Variational Bayes and beyond: Bayesian inference for big data

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Assistant Professor,
MIT

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

Bayesian inference

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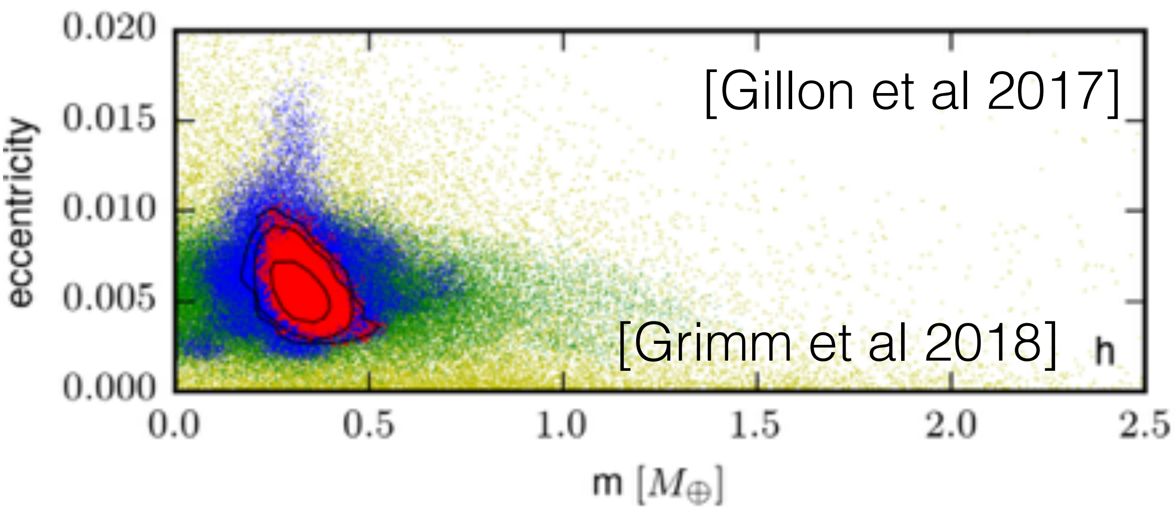

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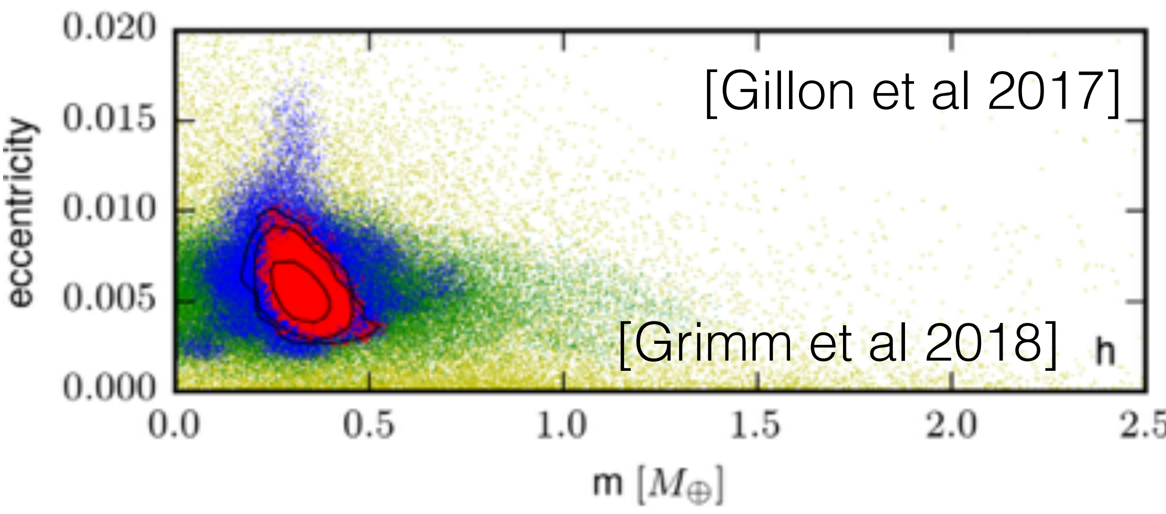

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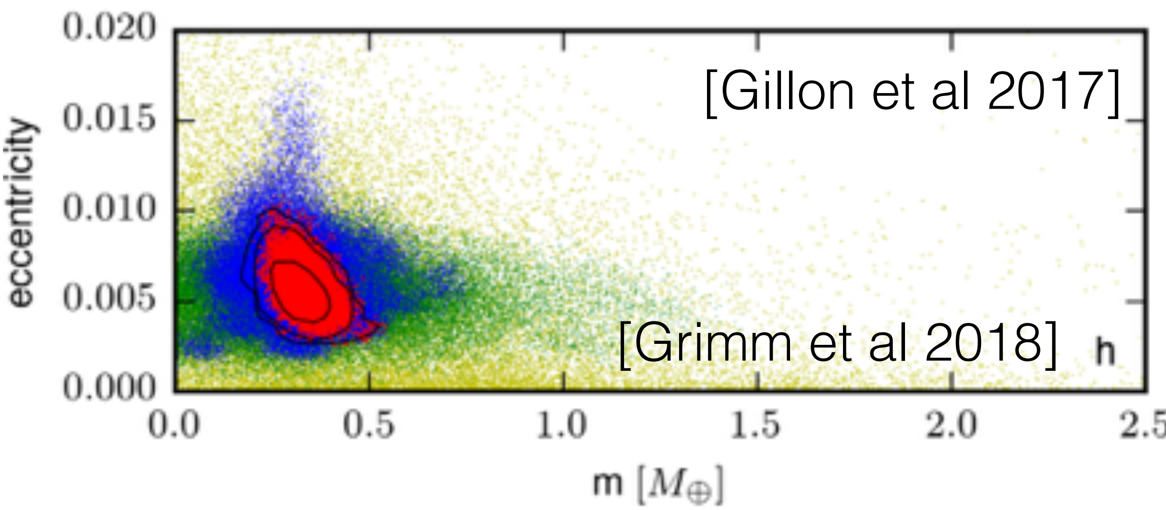

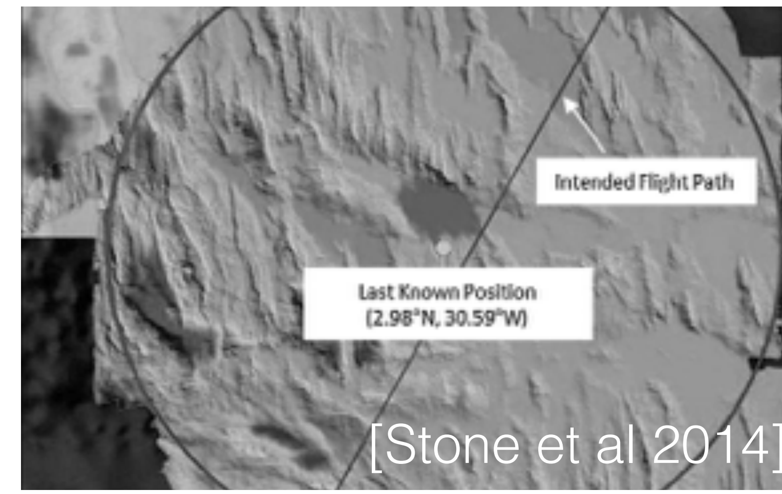

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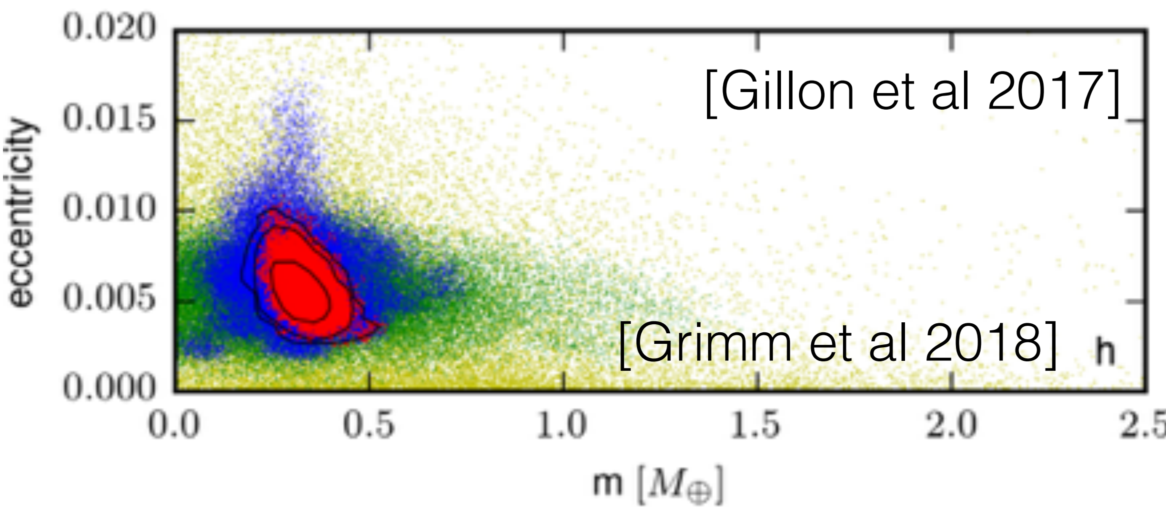

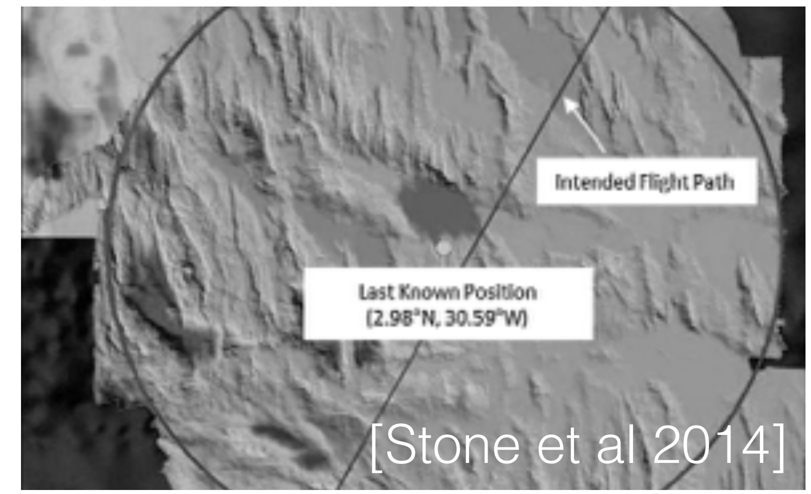

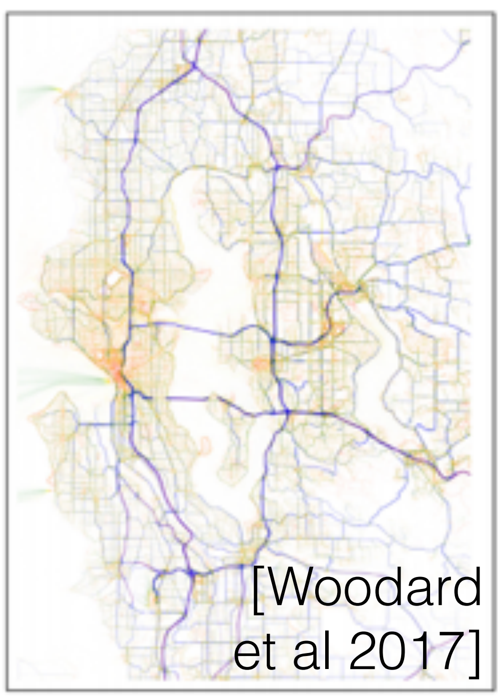

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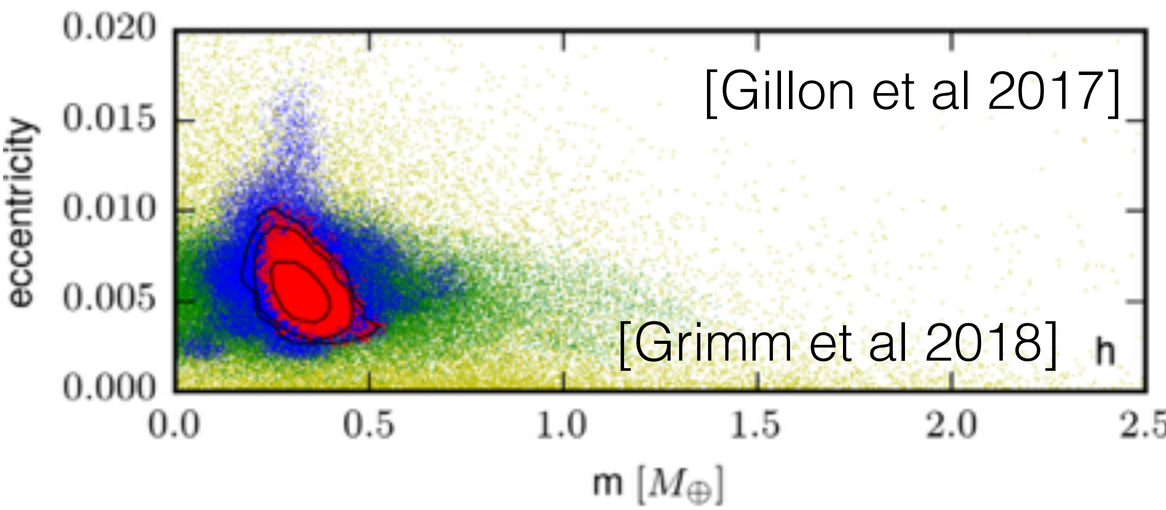

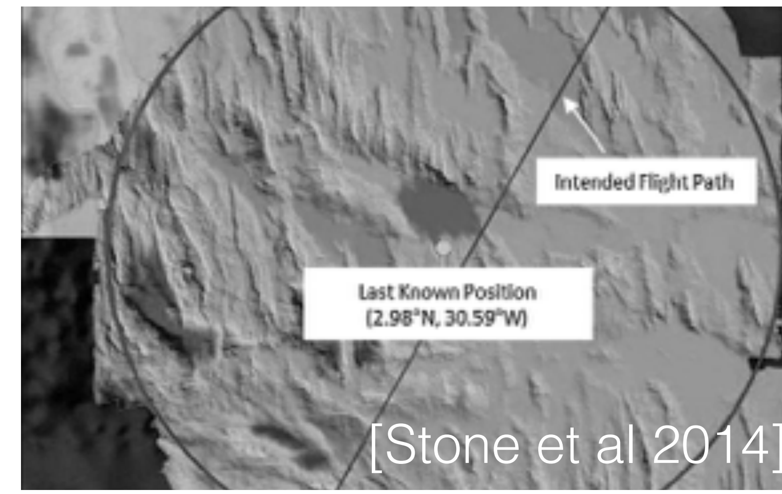

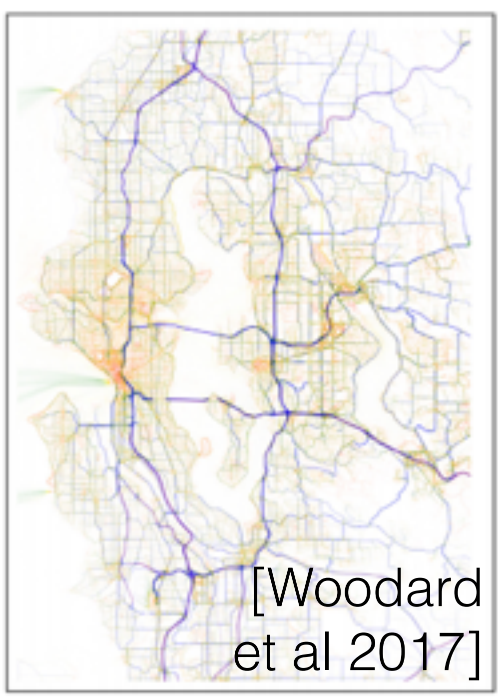

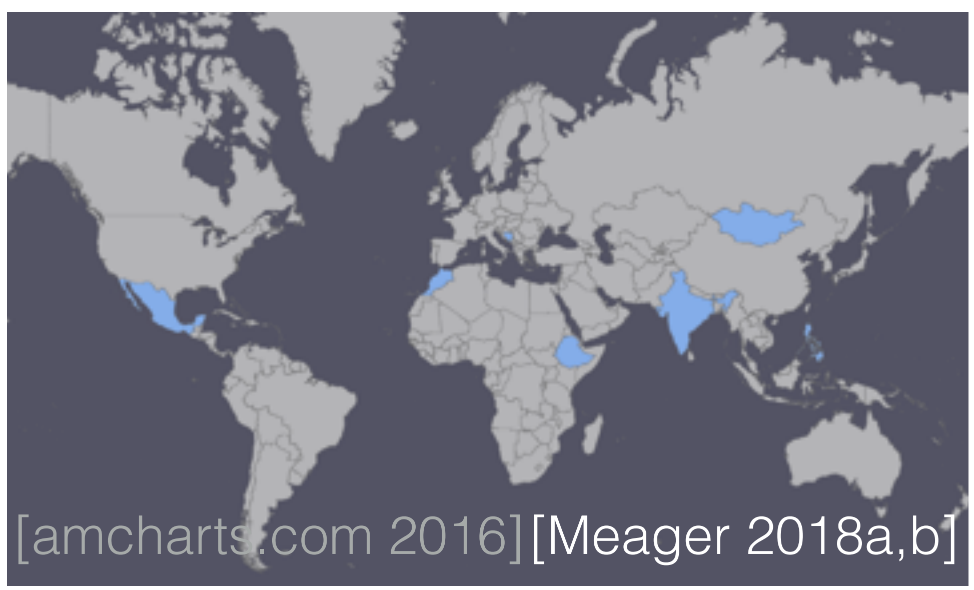

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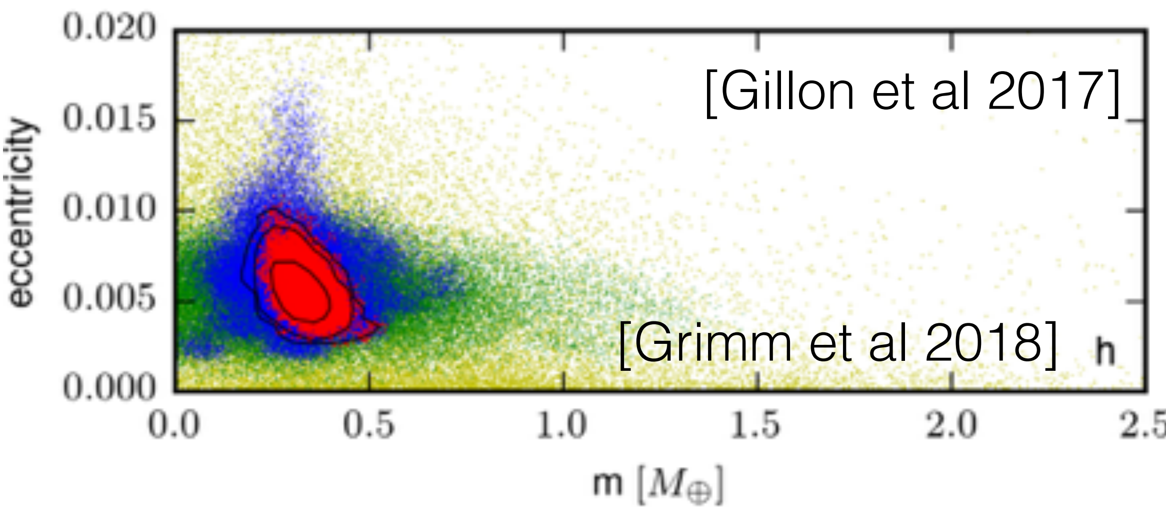

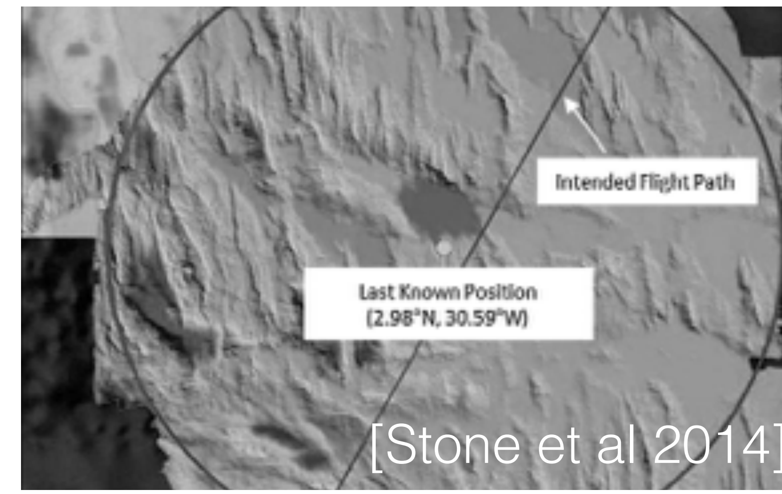

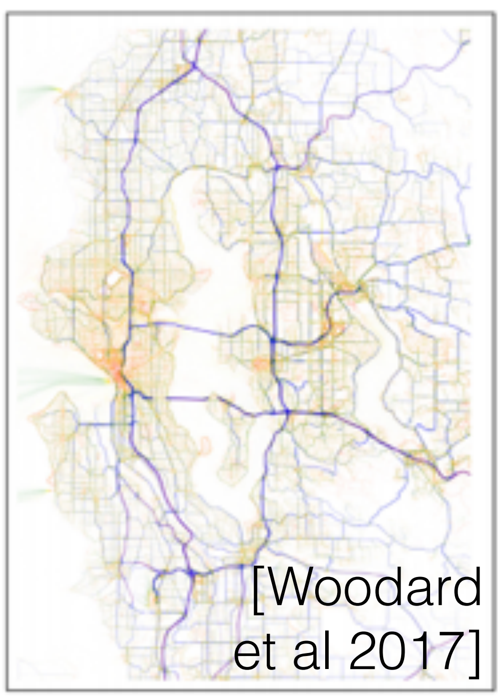

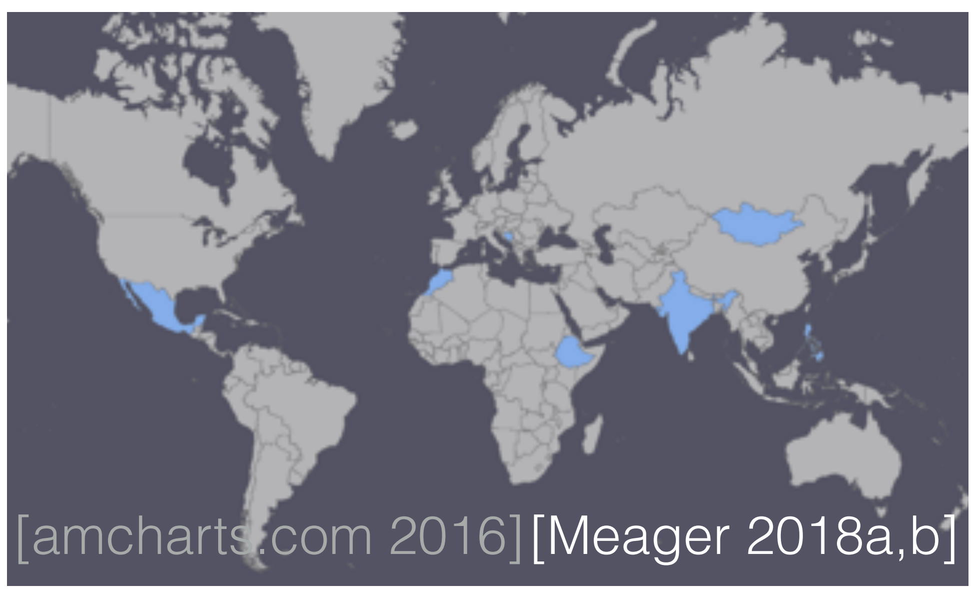

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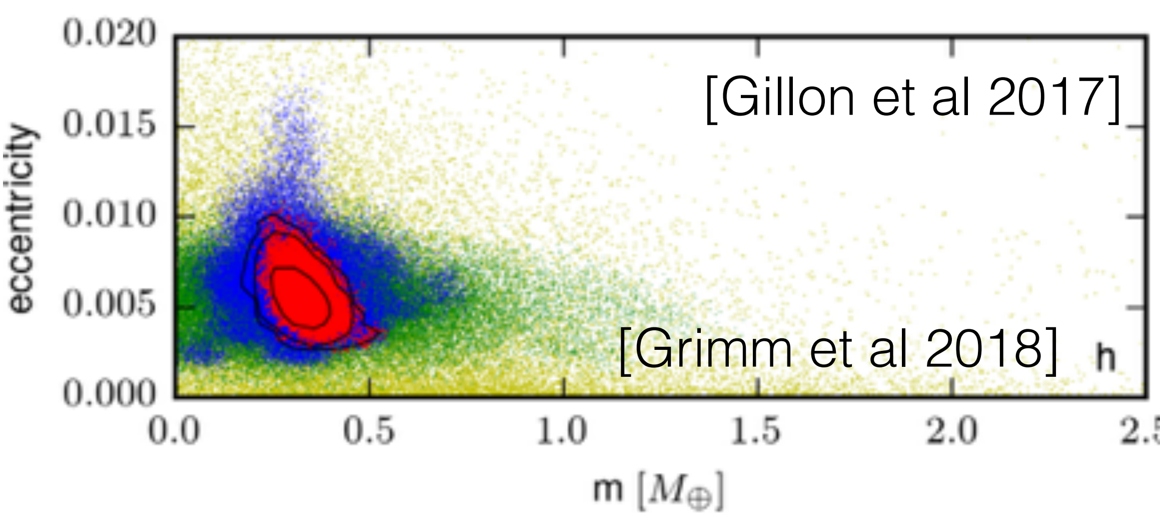
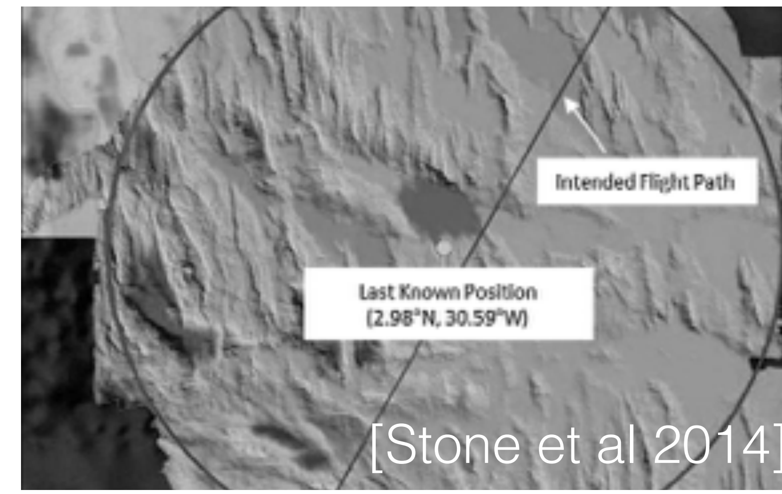
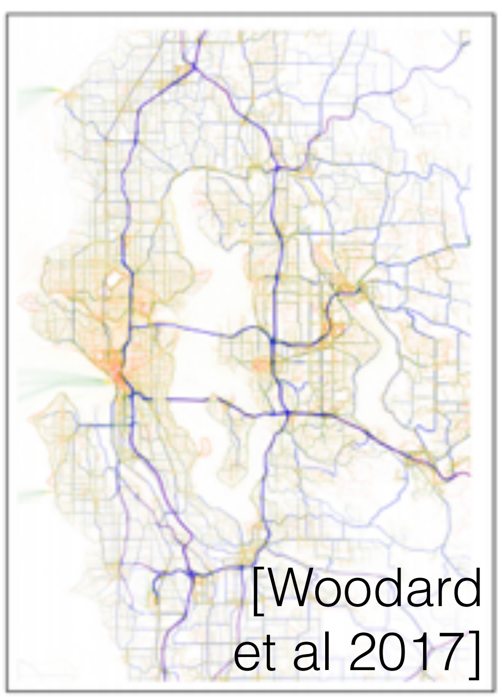
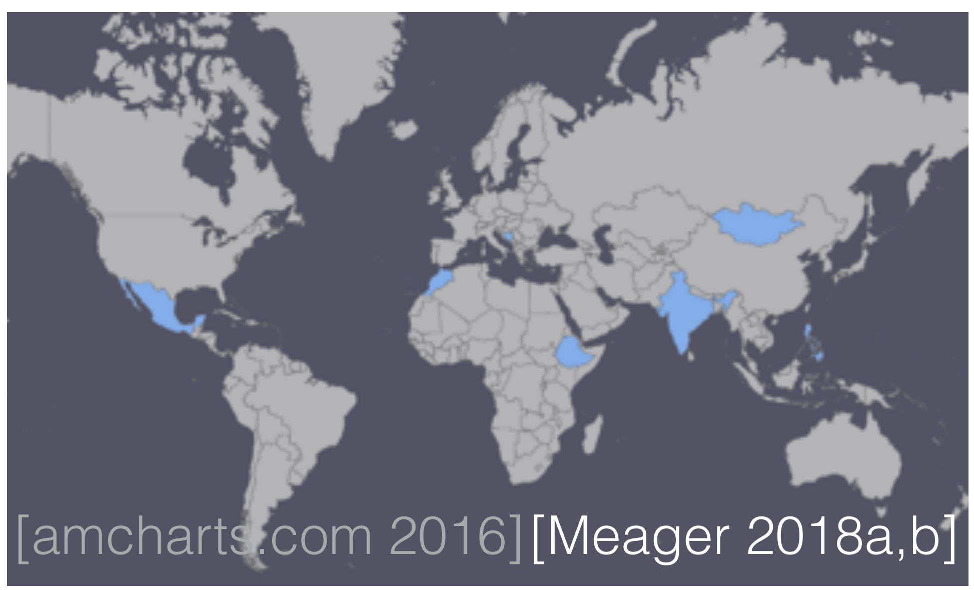


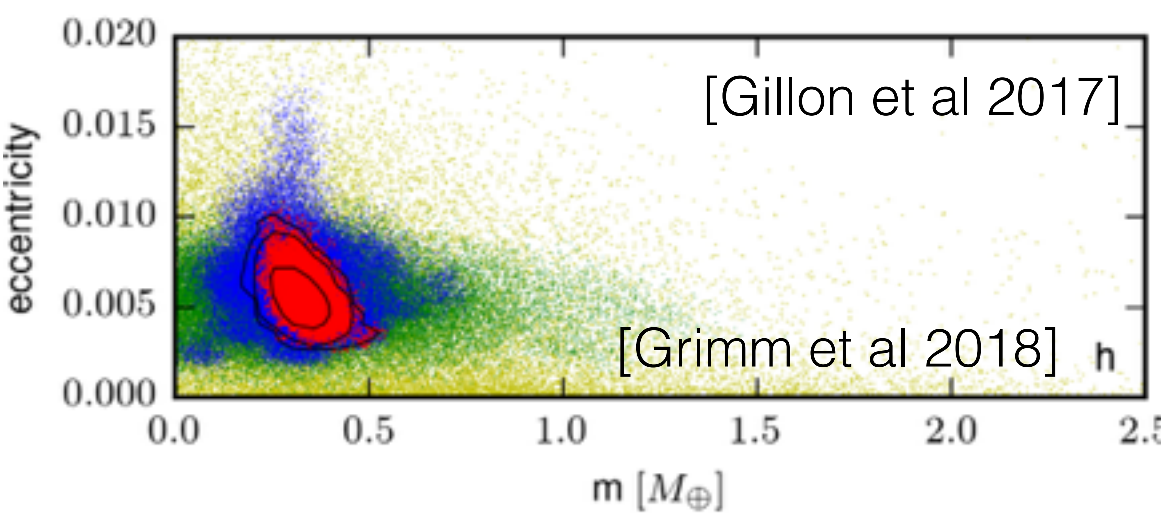


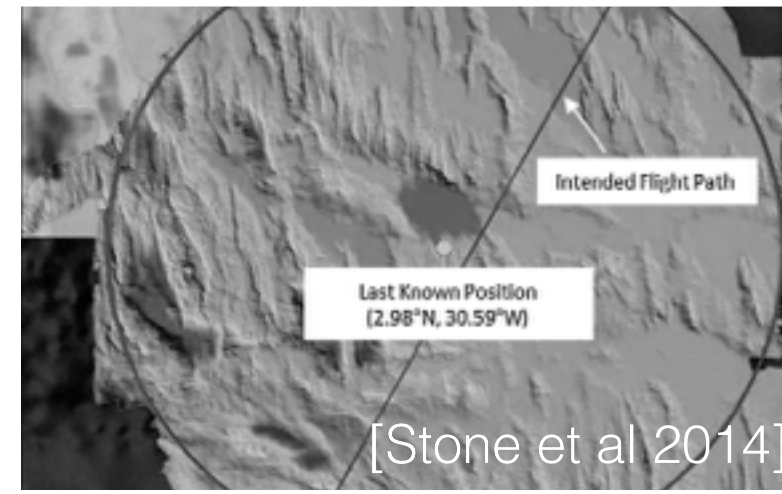


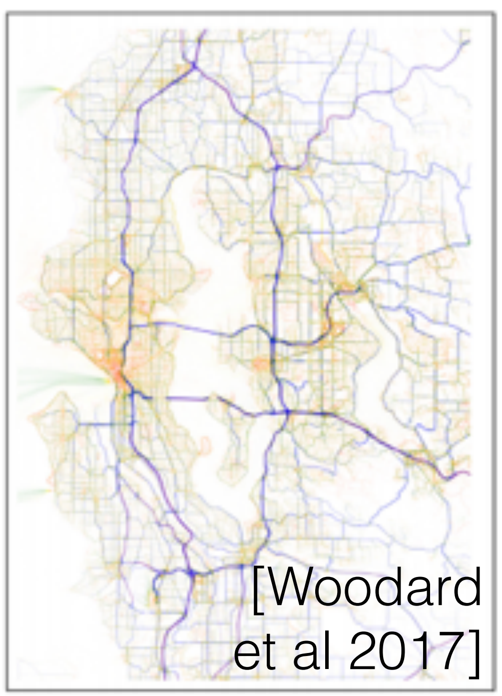


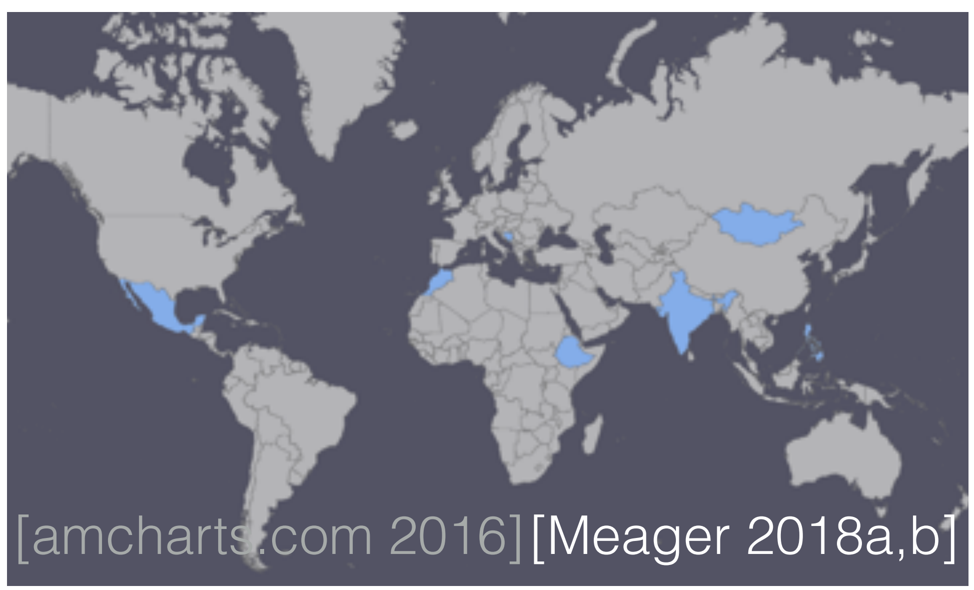
Bayesian inference

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









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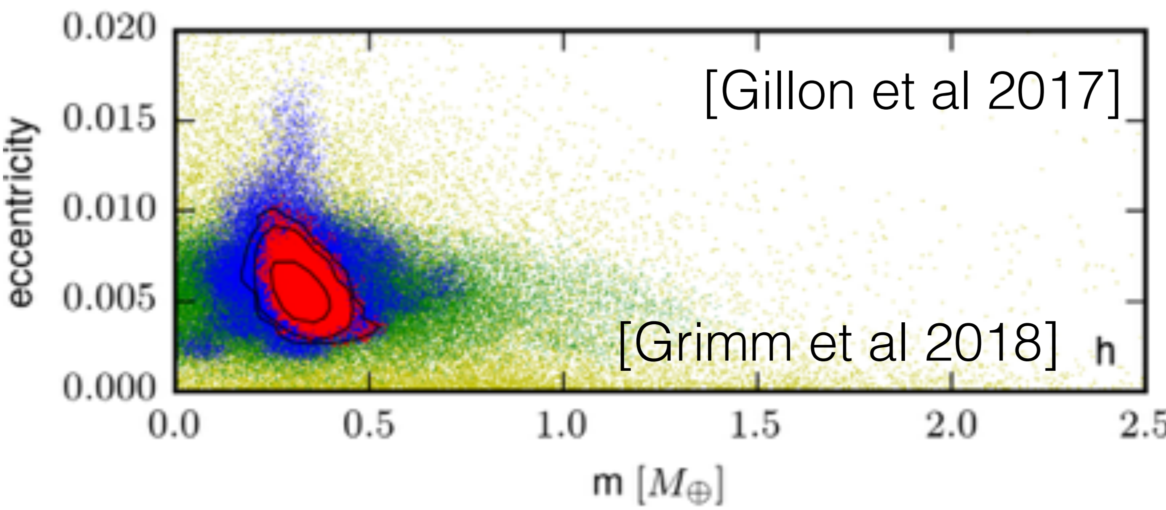
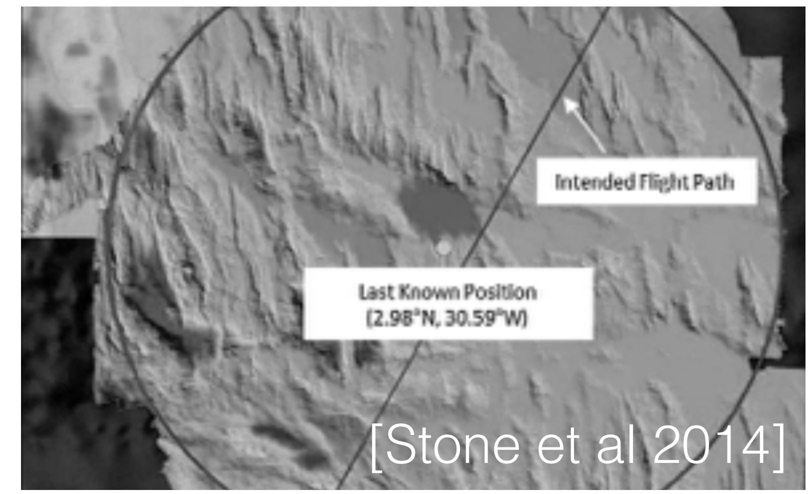


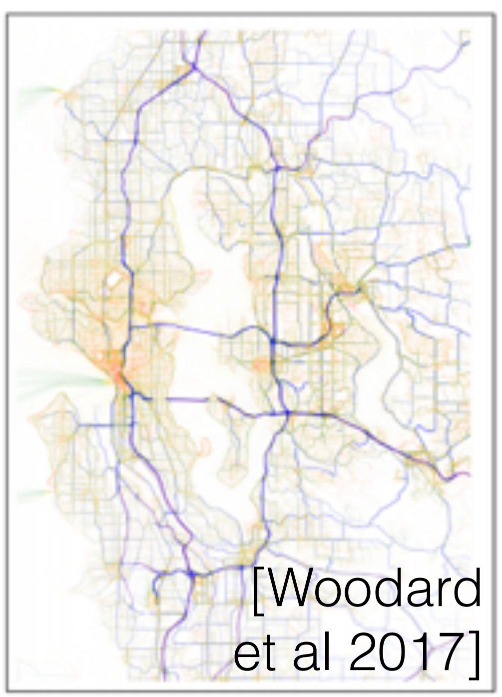
[Gillon et al 2017]

[Grimm et al 2018]

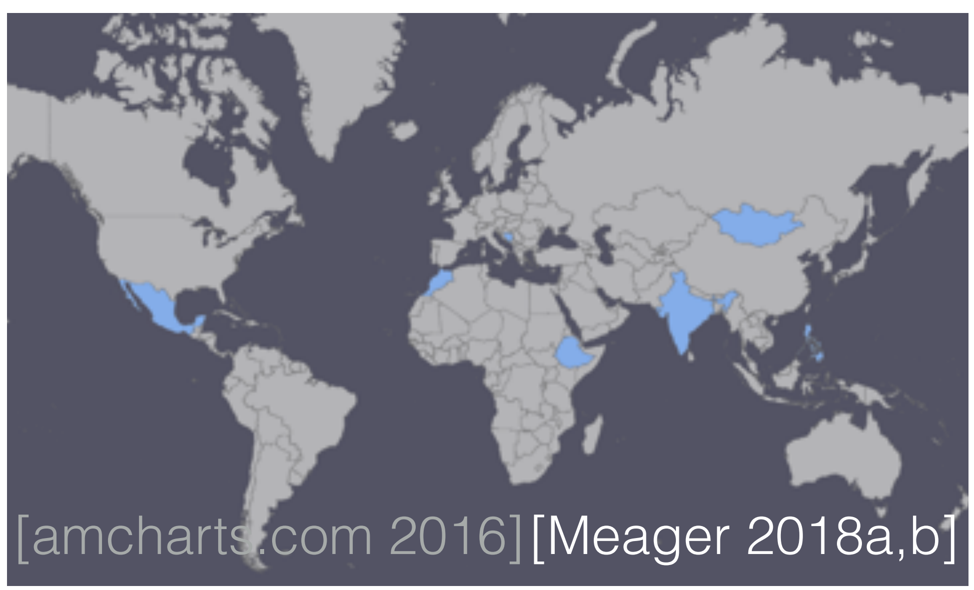
[ESO/ L. Calçada/ M. Kornmesser 2017] [Abbott et al 2016a,b]



[Stone et al 2014]



[Woodard et al 2017]



[amcharts.com 2016] [Meager 2018a,b]

[Kuikka et al 2014]
[Baltic Salmon Fund]

[Chati, Balakrishnan 2017]
[Julian Hertzog 2016]

[mc-stan.org]

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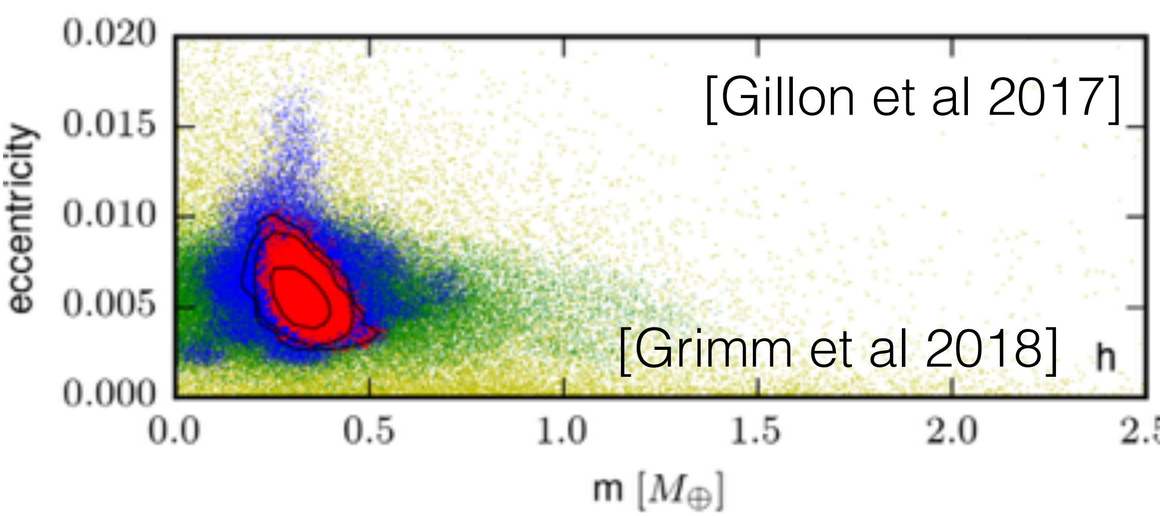

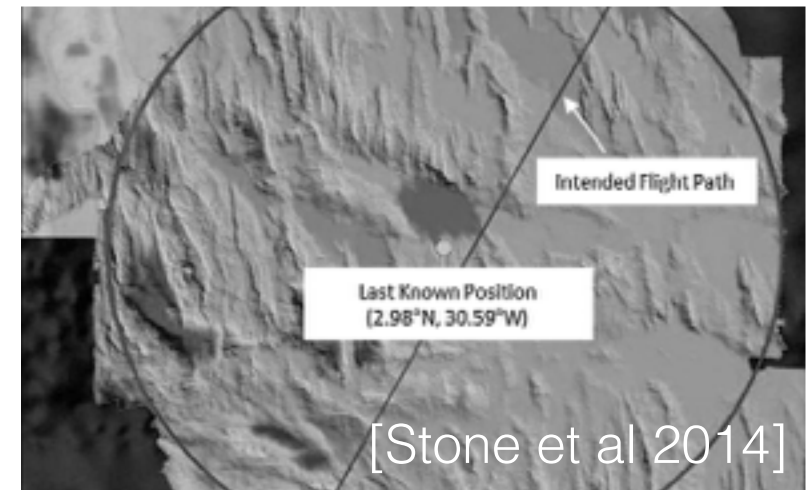

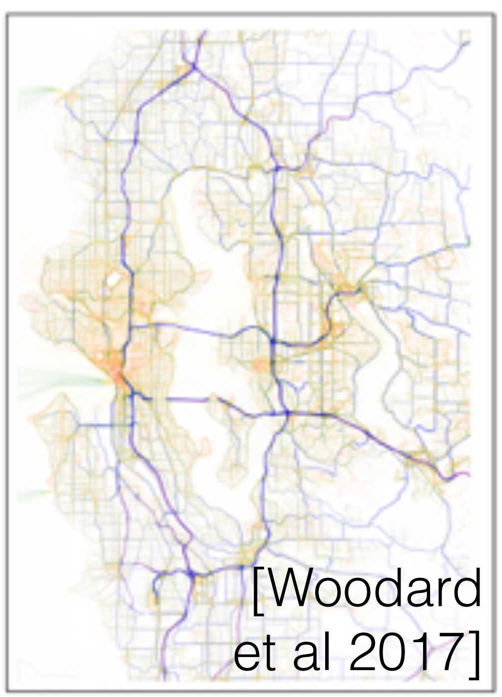

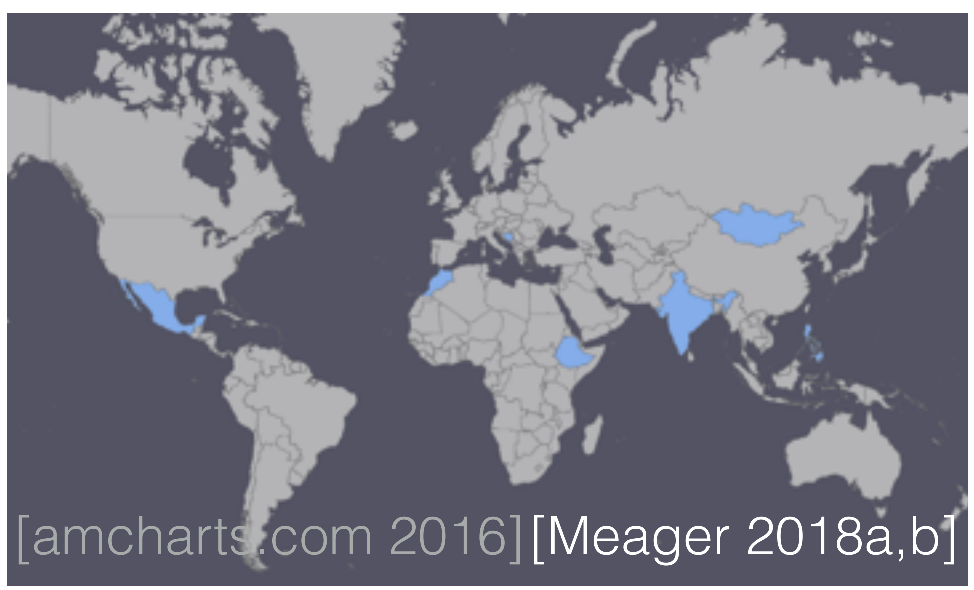

[mc-stan.org]

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

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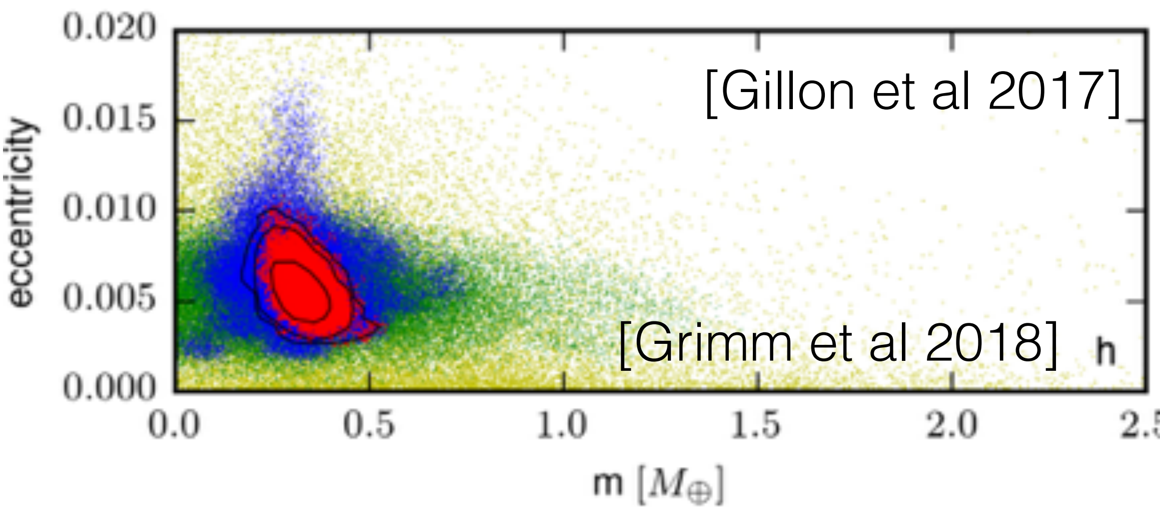

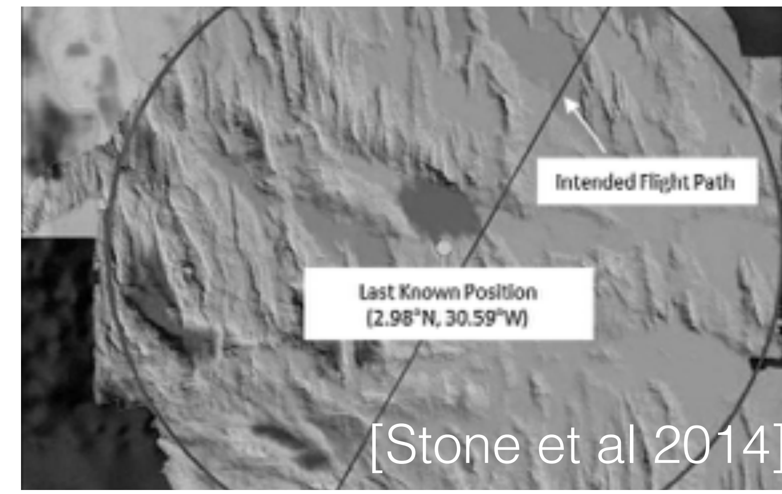

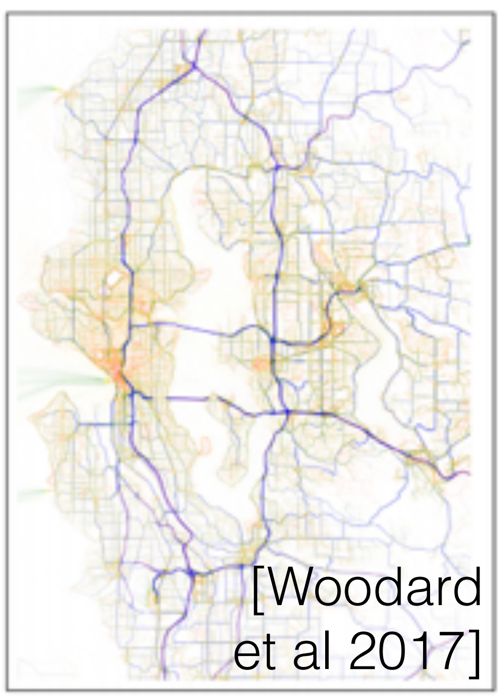

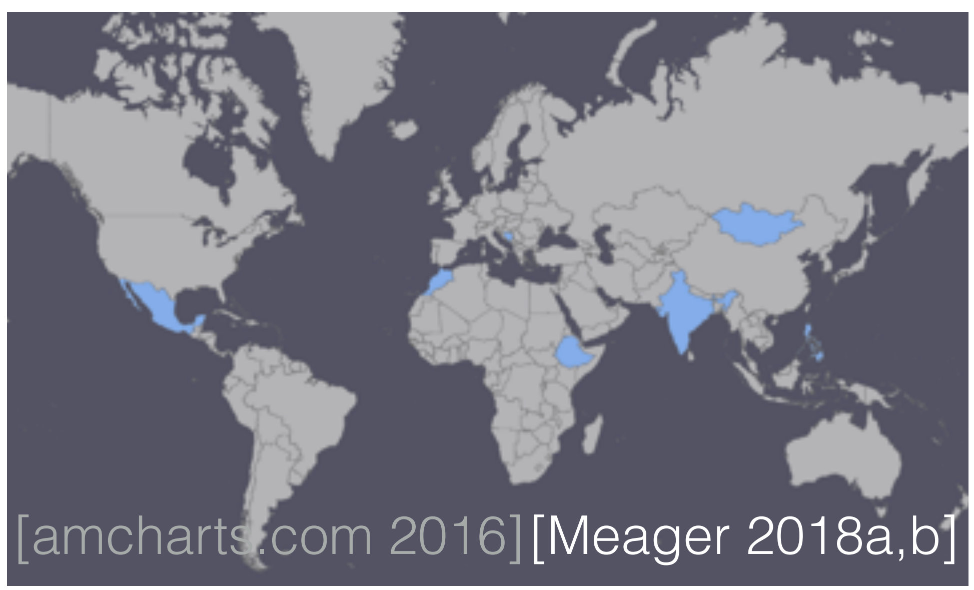

[mc-stan.org]

- Challenge: fast (compute, user), reliable inference
- Uncertainty doesn't have to disappear in large data sets

Variational Bayes

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- Modern problems: often large data, large dimensions

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[Blei et al 2003]

The William Randolph Hearst Foundation will give $1.25 million to Lincoln Center, Metropolitan Opera Co., New York Philharmonic and Juilliard School. “Our board felt that we had a real opportunity to make a mark on the future of the performing arts with these grants an act every bit as important as our traditional areas of support in health, medical research, education and the social services,” Hearst Foundation President Randolph A. Hearst said Monday in announcing the grants. Lincoln Center’s share will be $200,000 for its new building, which will house young artists and provide new public facilities. The Metropolitan Opera Co. and New York Philharmonic will receive $400,000 each. The Juilliard School, where music and the performing arts are taught, will get $250,000. The Hearst Foundation, a leading supporter of the Lincoln Center Consolidated Corporate Fund, will make its usual annual $100,000 donation, too.

