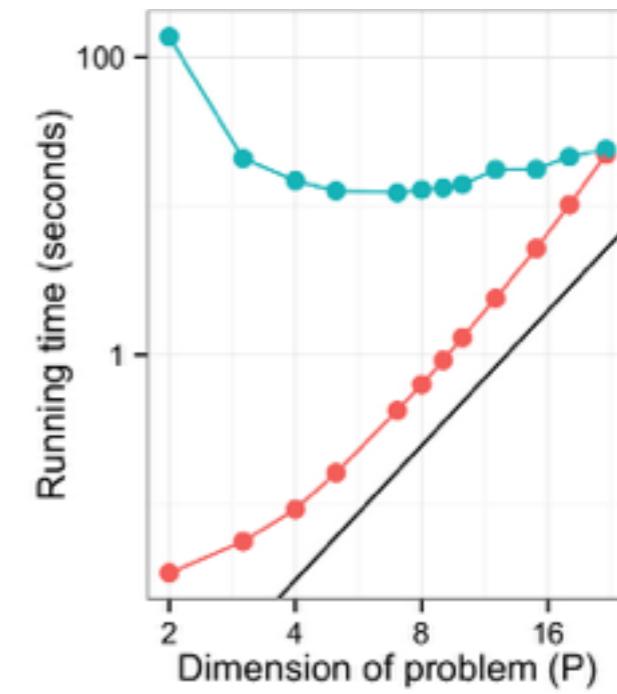
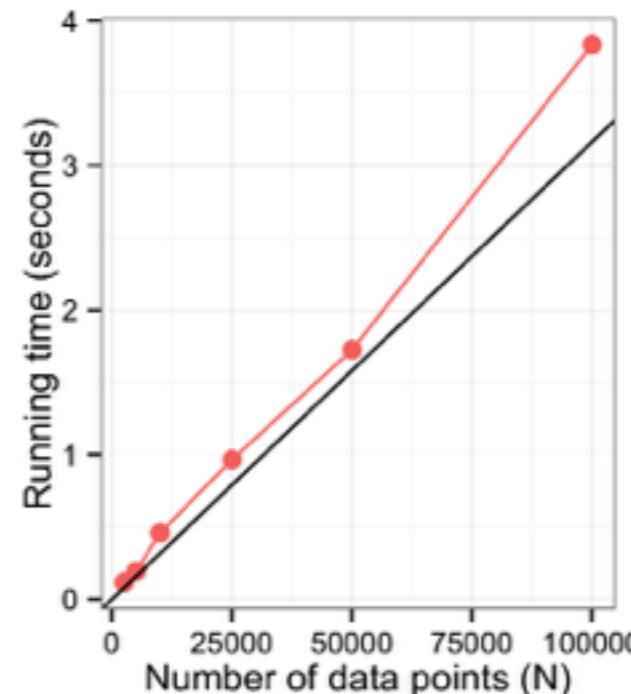
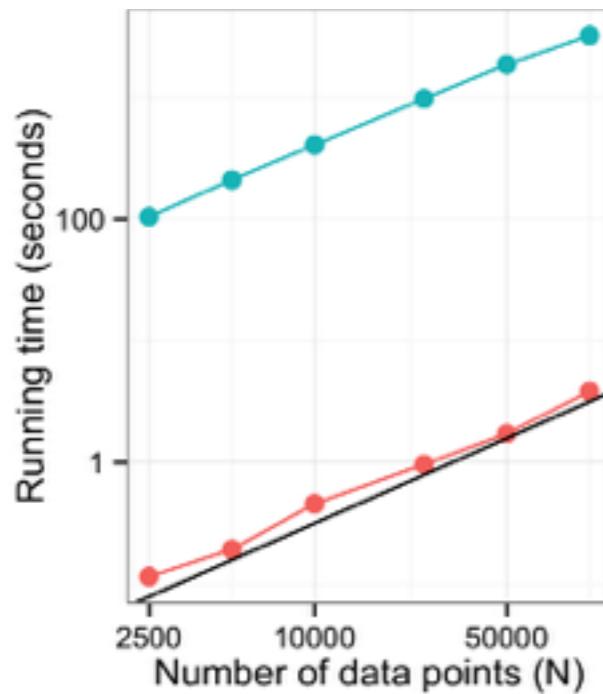
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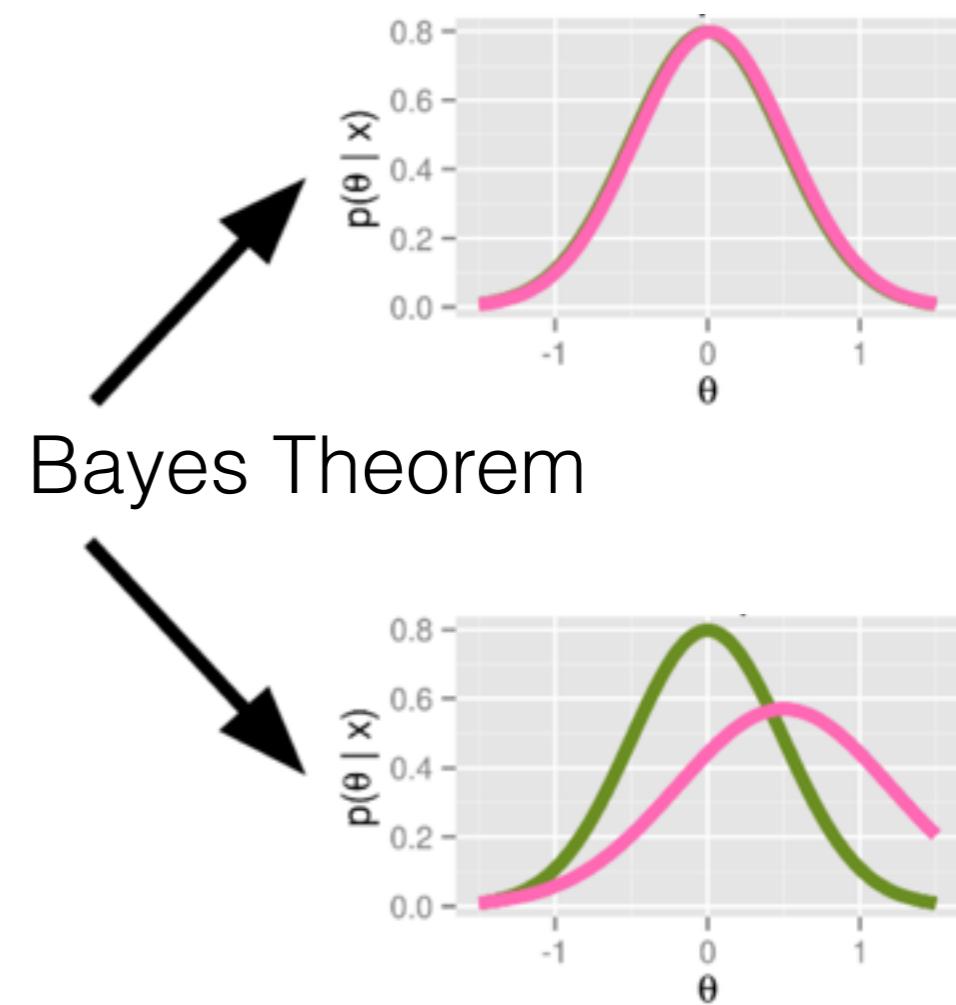
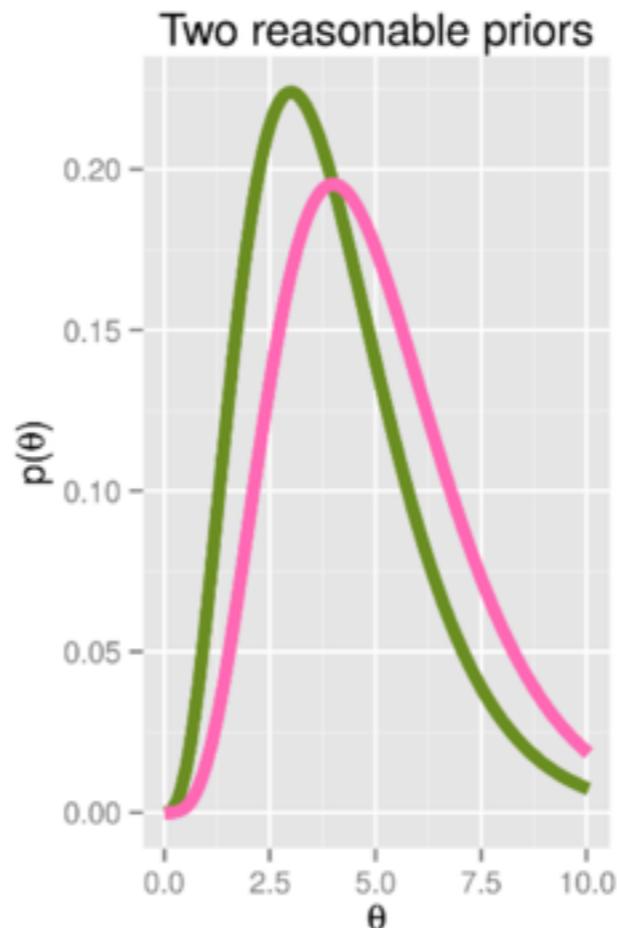
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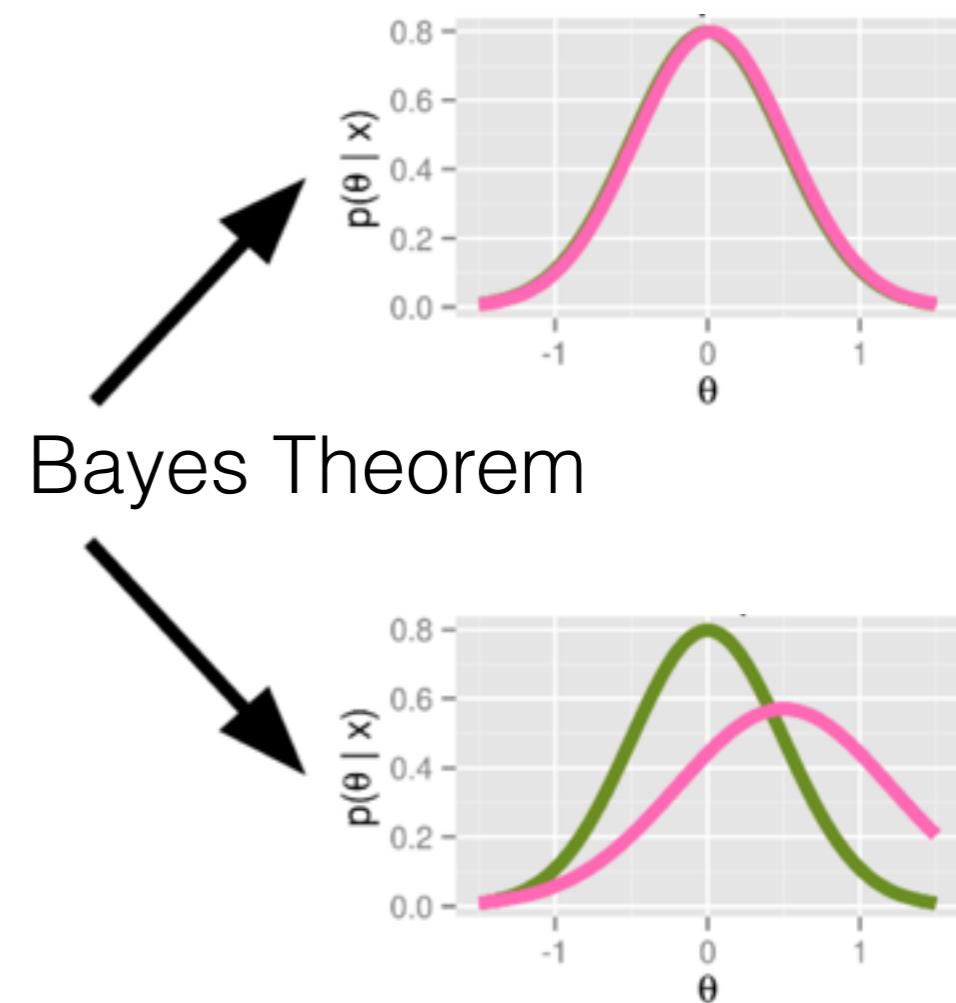
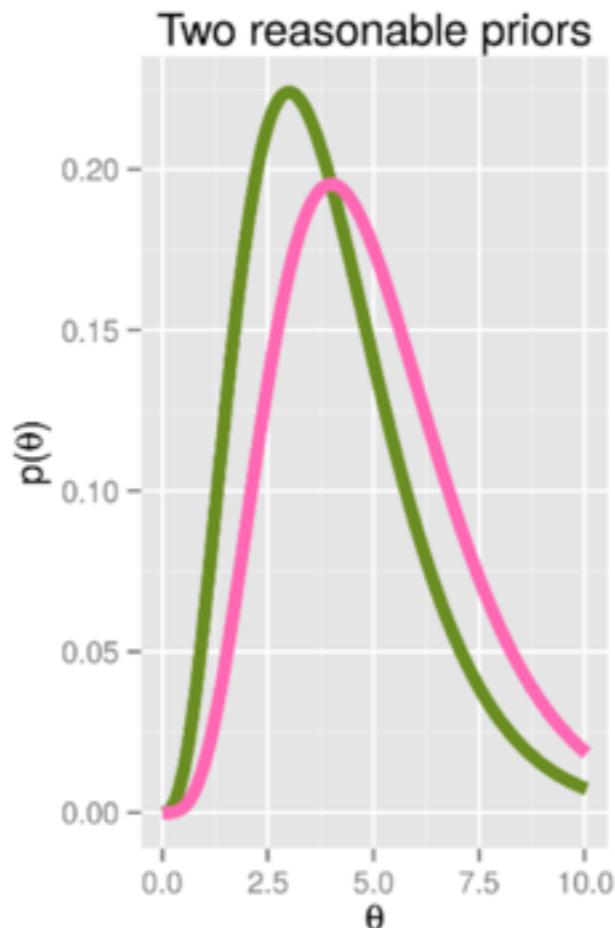
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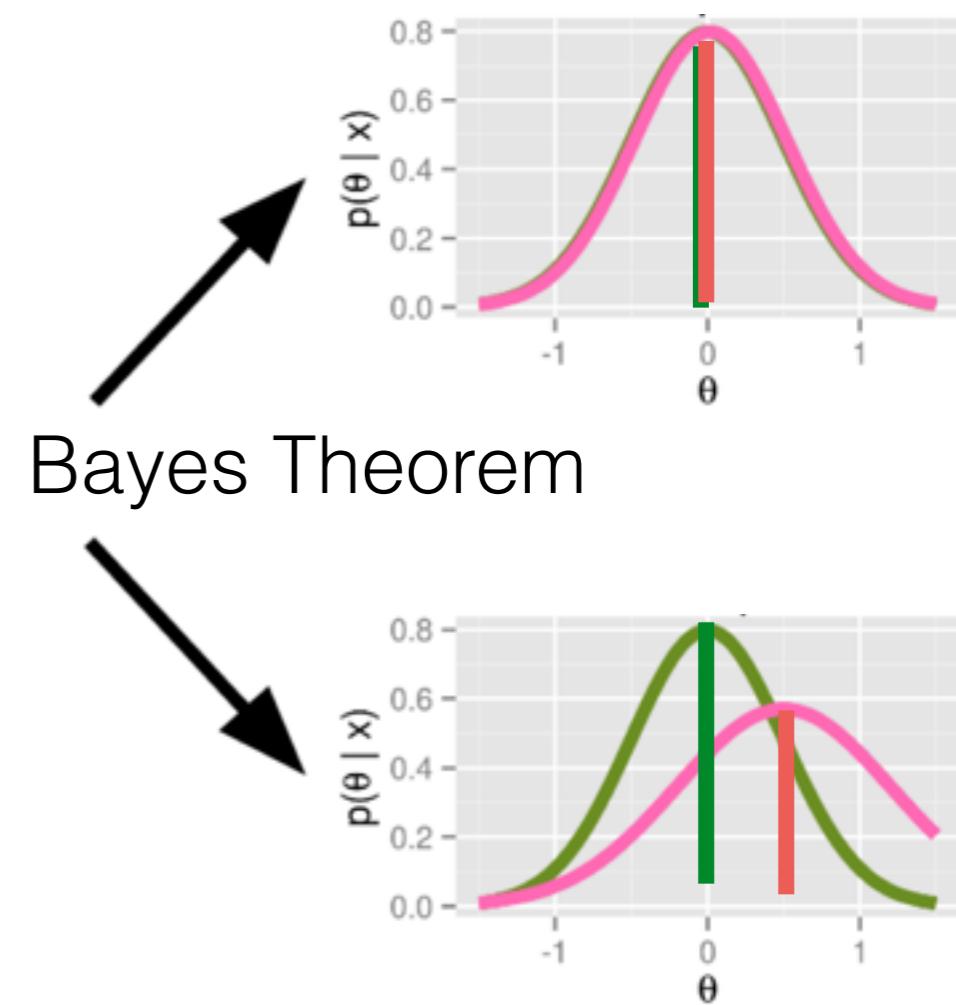
