Variational Bayes and beyond: Foundations of scalable Bayesian inference

Tamara Broderick
Associate Professor
MIT

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

Bayesian inference

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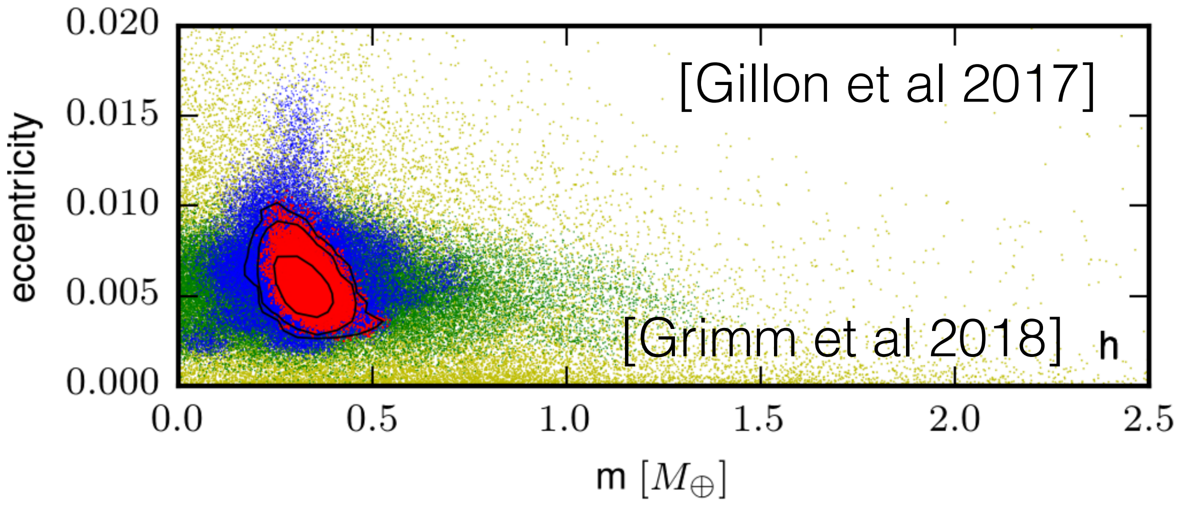

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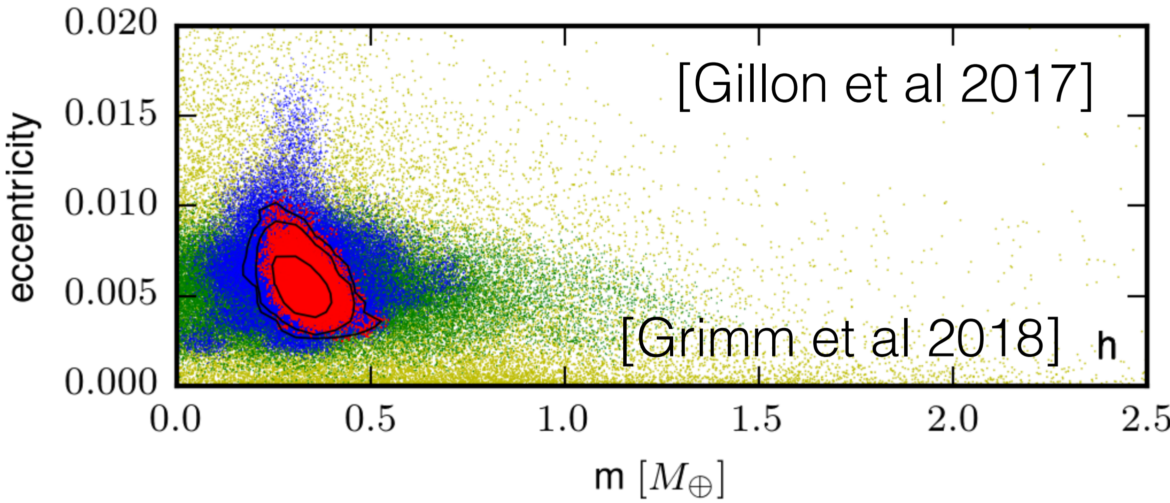

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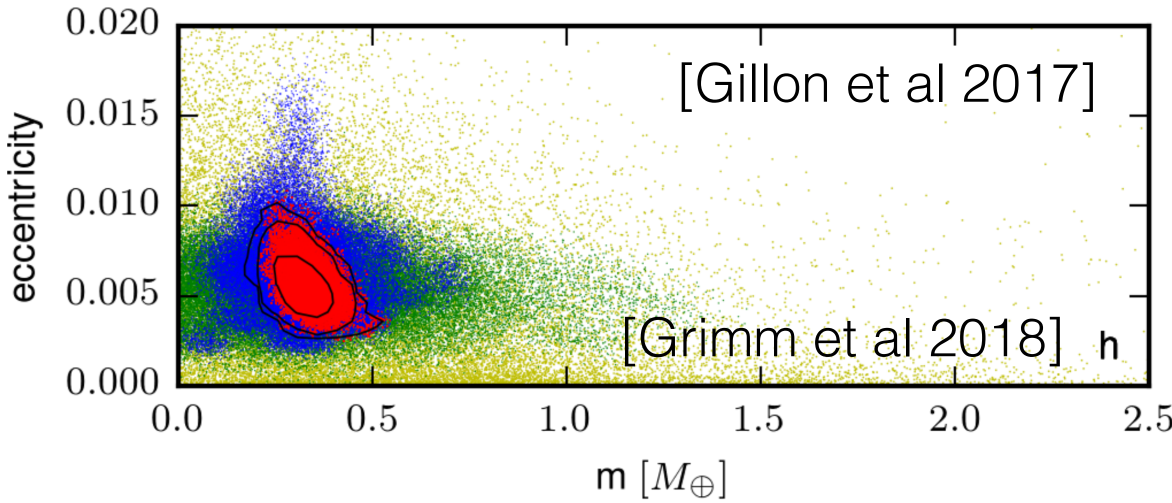

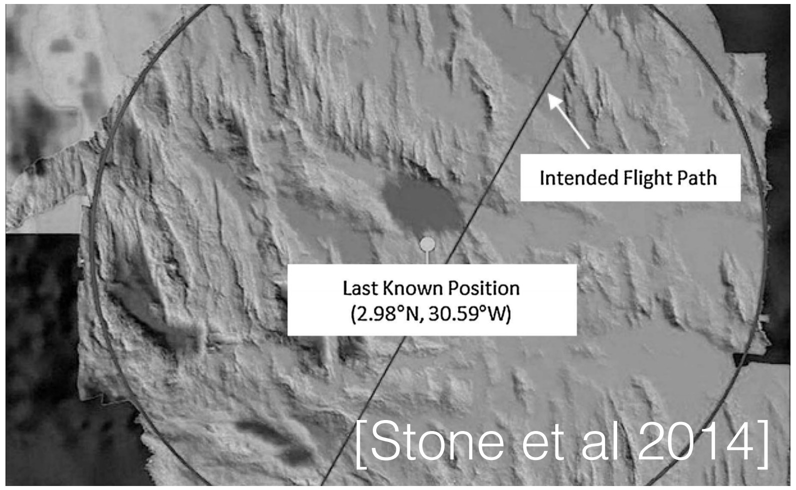

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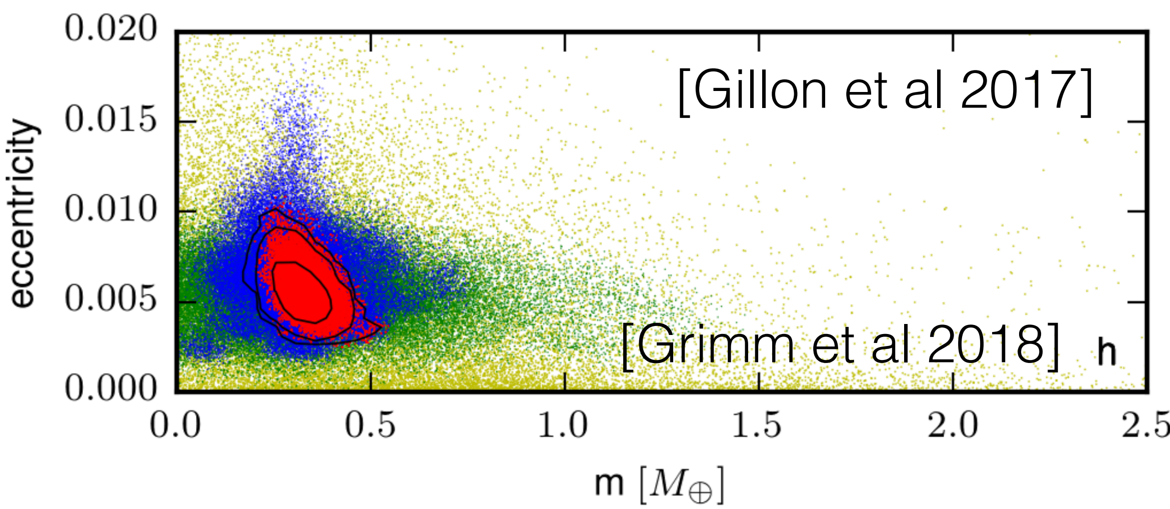

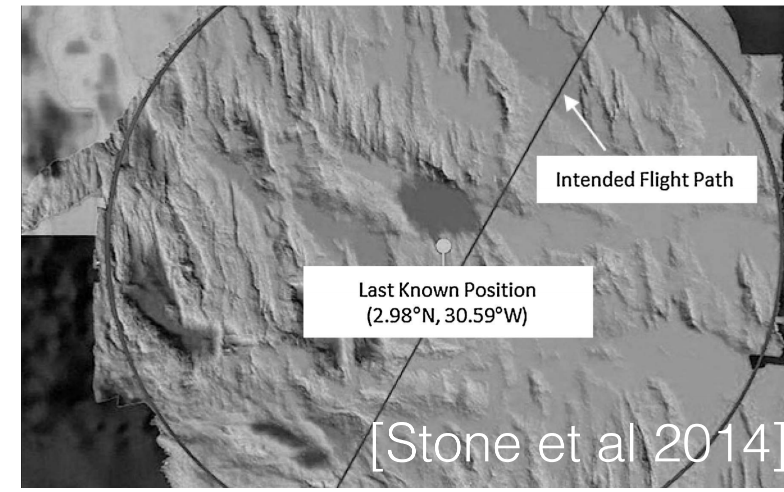

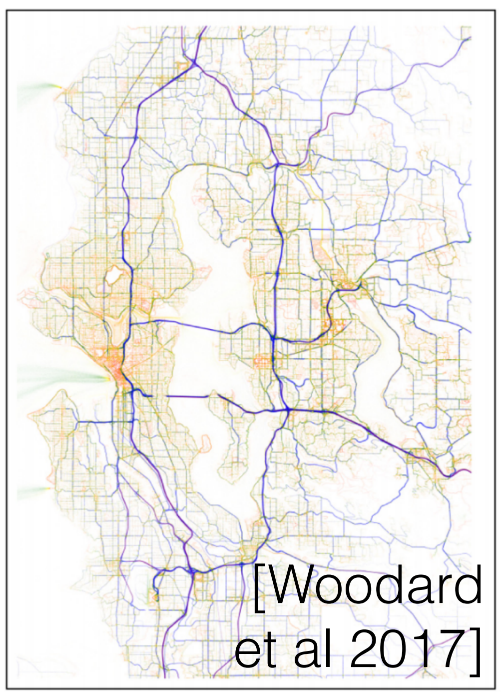

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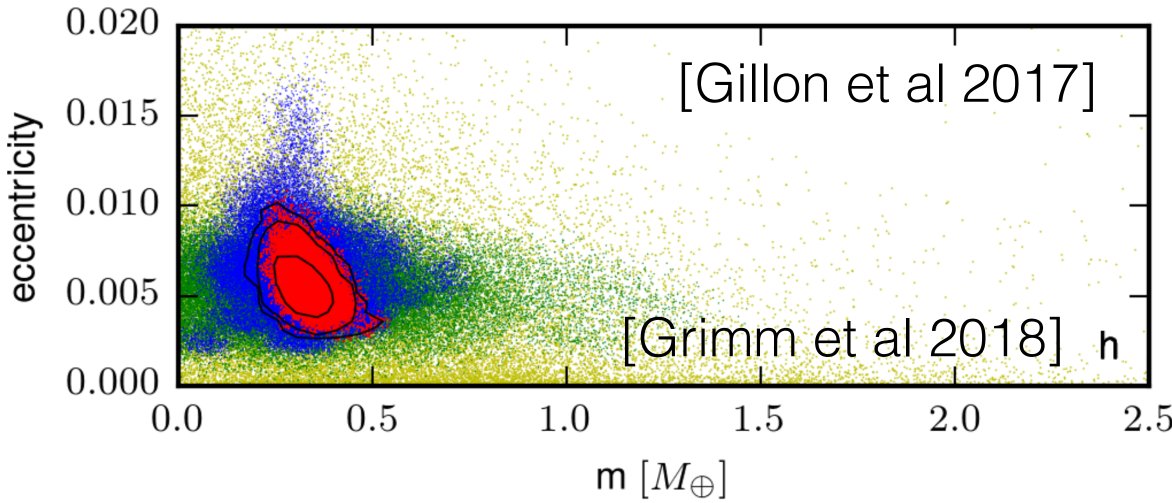

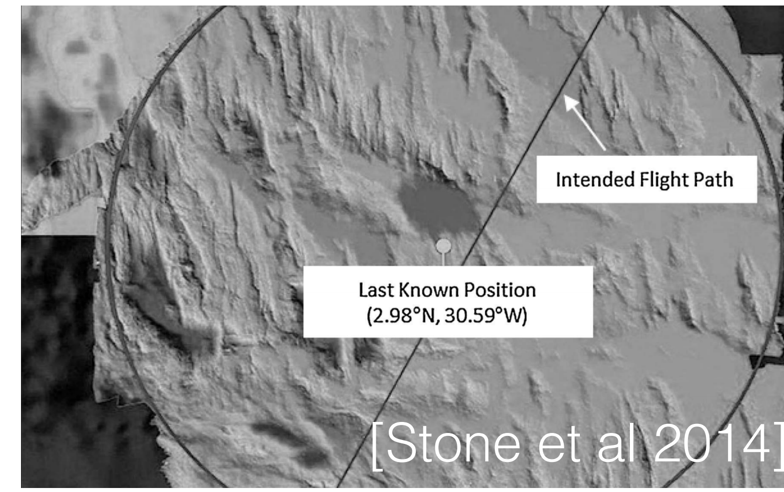

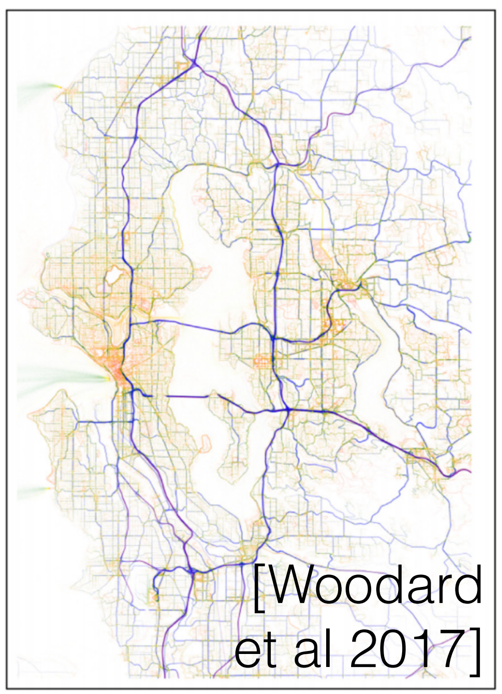

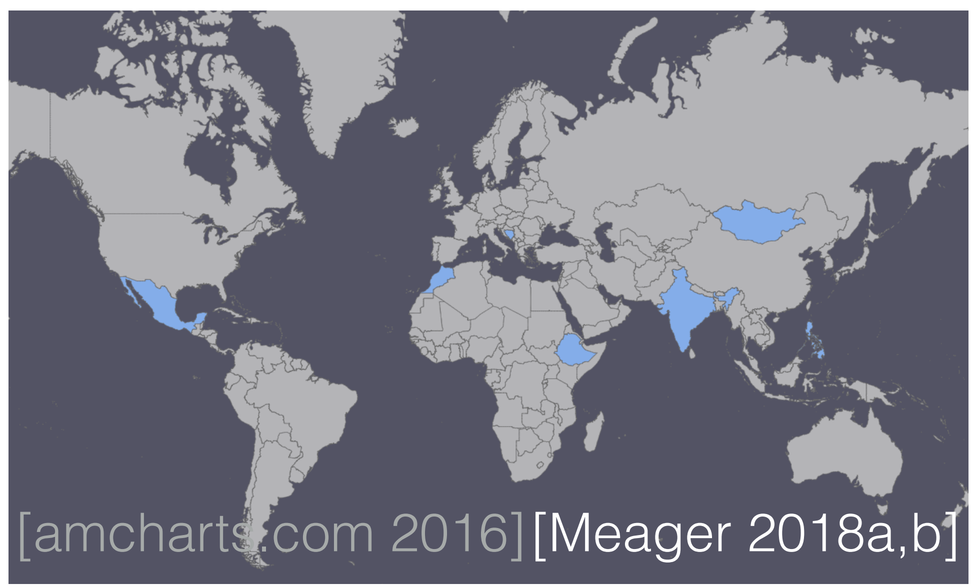

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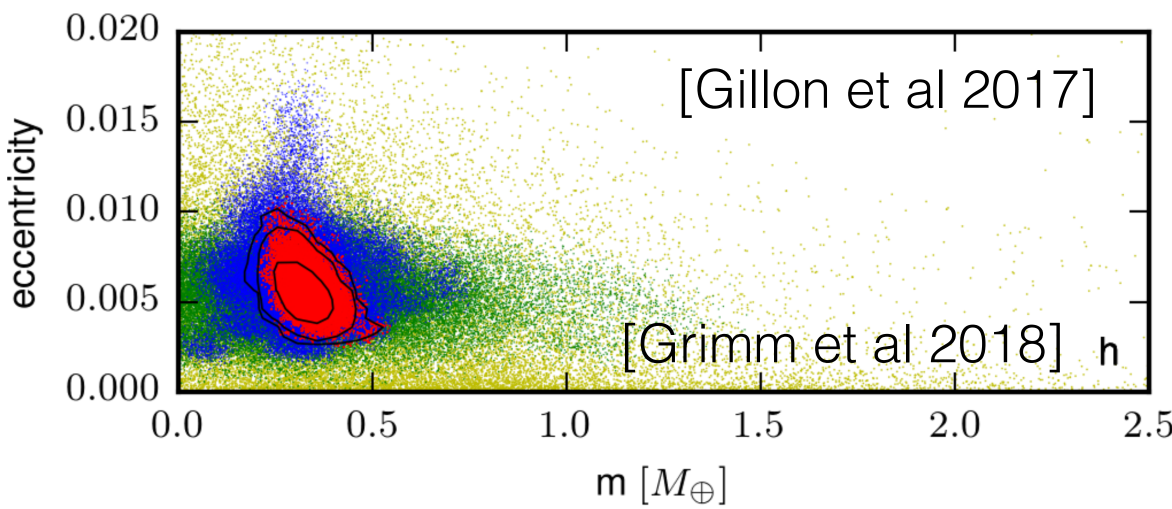

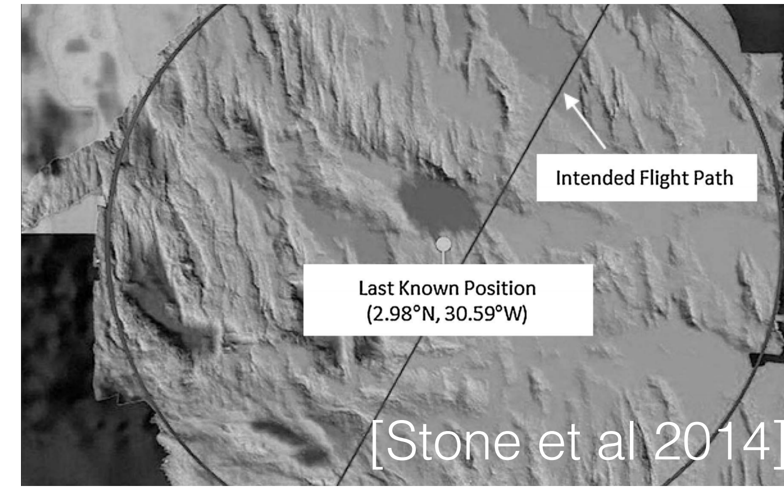

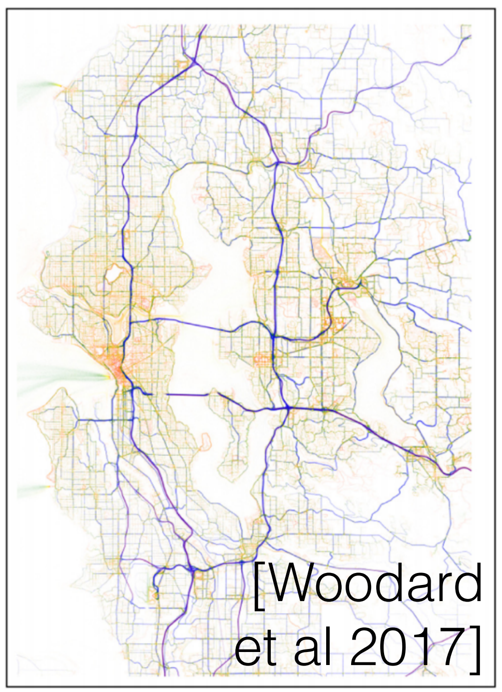

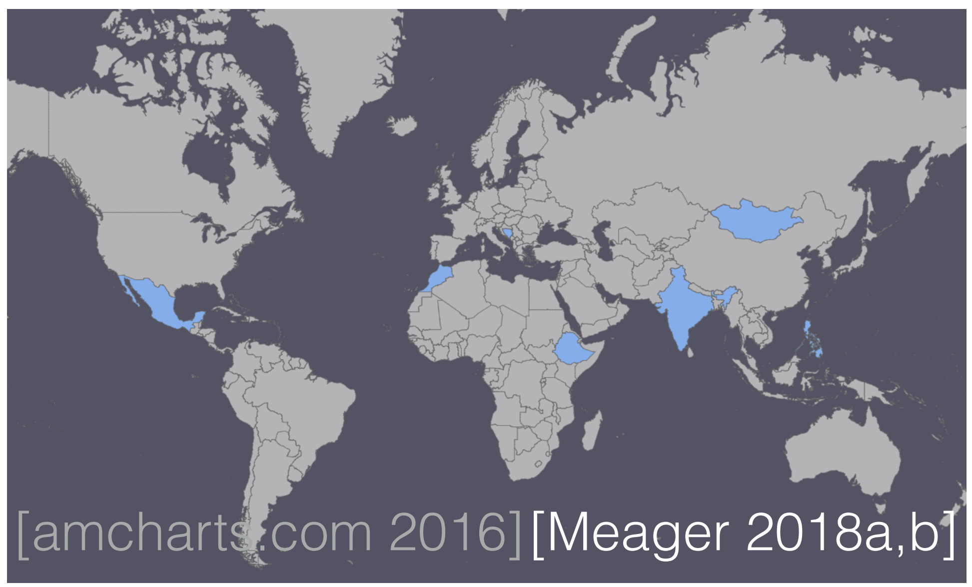

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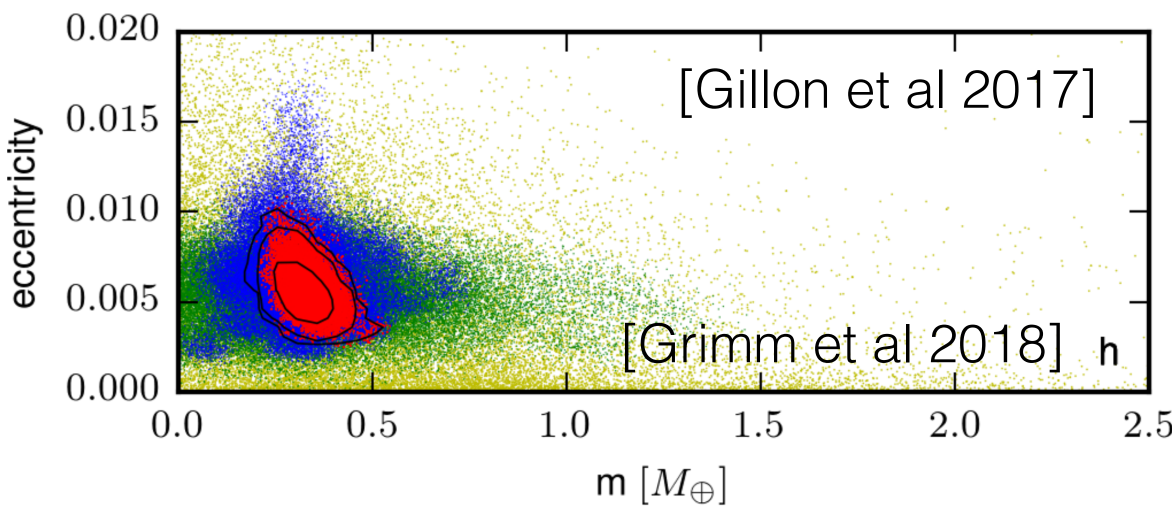

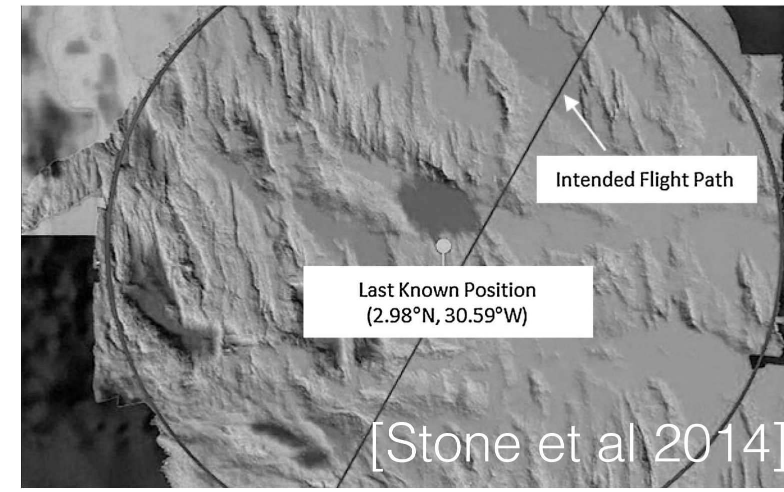

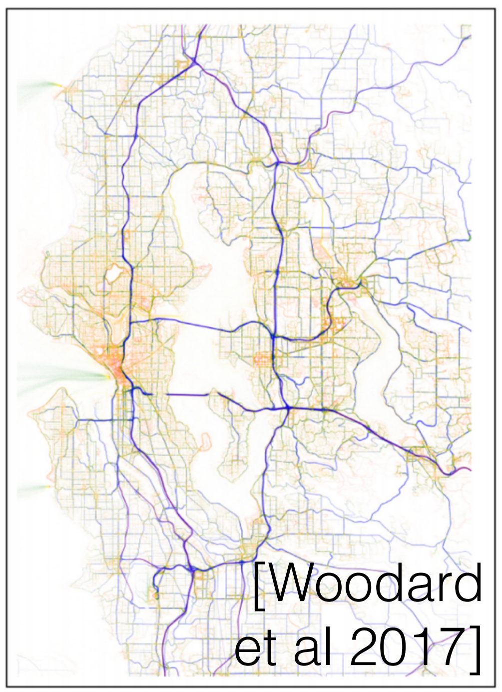

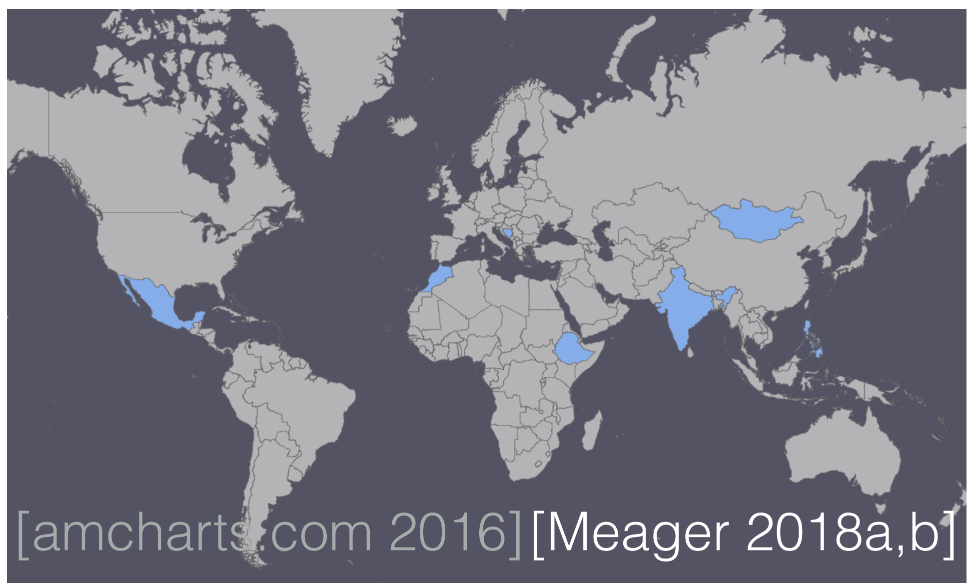

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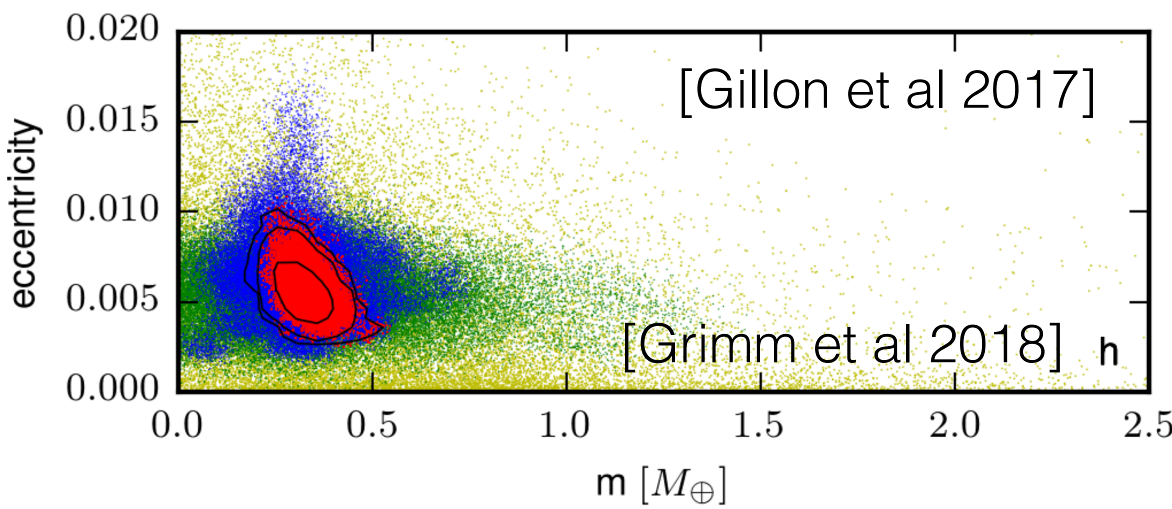

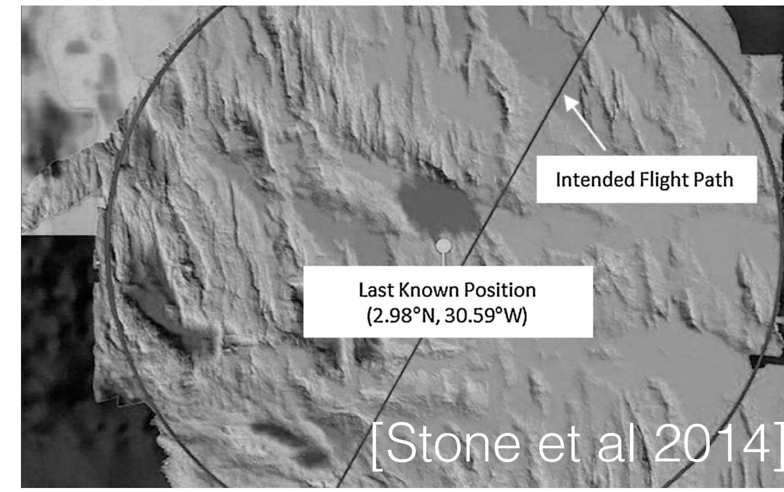

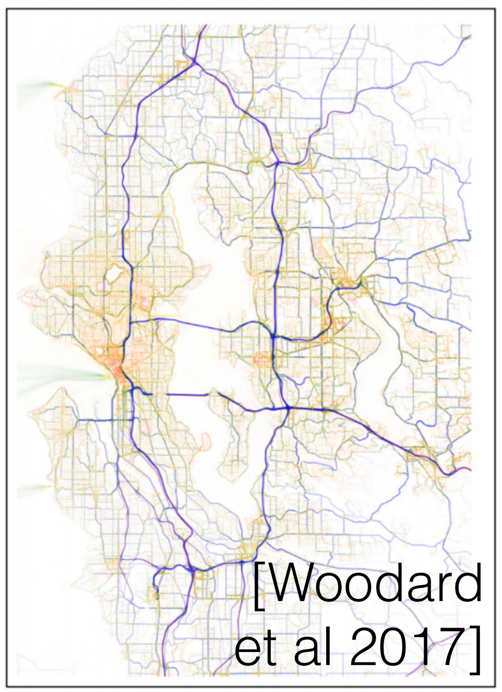

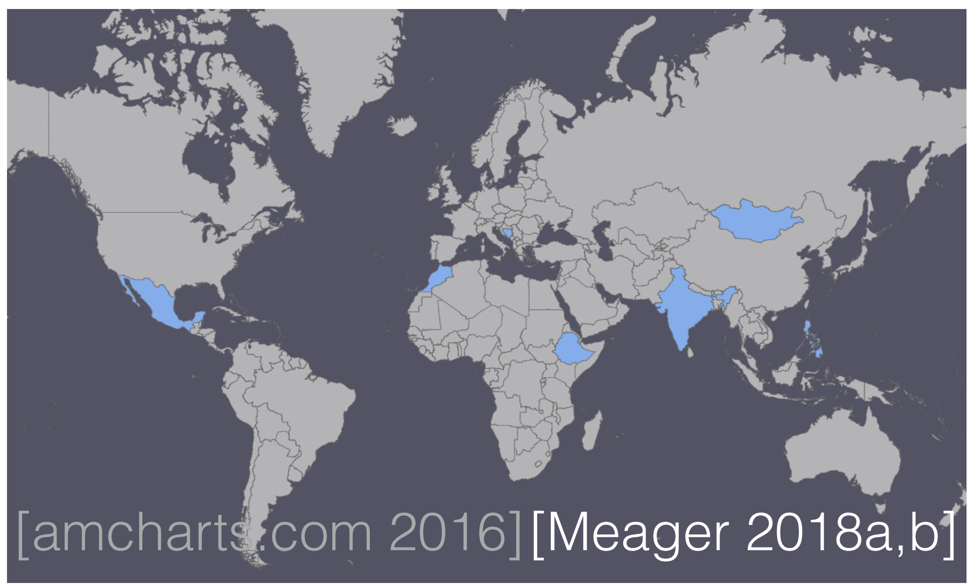

- Goals: good point estimates, uncertainty estimates

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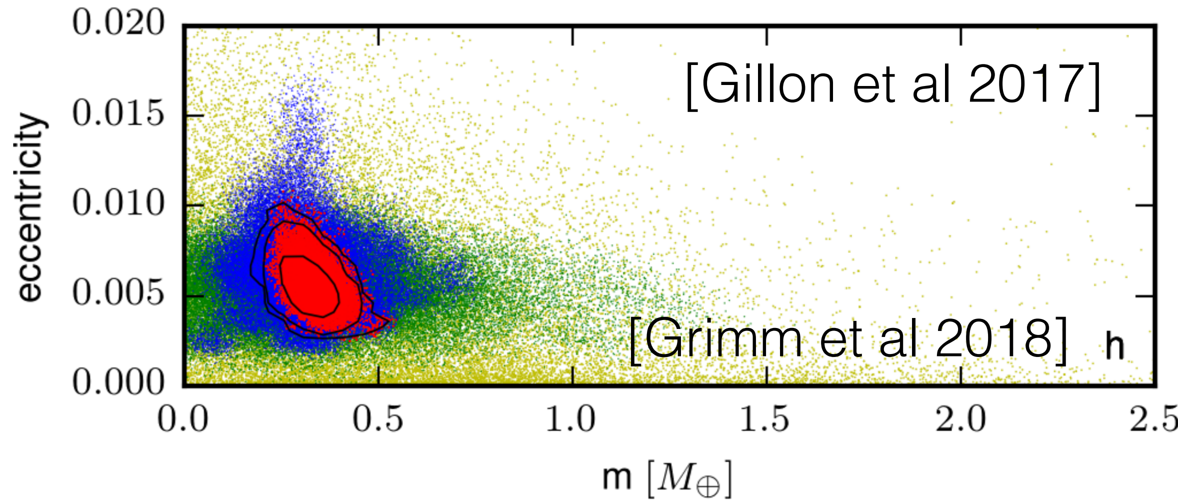
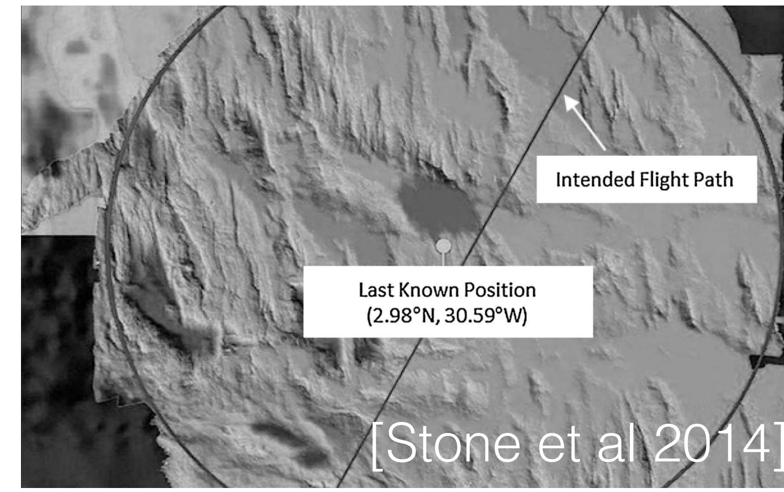
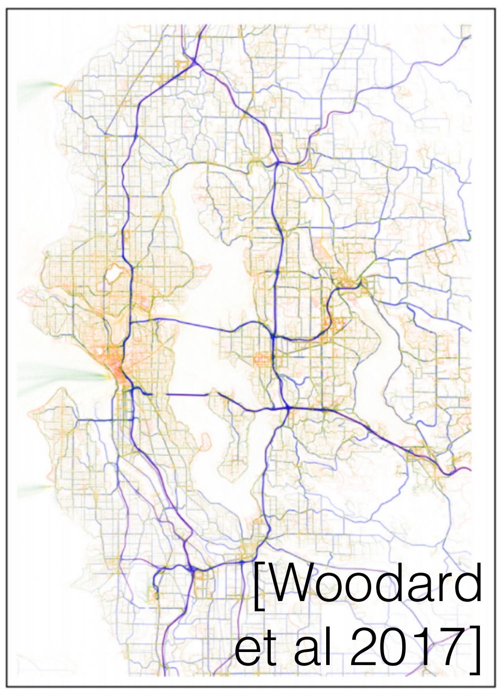
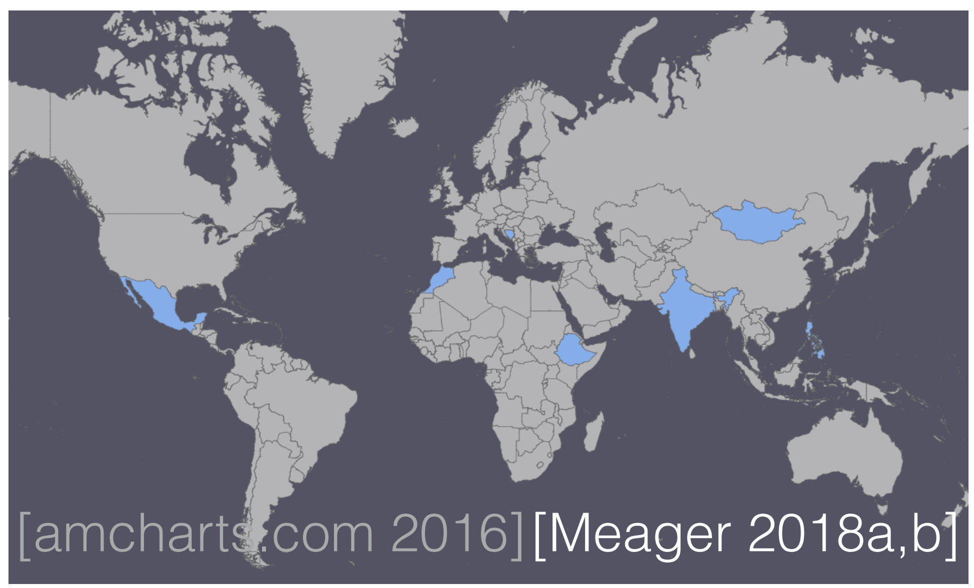