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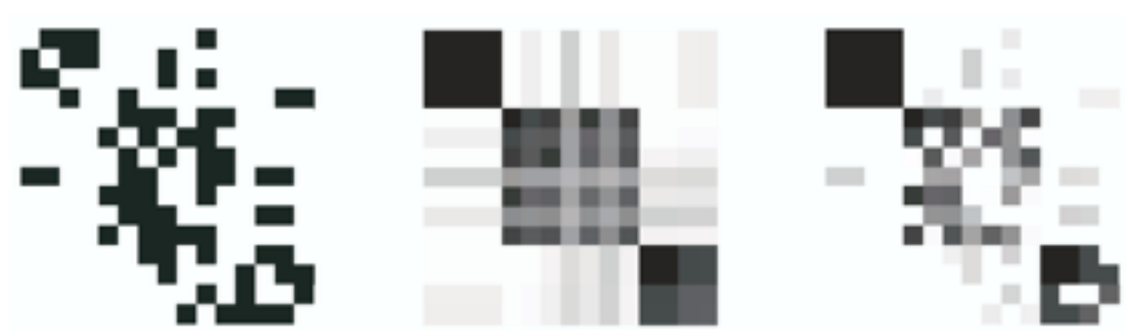

[Airoldi et al 2008]

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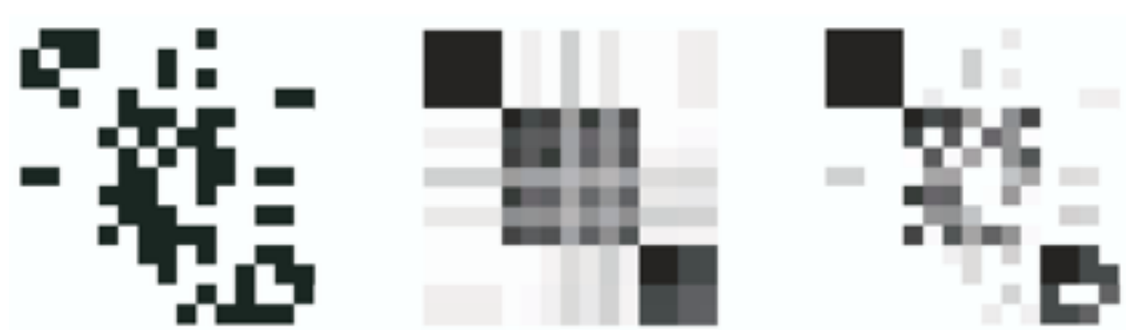

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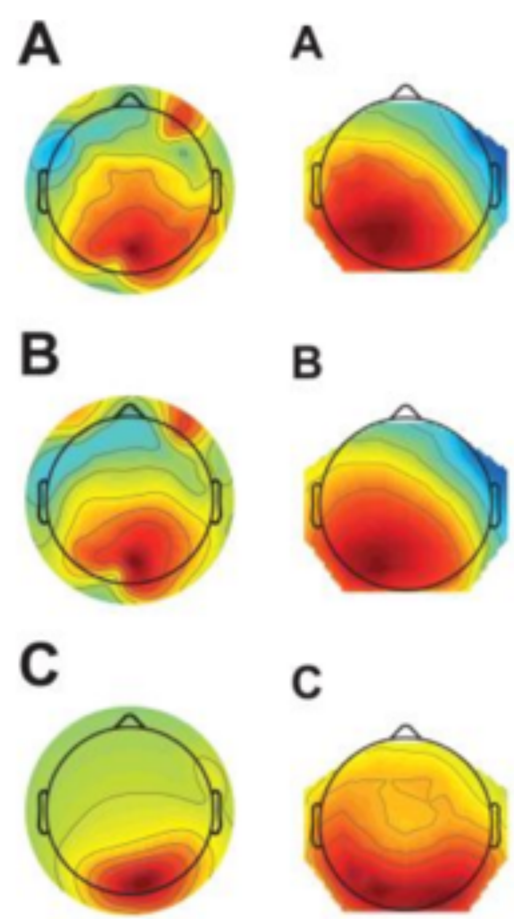

[Gershman et al 2014]

[Blei et al 2018]

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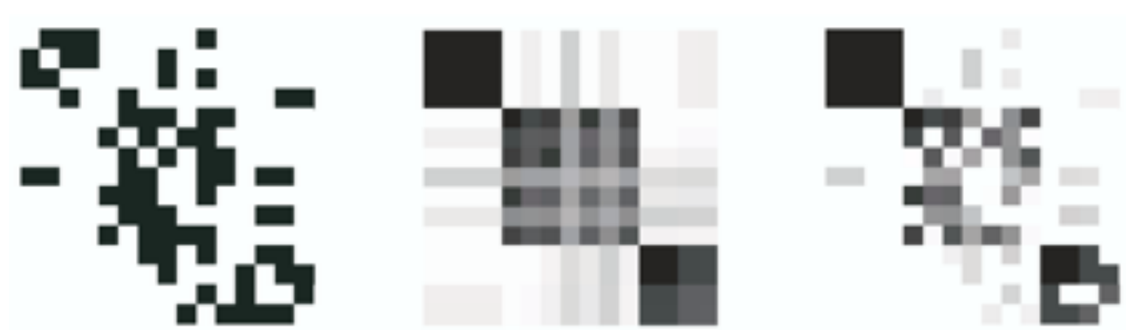

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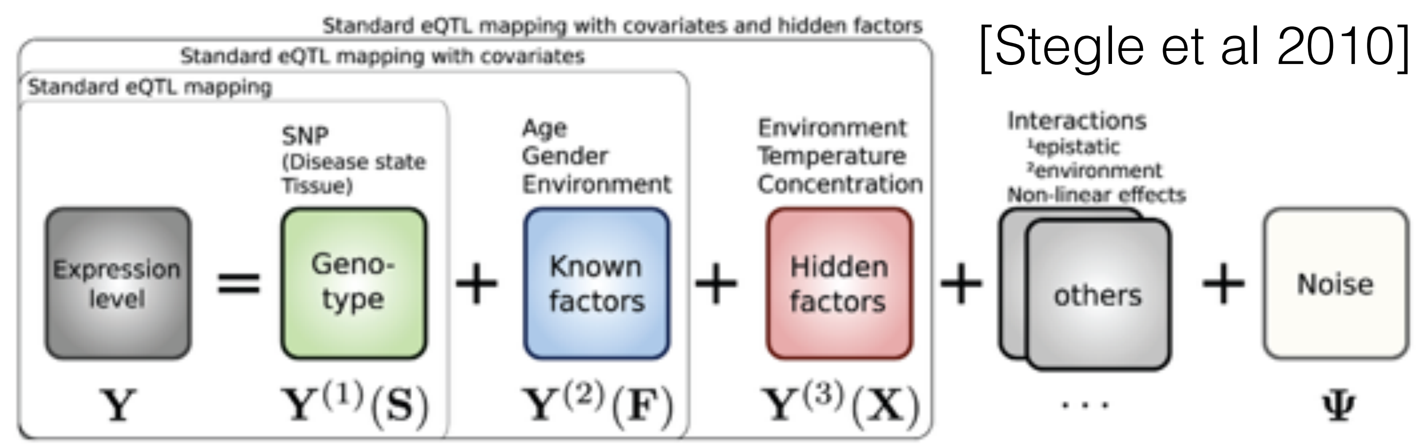
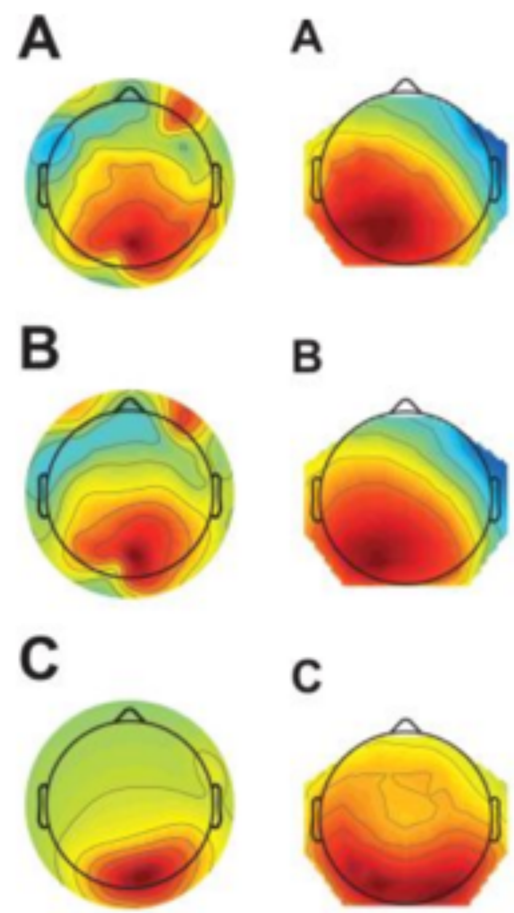


[Stegle et al 2010]



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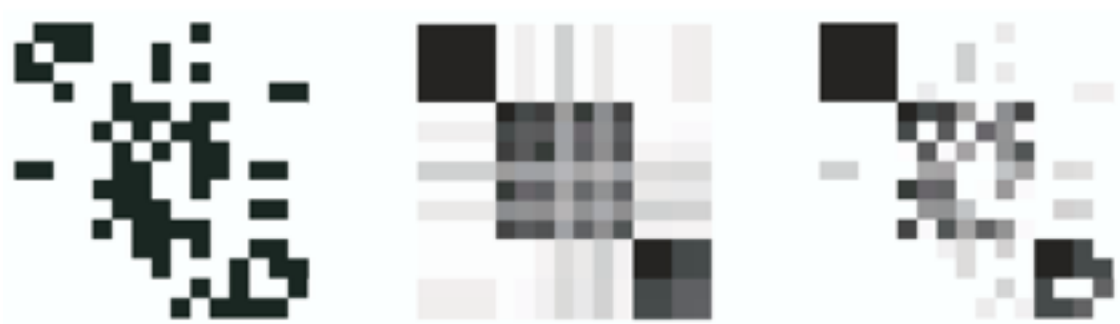

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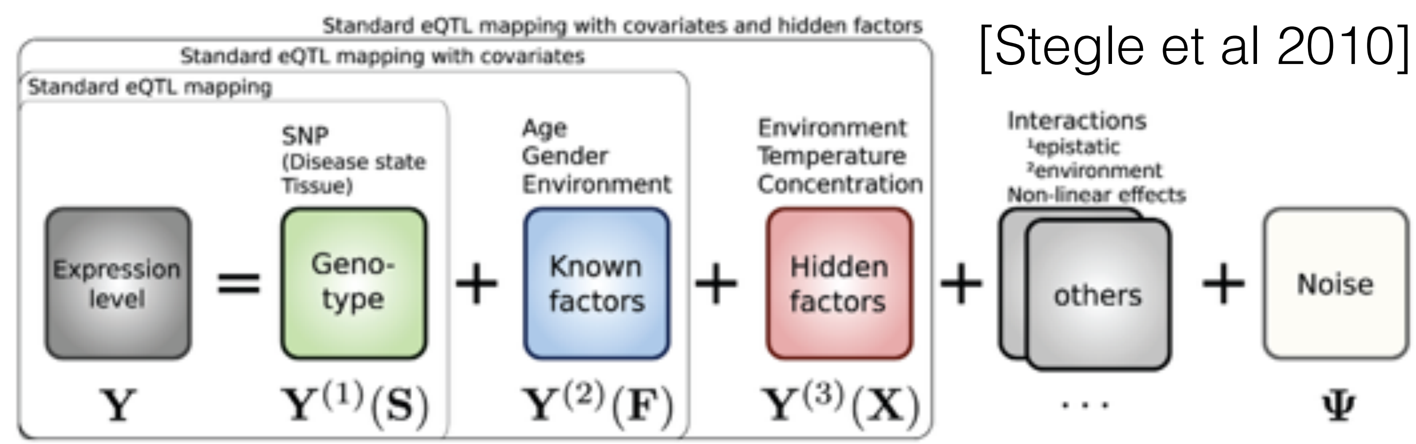

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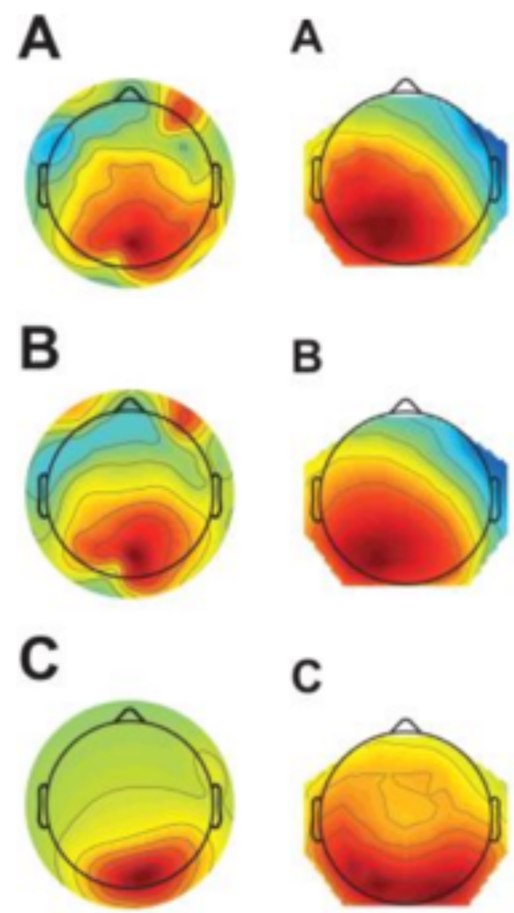

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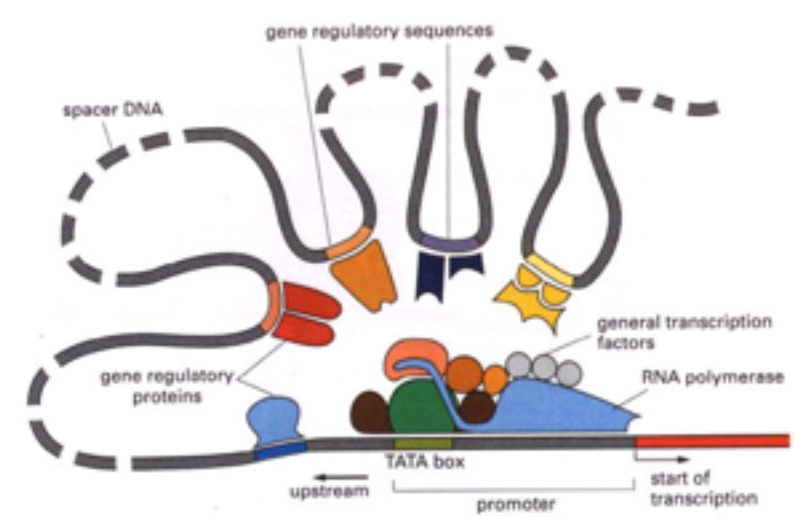

[Xing et al 2004]
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Roadmap

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

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parameters

$$p(\theta)$$

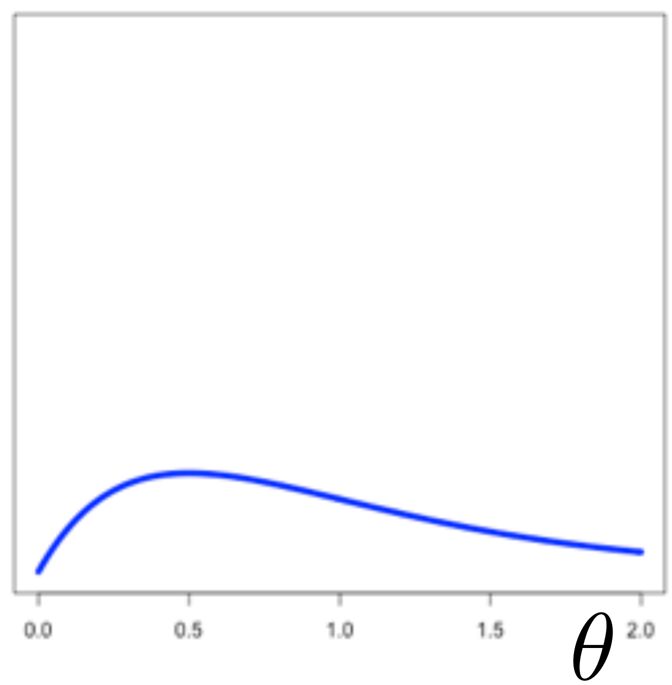
prior

Bayesian inference

parameters

$p(\theta)$

prior

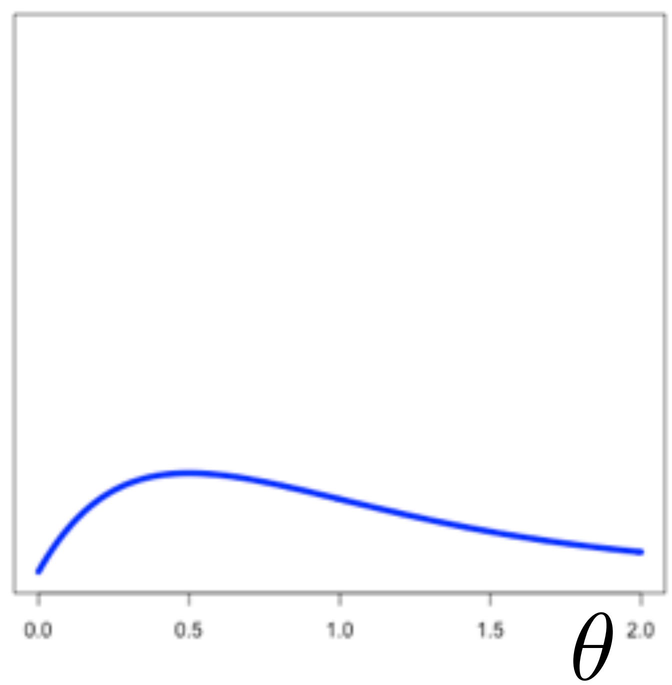


Bayesian inference

parameters

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

likelihood prior

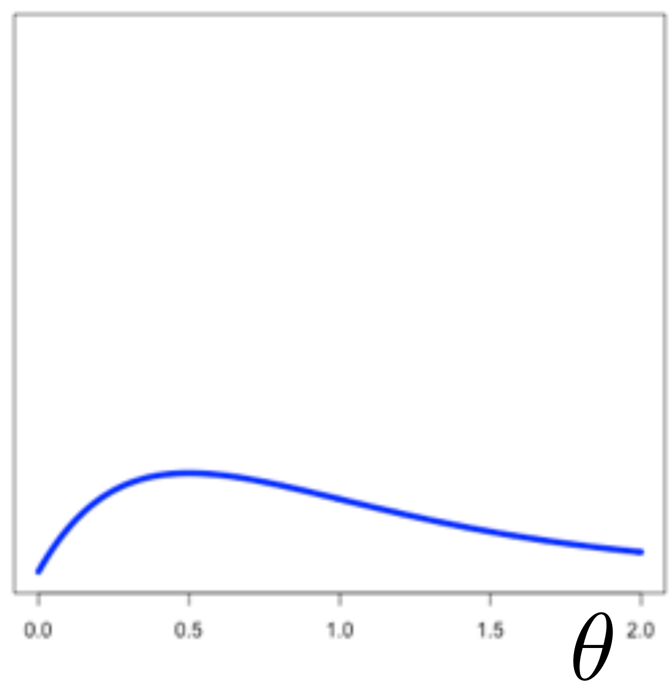


Bayesian inference

data parameters

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

likelihood prior

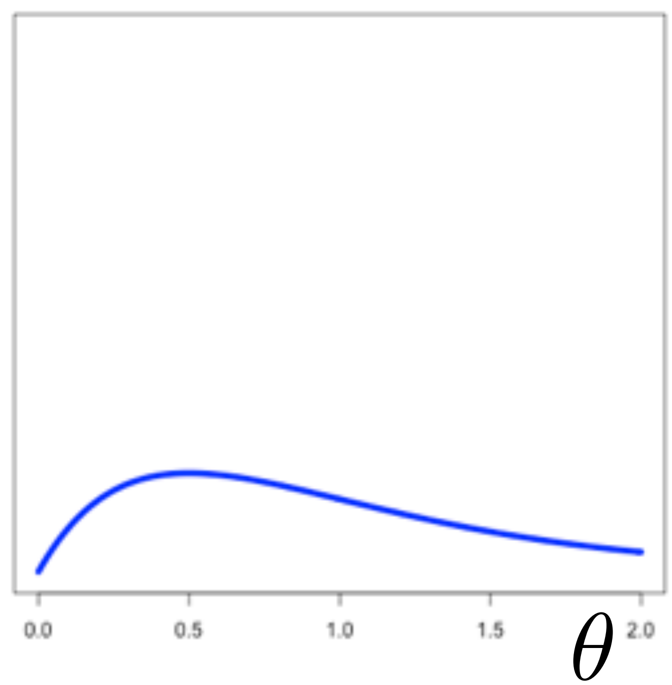


Bayesian inference

data parameters

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

posterior likelihood prior



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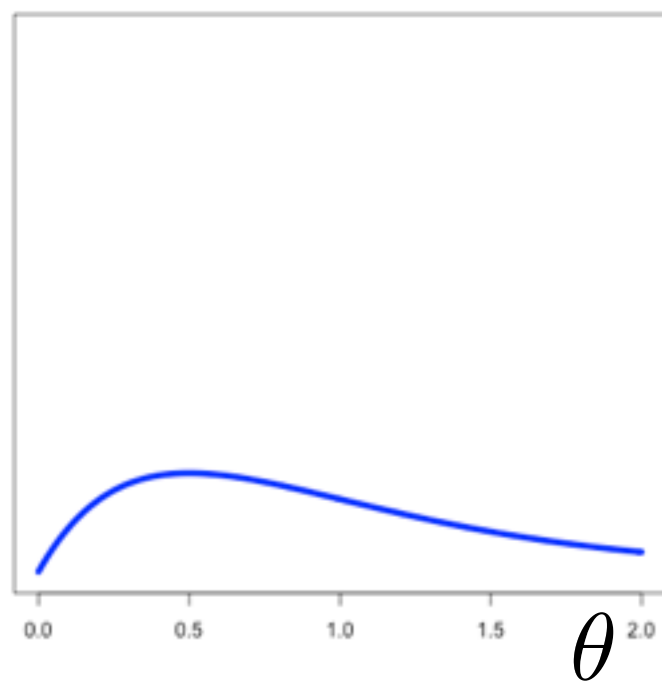

Bayes Theorem

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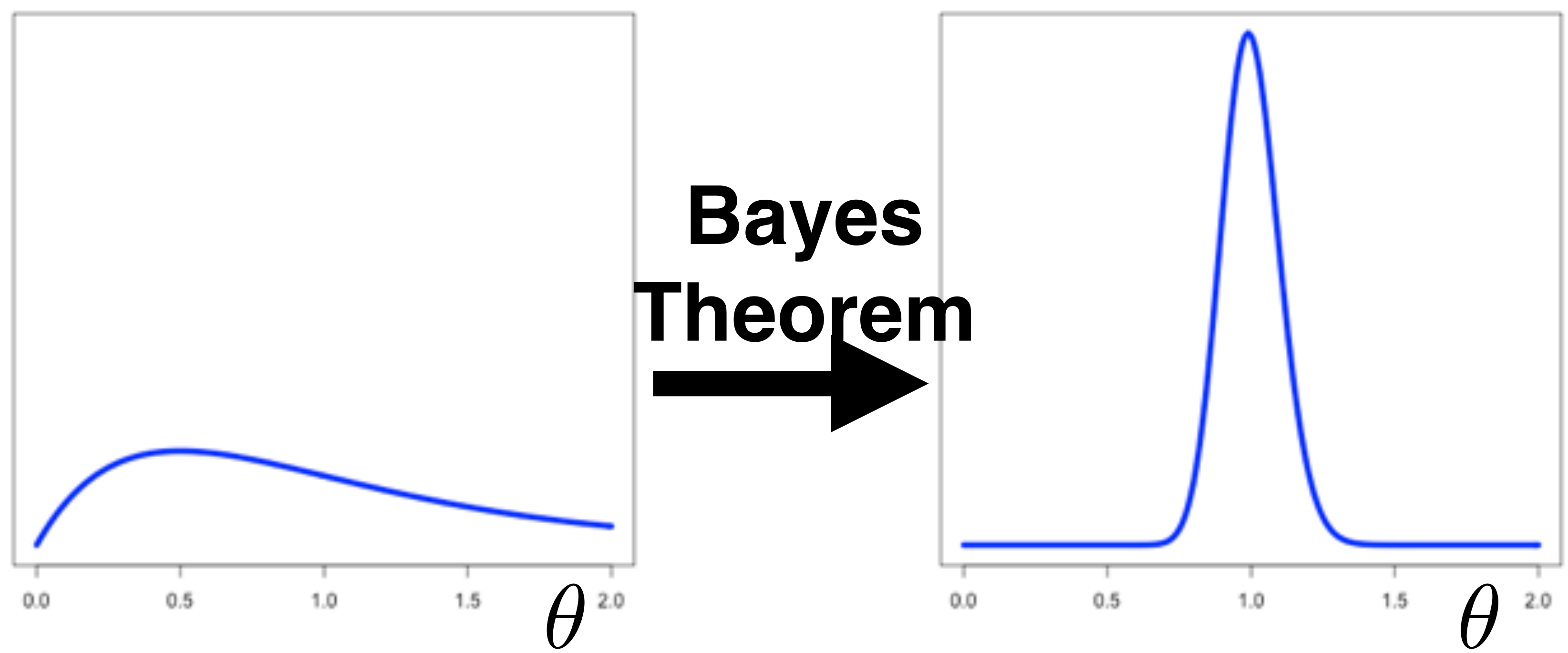

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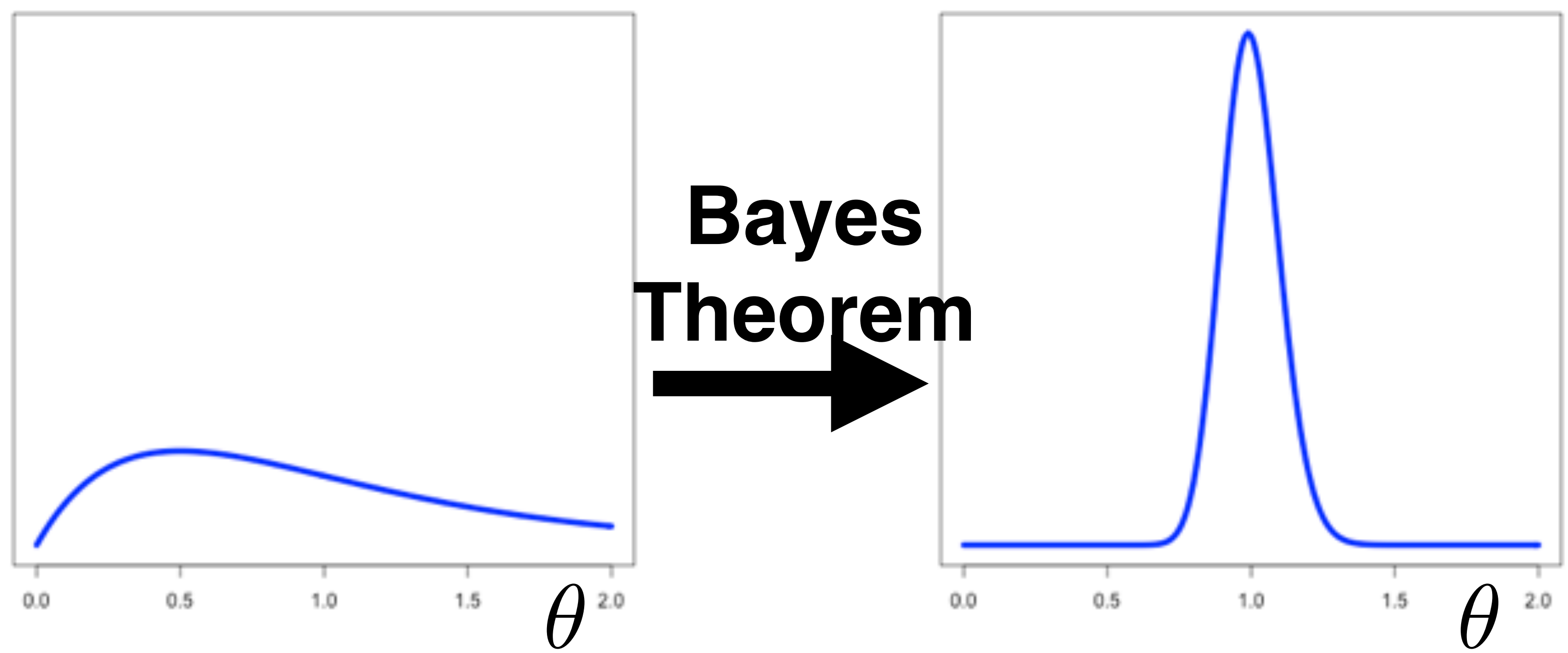

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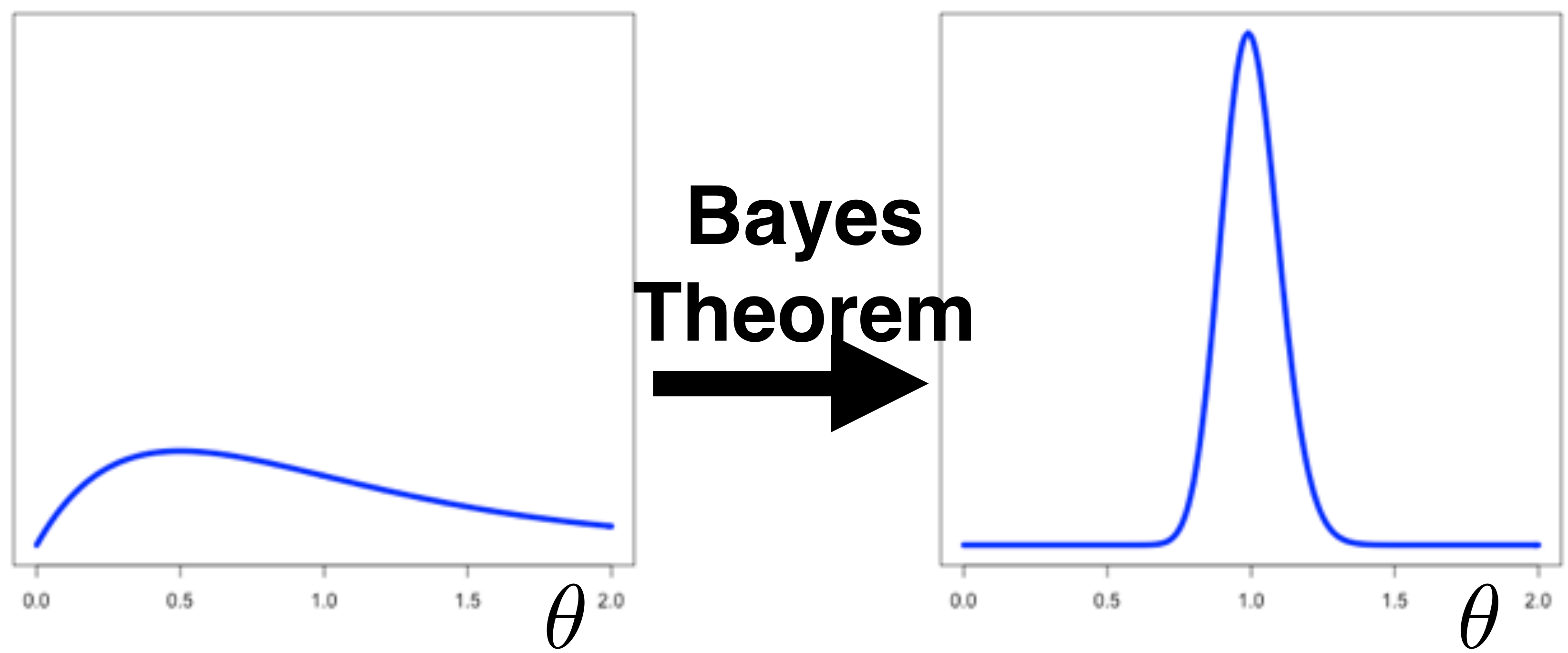

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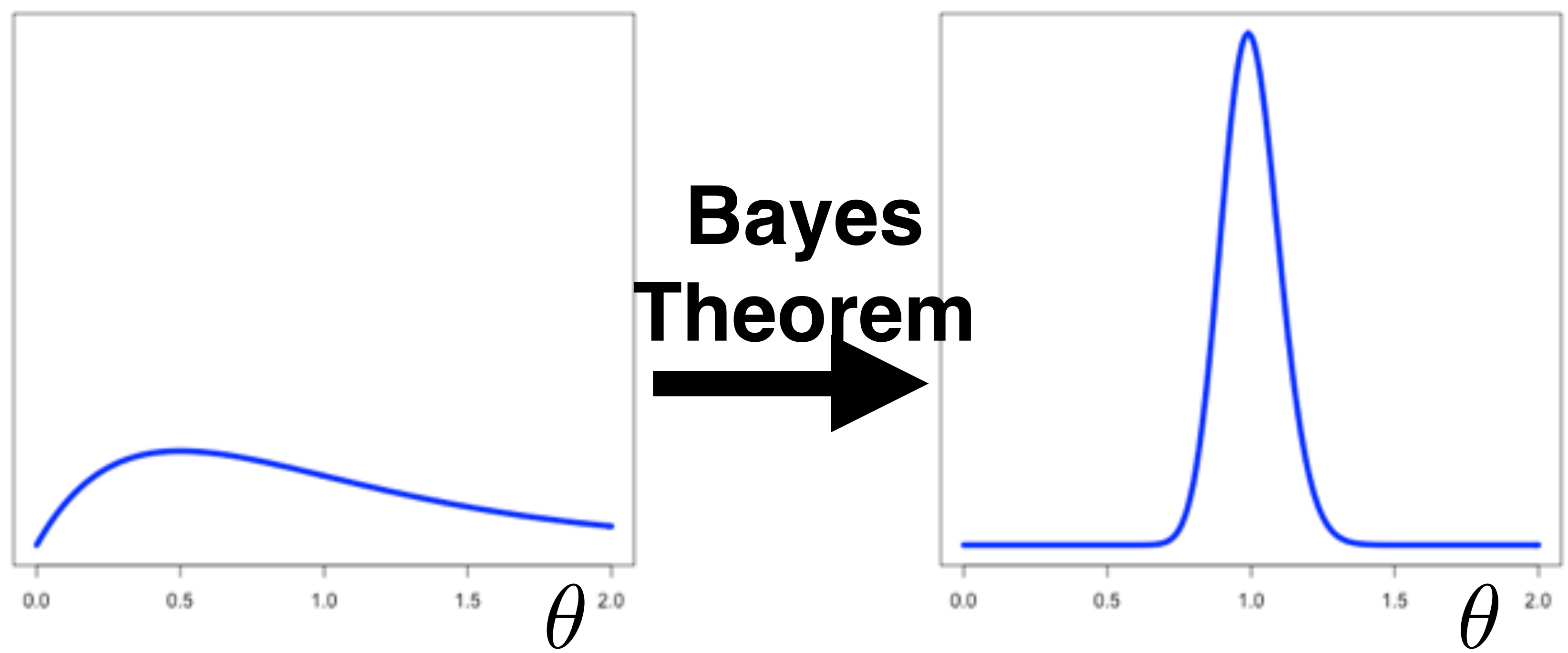

1. Build a model: choose prior & choose likelihood
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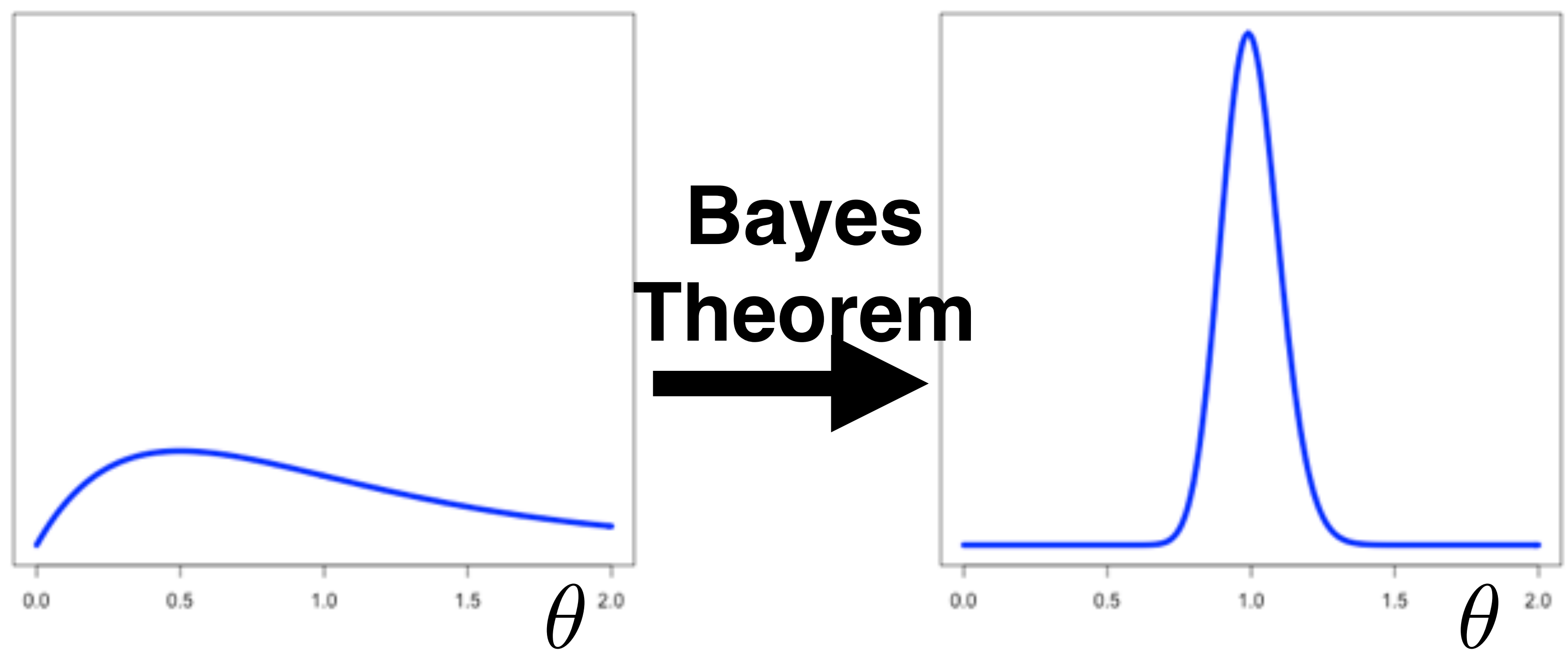

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- Why are steps 2 and 3 hard?

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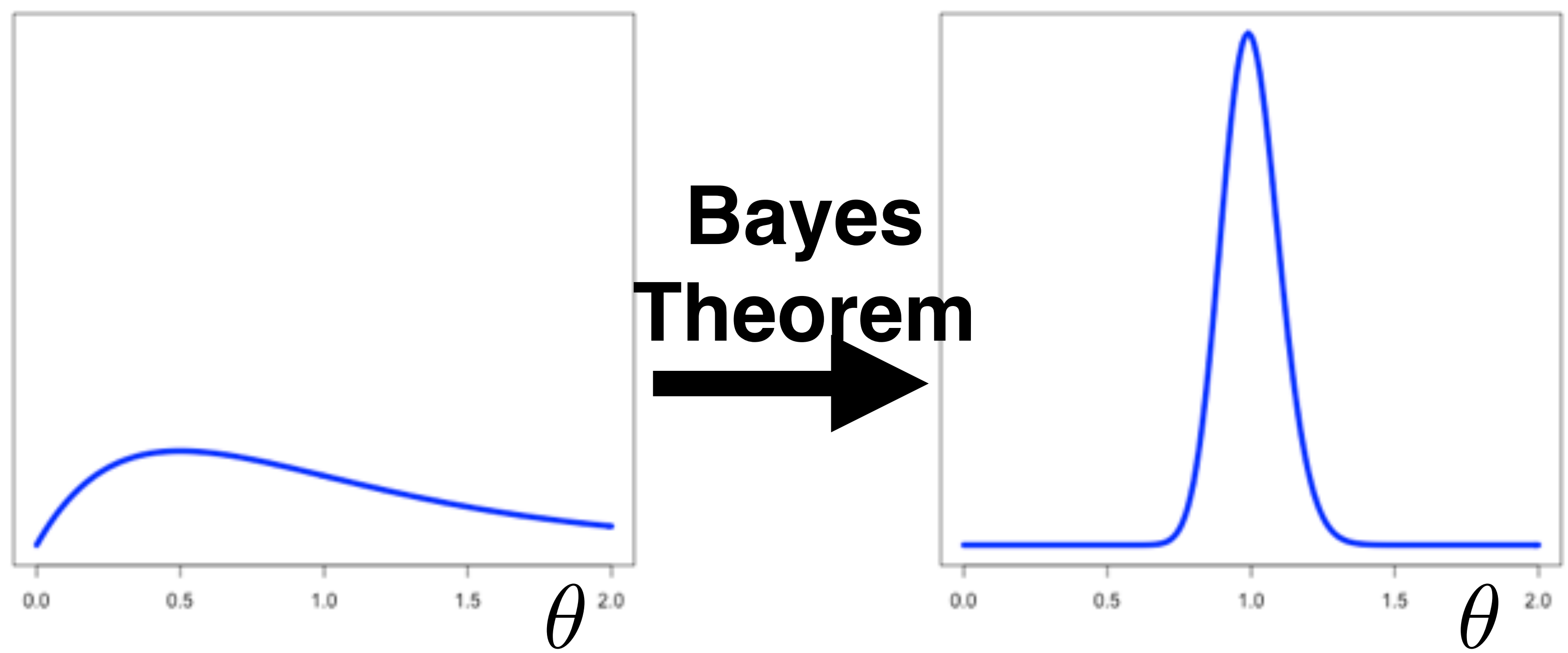

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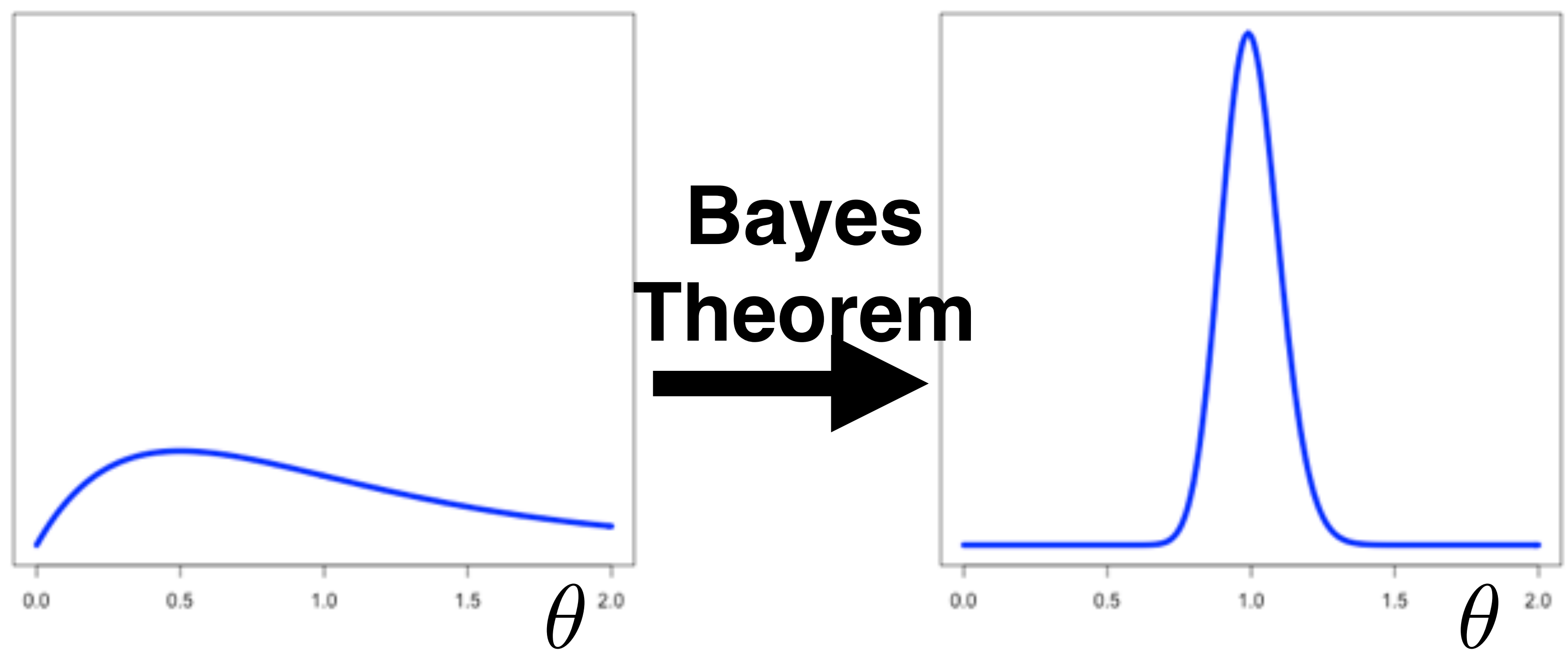

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Bayesian inference

data parameters

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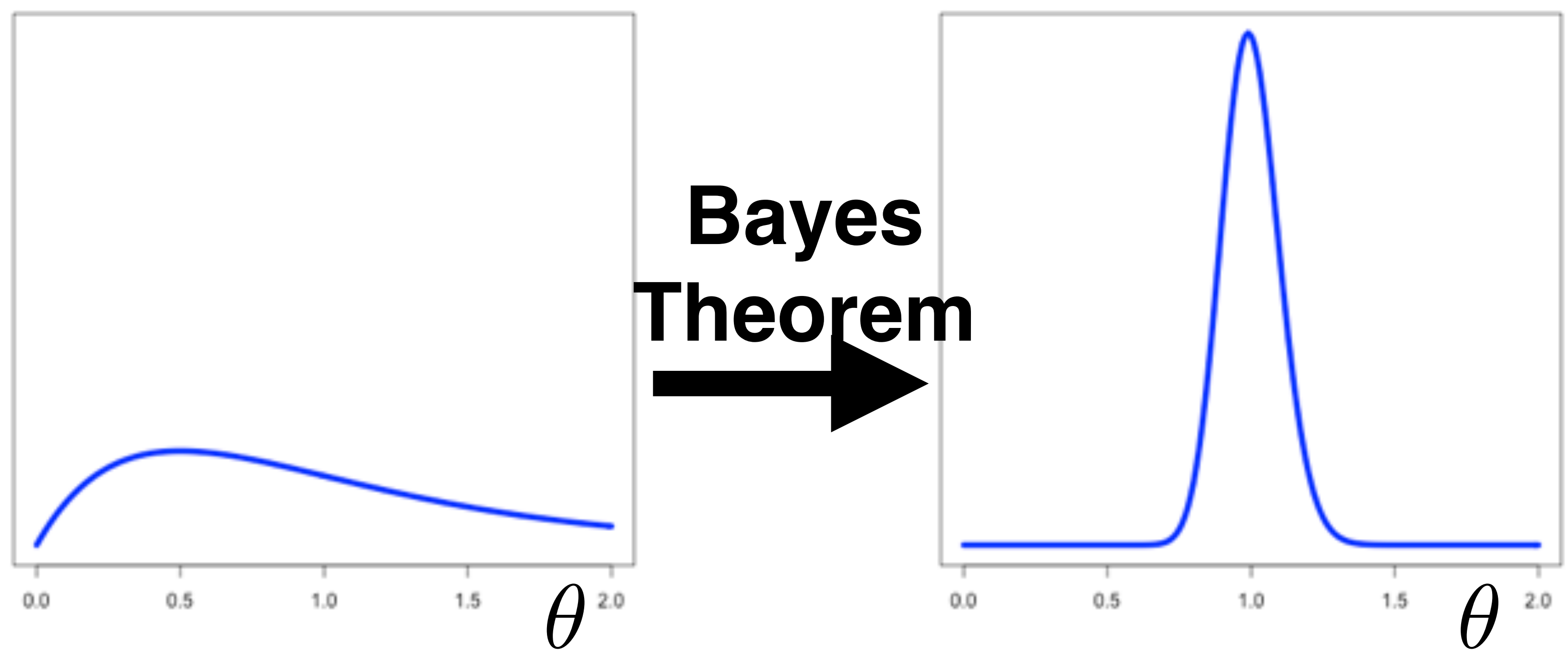
posterior likelihood prior



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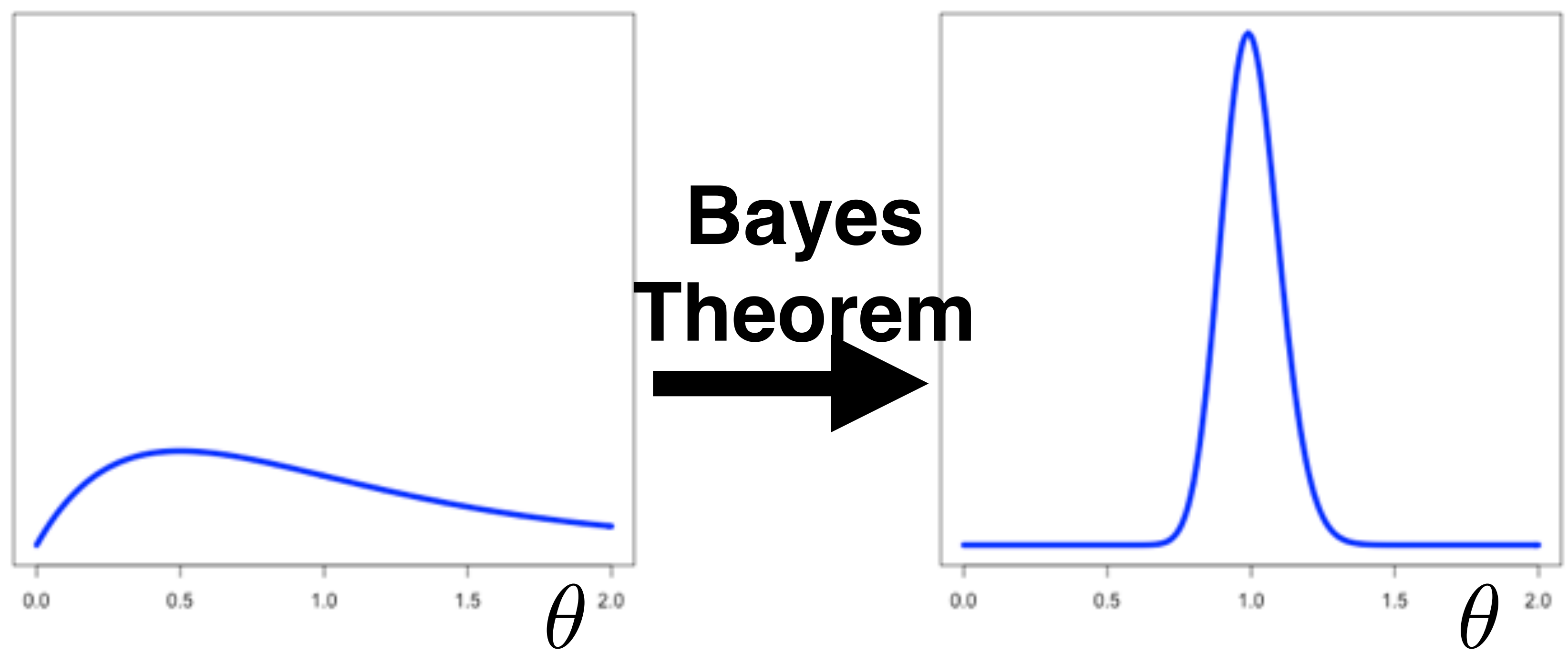

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Bayesian inference

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

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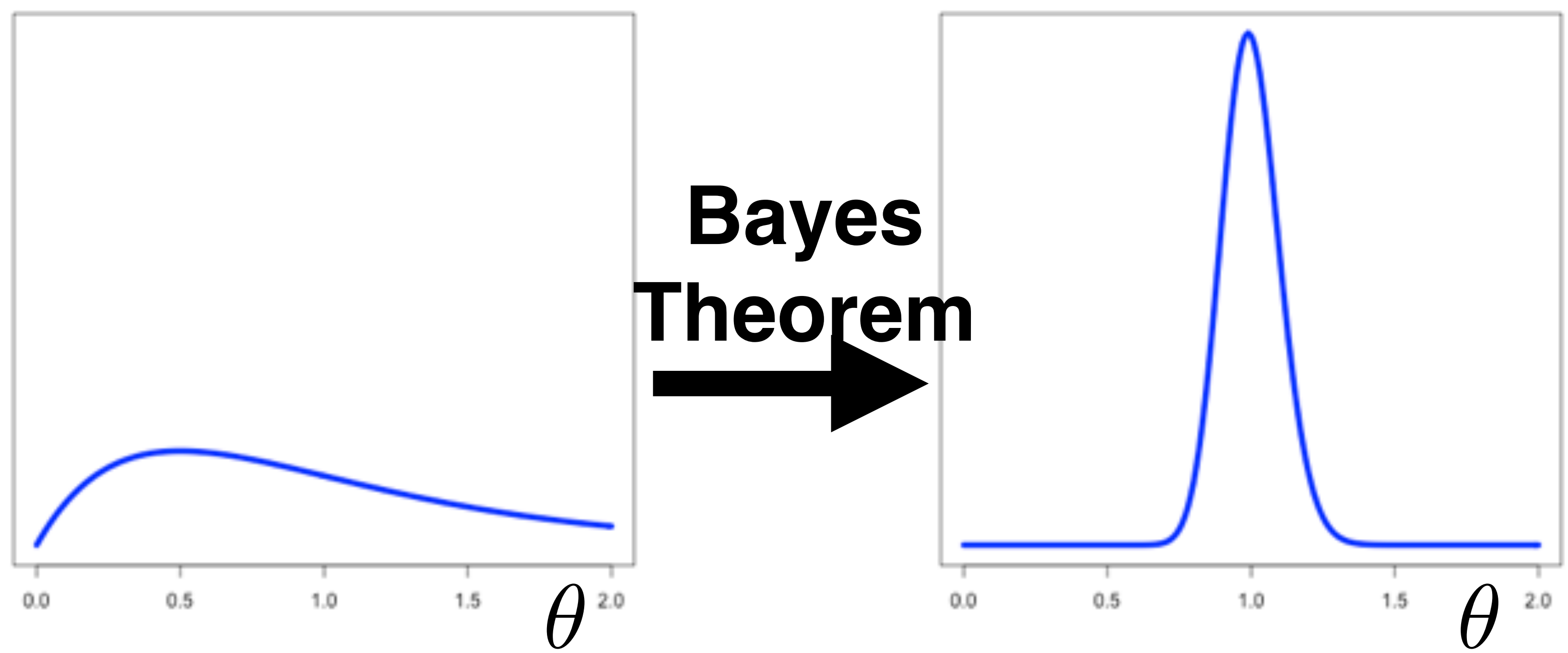

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- Gold standard: Markov Chain Monte Carlo (MCMC)

[Bardenet, Doucet, Holmes 2017]

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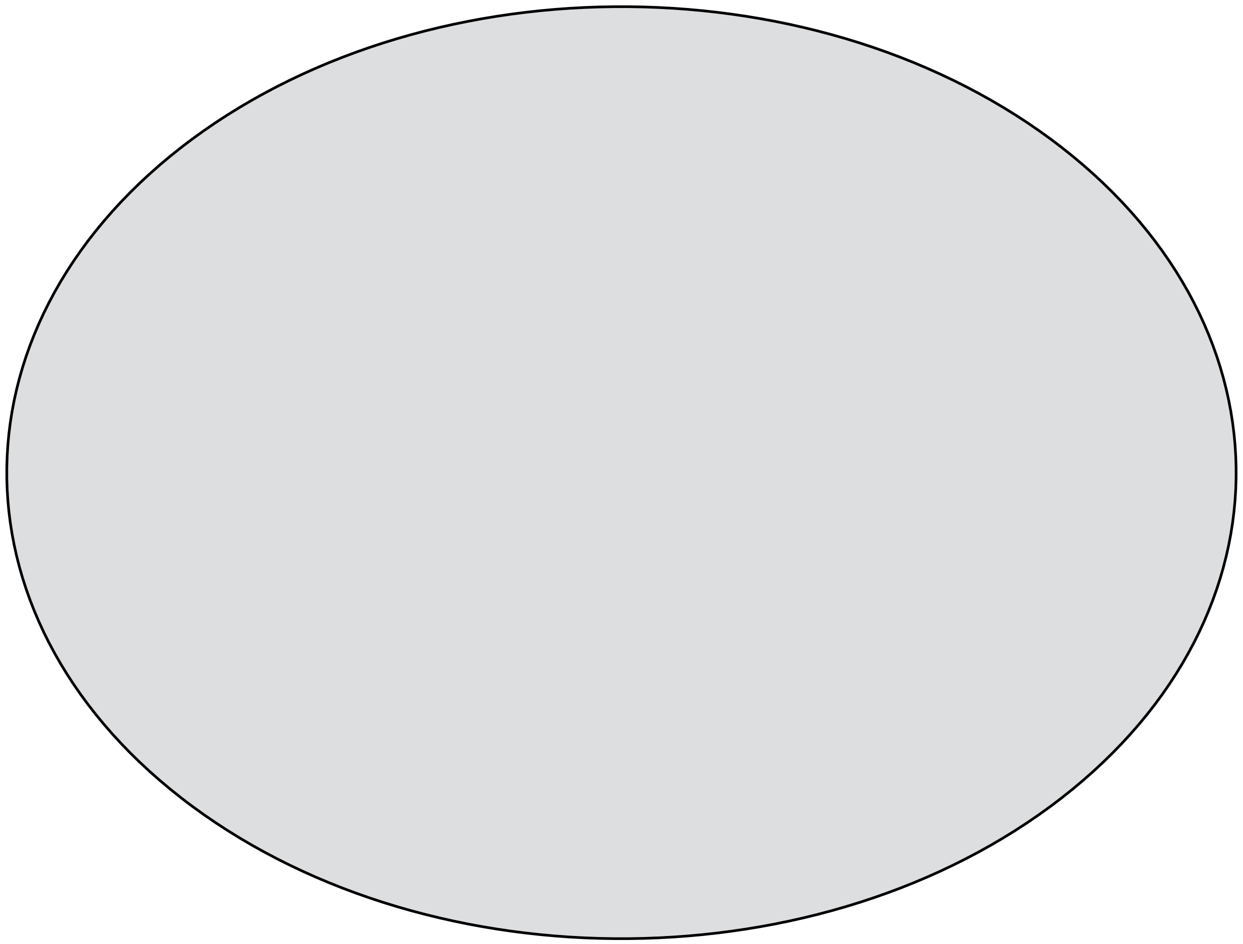