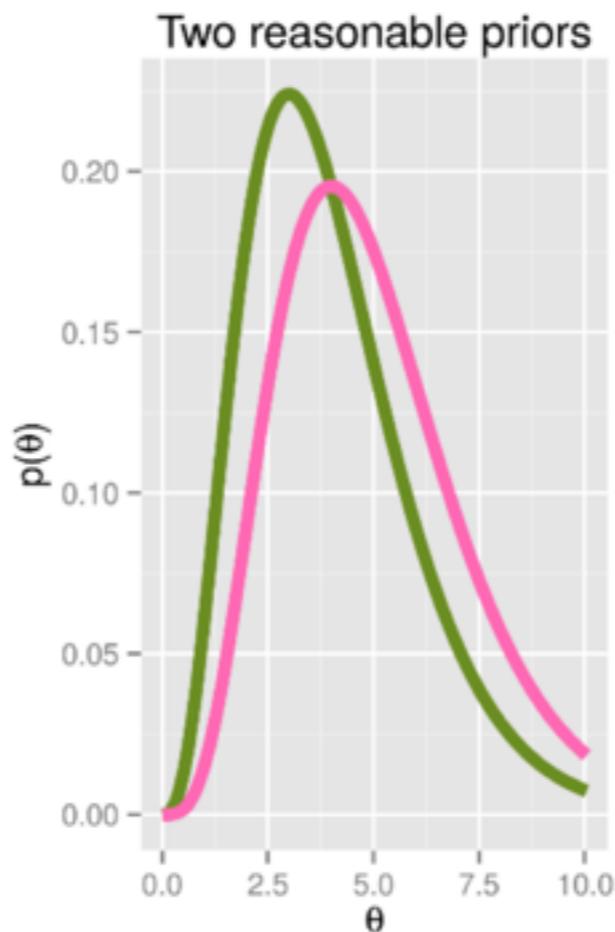
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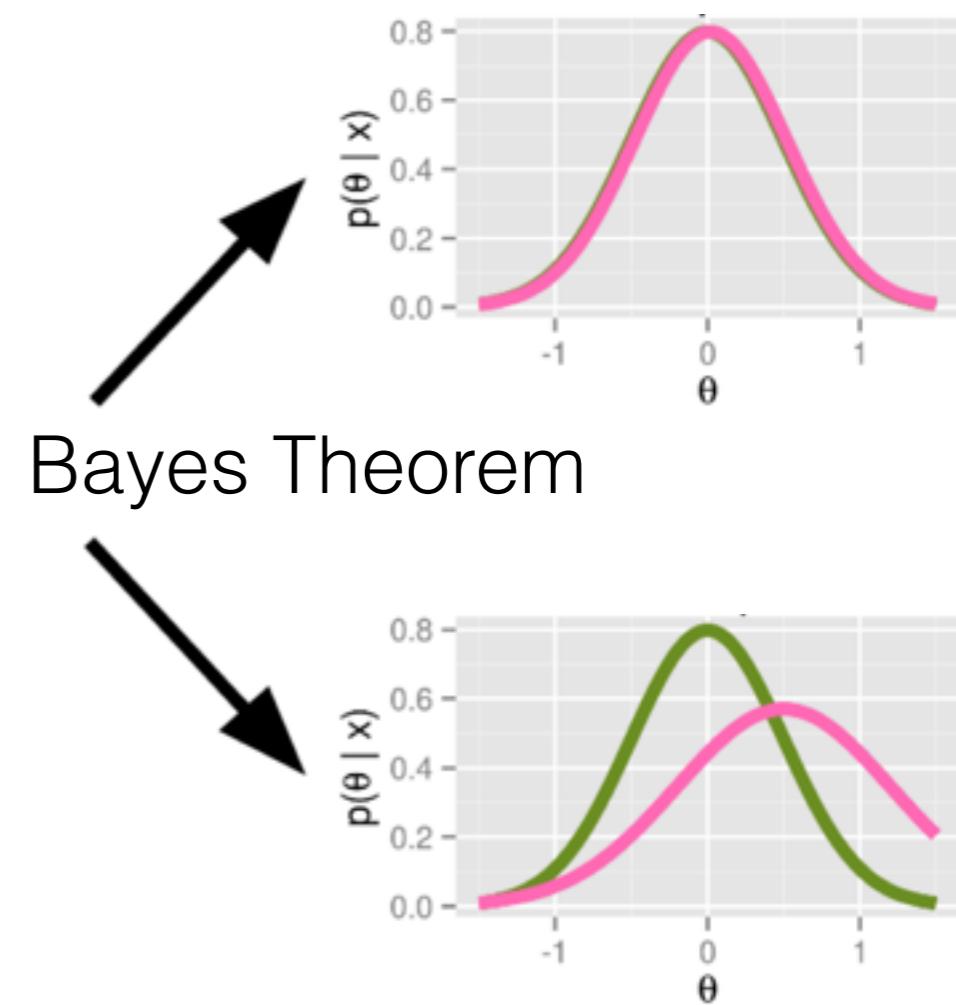
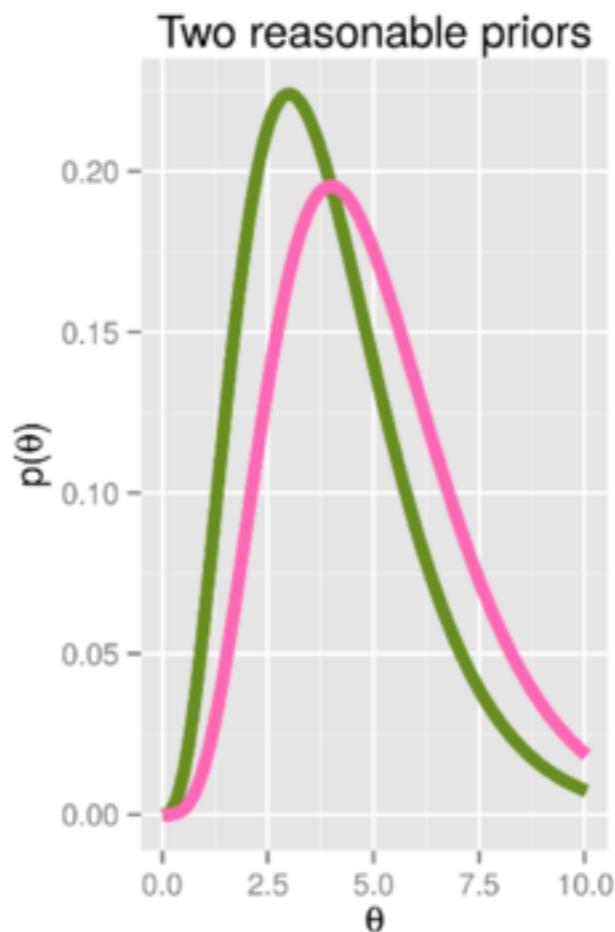
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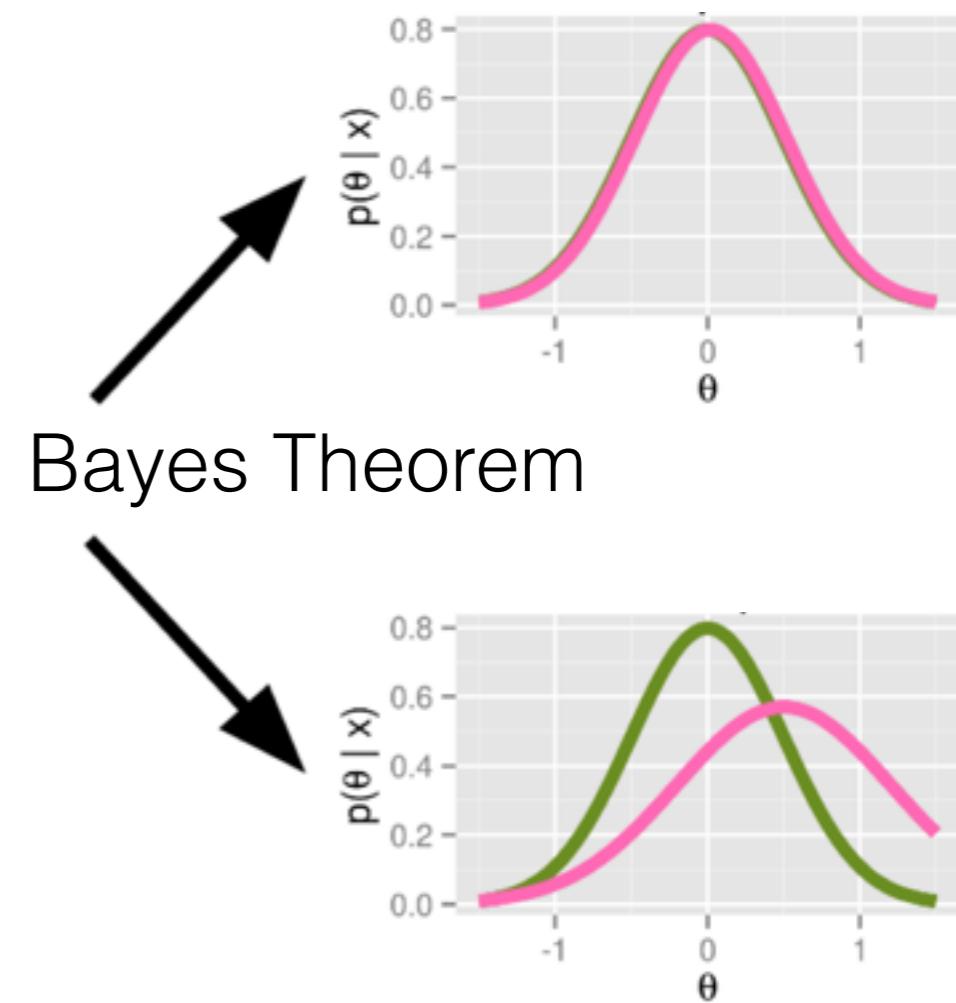
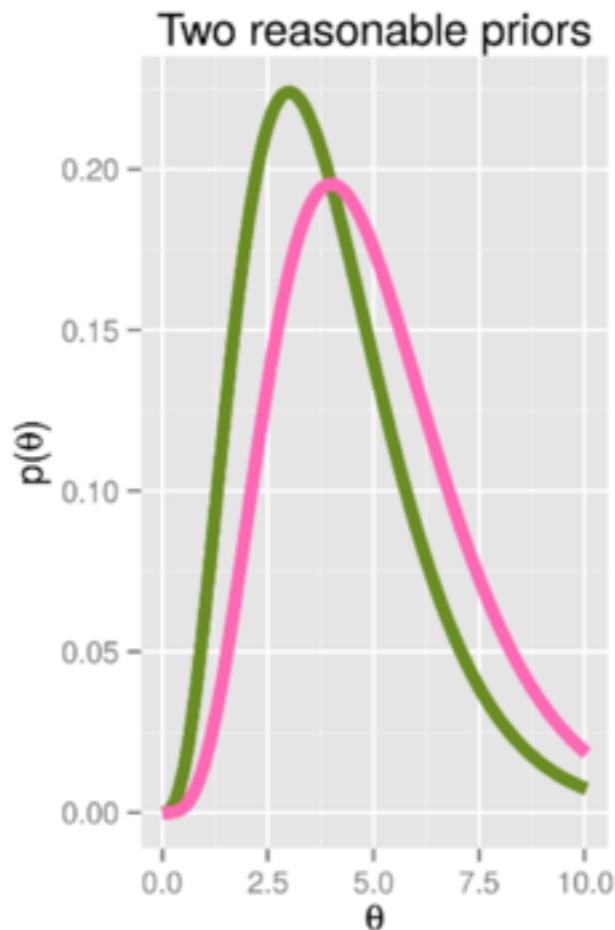
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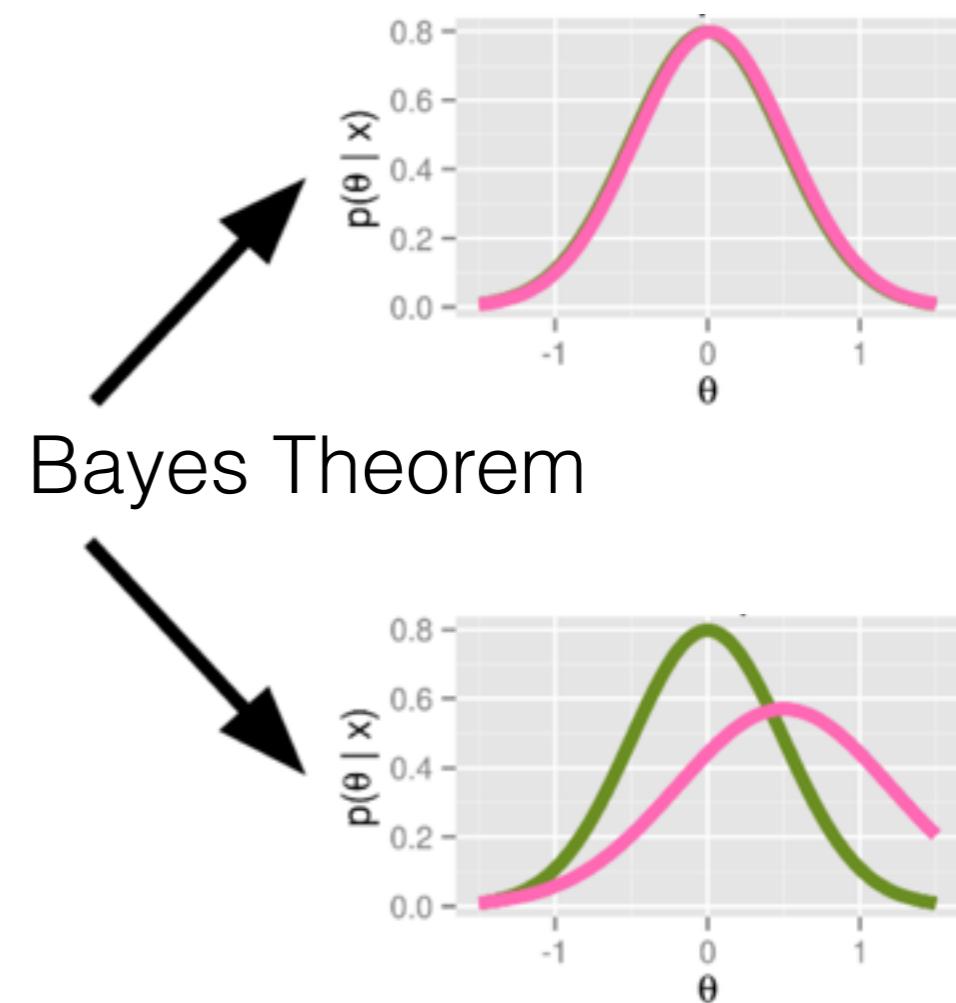
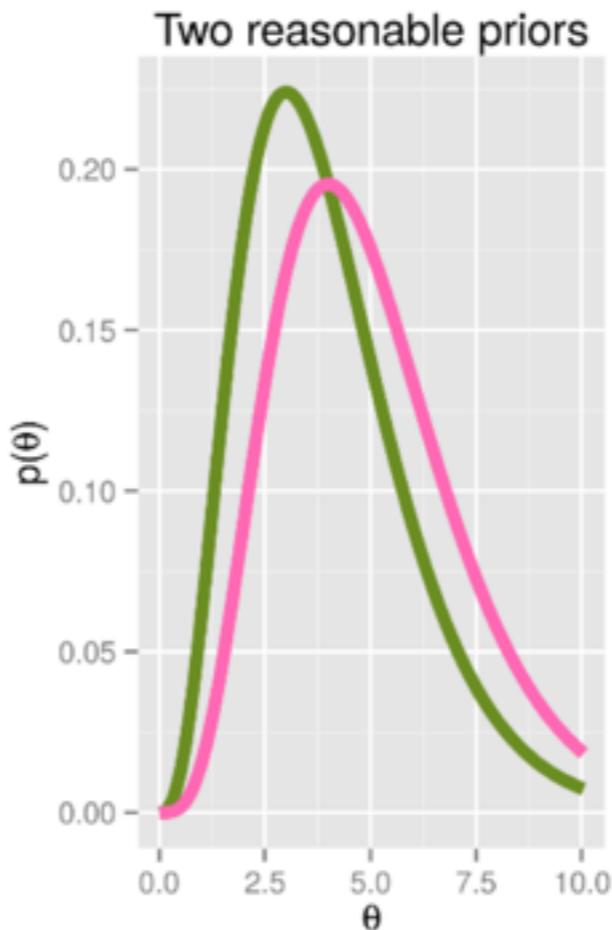