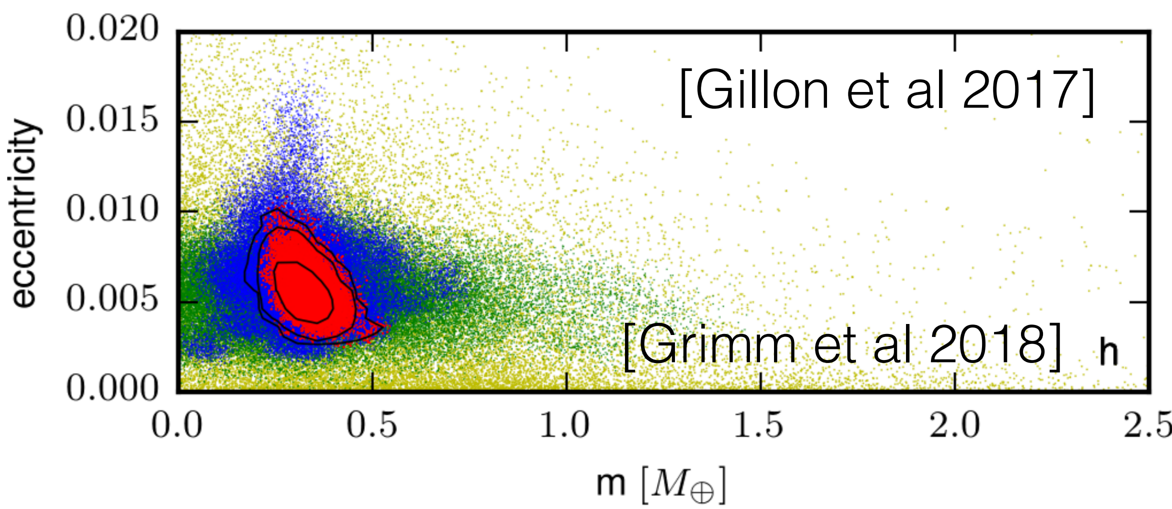


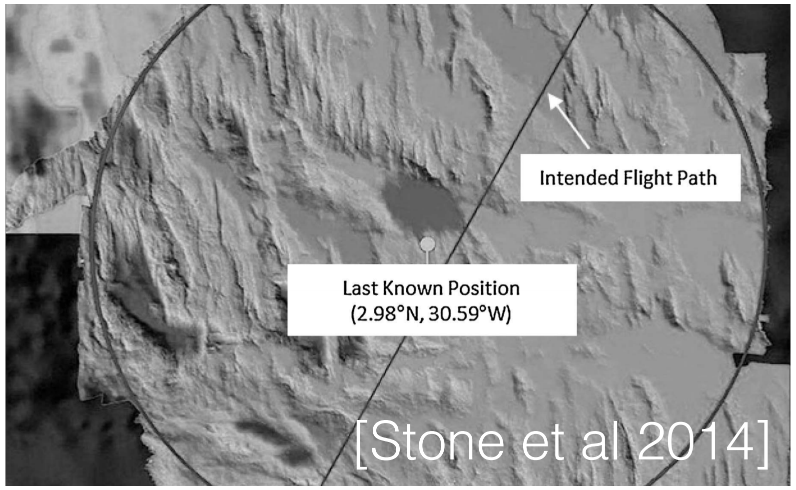


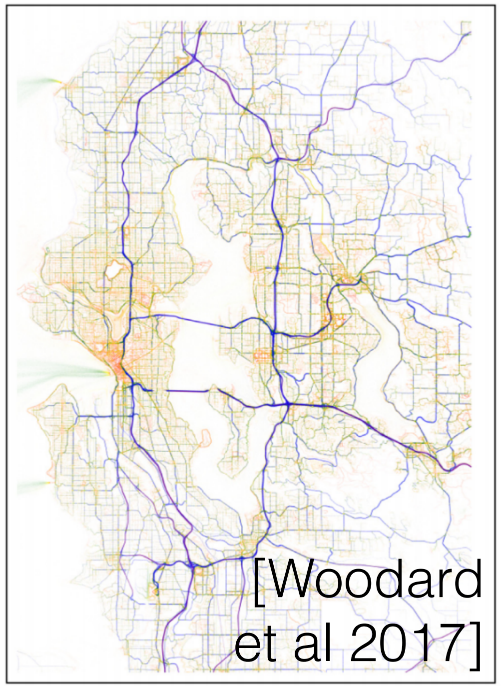


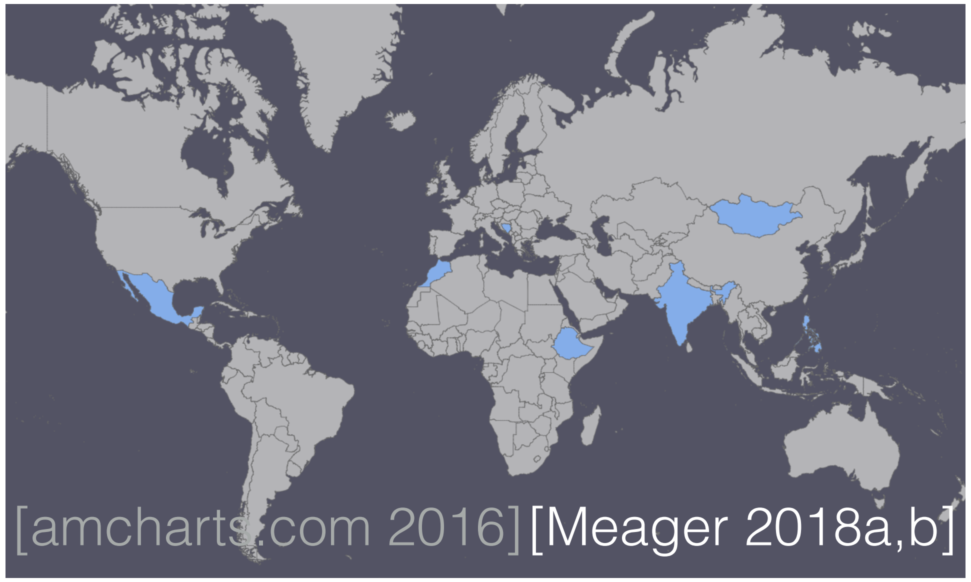
- Goals: good point estimates, uncertainty estimates
  - More: interpretable, modular, expert info

Bayesian inference









[mc-stan.org]

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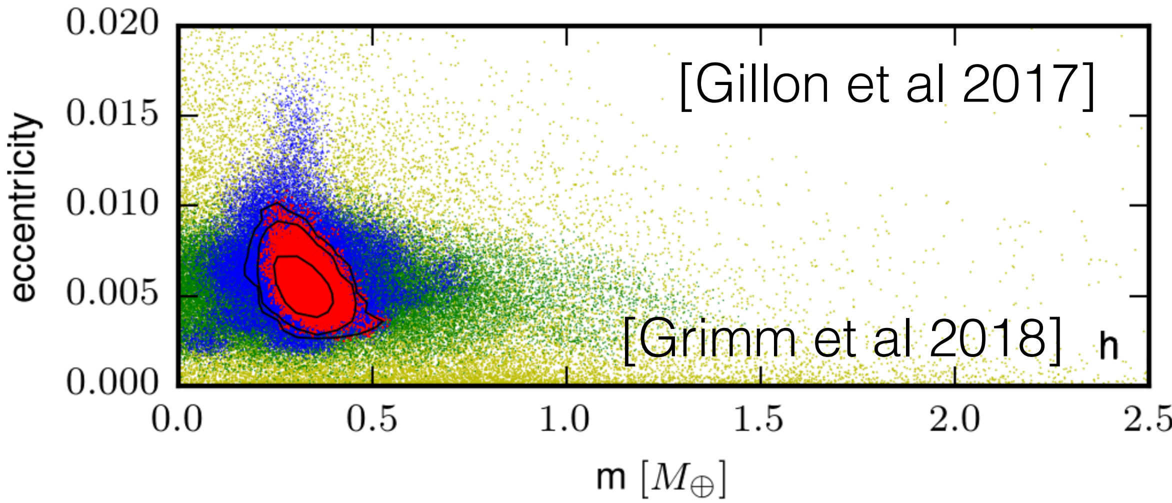

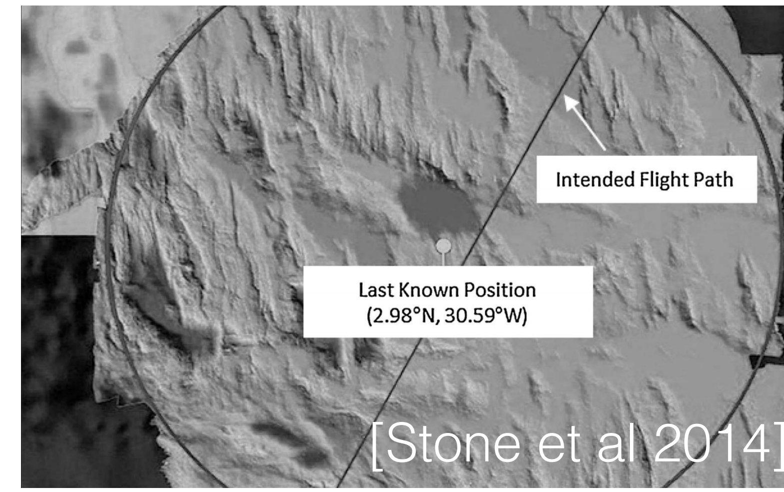

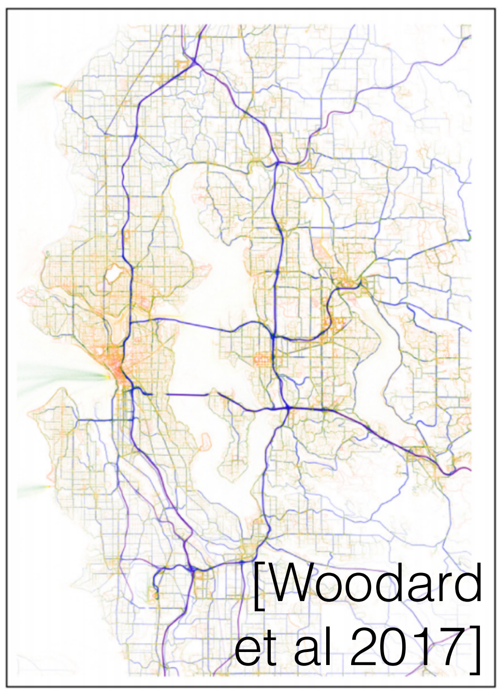

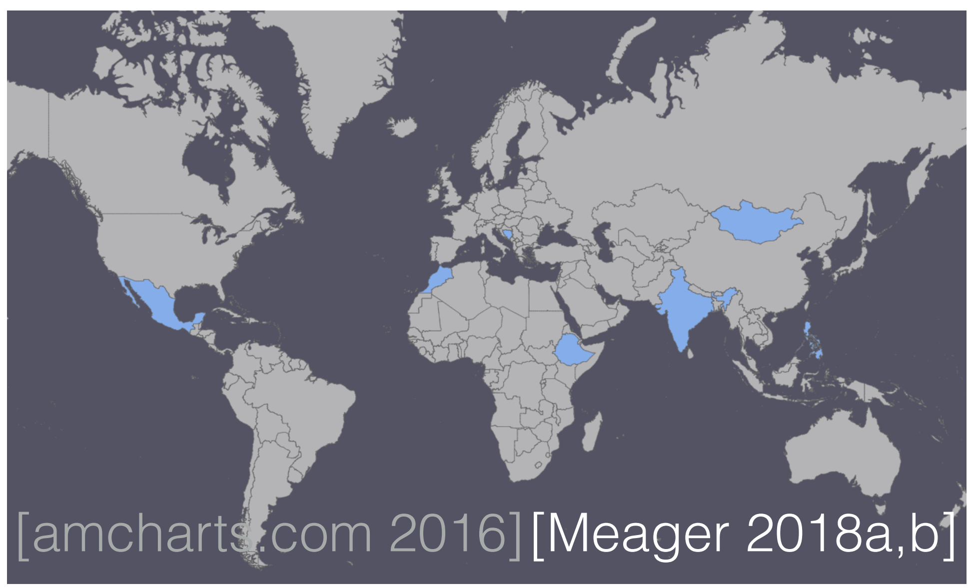

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- Goals: good point estimates, uncertainty estimates
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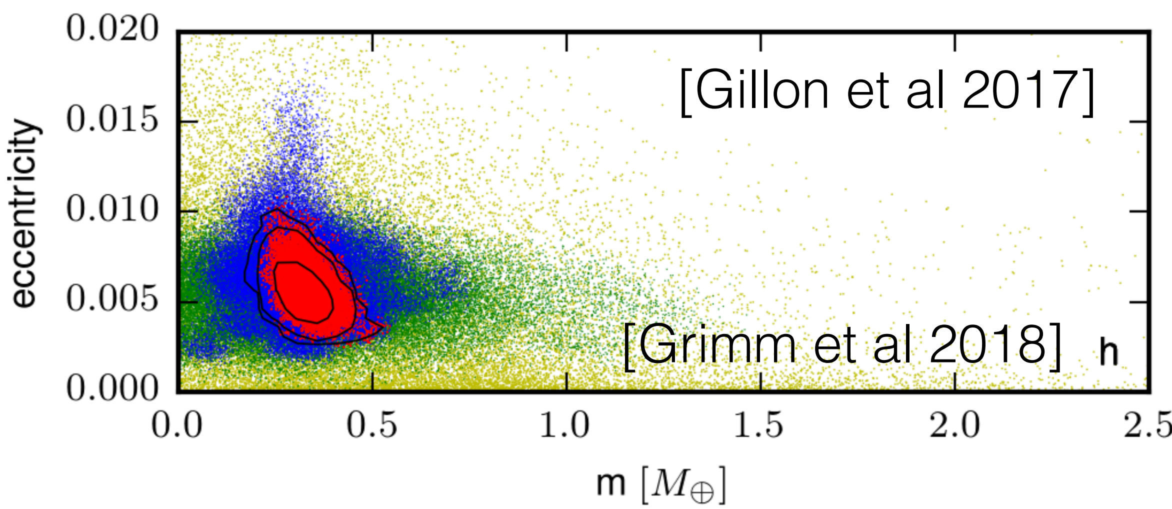
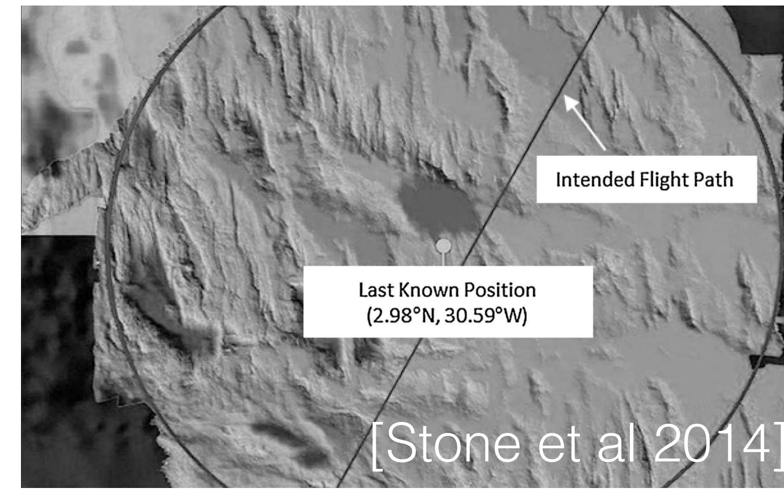
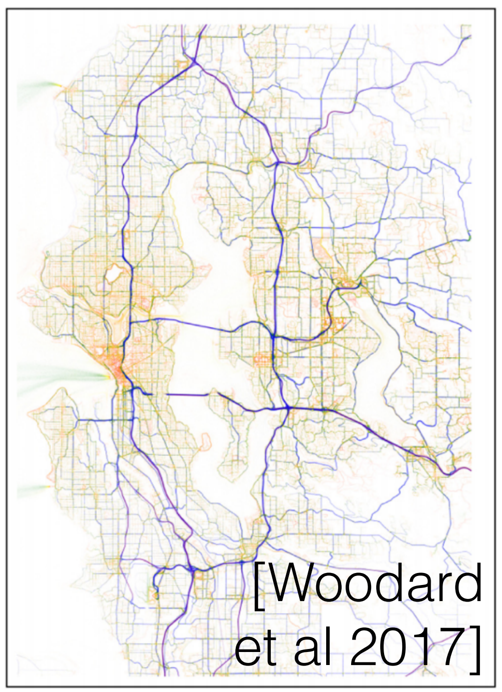
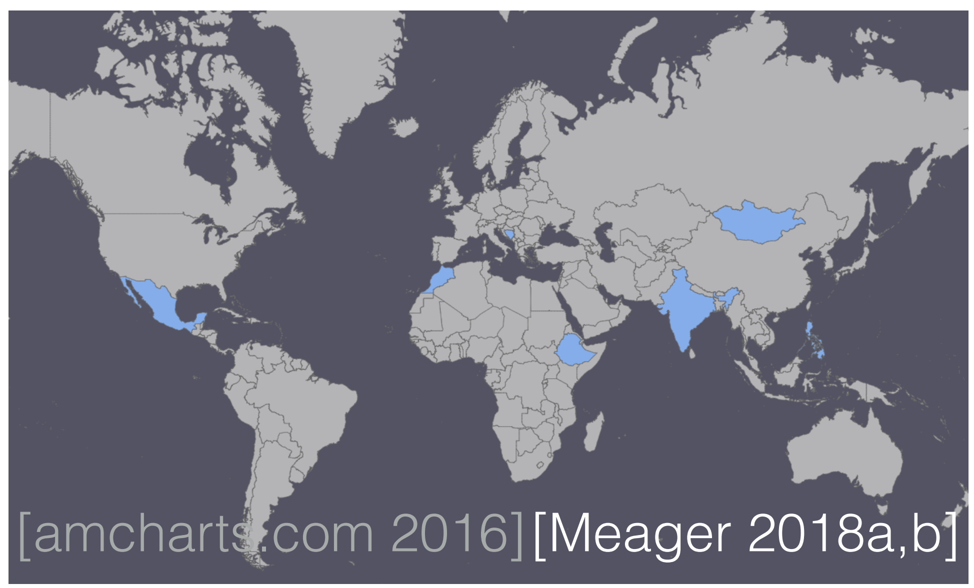
- Challenge: speed (compute, user), reliable inference

Bayesian inference









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- 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]

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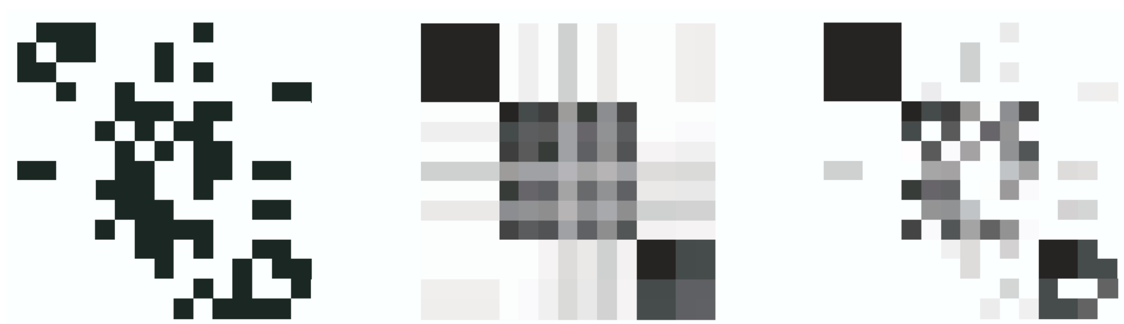

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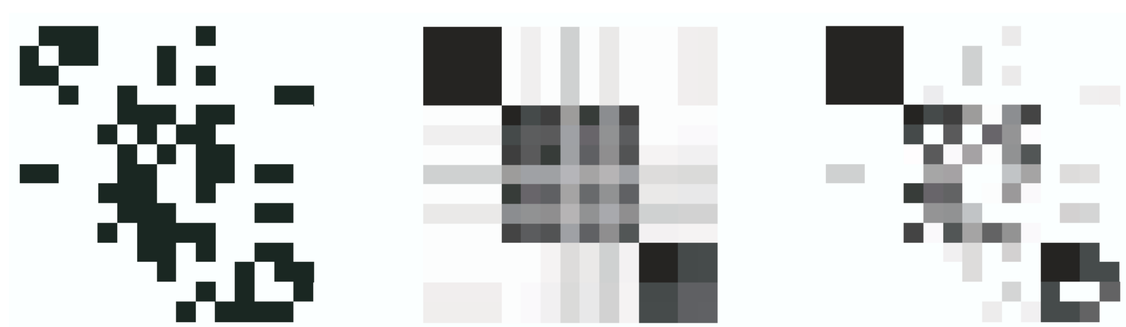

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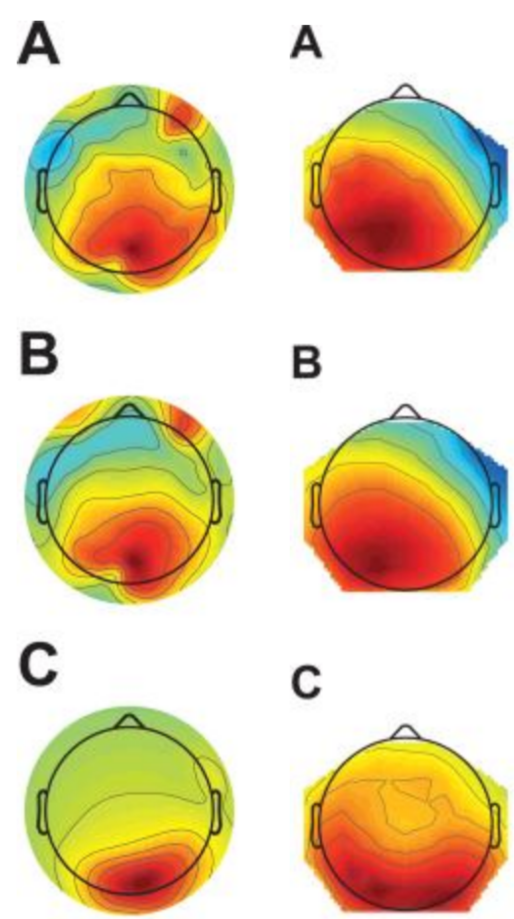

[Gershman et al 2014]

[Blei et al 2018]

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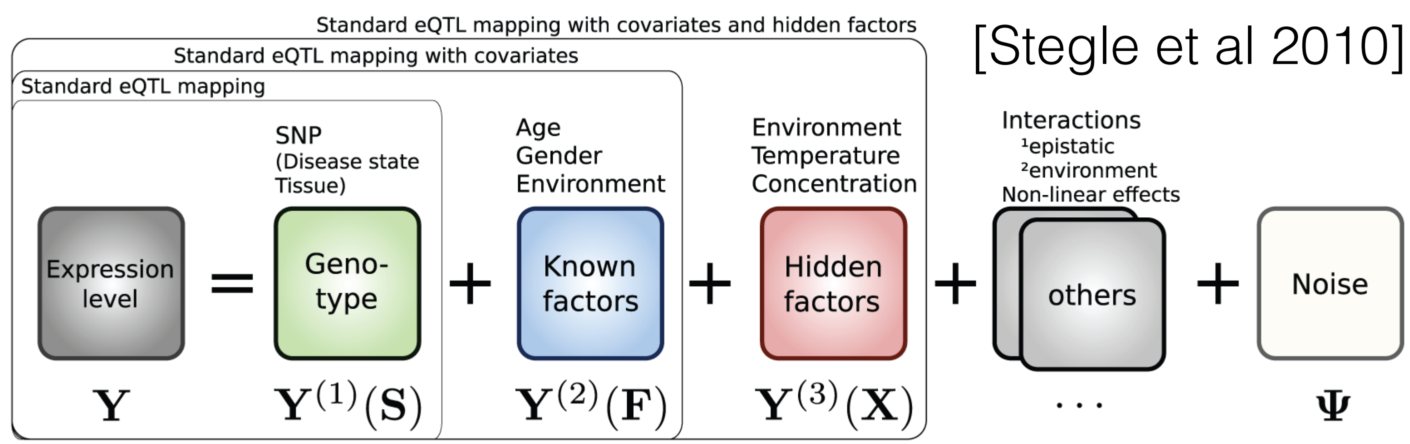
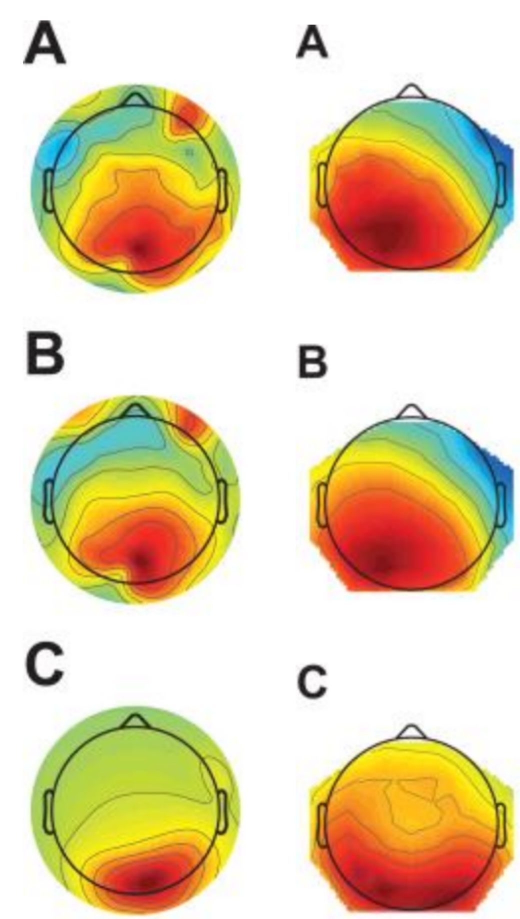
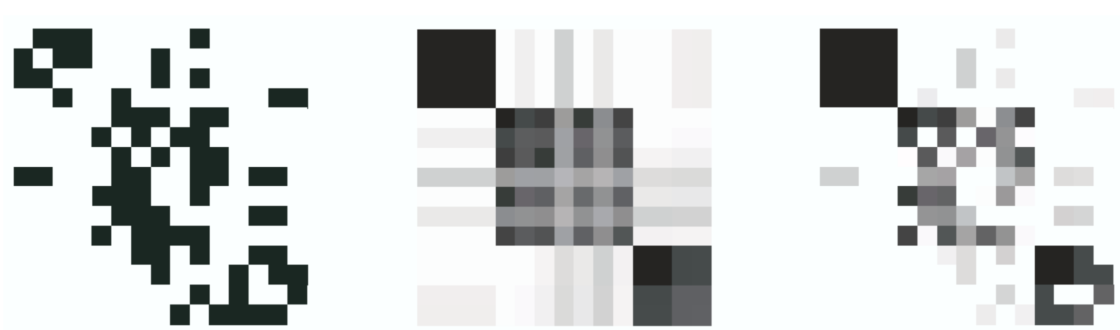


[Stegle et al 2010]





[Airoldi et al 2008] [Gershman et al 2014] [Blei et al 2018]

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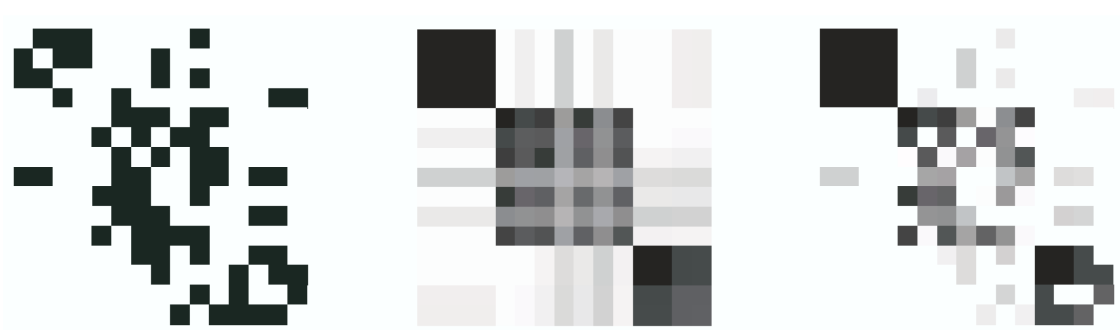

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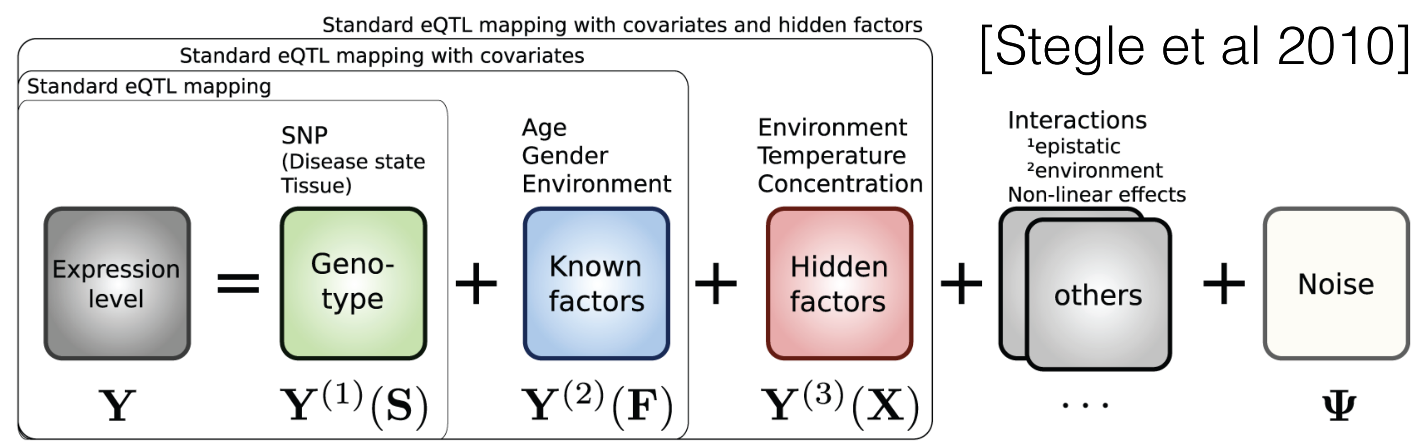

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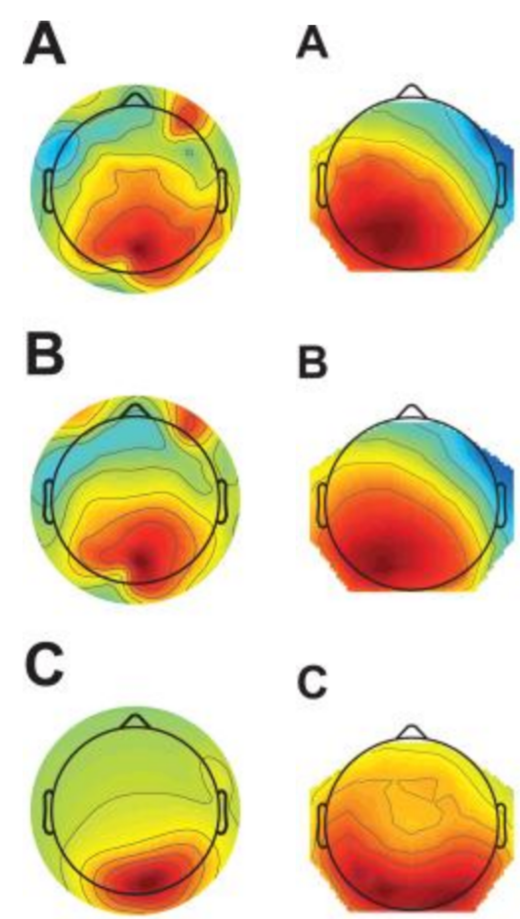

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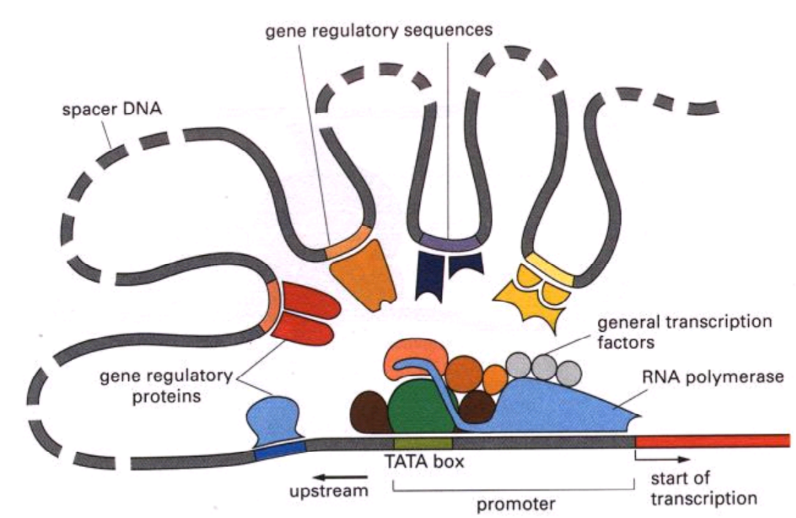

[Xing et al 2004]
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[Blei et al 2018]

Roadmap

- Bayes & Approximate Bayes review

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- What is:
    - Variational Bayes (VB)
    - Mean-field variational Bayes (MFVB)

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- When can we trust VB?
- Where do we go from here?