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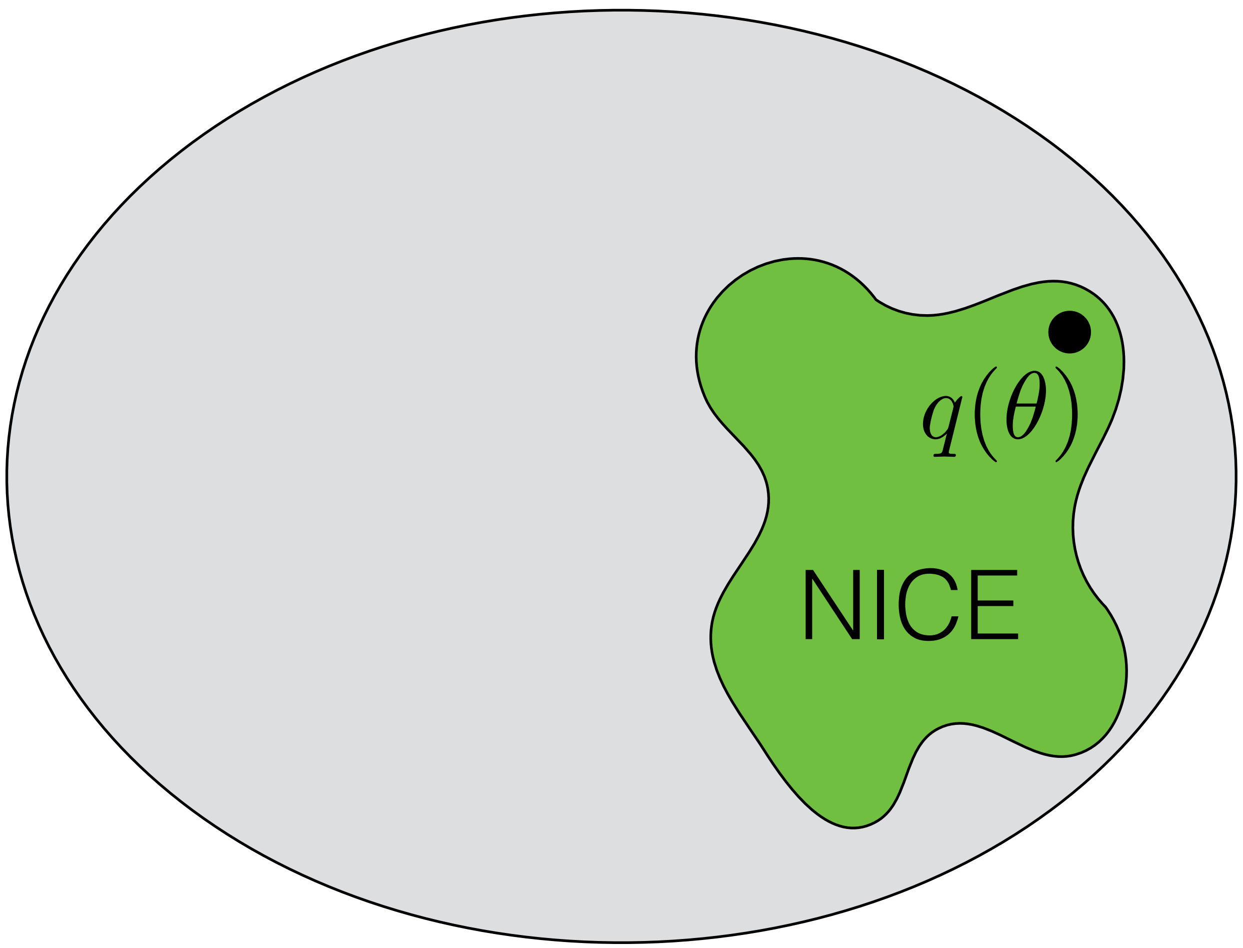

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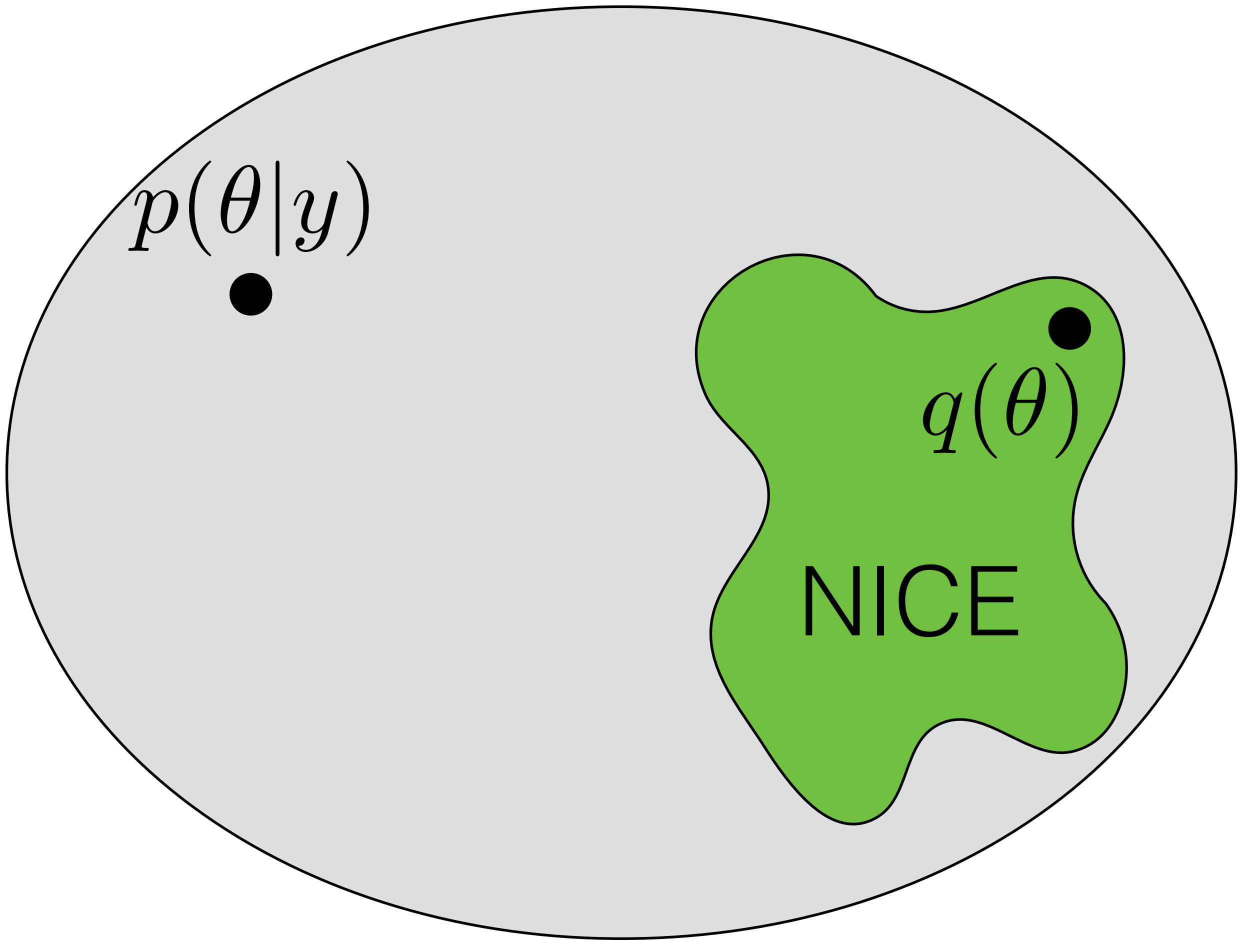

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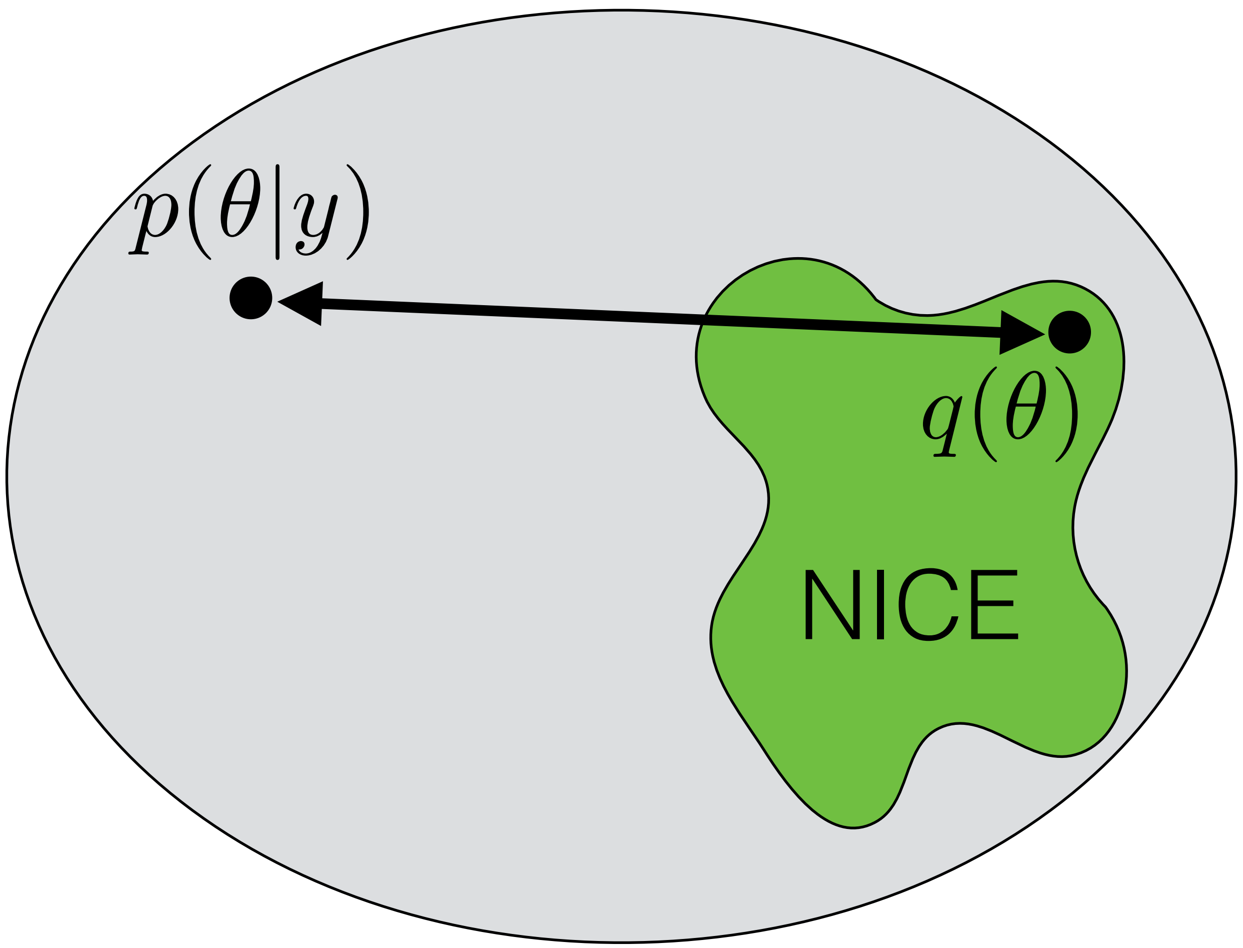

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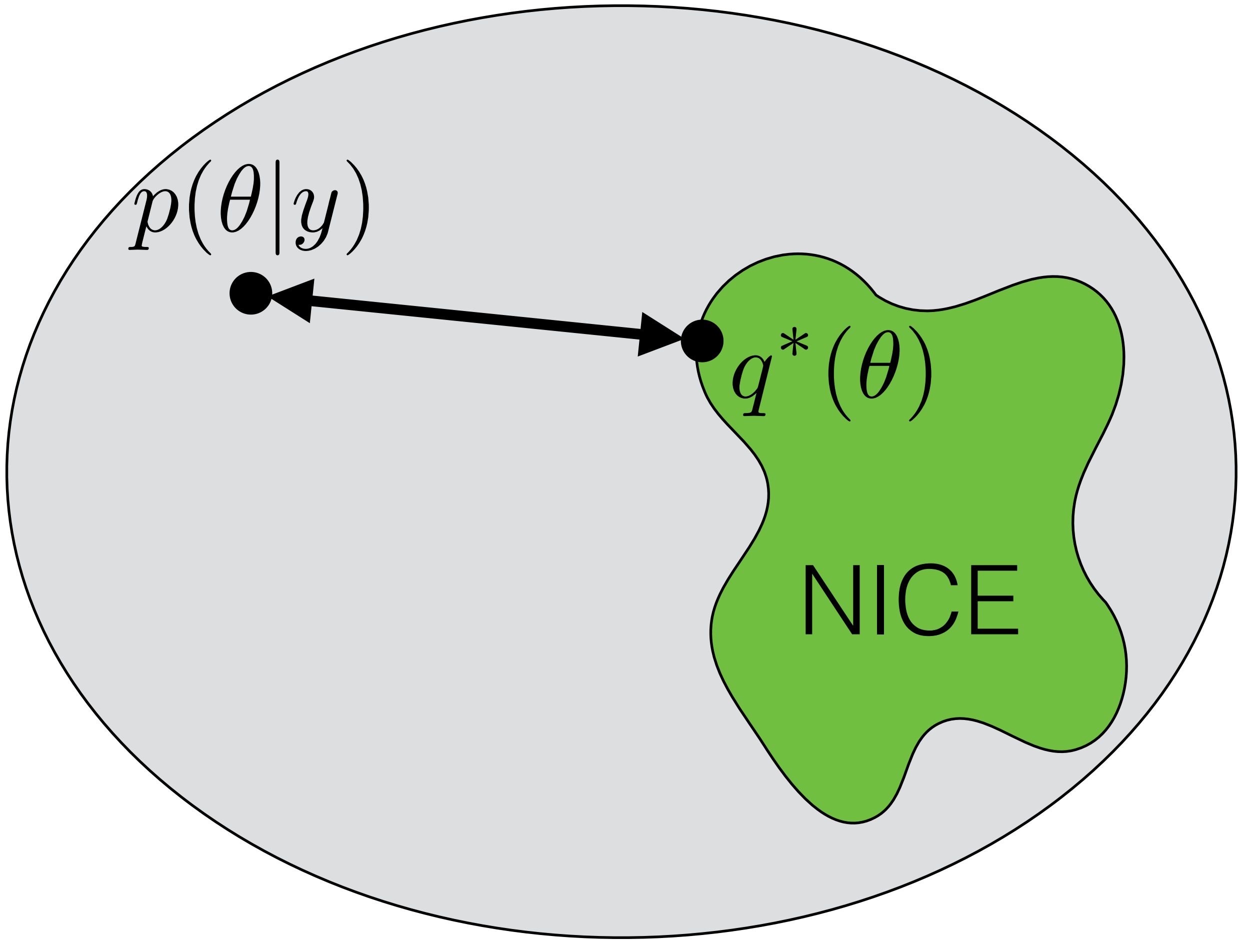

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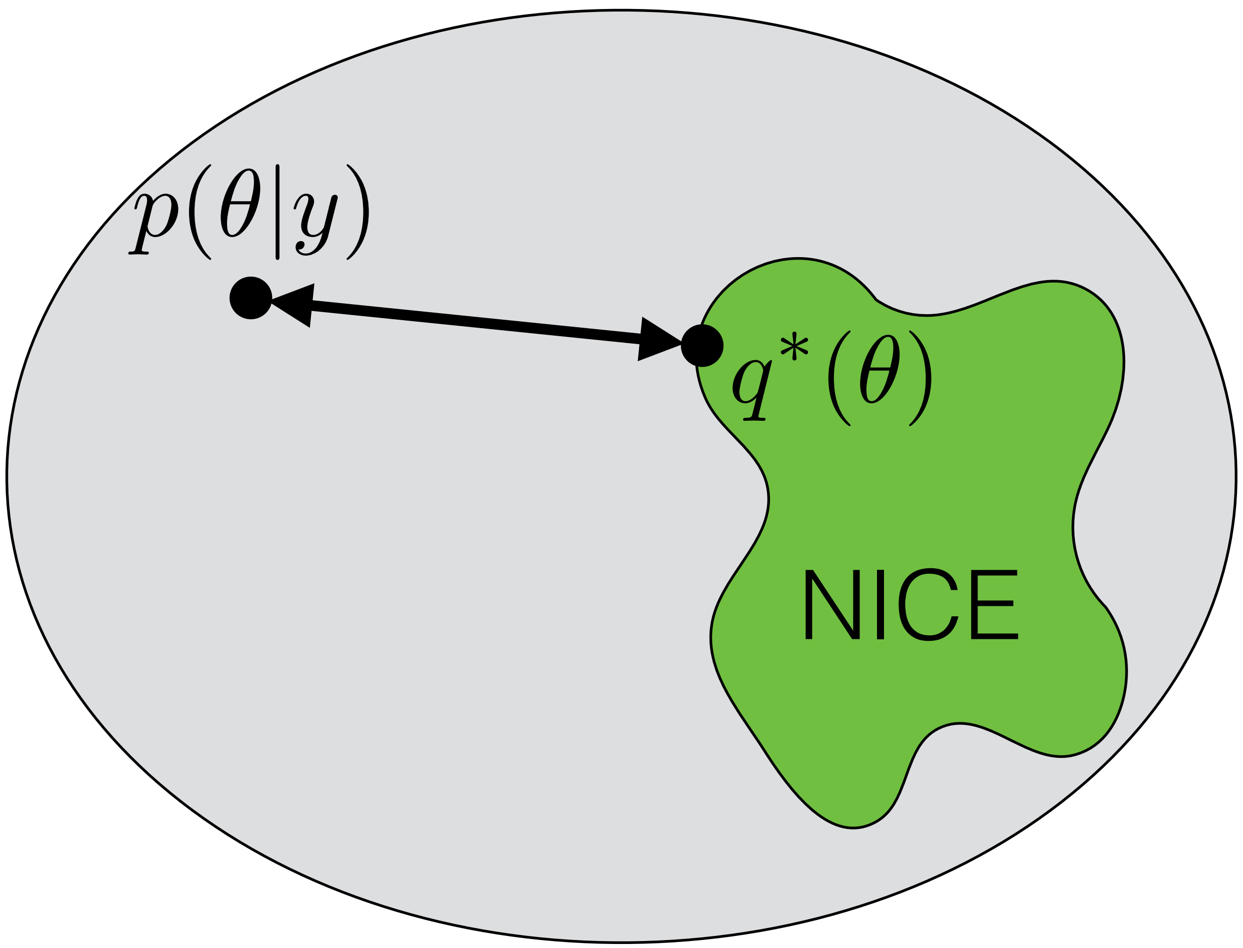

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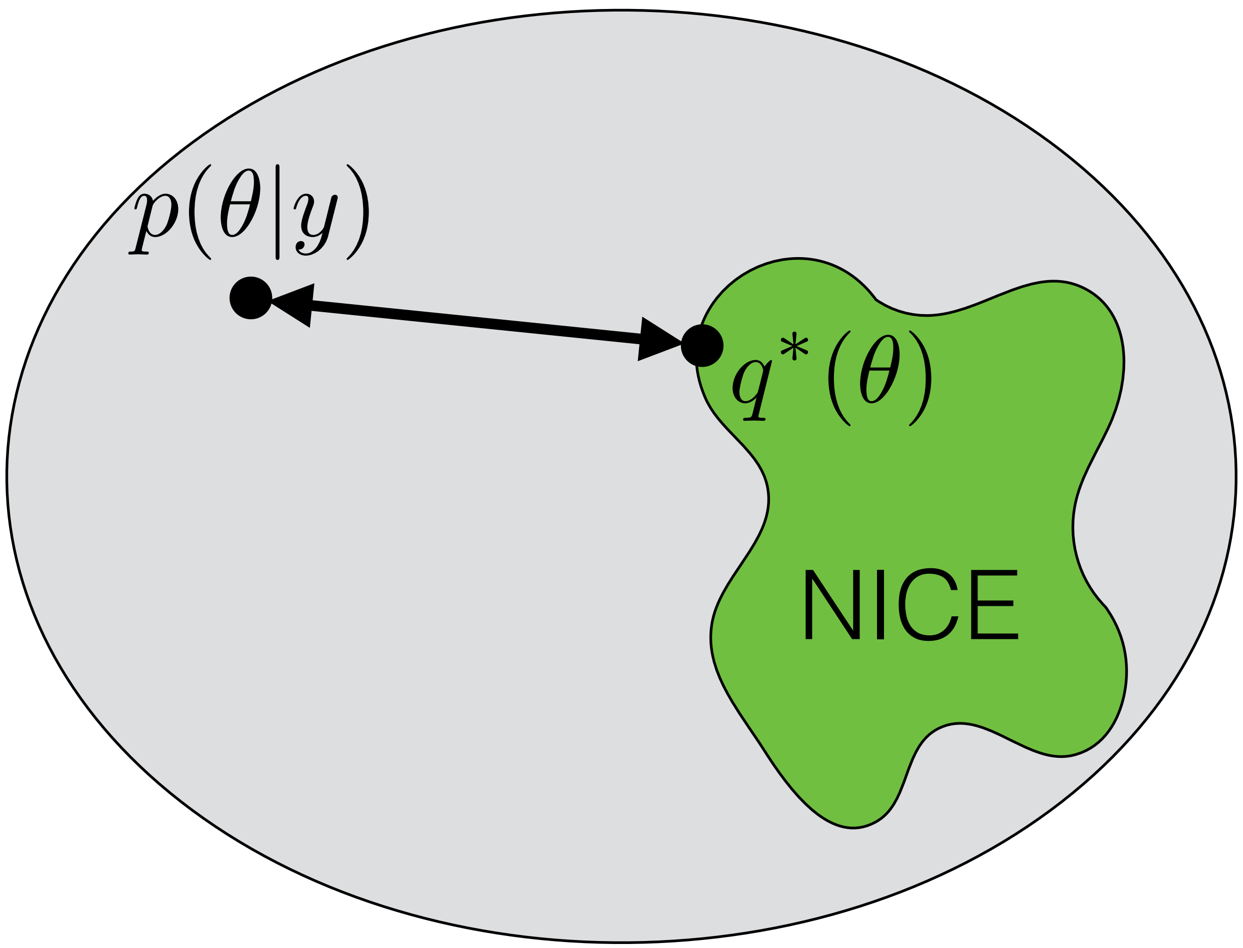

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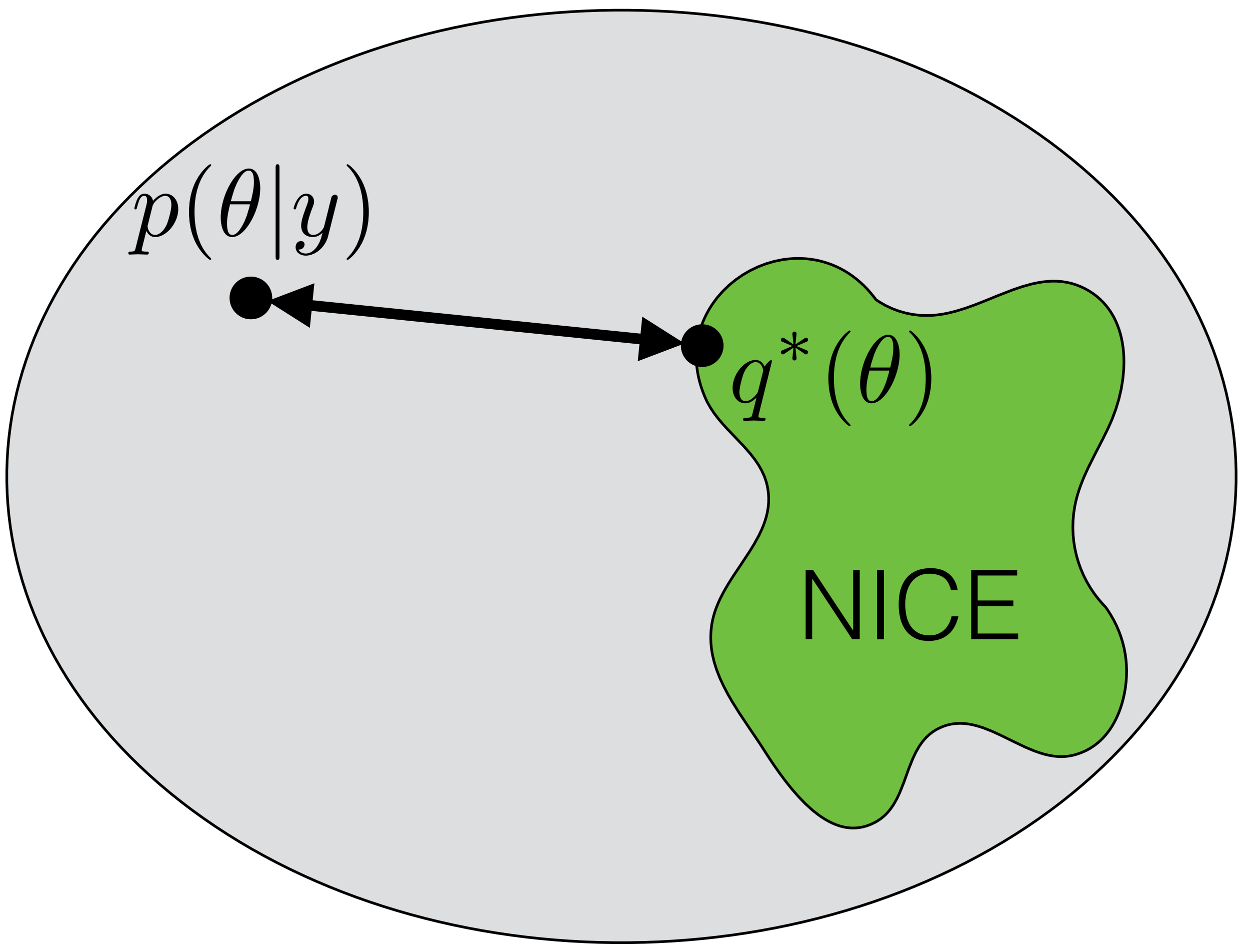

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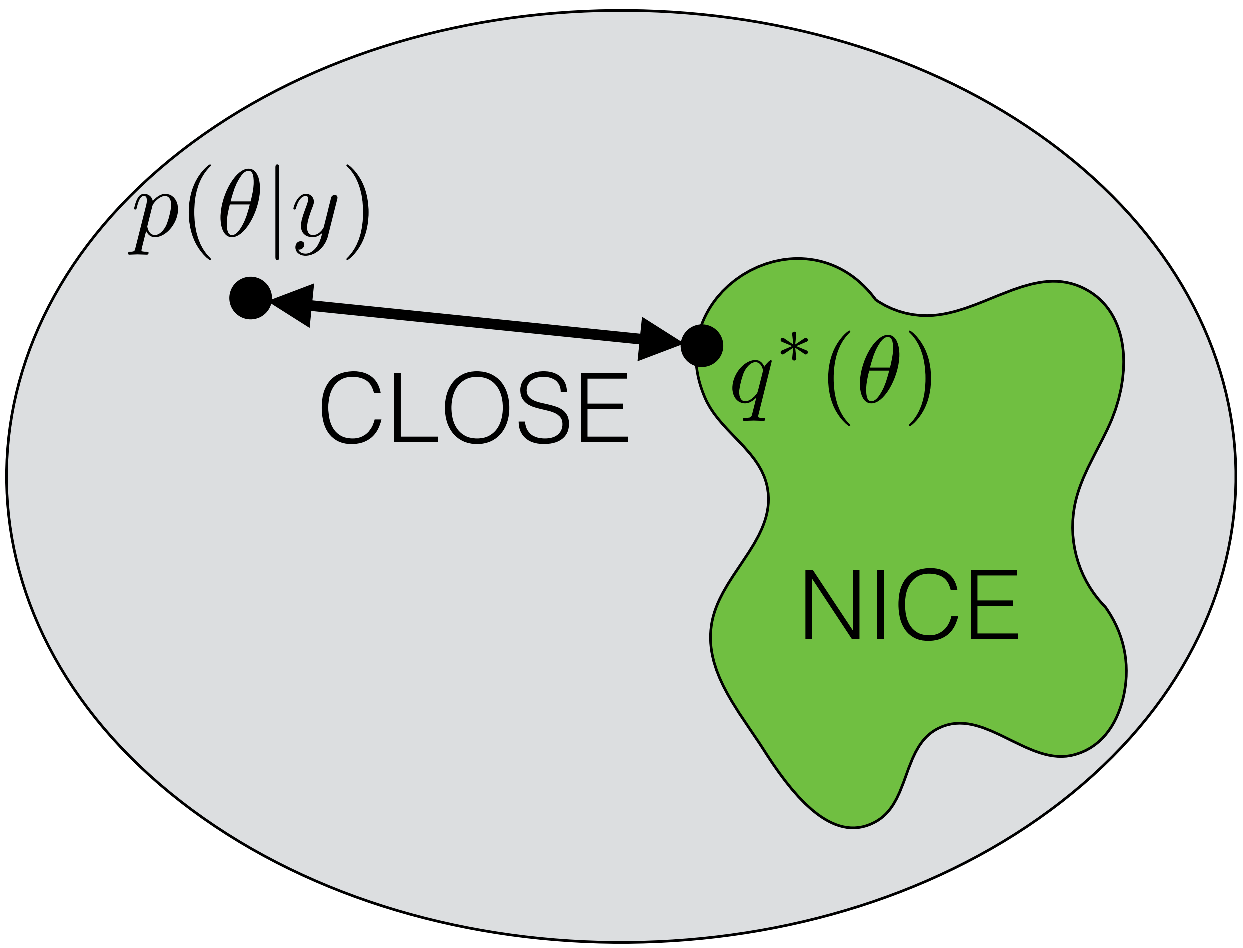

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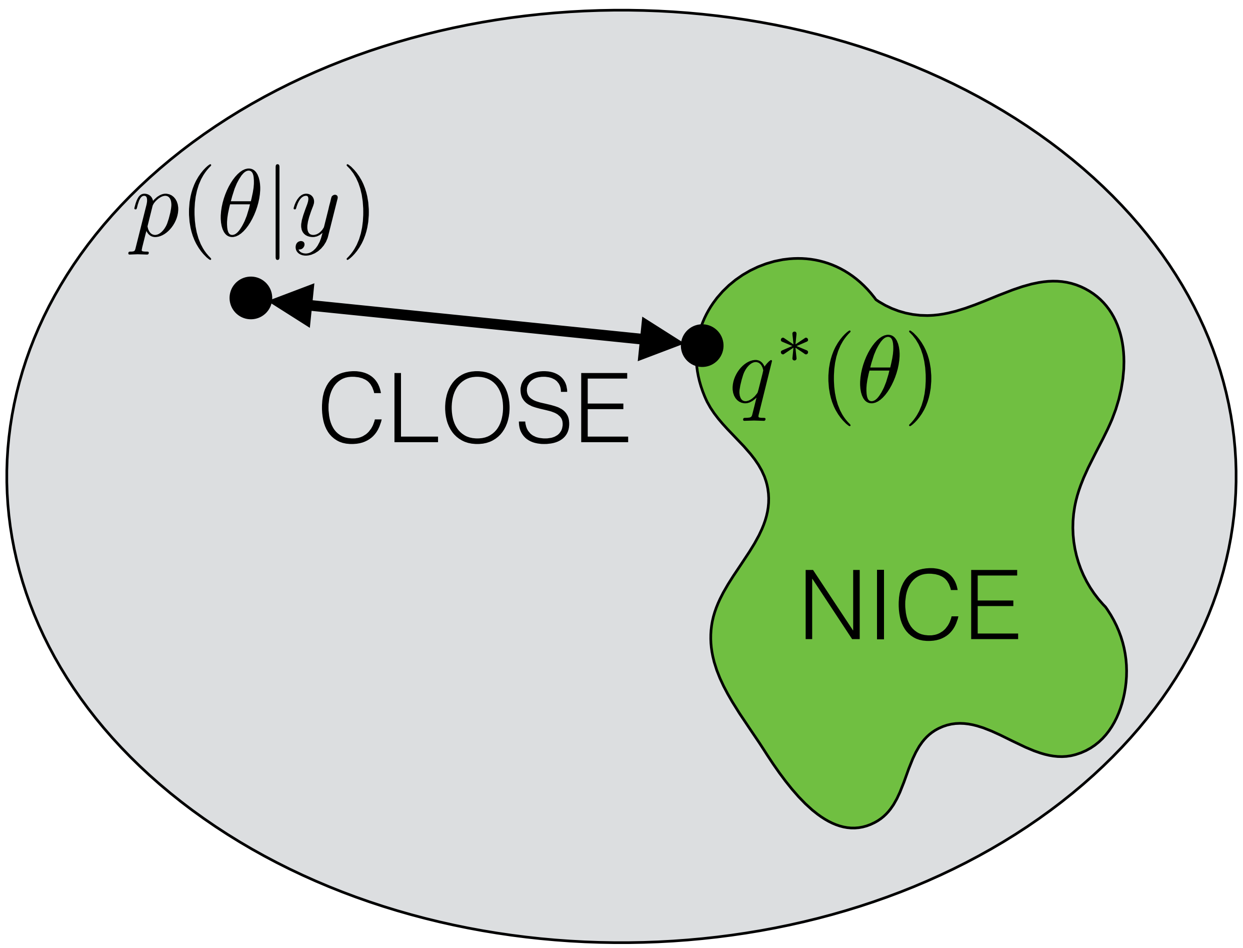

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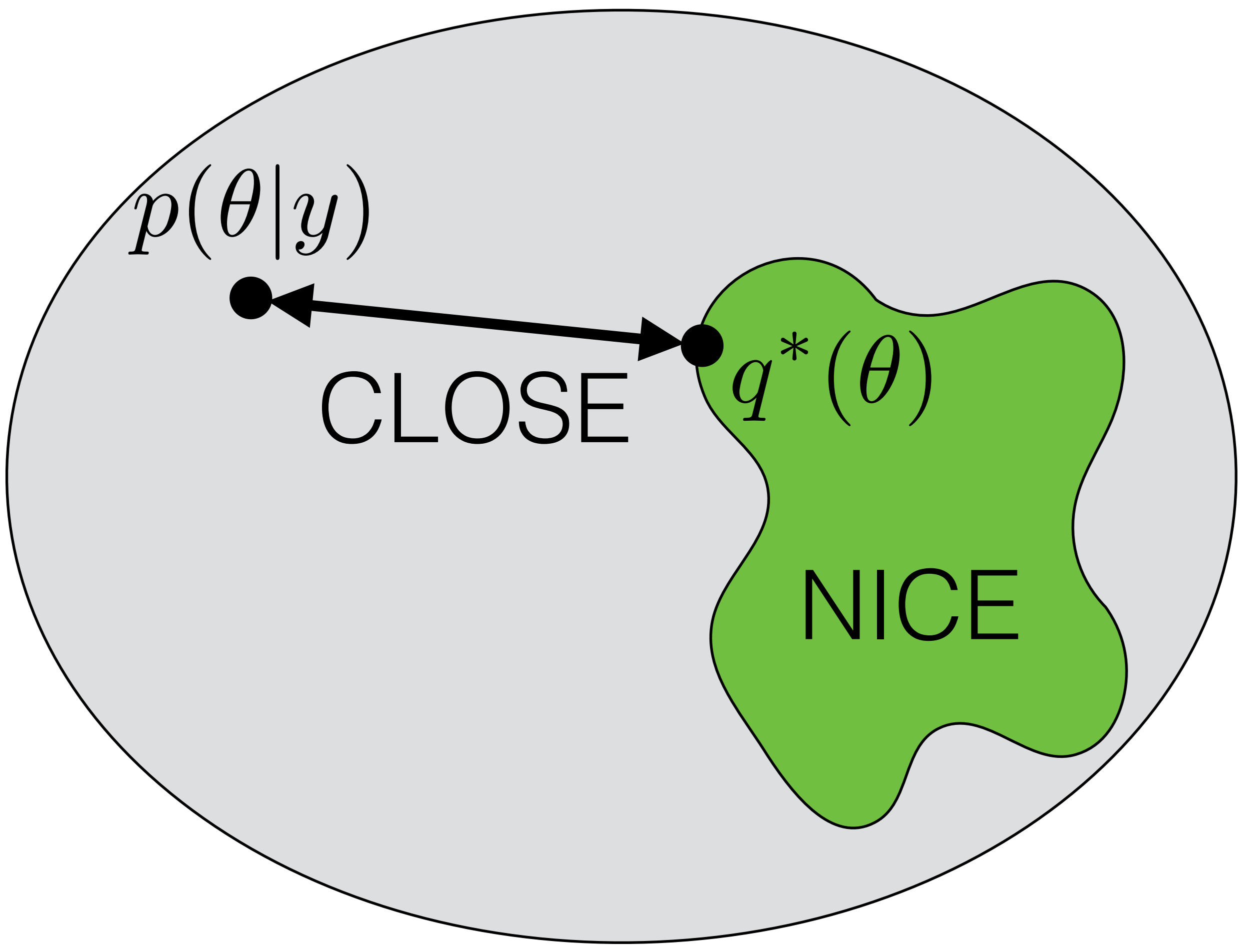

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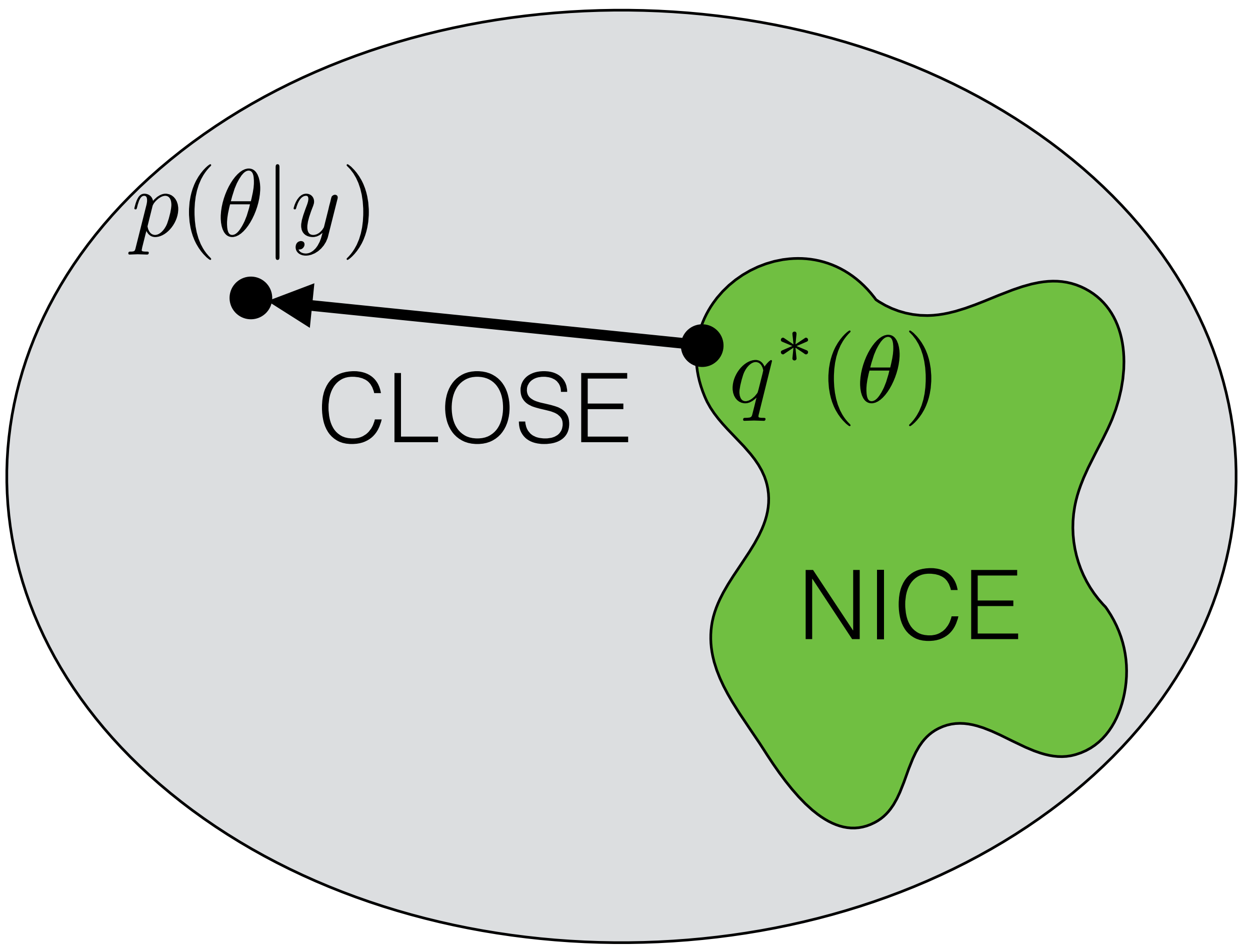

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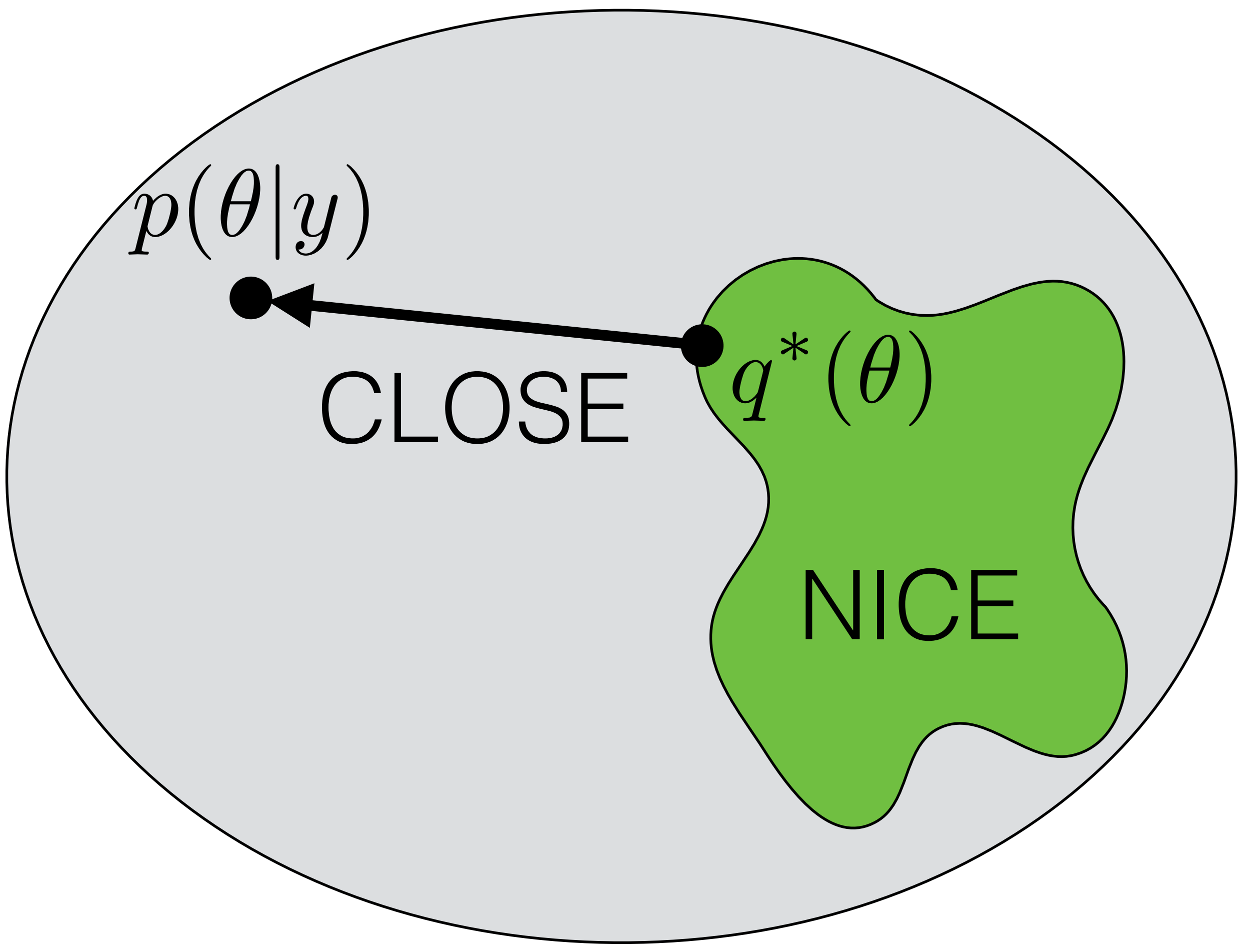

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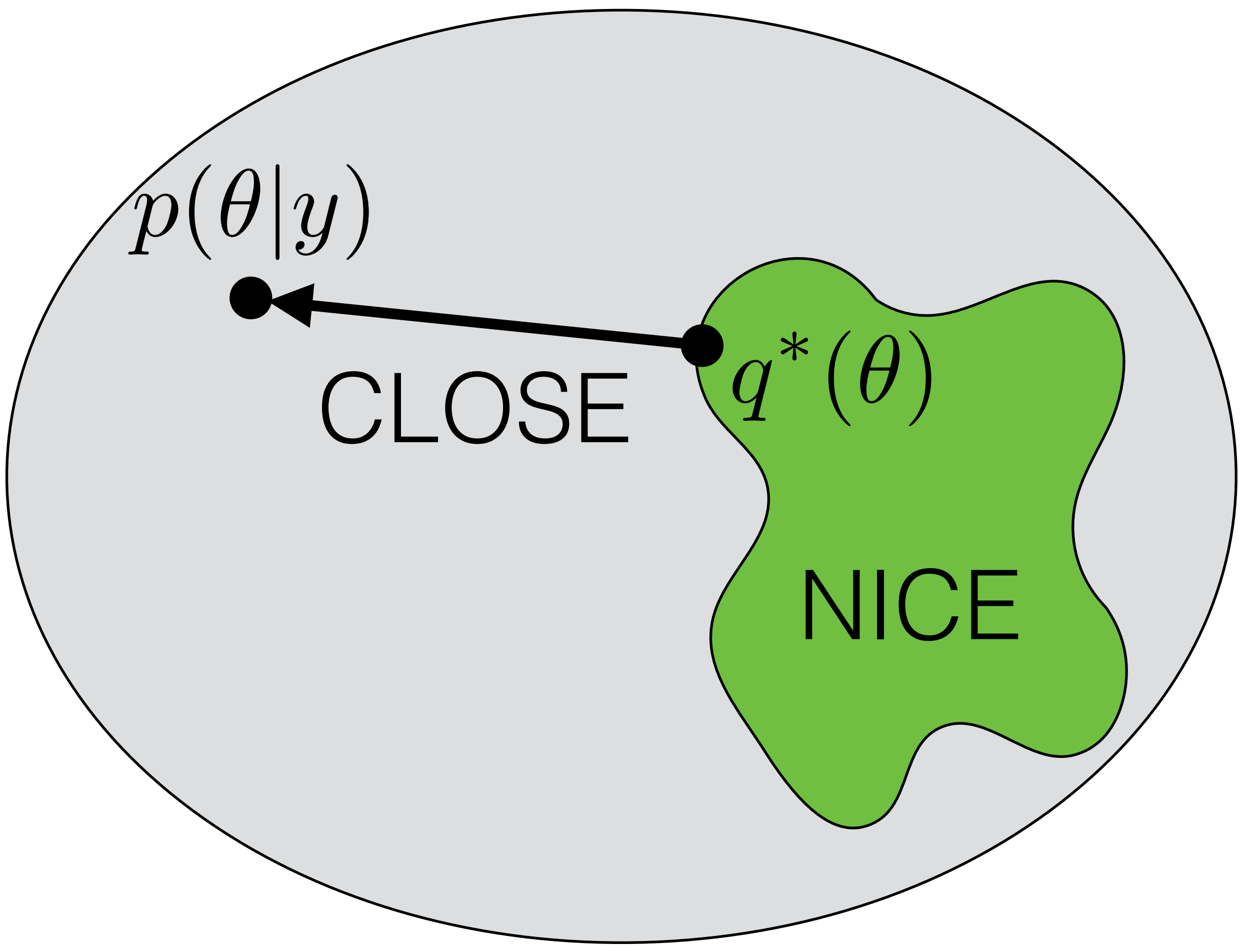

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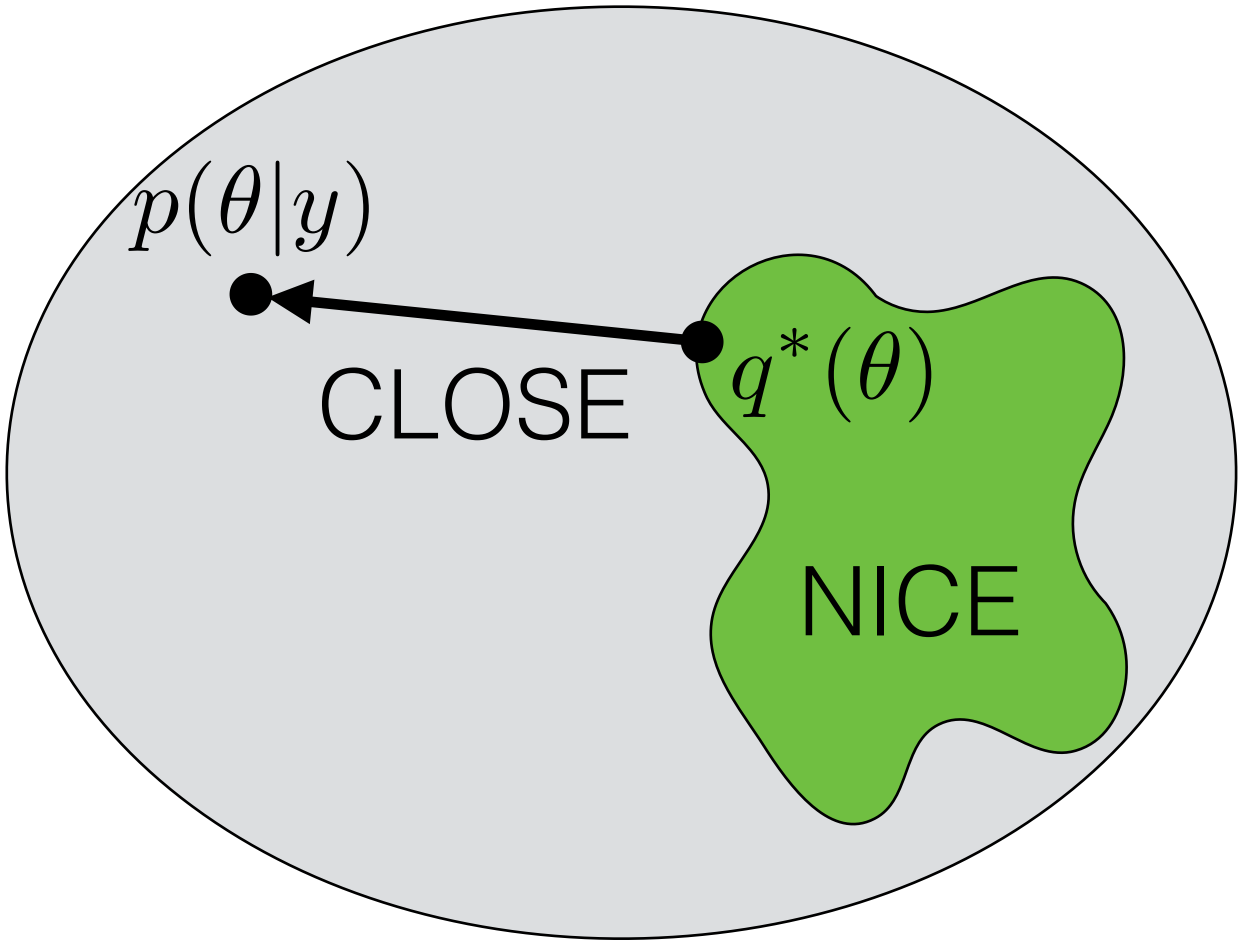

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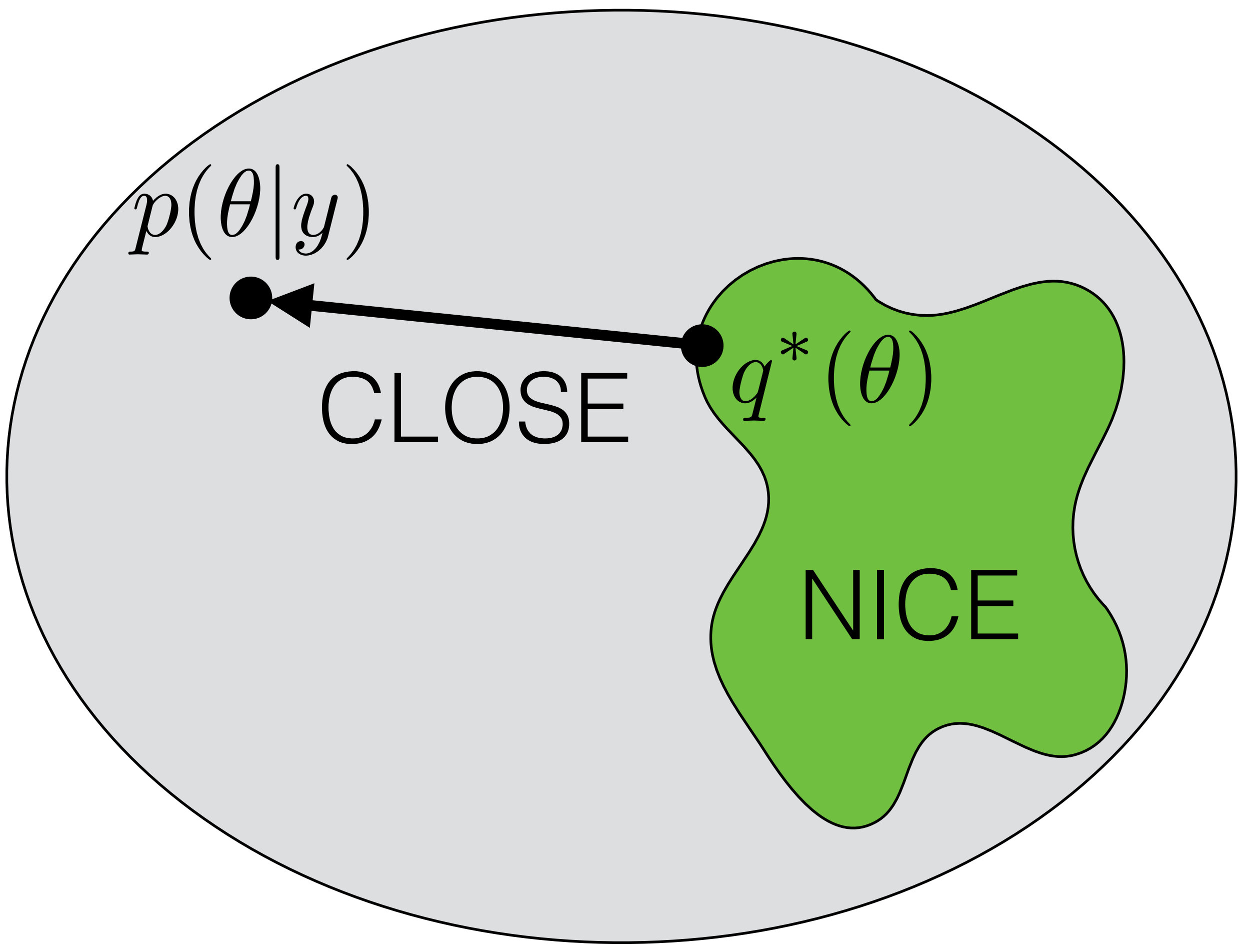

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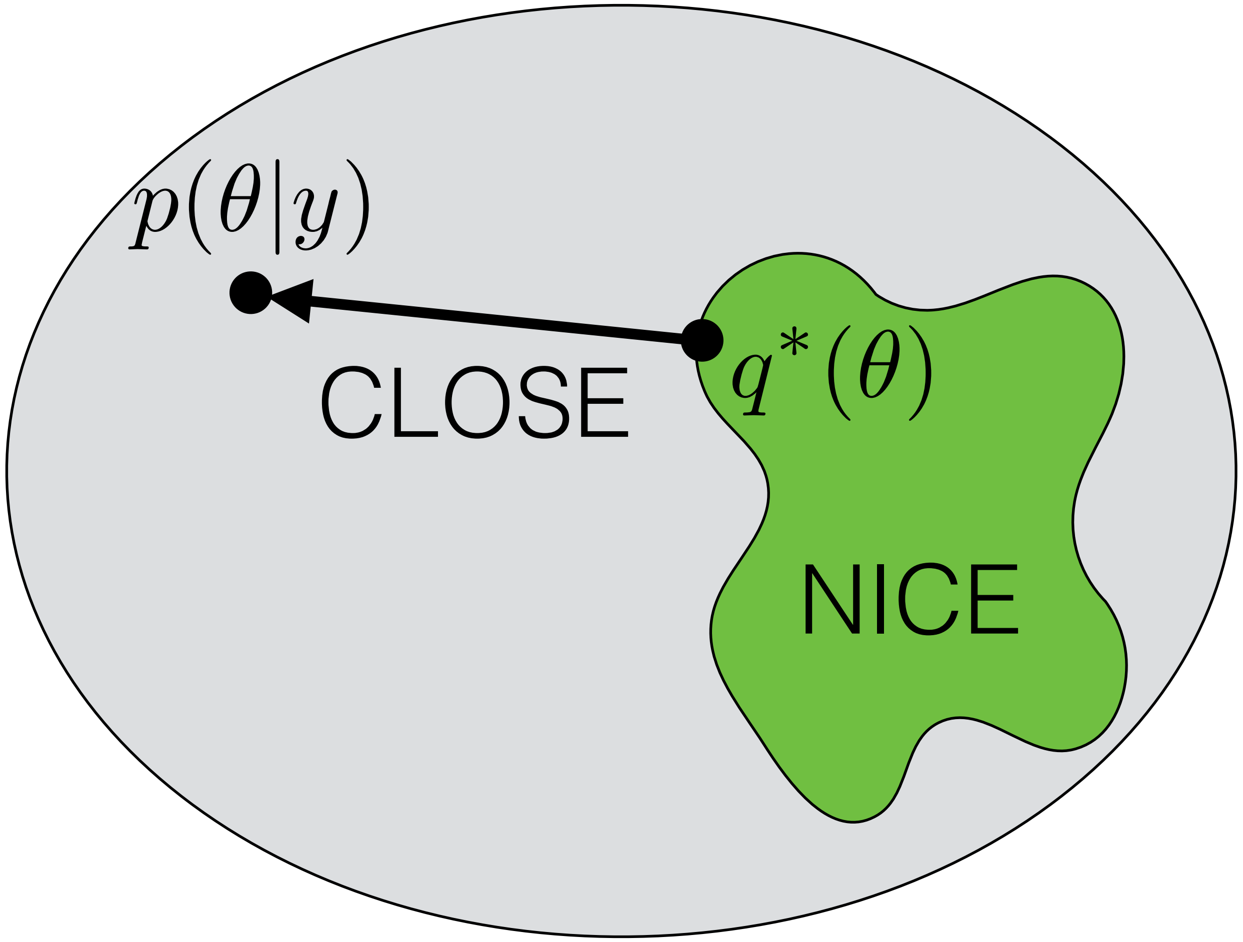
- VB practical success: point estimates and prediction, fast, streaming, distributed (3.6M Wikipedia, 350K Nature)

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

Why KL?