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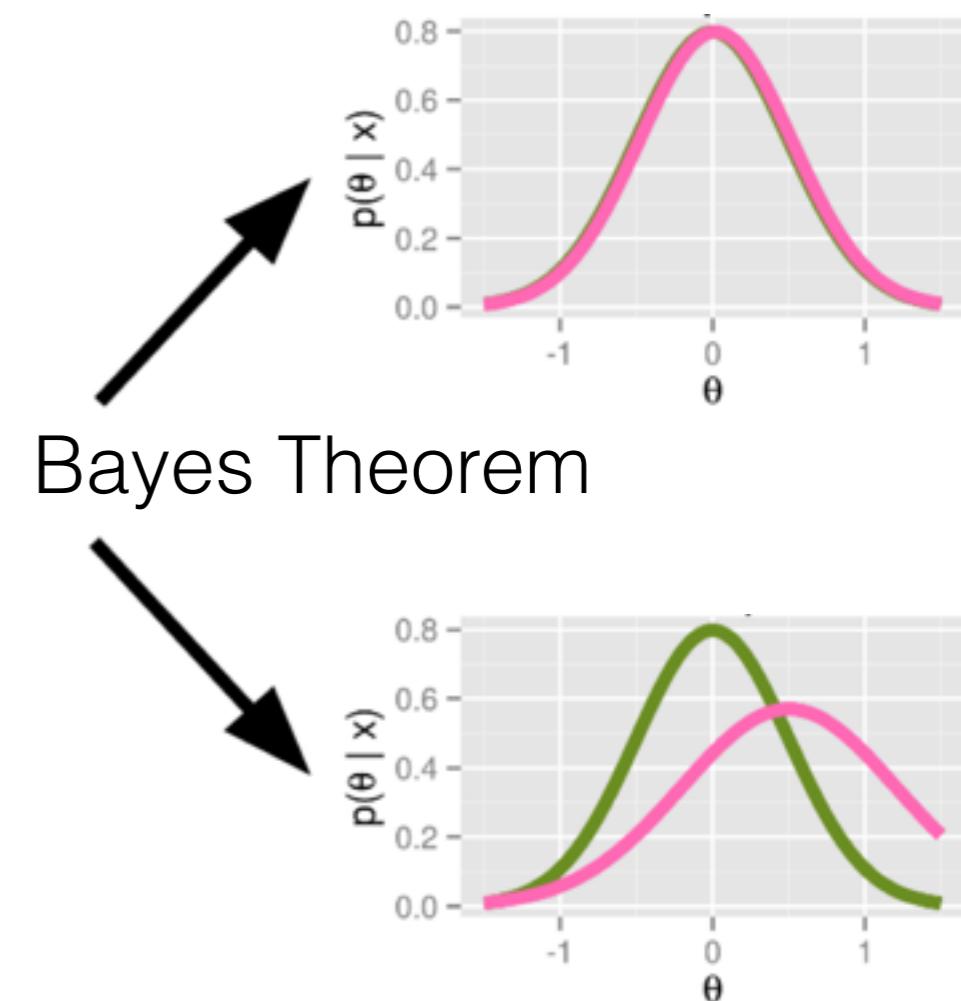
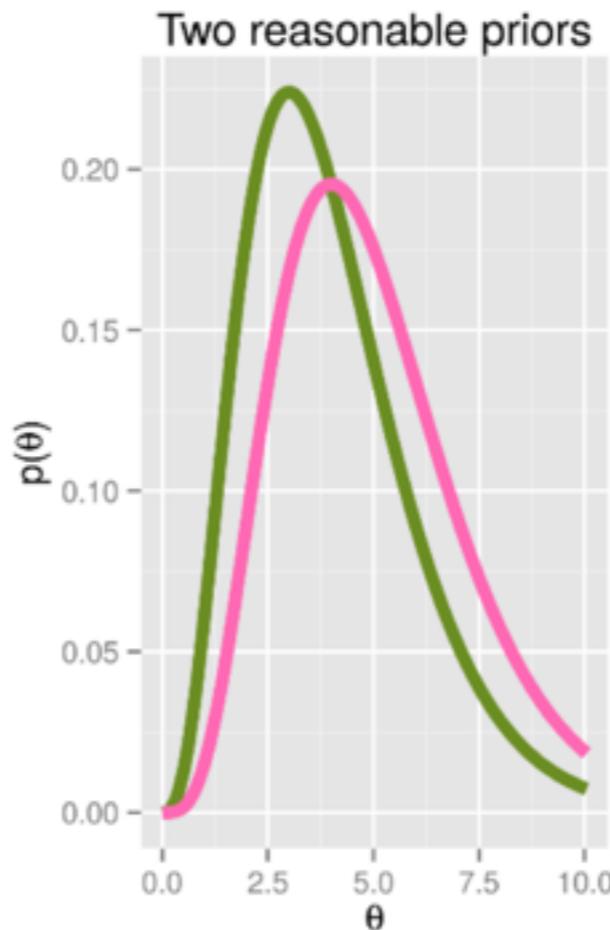
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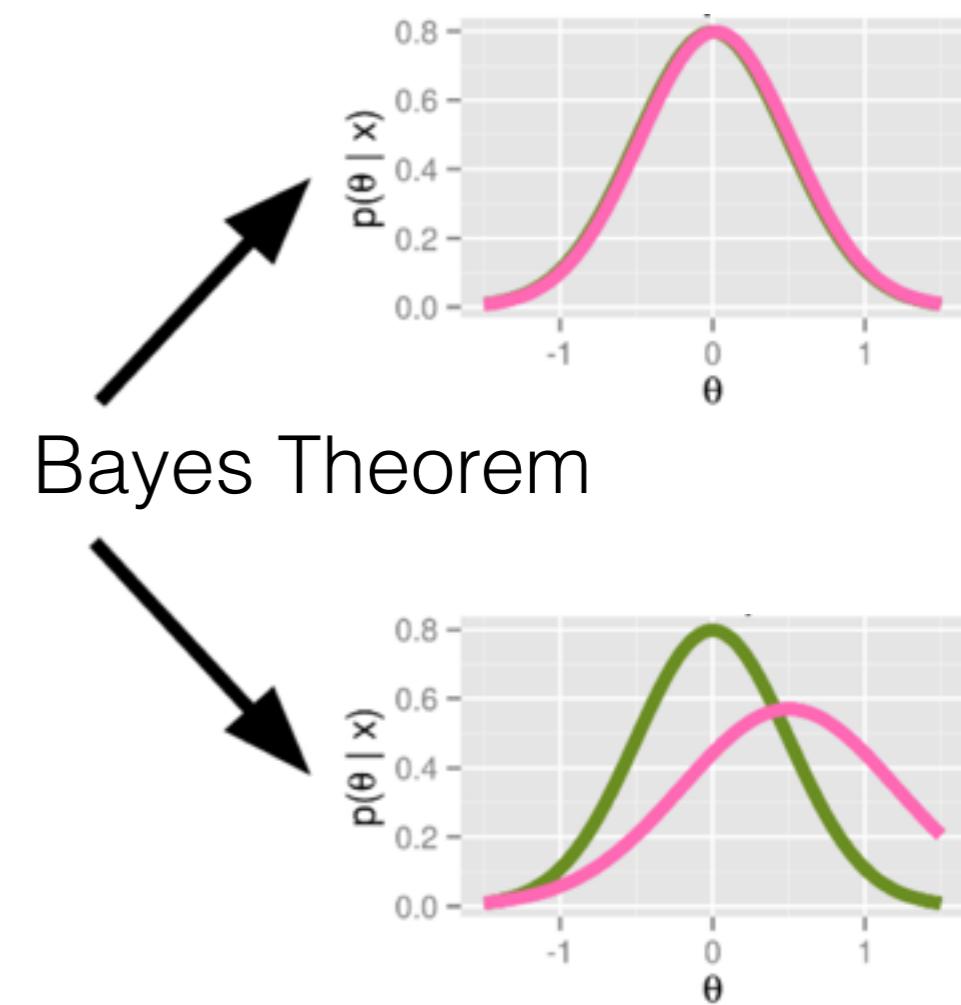
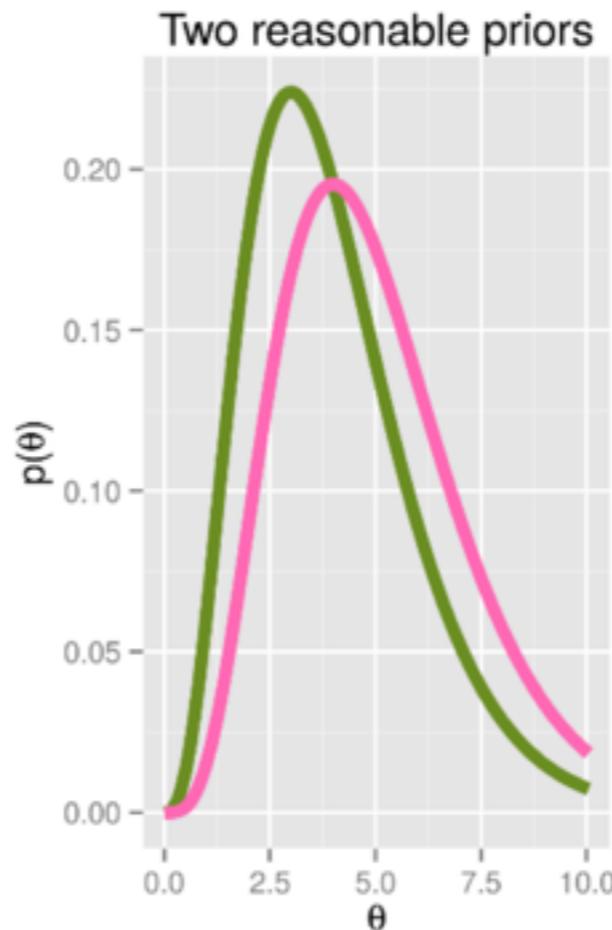
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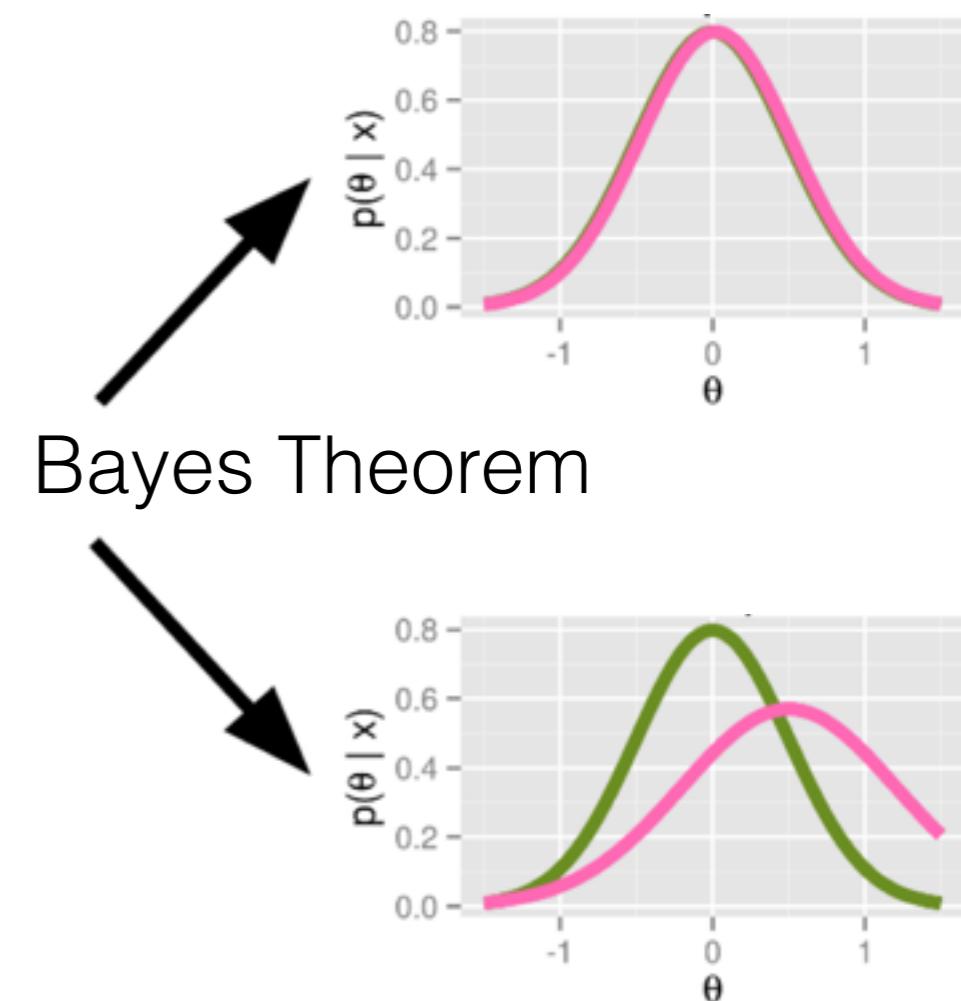
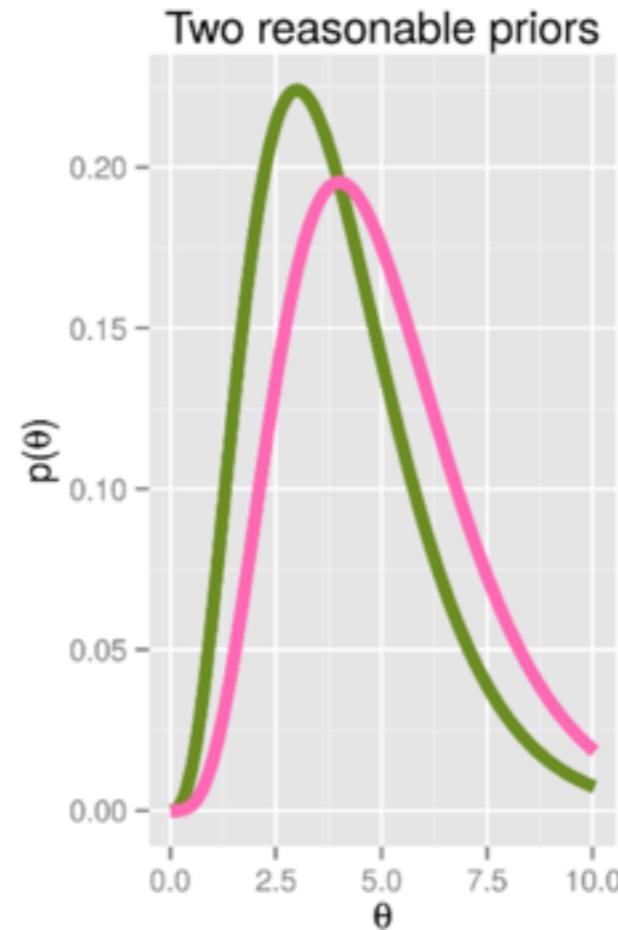
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$$p_\alpha(\theta) := p(\theta|x, \alpha)$$