Roadmap

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

Bayesian inference

Bayesian inference

parameters

θ

Bayesian inference

parameters

$$p(\theta)$$

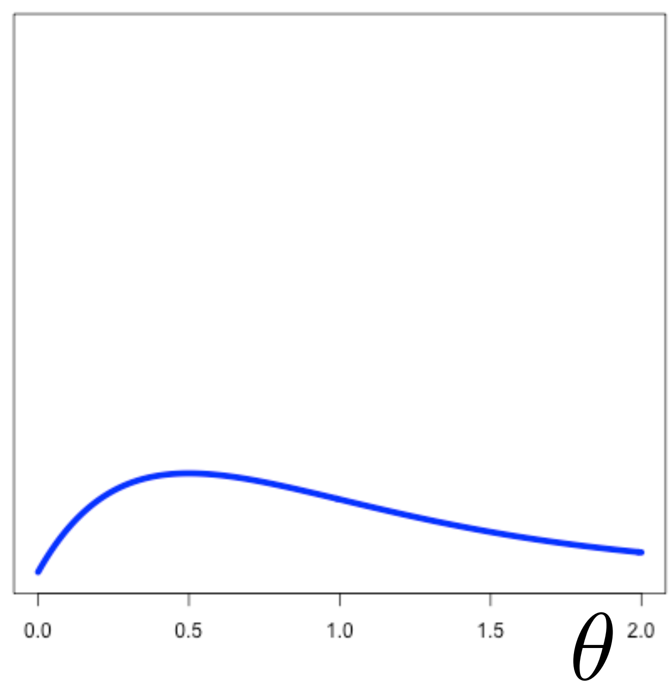
prior

Bayesian inference

parameters

$p(\theta)$

prior

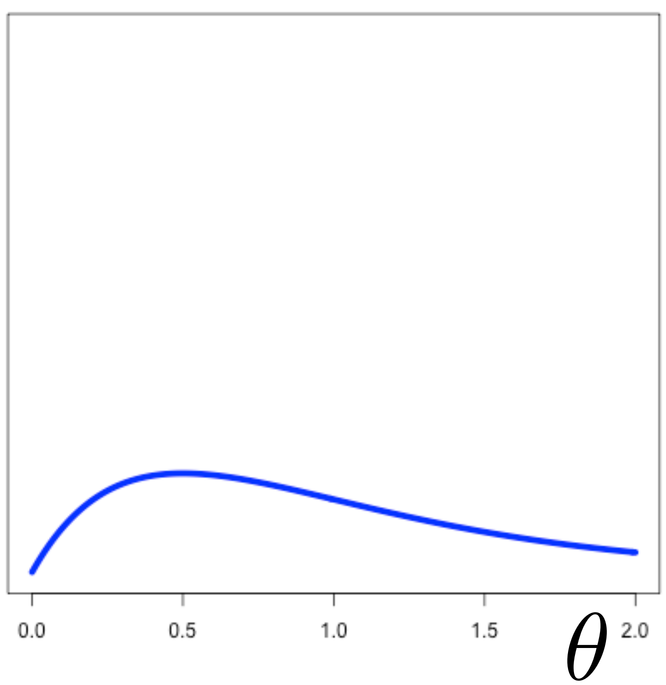


Bayesian inference

parameters

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

likelihood prior



Bayesian inference

data parameters

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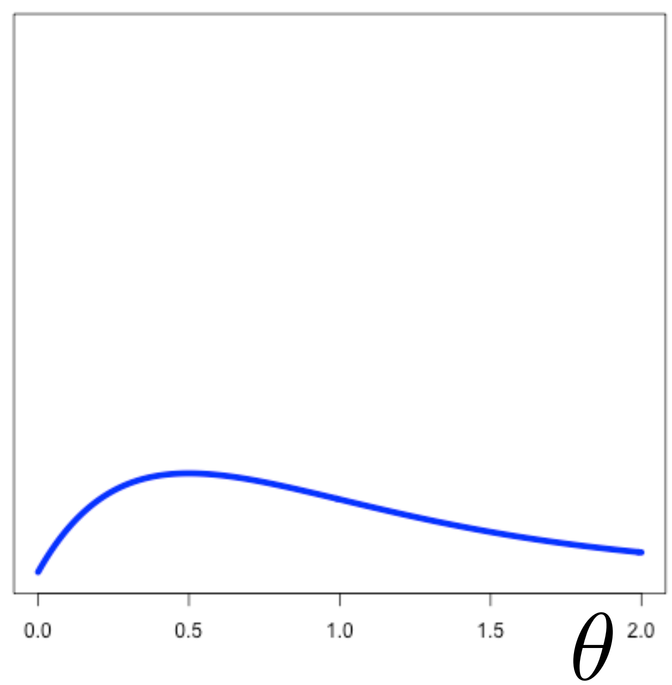


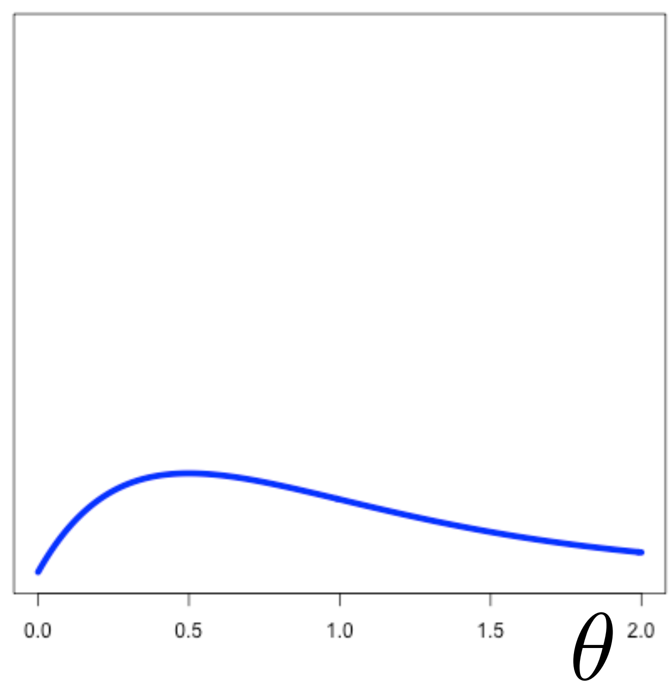
Bayesian inference

data

parameters

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

posterior likelihood prior



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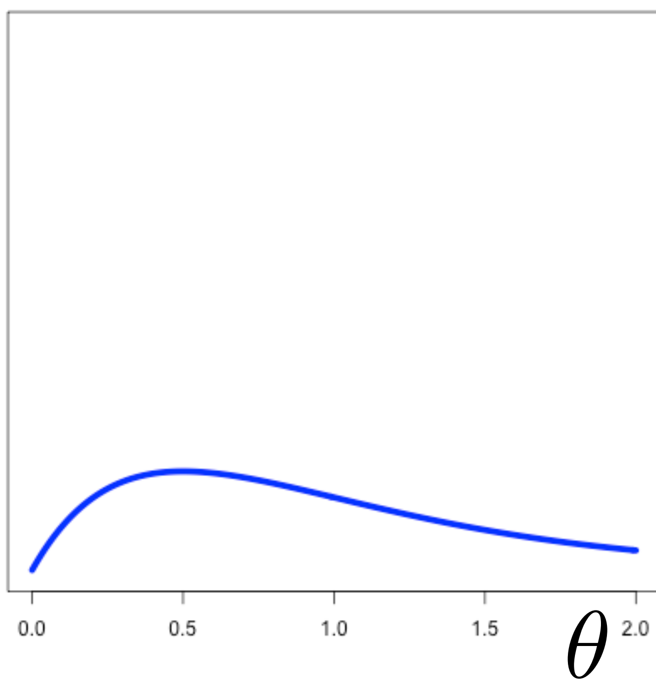

Bayes Theorem

Bayesian inference

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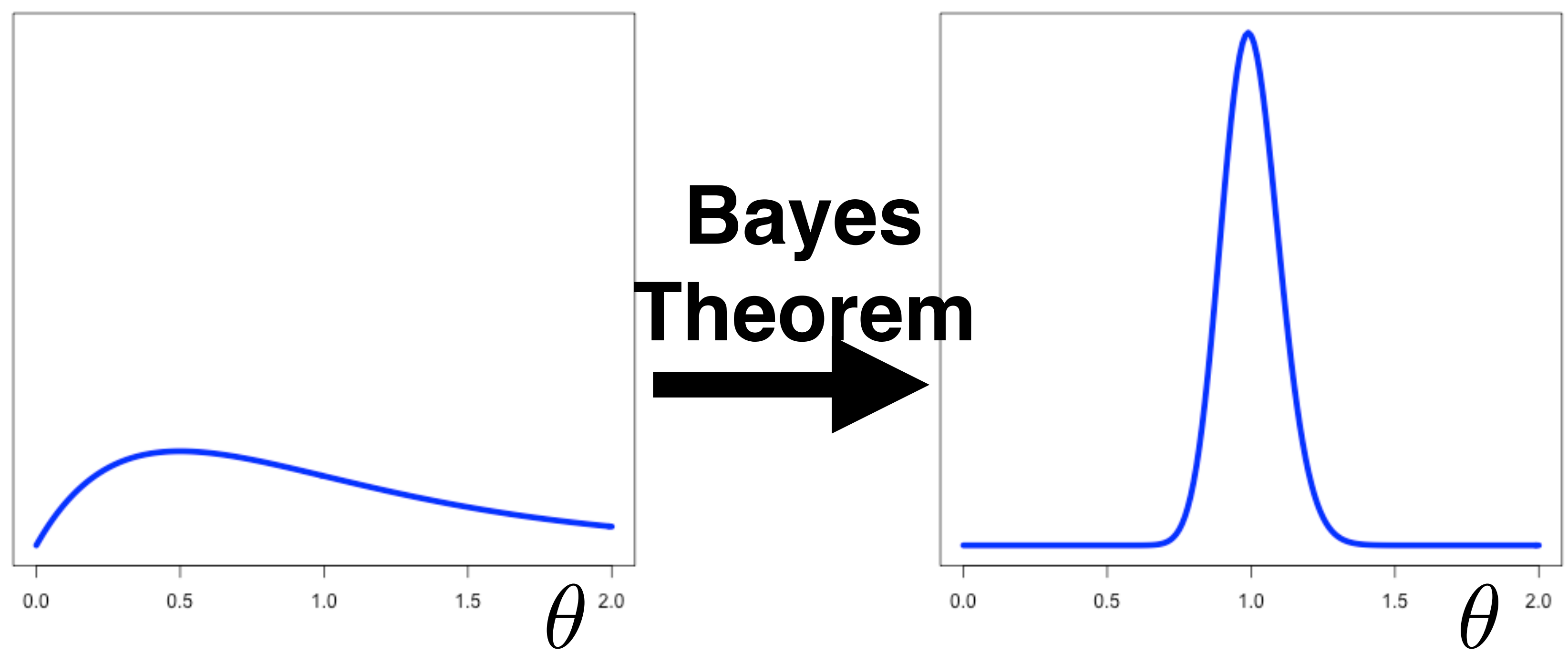

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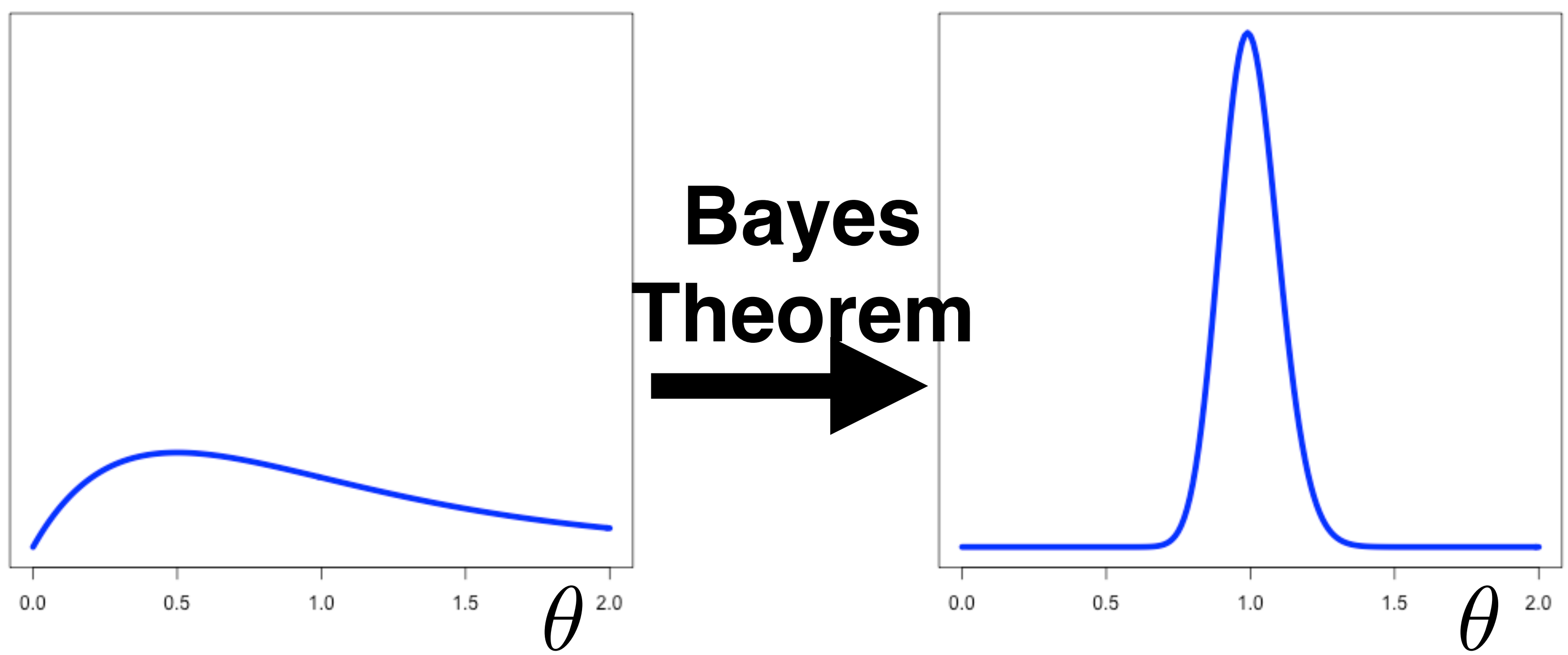

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Bayesian inference

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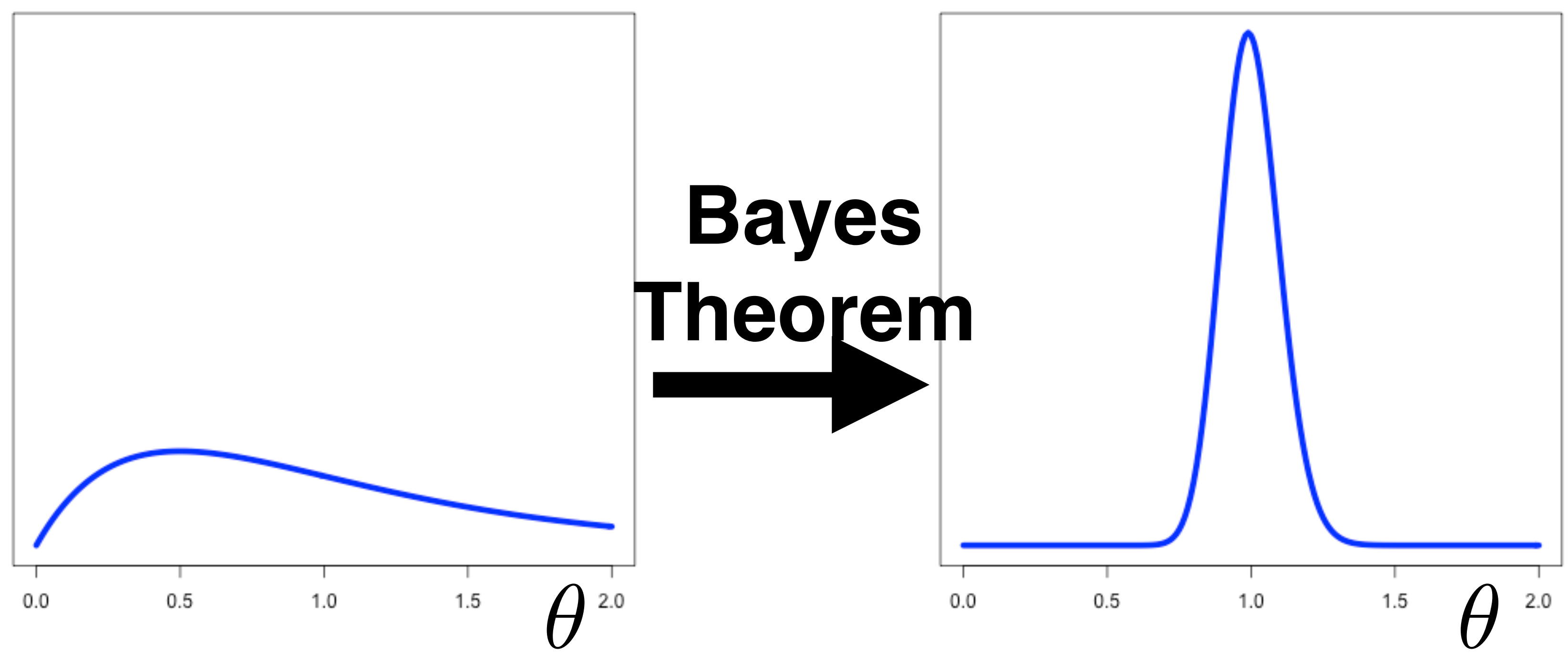

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Bayesian inference

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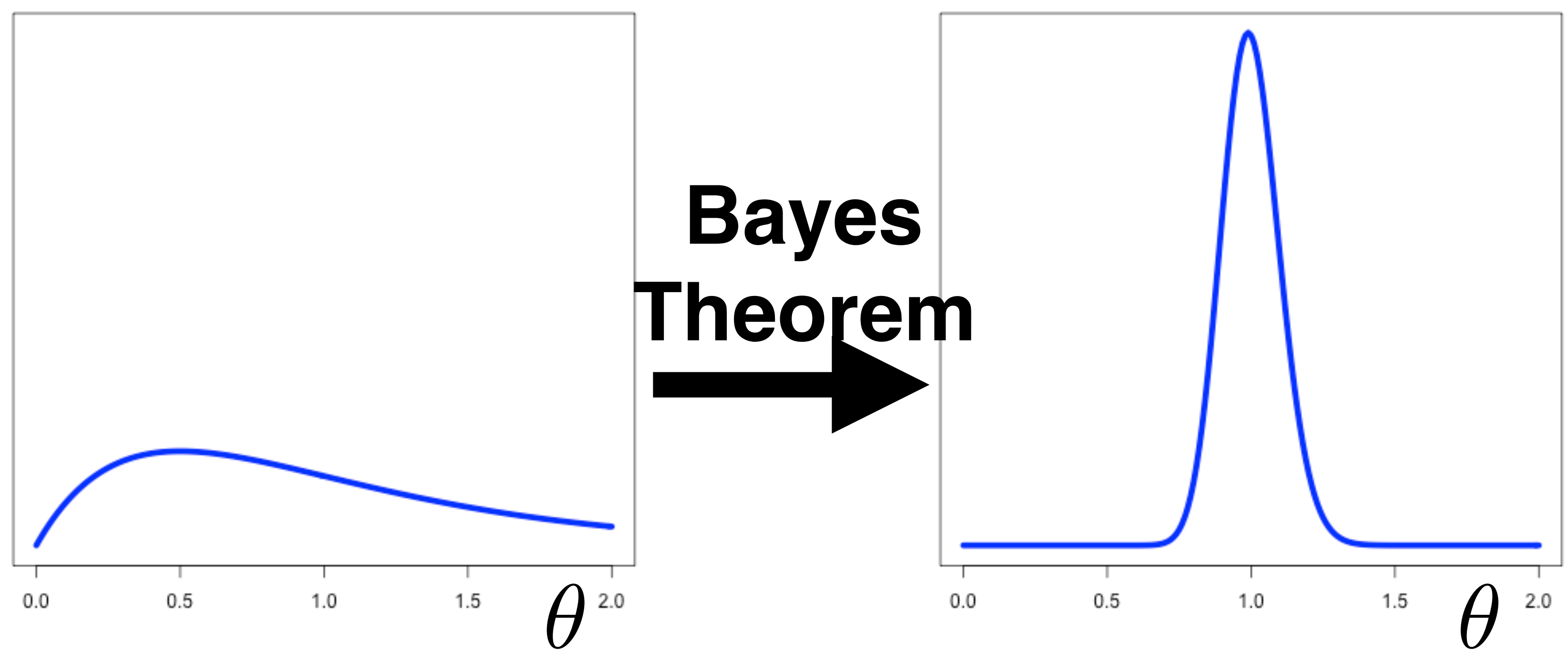

1. Build a model: choose prior & choose likelihood
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3. Report a summary, e.g. posterior means and (co)variances

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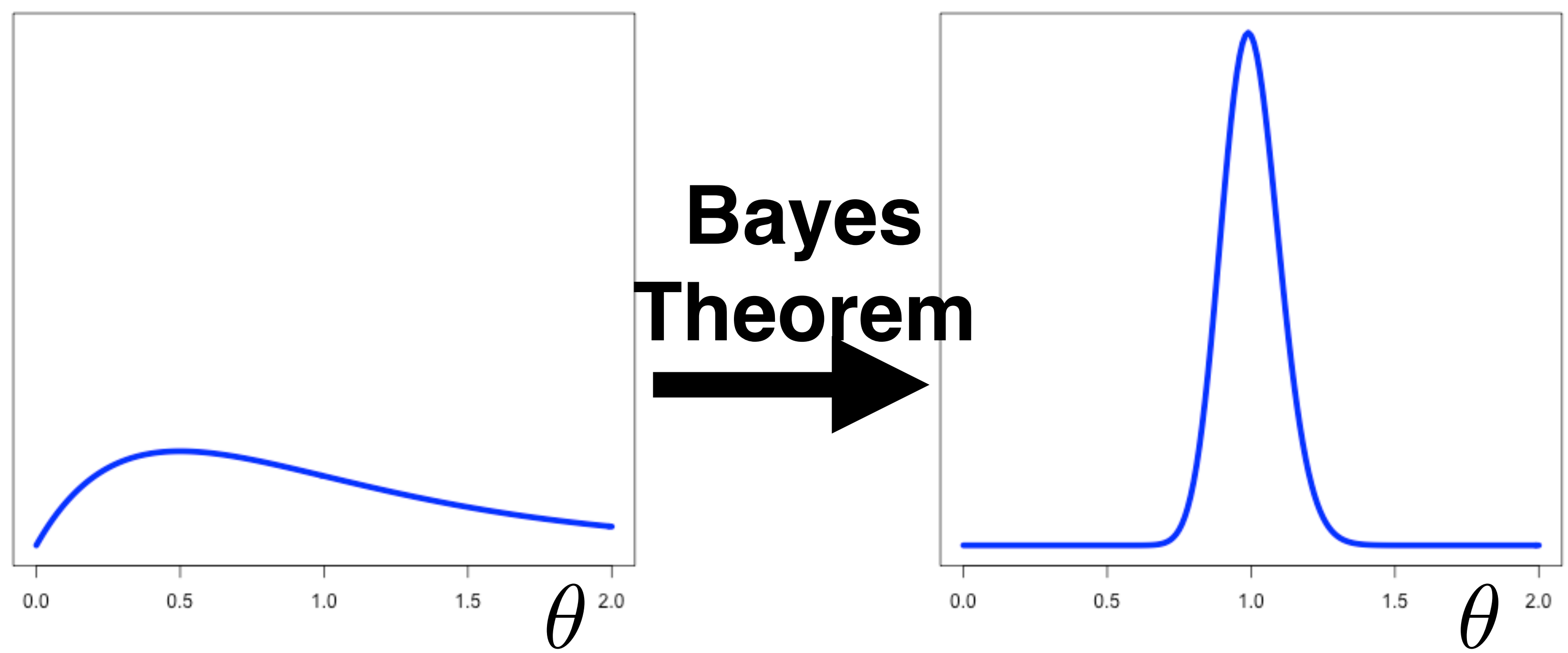

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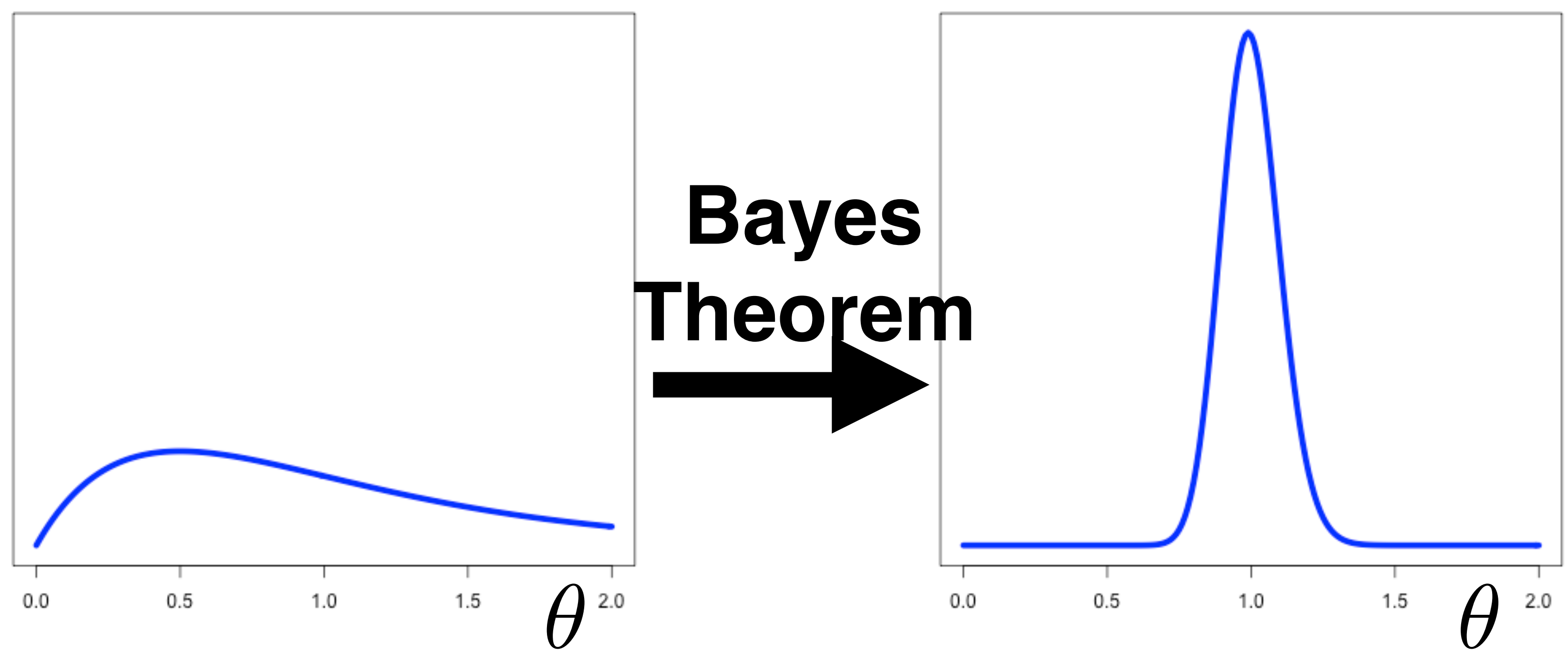

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  - Typically no closed form

Bayesian inference

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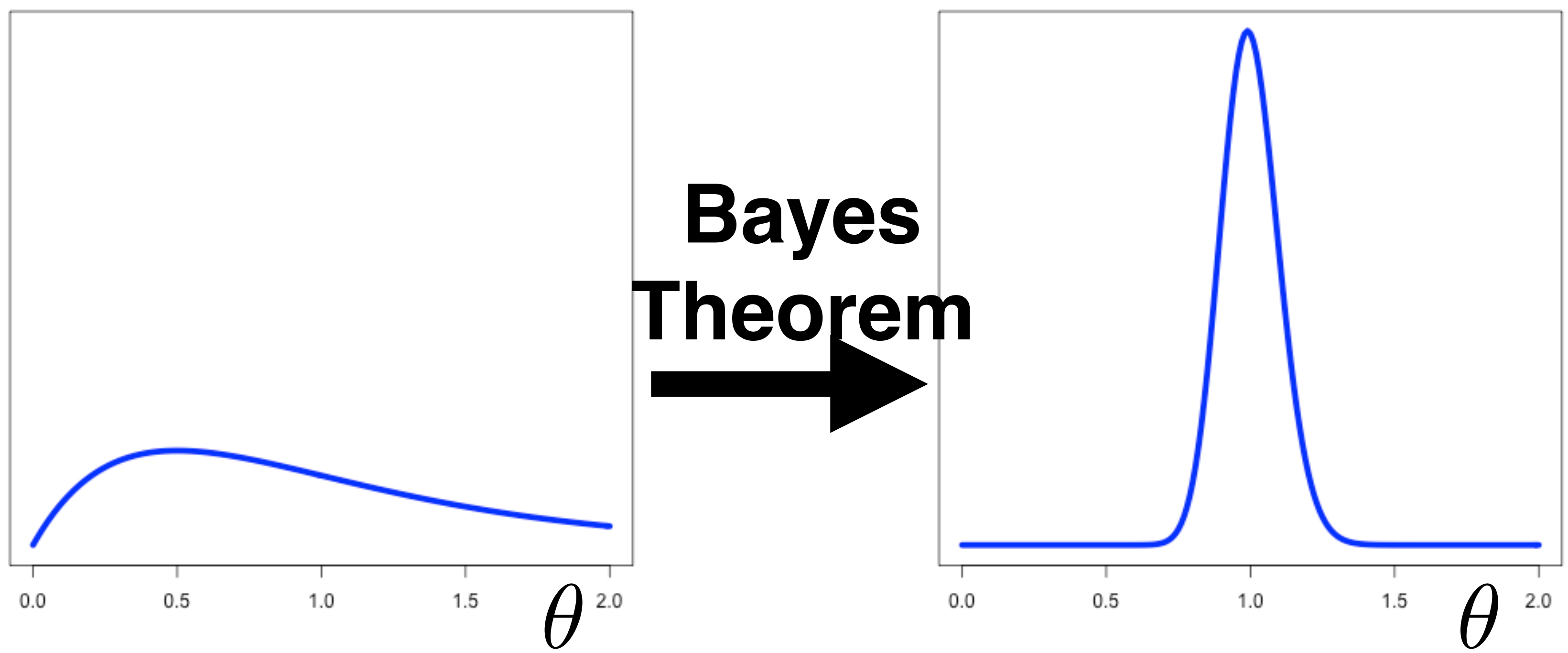
data — parameters

posterior — likelihood — prior



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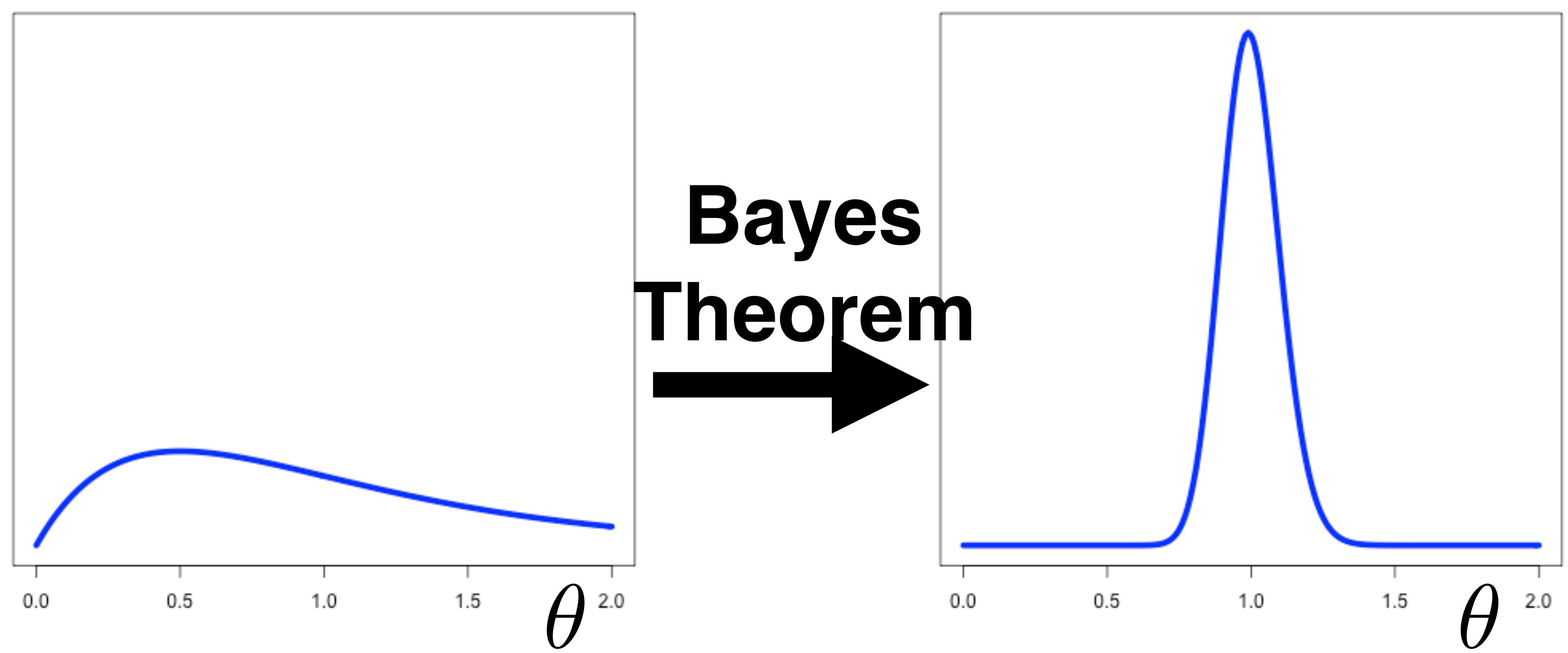
Bayesian inference

data parameters

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

posterior likelihood prior



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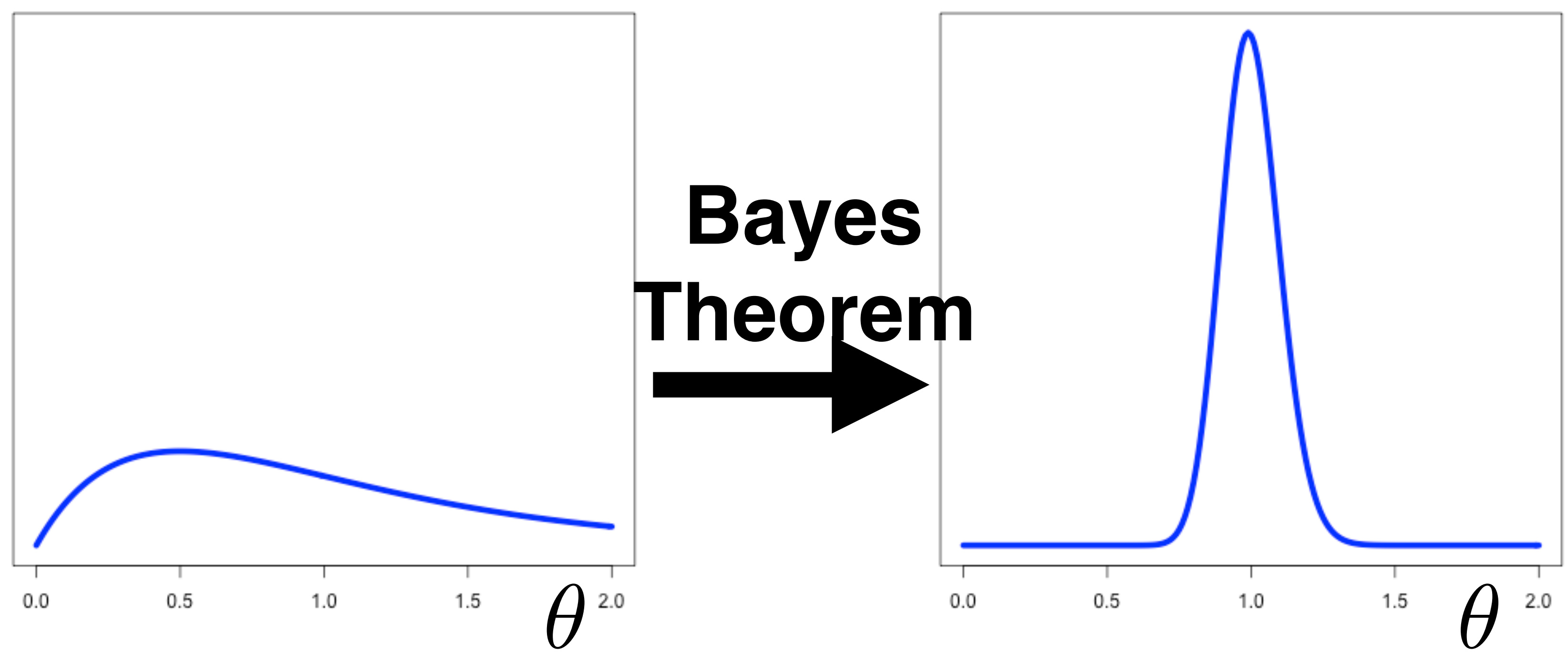
posterior likelihood prior evidence



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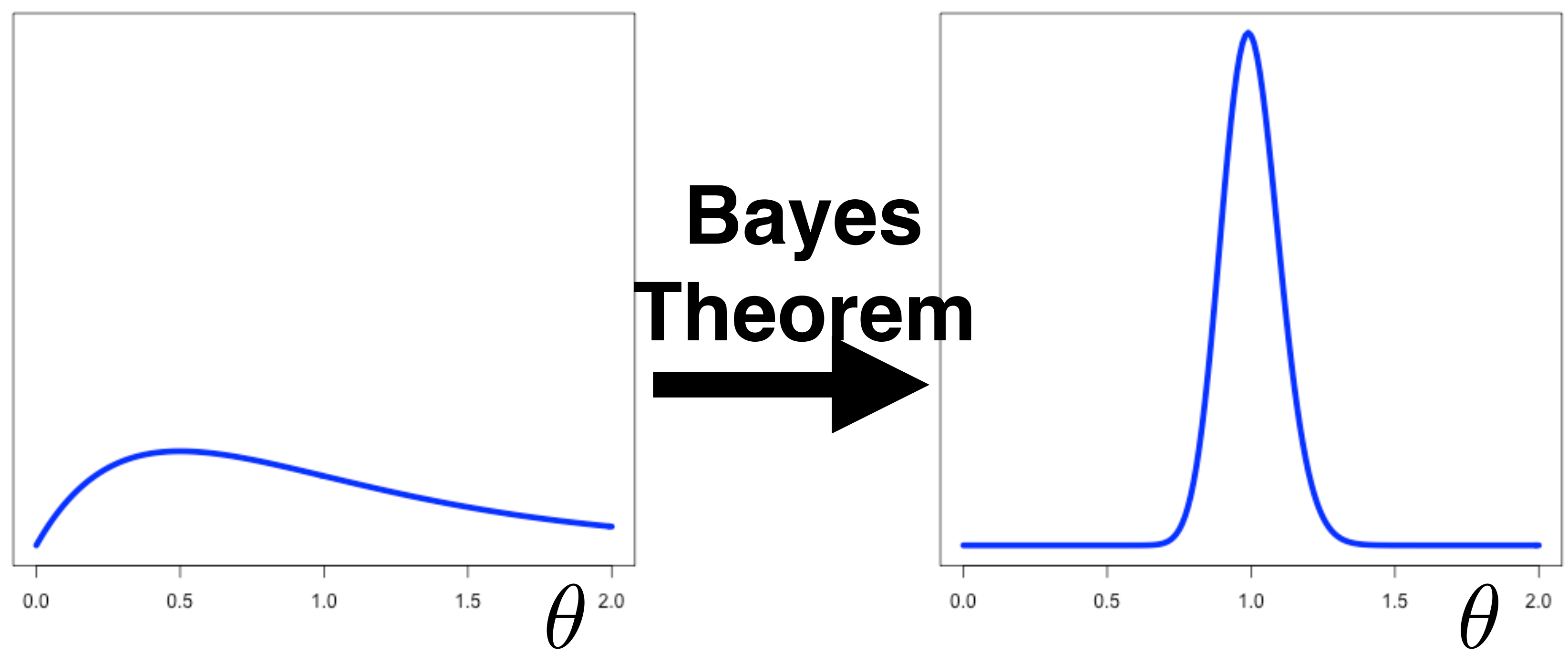
Bayesian inference

data

parameters

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

posterior likelihood prior evidence



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- Gold standard: Markov Chain Monte Carlo (MCMC)

[Bardenet, Doucet, Holmes 2017]

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Instead: an optimization approach

- Approximate posterior with q^*

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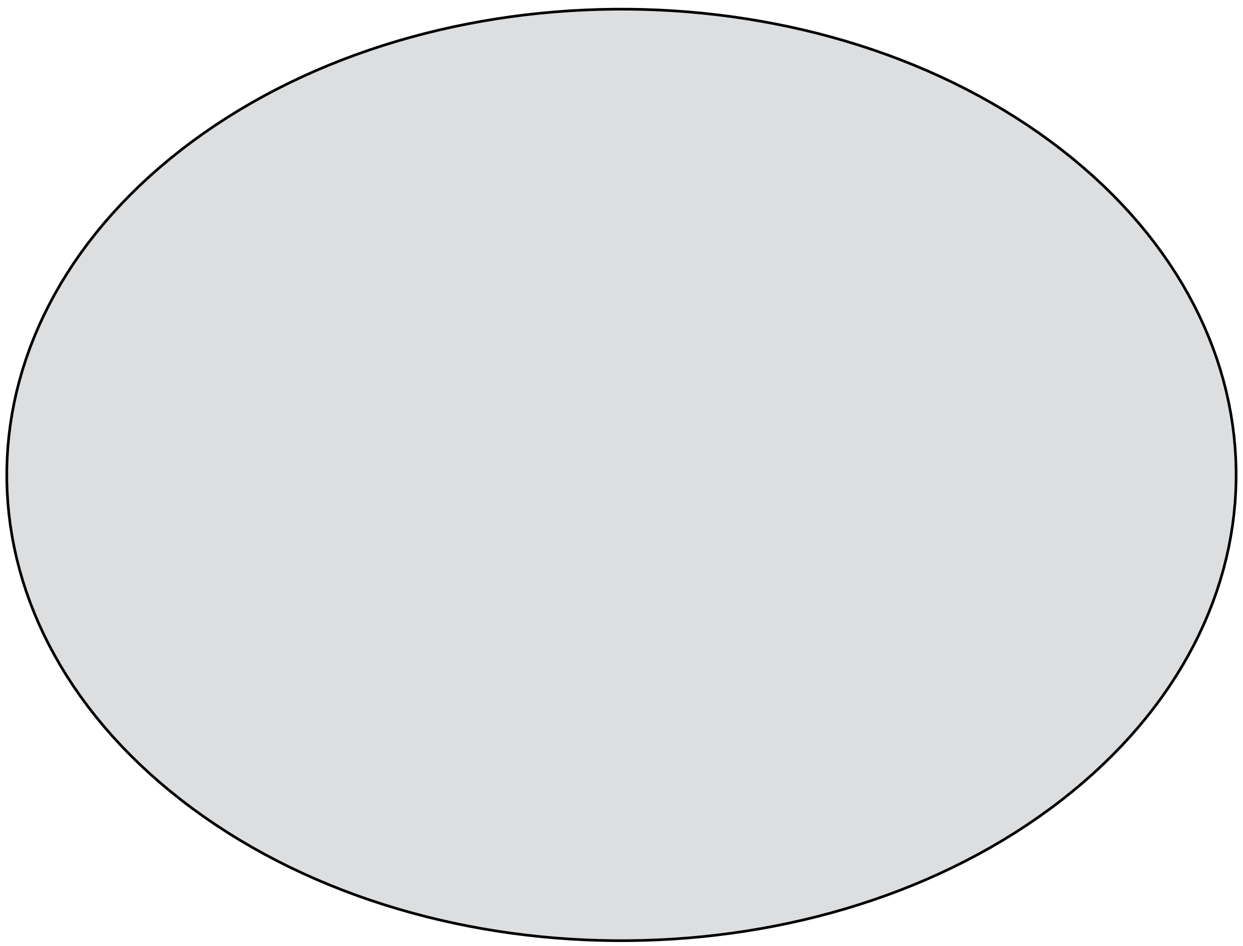