- Variational Bayes

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



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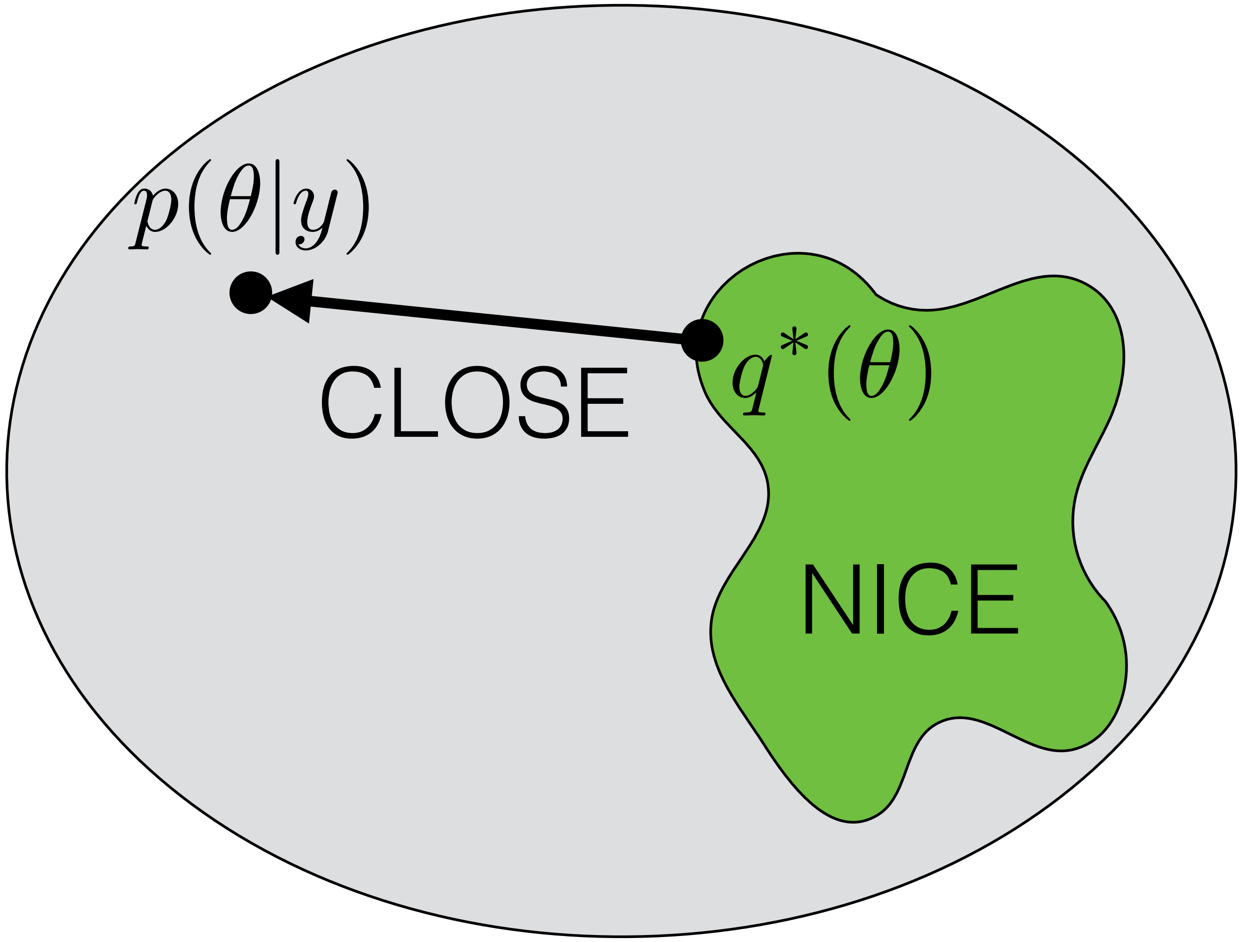

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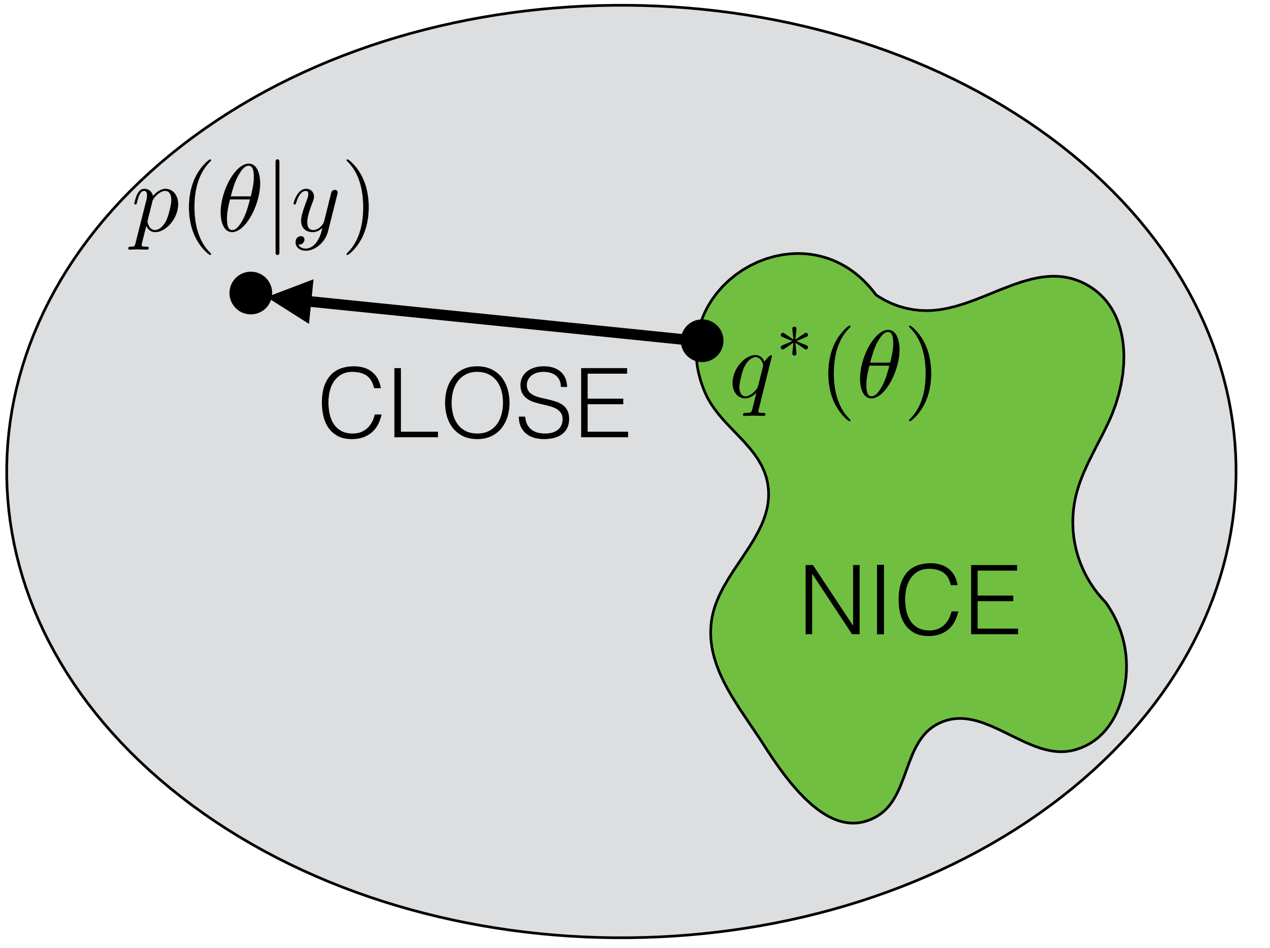

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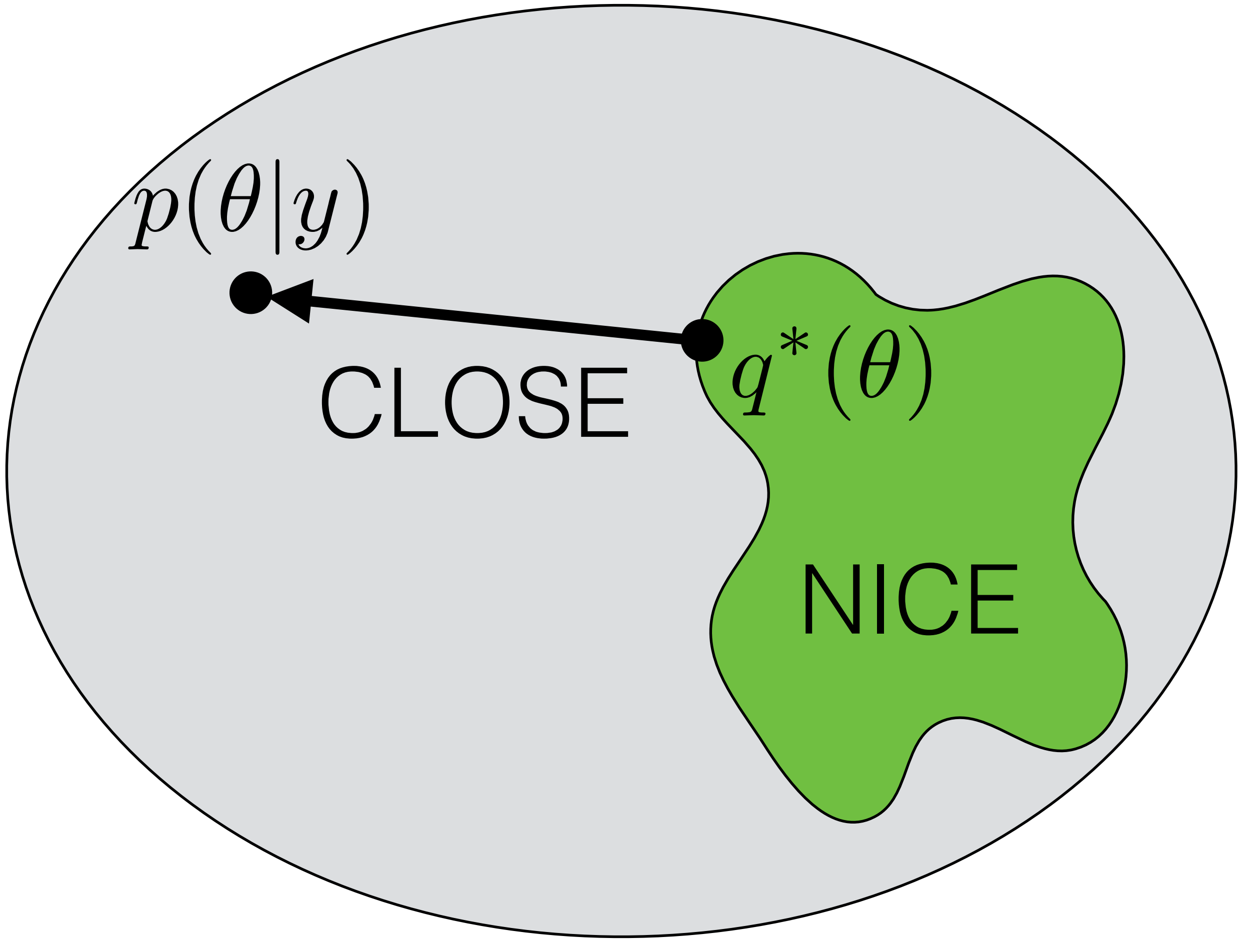

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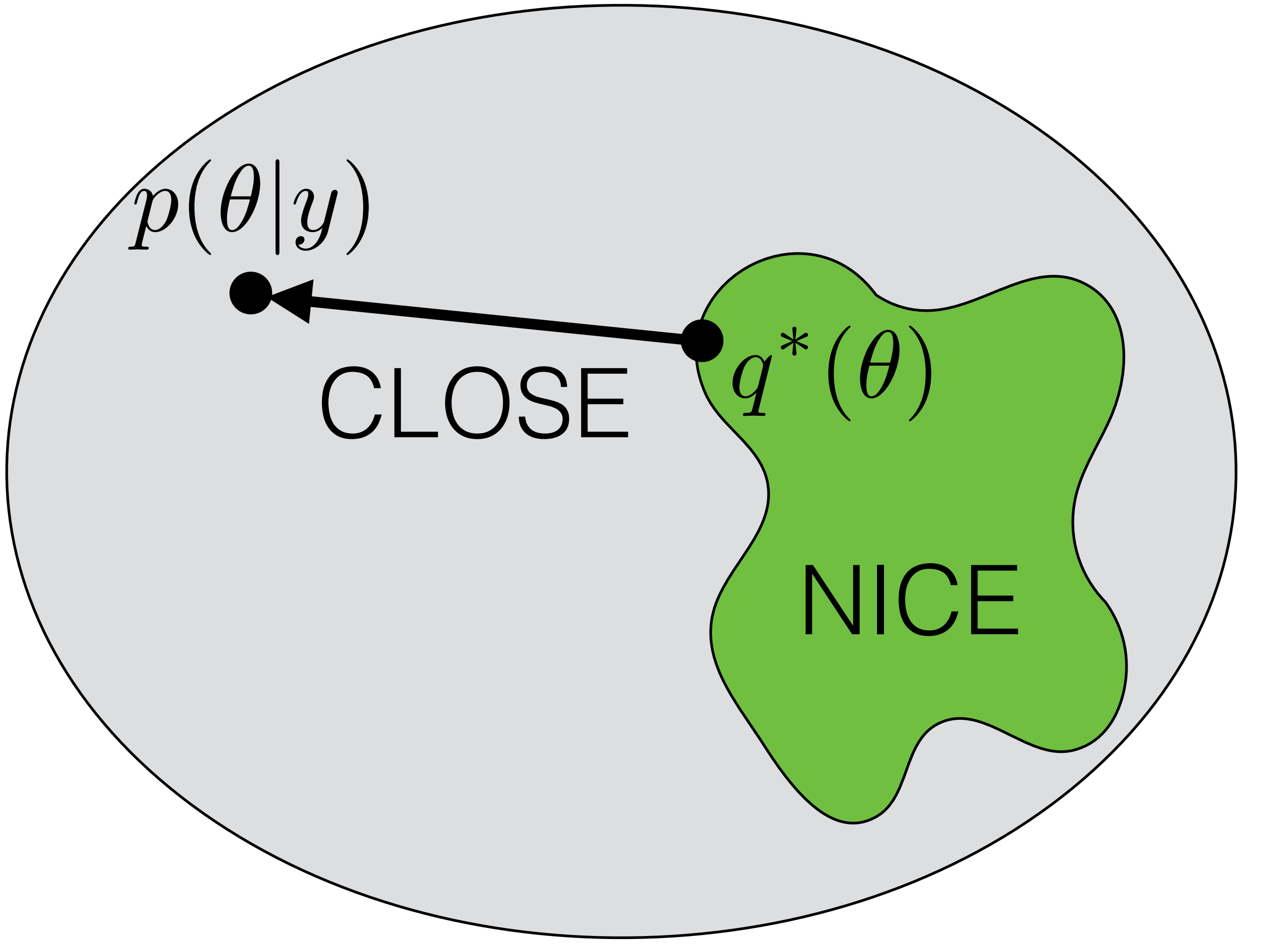

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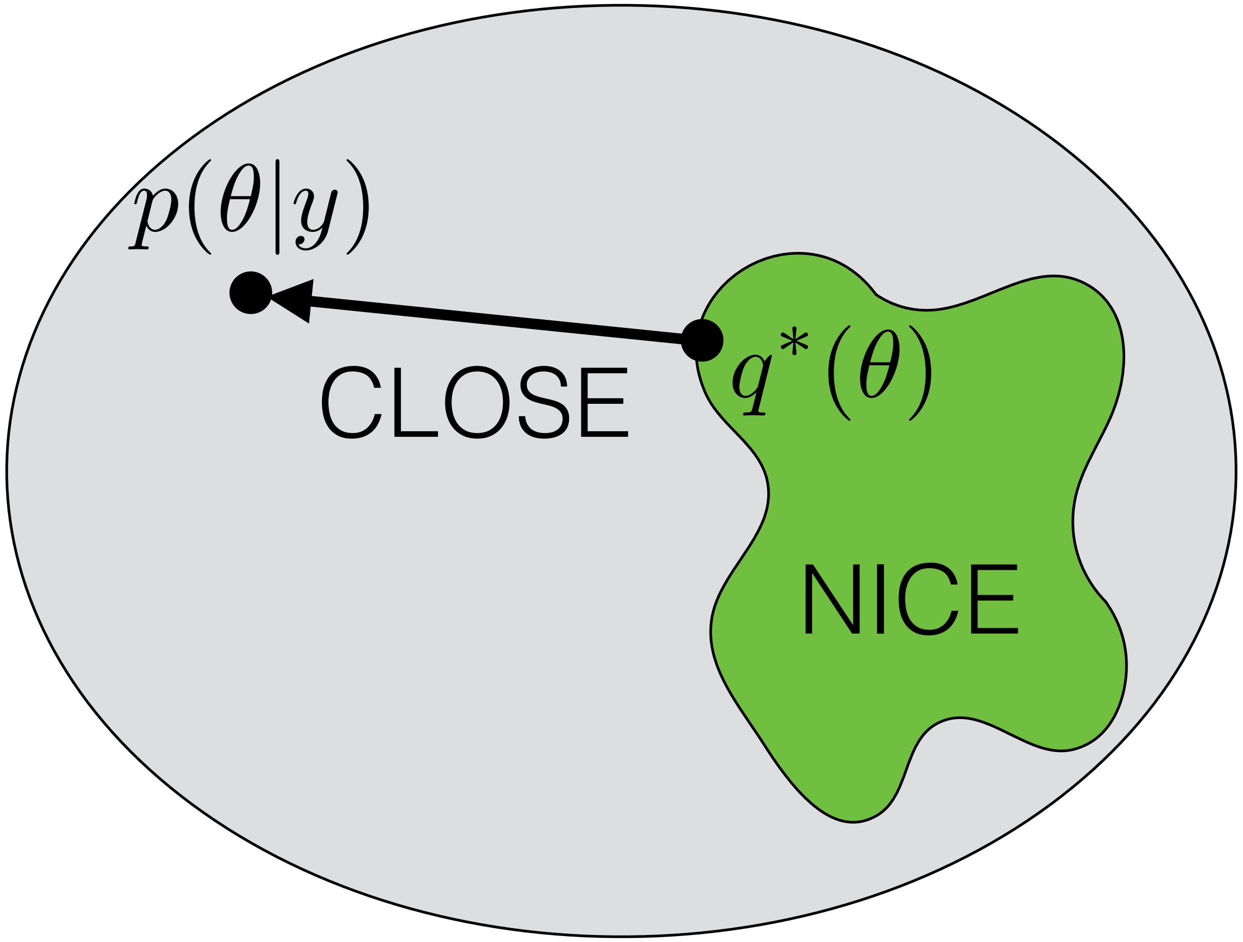

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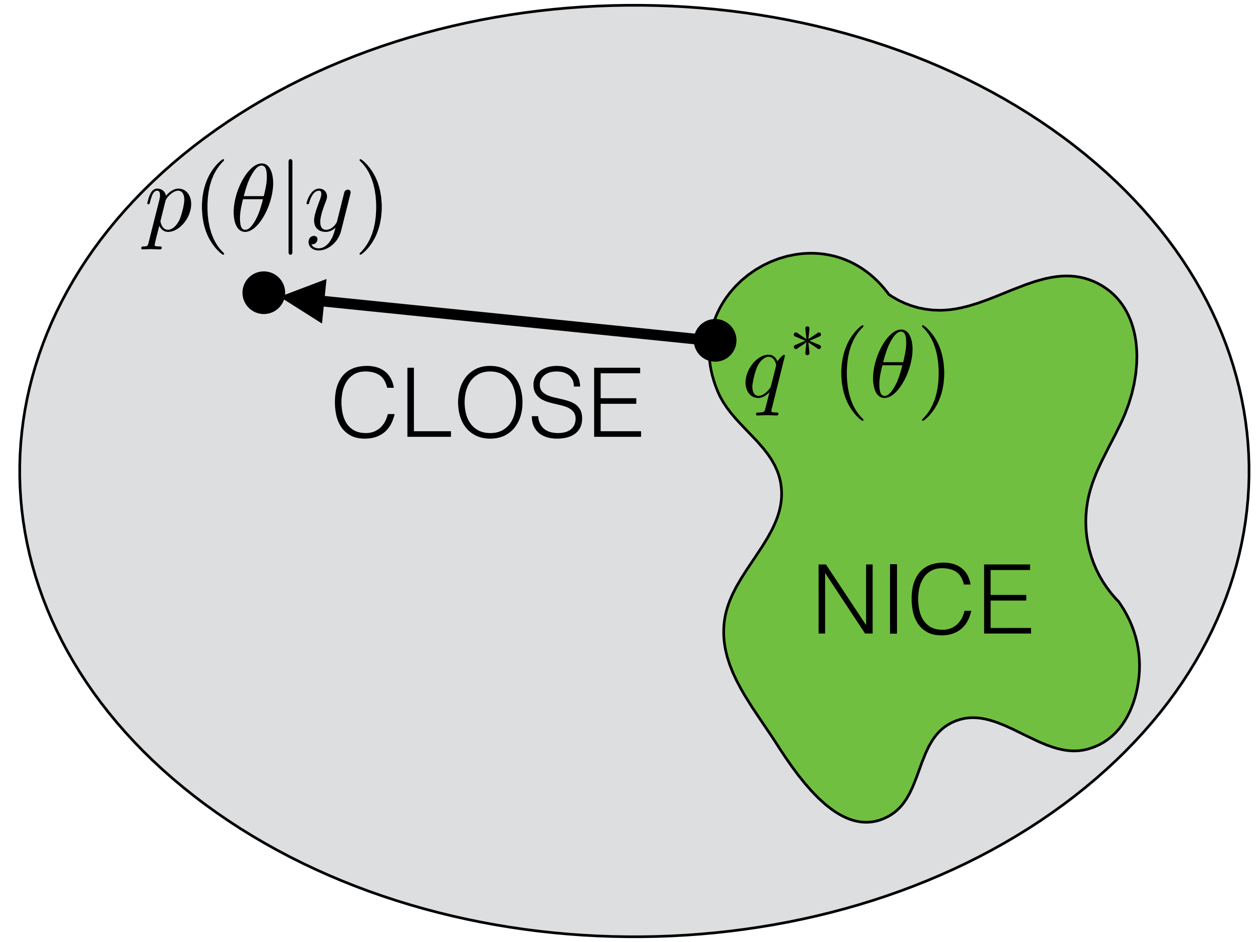

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"Evidence lower bound" (ELBO)

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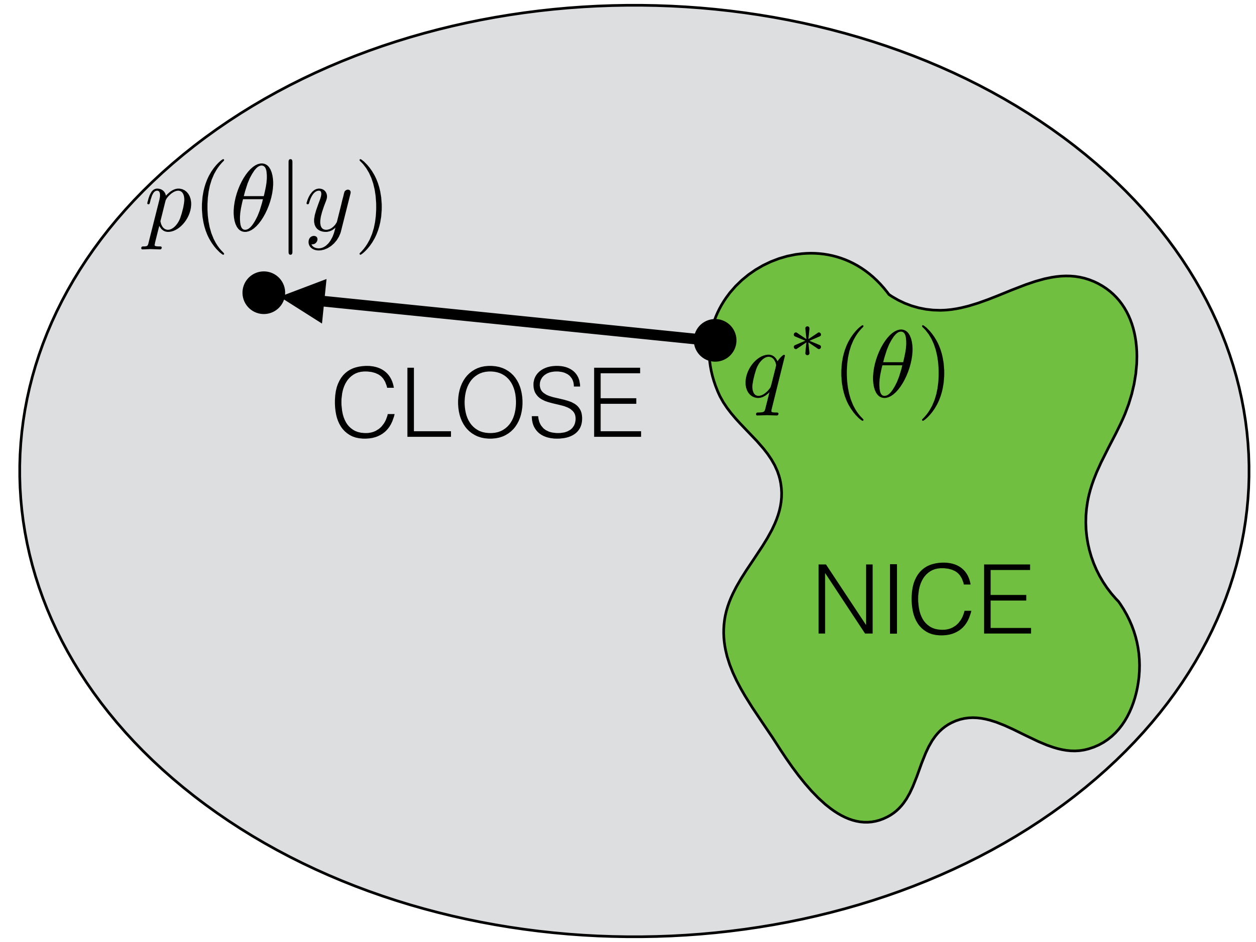

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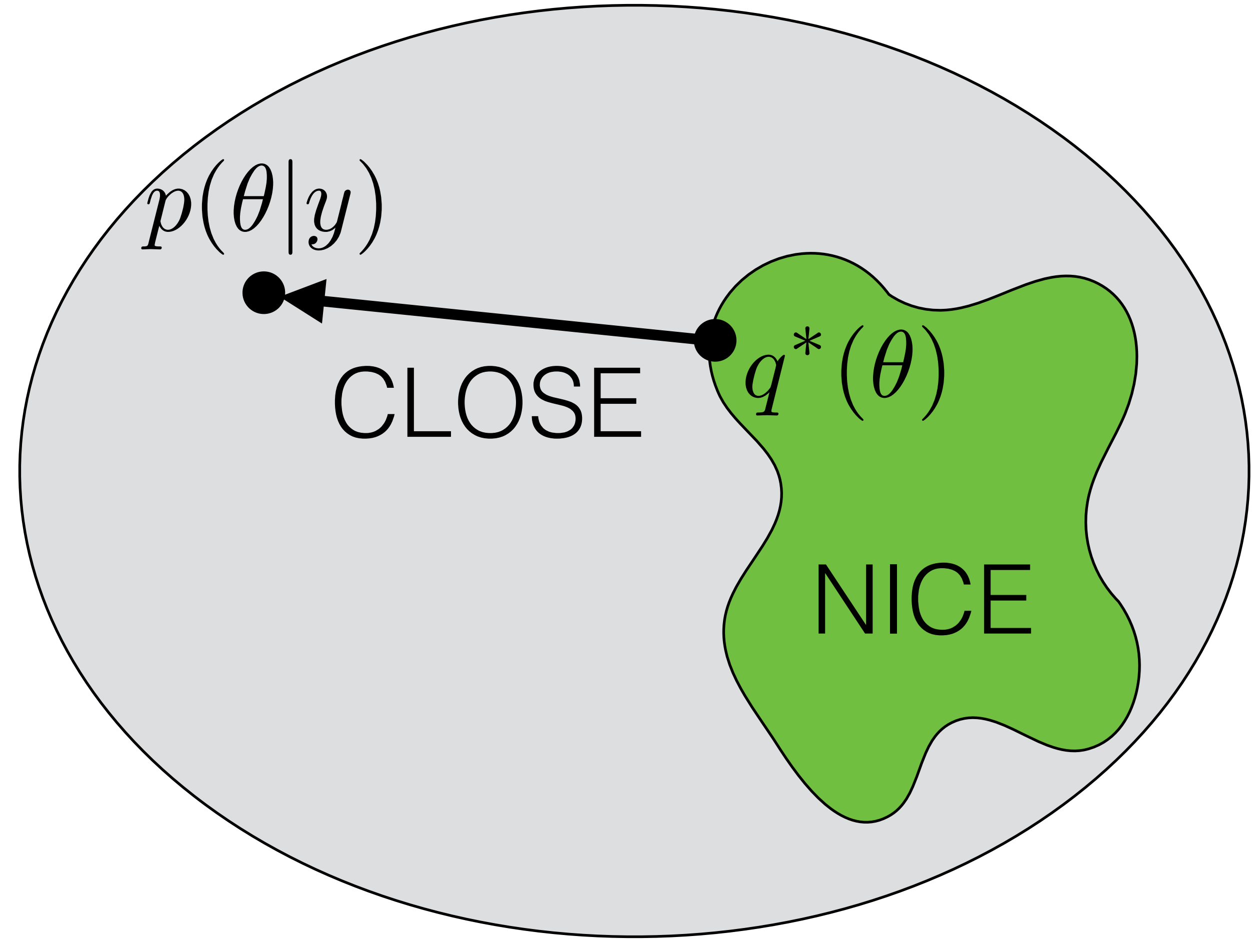

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- Exercise: Show $\text{KL} \geq 0$ [Bishop 2006, Sec 1.6.1]

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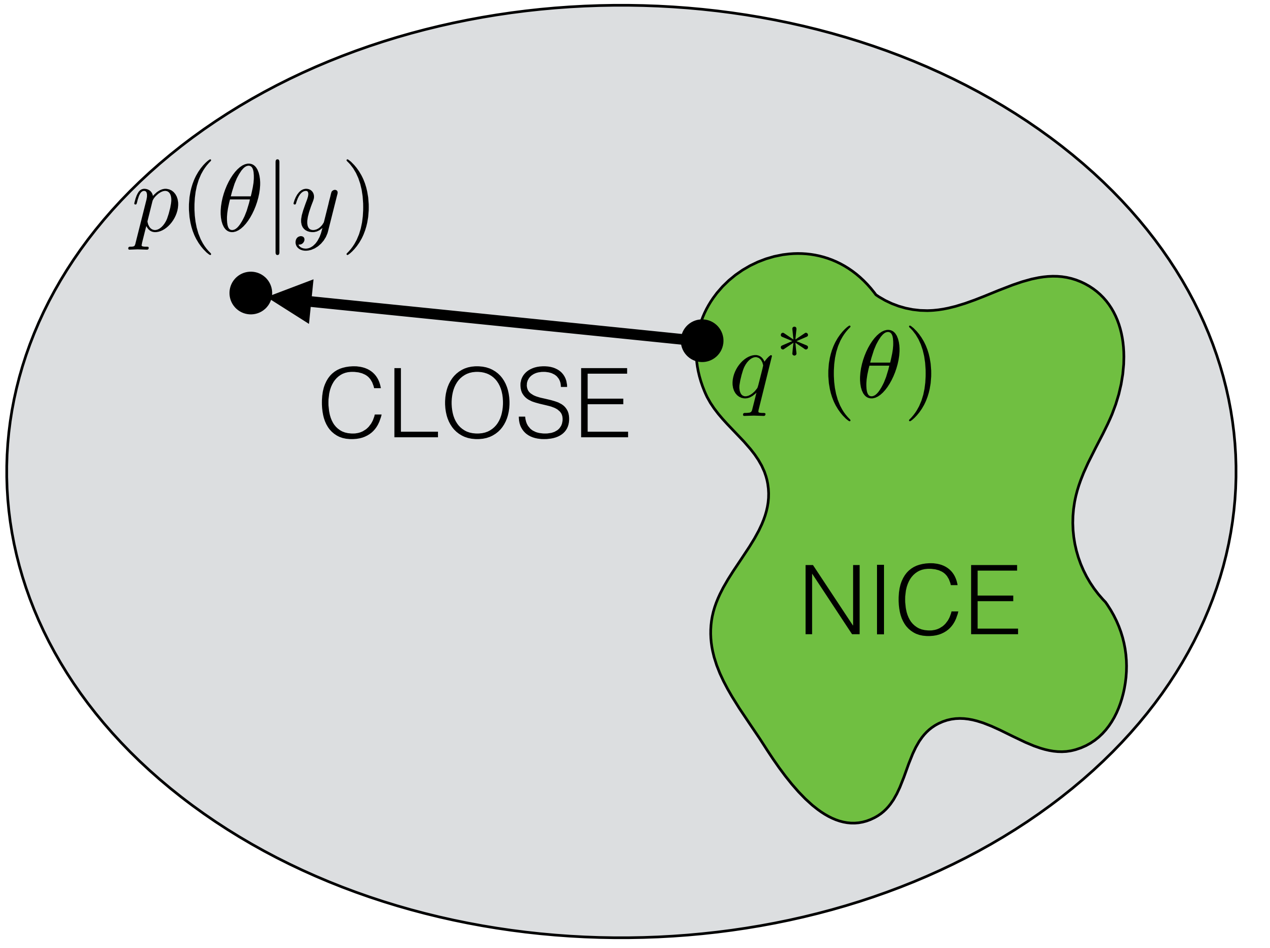

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"Evidence lower bound" (ELBO)

- Exercise: Show $\mathrm{KL} \geq 0$ [Bishop 2006, Sec 1.6.1]
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Why KL?

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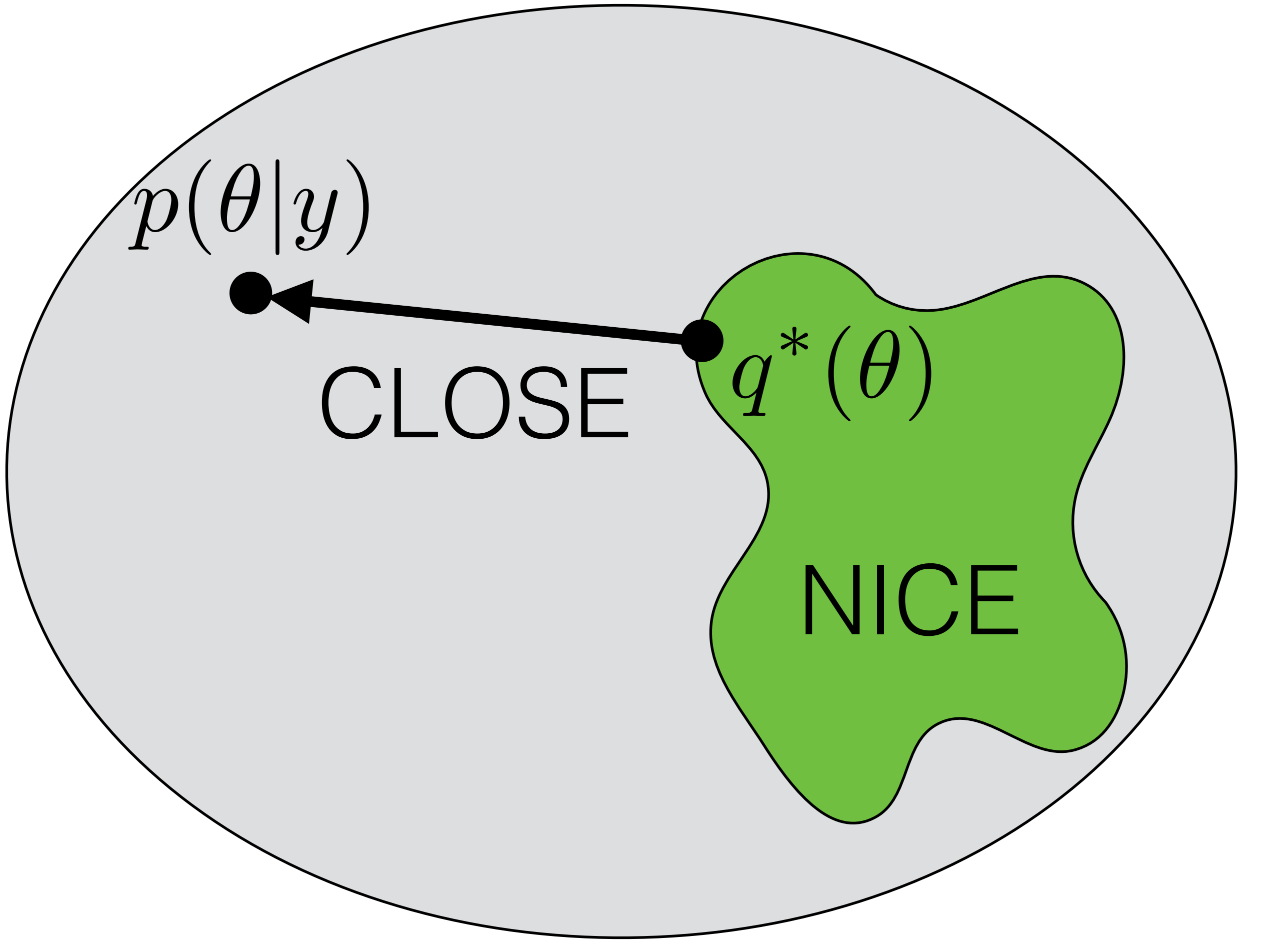

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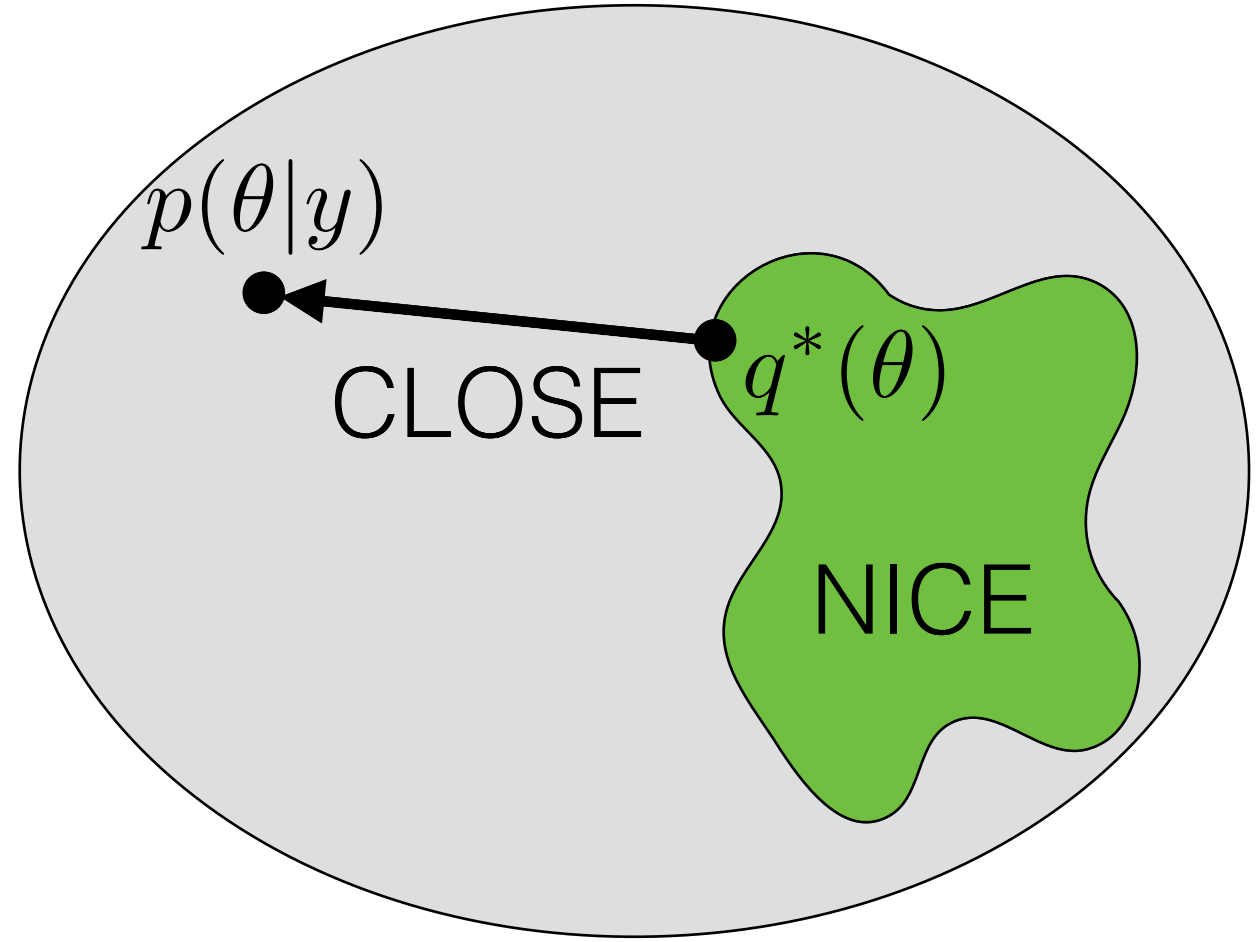

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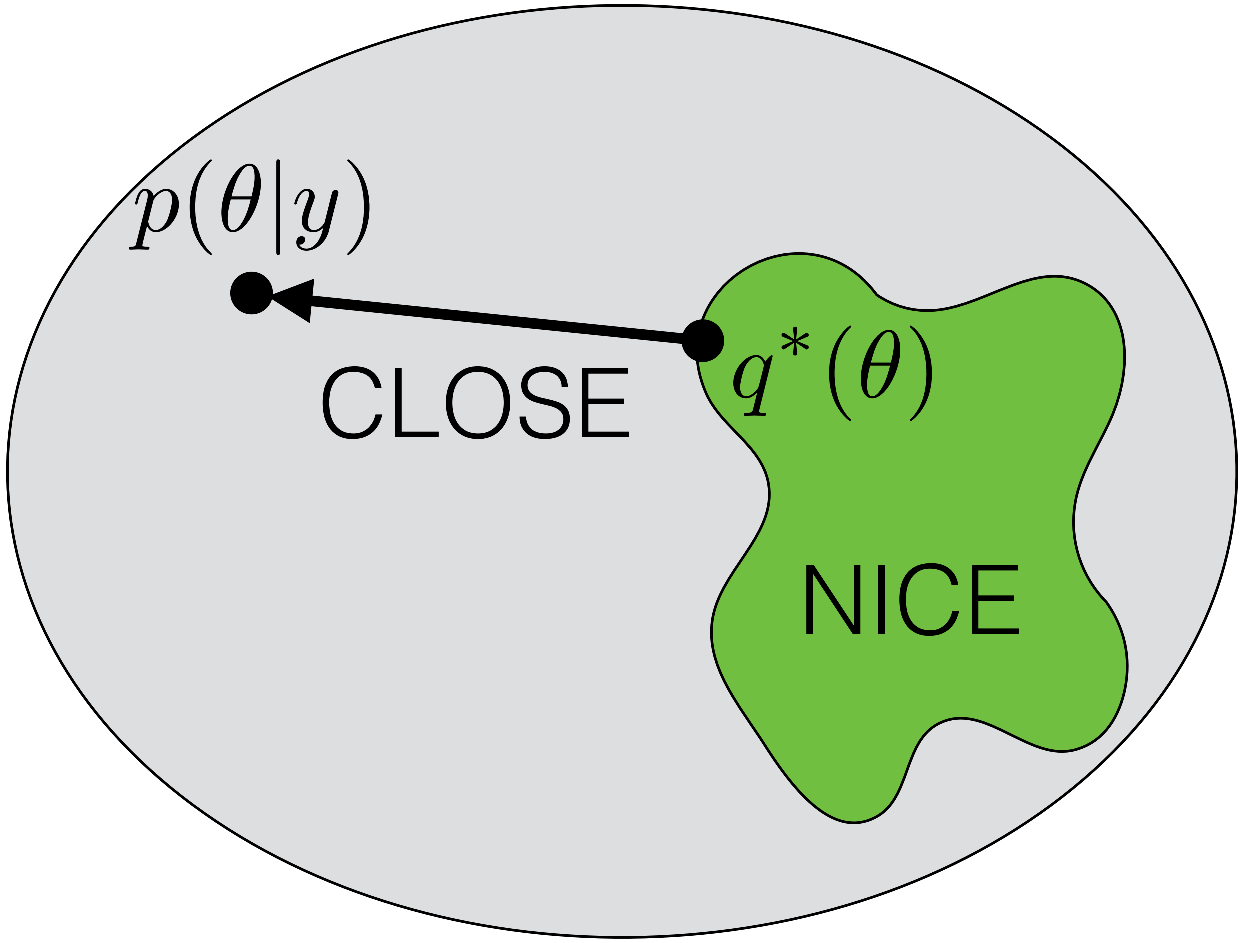

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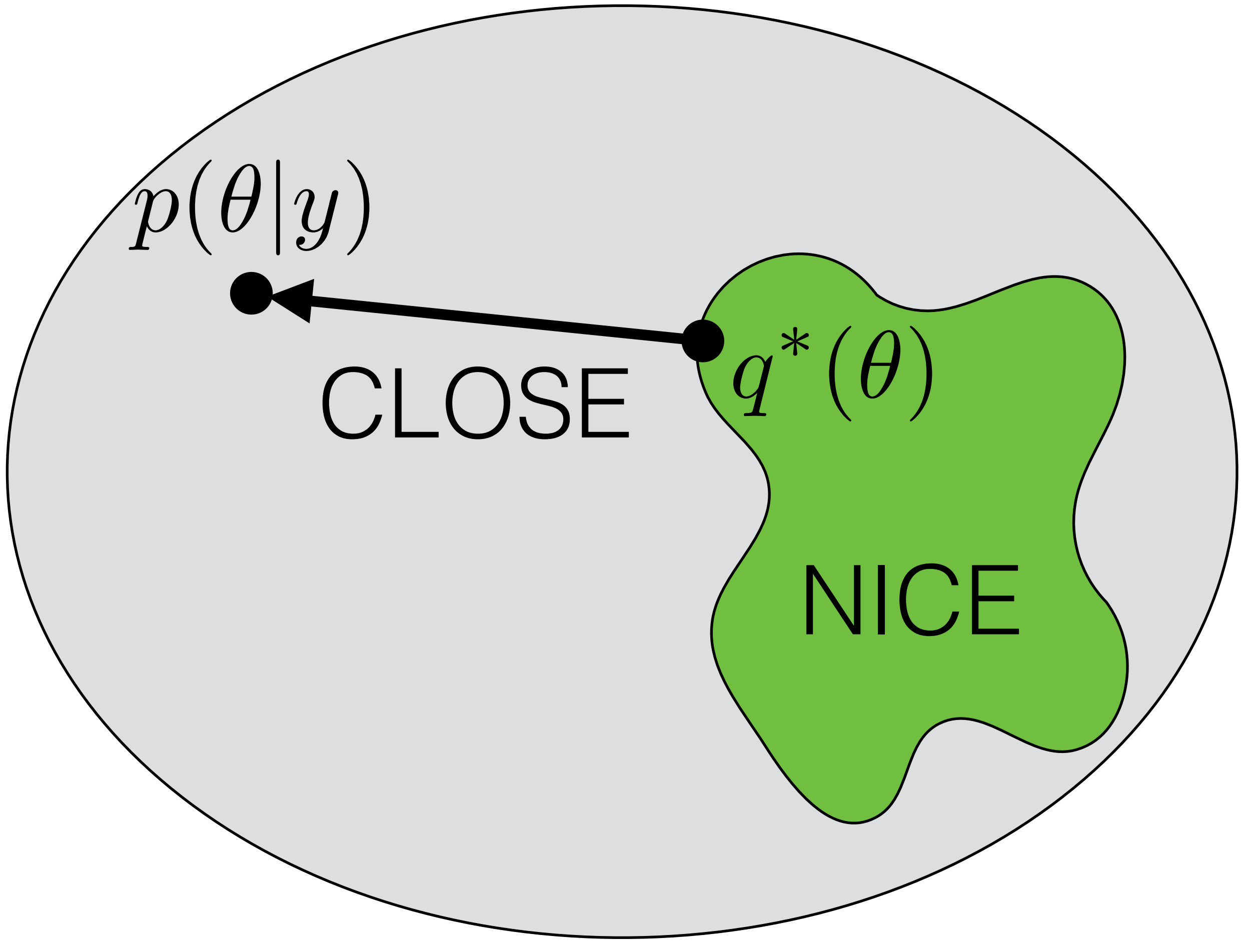

Choose "NICE" distributions

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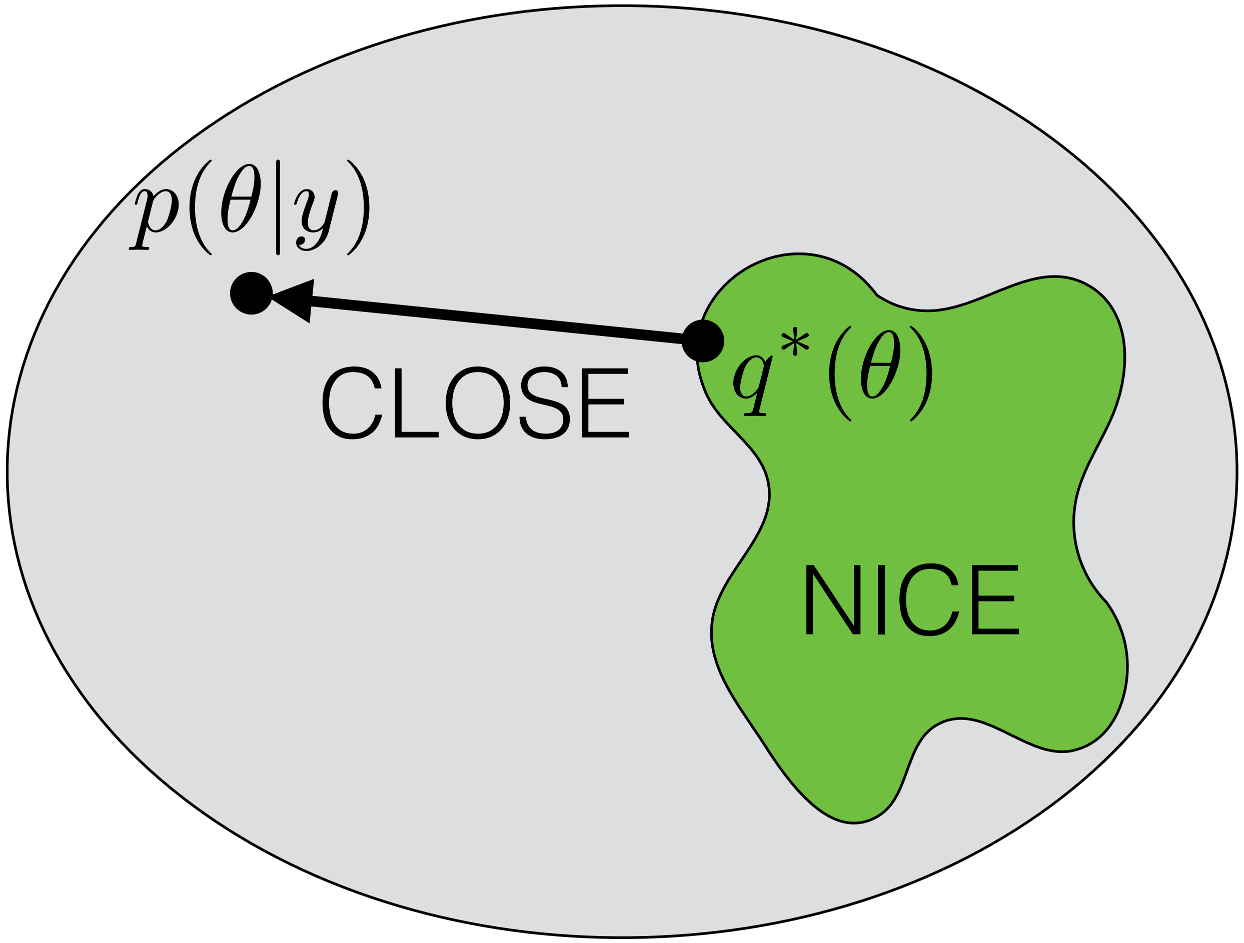

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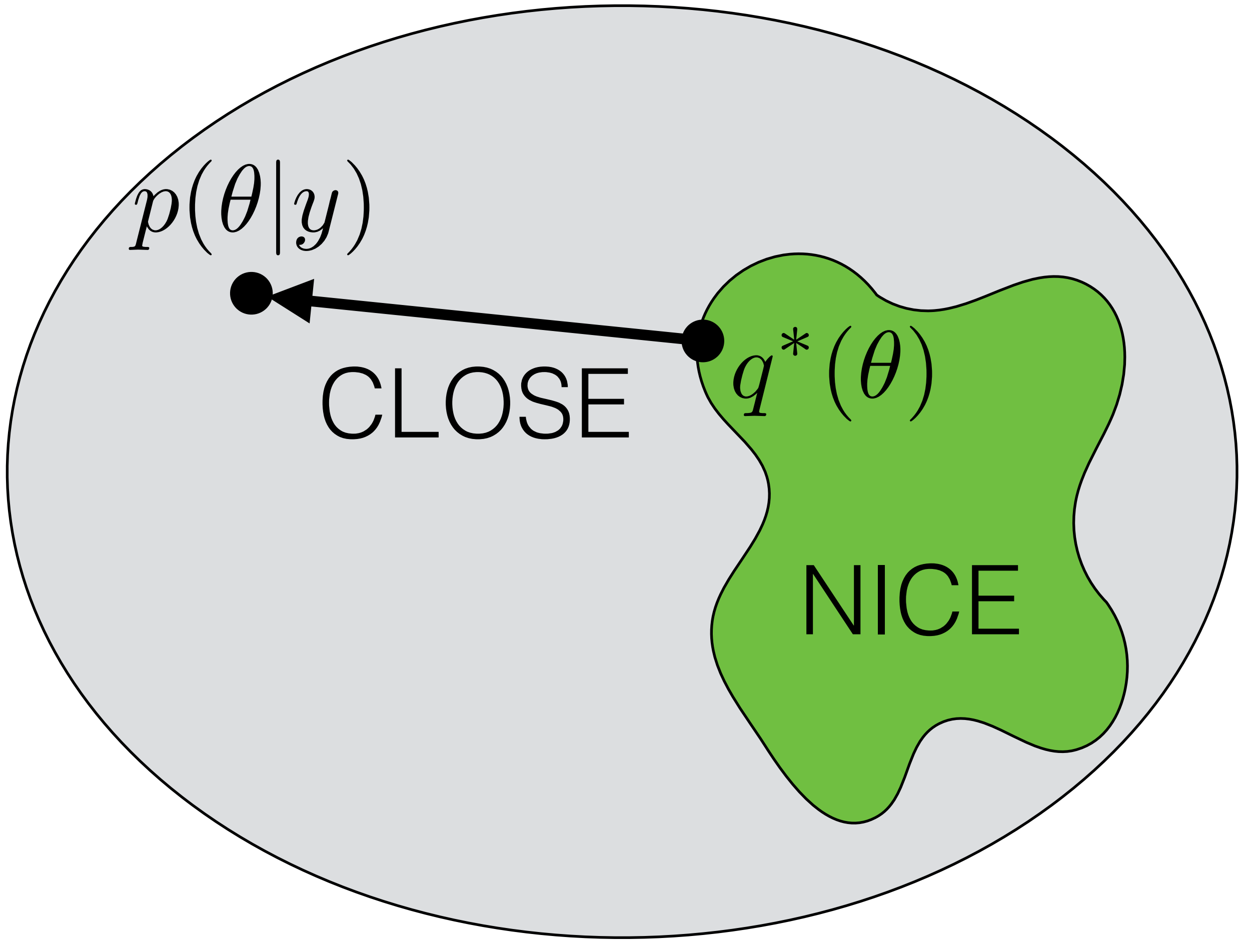