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

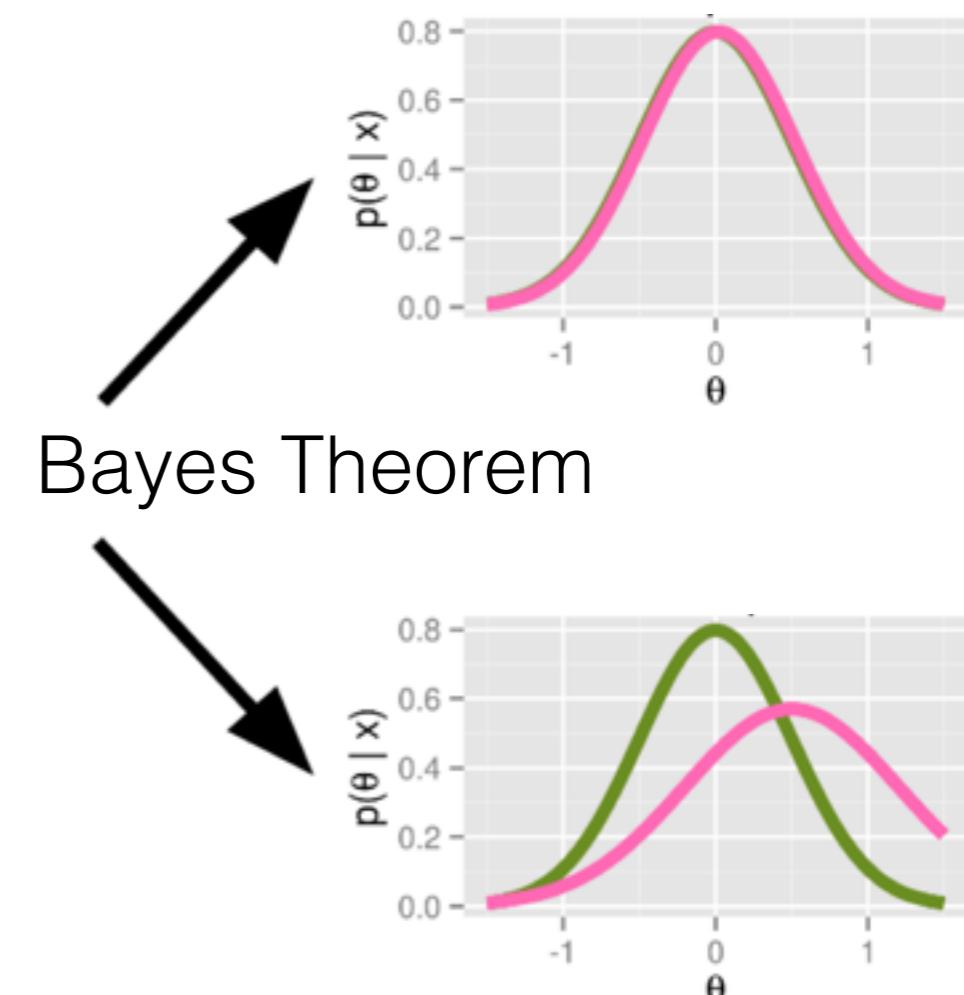
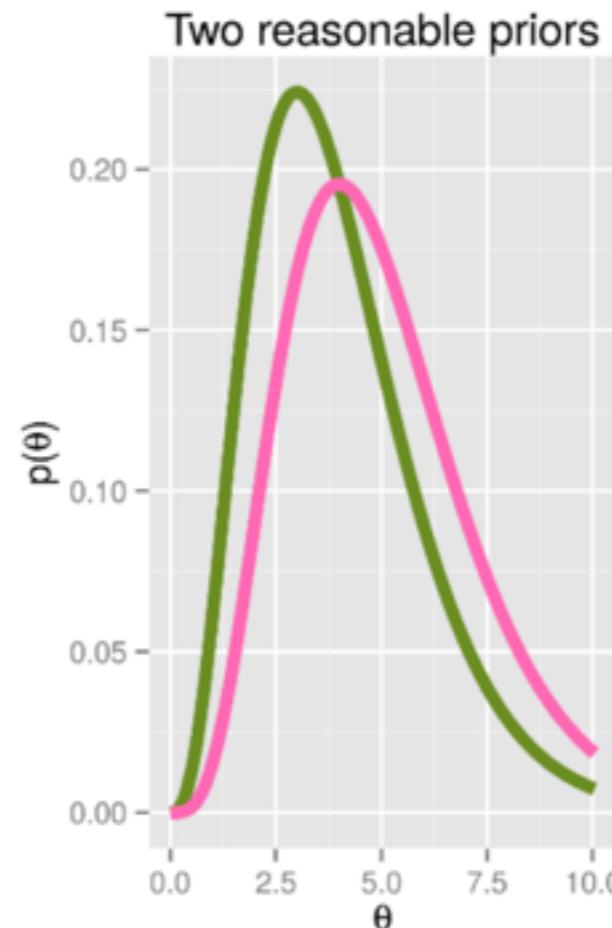
- Sensitivity