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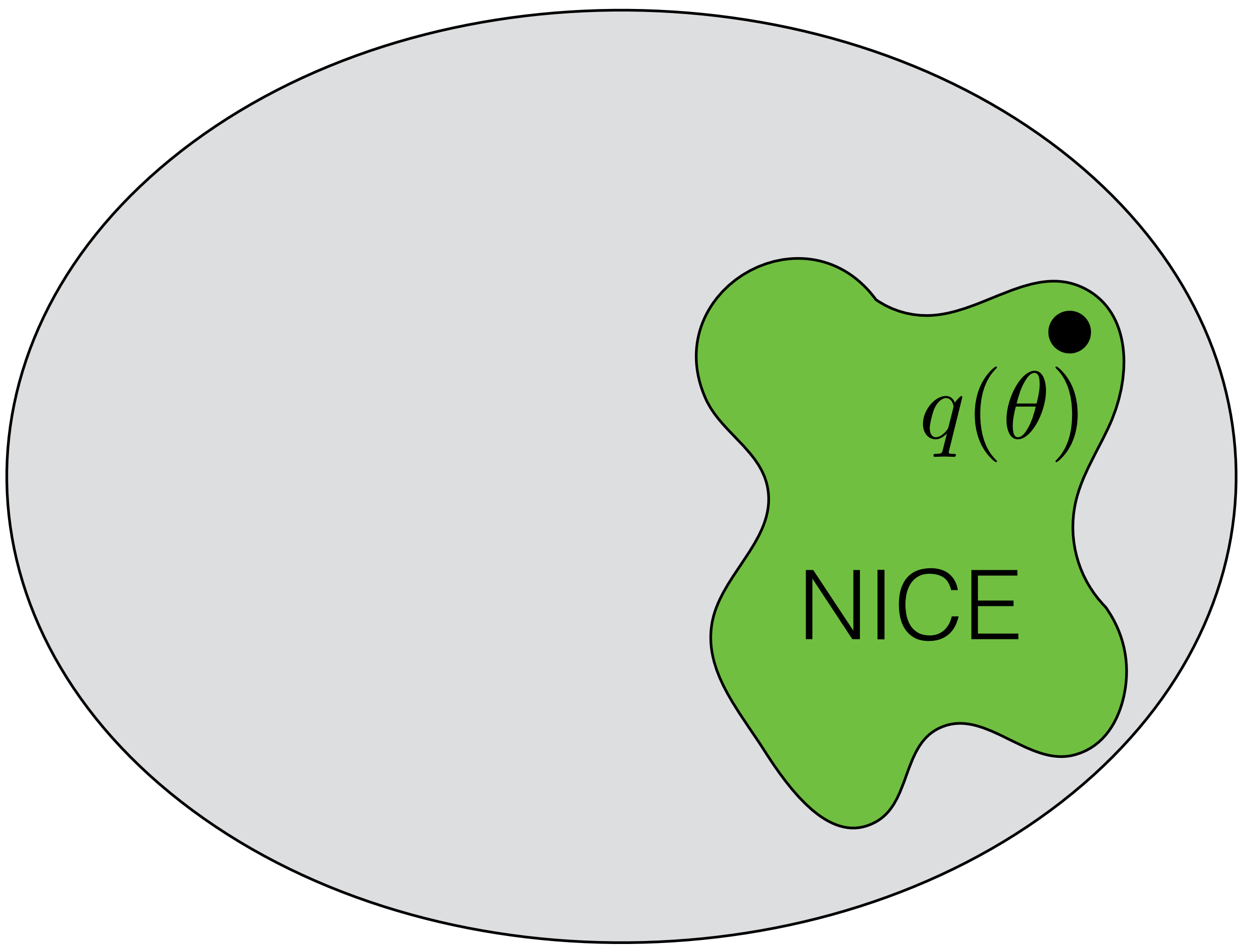

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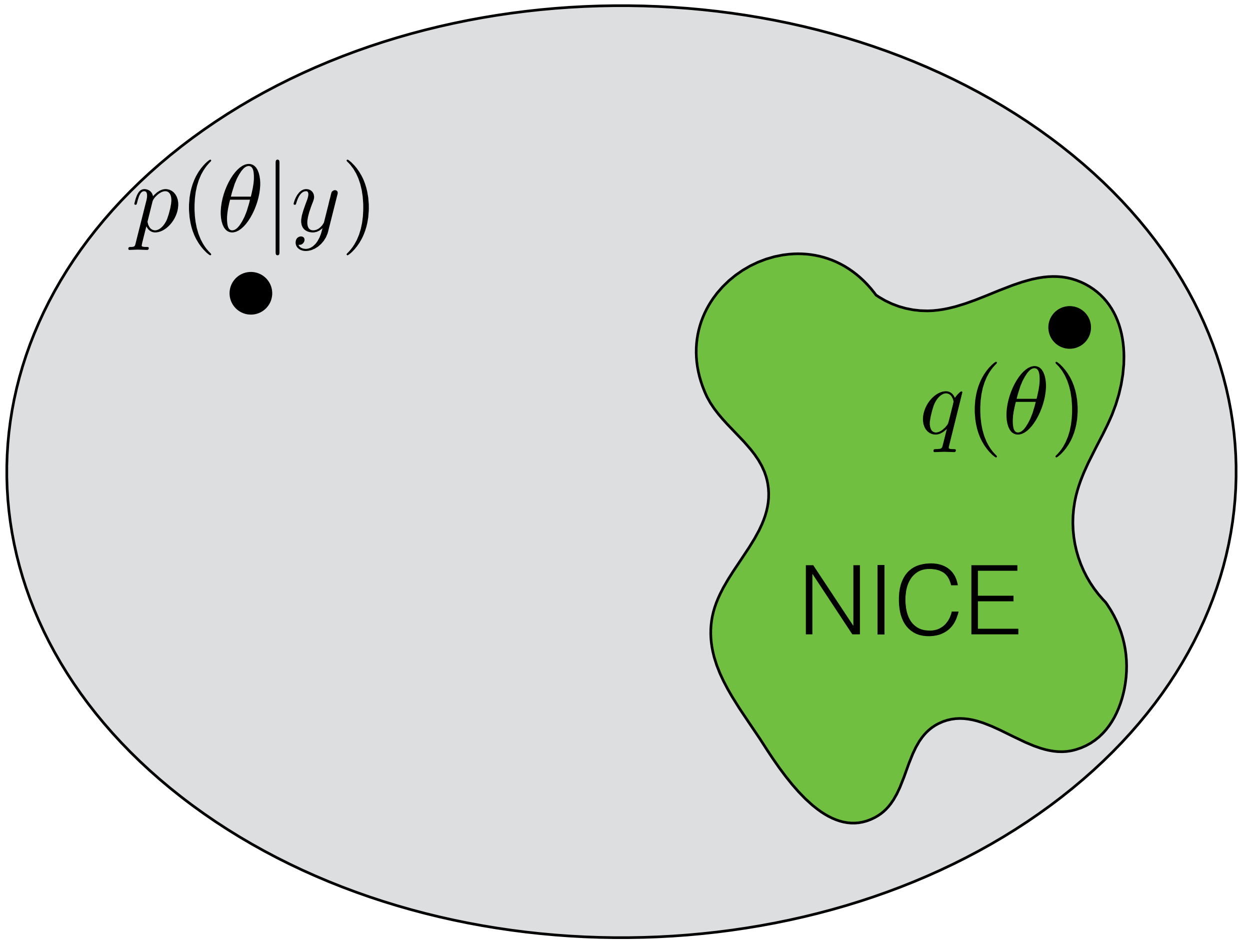

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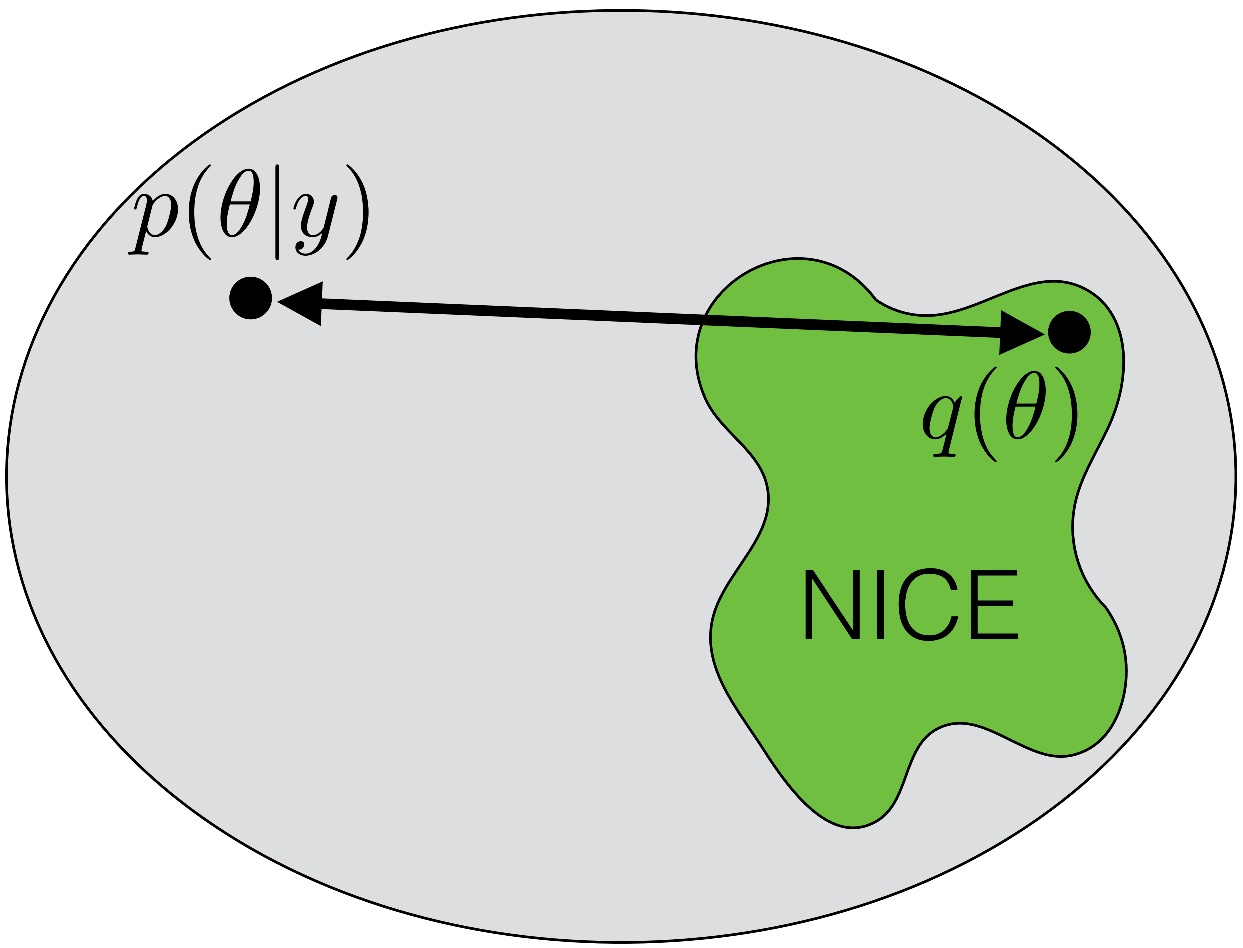

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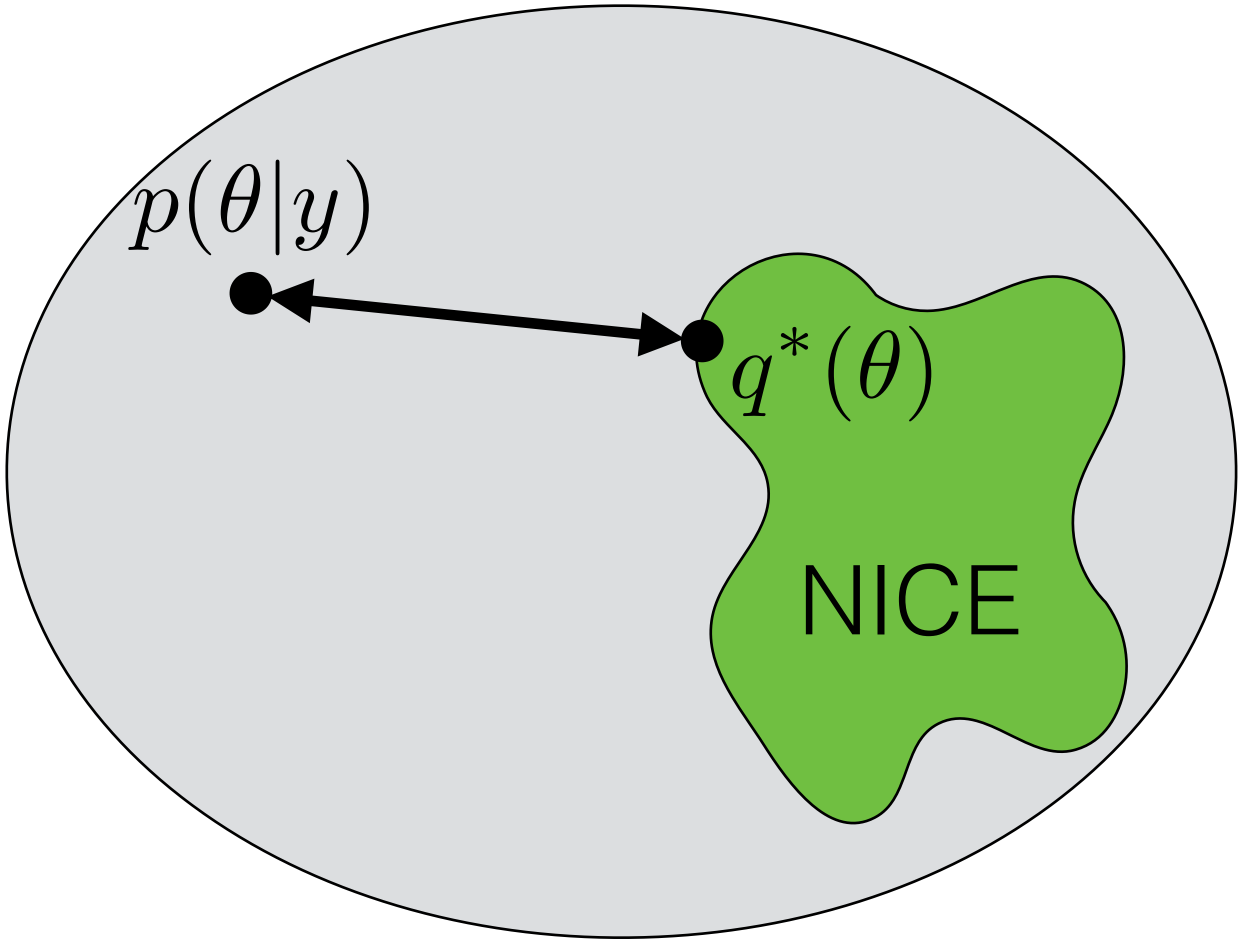

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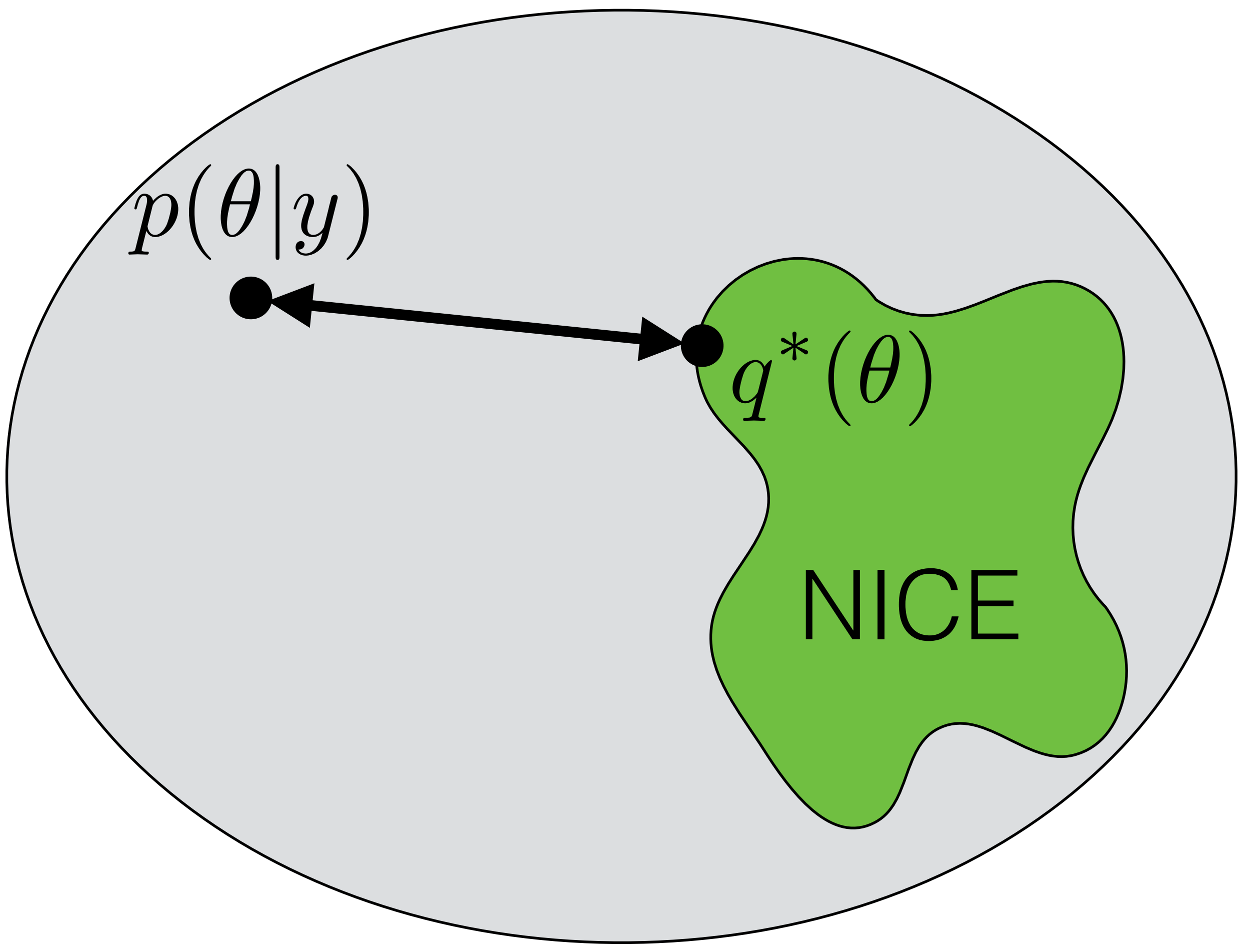

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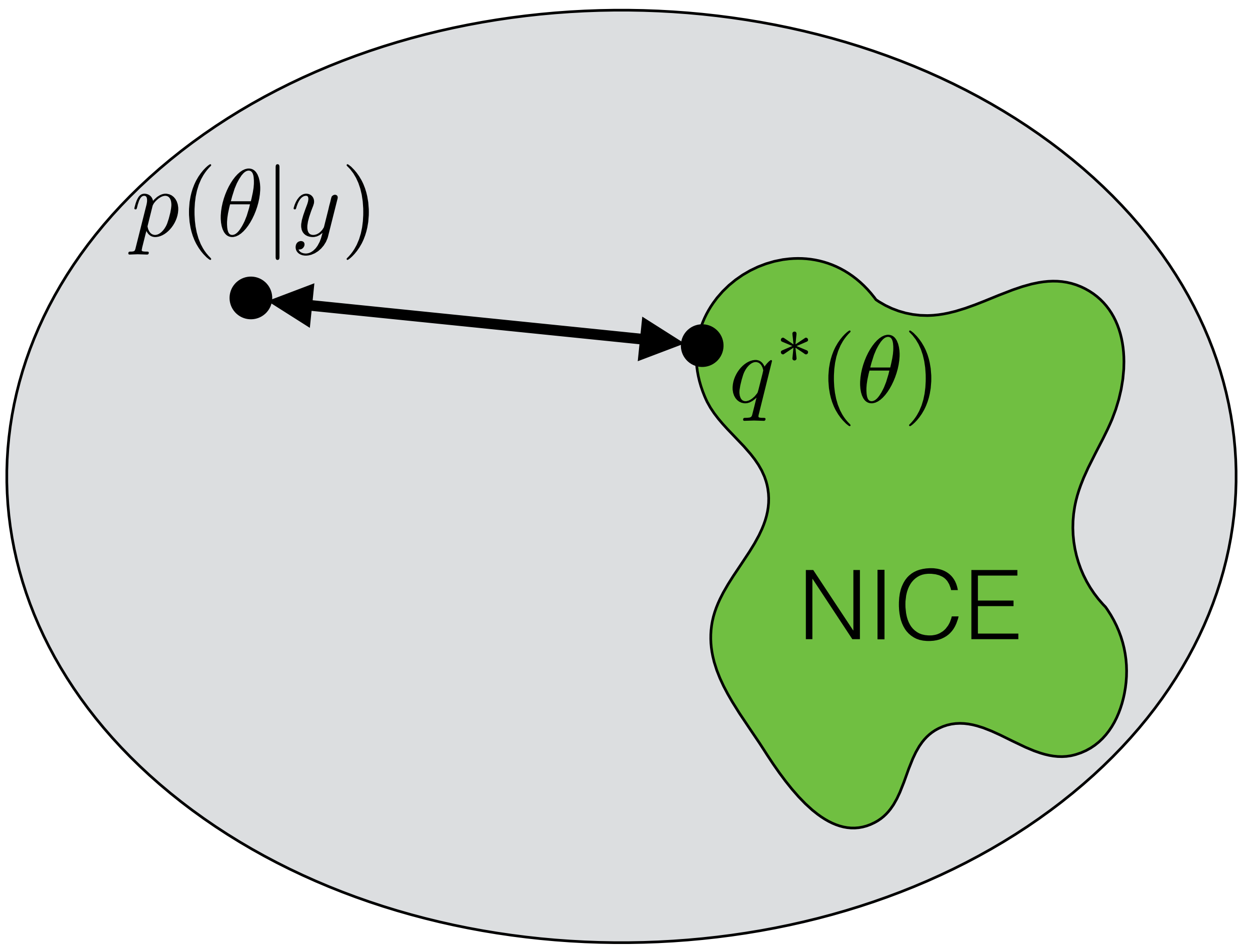

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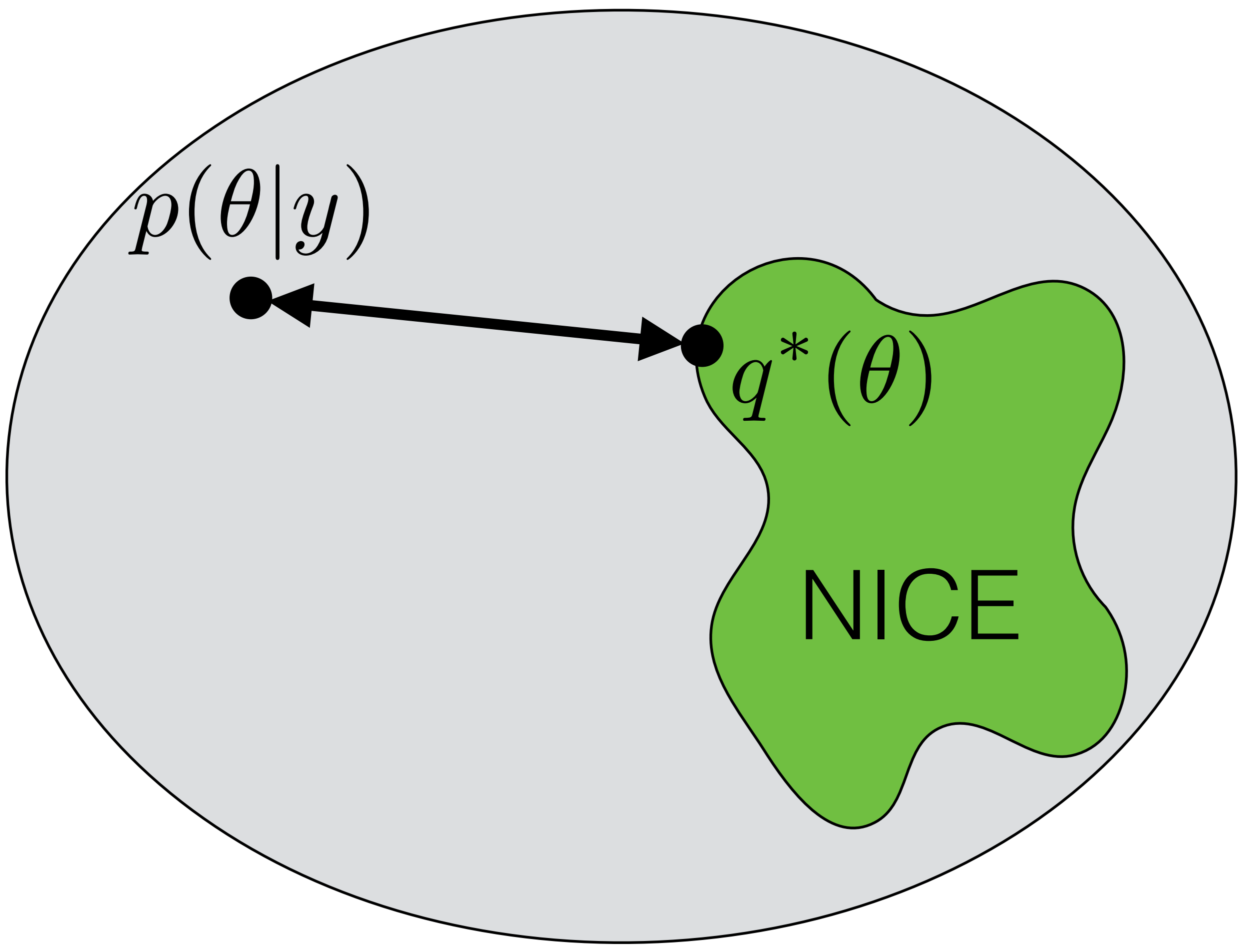

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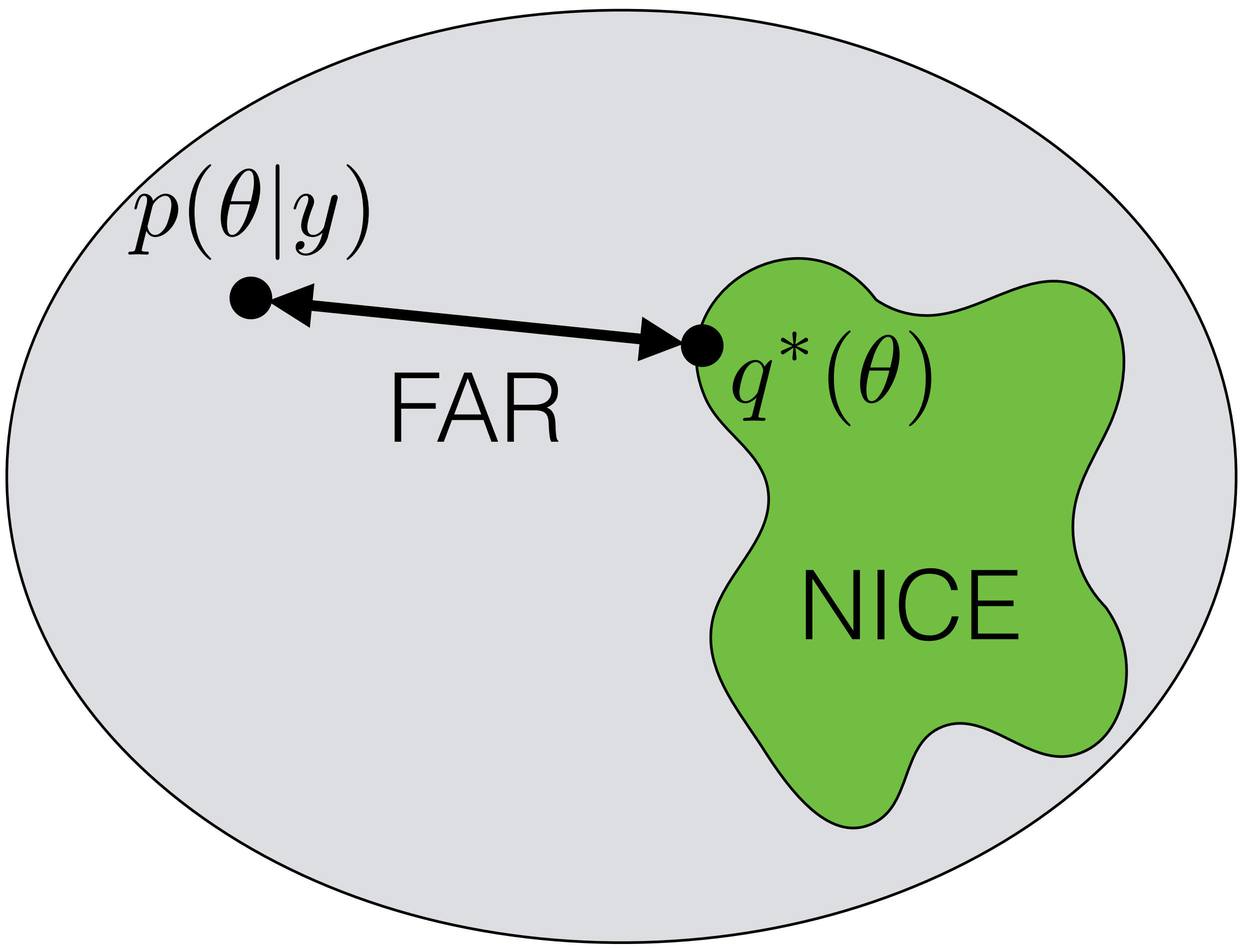

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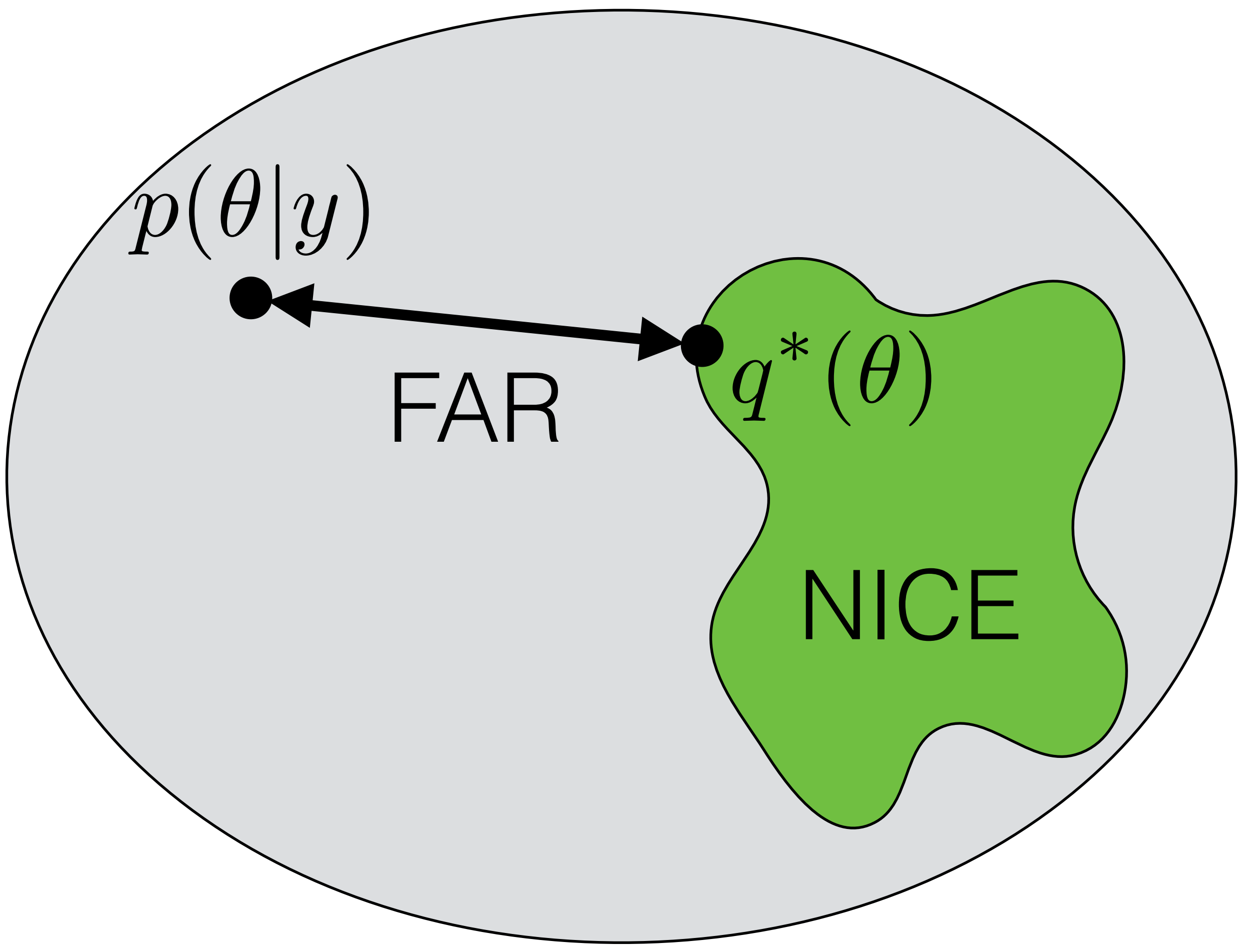

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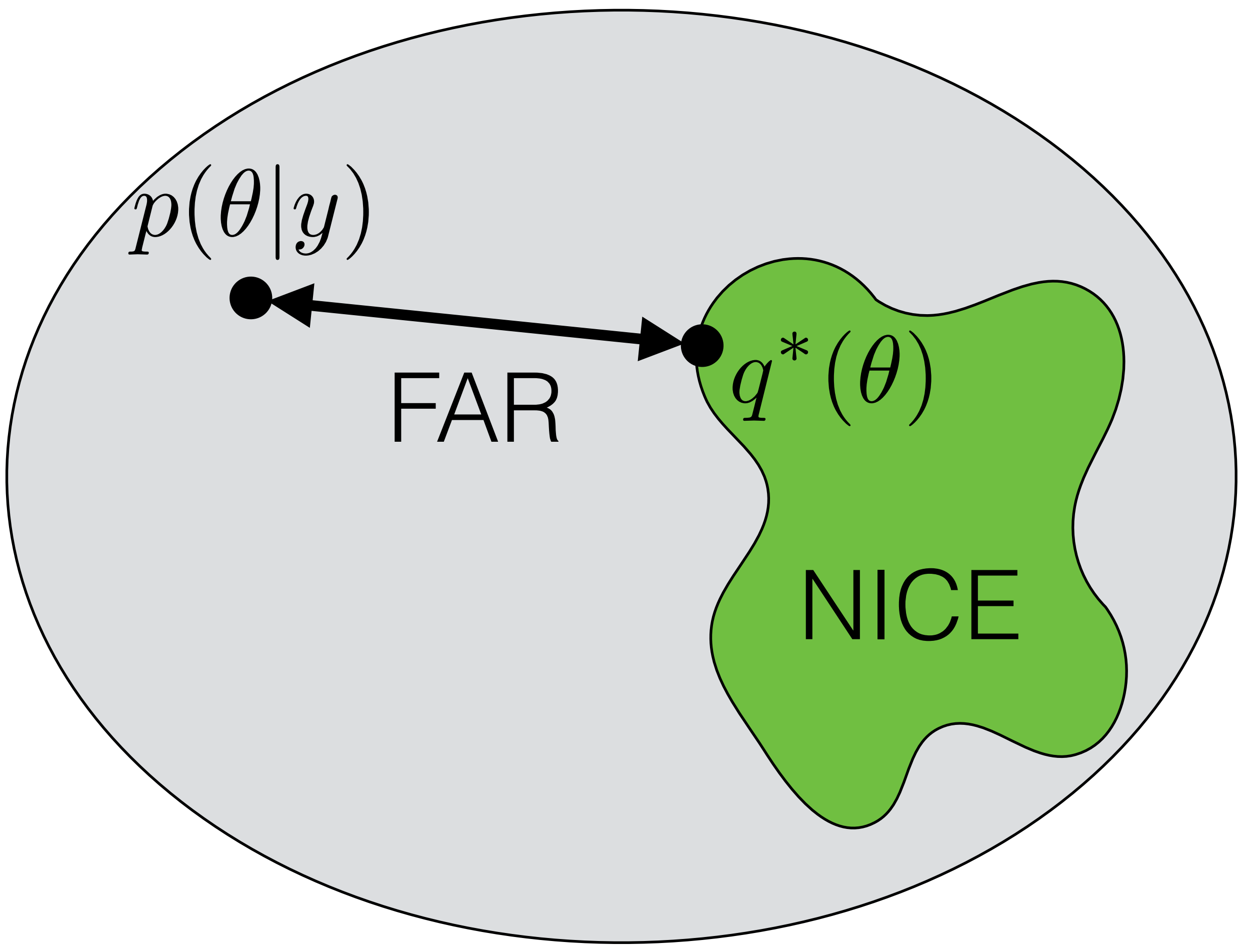

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$$KL(q(\cdot)||p(\cdot|y))$$