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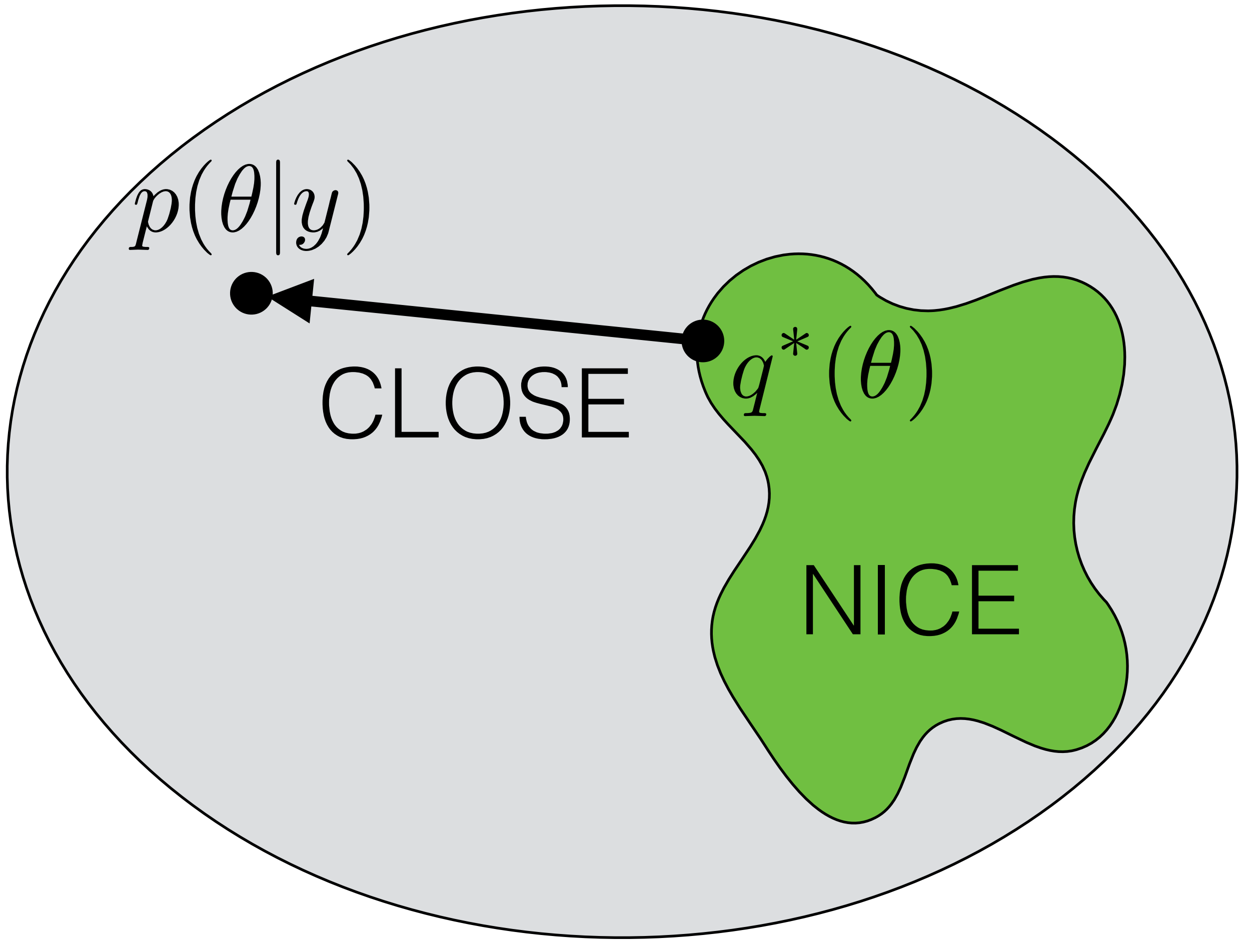

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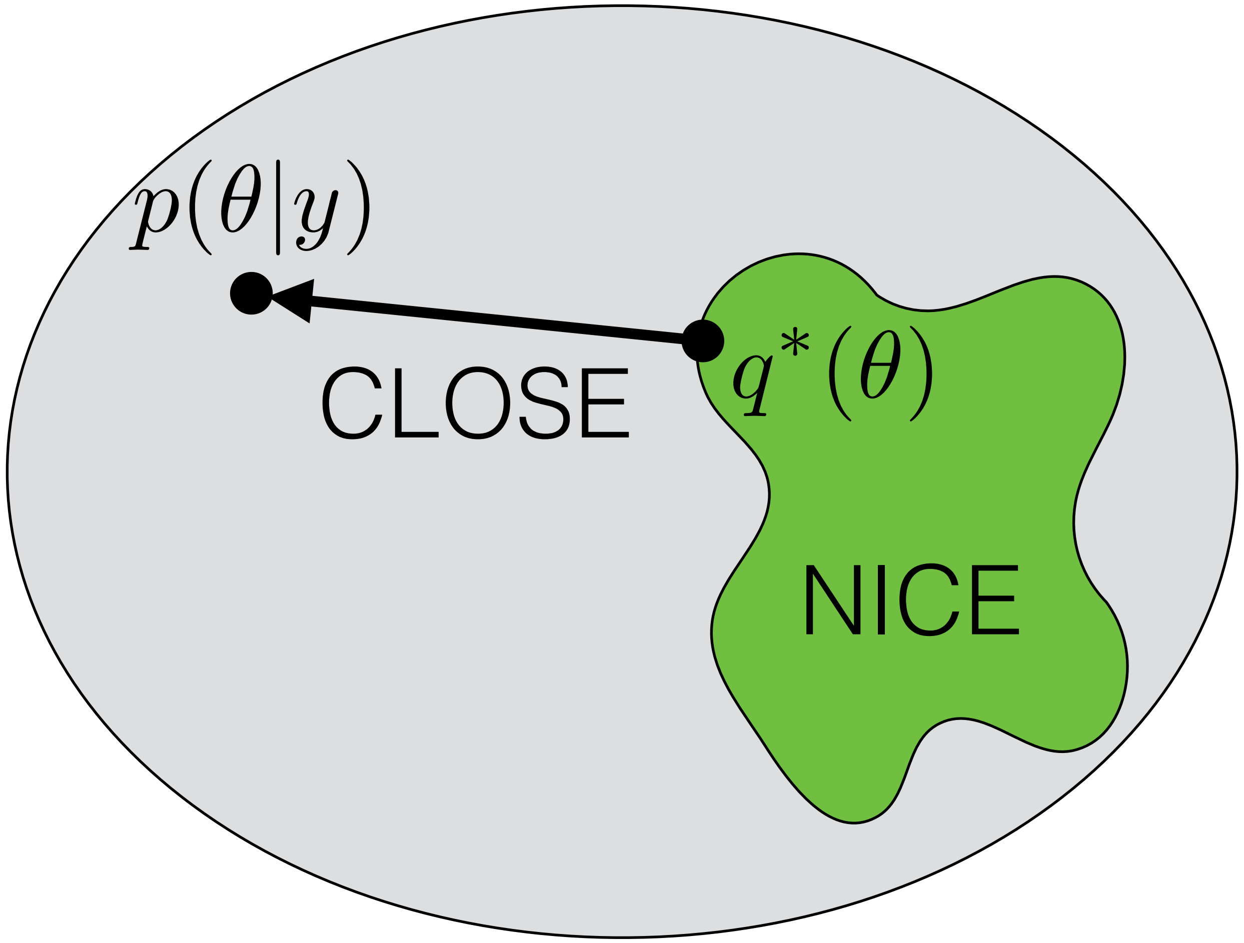

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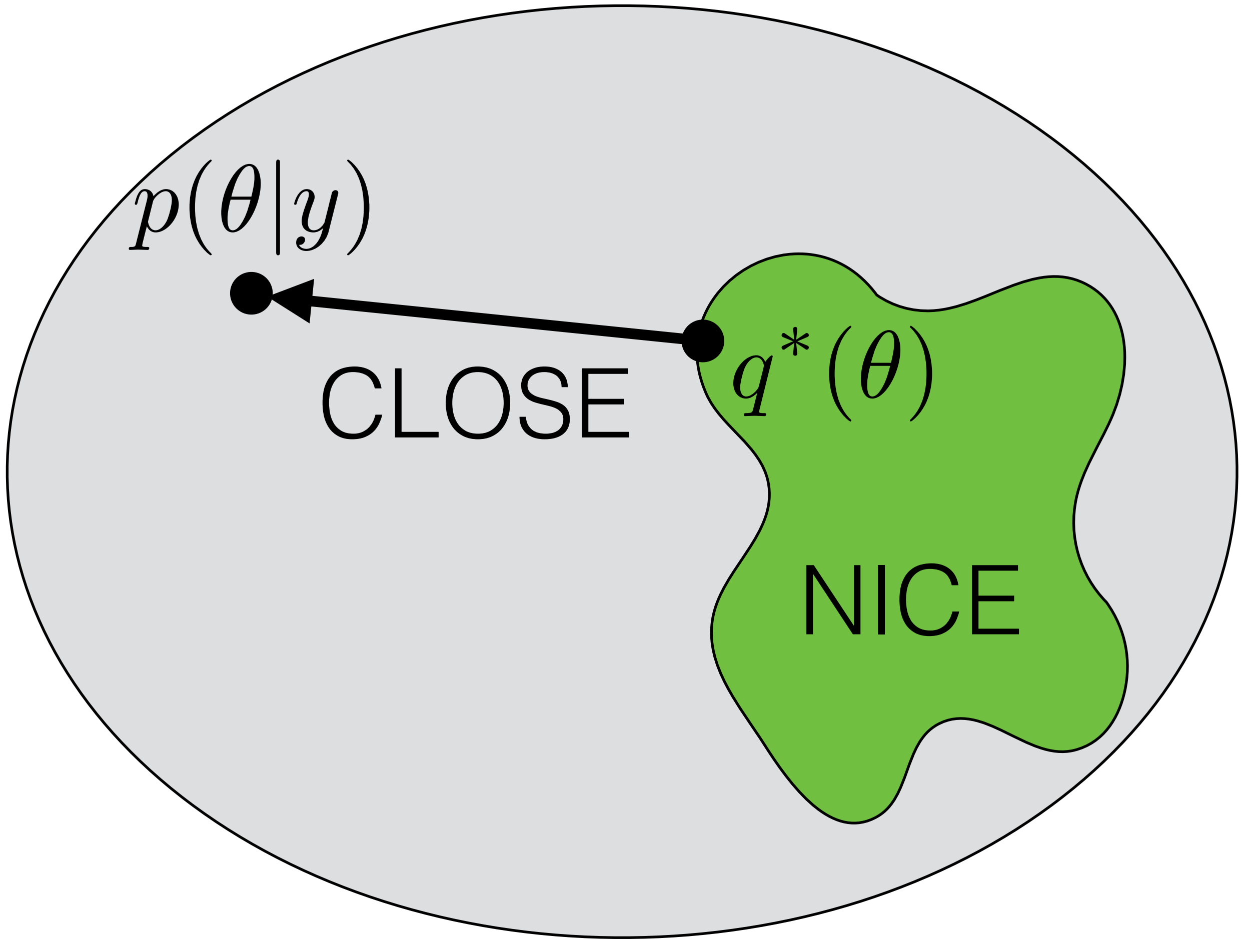

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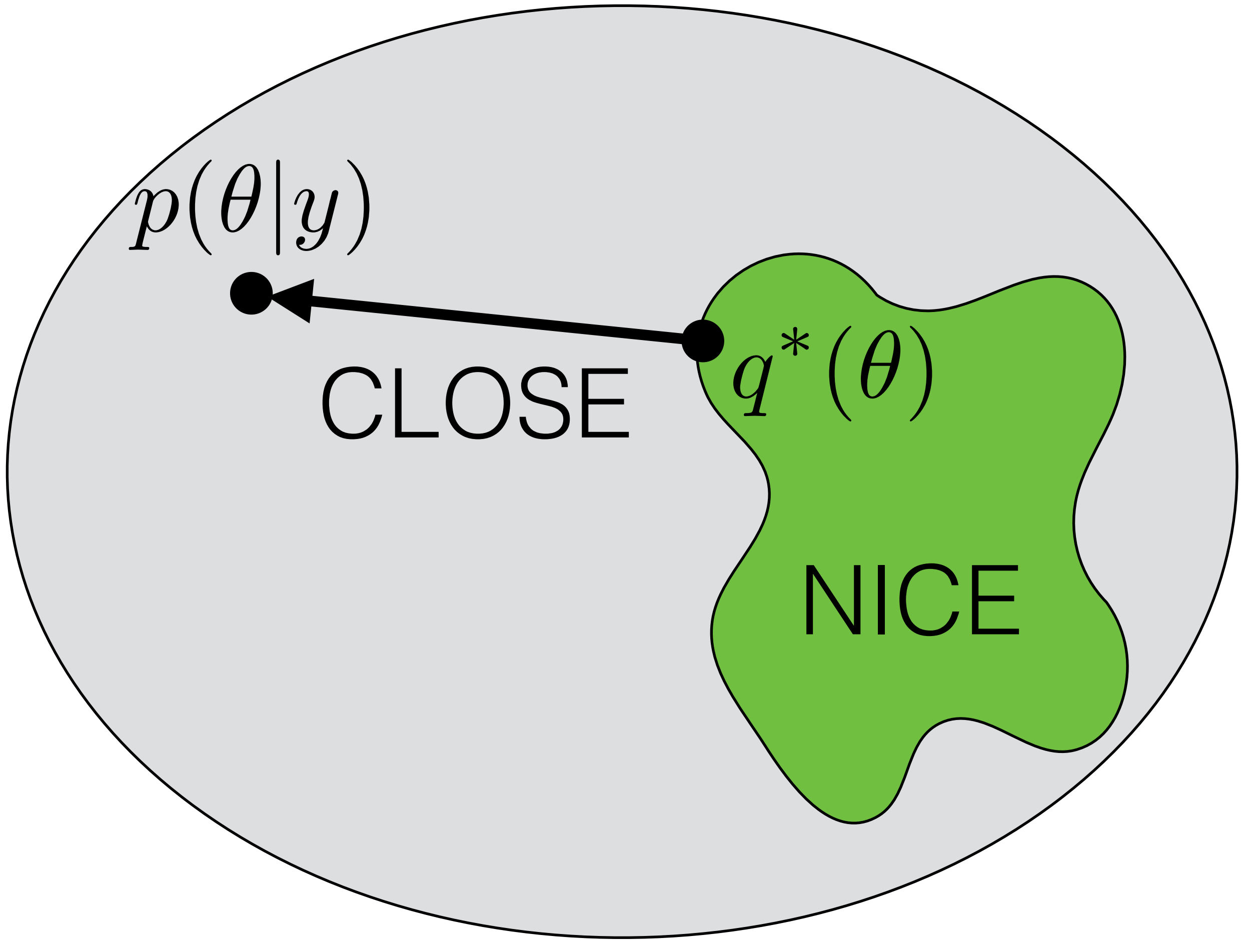

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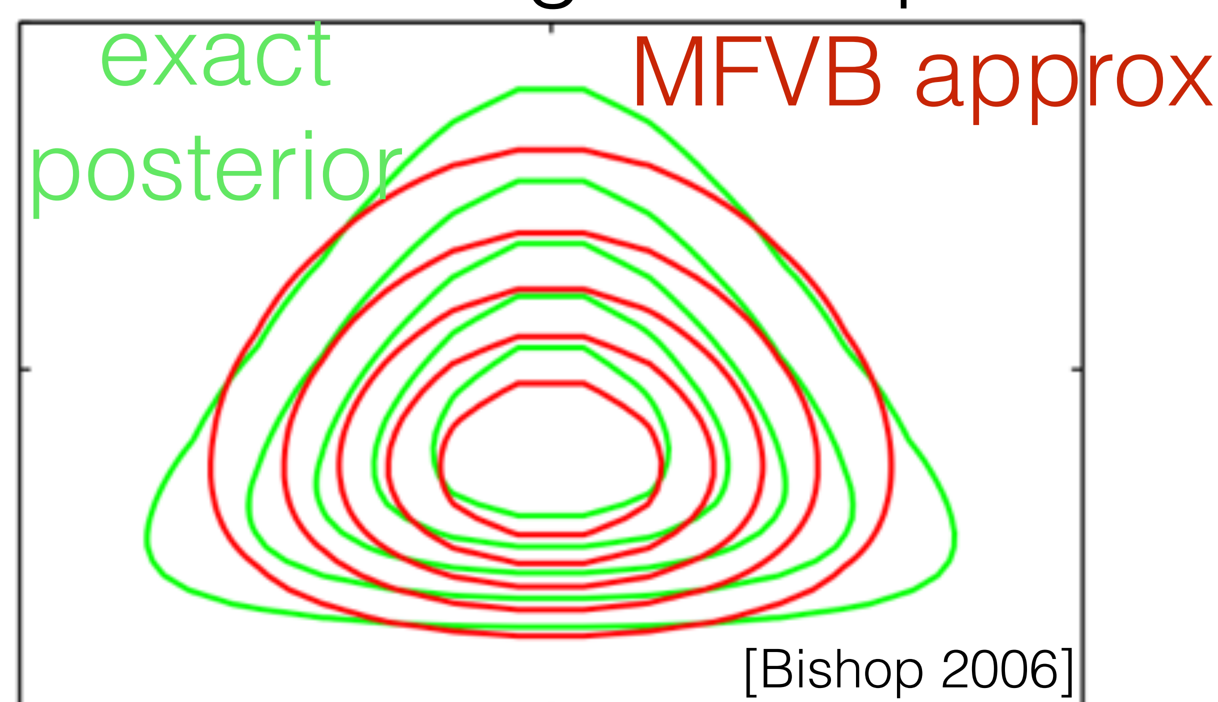

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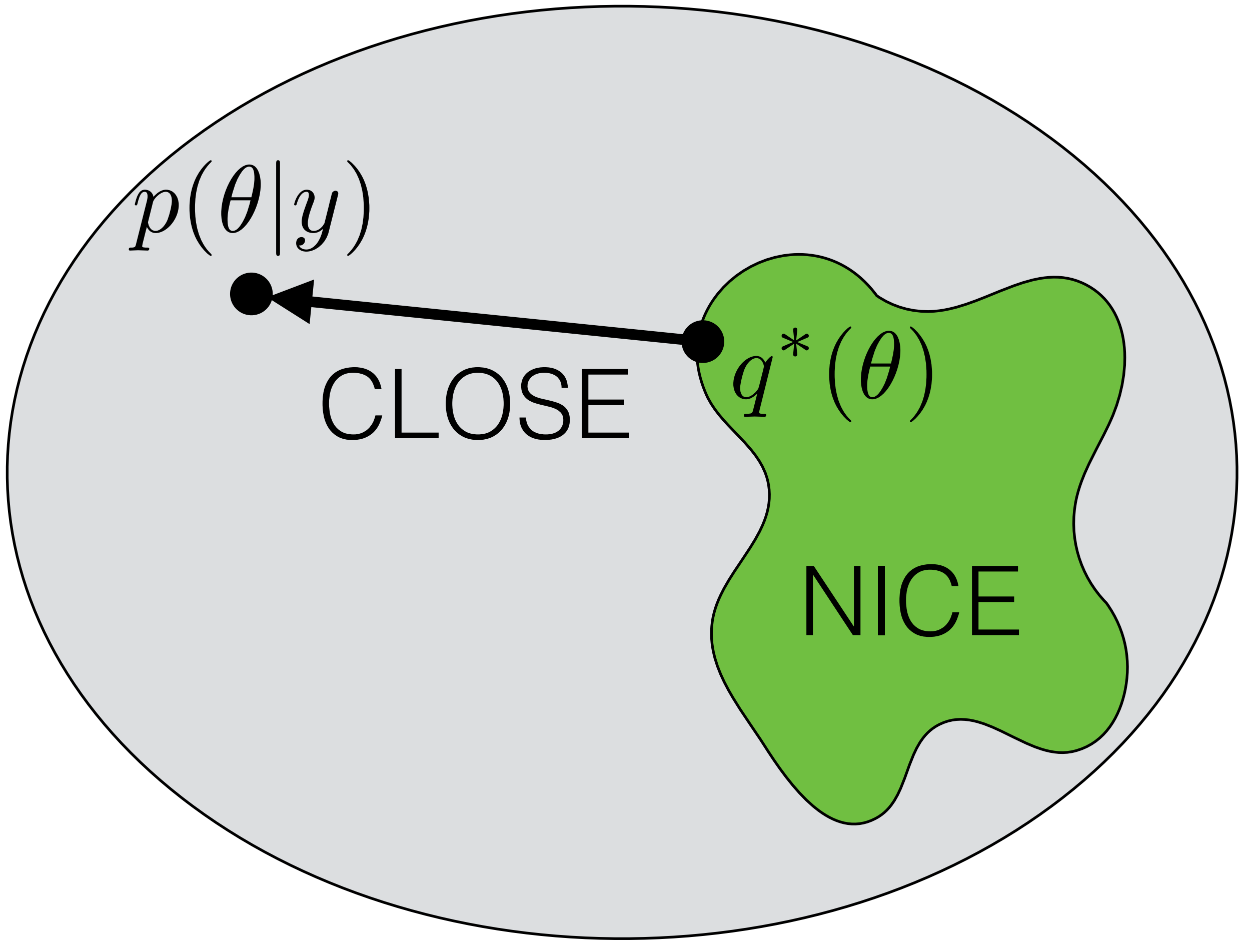

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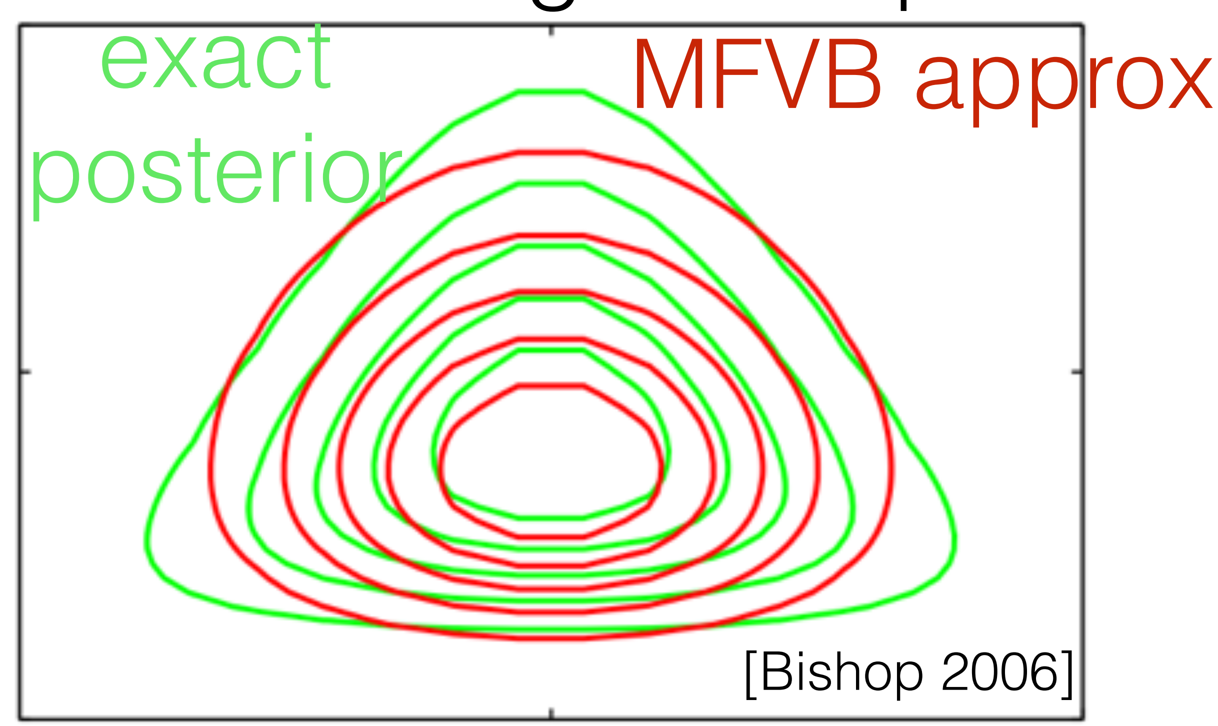

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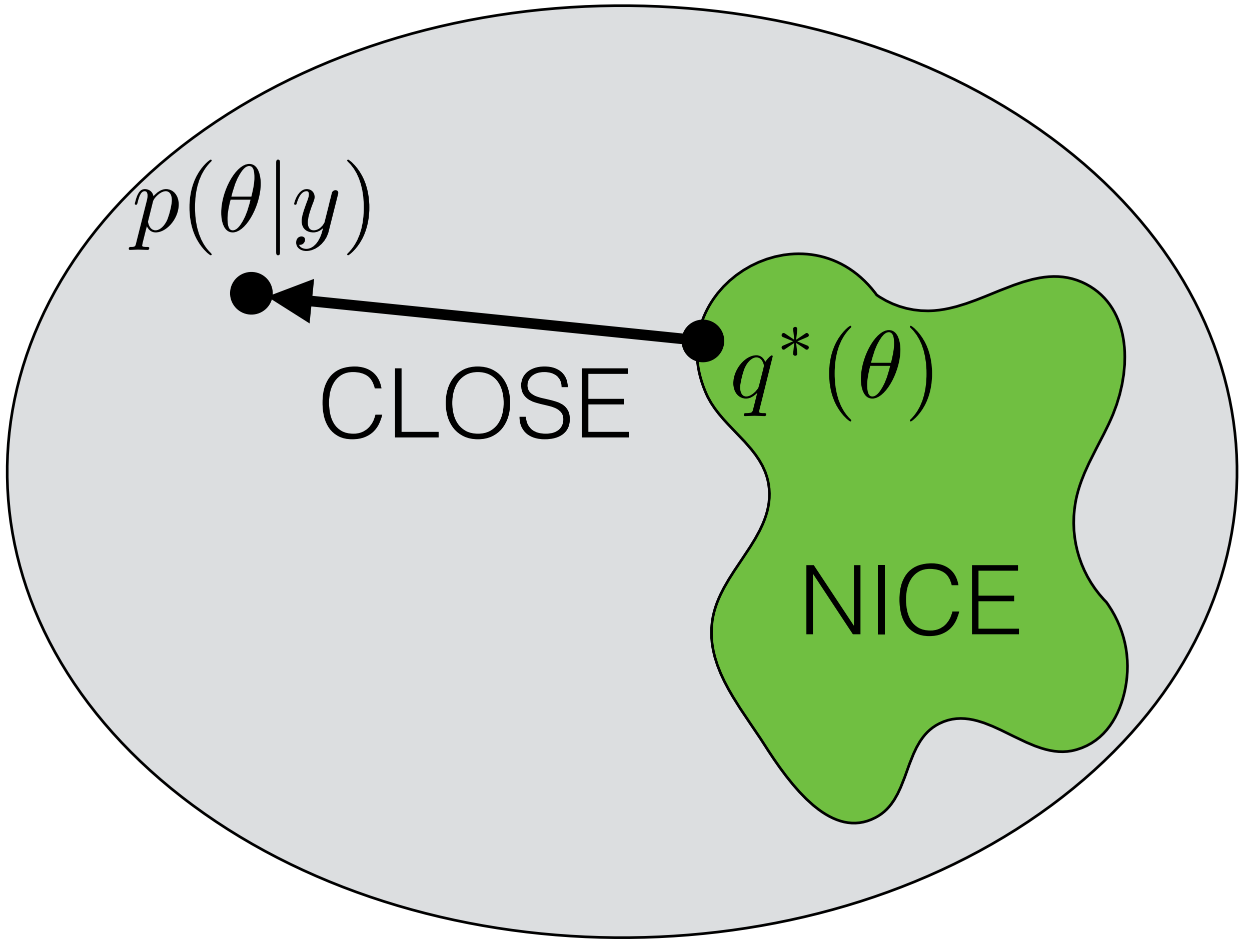

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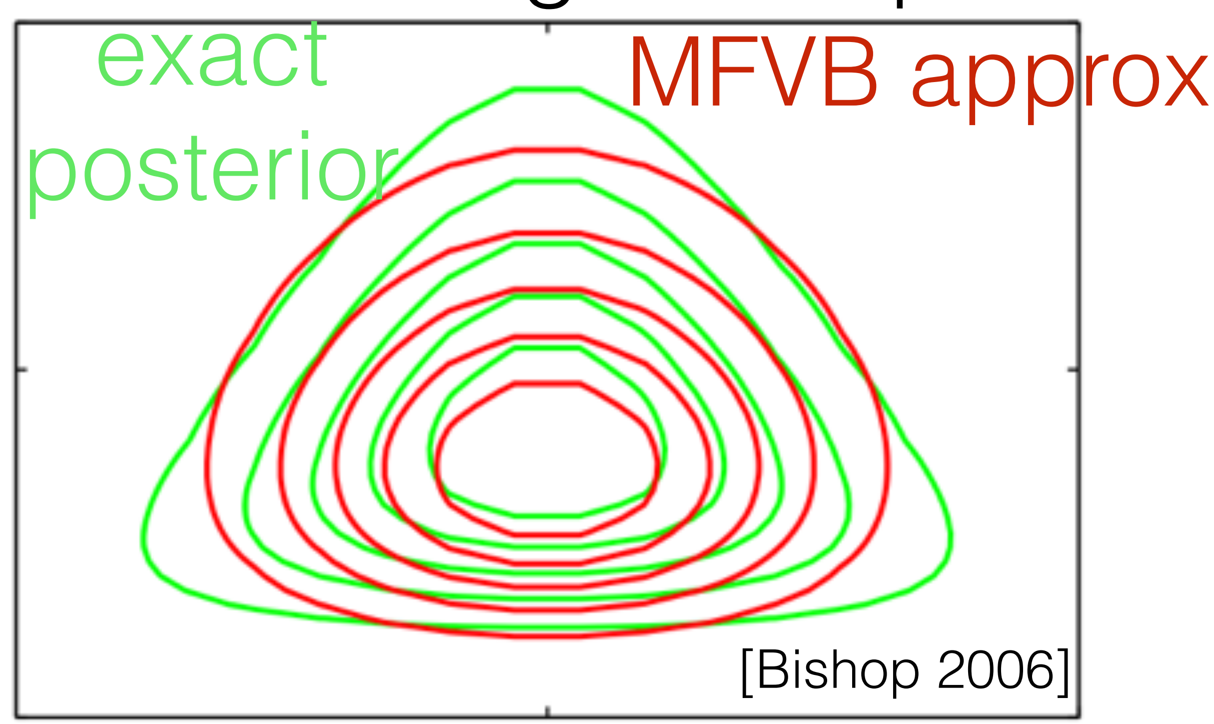

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- One option: Coordinate descent in $q_1, \ldots, q_J$

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

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- Automatic differentiation variational inference (ADVI) [Kucukelbir et al 2015, 2017]

Roadmap

- Bayes & Approximate Bayes review
- What is:
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- Why use MFVB?
- When can we trust MFVB?
- Where do we go from here?

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Midge wing length

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

[CSIRO 2004]

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

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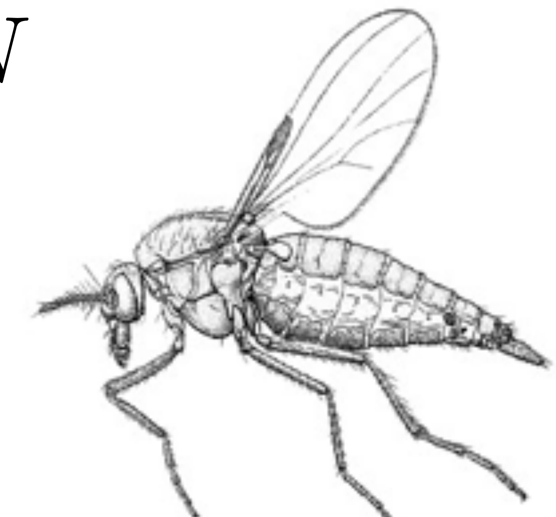

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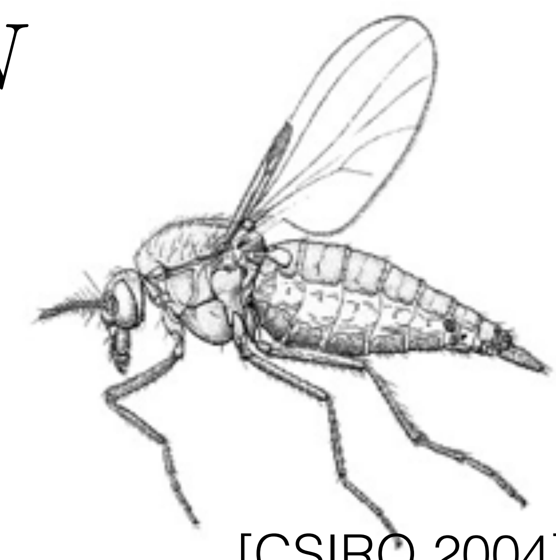

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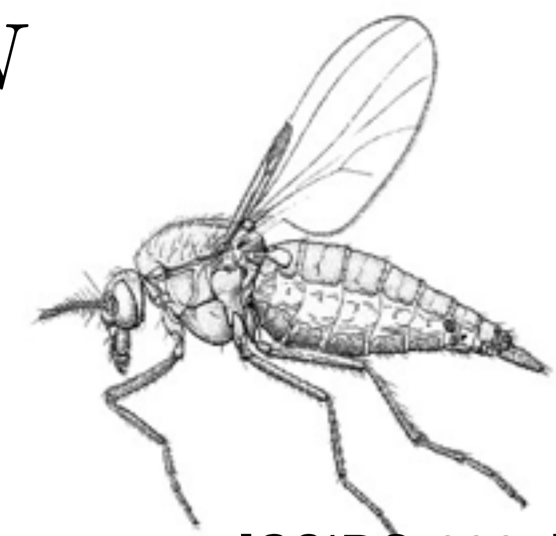

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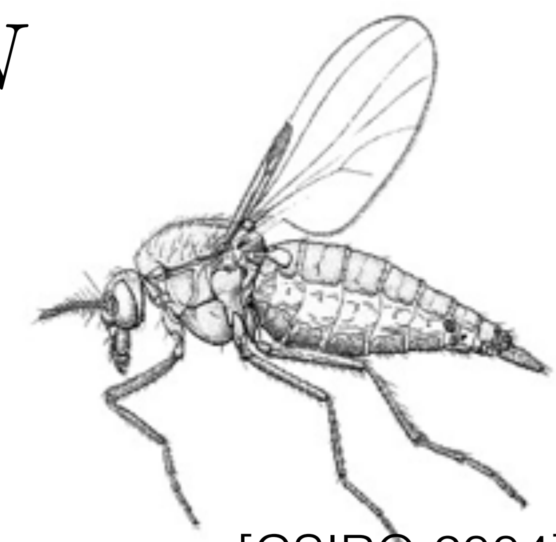

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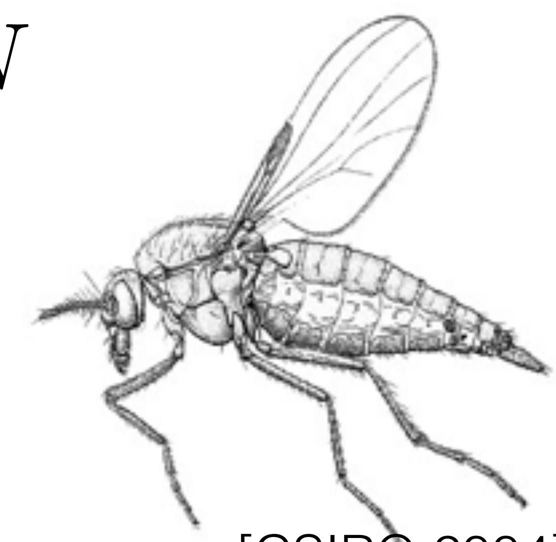

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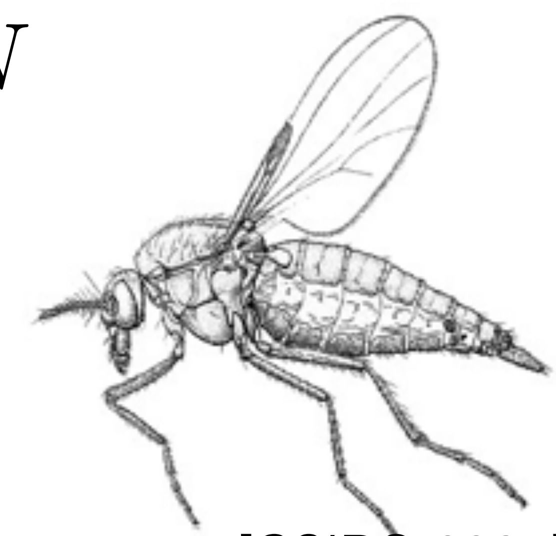

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"variational parameters"

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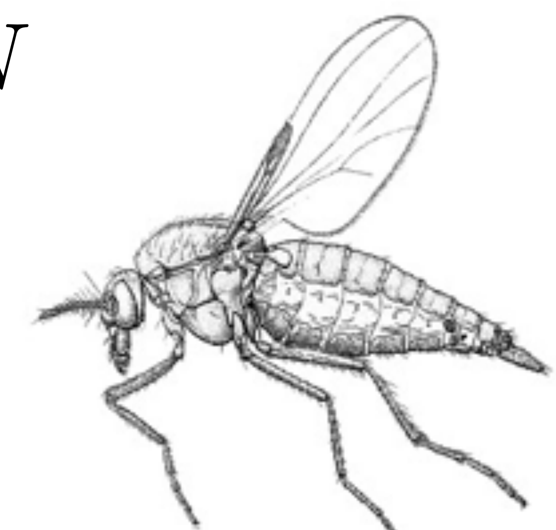

[CSIRO 2004]

- Exercise: check $p(\mu, \tau|y) \neq f_1(\mu, y) f_2(\tau, y)$
- MFVB approximation:

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

- Coordinate descent [Exercise: derive this] [Bishop 2006, Sec 10.1.3]

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

  - Iterate: $(\mu_N, \rho_N) = f(a_N, b_N)$
    $(a_N, b_N) = g(\mu_N, \rho_N)$

"variational parameters"

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

Midge wing length

- Catalogued midge wing lengths (mm) $y = (y_1, \ldots, y_N)$
- Parameters of interest: population mean and precision $\theta = (\mu, \tau)$
- Model (conjugate prior): [Exercise: find the posterior]

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

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

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

[CSIRO 2004]

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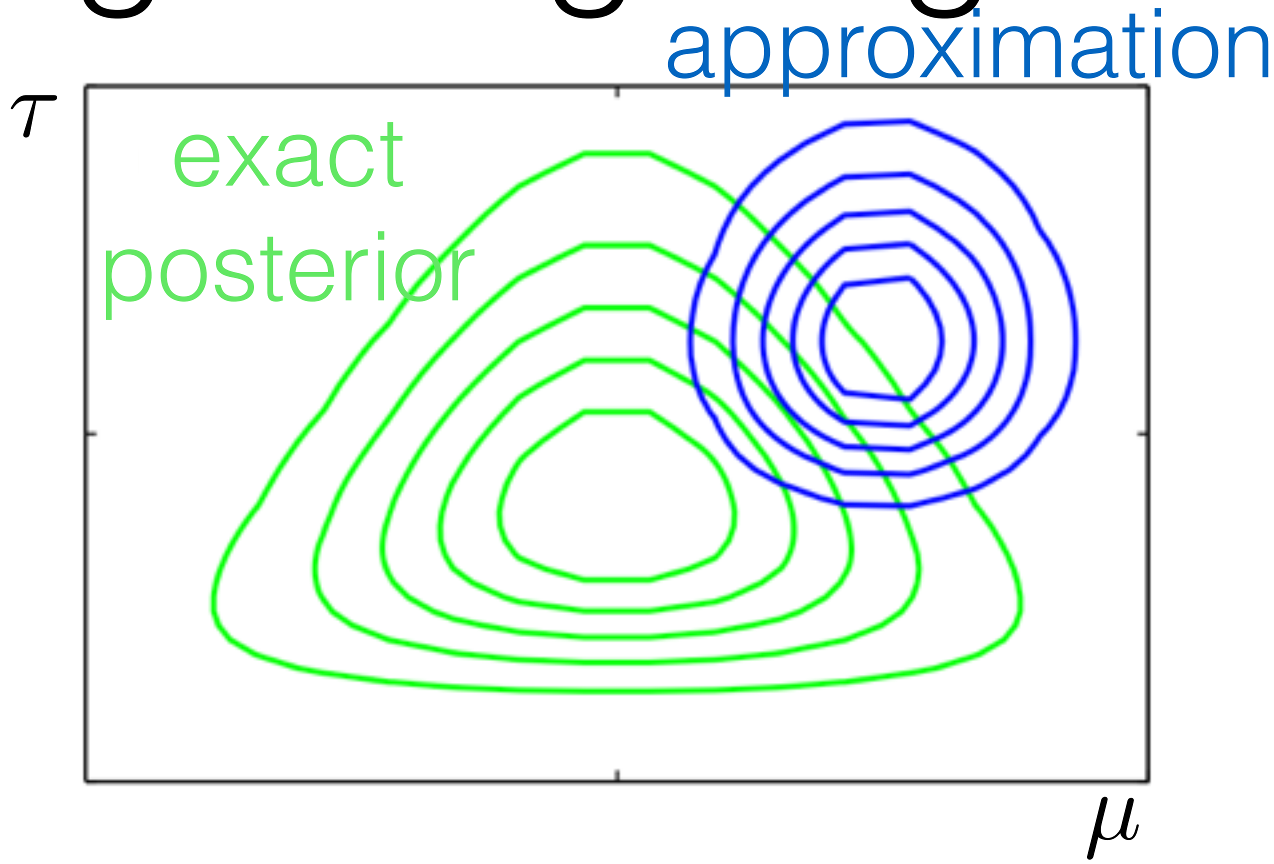

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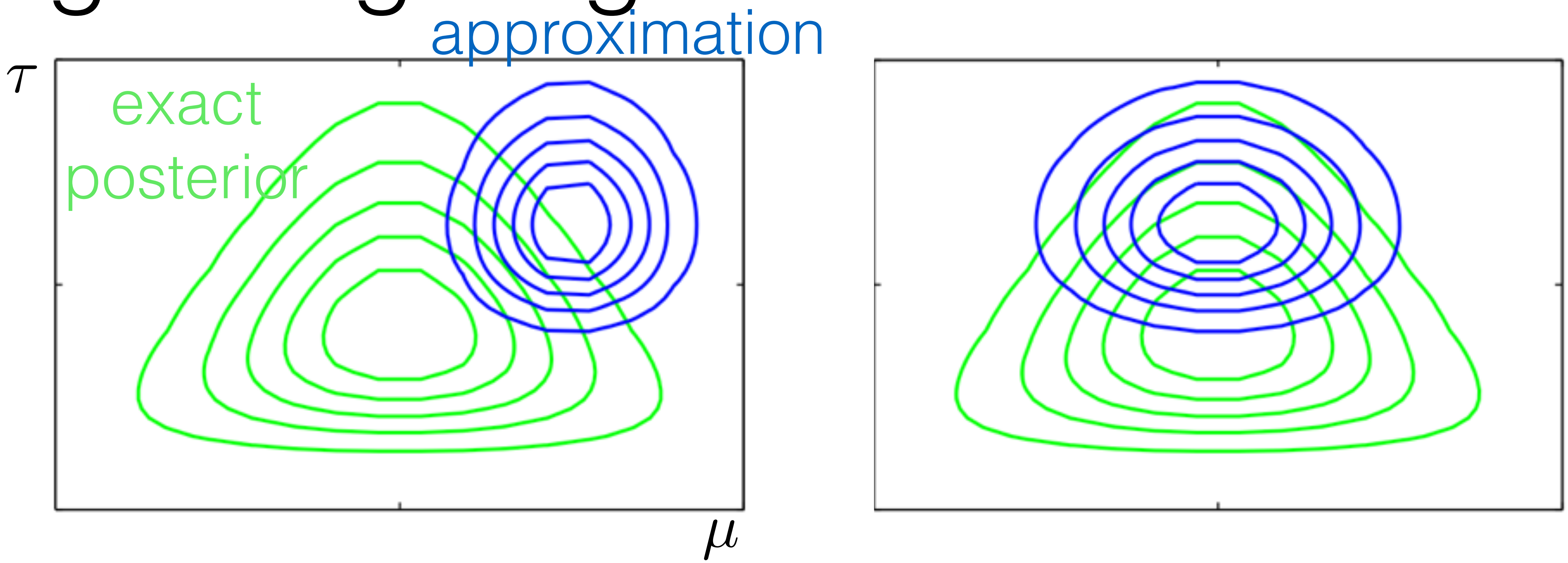

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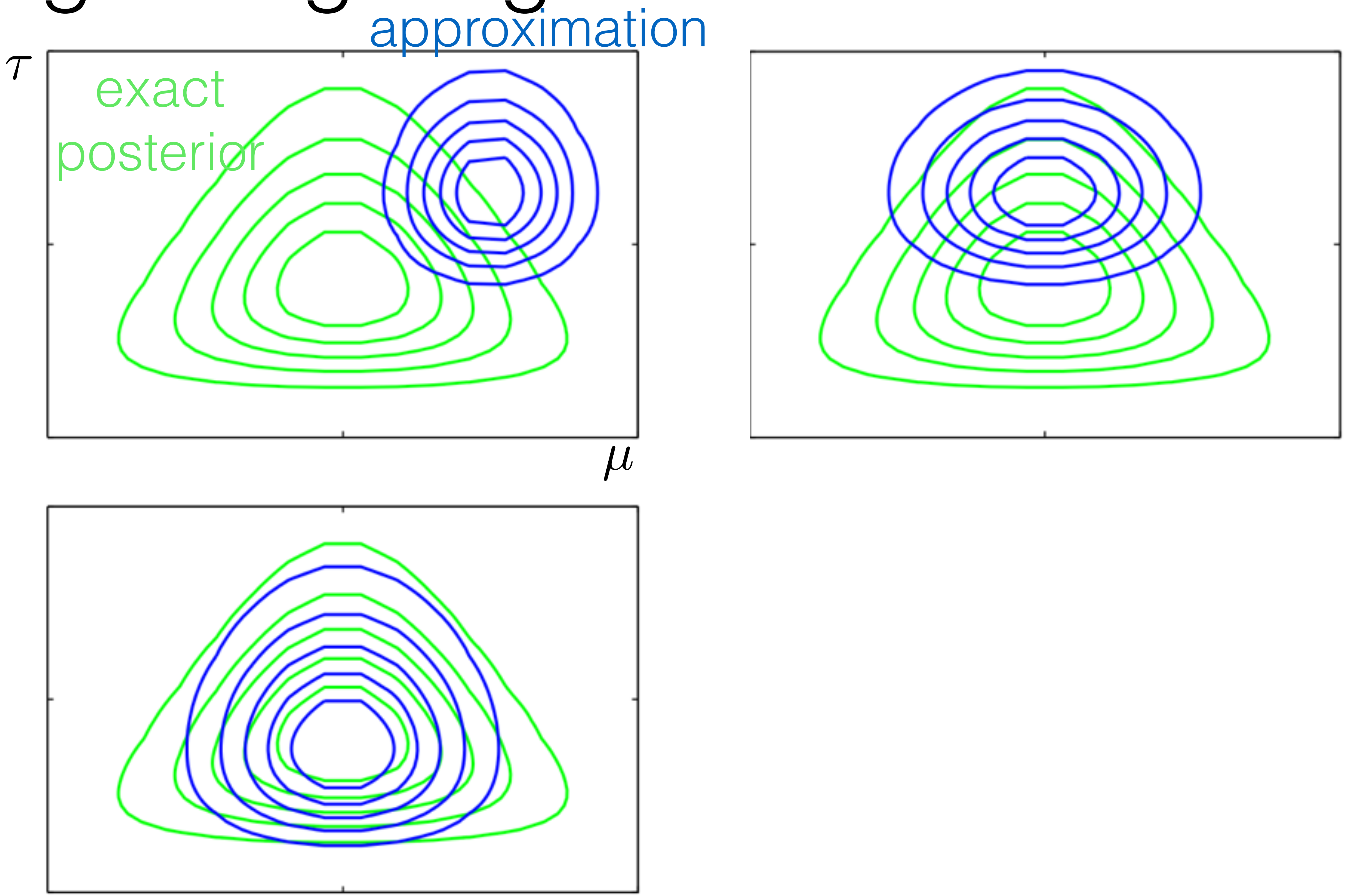

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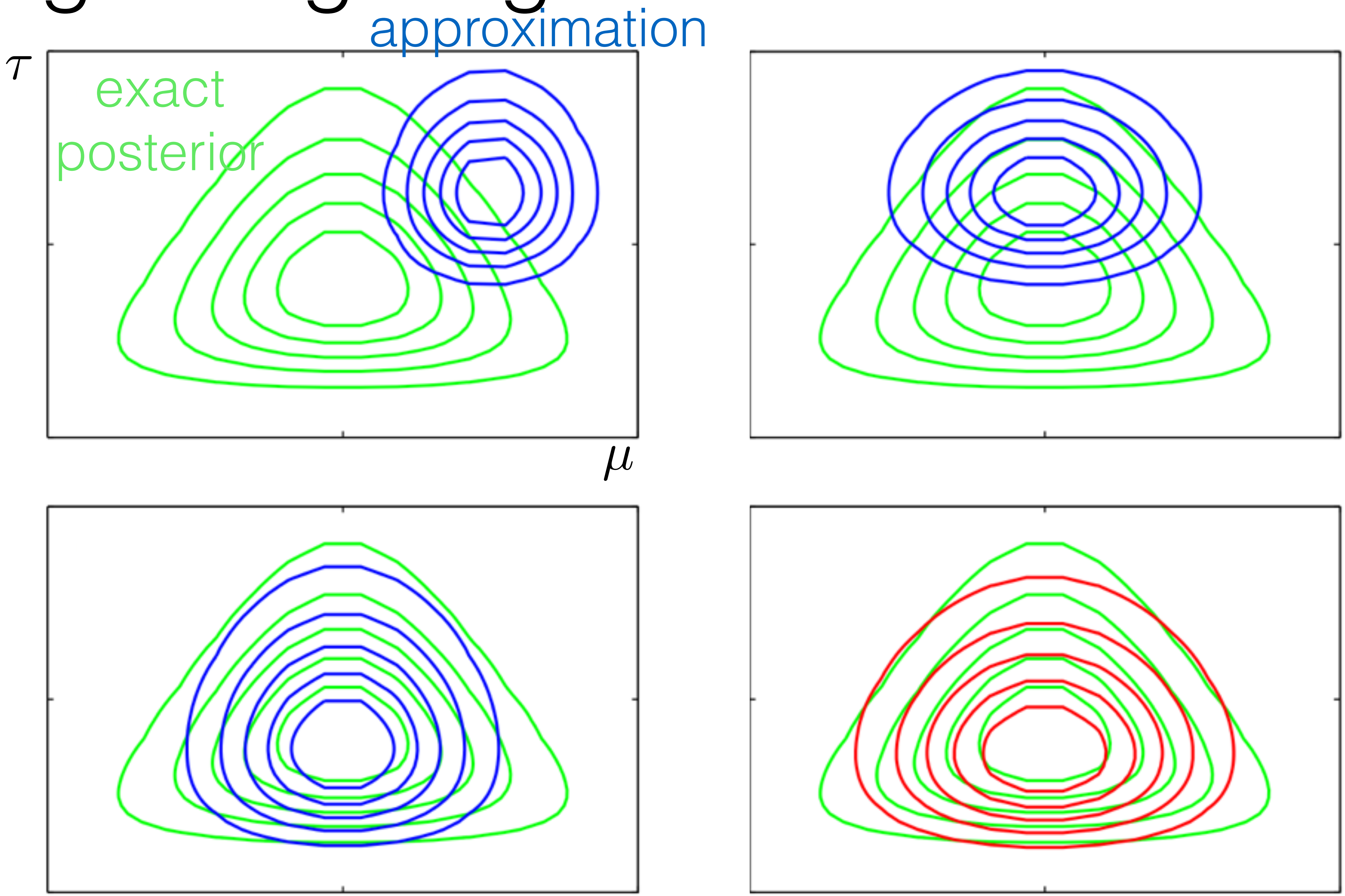

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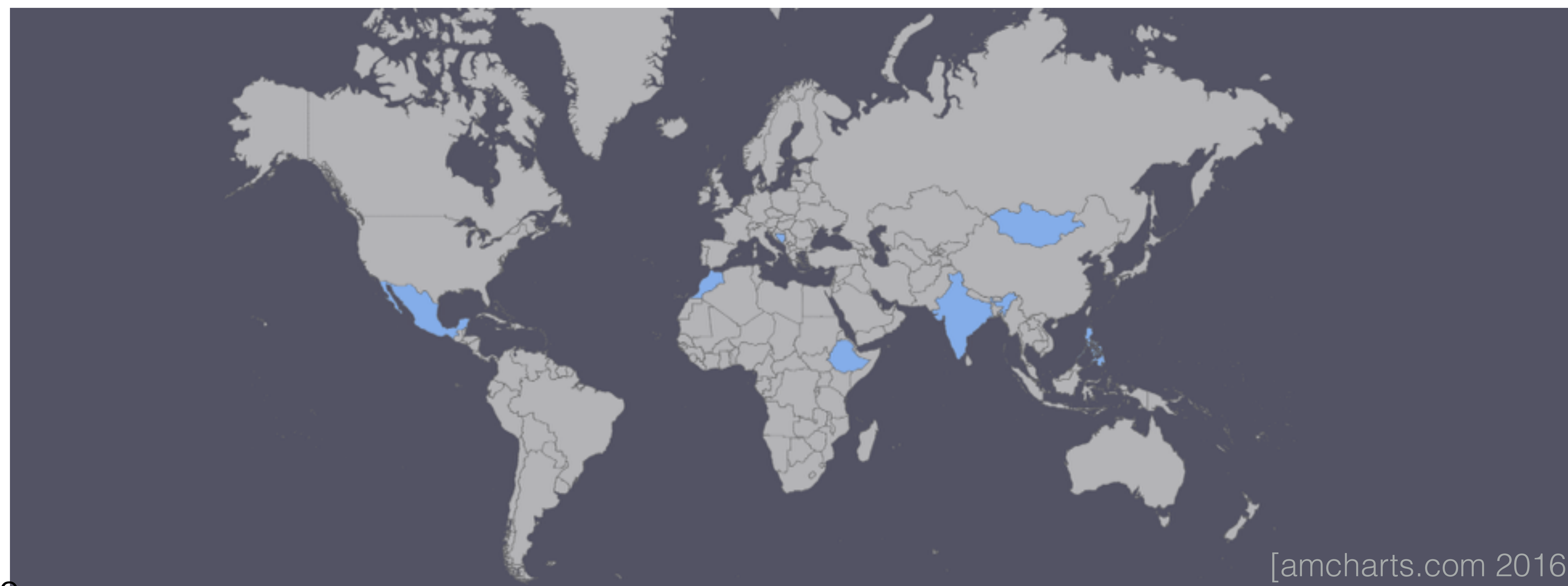
Microcredit Experiment



Microcredit Experiment

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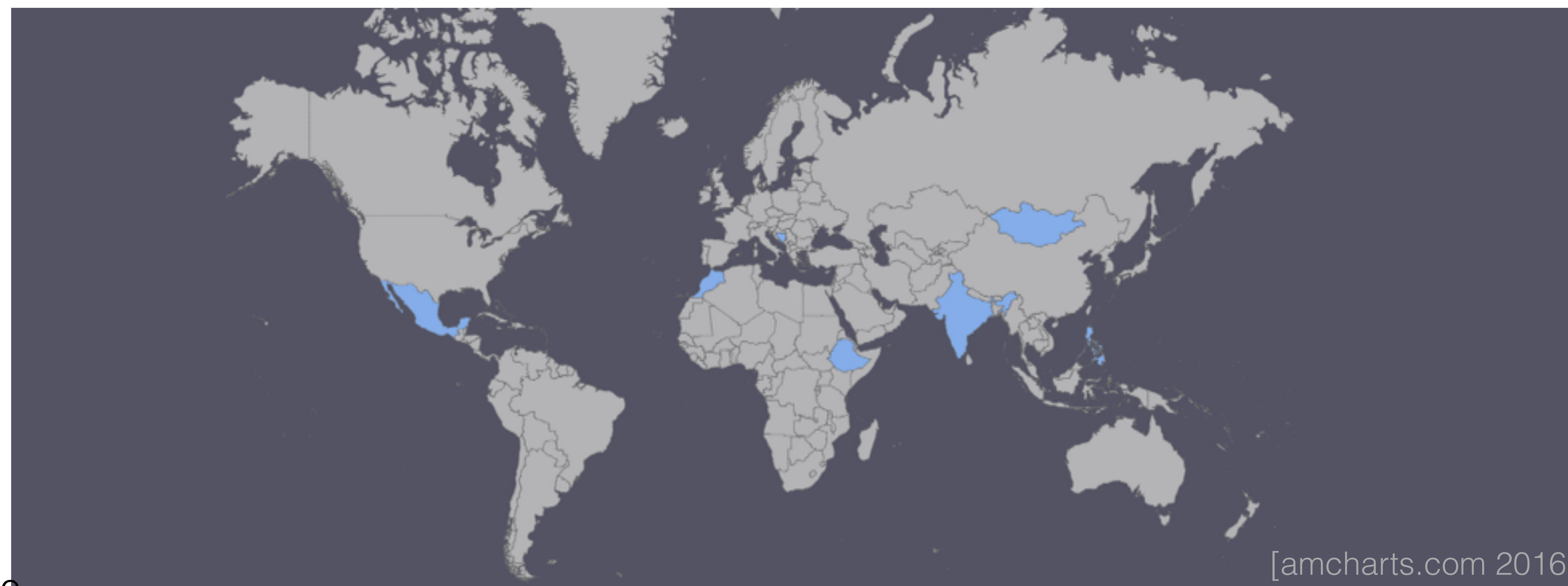