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

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

- When q_α^* in exponential family

$$\hat{S} = A \left(\left. \frac{\partial^2 KL}{\partial m \partial m^T} \right|_{m=m^*} \right)^{-1} B$$



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

- Priors and hyperpriors:

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

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

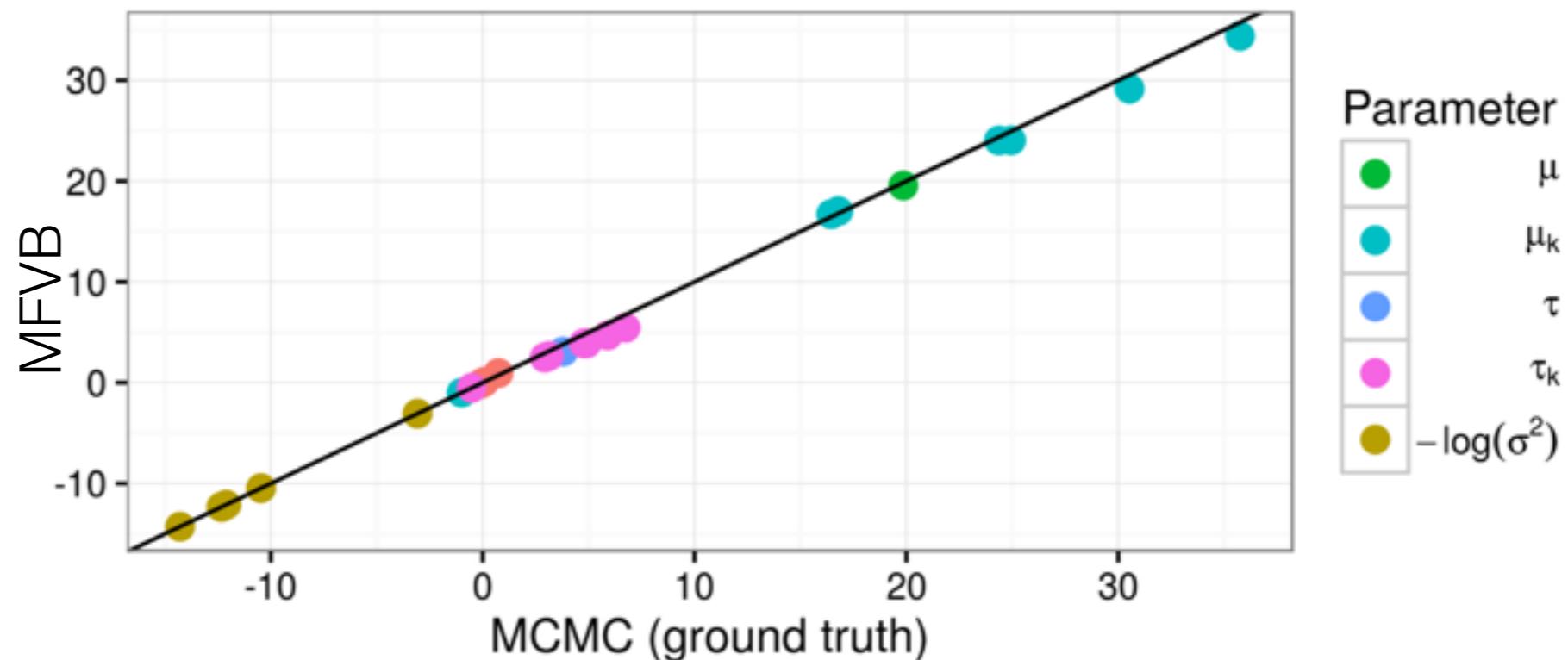
$$\sigma_k^{-2} \stackrel{iid}{\sim} \Gamma(a, b)$$

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

Microcredit Experiment

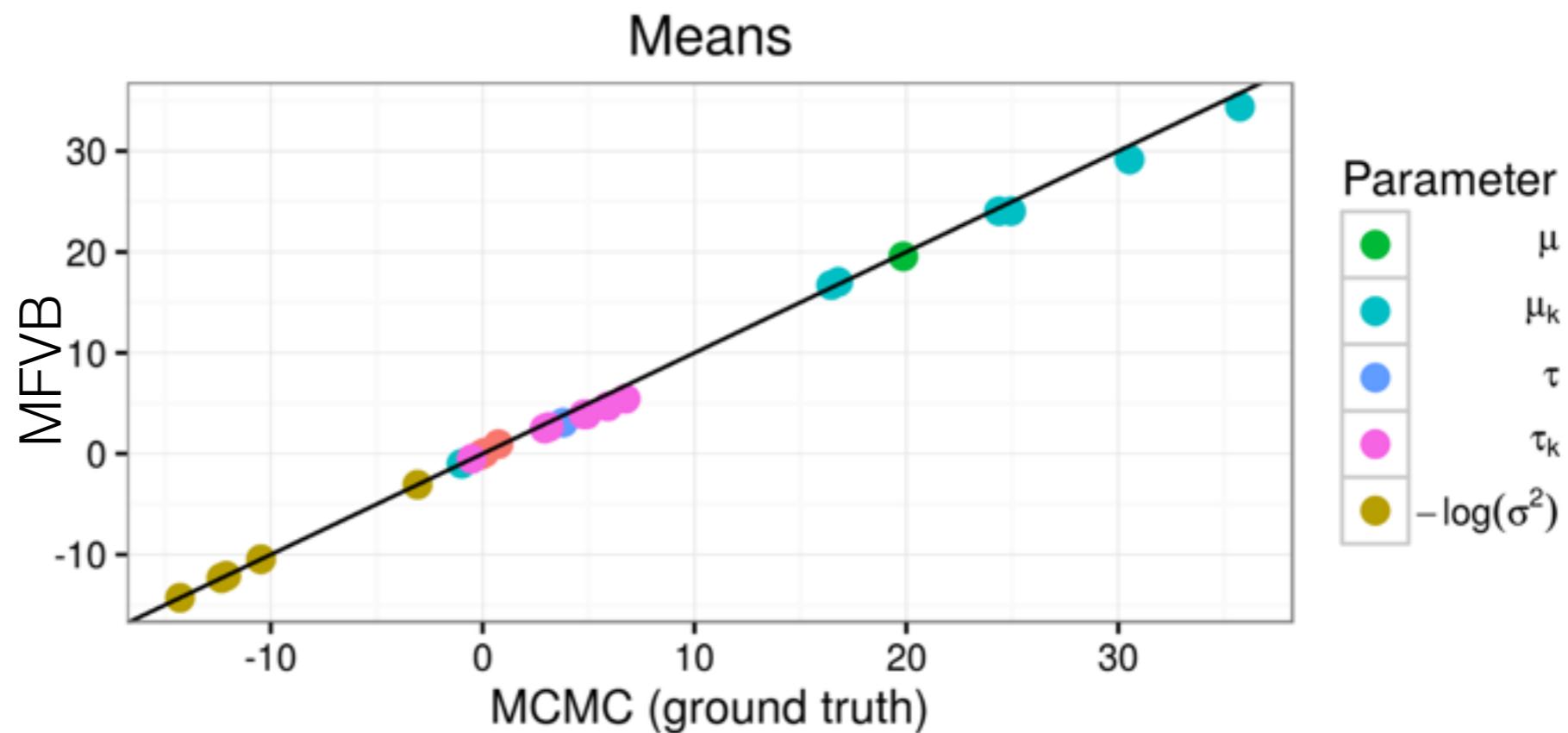
Microcredit Experiment

Means



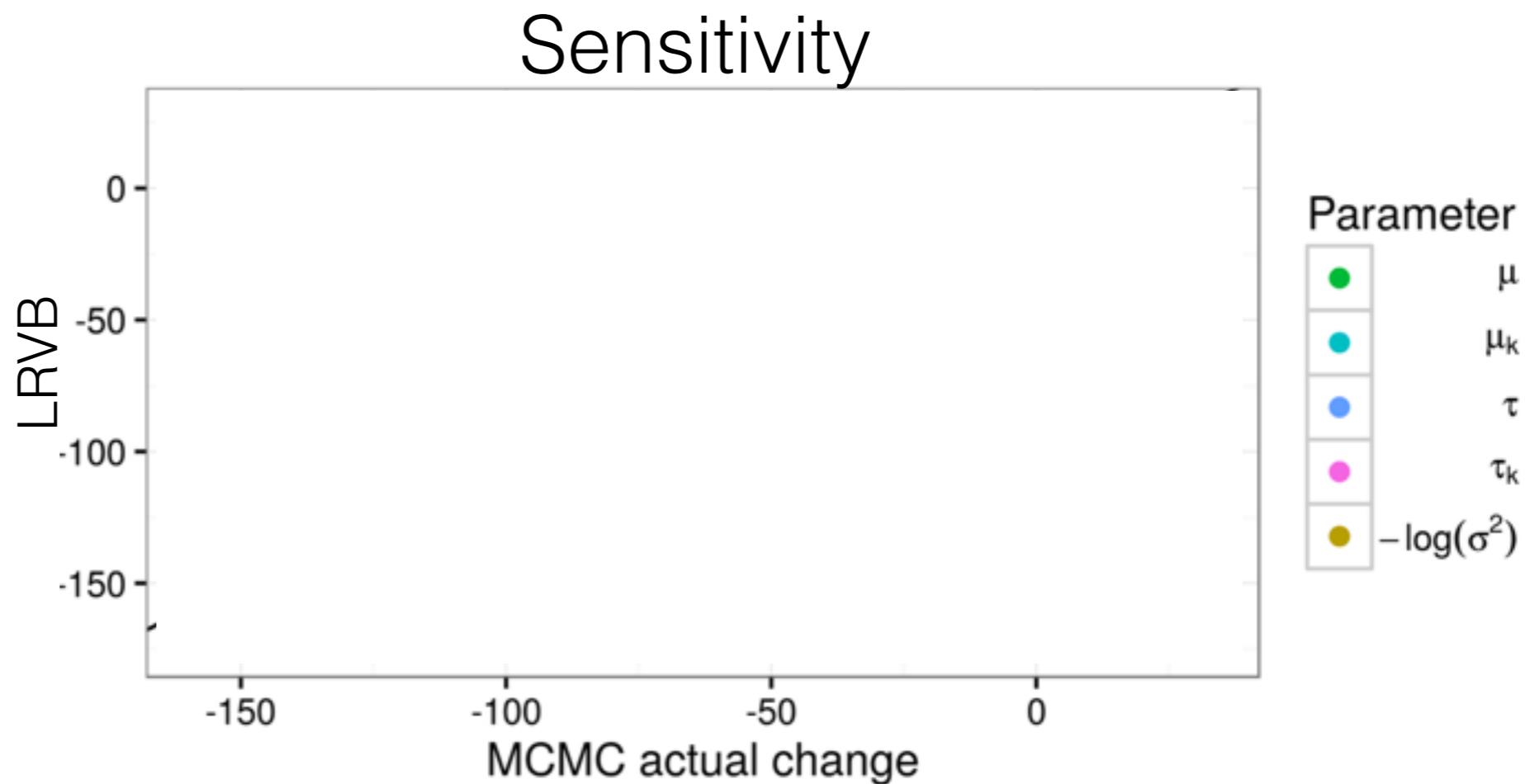
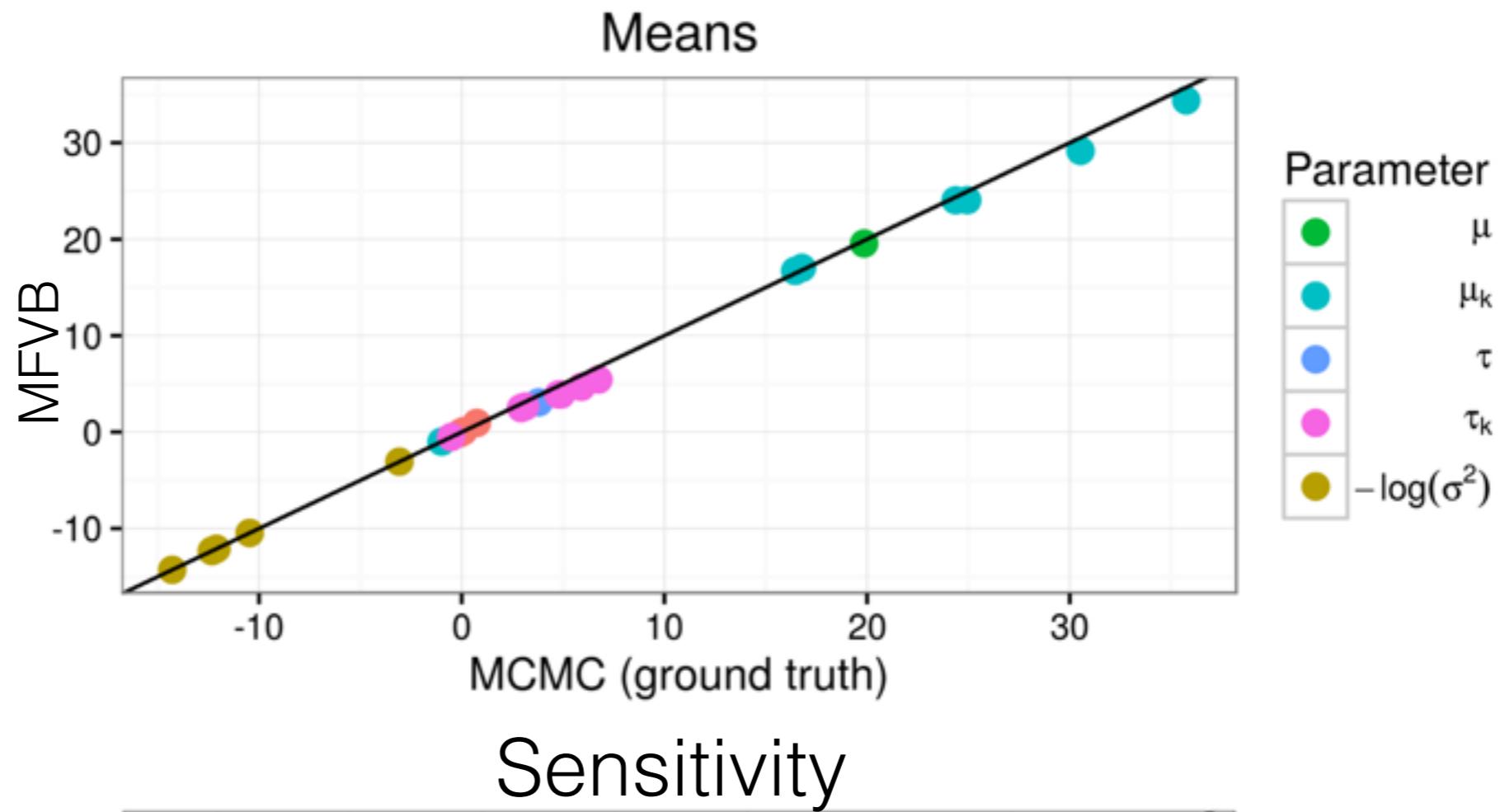
Microcredit Experiment