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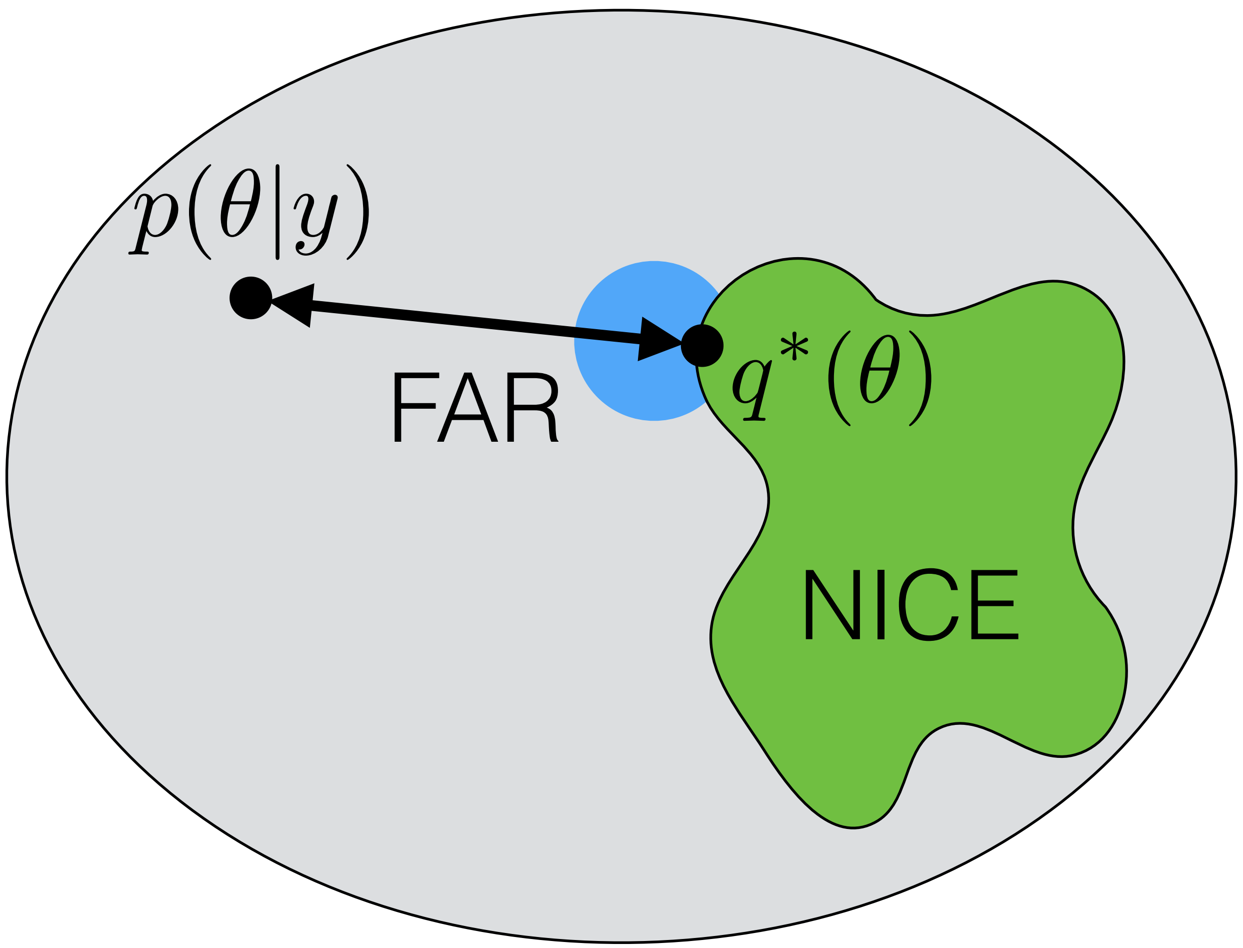

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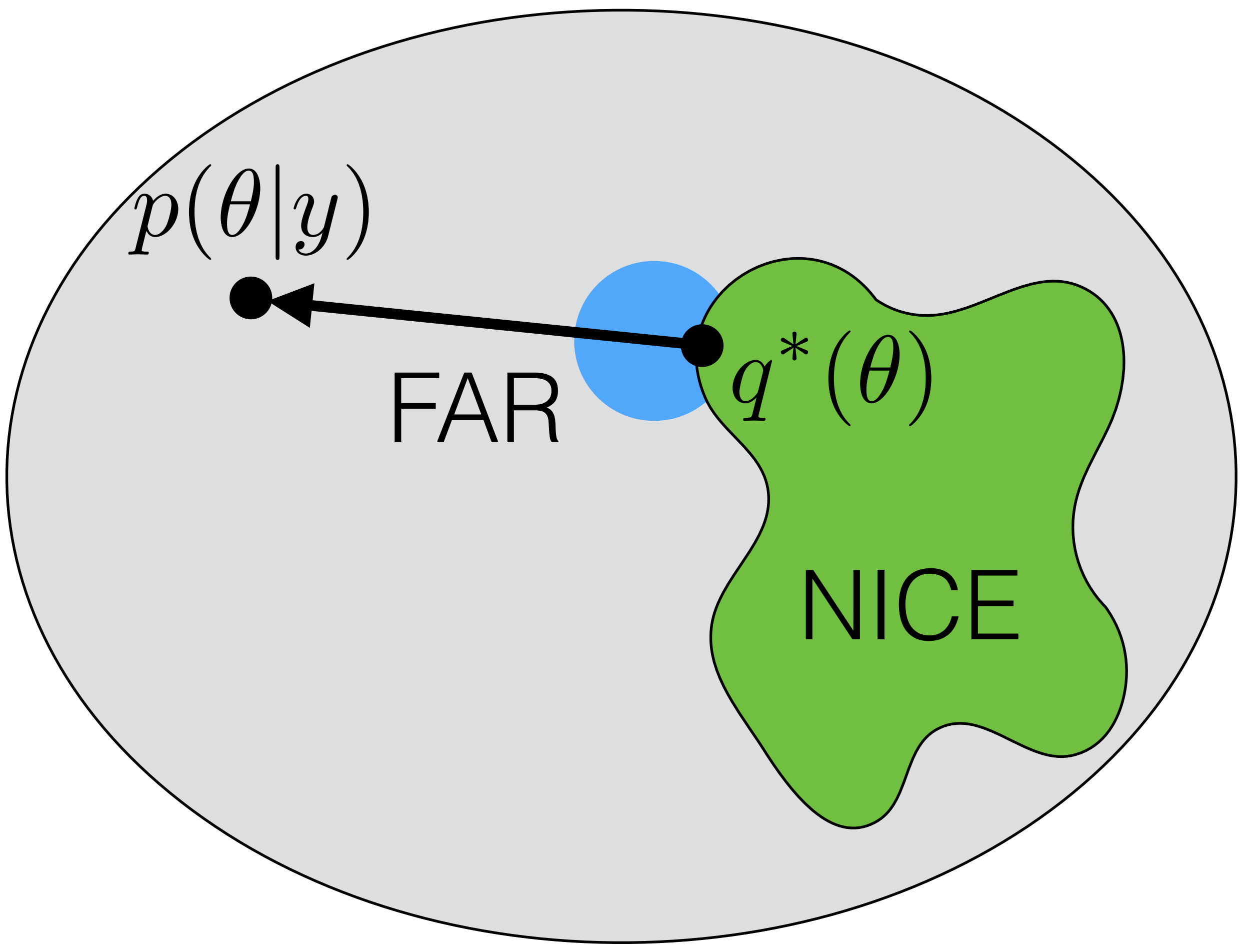

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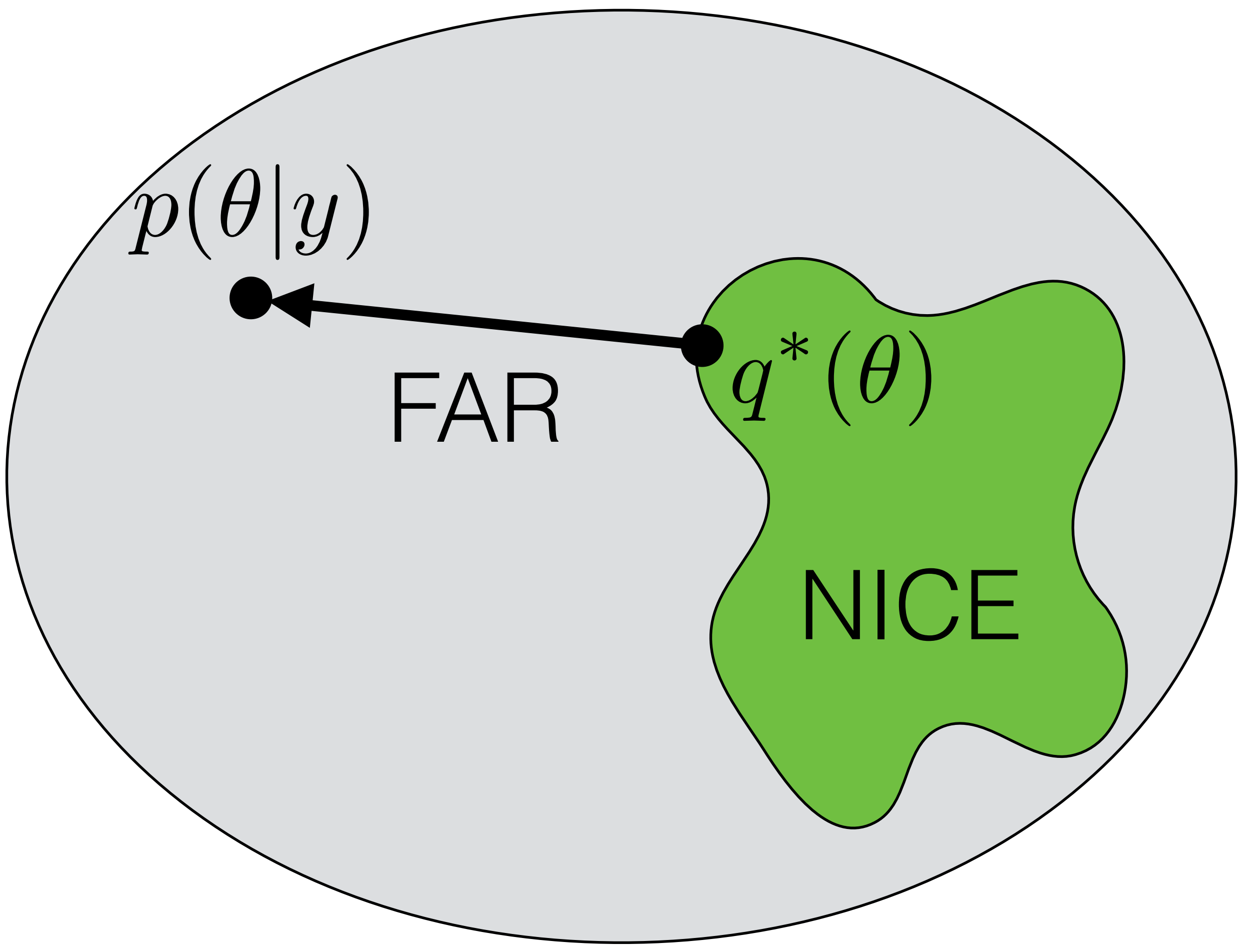

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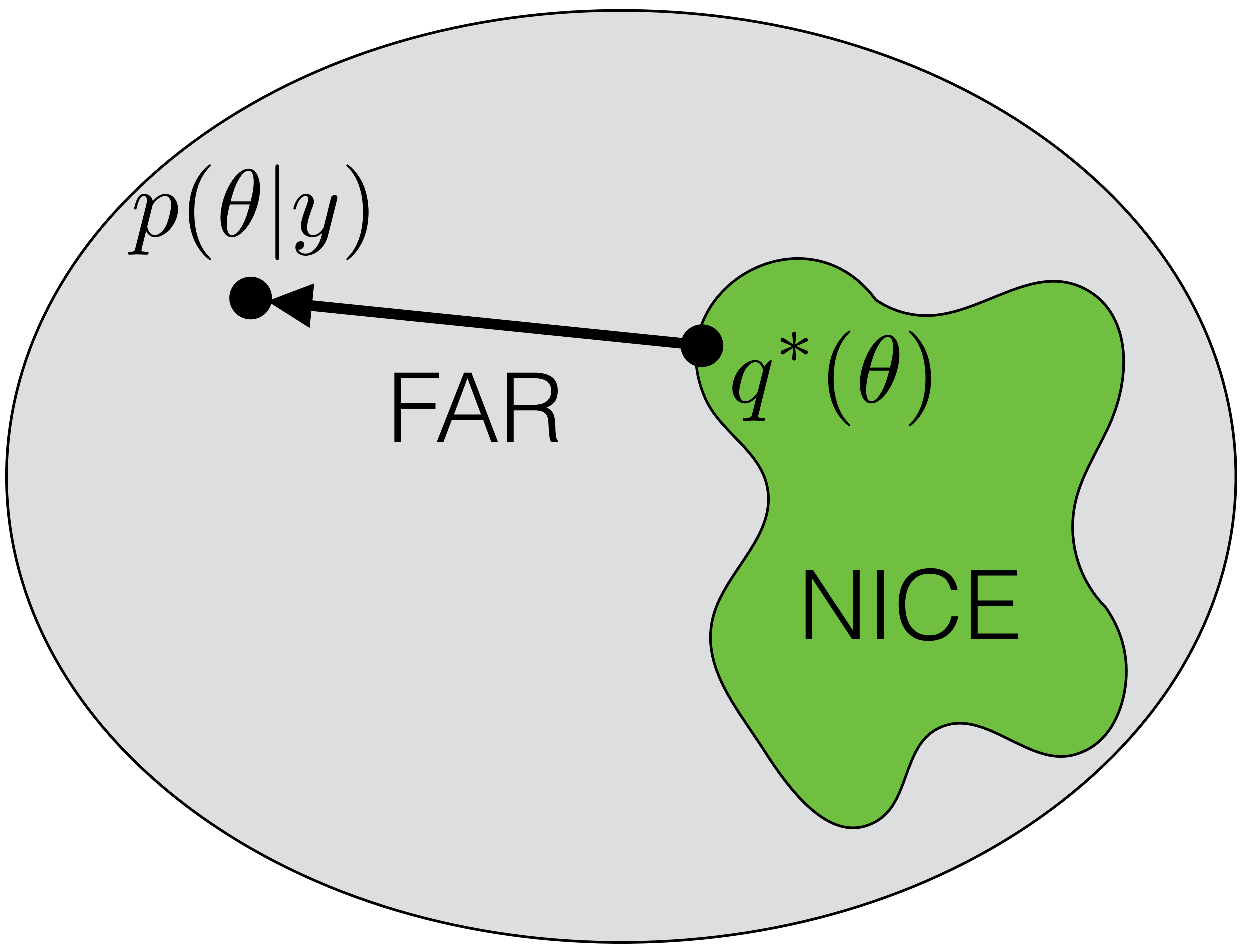

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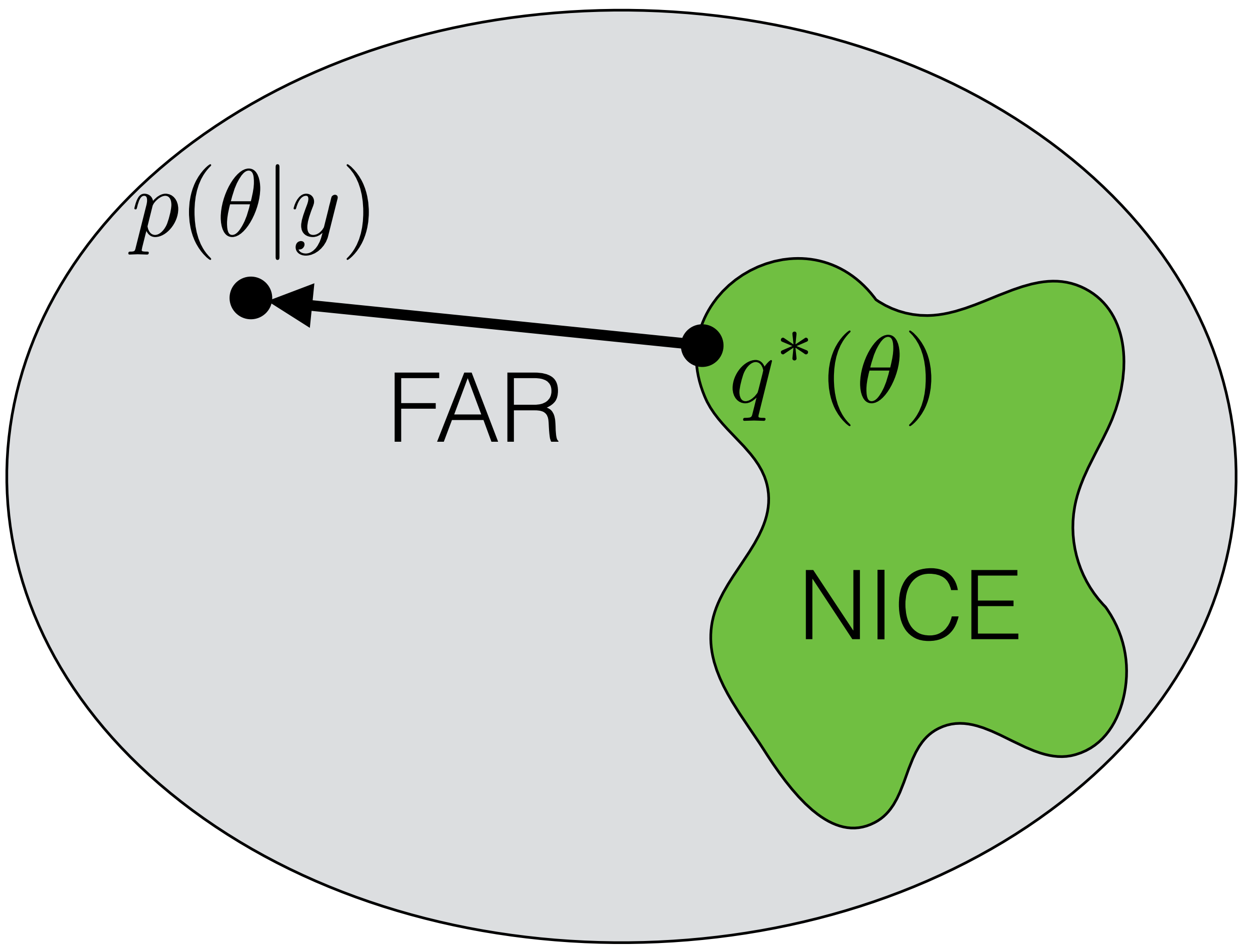

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- VB practical success: point estimates and prediction

Approximate Bayesian Inference

[Bardenet, Doucet, Holmes 2017]

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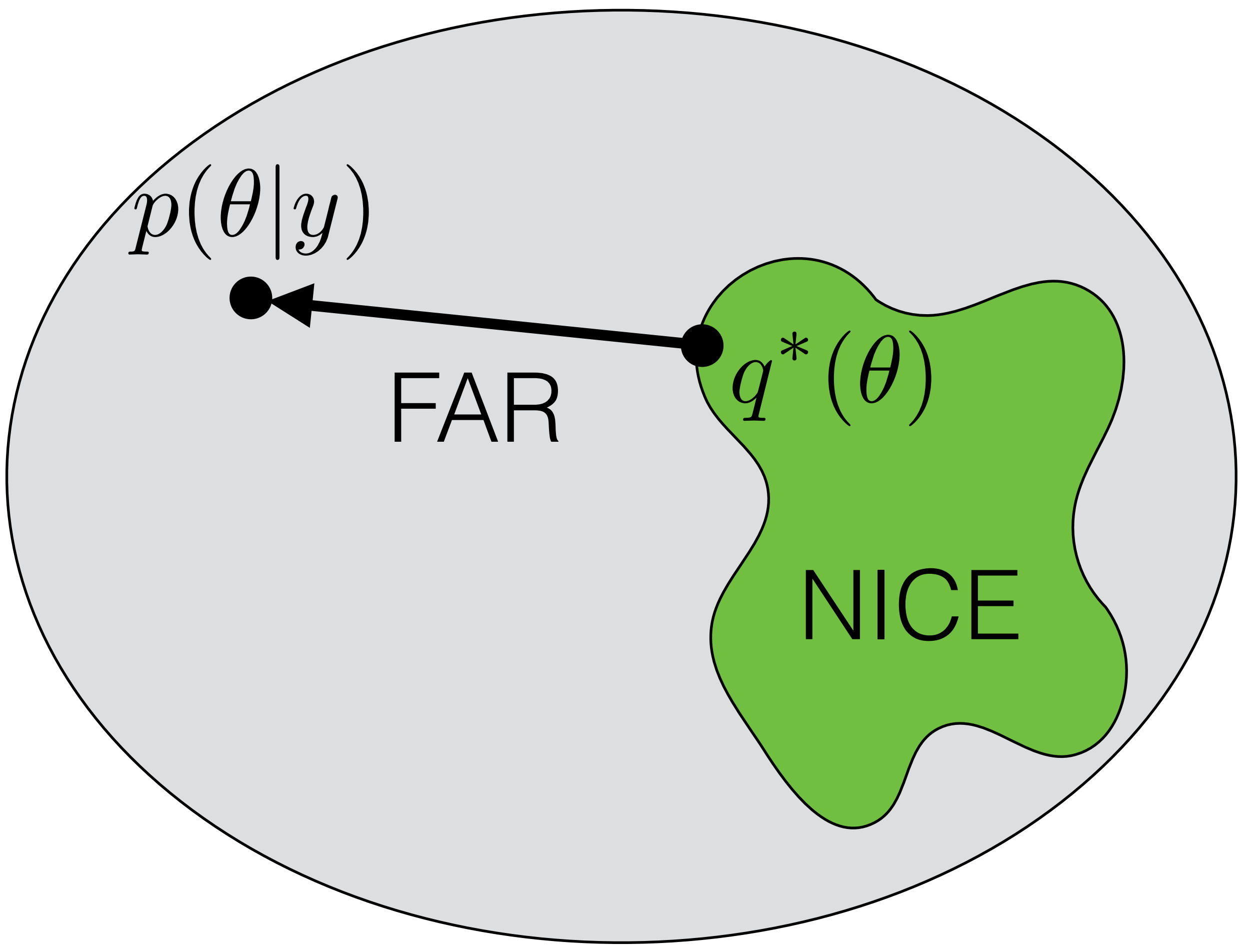

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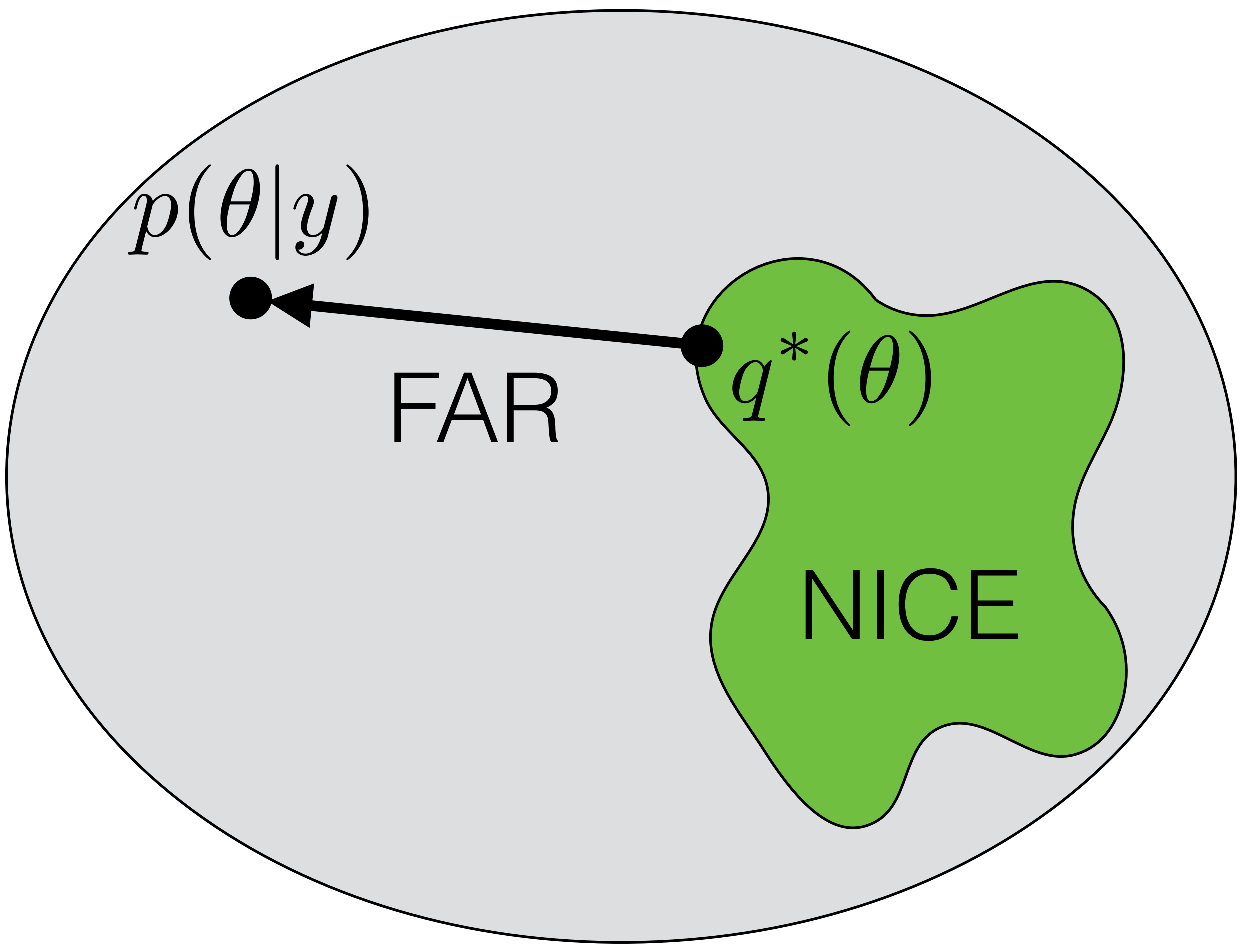

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$$KL(q(\cdot)||p(\cdot|y))$$

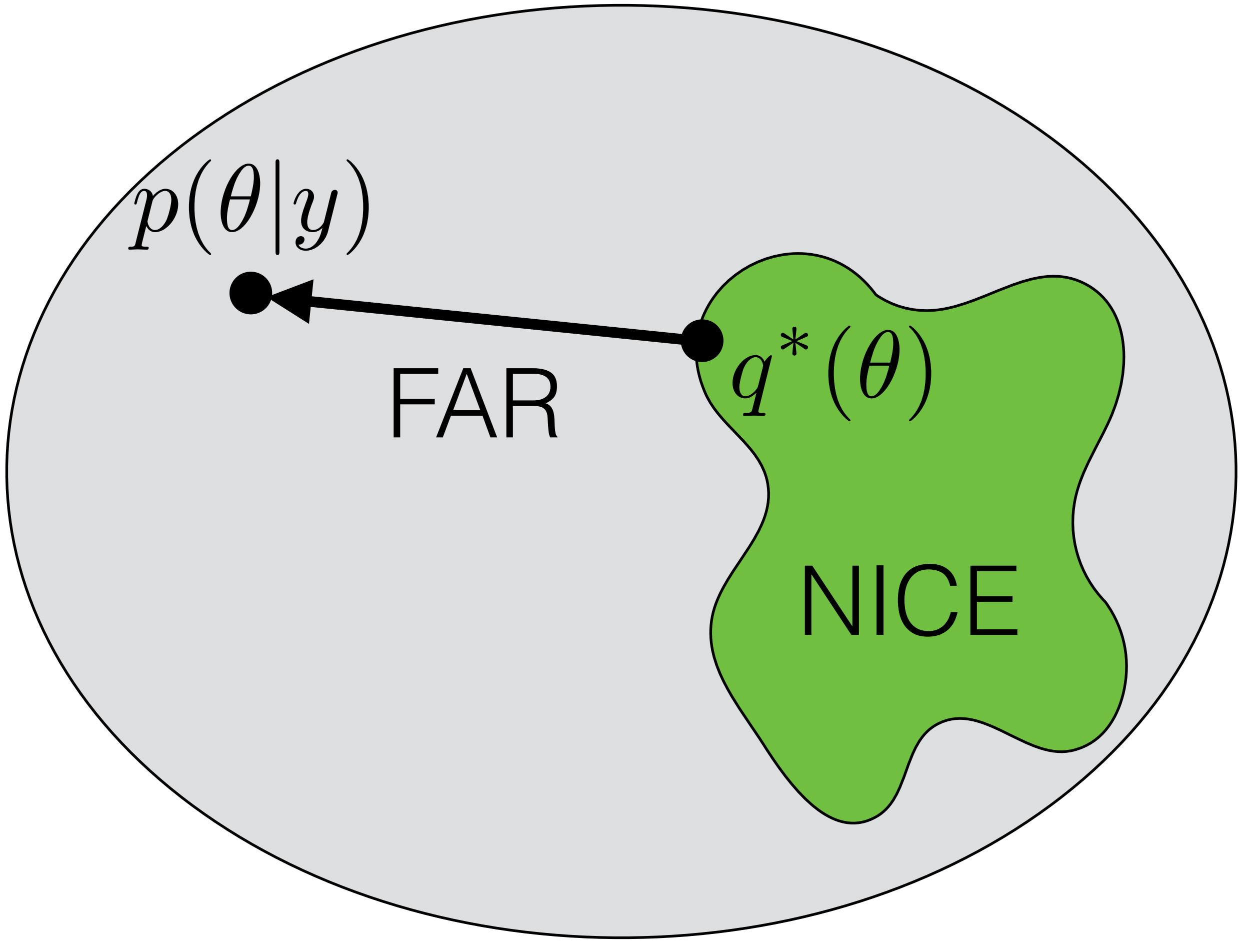
- VB practical success: point estimates and prediction, fast, streaming, distributed (3.6M Wikipedia, 350K Nature)

[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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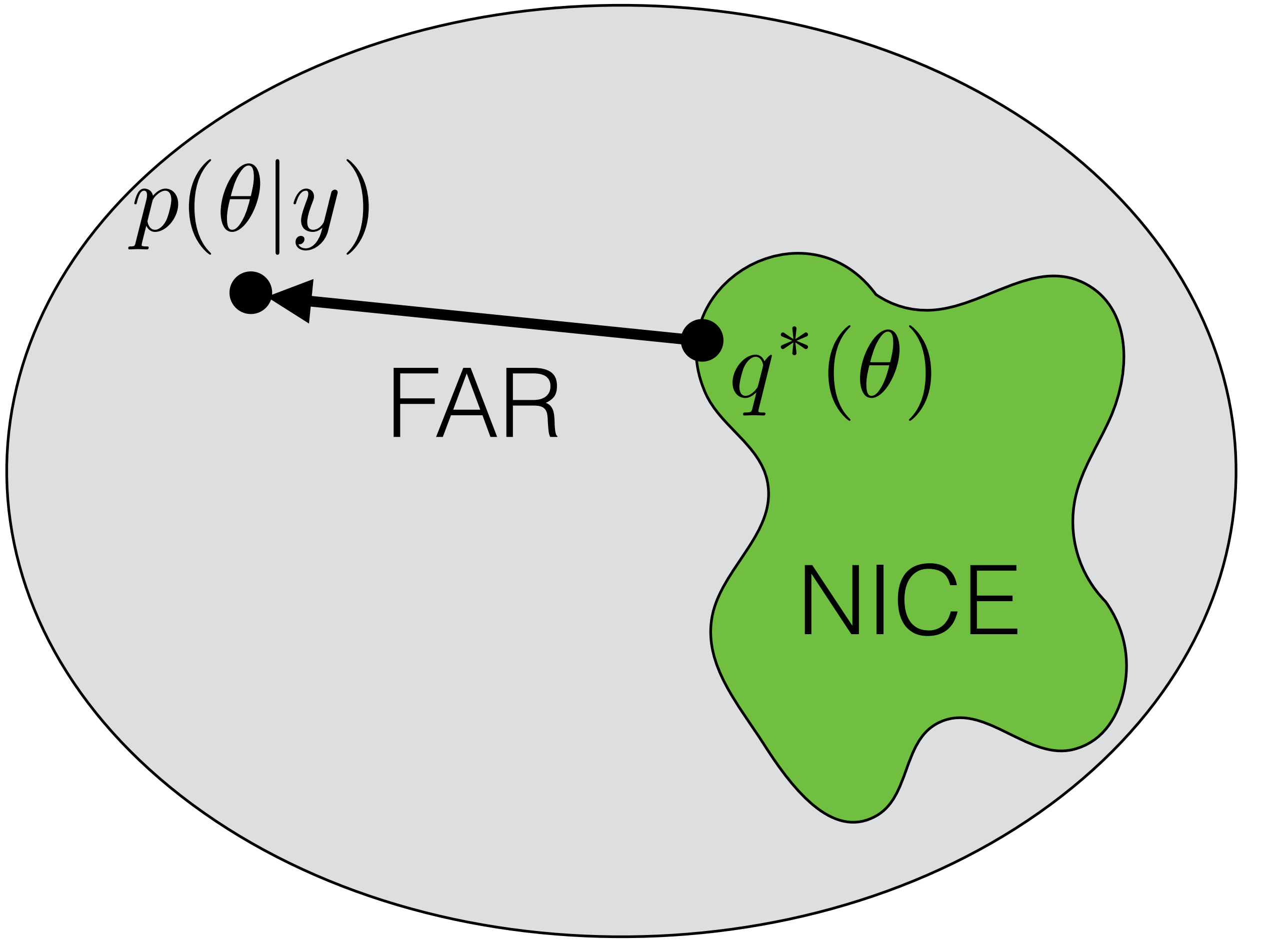

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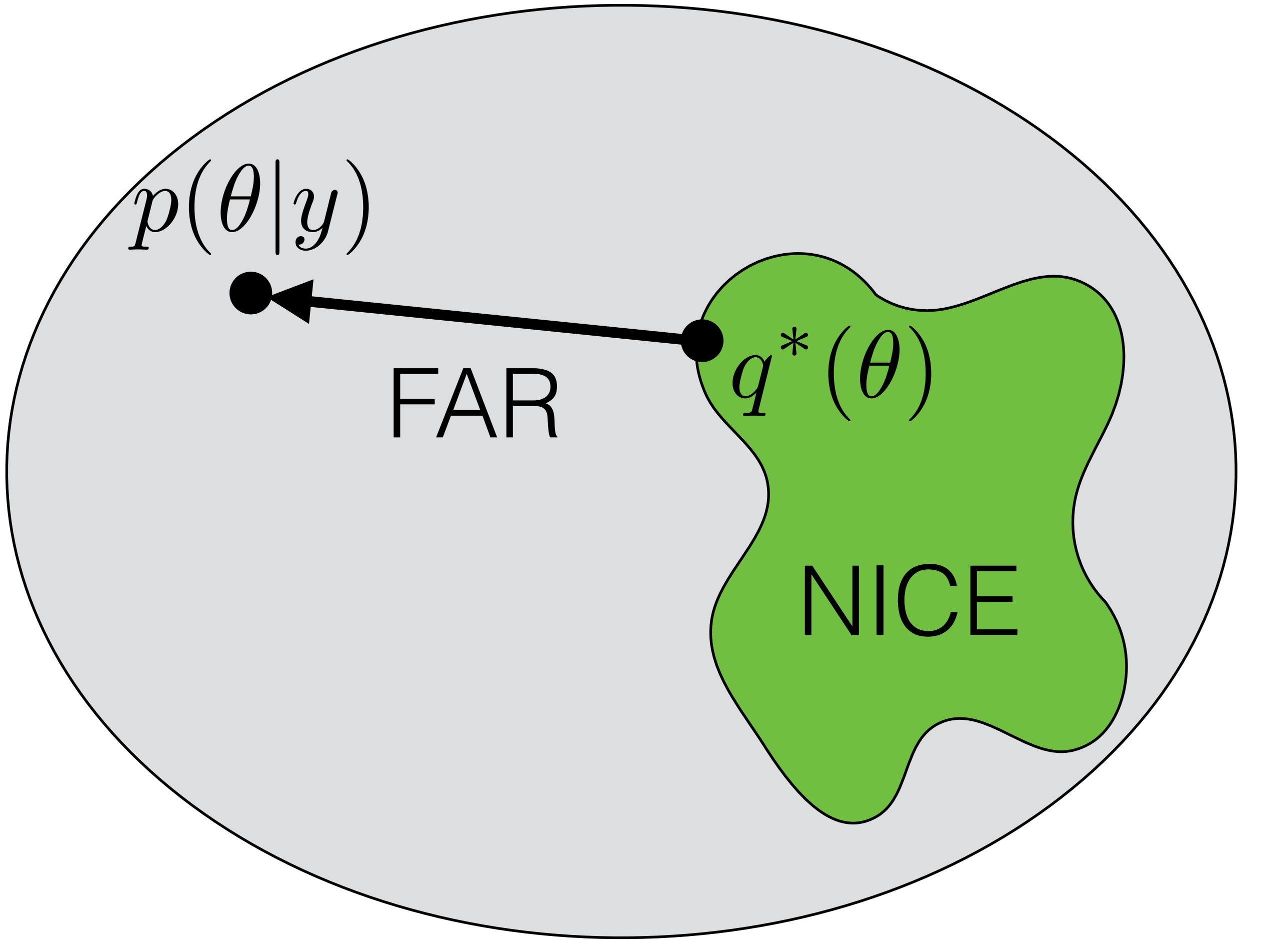

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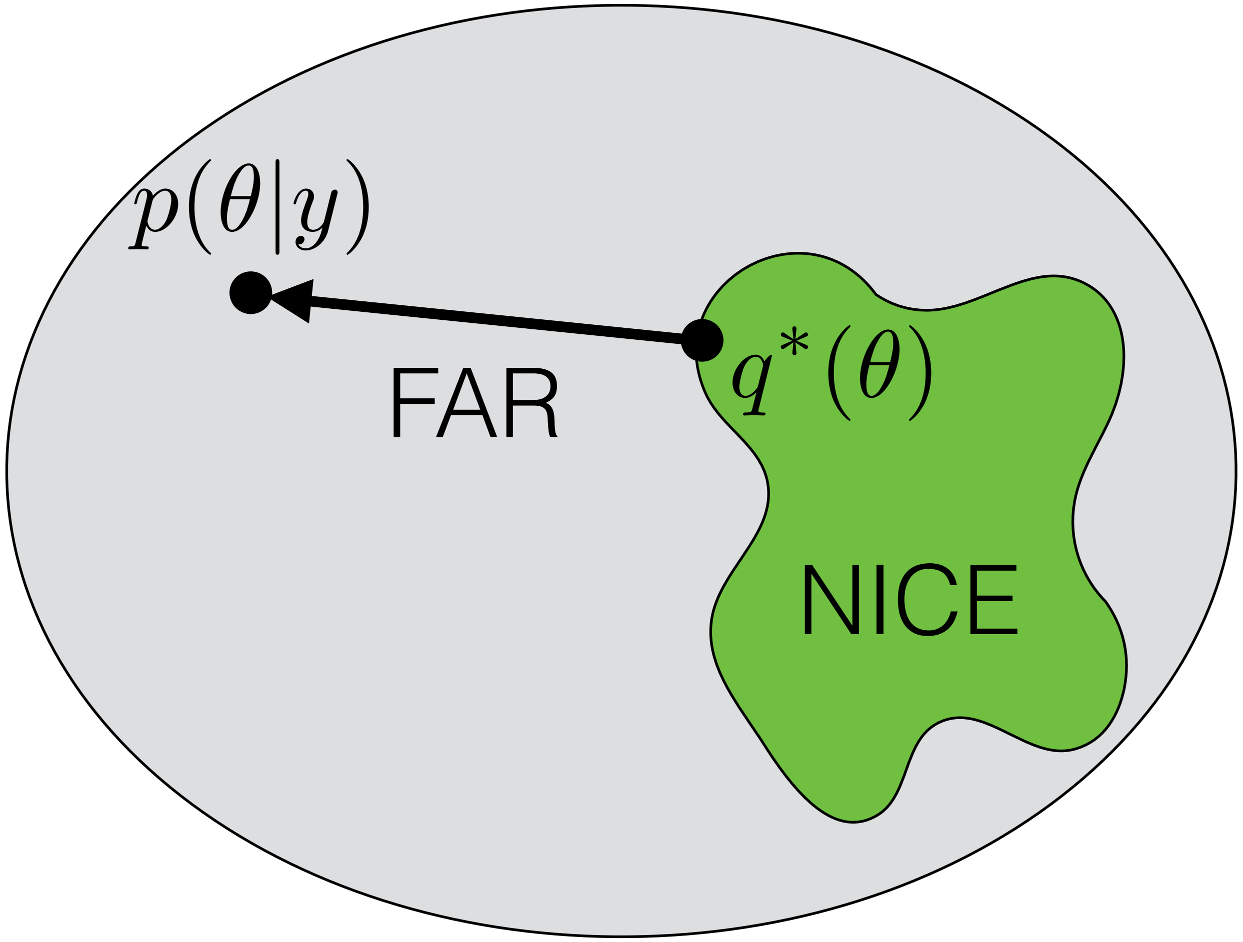