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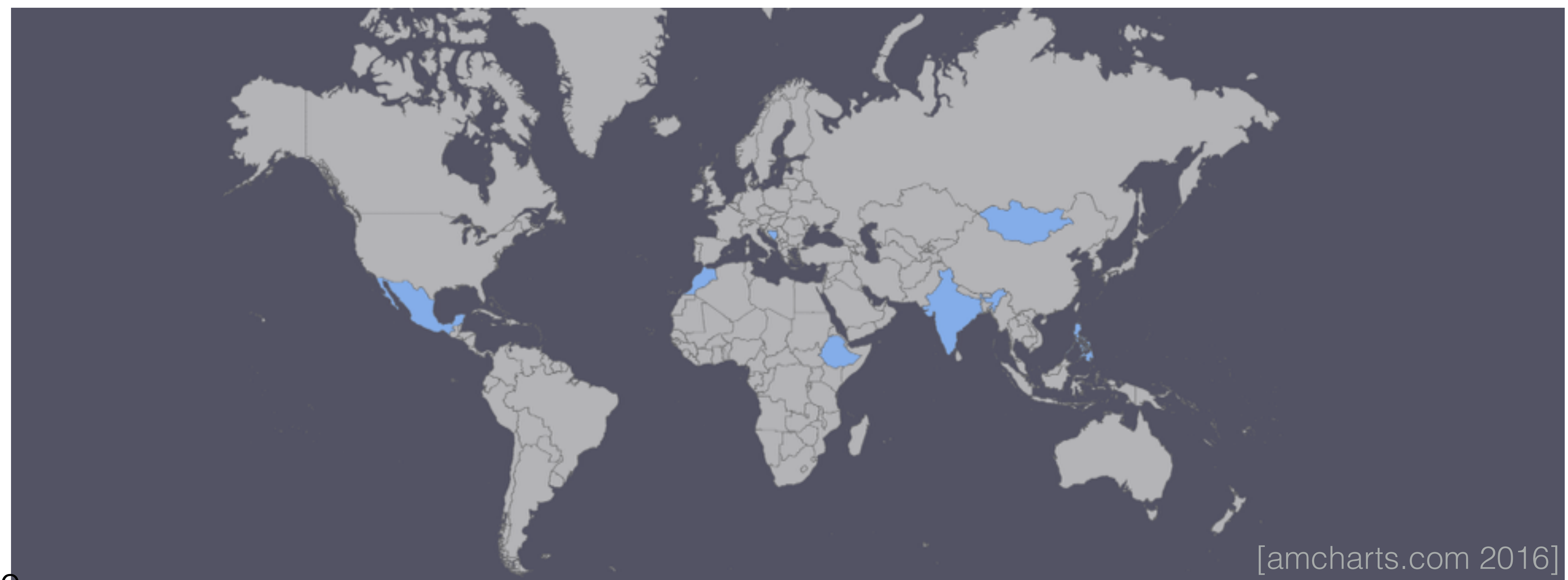

Microcredit Experiment

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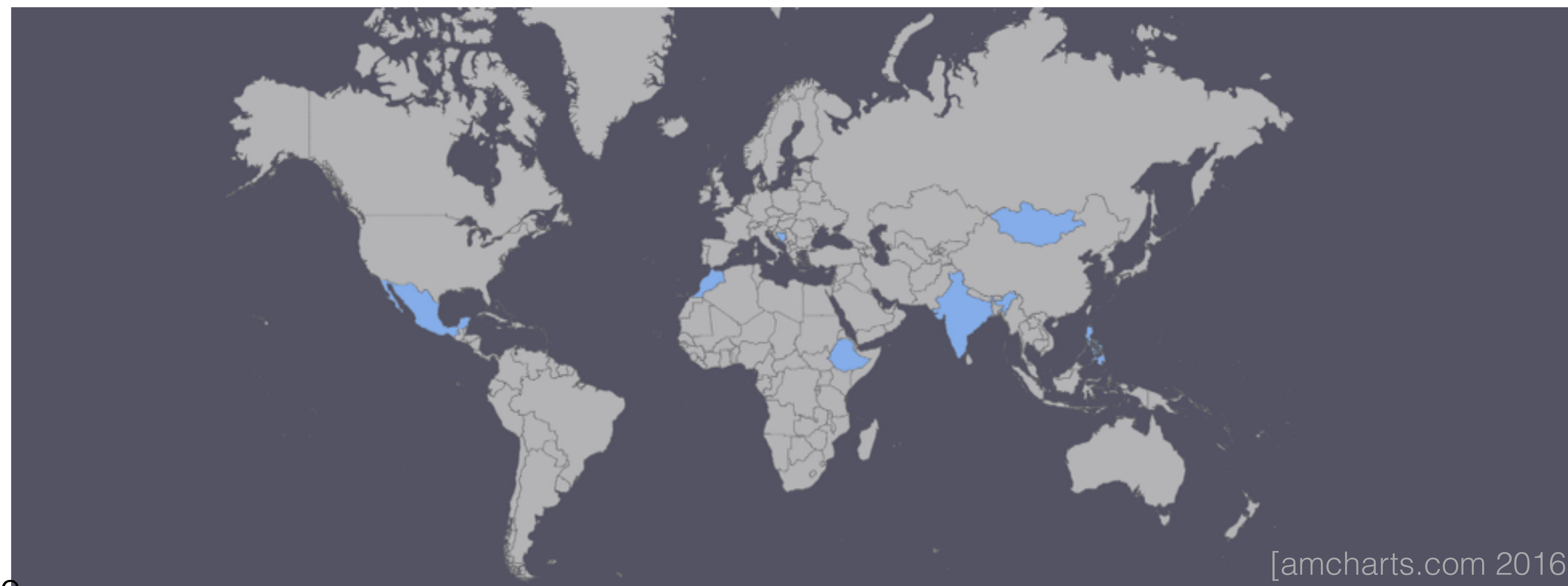

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$$y_{kn}$$

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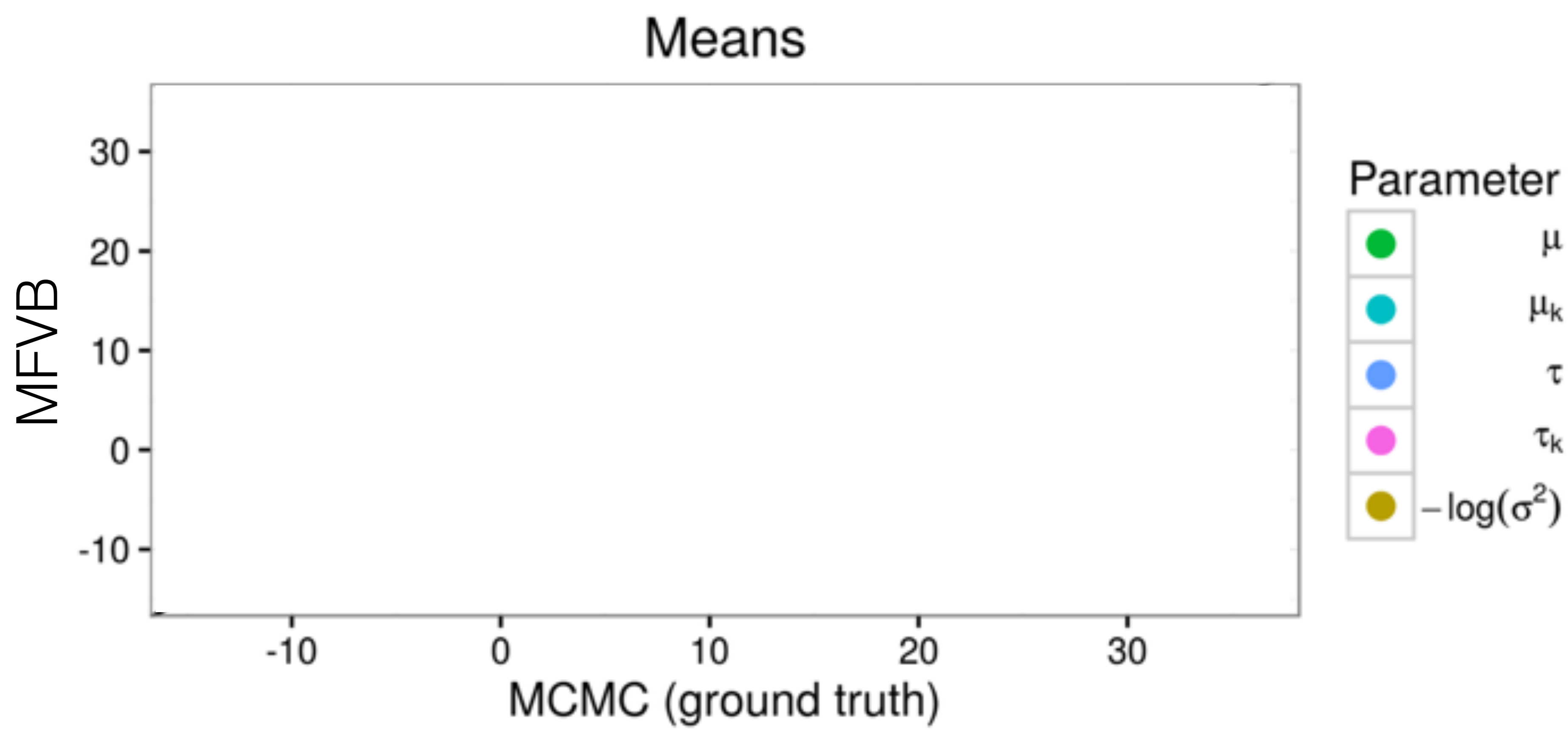
$$\sigma_k^{-2} \overset{iid}{\sim} \Gamma(a, b) \qquad C \sim \mathrm{Sep\&LKJ}(\eta, c, d)$$

Microcredit

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

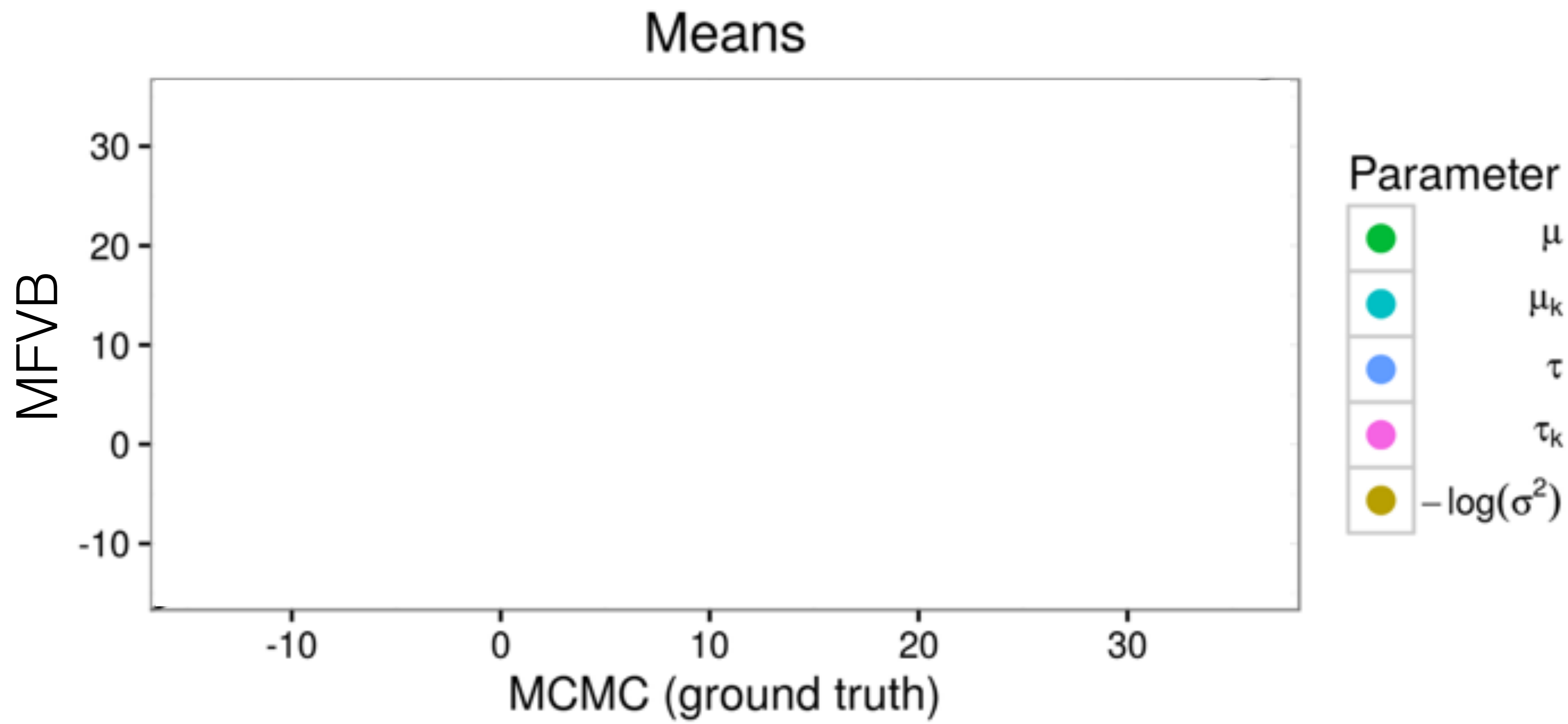
Microcredit



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

Microcredit

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



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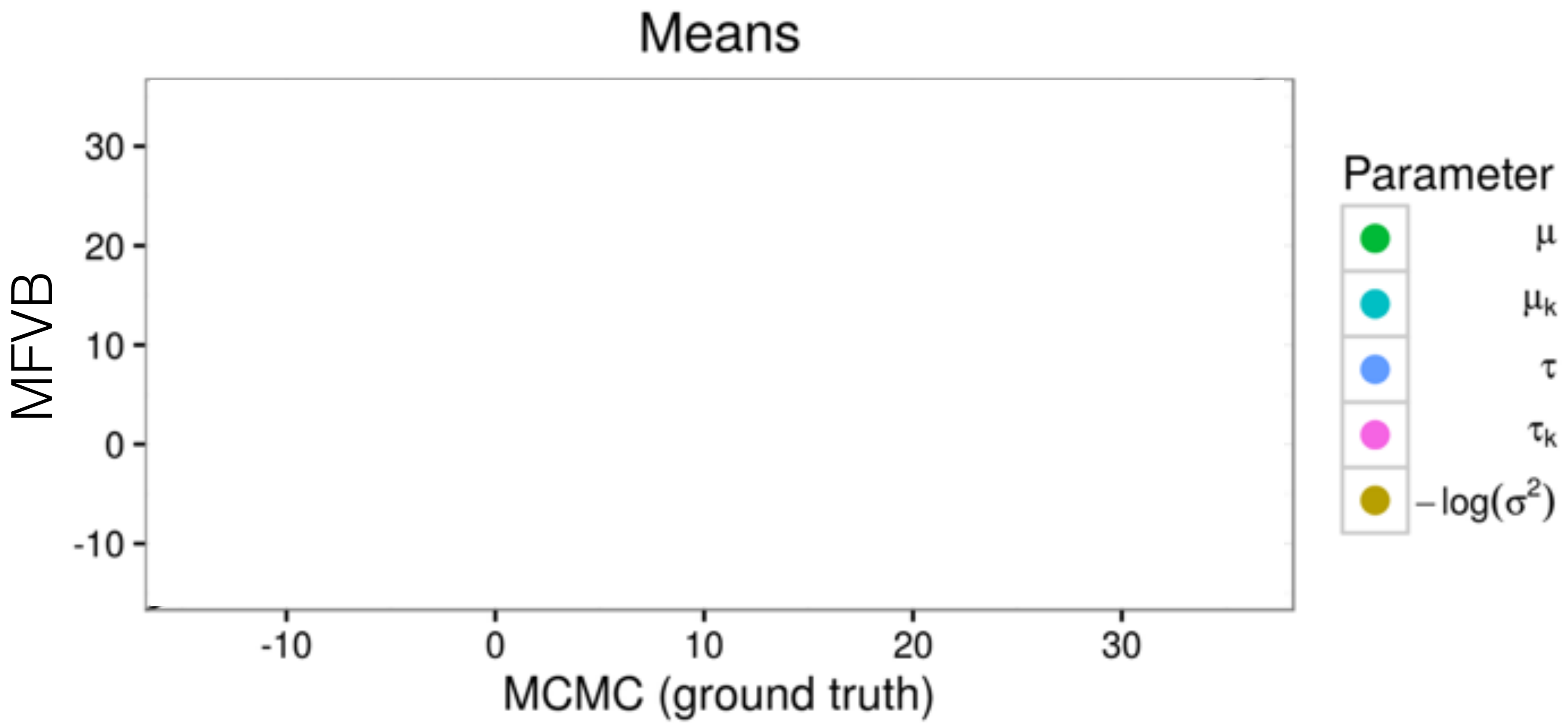

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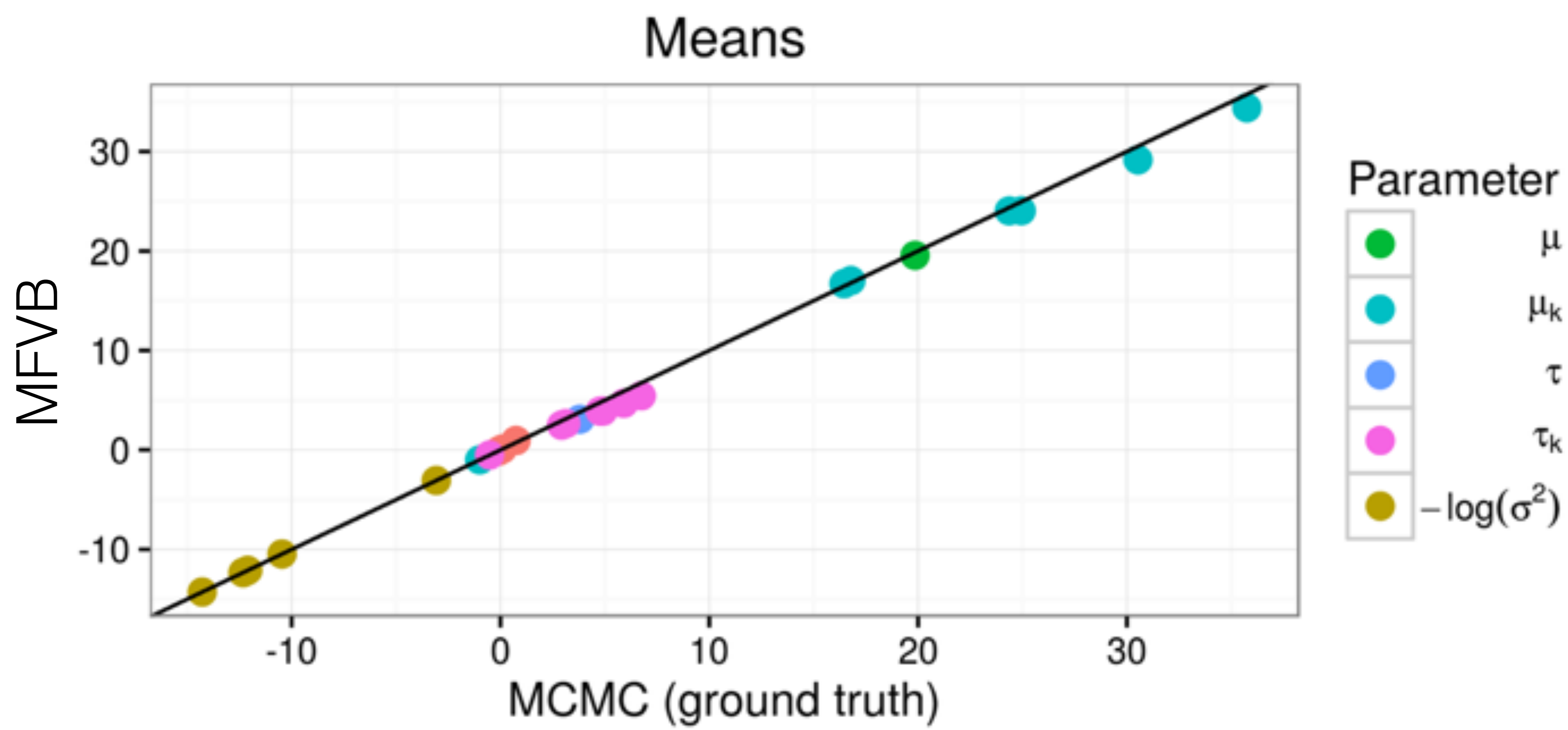

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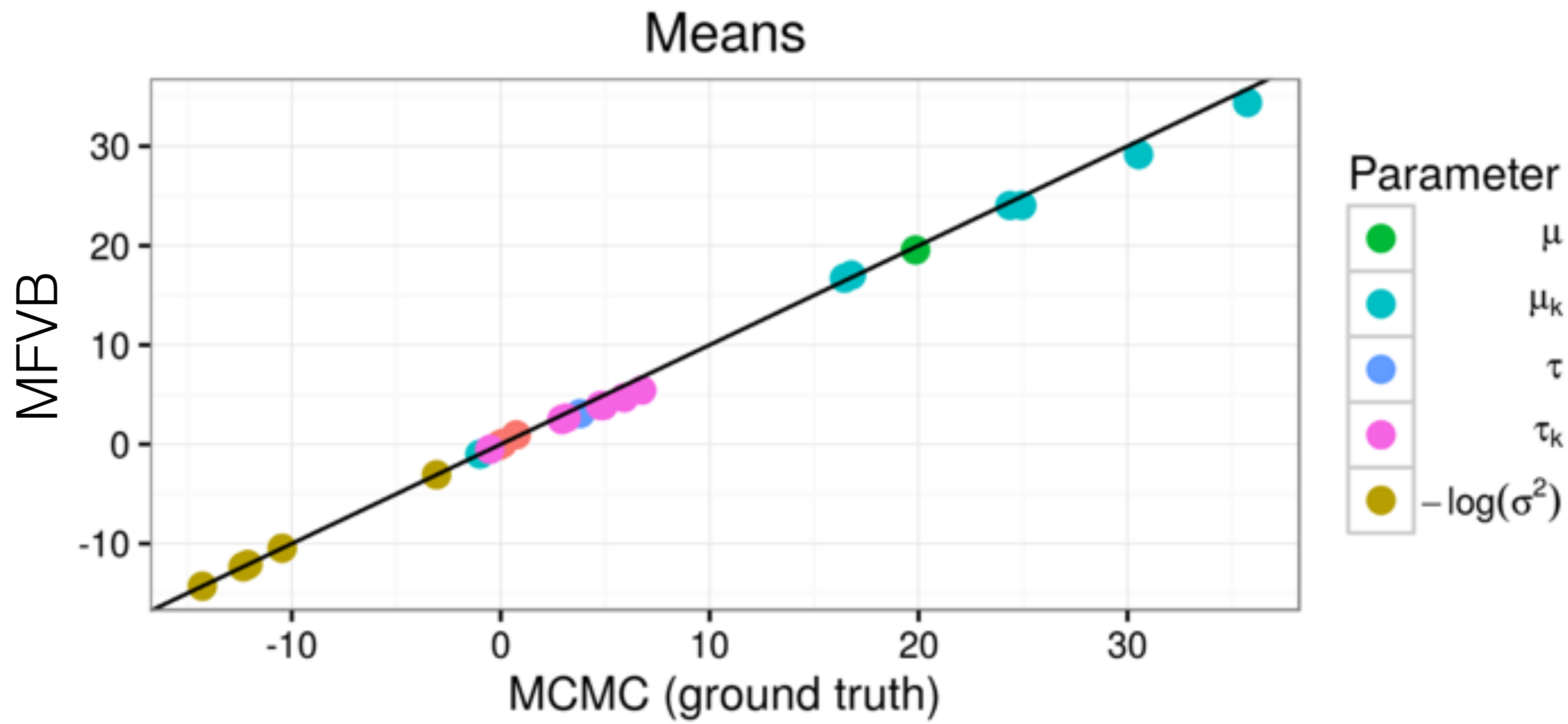

Criteo Online Ads Experiment

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

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

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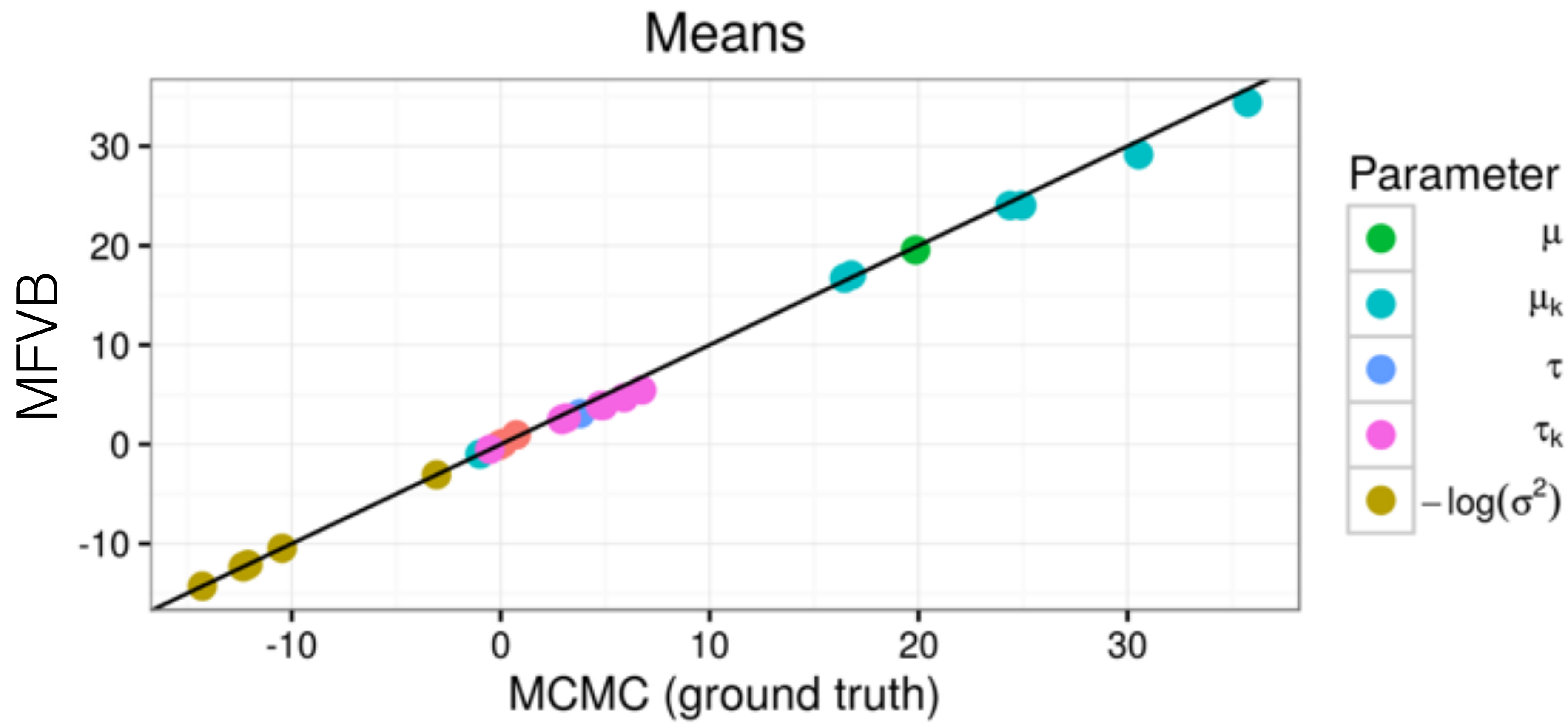

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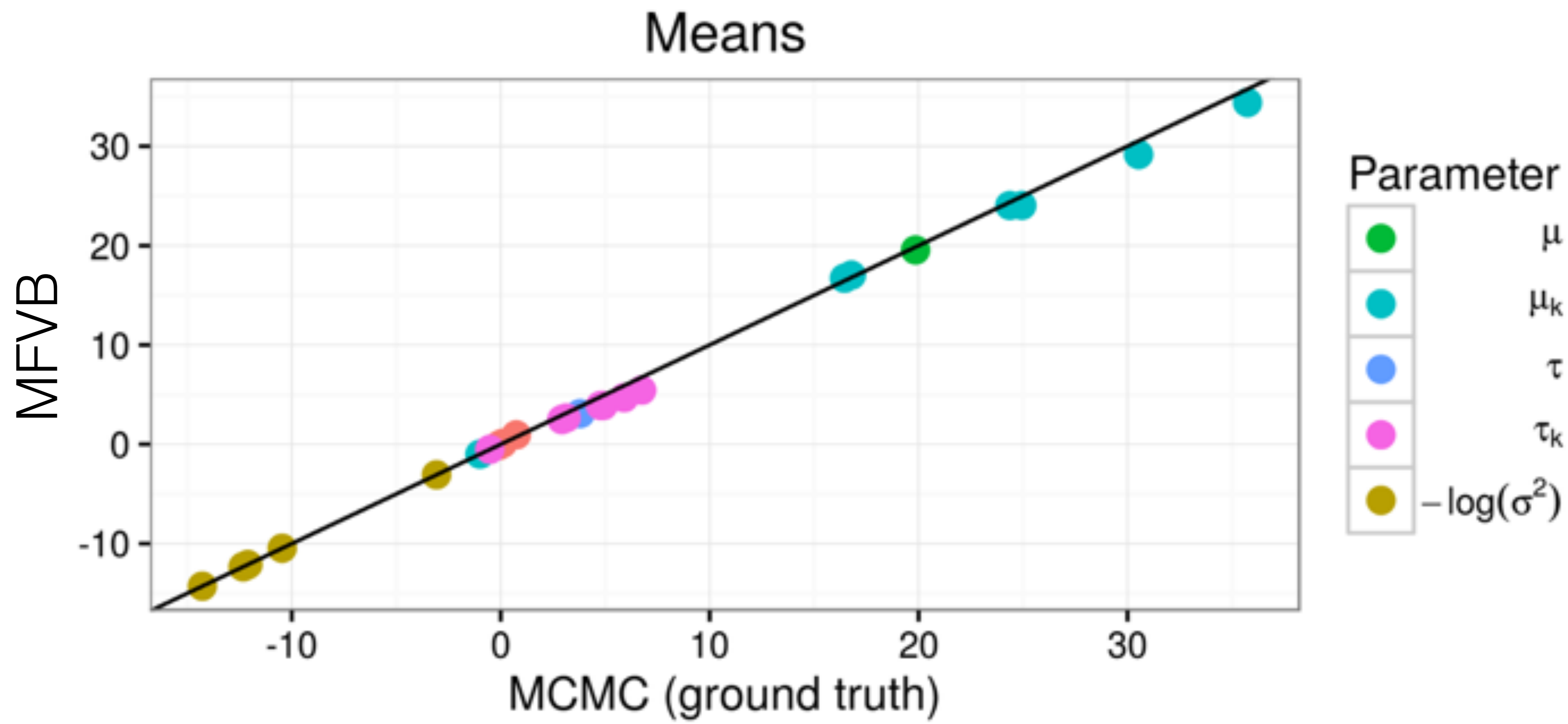

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[Giordano, Broderick, Meager, Huggins, Jordan 2016; Giordano, Broderick, Jordan 2018]

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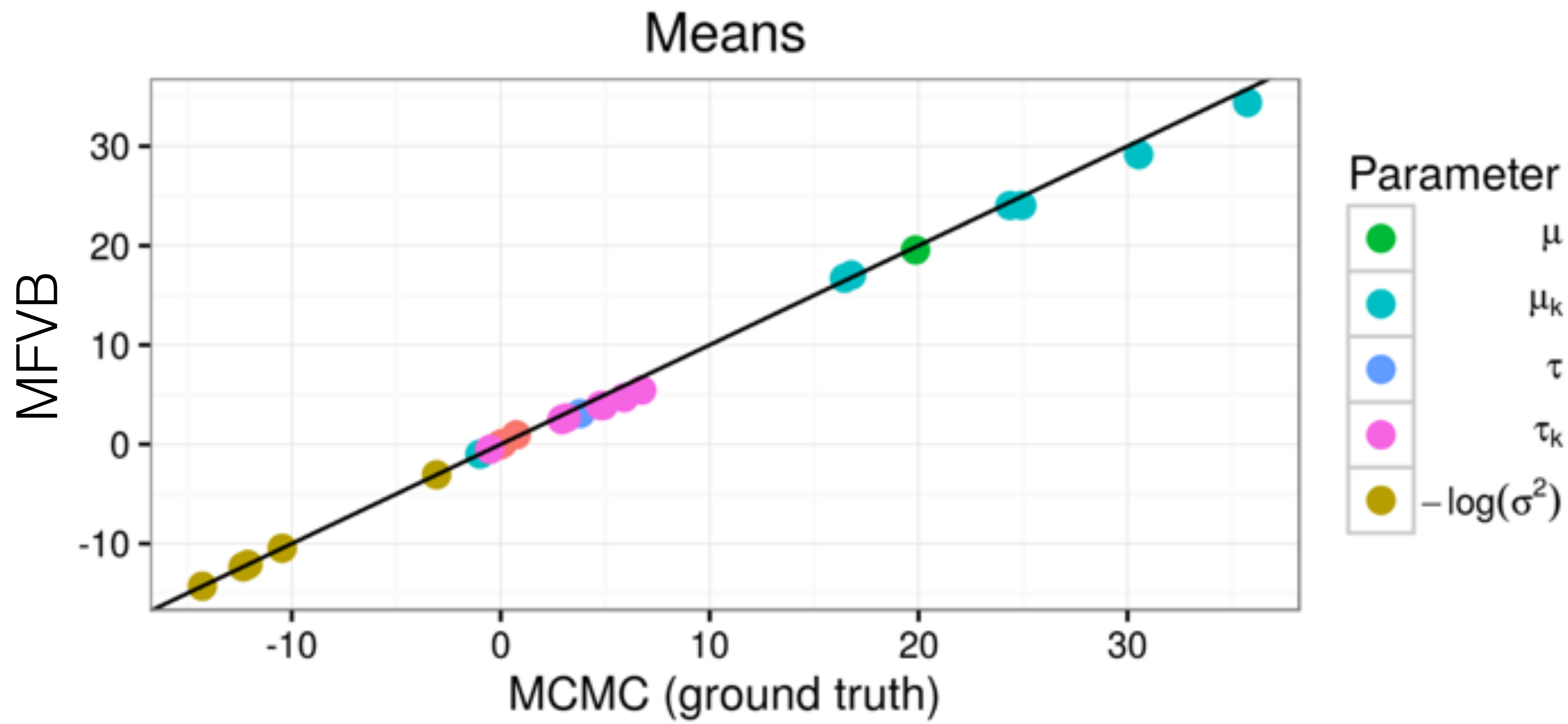

Criteo Online Ads Experiment

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- Logistic GLMM; N = 61,895 subset to compare to MCMC

[Giordano, Broderick, Meager, Huggins, Jordan 2016; Giordano, Broderick, Jordan 2018]

Criteo Online Ads Experiment

[Giordano, Broderick, Jordan 2018]

Criteo Online Ads Experiment

- MAP: **12 s**

[Giordano, Broderick, Jordan 2018]

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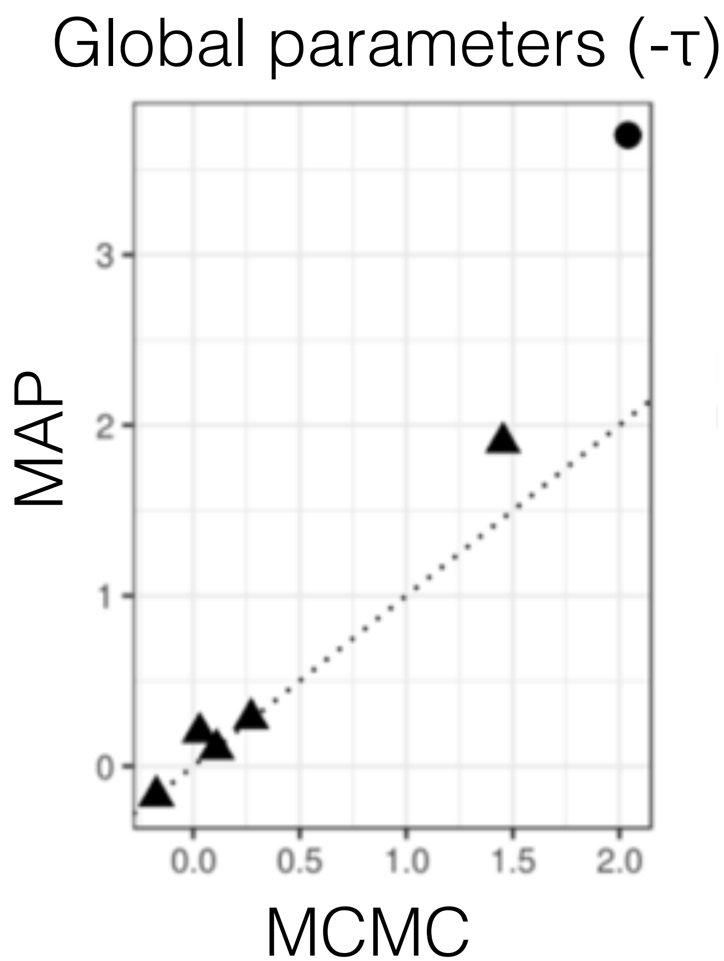

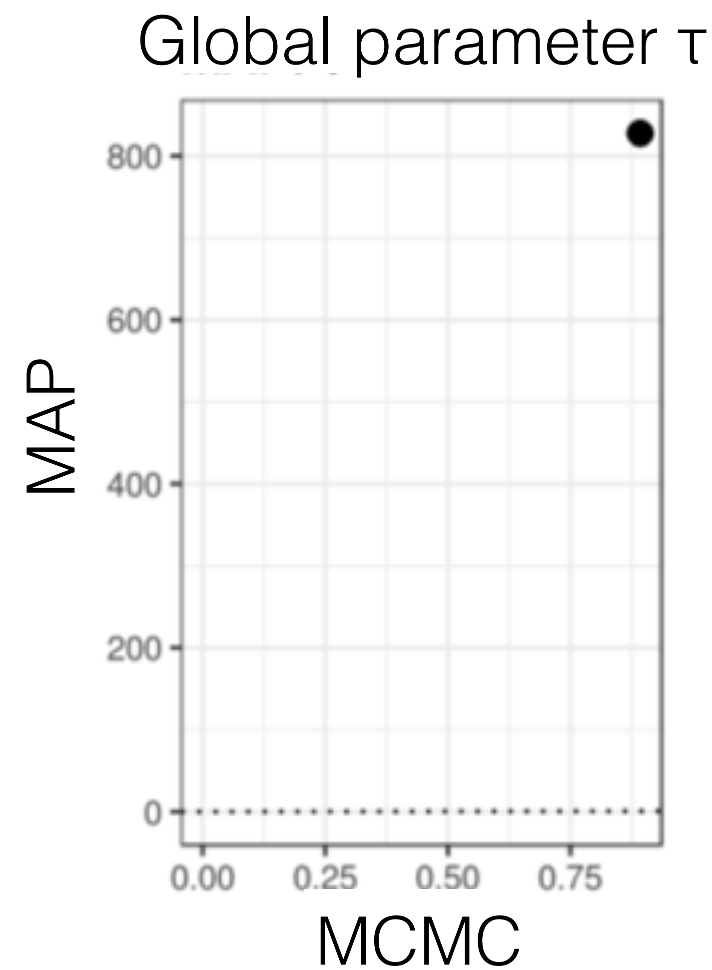

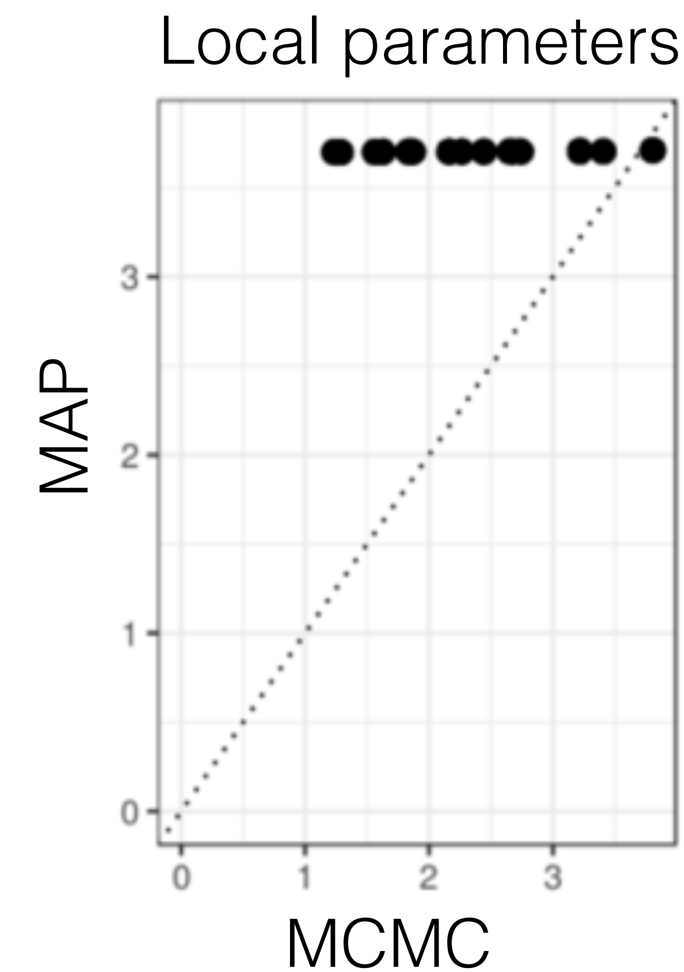

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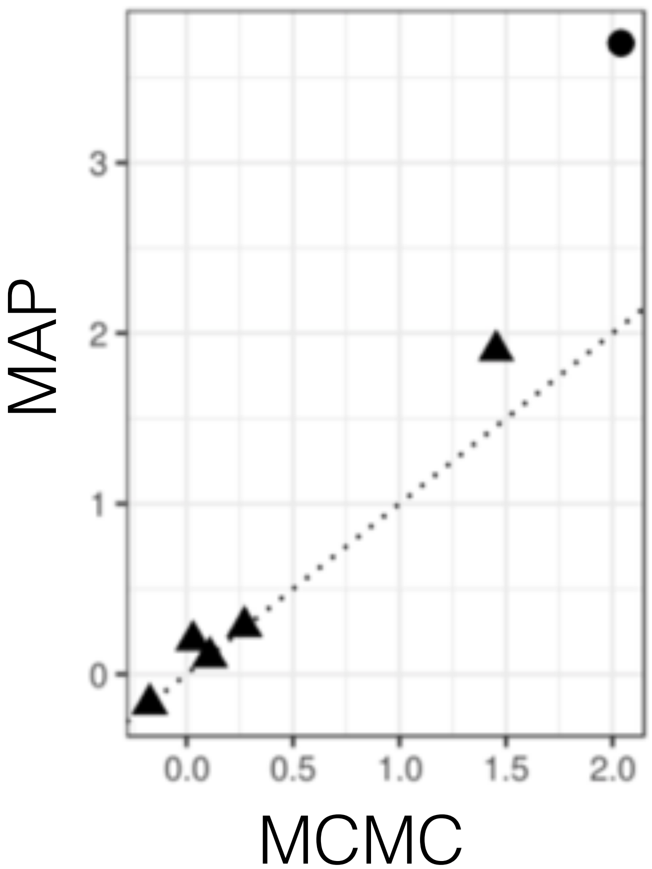
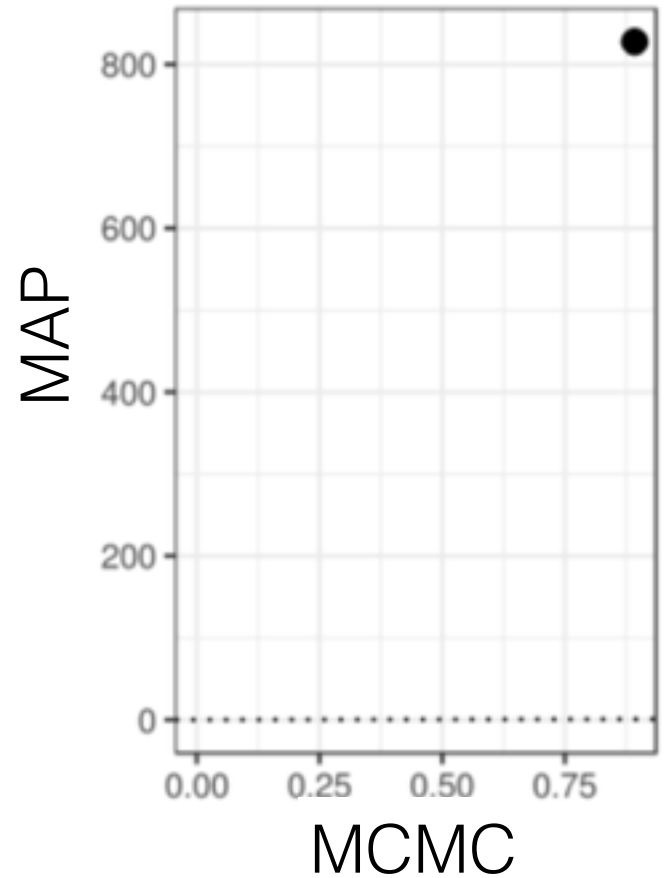
[Giordano, Broderick, Jordan 2018]

Criteo Online Ads Experiment

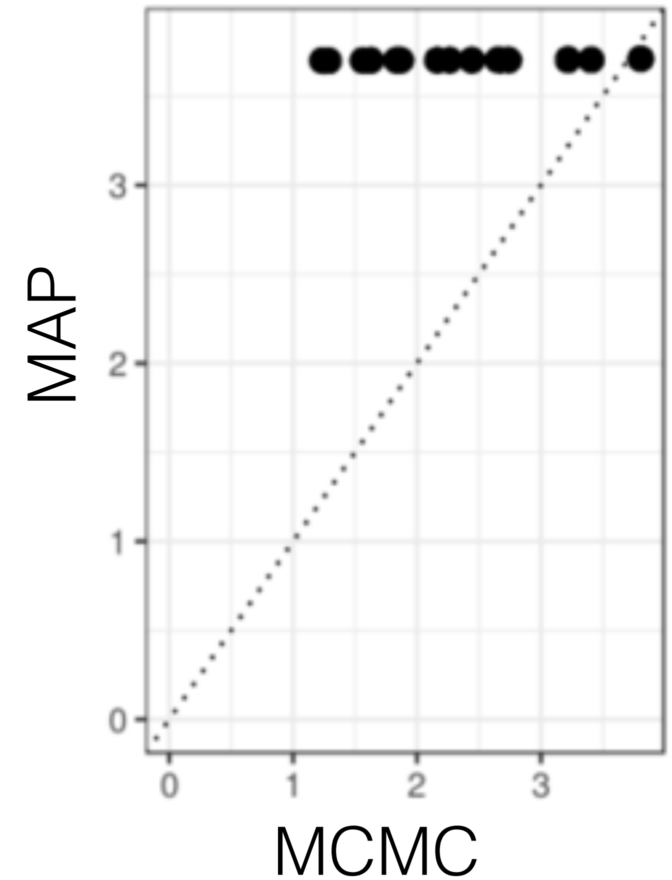
Global parameters (-τ)



Global parameter τ



Local parameters



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

[Giordano, Broderick, Jordan 2018]

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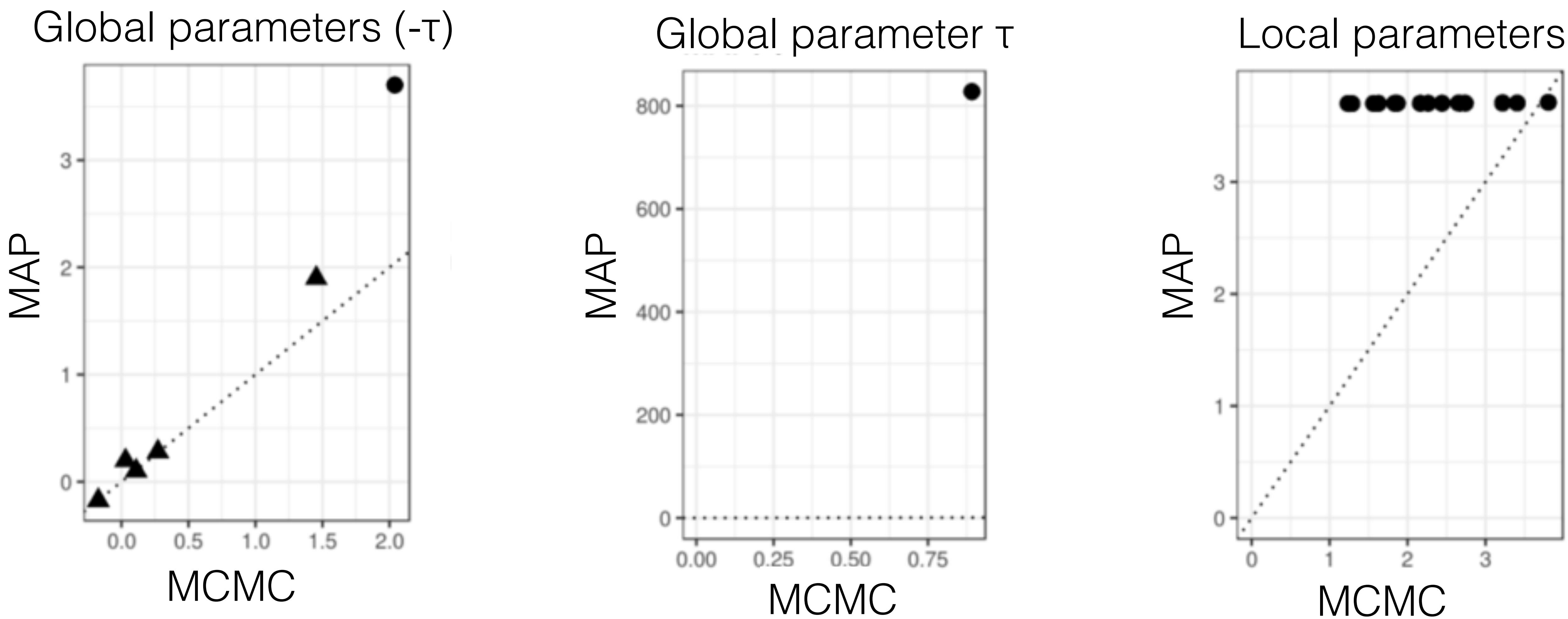

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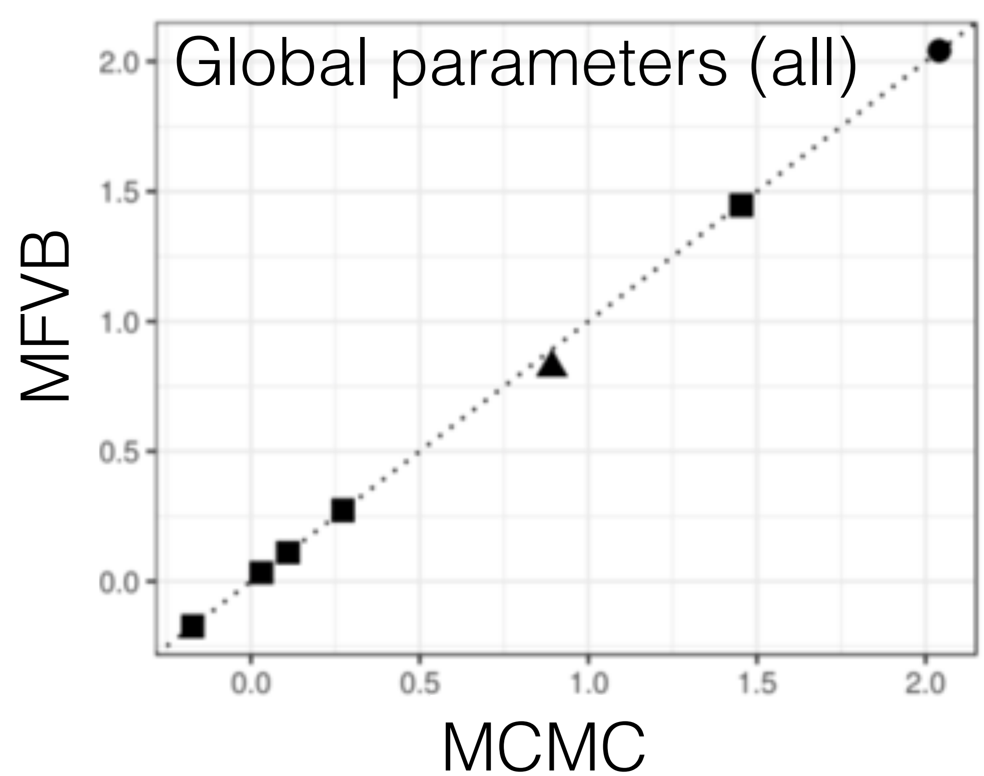

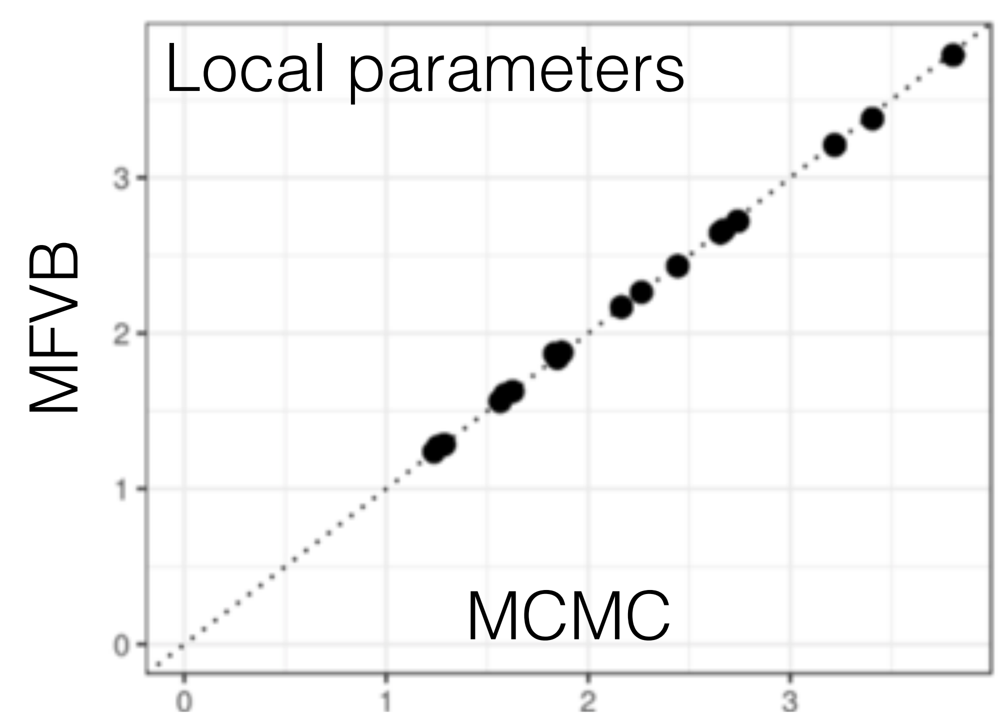

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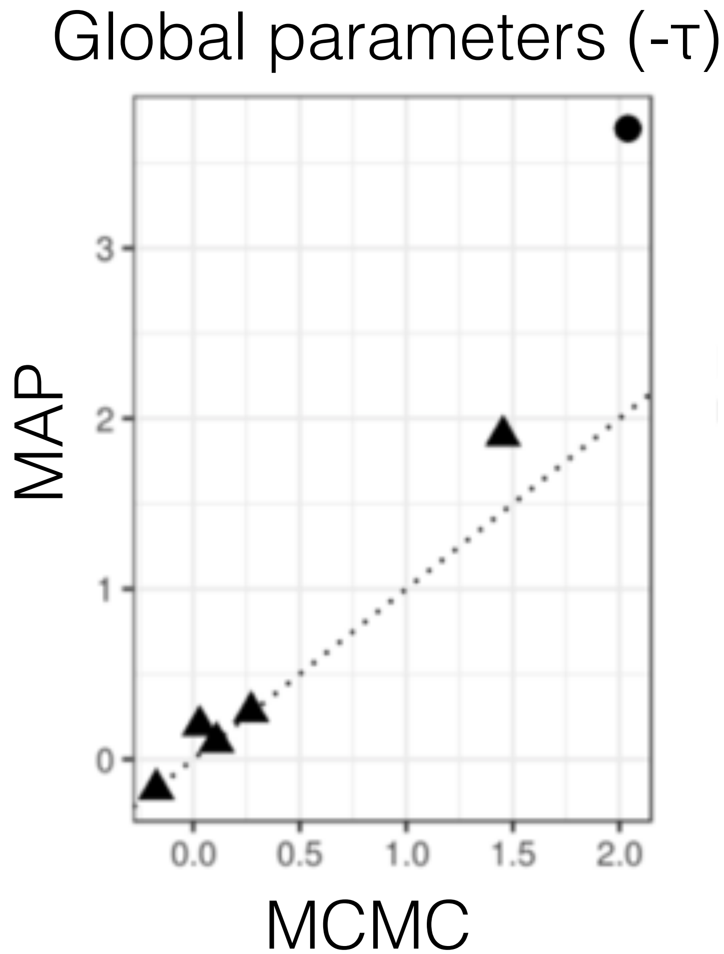
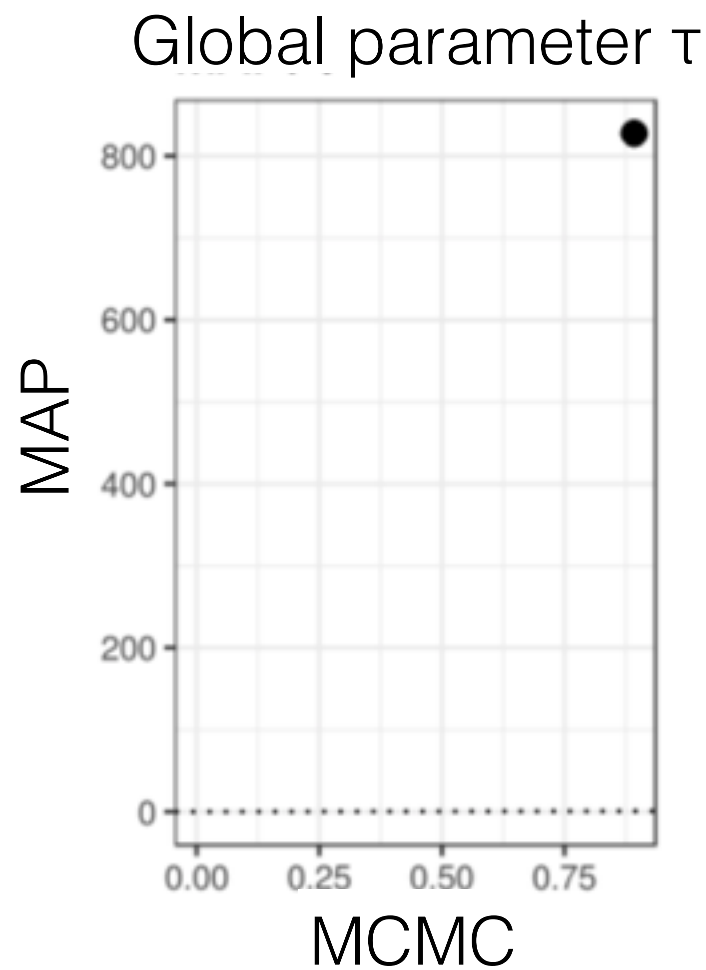
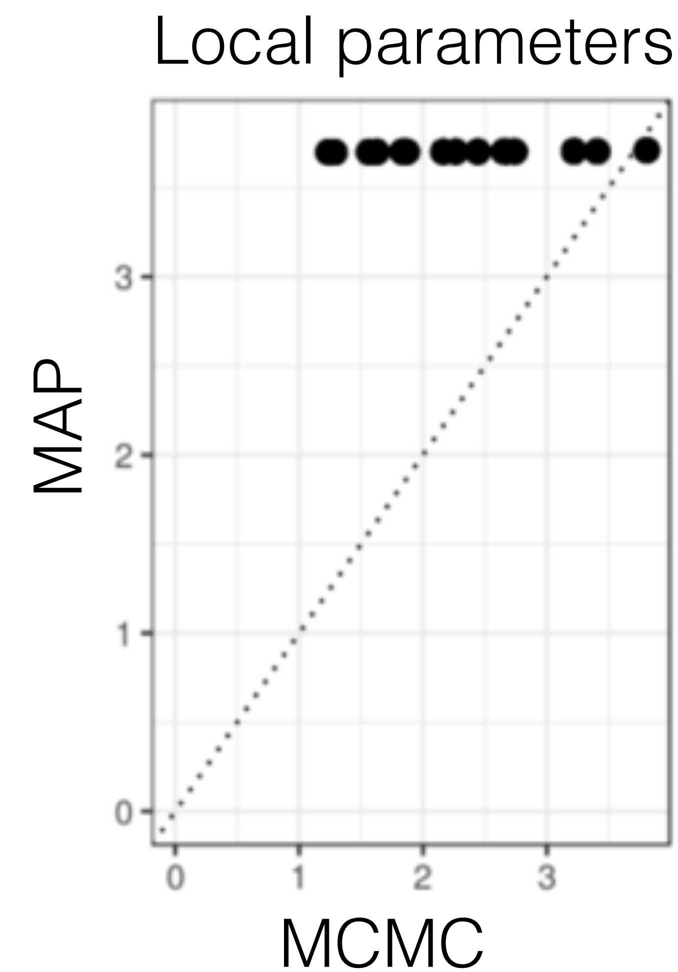
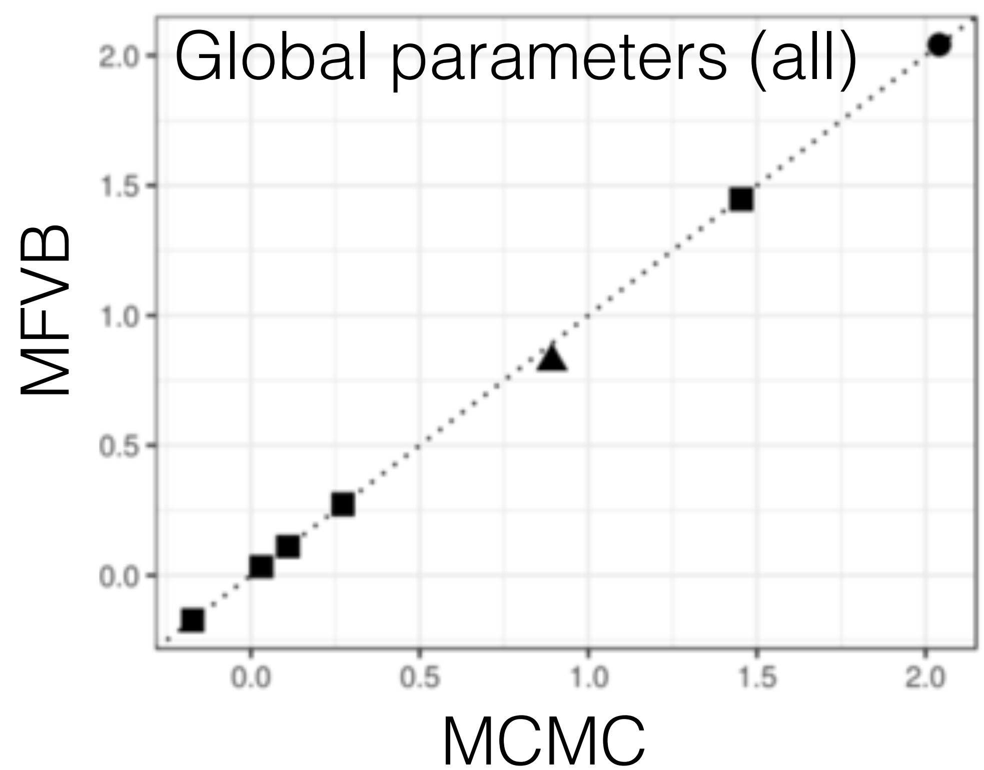
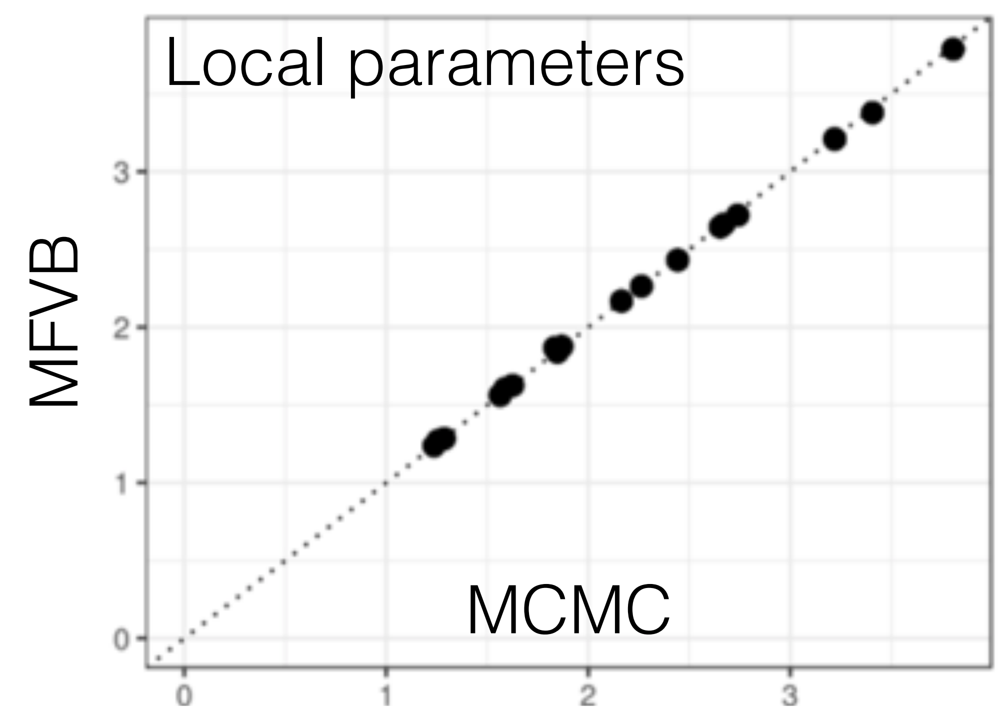






- MAP: **12 s**
- MFVB: **57 s**
- MCMC (5K samples): 21,066 s (**5.85 h**)





[Giordano, Broderick, Jordan 2018]

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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What about uncertainty?