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



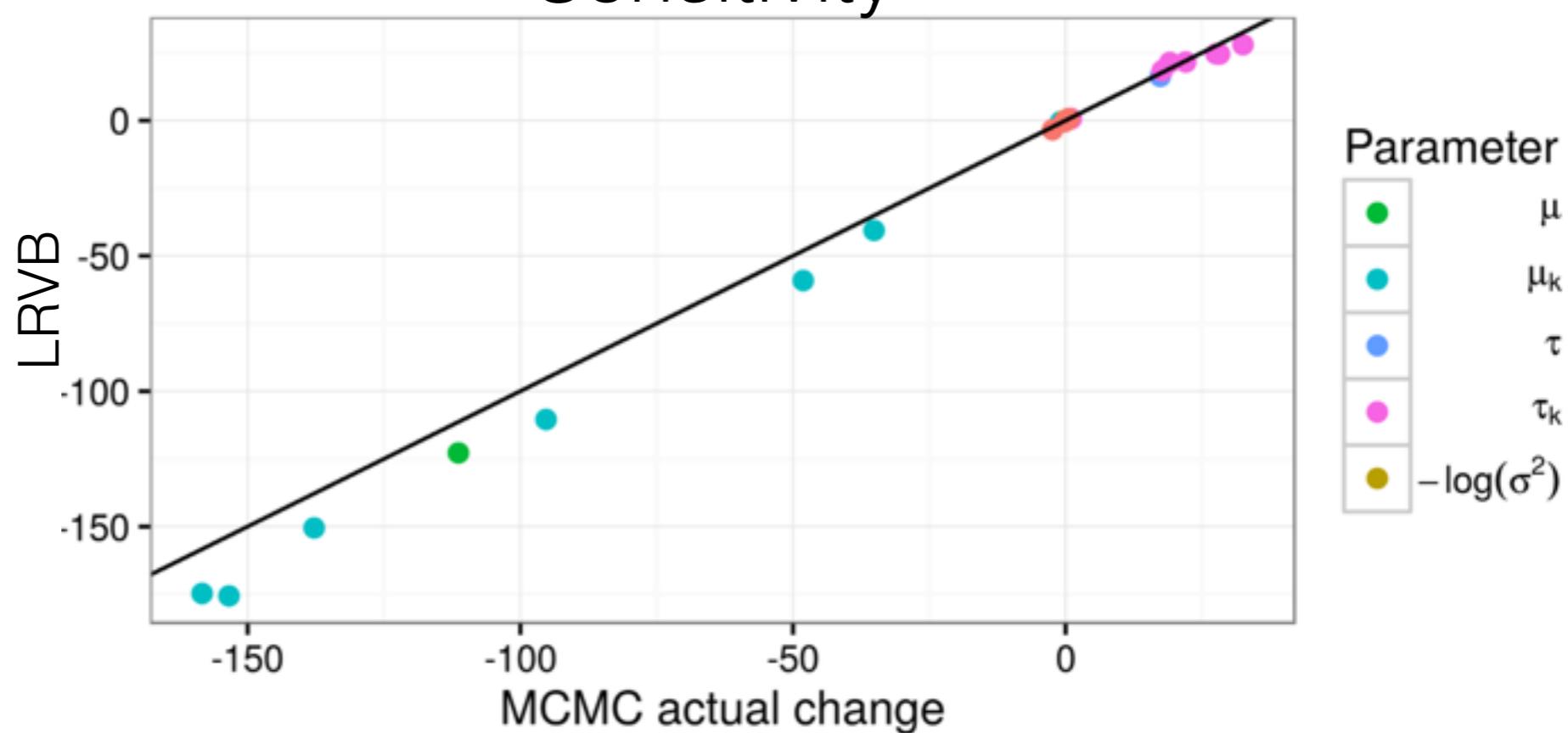
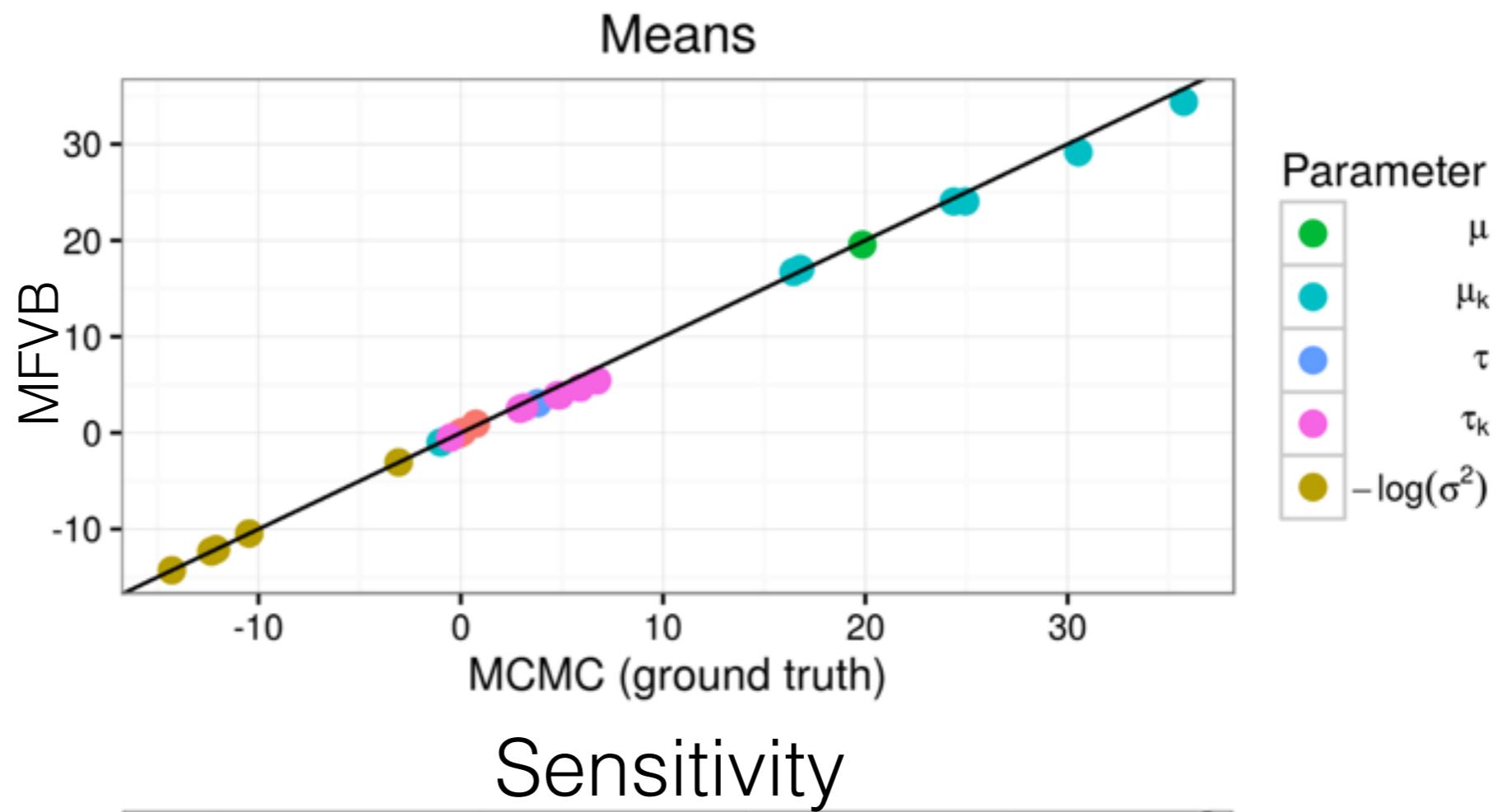
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Microcredit Experiment

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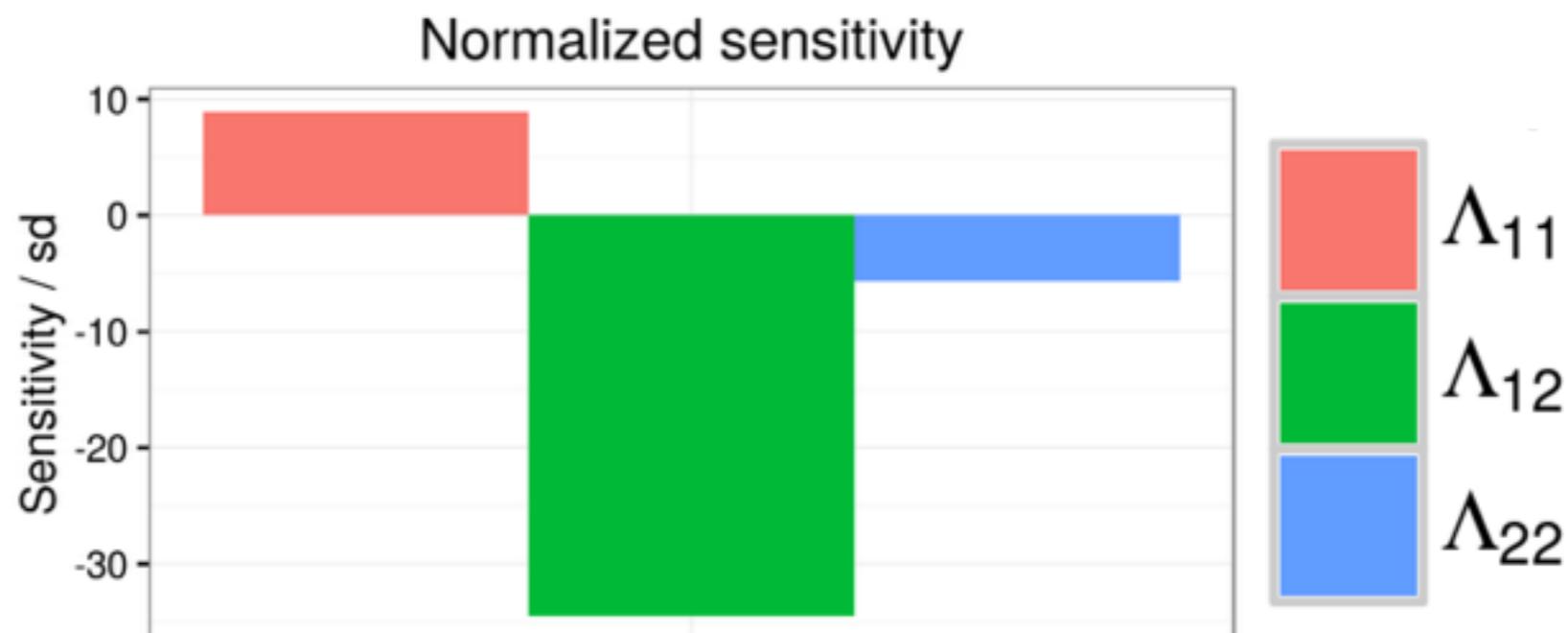
- Sensitivity of the expected microcredit effect (τ)

Microcredit Experiment

- Sensitivity of the expected microcredit effect (τ)
- Normalized to be on scale of τ std devs