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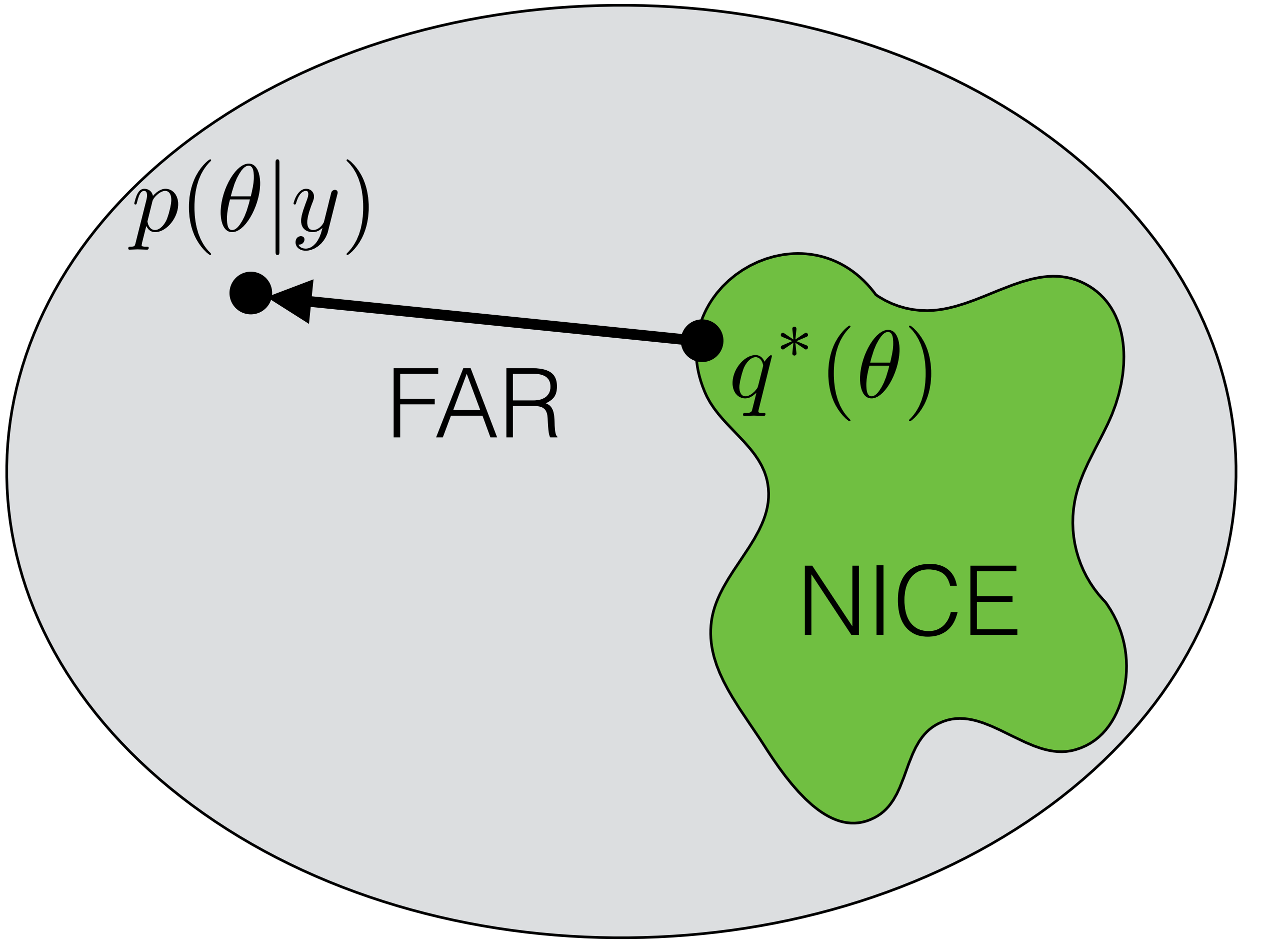

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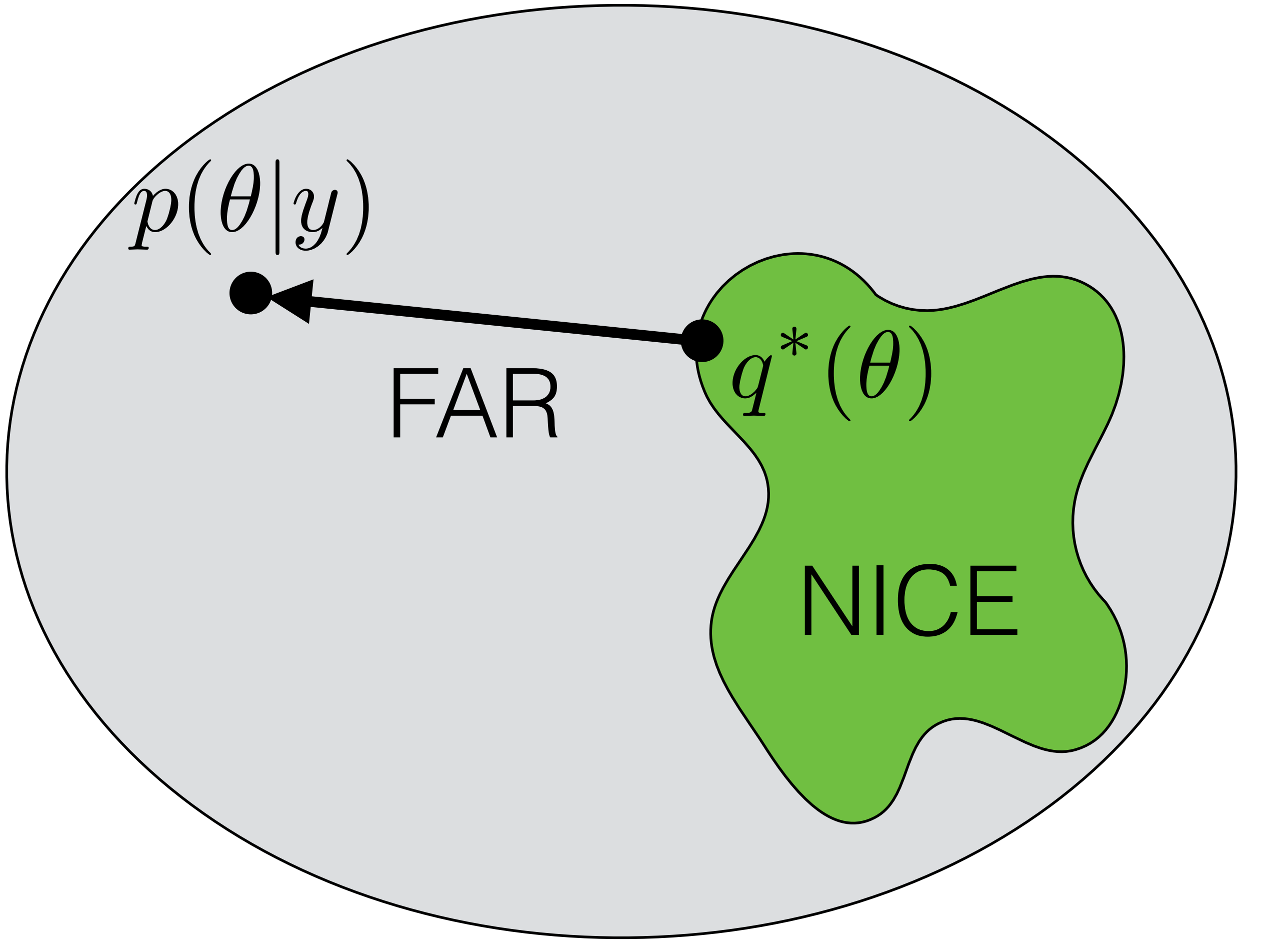

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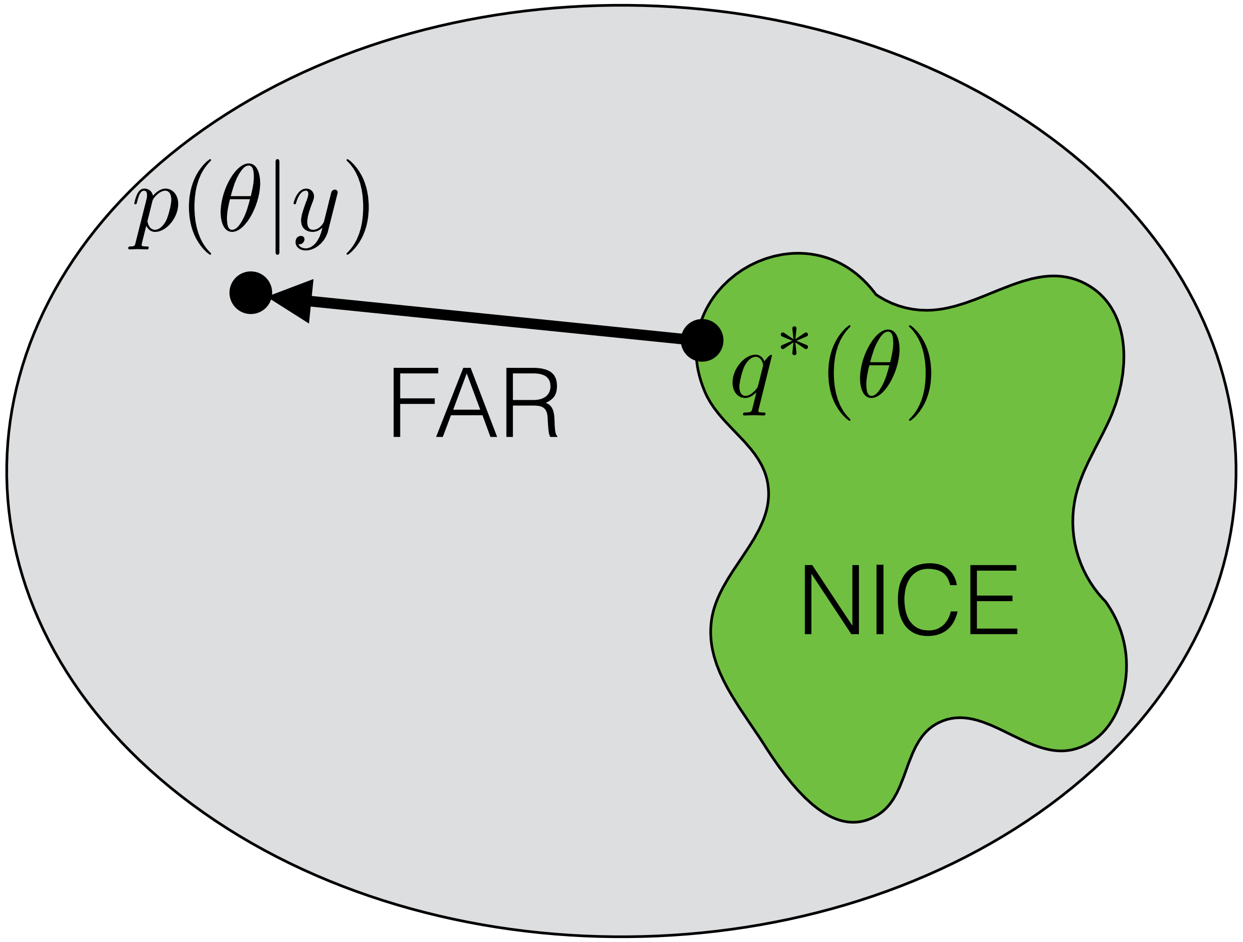

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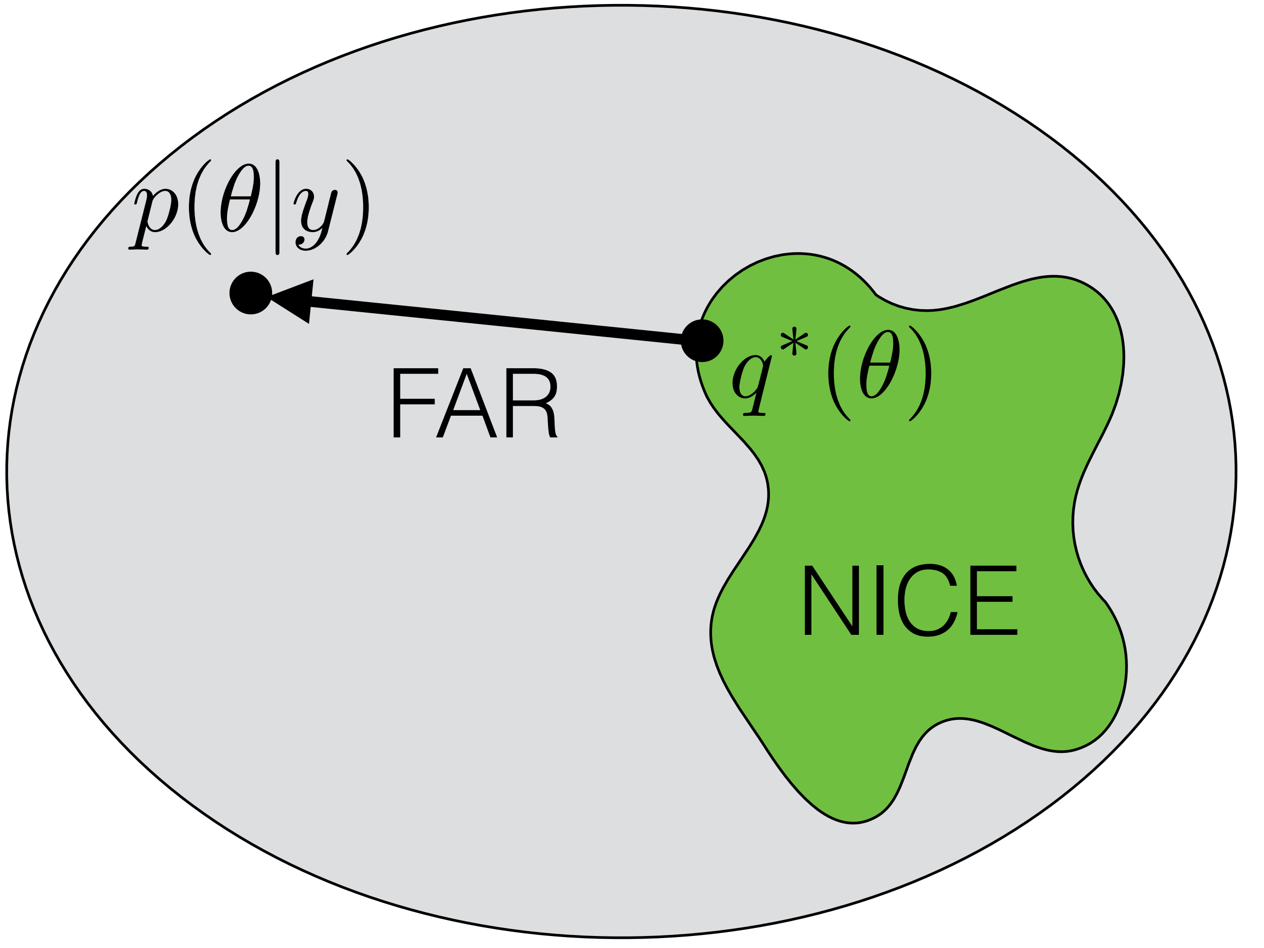

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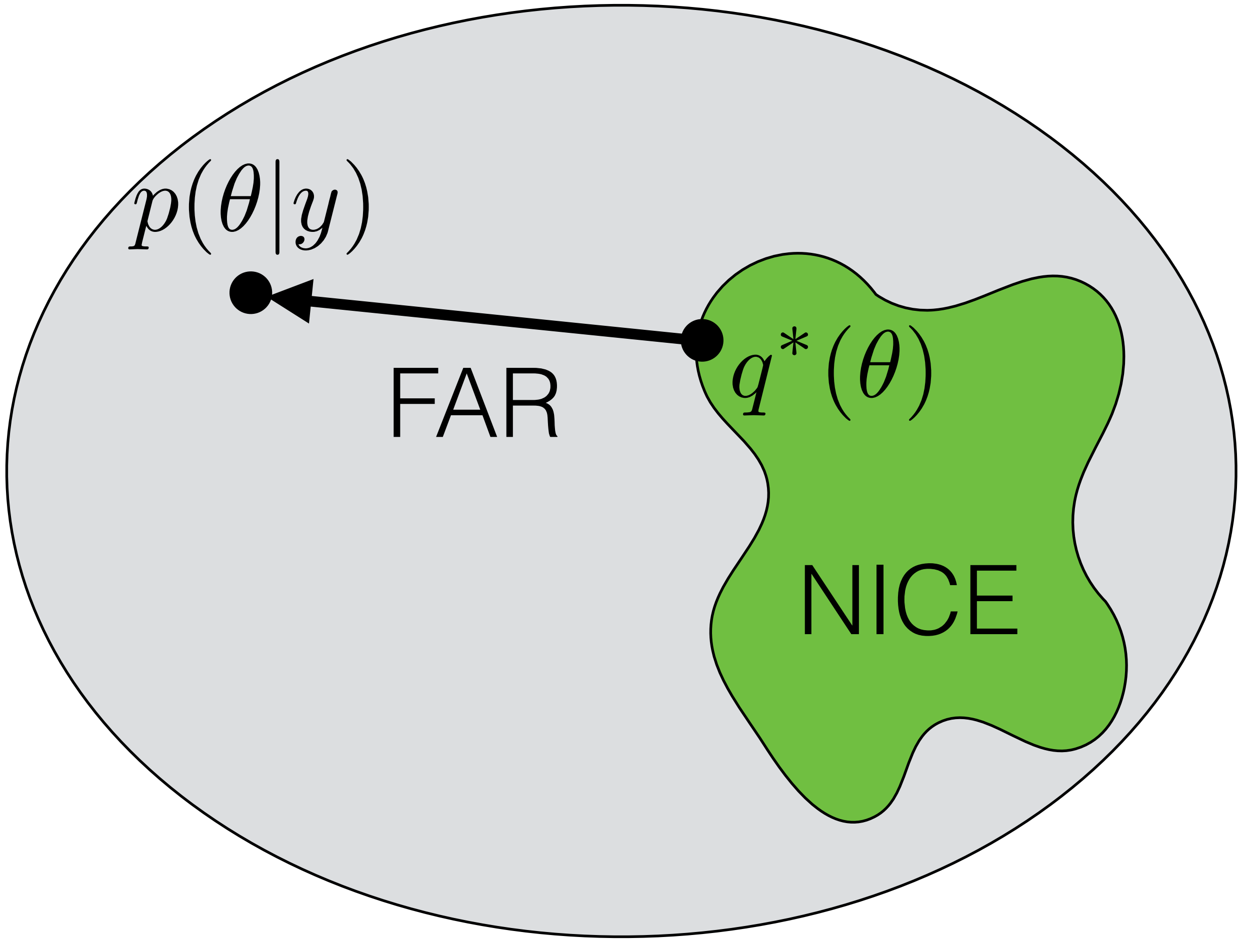

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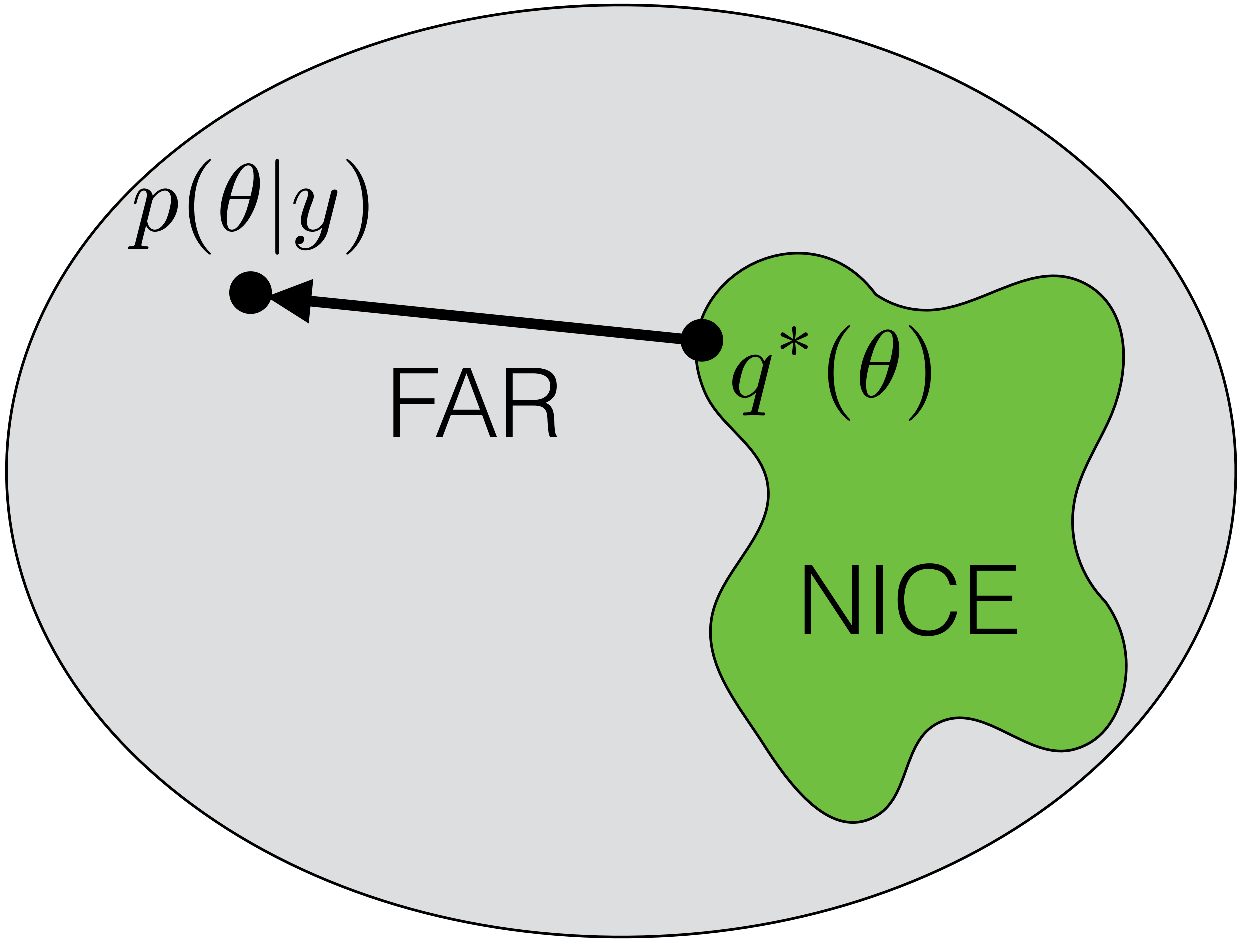

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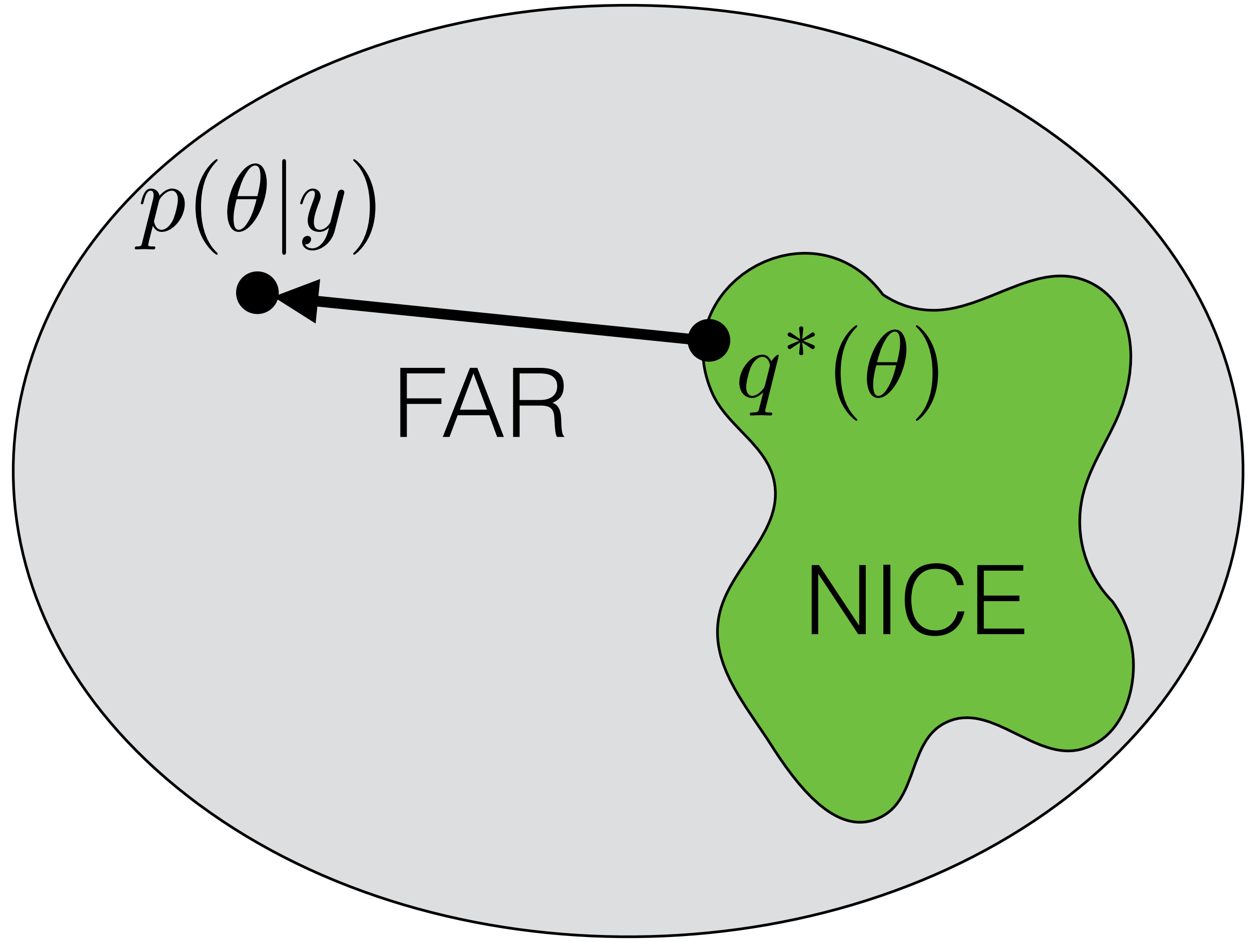

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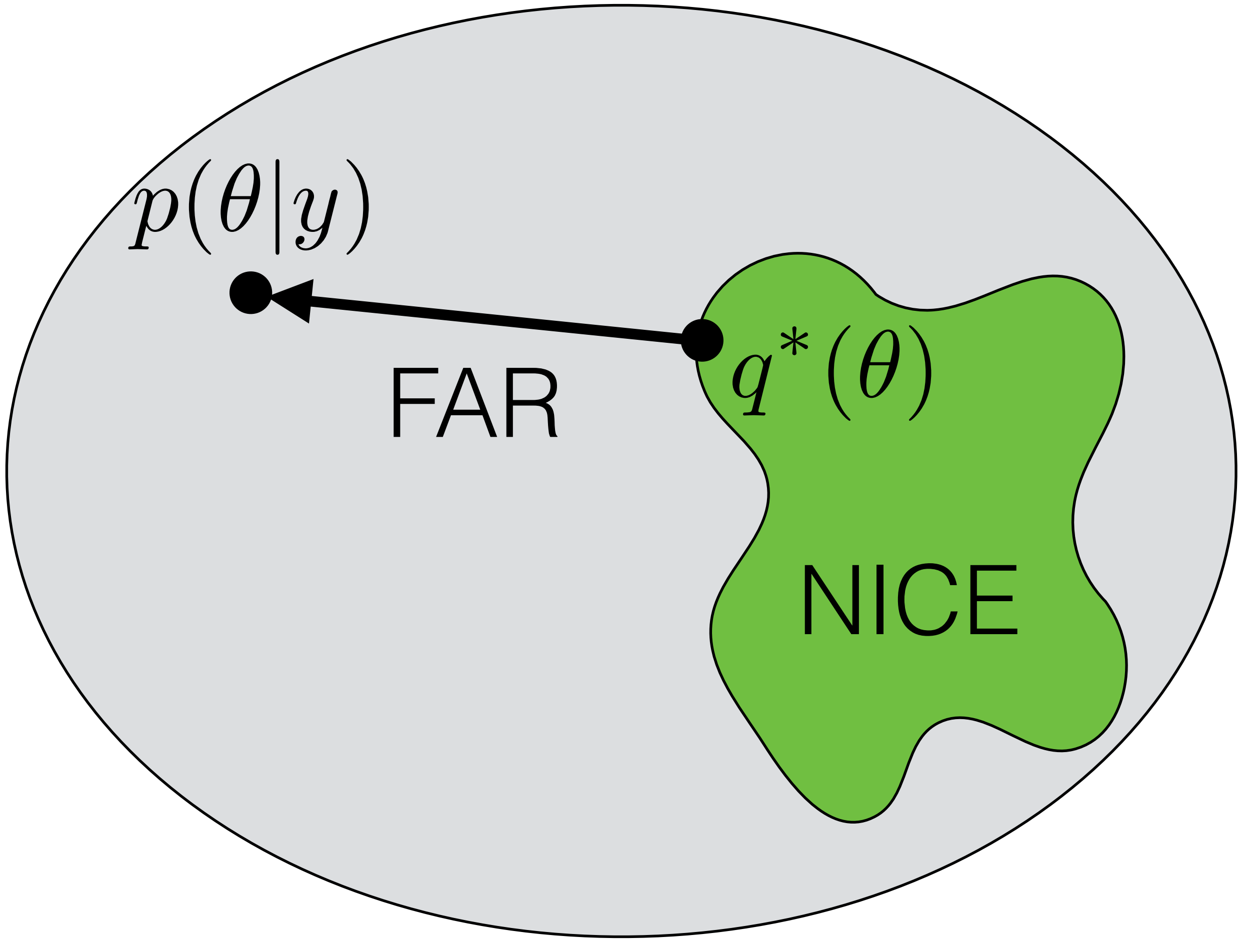

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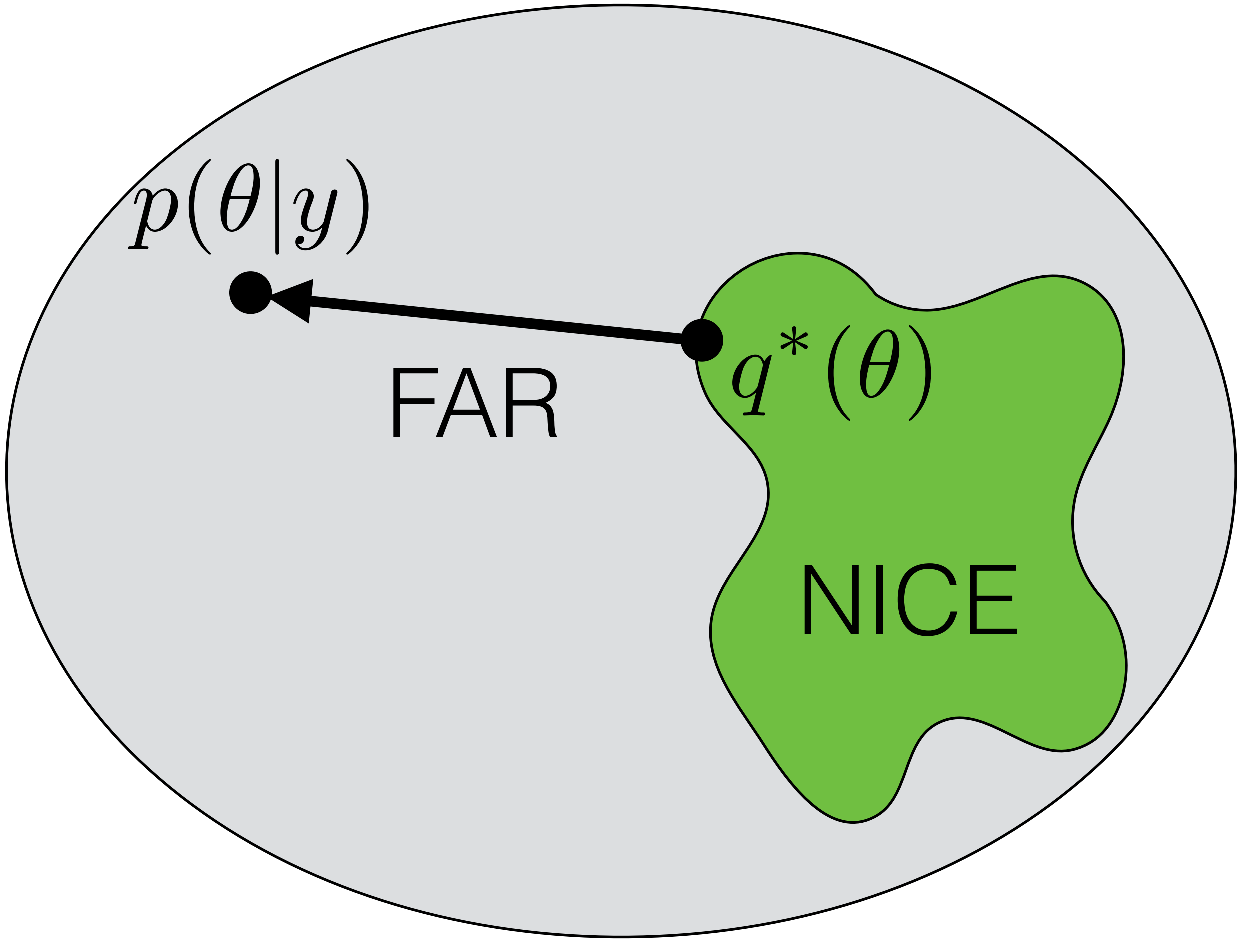

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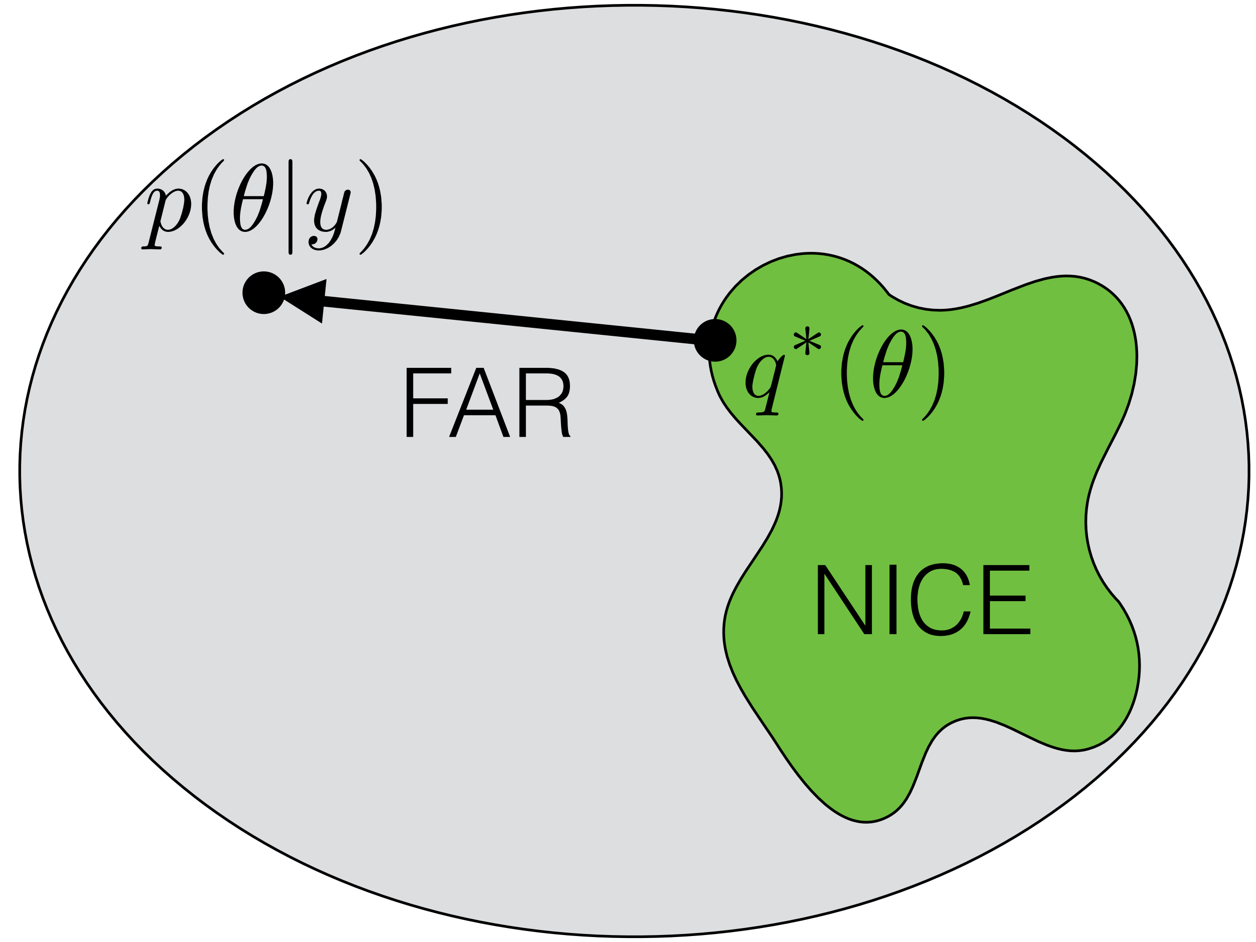

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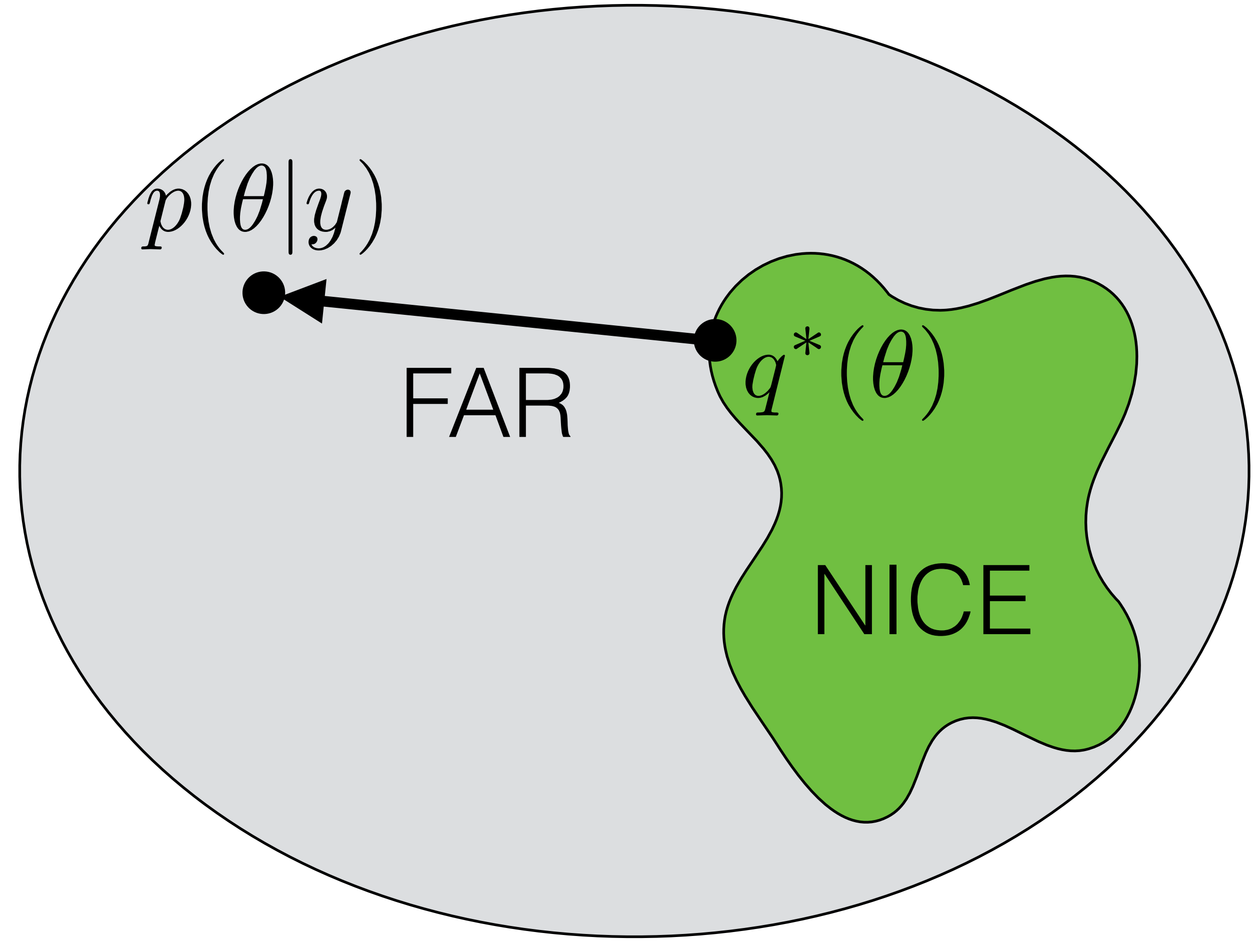