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

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

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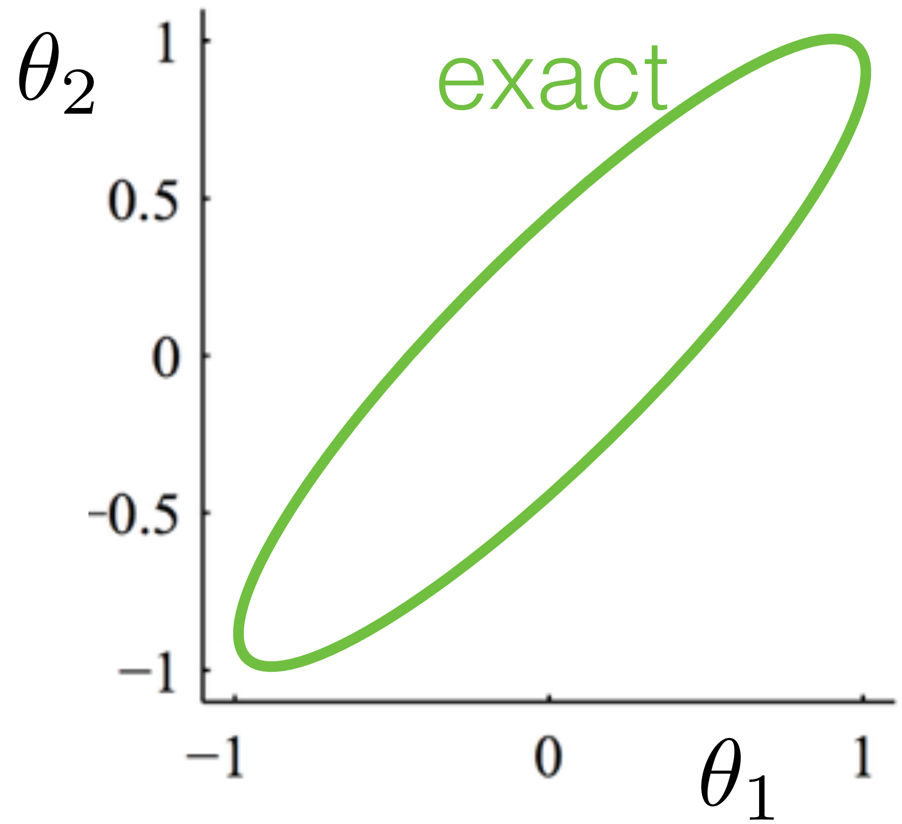

[Turner & Sahani 2011; MacKay 2003; Bishop 2006; Wang, Titterington 2004]

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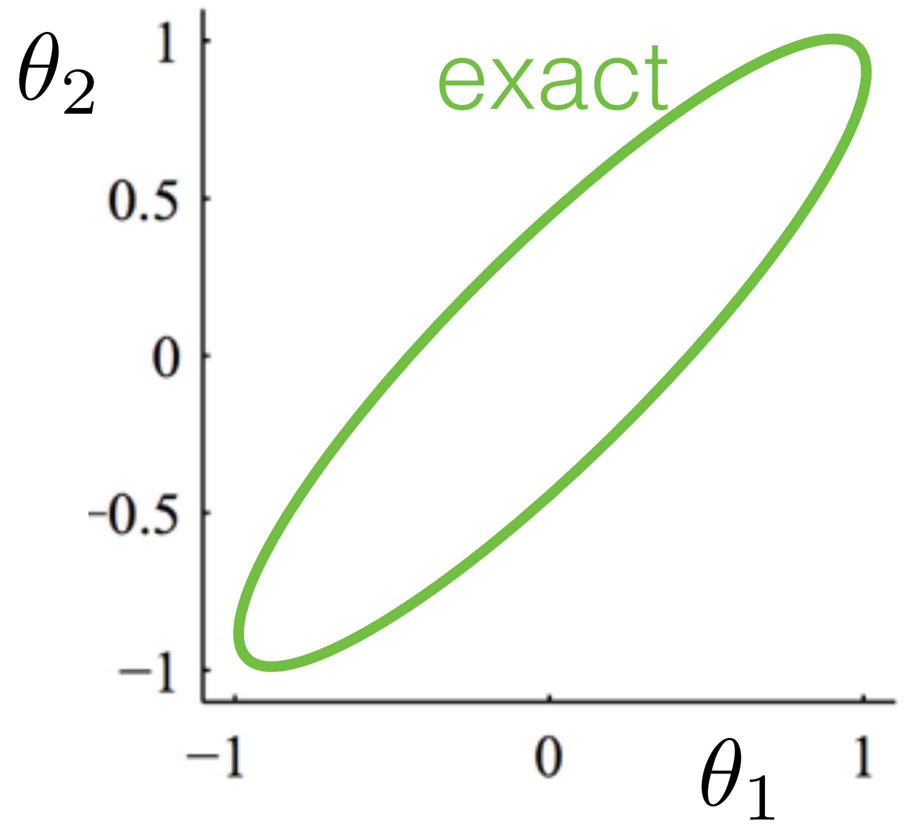

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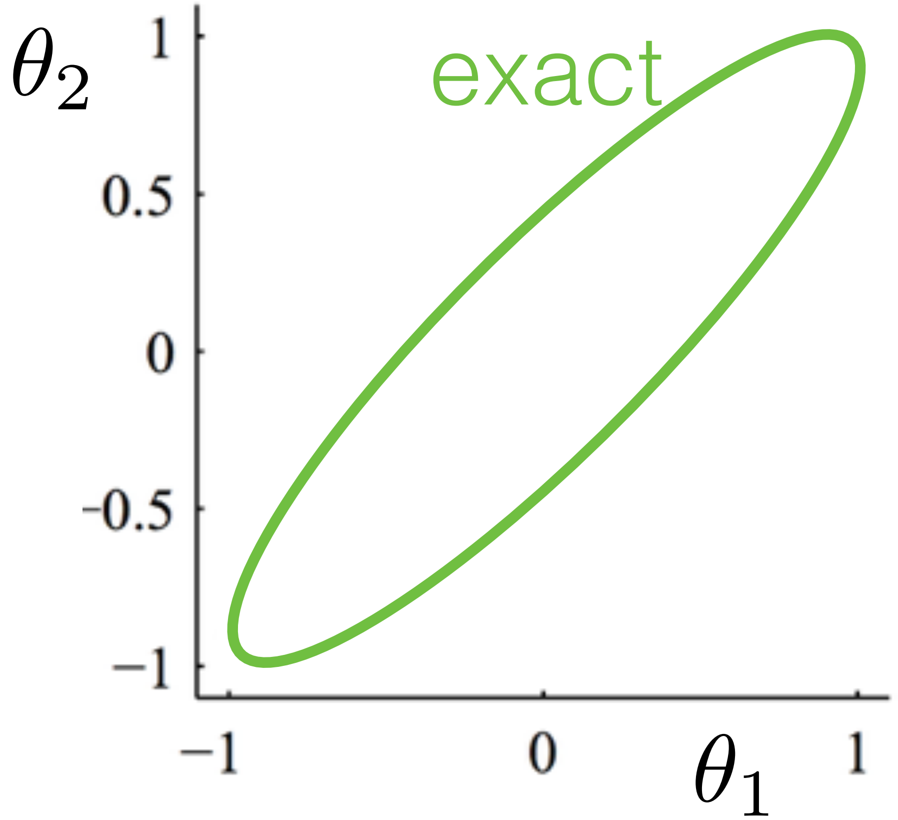

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- Conjugate linear regression
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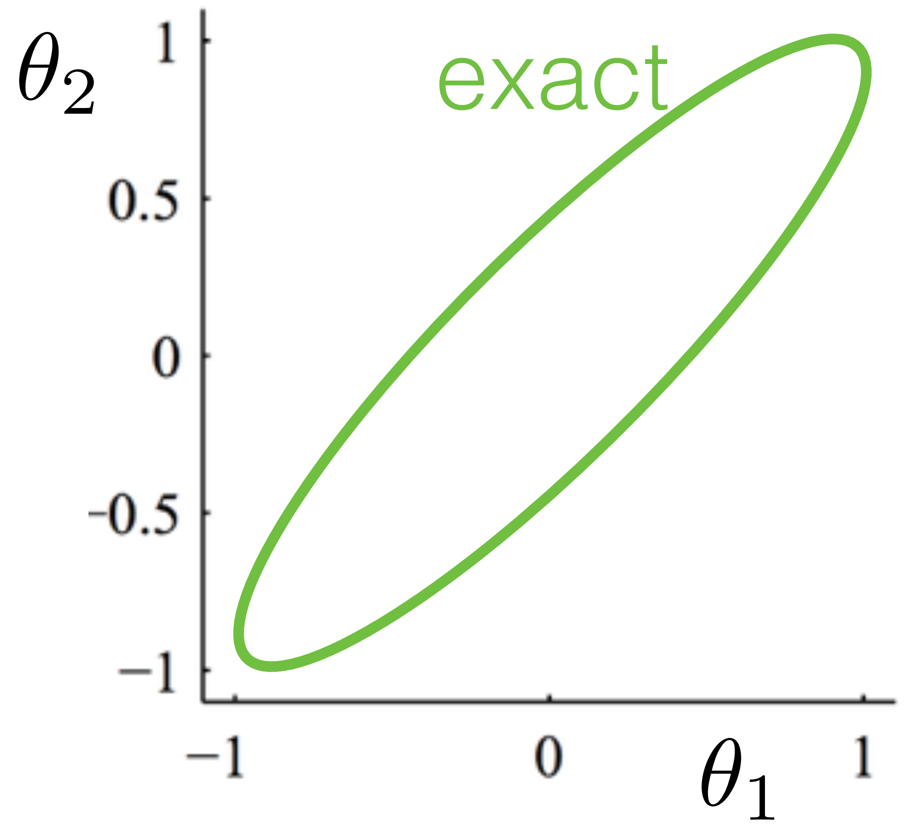

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[Exercise: derive the MFVB-CA steps. Hint: use precision matrix.]

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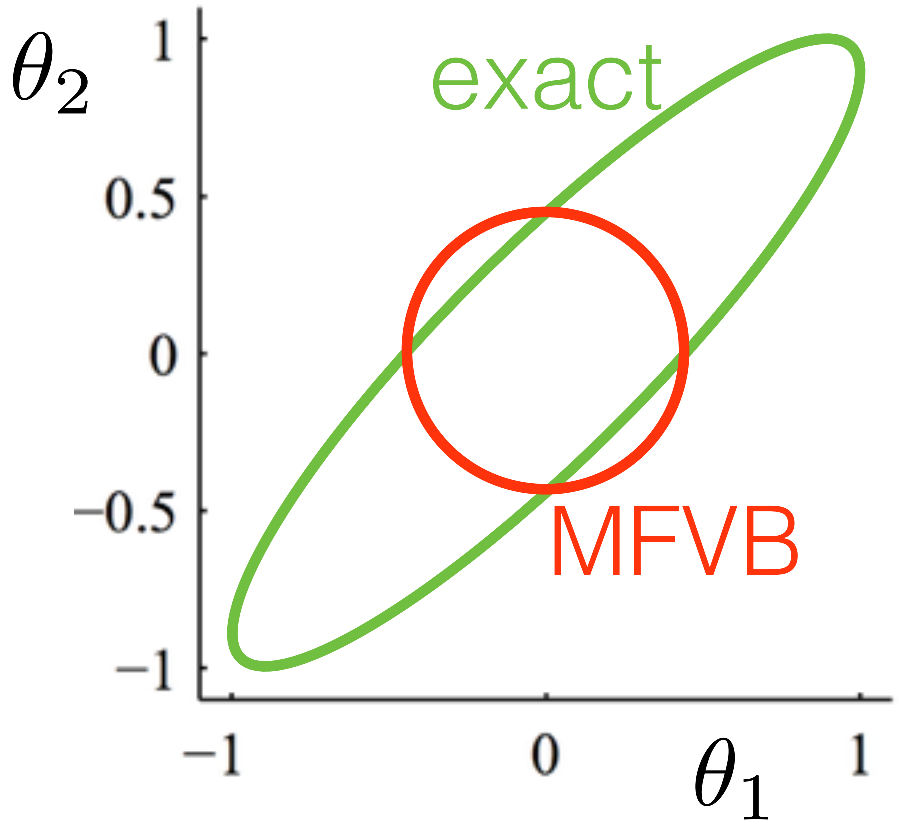

[Turner & Sahani 2011; MacKay 2003; Bishop 2006; Wang, Titterington 2004]

- Conjugate linear regression
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[Exercise: derive the MFVB-CA steps. Hint: use precision matrix.]

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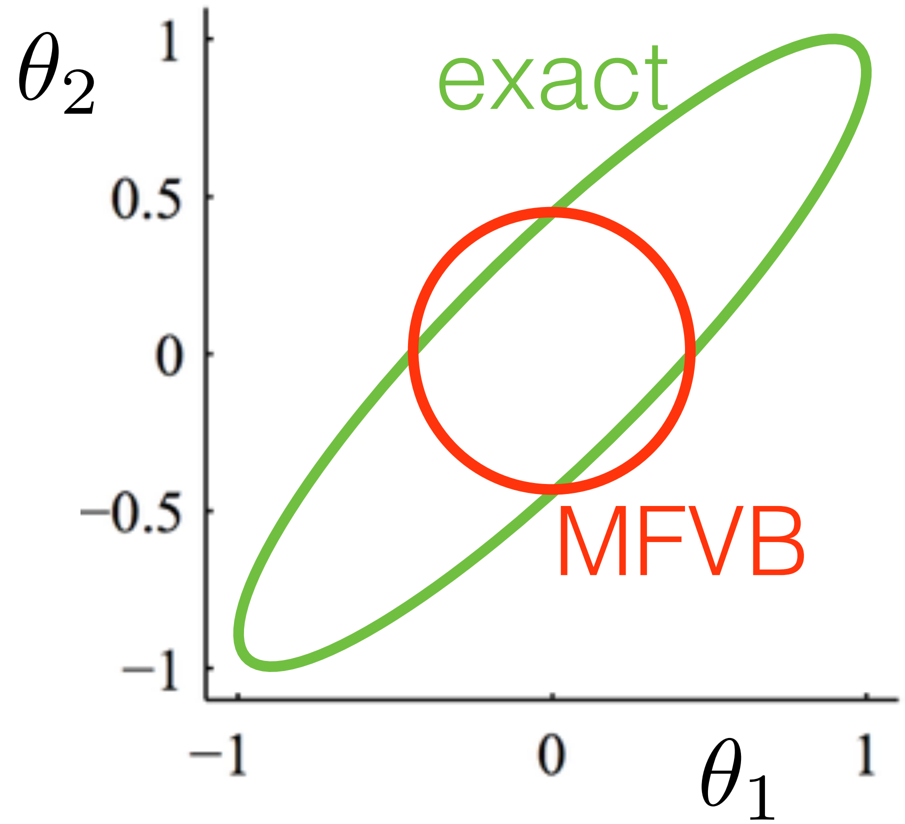

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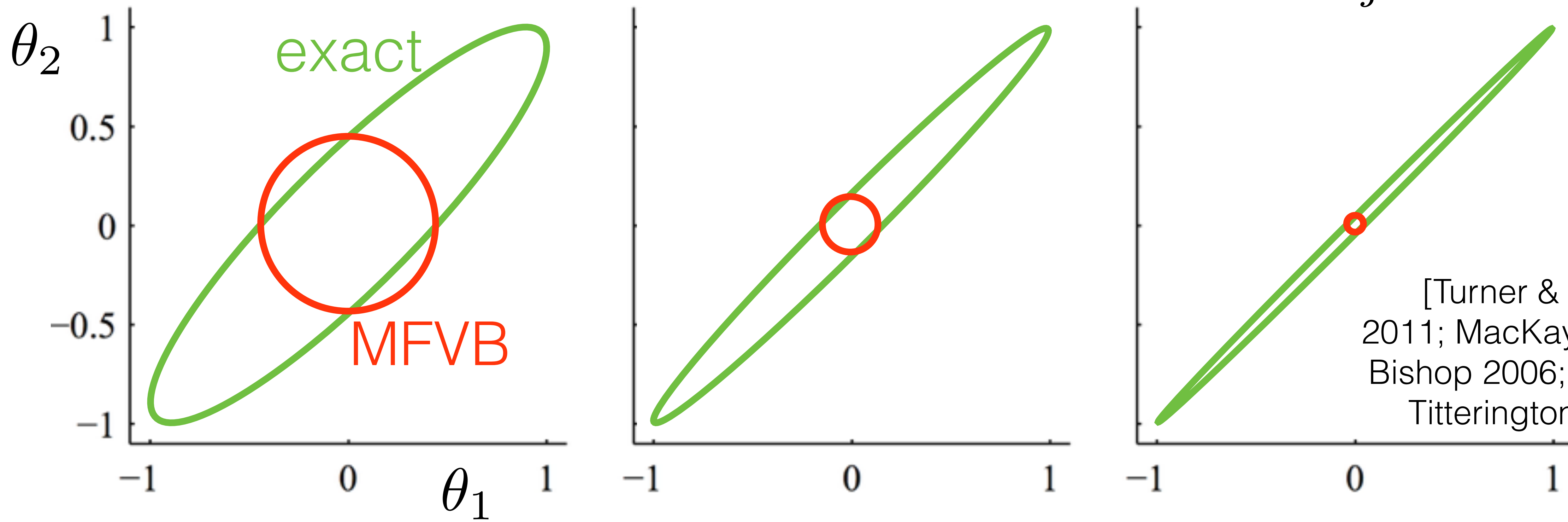

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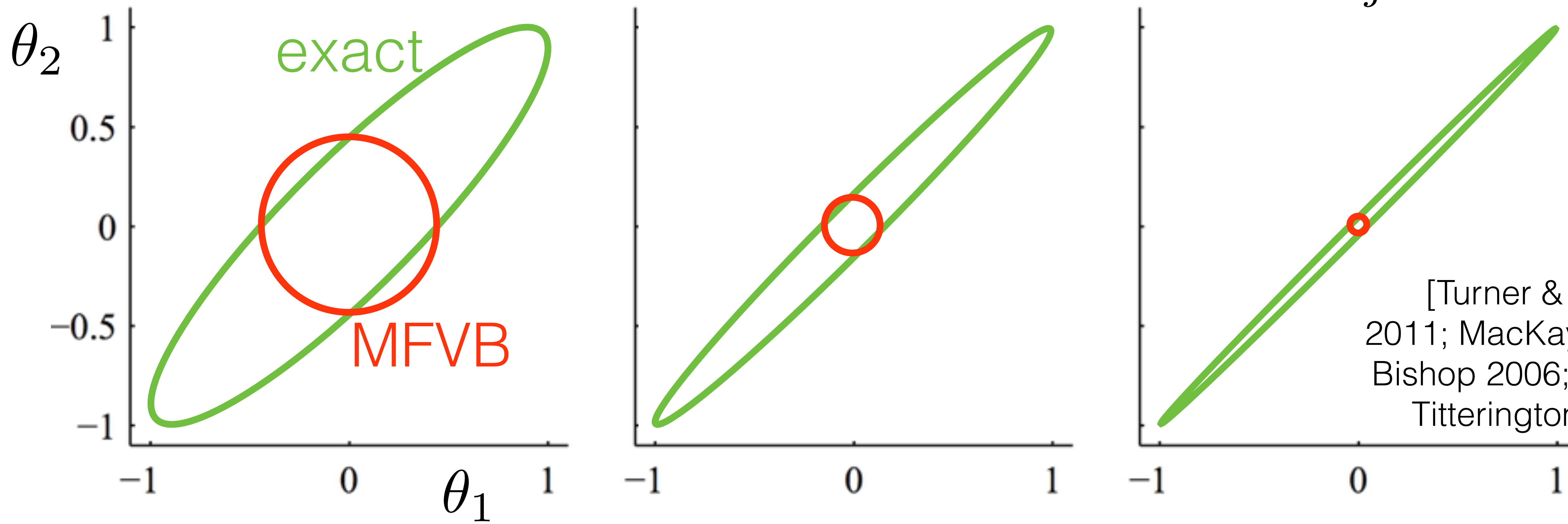

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- Underestimates variance (sometimes severely)
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What about uncertainty?

- Microcredit

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

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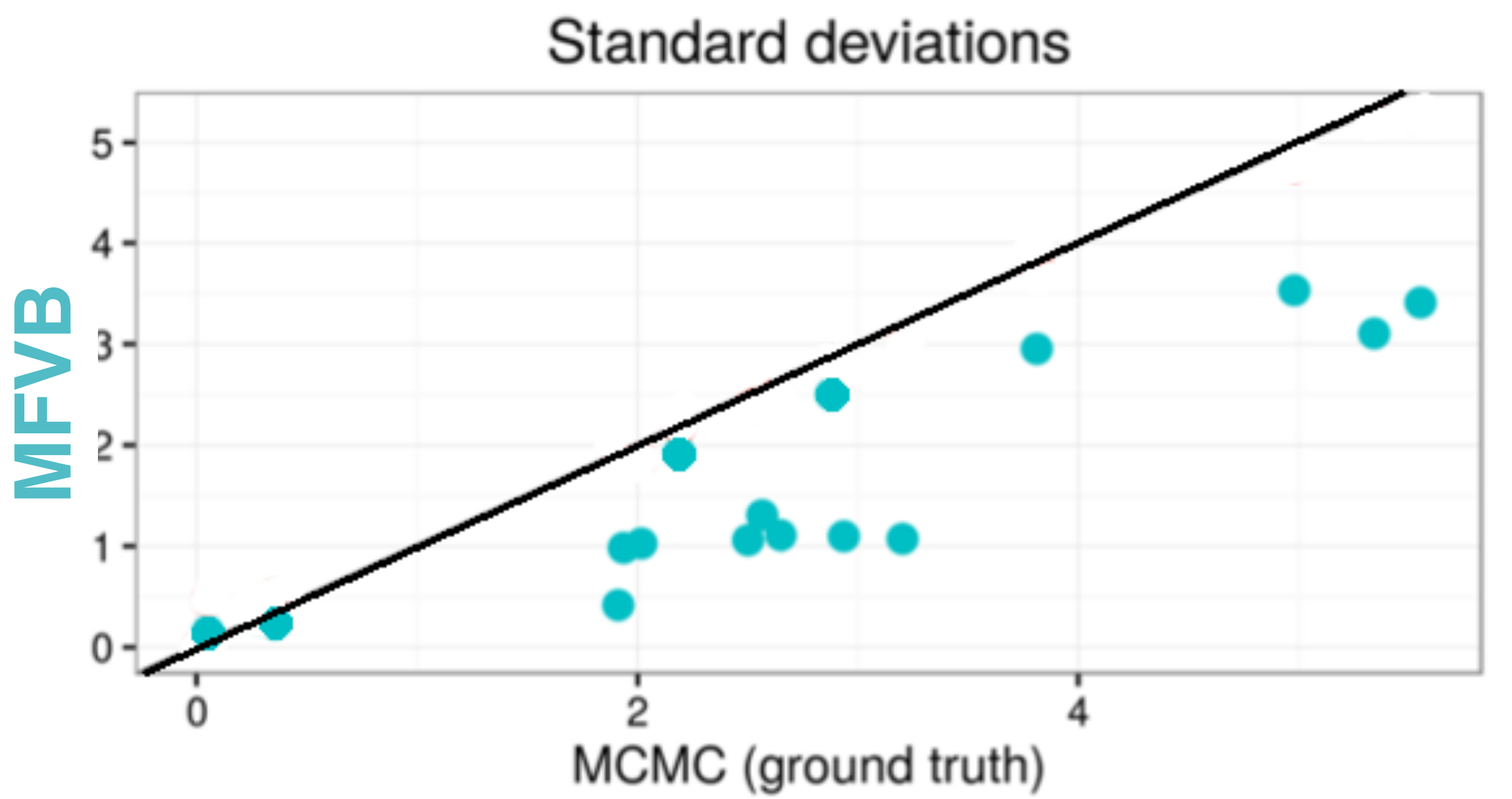
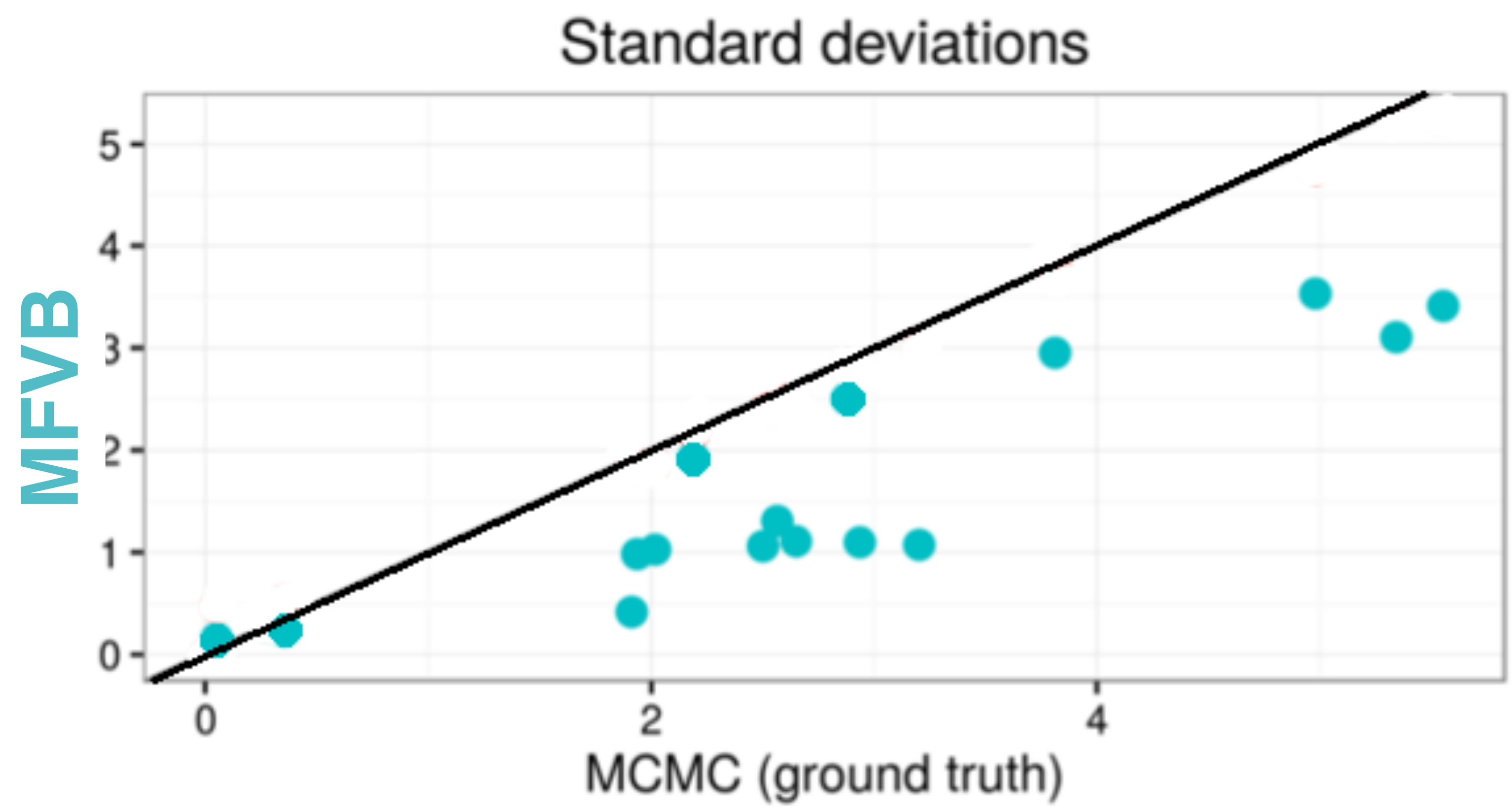


[Giordano, Broderick, Meager, Huggins, Jordan 2016]

What about uncertainty?

- Microcredit effect
- τ mean: 3.08 USD PPP



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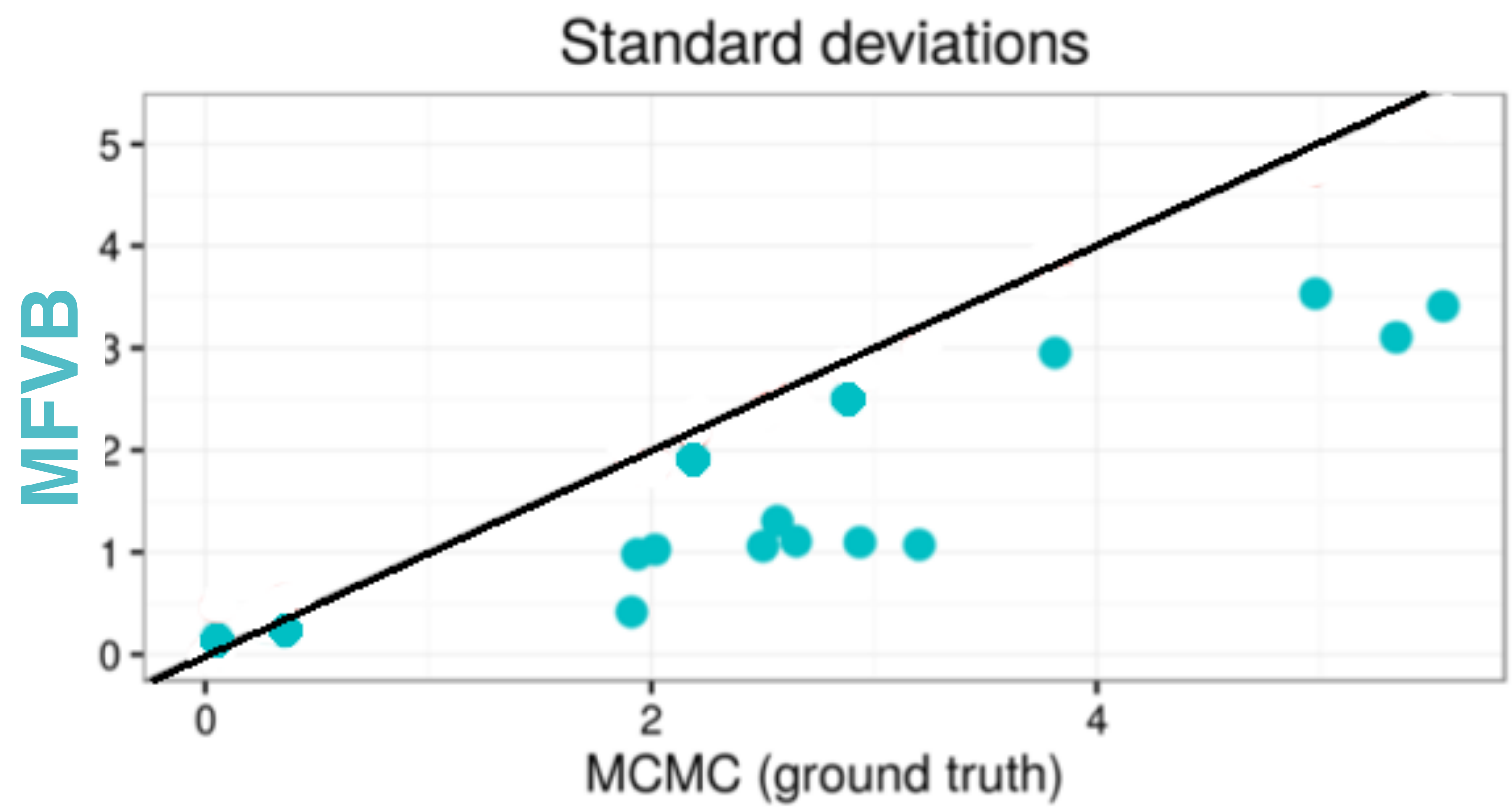

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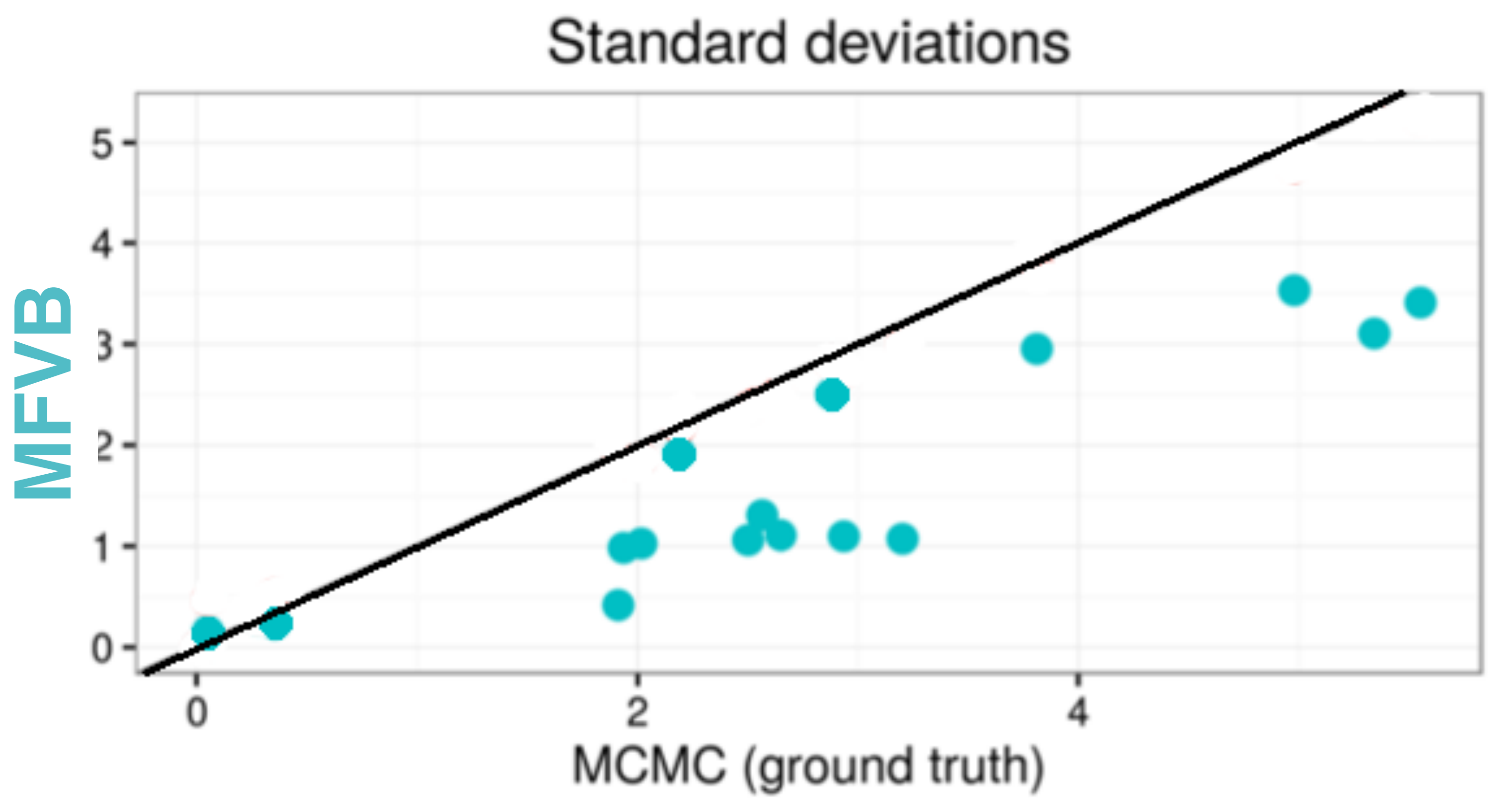

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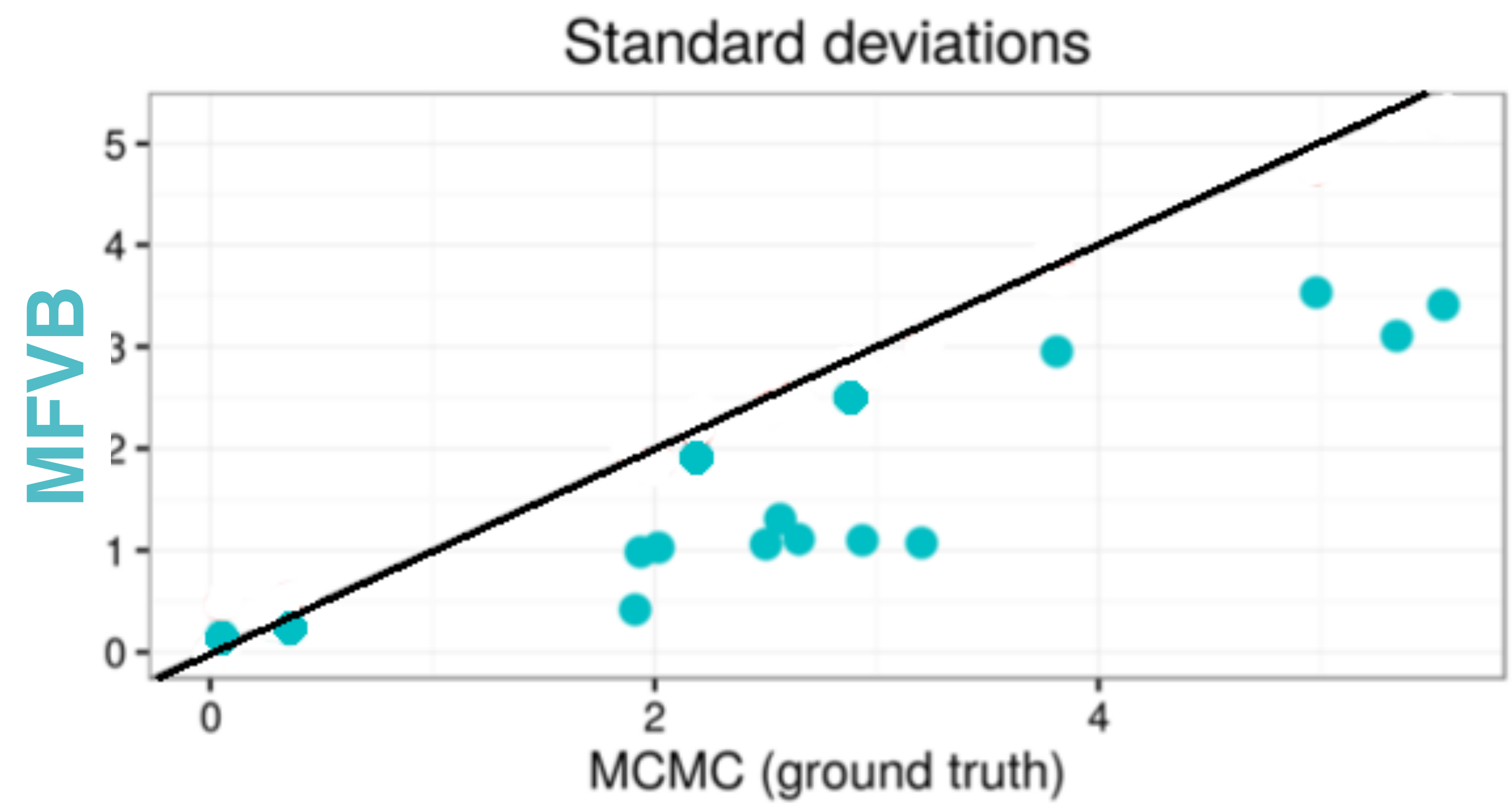
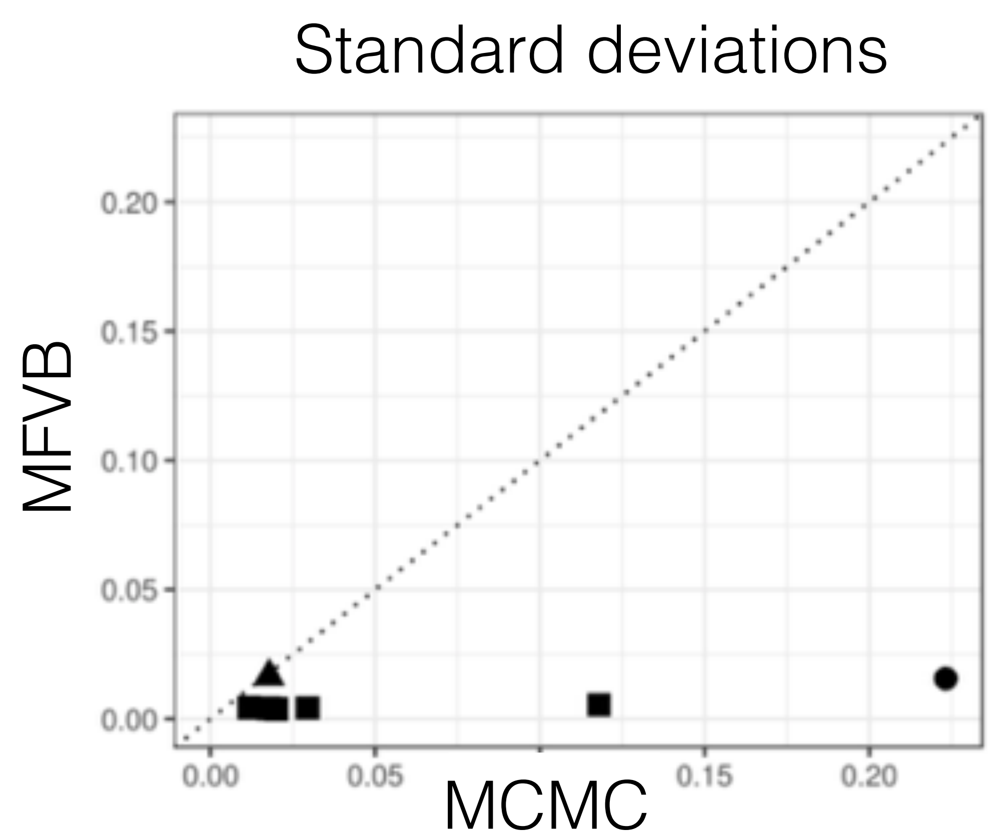


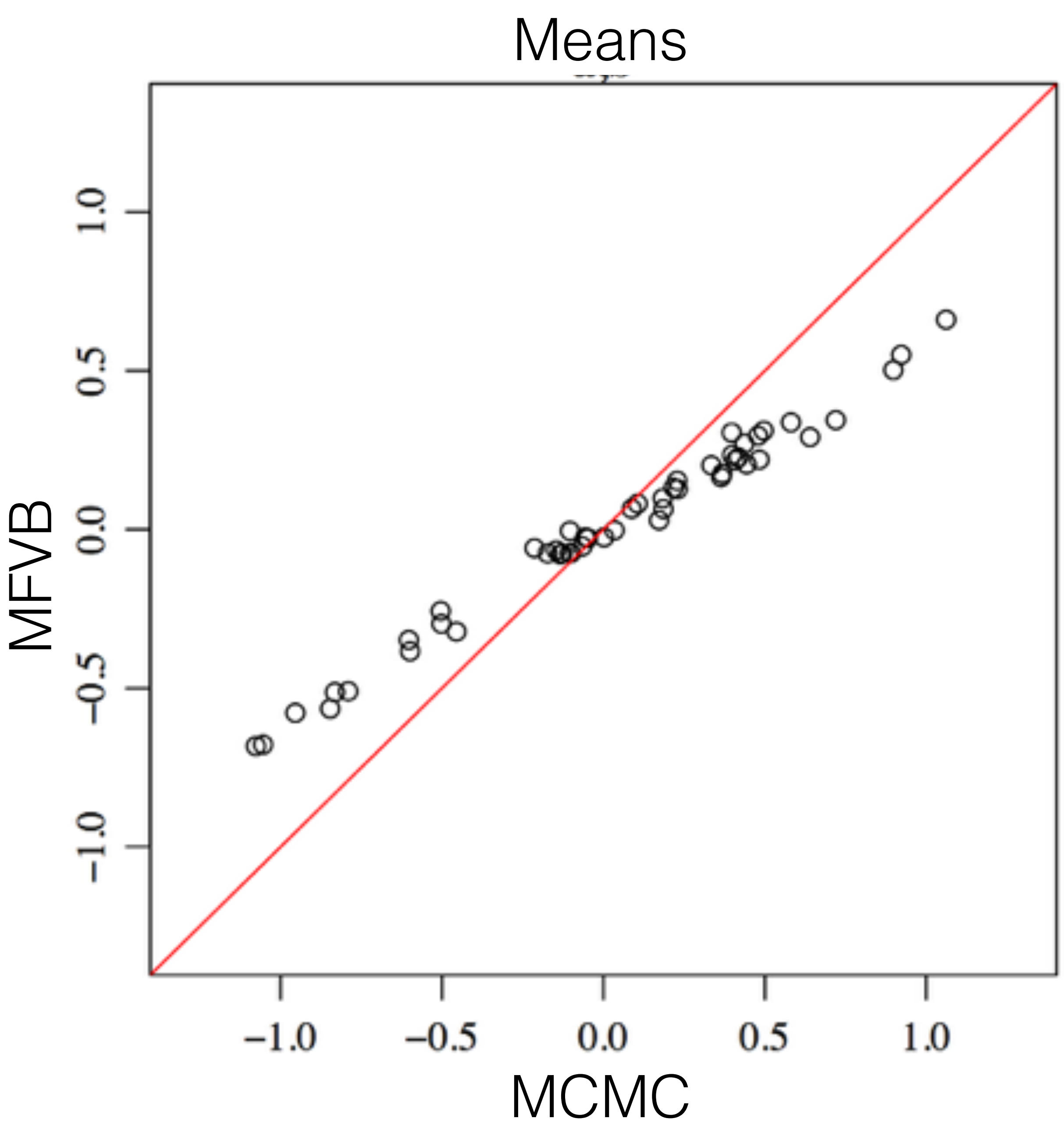
- Criteo online ads experiment

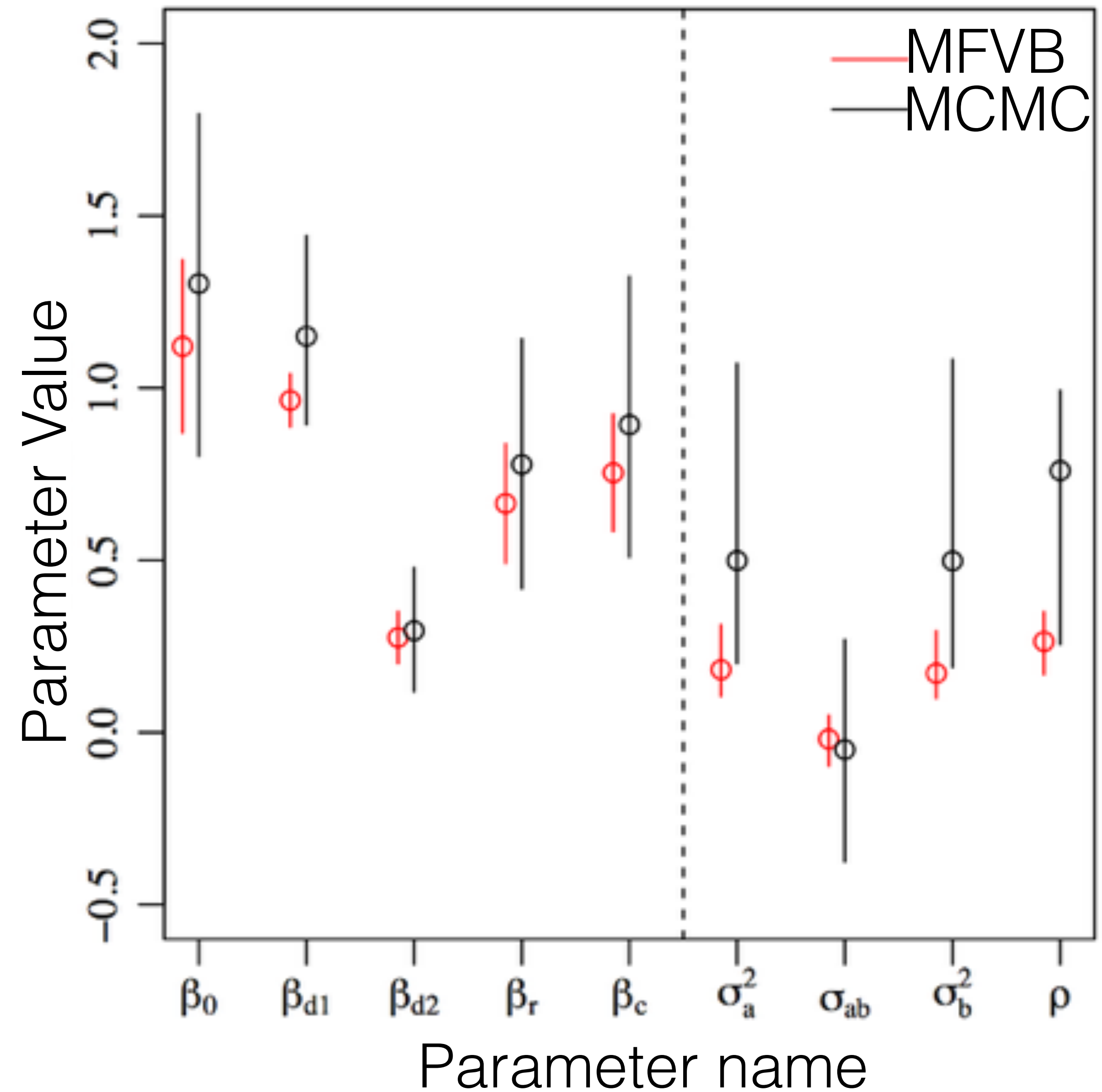


[Giordano, Broderick, Meager, Huggins, Jordan 2016; Giordano, Broderick, Jordan 2018]

What about means?