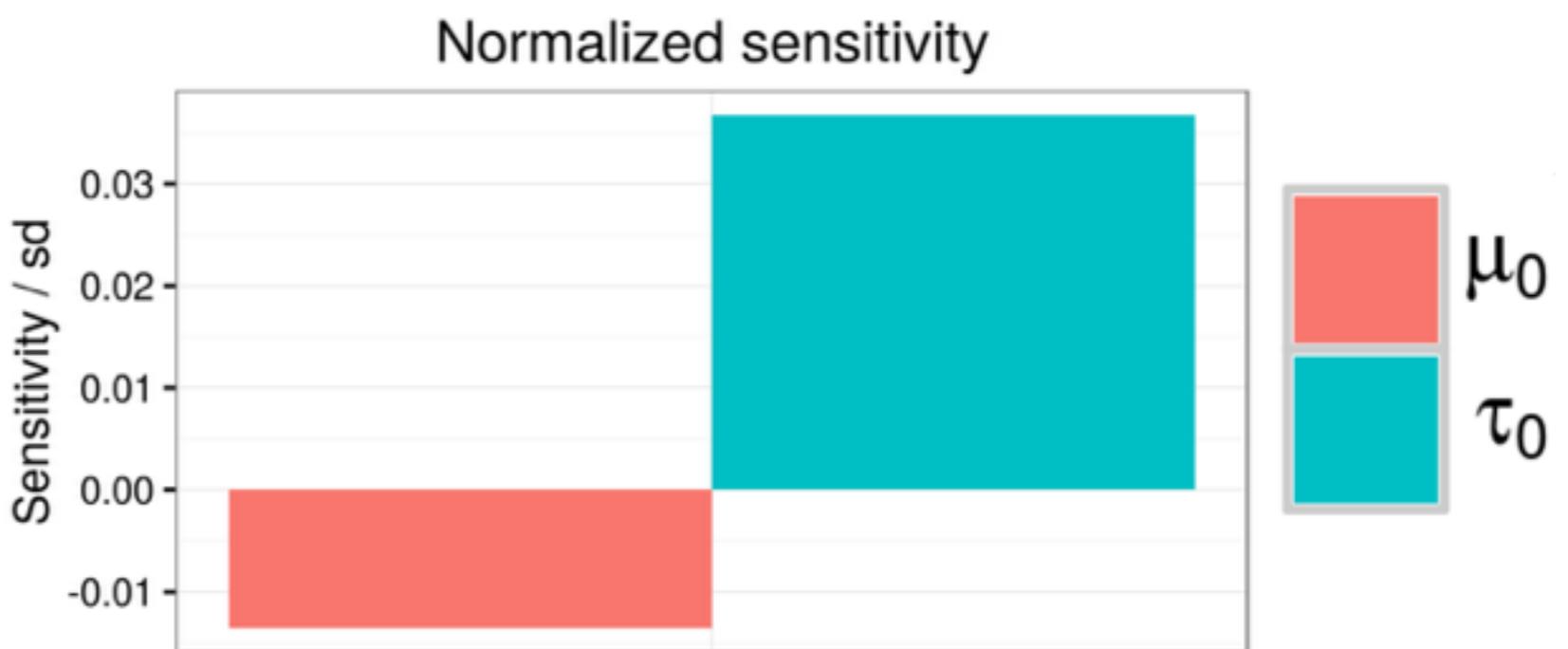
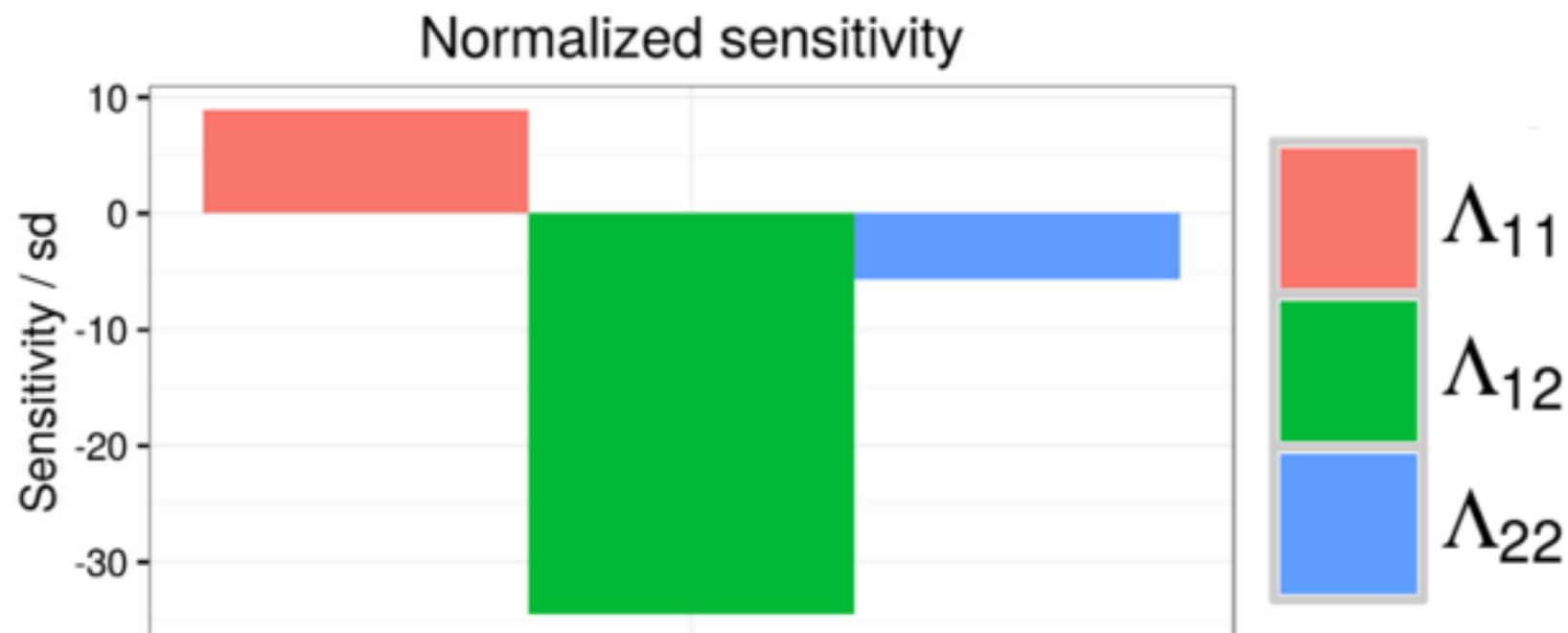
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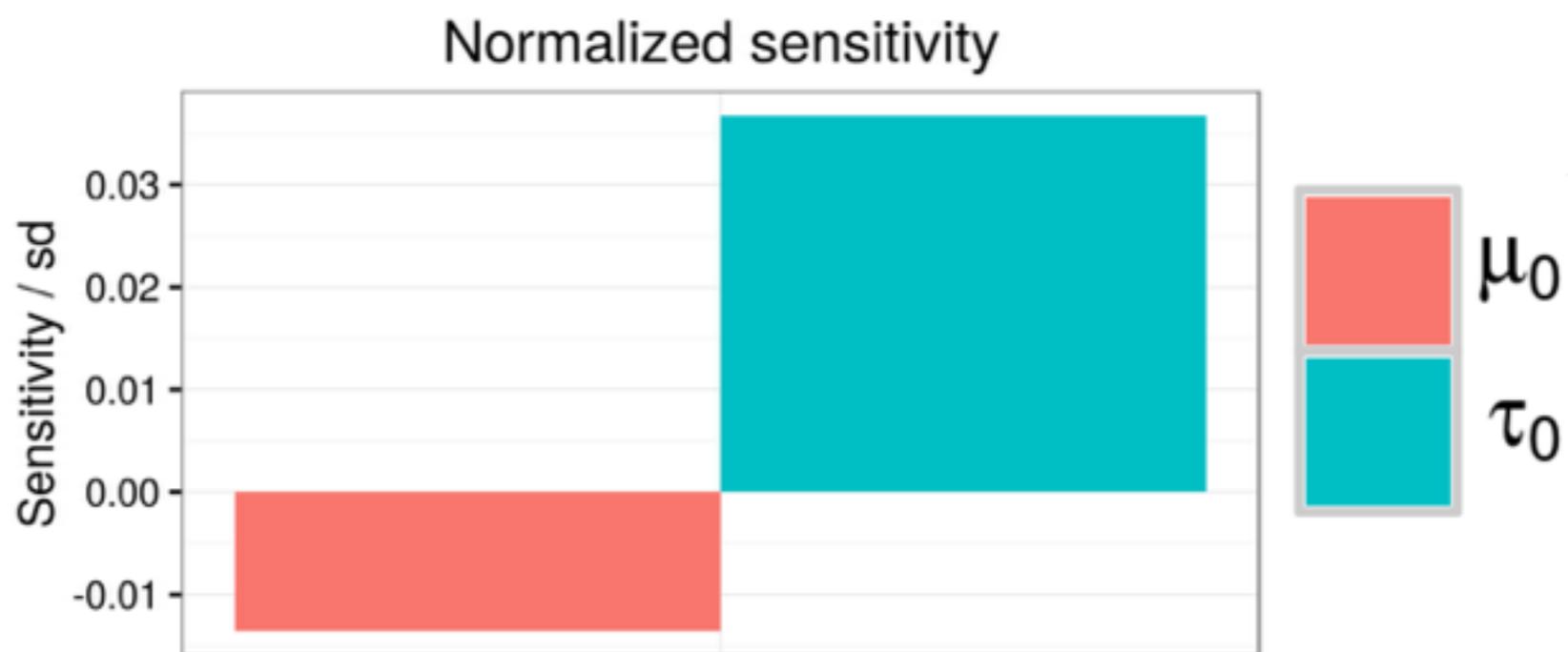
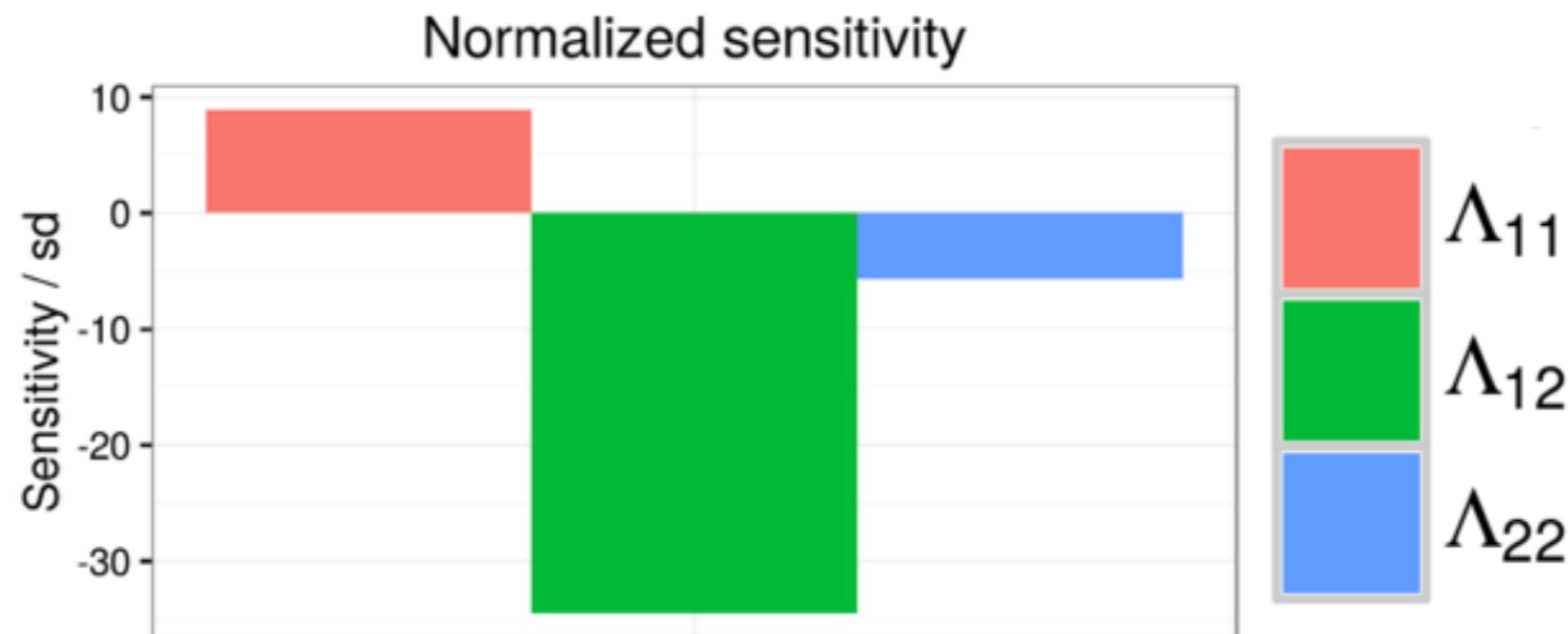
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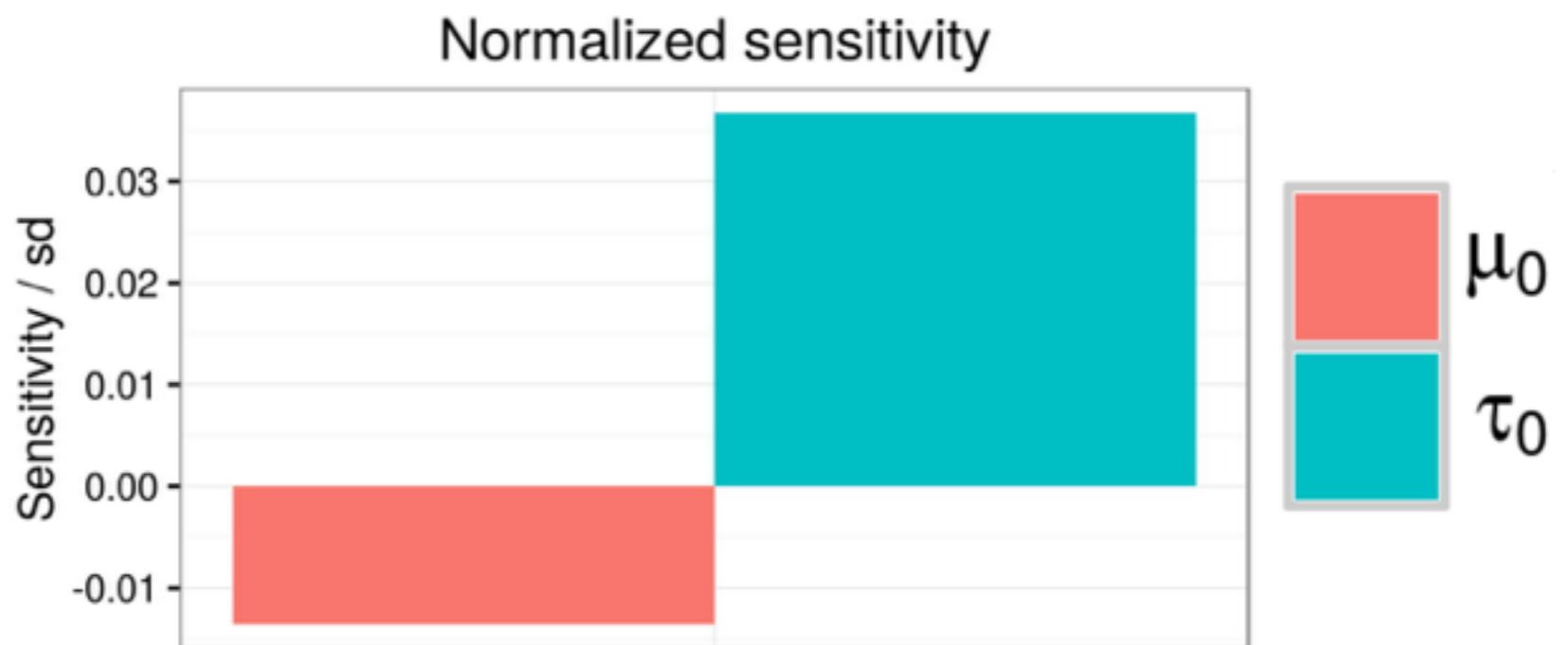
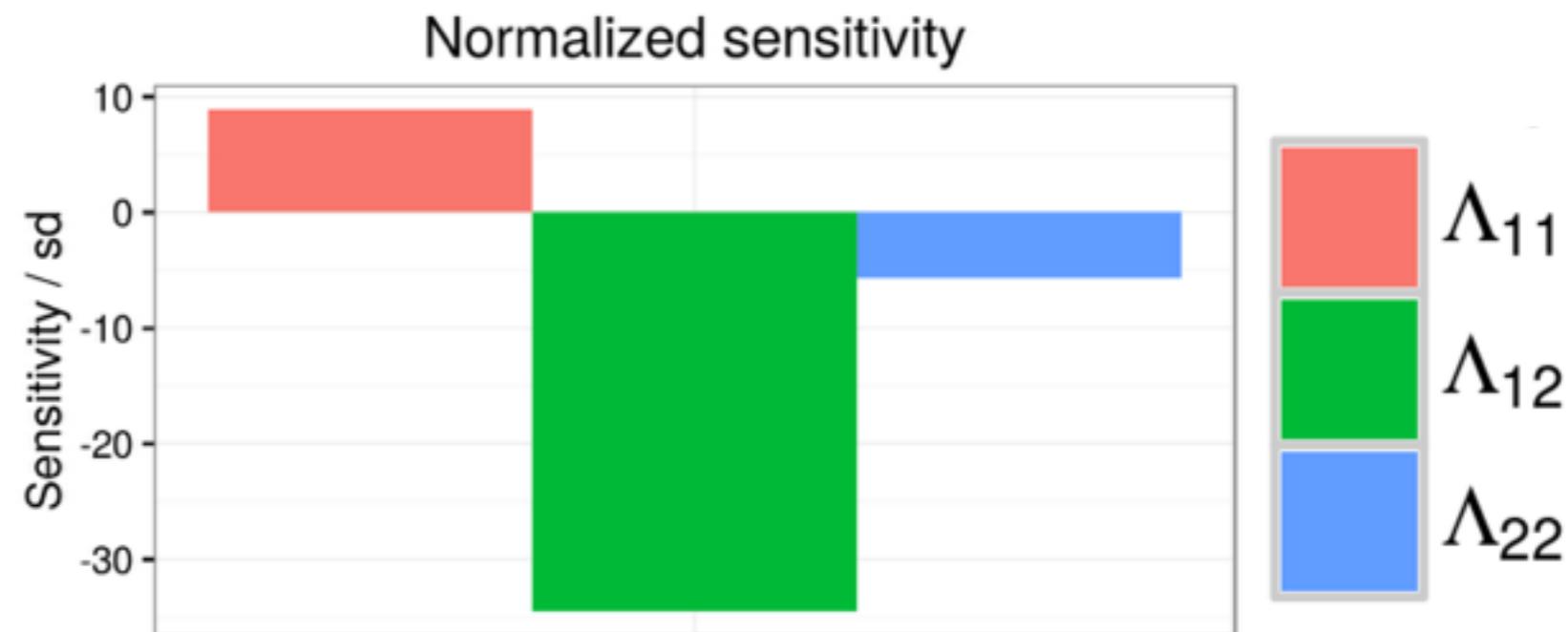
Microcredit Experiment