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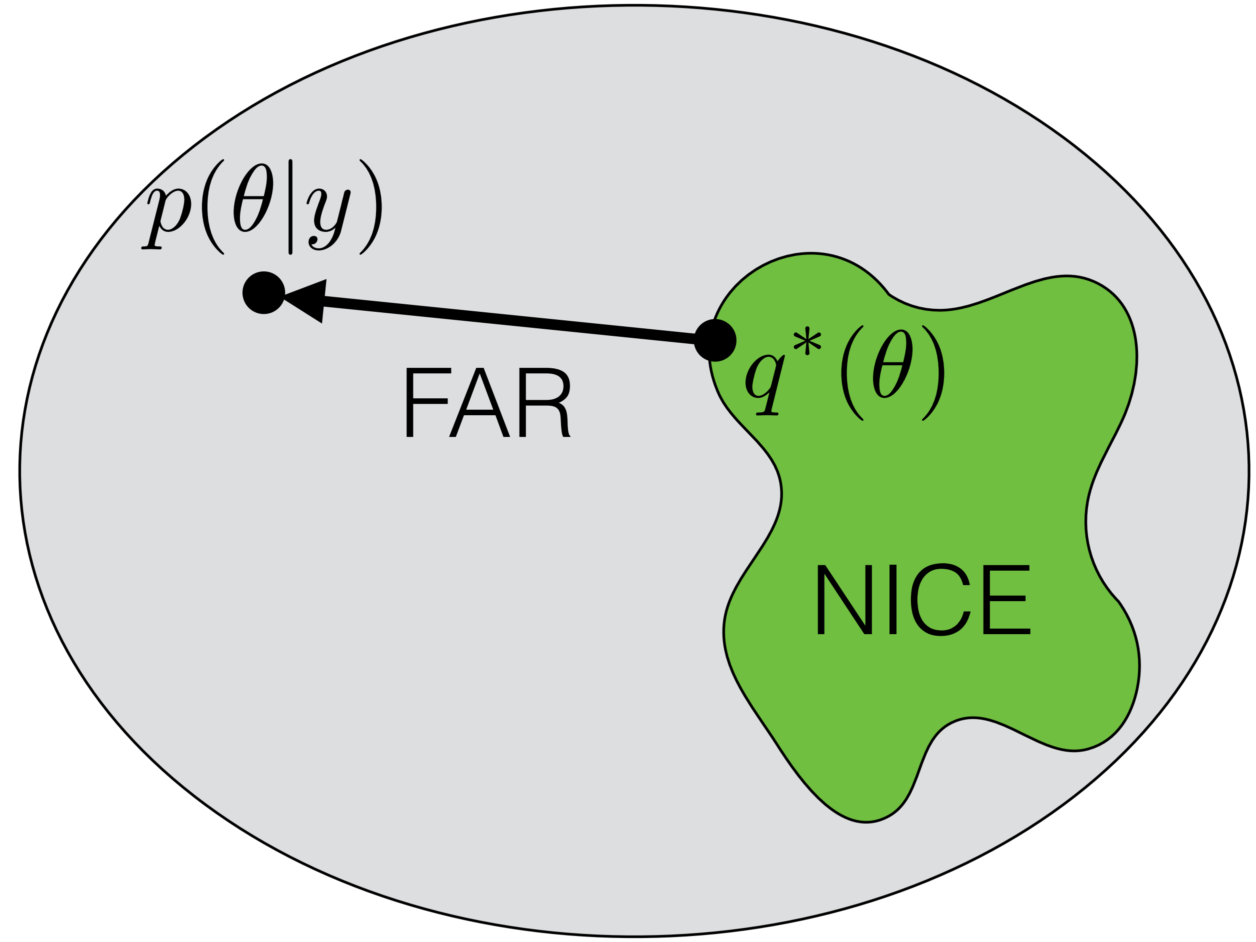

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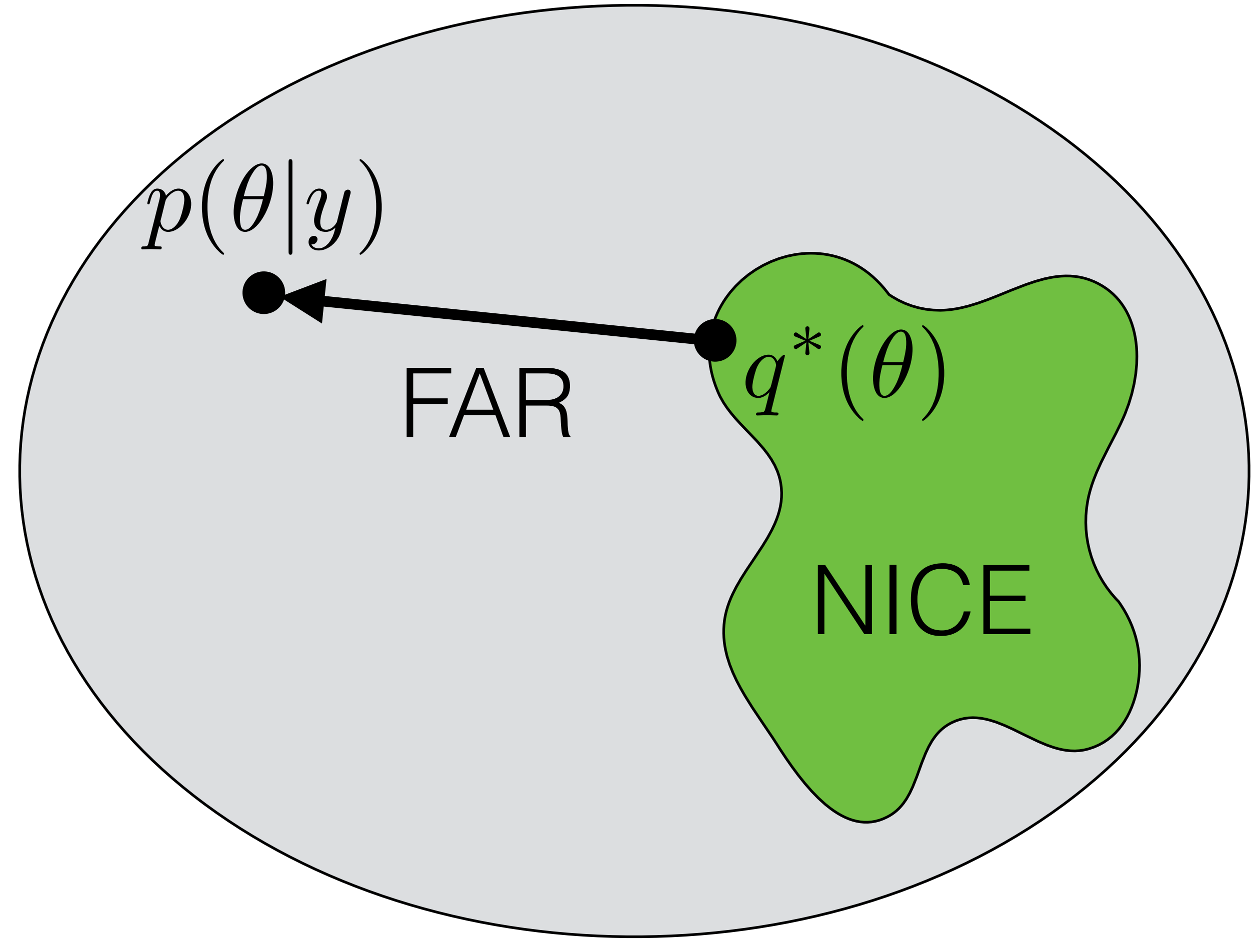

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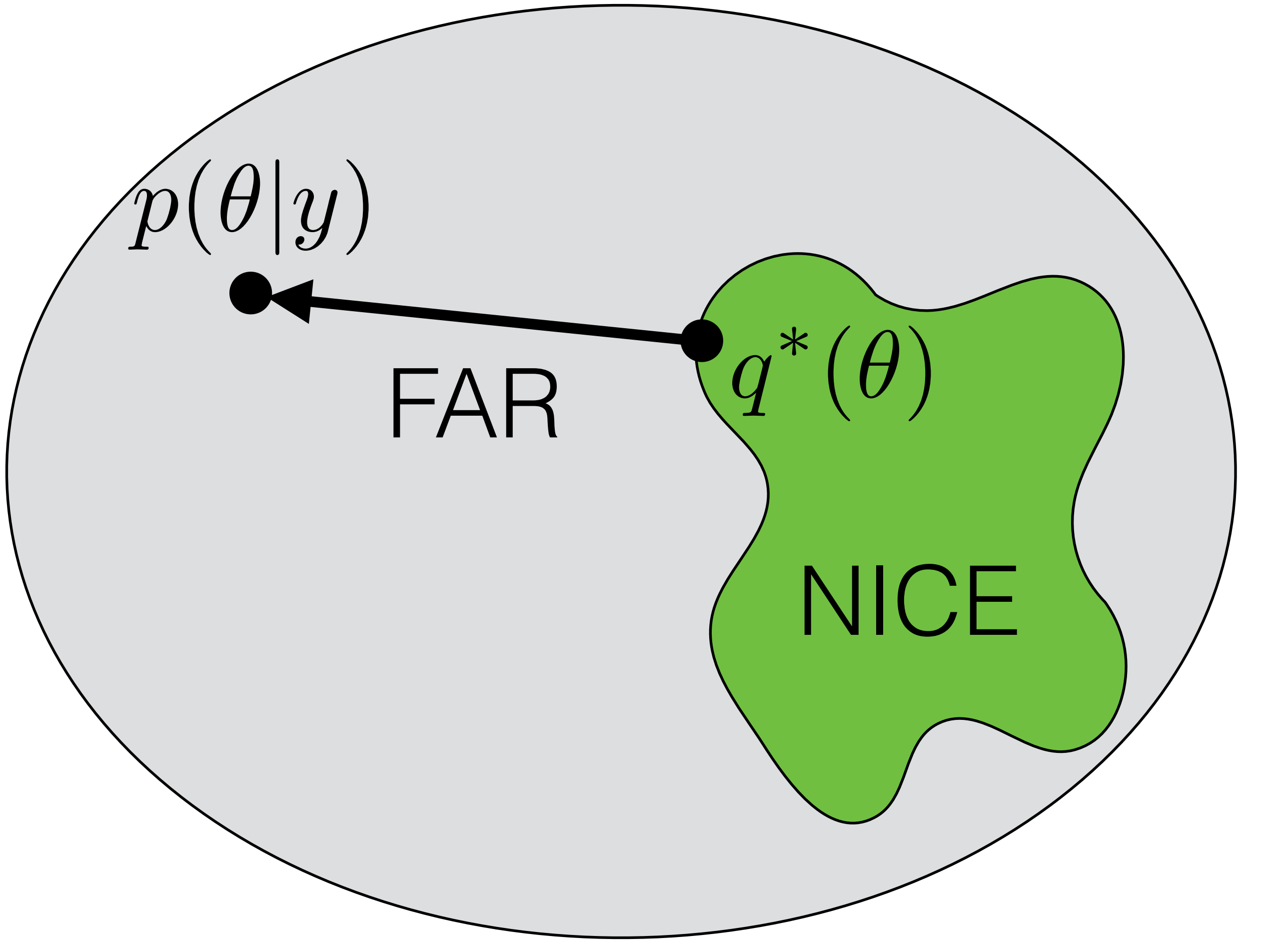

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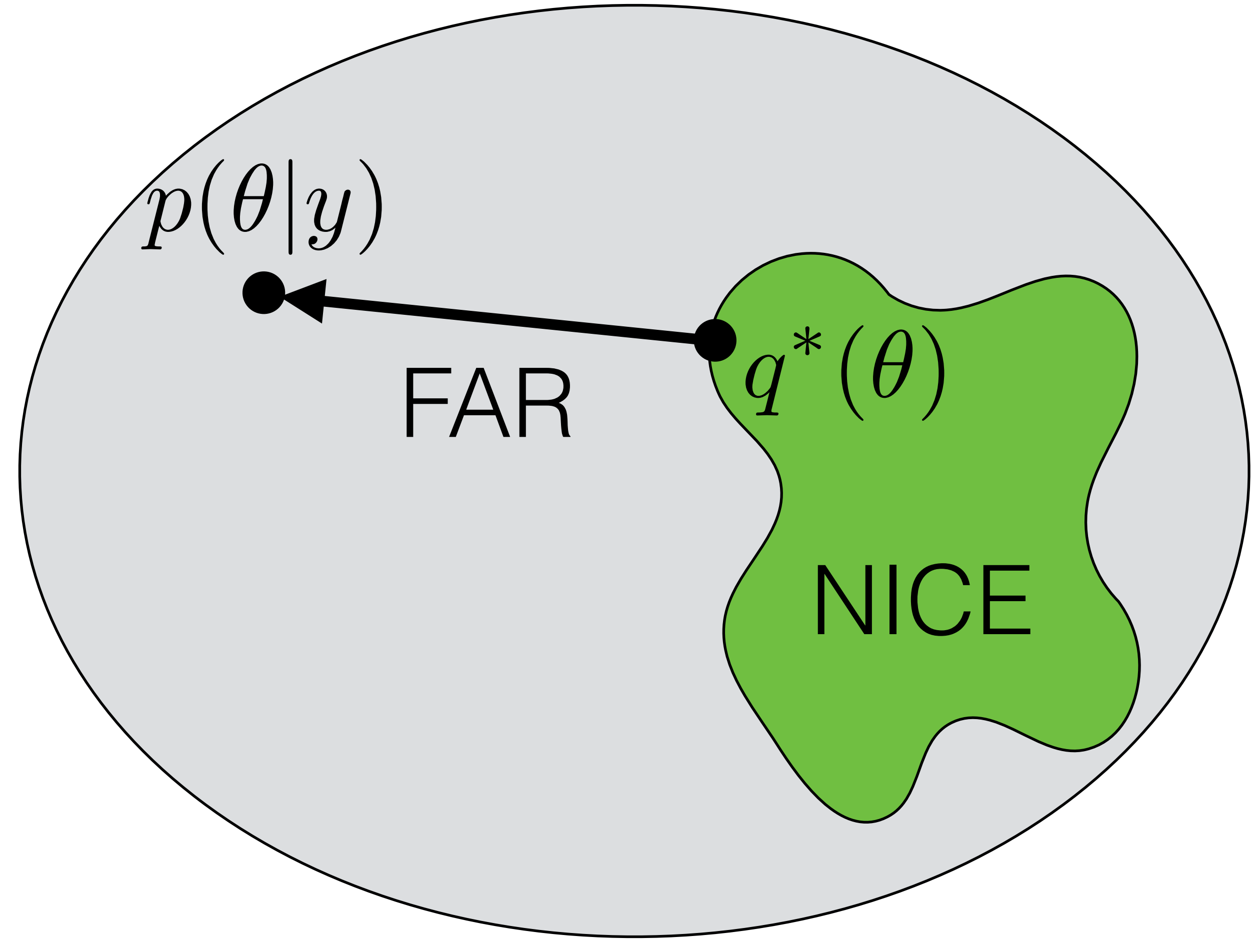

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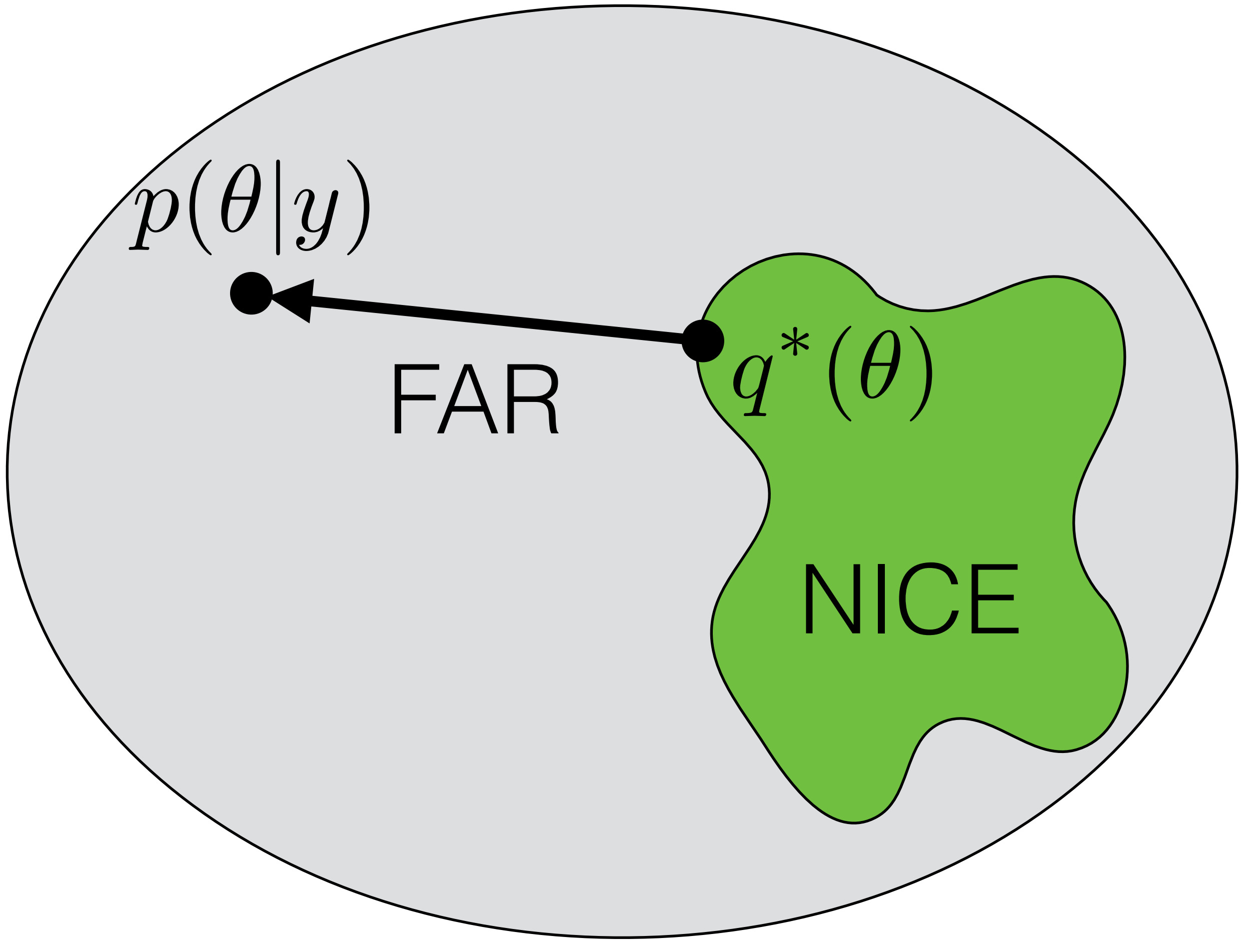

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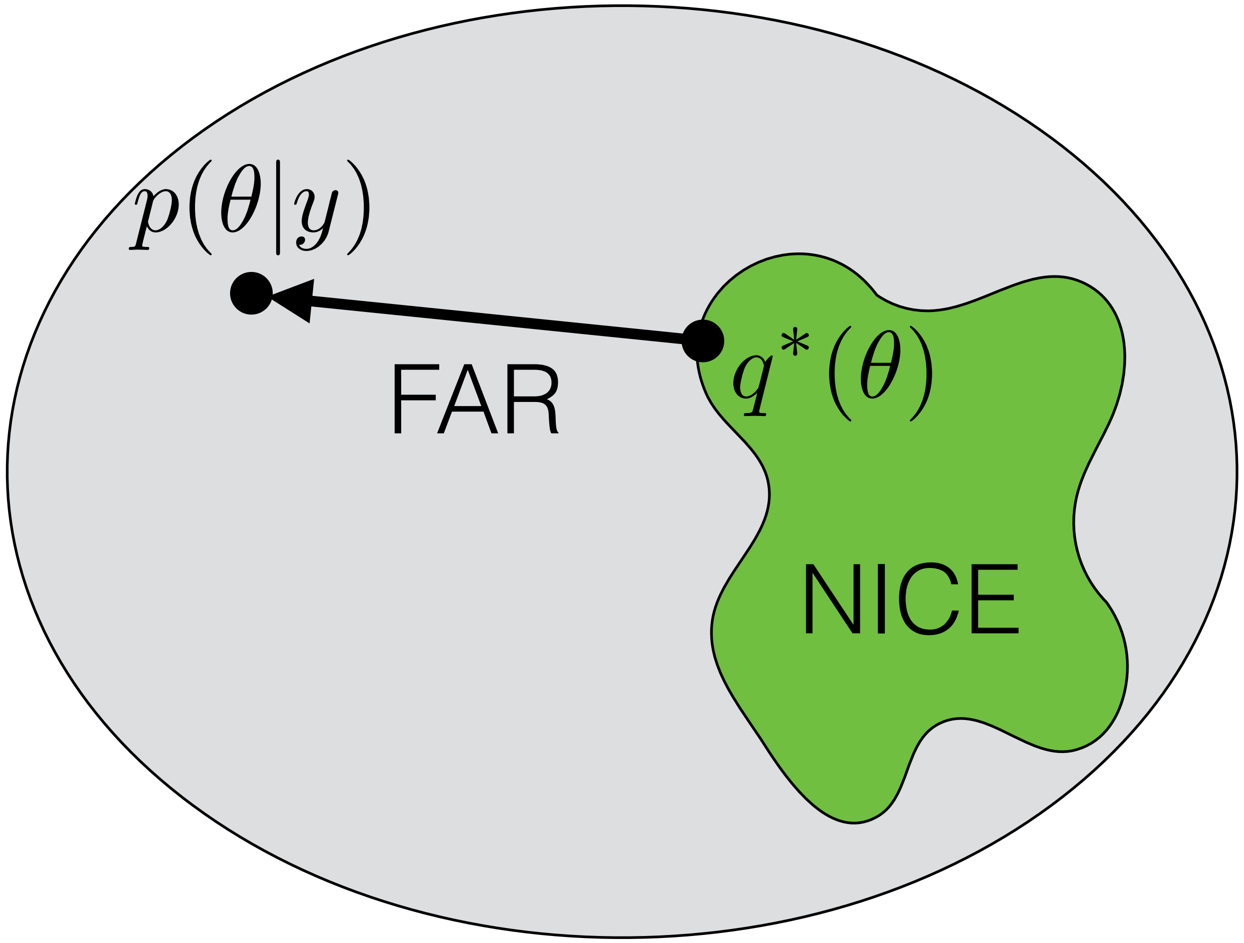

Choose "NICE" distributions

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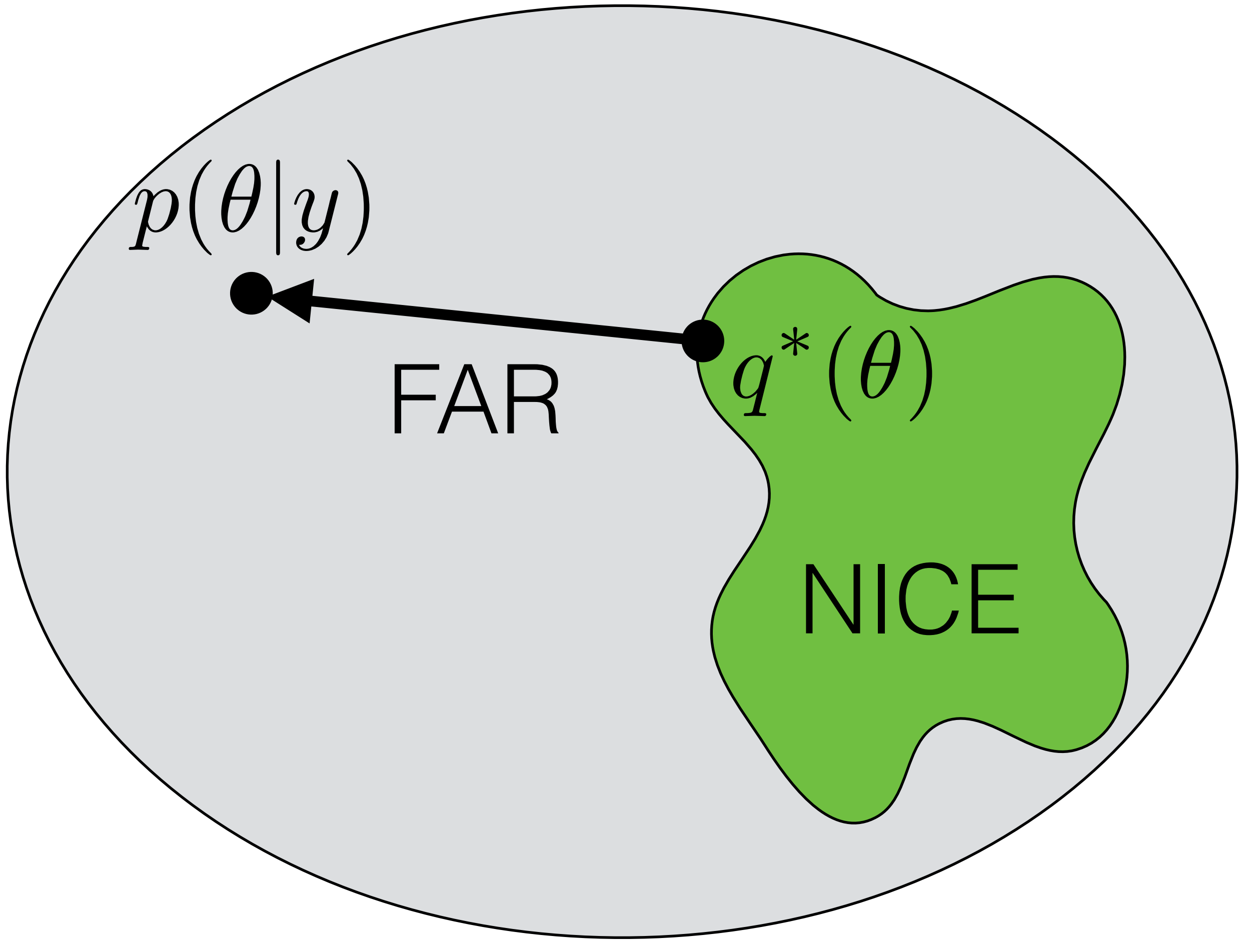

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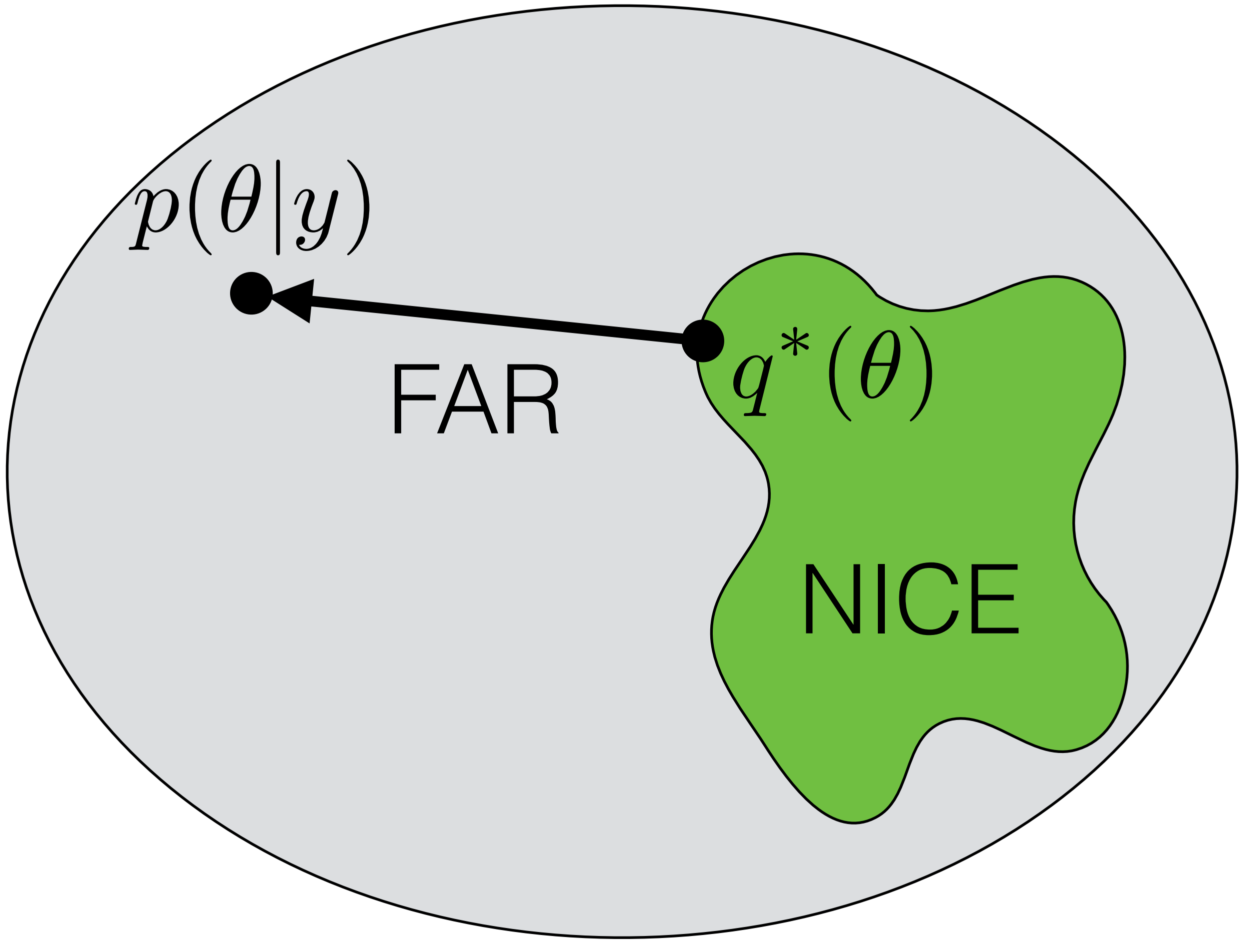

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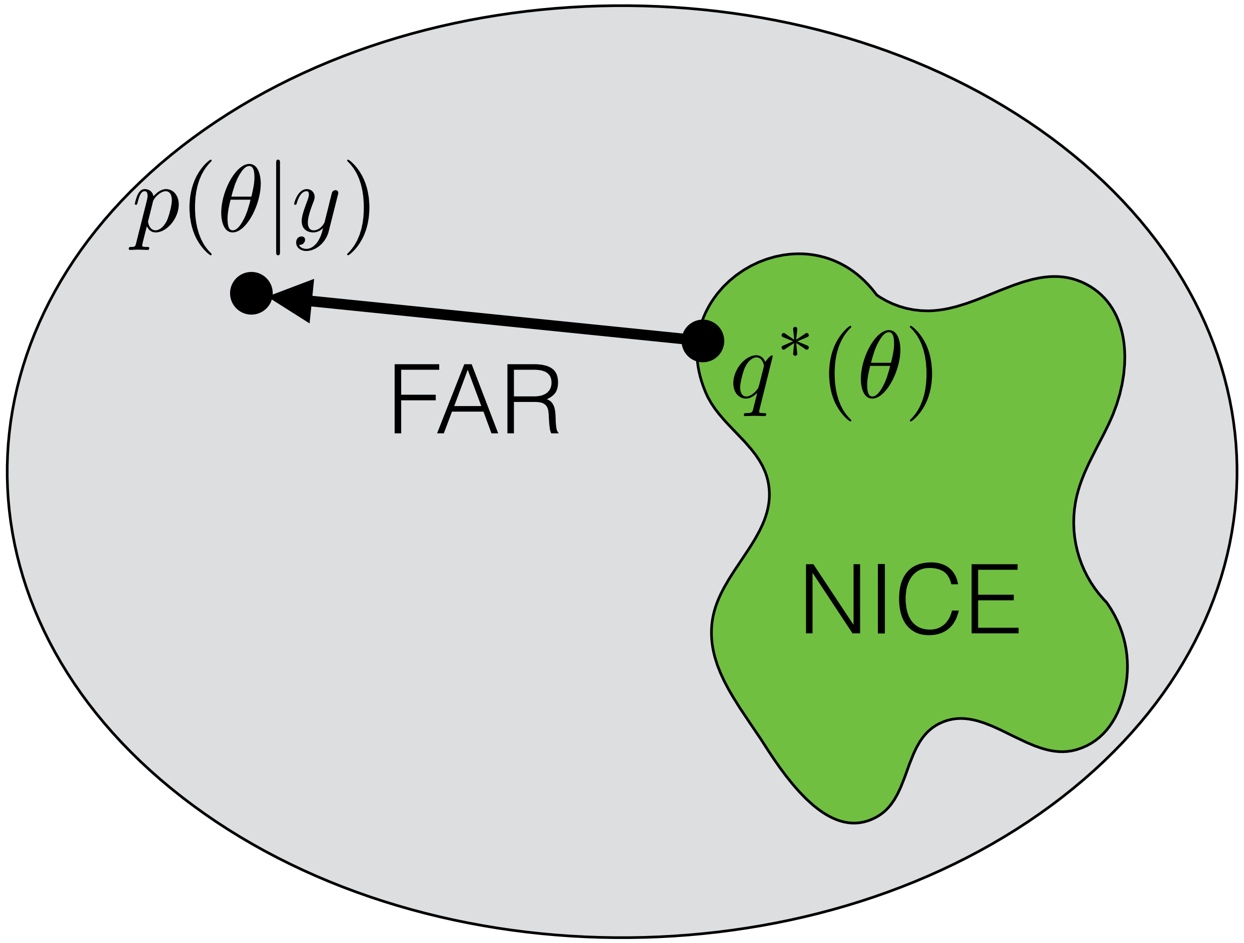

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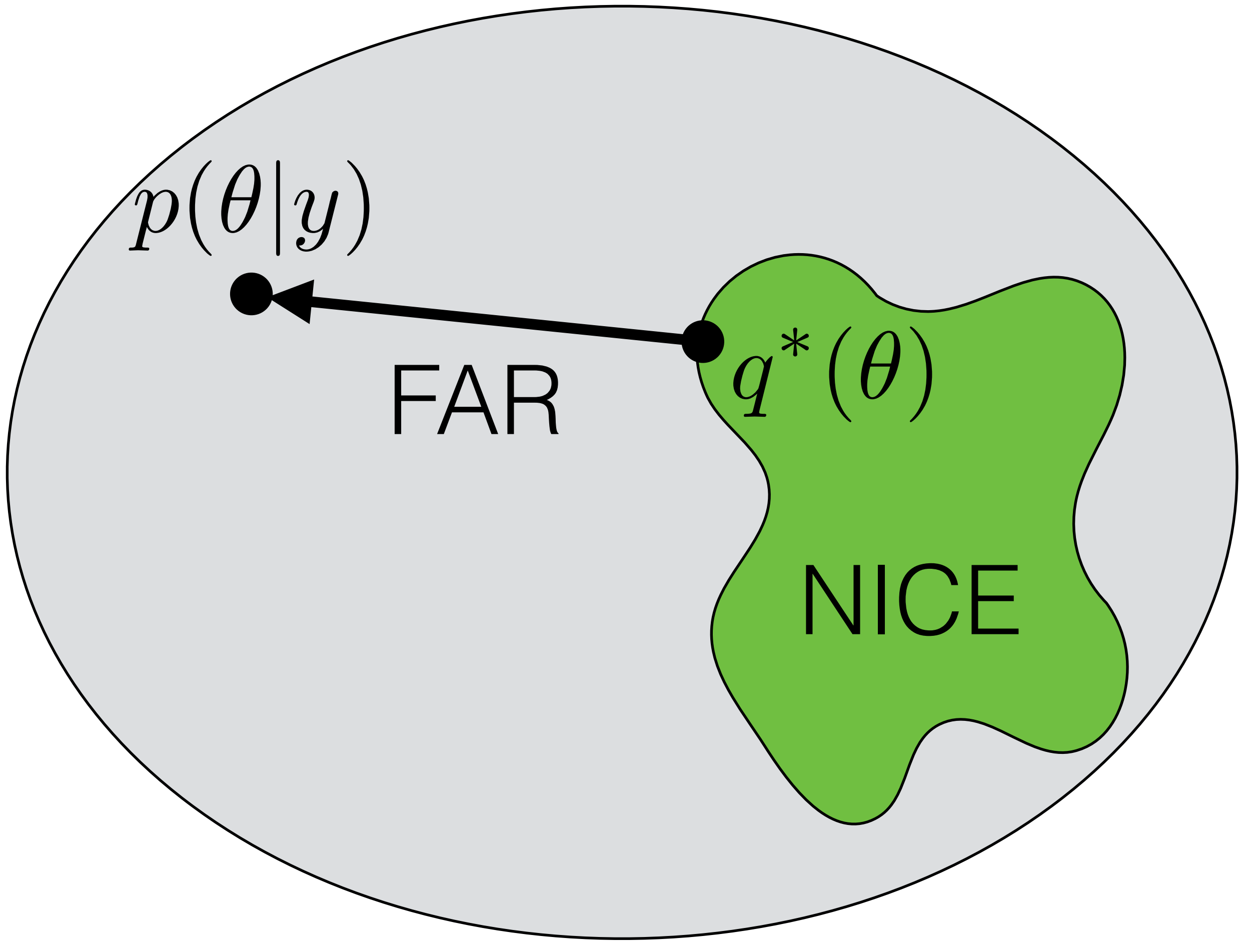