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





[Fosdick 2013, Ch 4, Fig 4.3]

Posterior means: revisited

- Want to predict college GPA y_n

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

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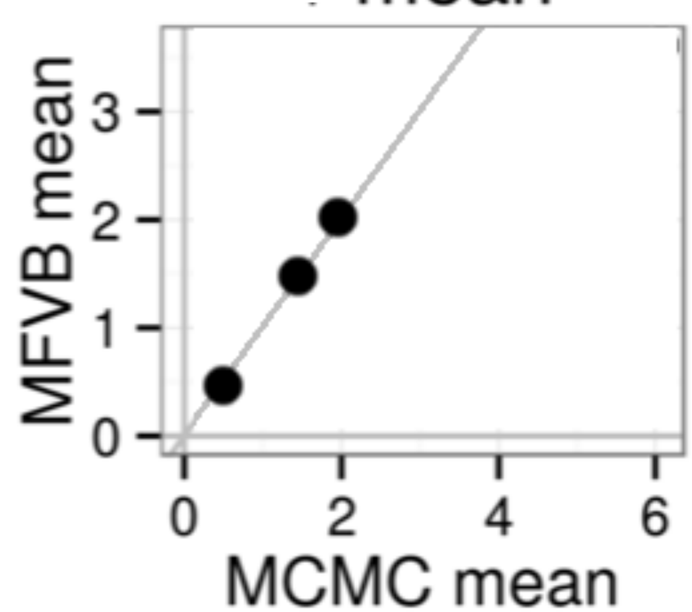

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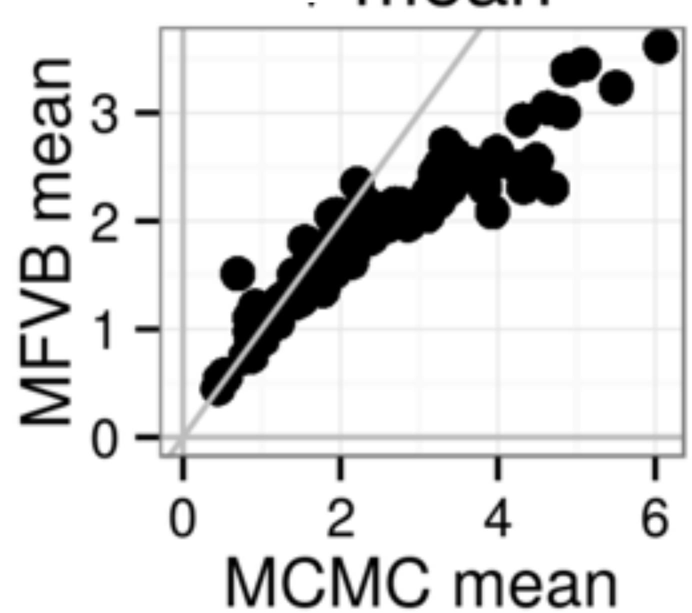

[Giordano, Broderick, Jordan 2015]

Roadmap

- Bayes & Approximate Bayes review
- What is:
  - Variational Bayes (VB)
  - Mean-field variational Bayes (MFVB)
- Why use MFVB?
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Is it just MFVB?

[Huggins, Karsprzak, Campbell, Broderick 2018]

Is it just MFVB?

Can have small KL and arbitrarily bad variance estimate

Proposition (HKCB). For any $t > 1$, there exist zero-mean, unimodal distributions q^* and p such that

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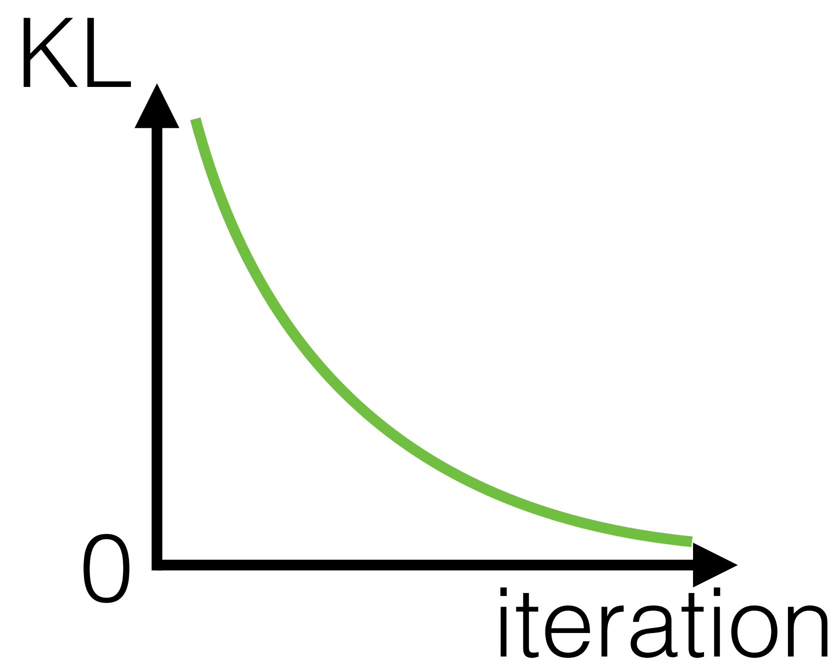

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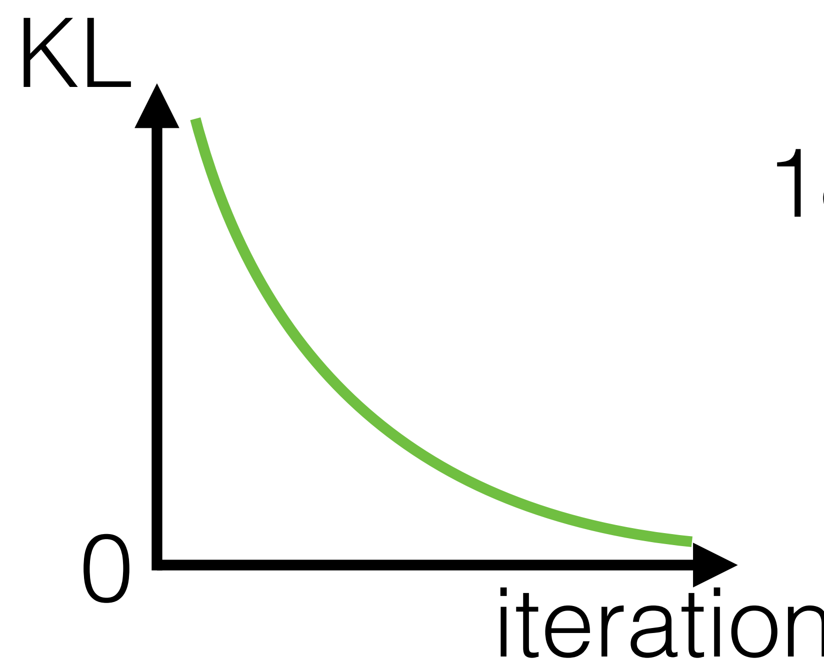

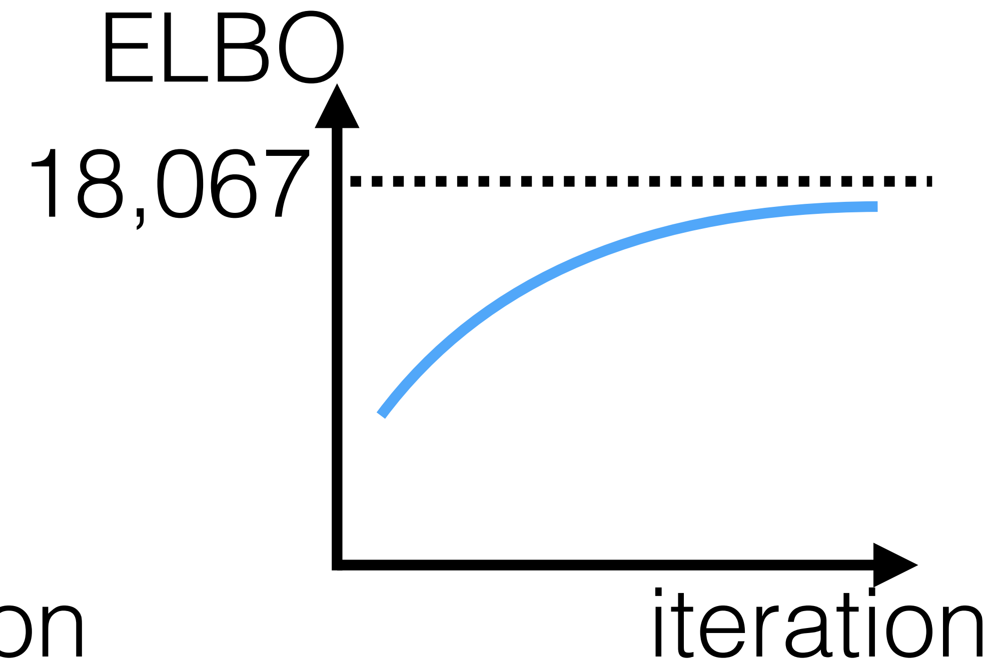

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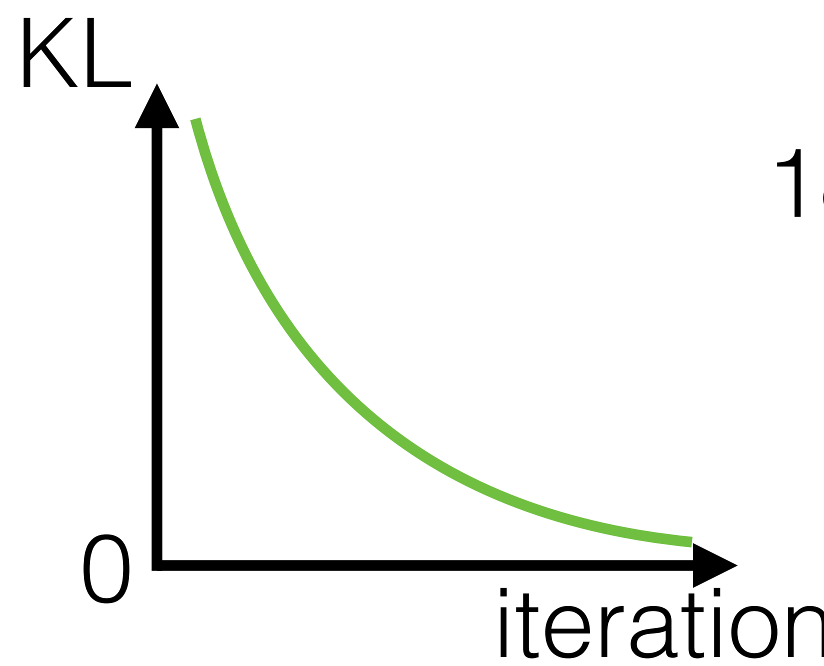

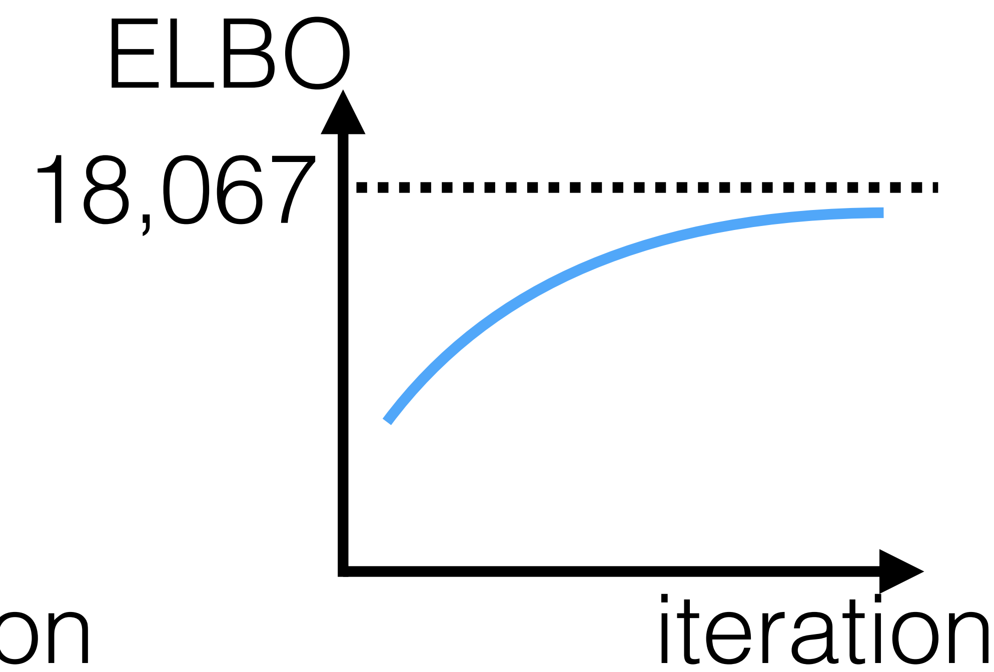

"Yes, but did it work? Evaluating variational inference" ICML 2018

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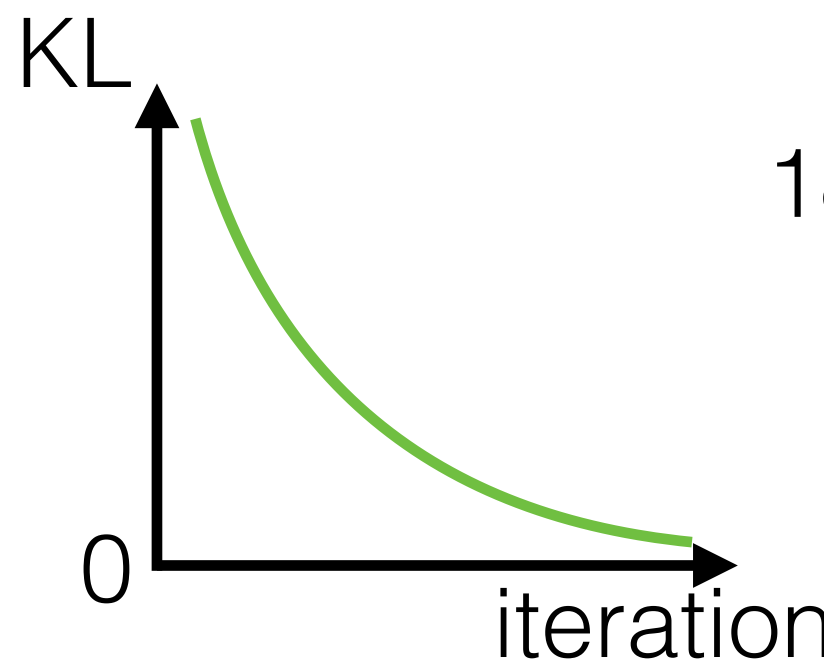

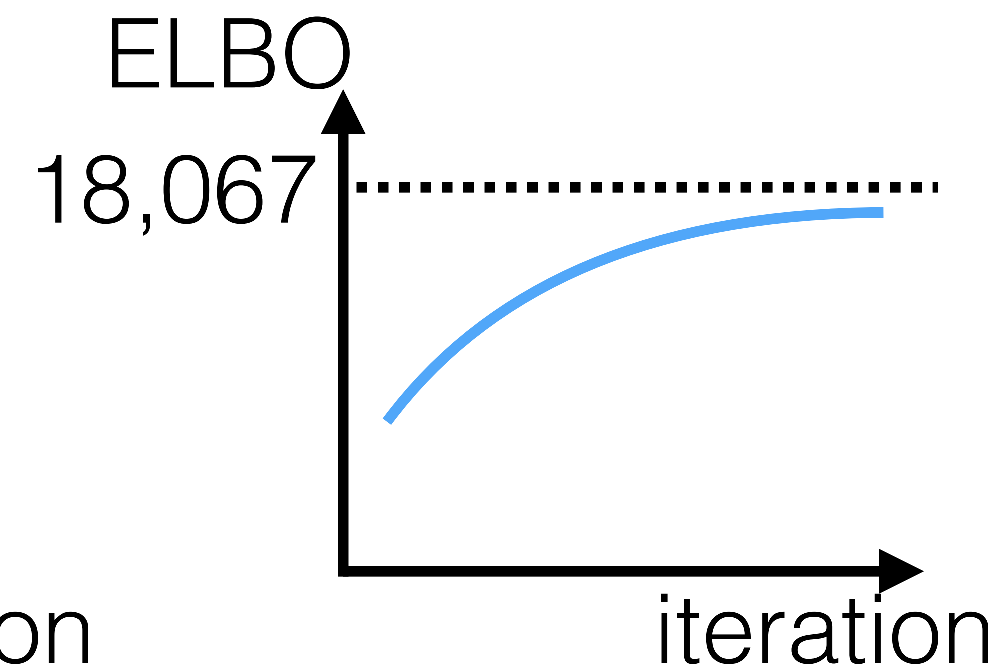

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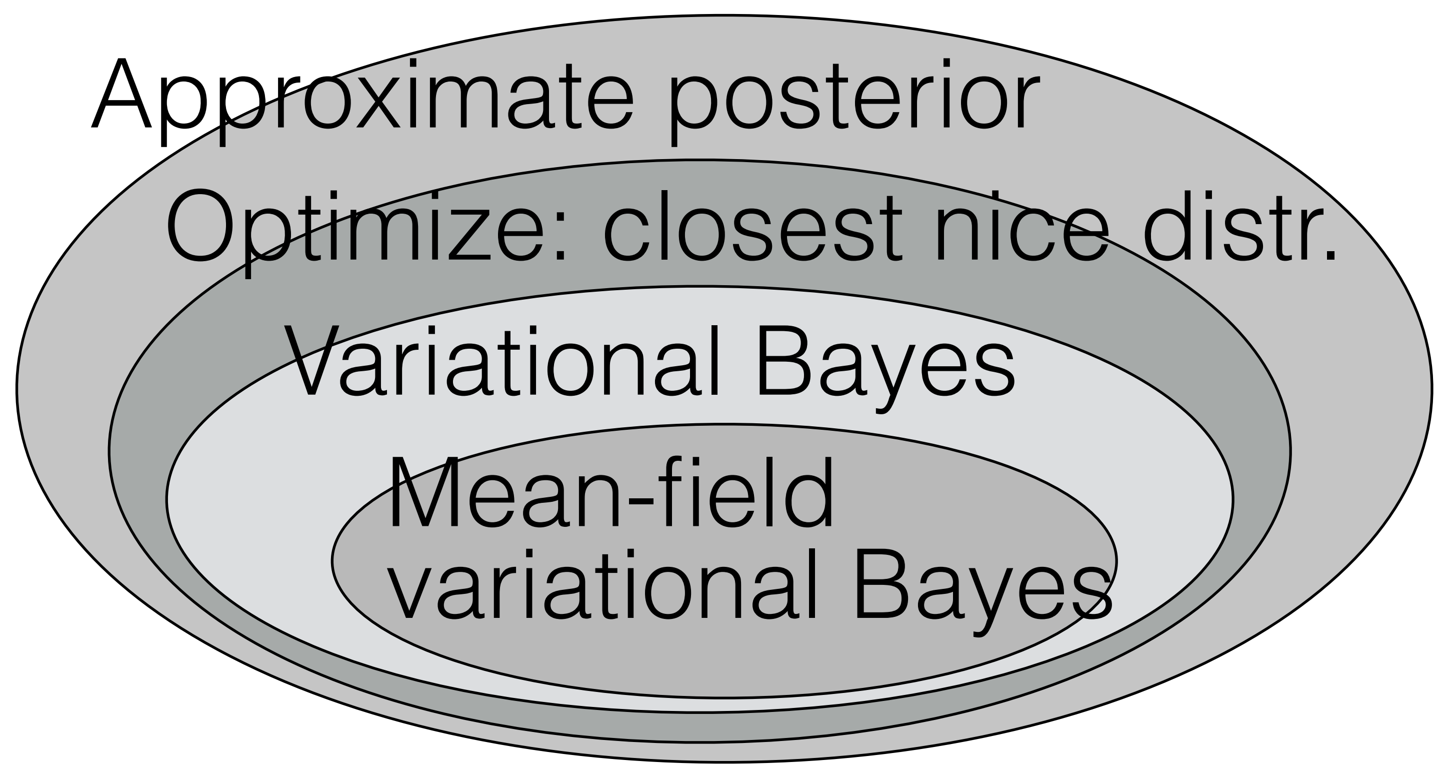

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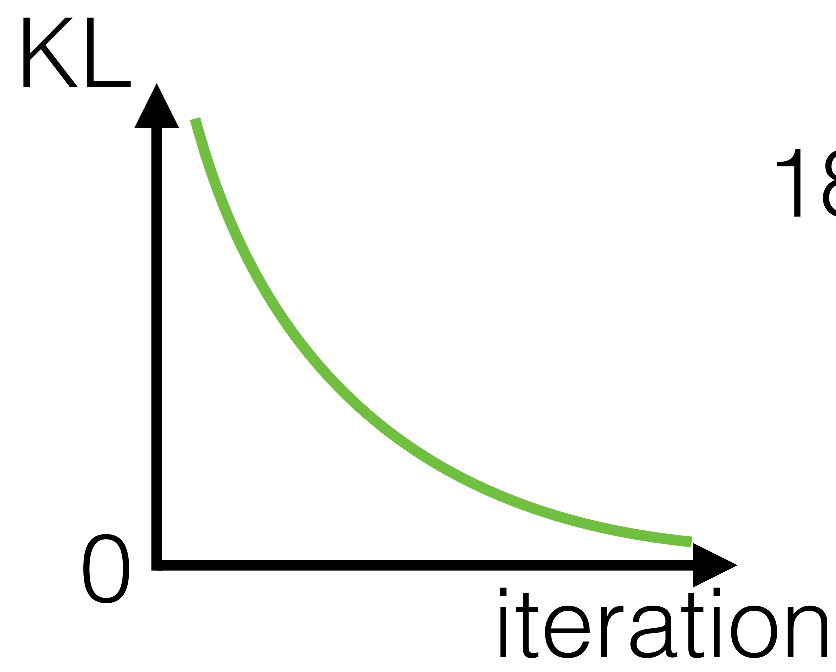

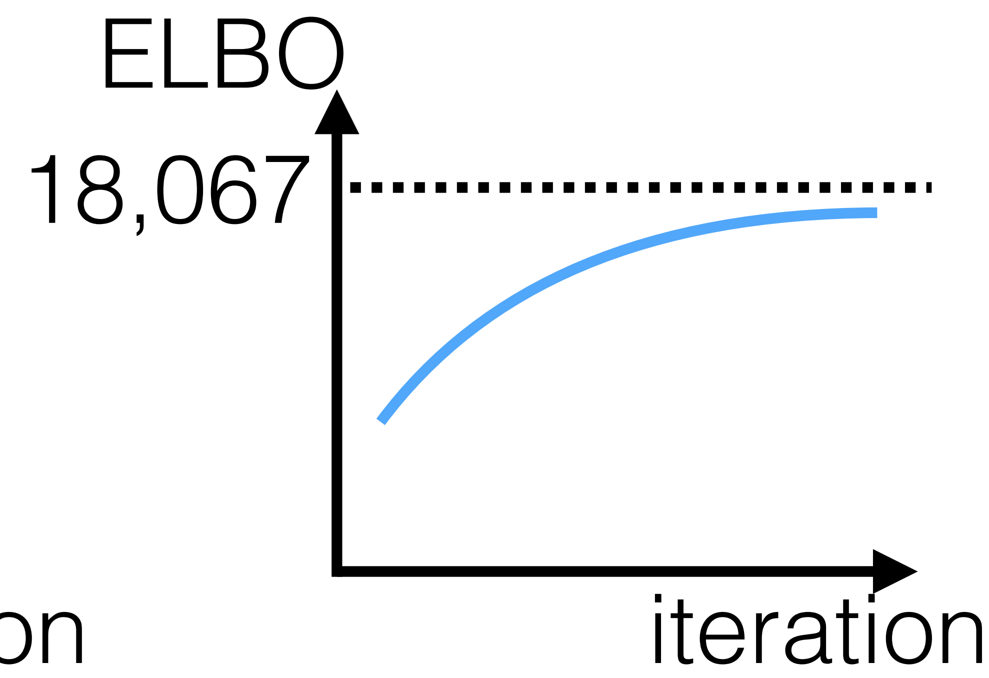

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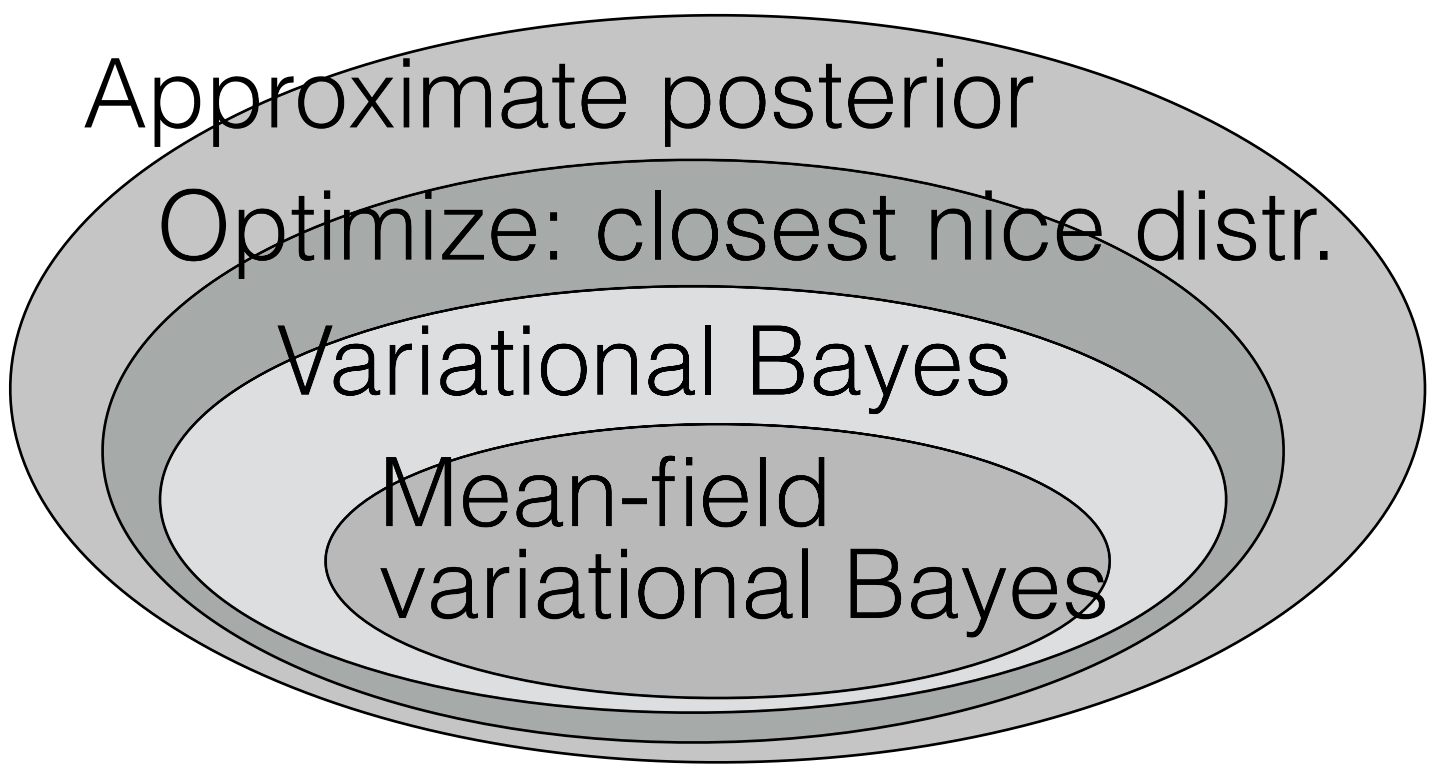
- Richer "nice" set; alternative divergences



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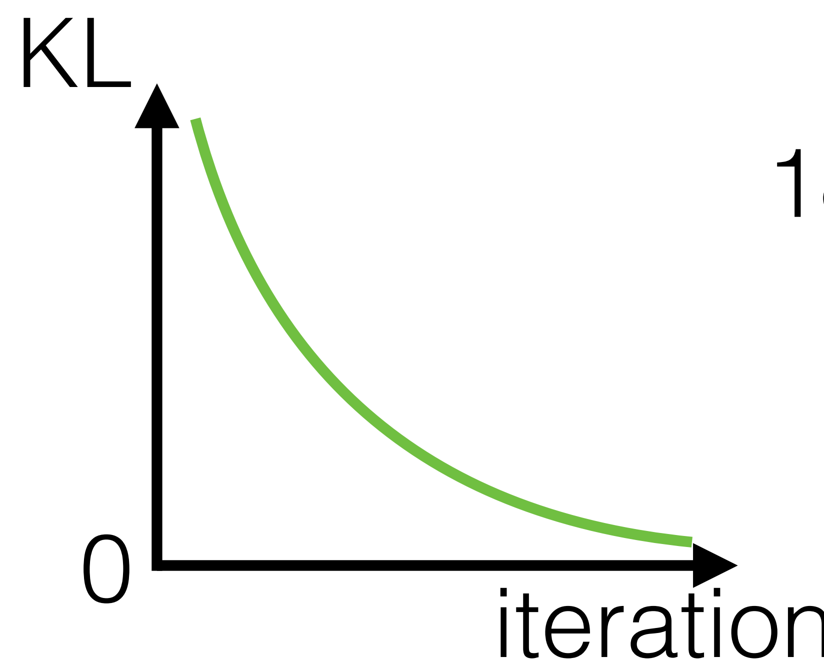

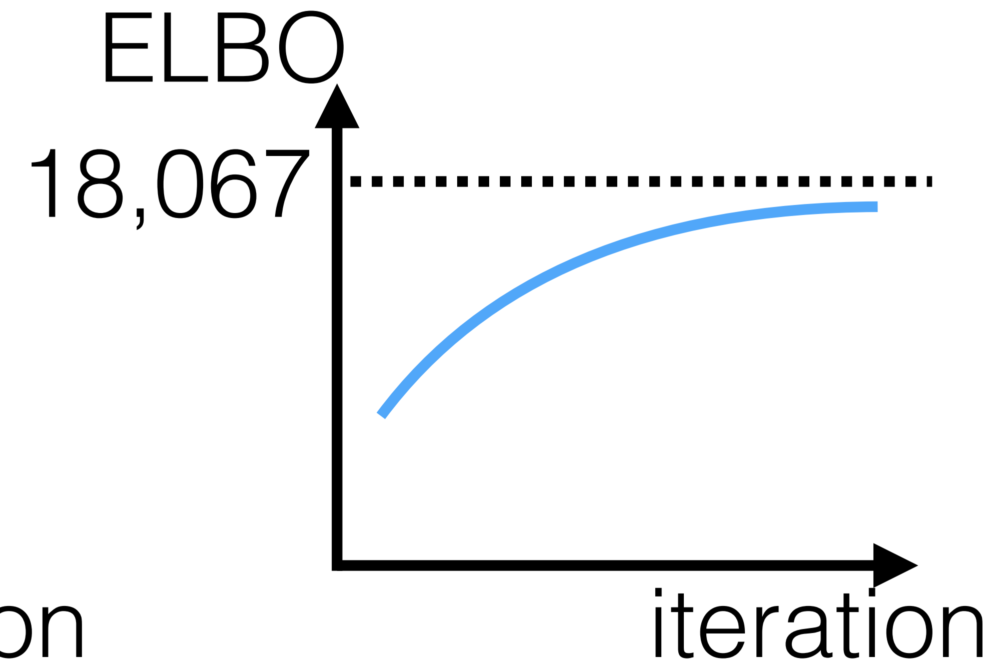

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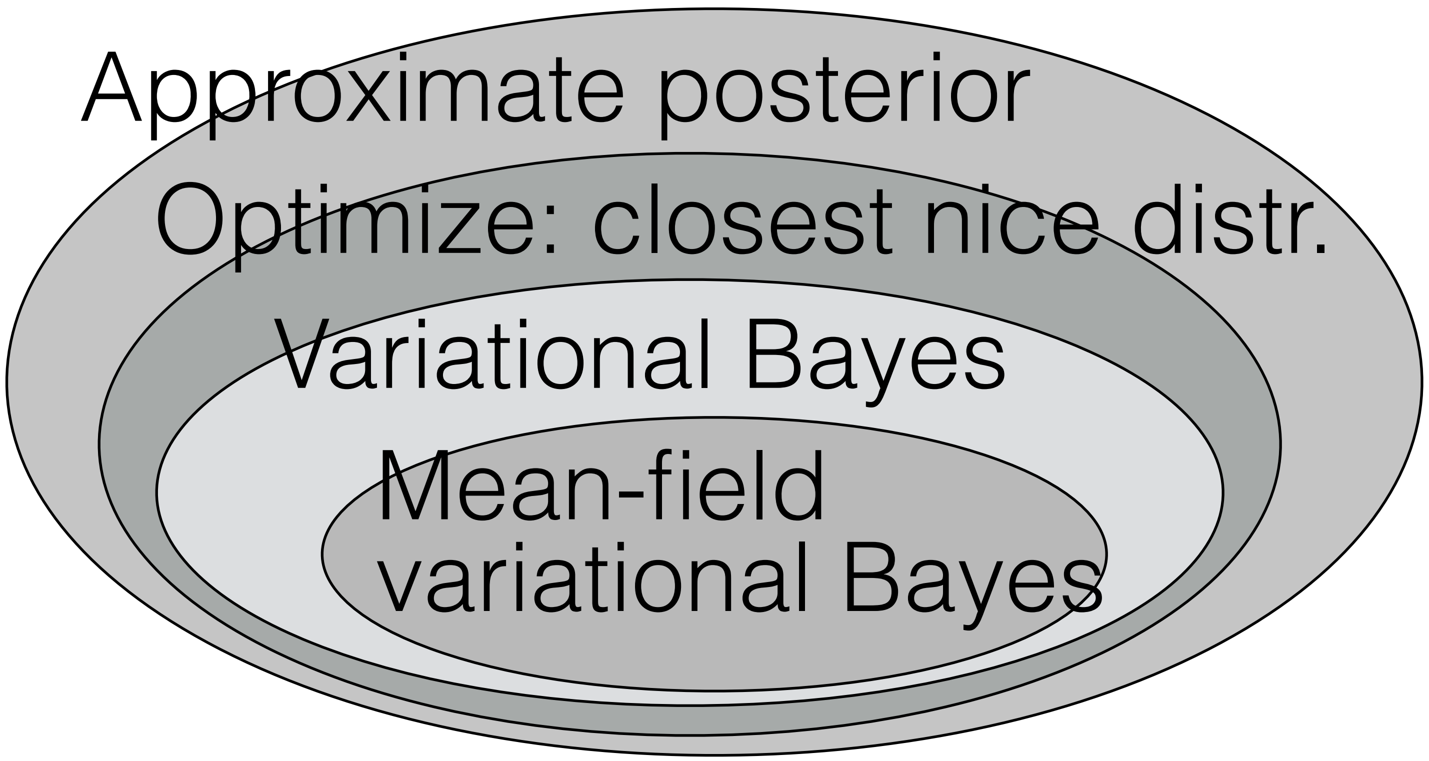

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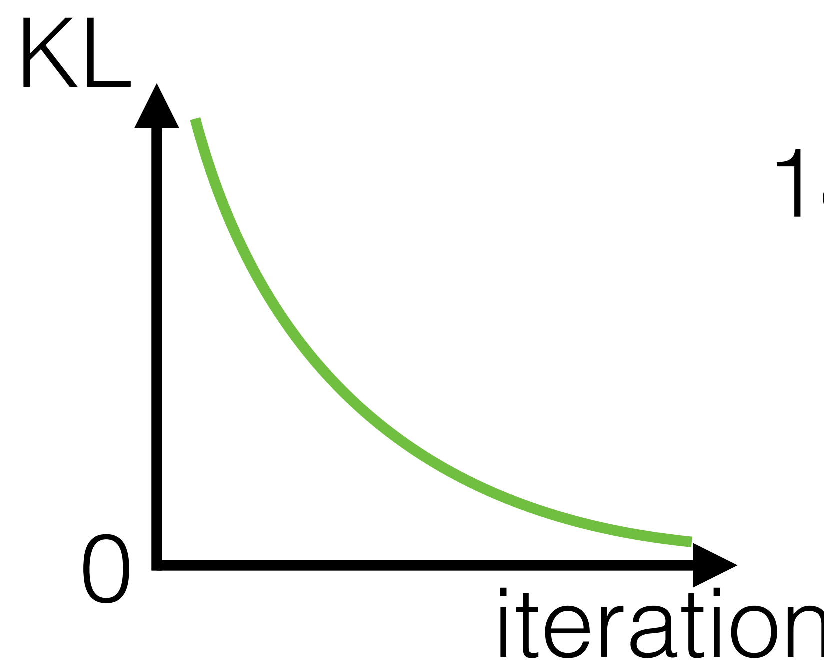

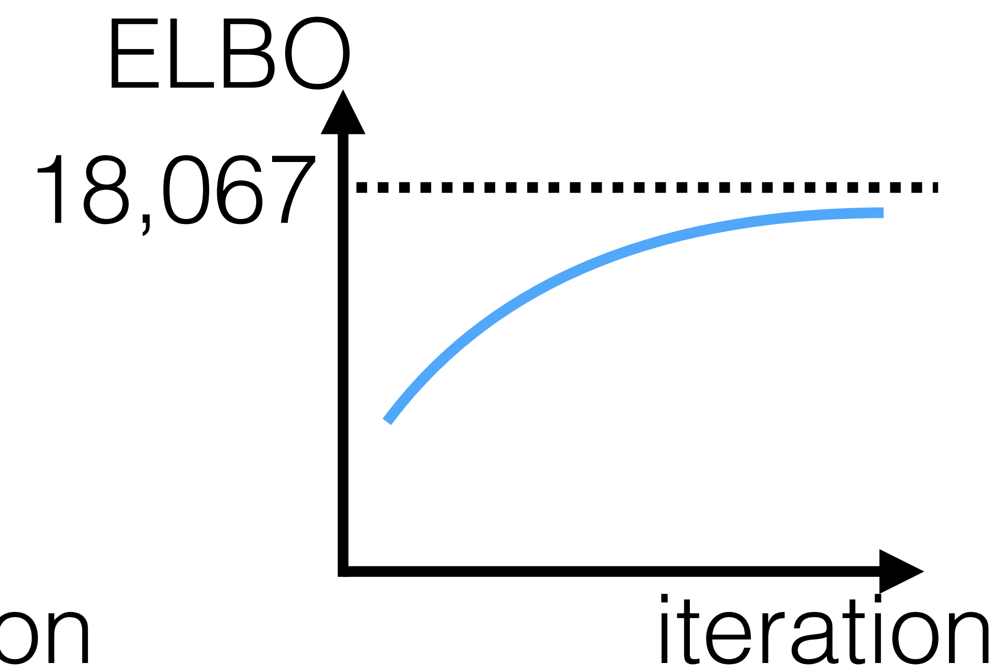

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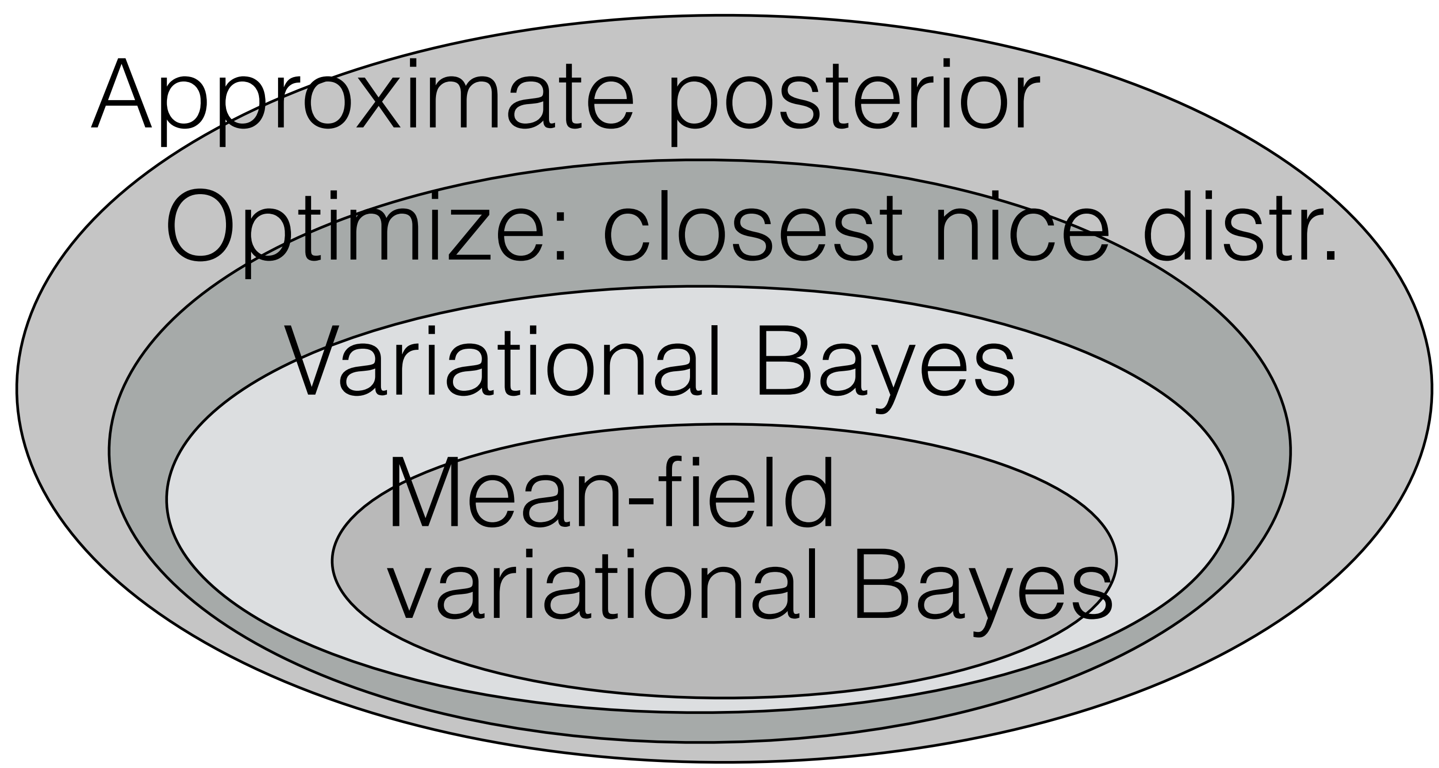

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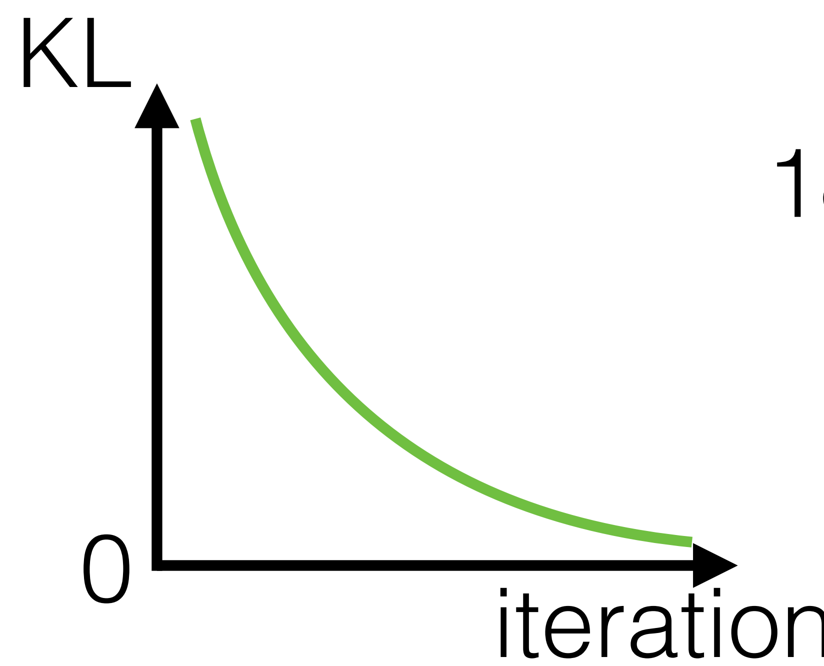

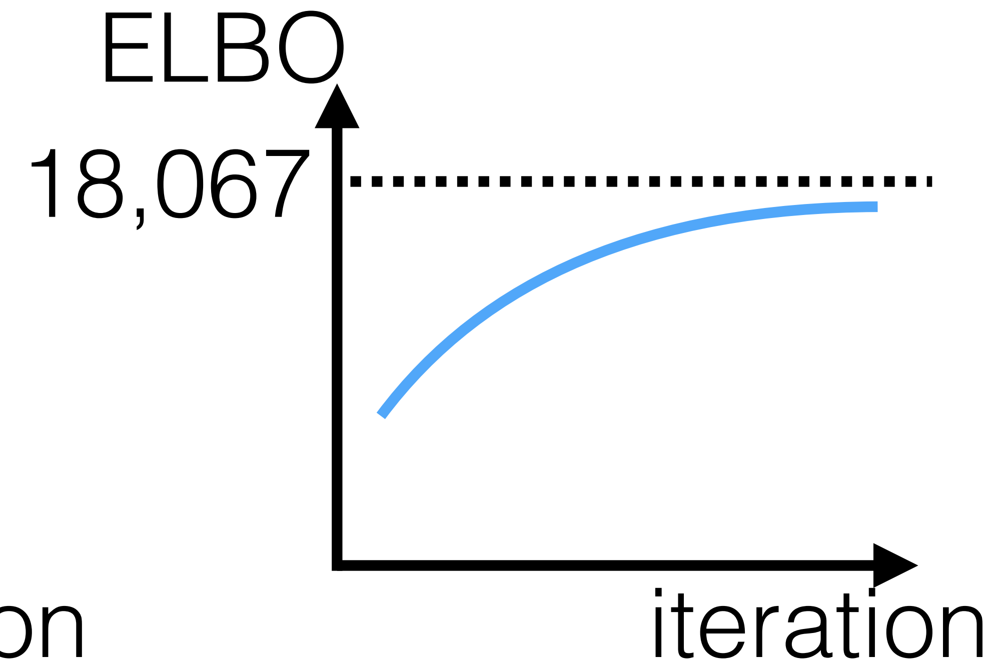

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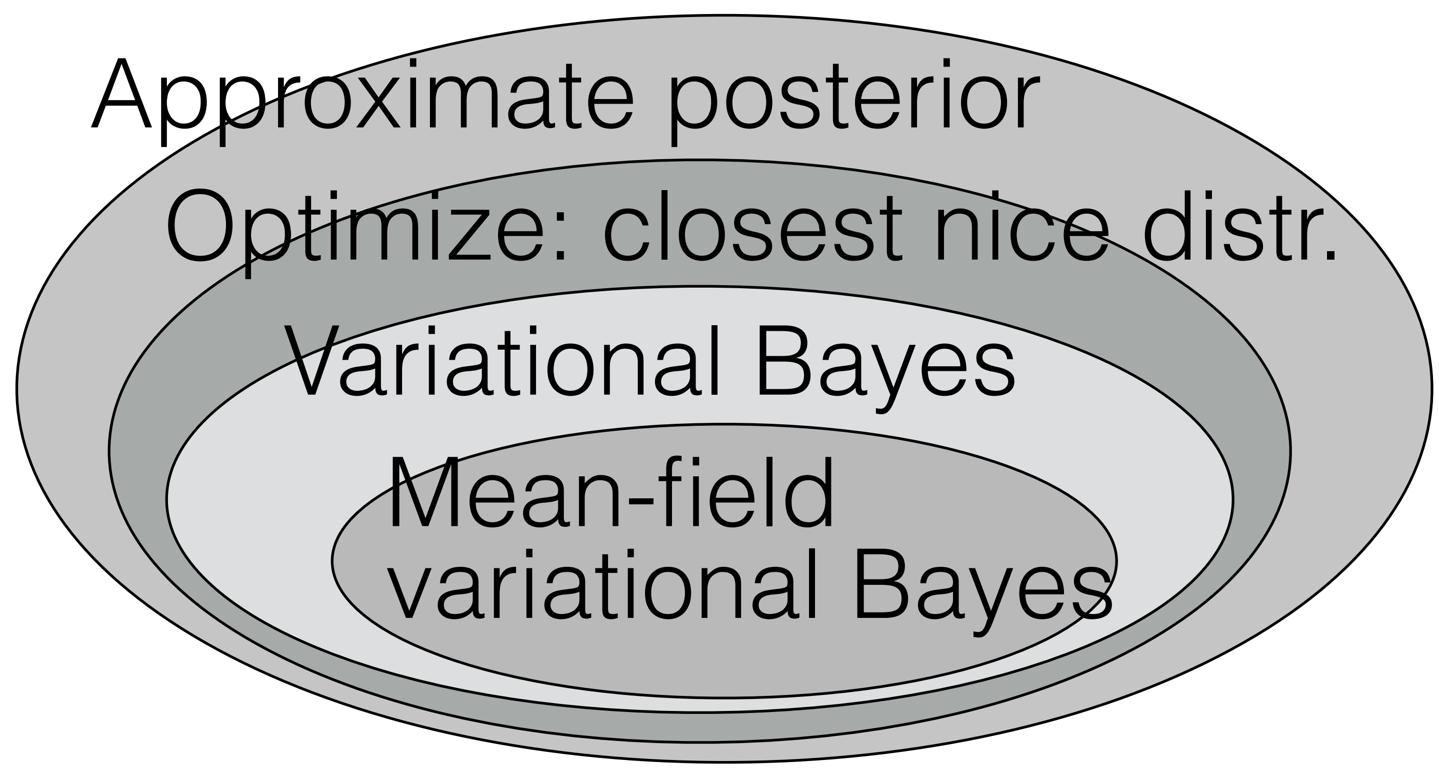

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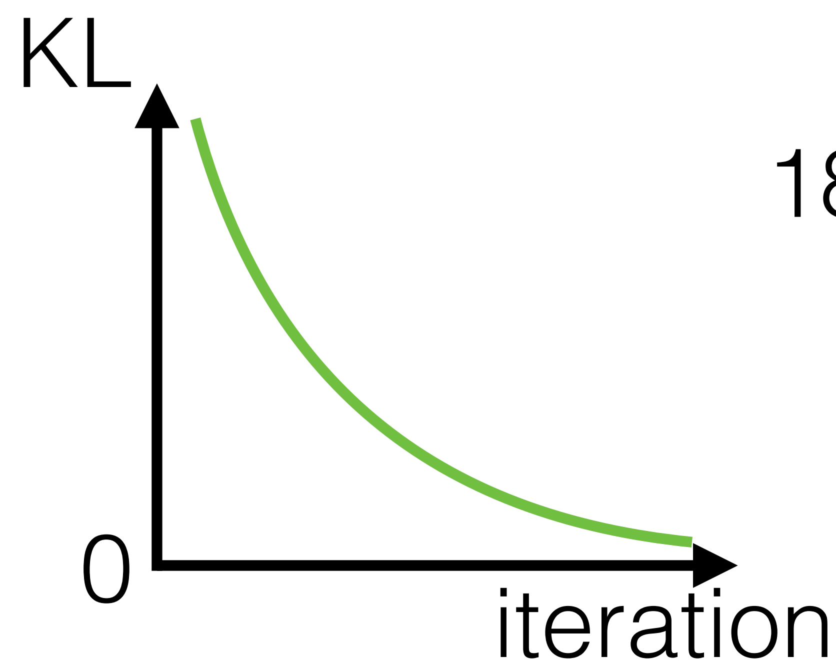

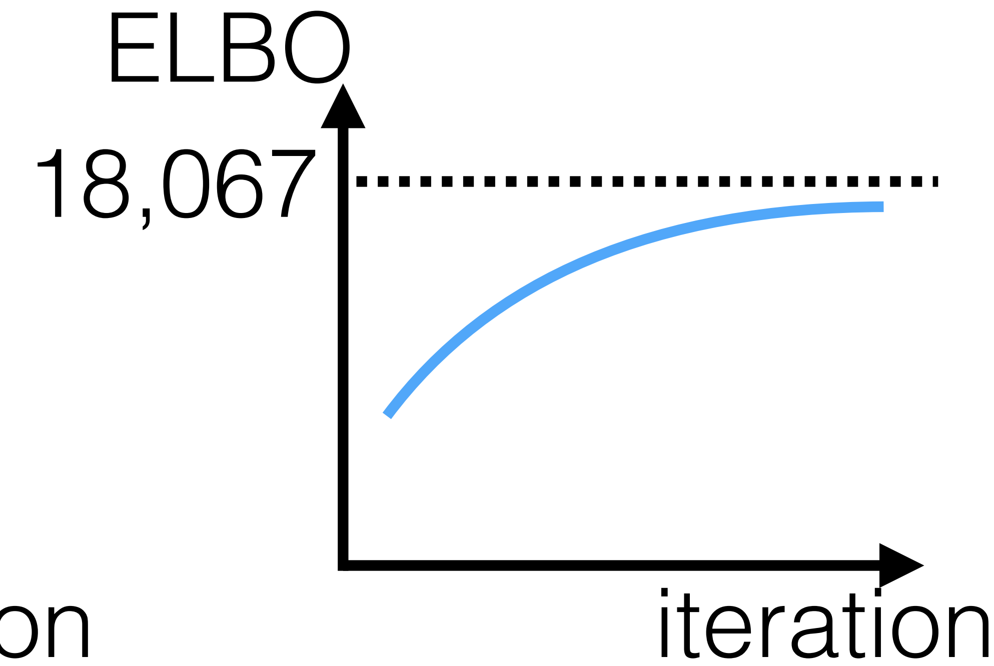

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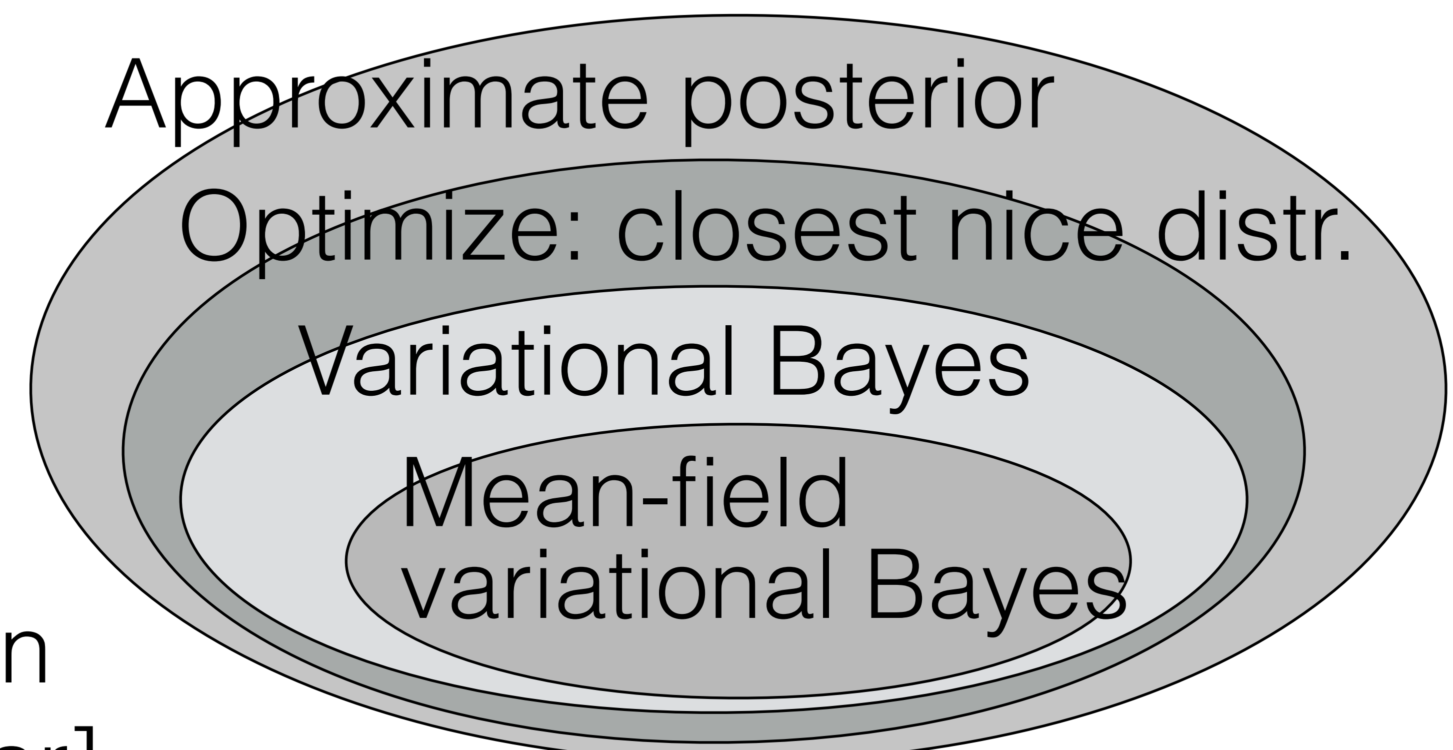

What to read next

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. *NeurIPS* 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*, 2018.
- J Huggins, T Campbell, M Kasprzak, T Broderick. Practical bounds on the error of Bayesian posterior approximations: A nonasymptotic approach, 2018. ArXiv: 1809.09505.

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AG Baydin, BA Pearlmutter, AA Radul, and JM Siskind. "Automatic differentiation in machine learning: a survey." ArXiv:1502.05767v4 (2018).

DM Blei, A Kucukelbir, and JD McAuliffe. "Variational inference: A review for statisticians." *Journal of the American Statistical Association* 112.518 (2017): 859-877.

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