- Sensitivity of the expected microcredit effect (τ)
- Normalized to be on scale of τ std devs
- τ mean (MFVB): 3.08 USD PPP
- τ std dev (LRVB): 1.83 USD PPP
- Mean is 1.68 std dev from 0



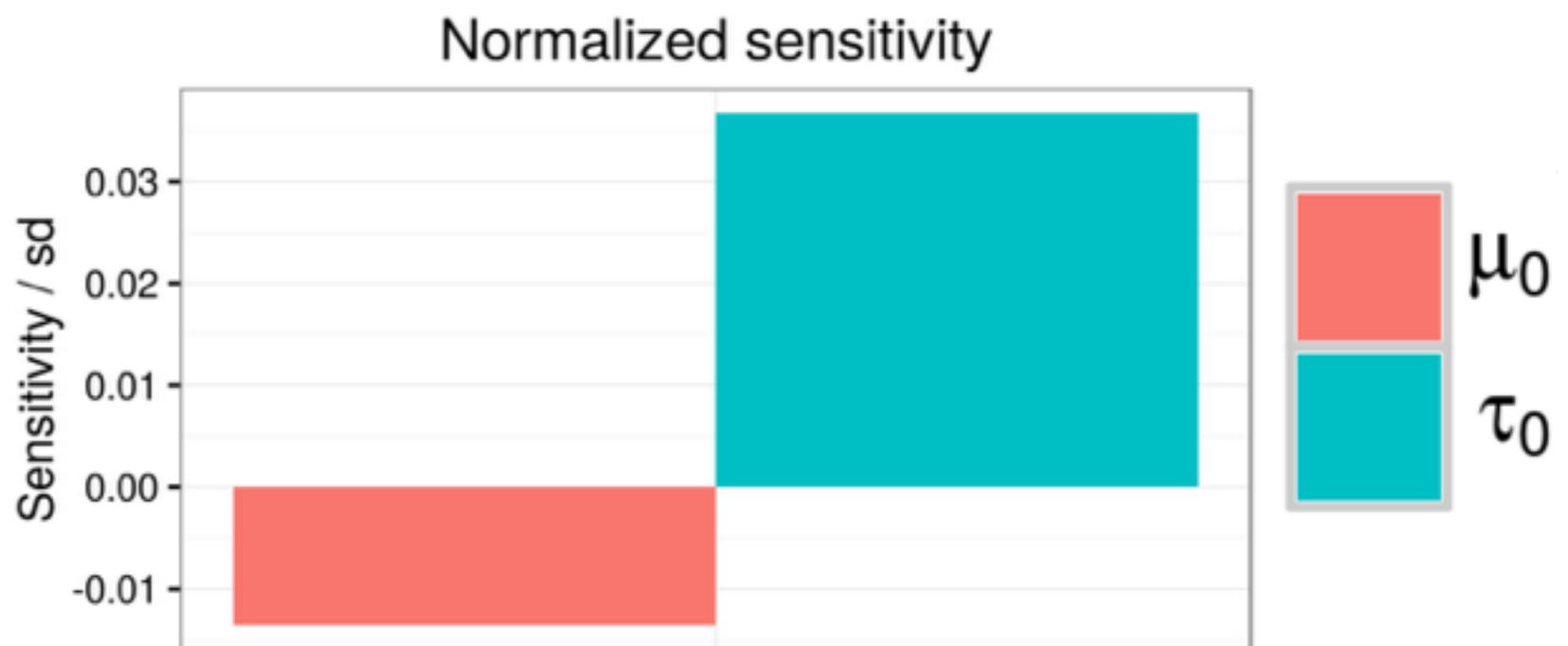
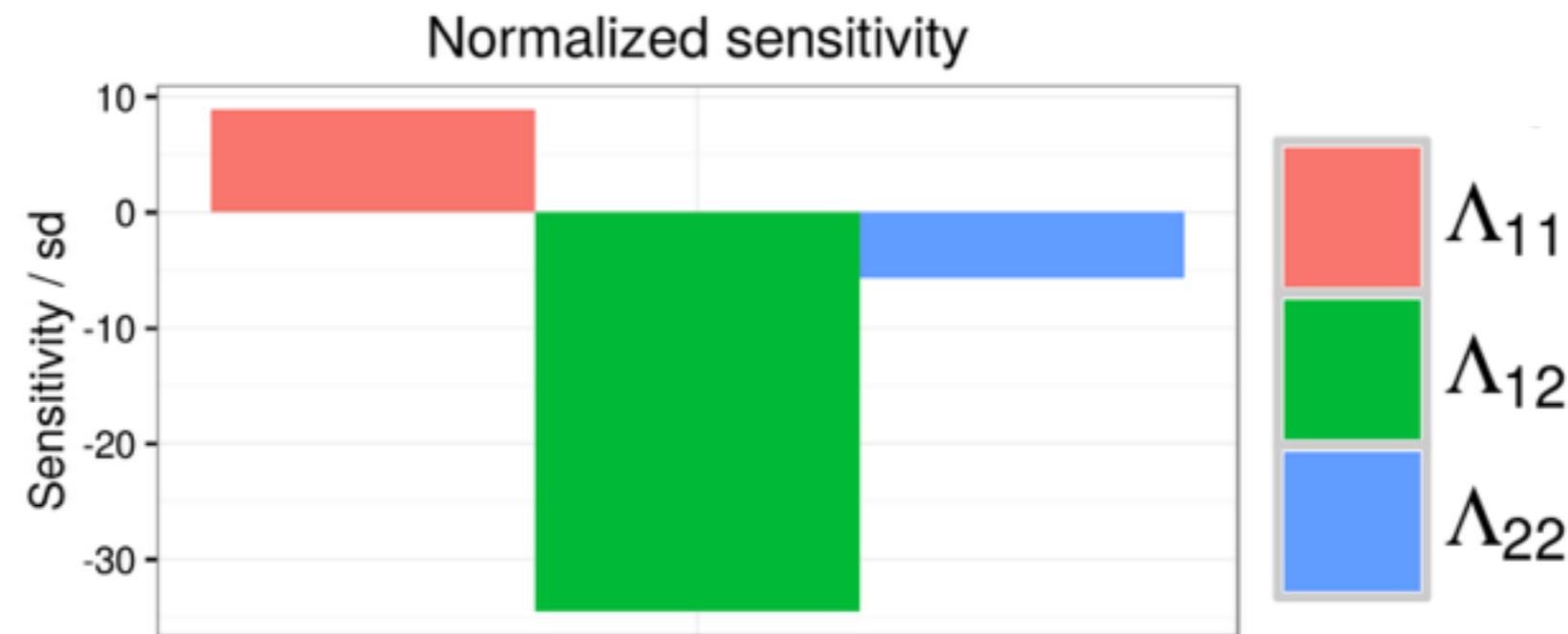
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Microcredit Experiment

- Sensitivity of the expected microcredit effect (τ)
- Normalized to be on scale of τ std devs
- τ mean (MFVB): 3.08 USD PPP
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- Mean is 1.68 std dev from 0
- $\Lambda_{11} += 0.04$
⇒ Mean > 2 std dev



Conclusions

- We provide *linear response variational Bayes*: supplements MFVB for fast & accurate **covariance** estimate
- More from LRVB: fast & accurate **robustness** quantification
- Interested in your data and models:
 - Sensitivity to prior perturbations
 - Sensitivity to likelihood, data perturbations

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