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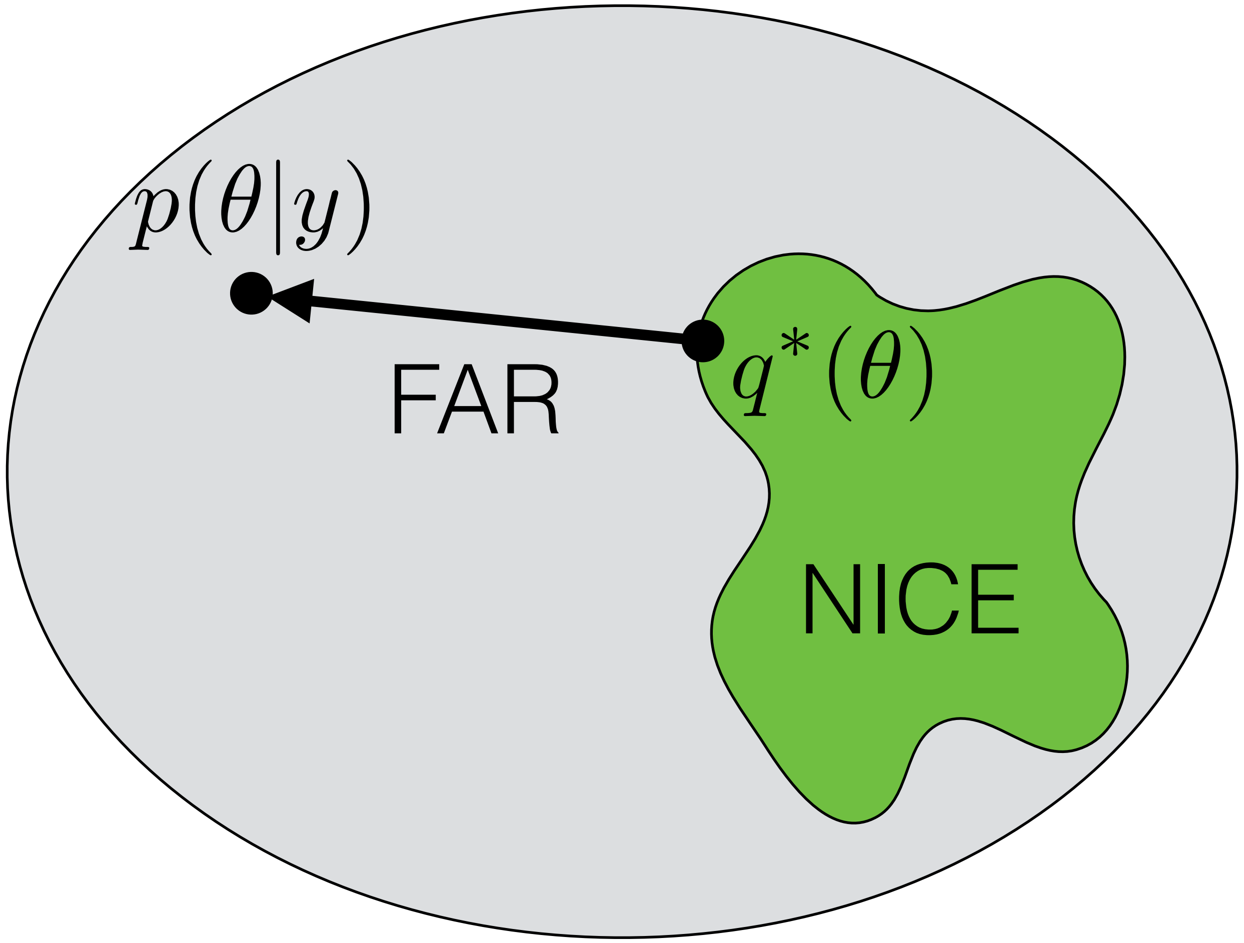

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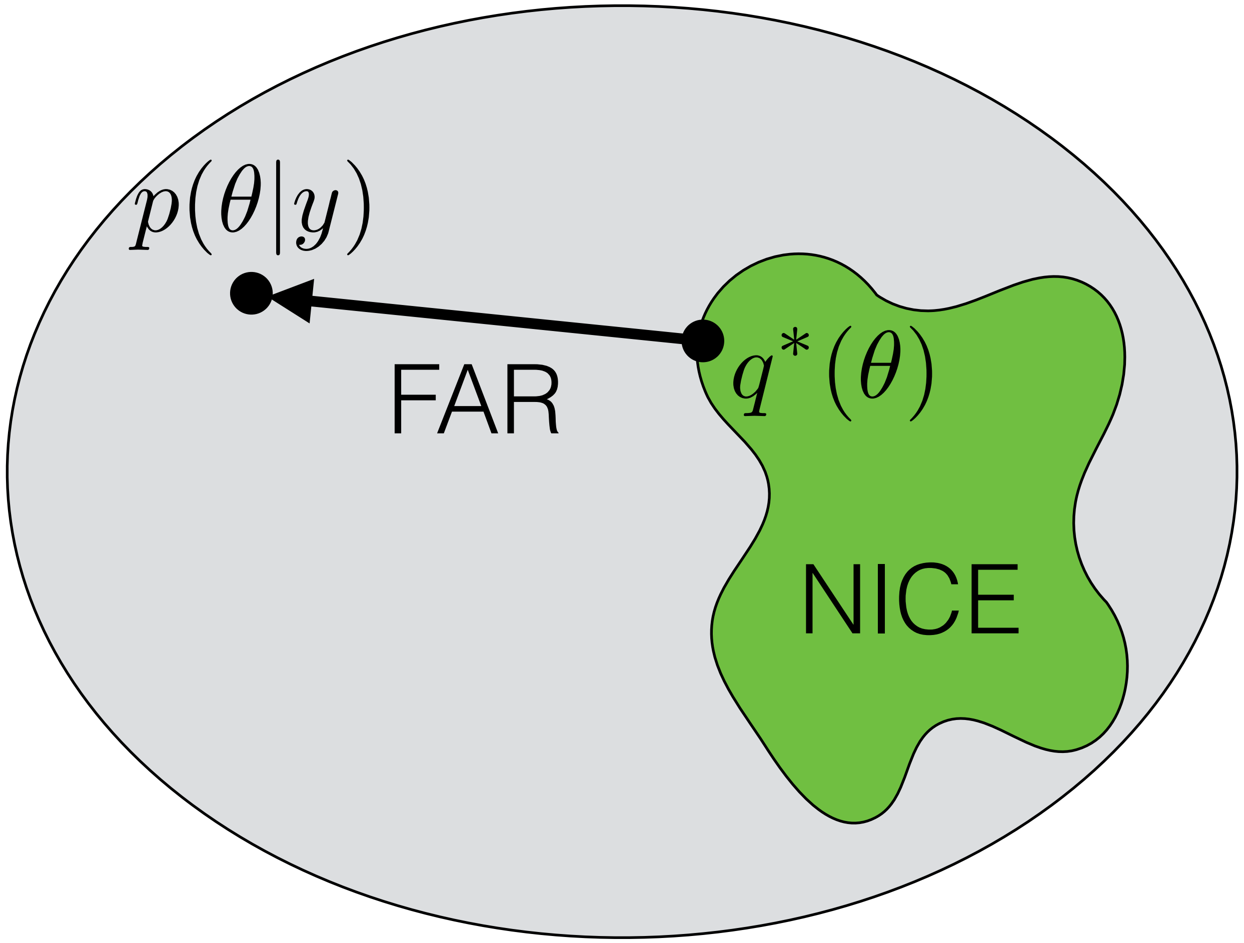

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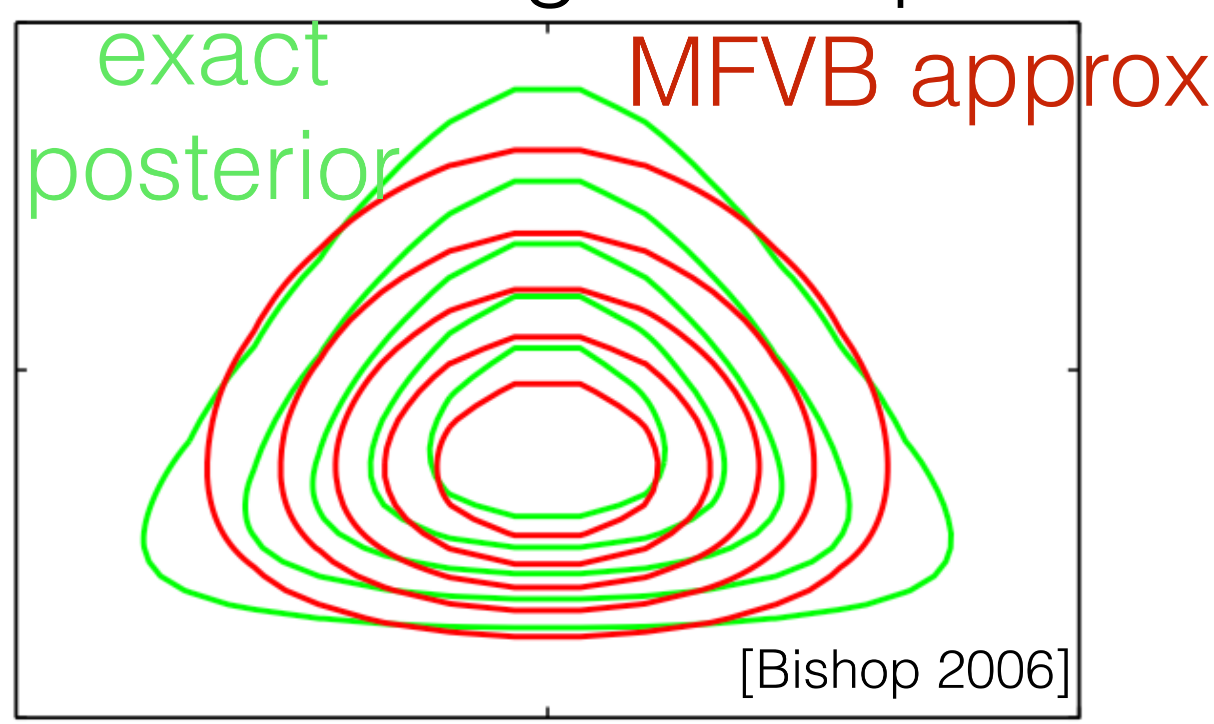

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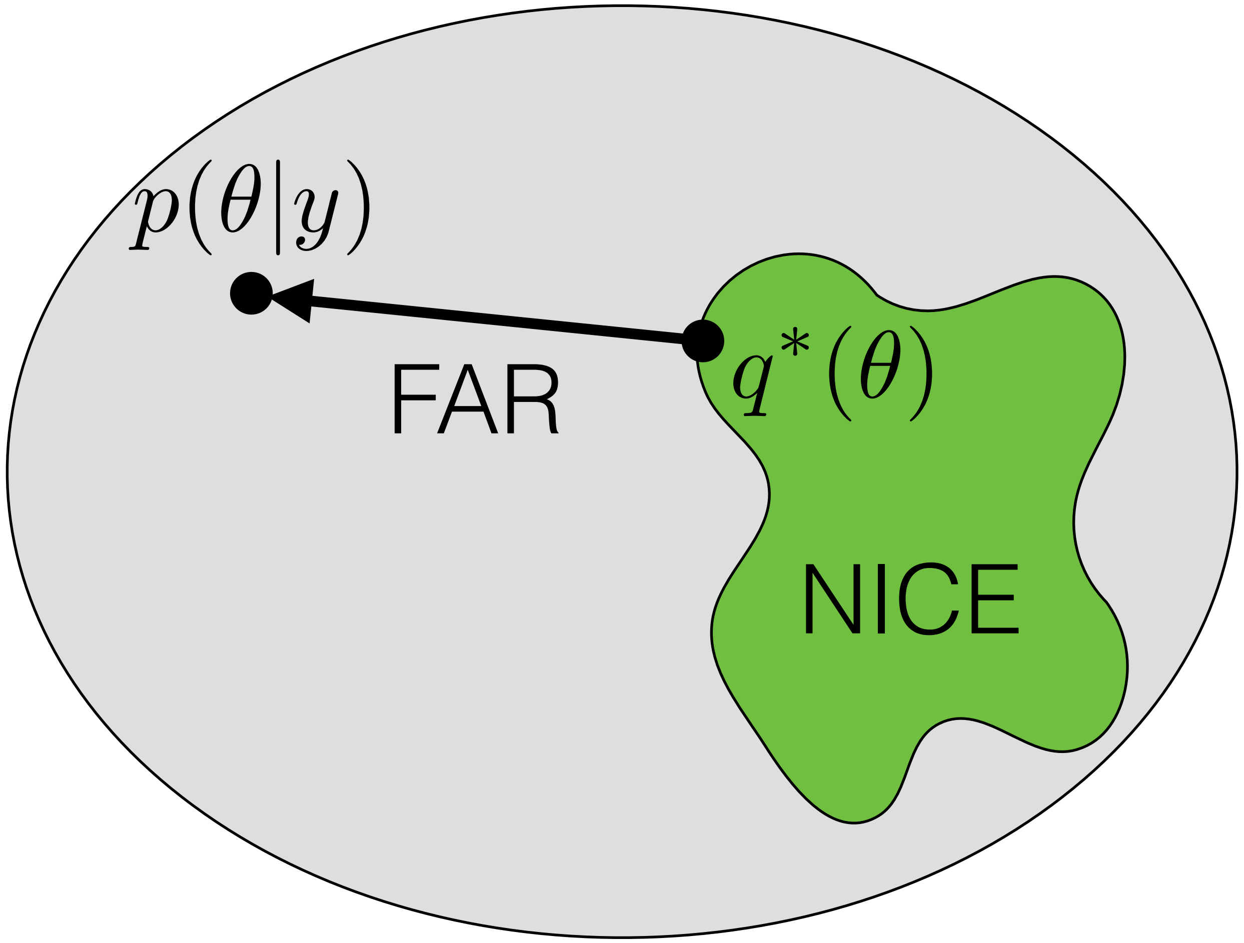

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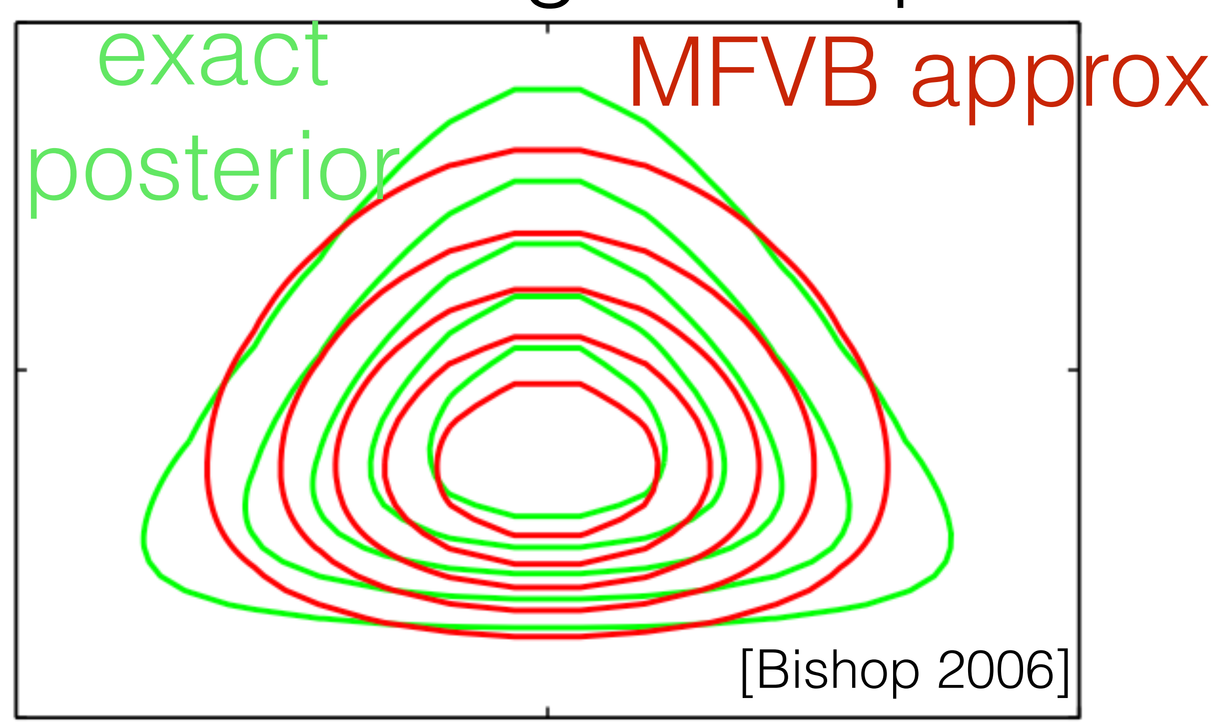

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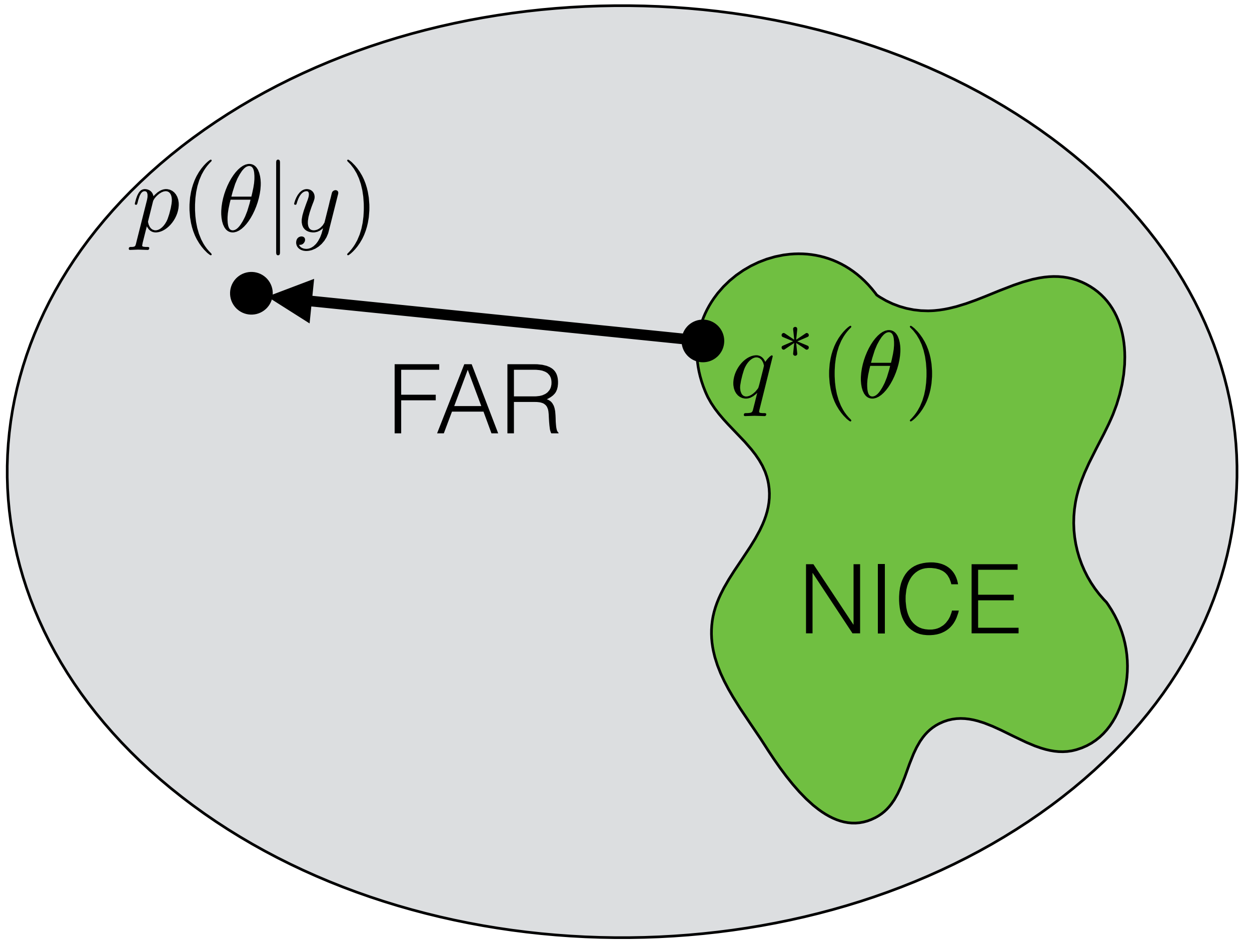

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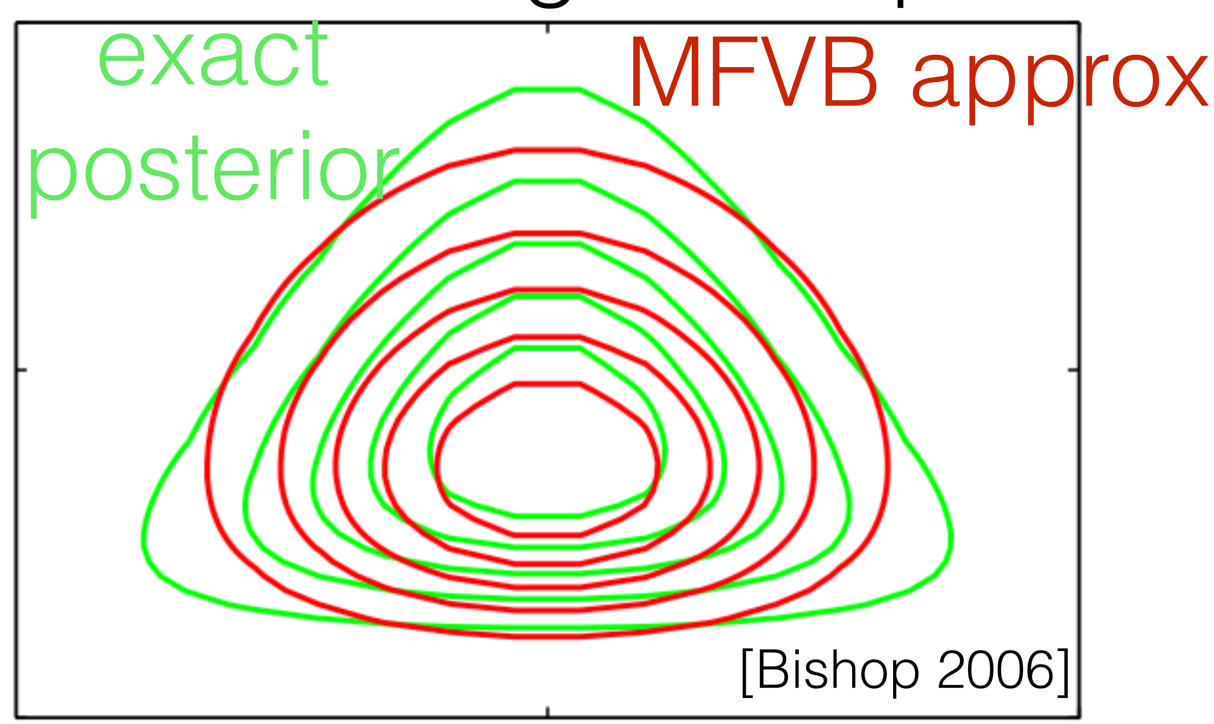

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- One option: Coordinate descent in $q_1, \ldots, q_J$

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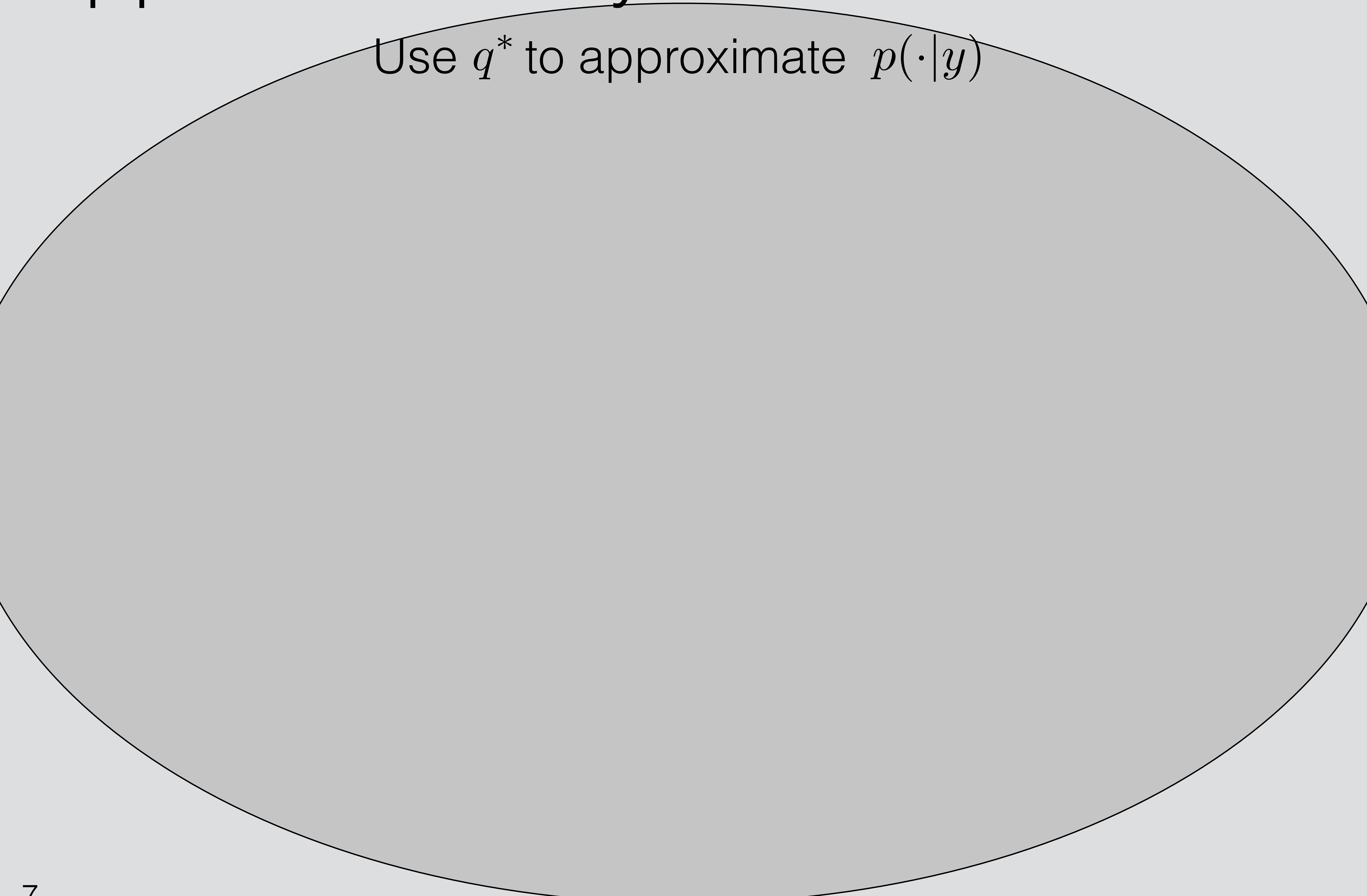

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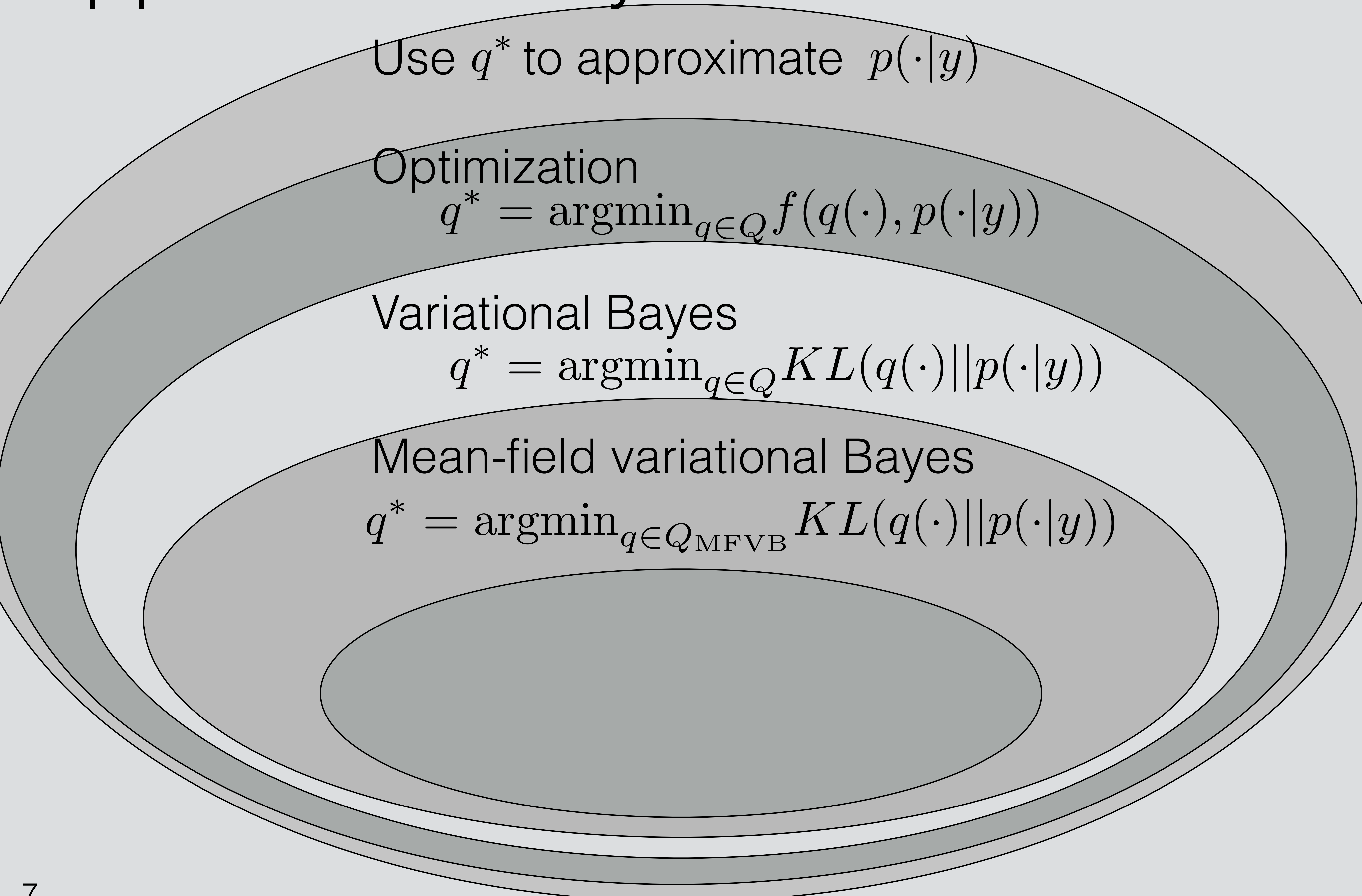

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  - Variational Bayes (VB)
  - Mean-field variational Bayes (MFVB)
- Why use VB?
- When can we trust VB?
- Where do we go from here?

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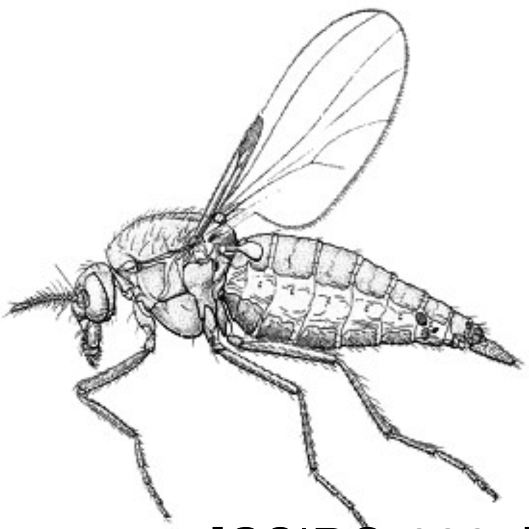
Midge wing length

- 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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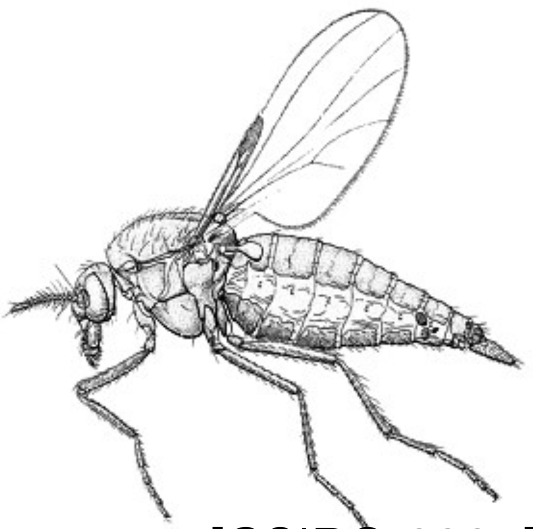
- Model:

$$p(y|\theta): \quad y_n \overset{iid}{\sim} \mathcal{N}(\mu, \sigma^2), \quad n = 1, \ldots, N$$



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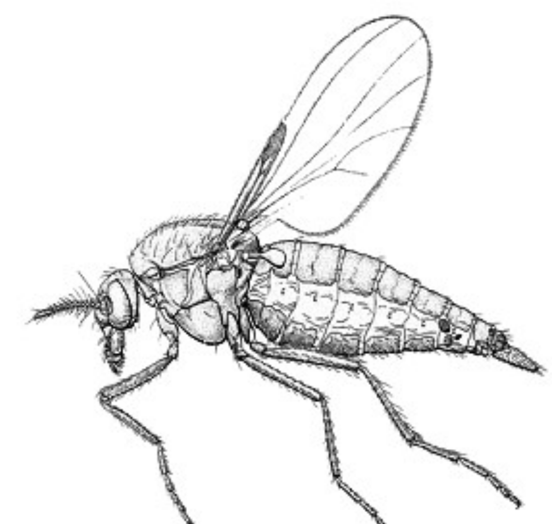

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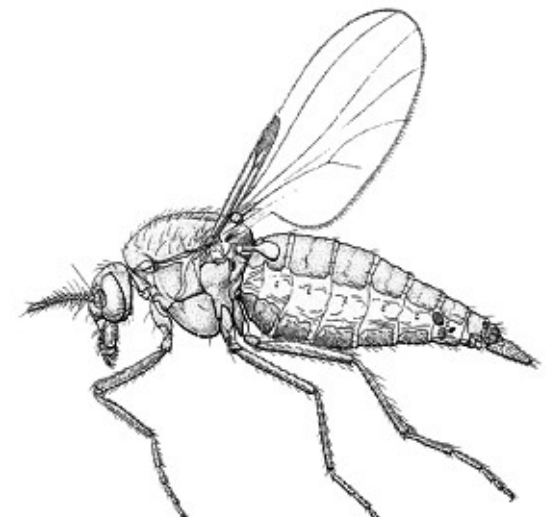

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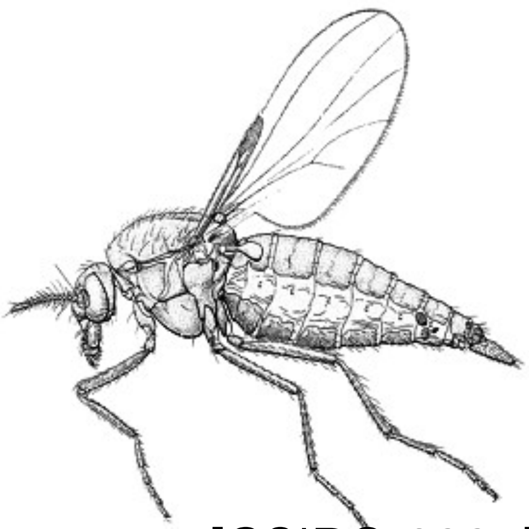

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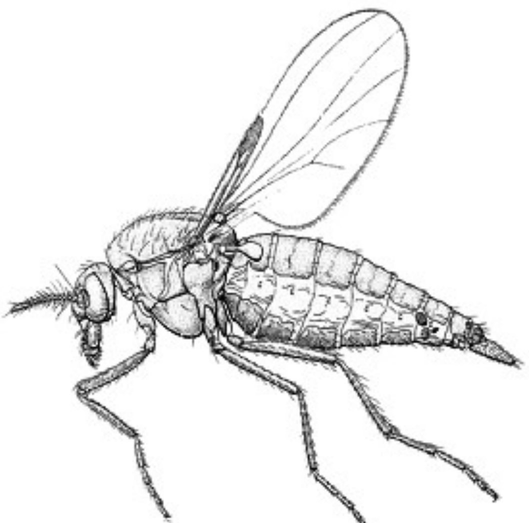

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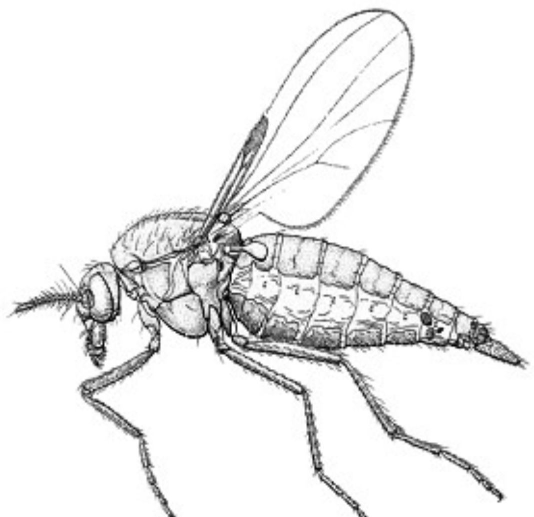

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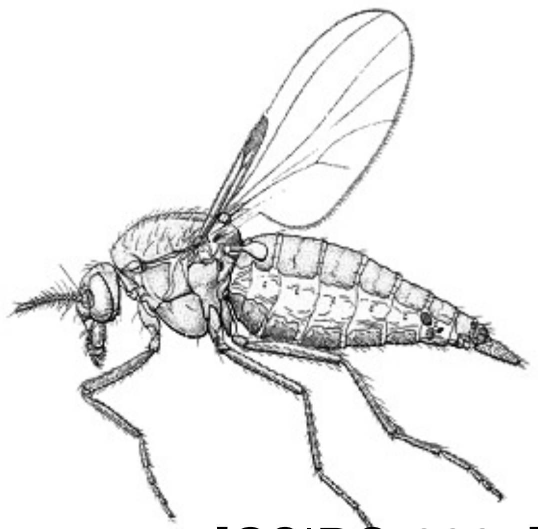

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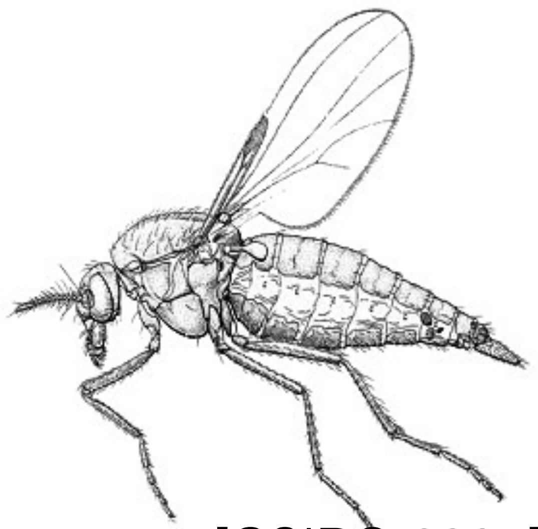

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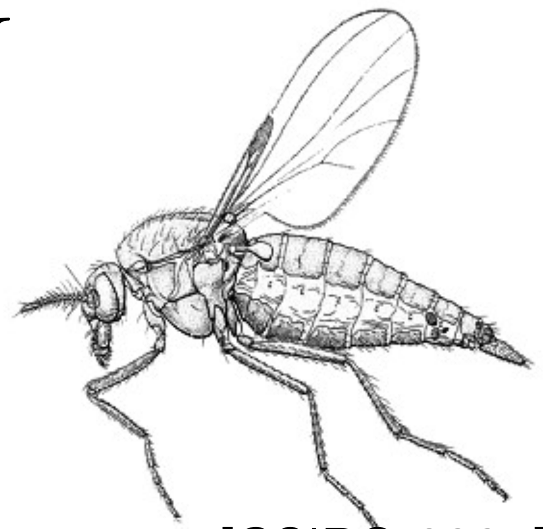

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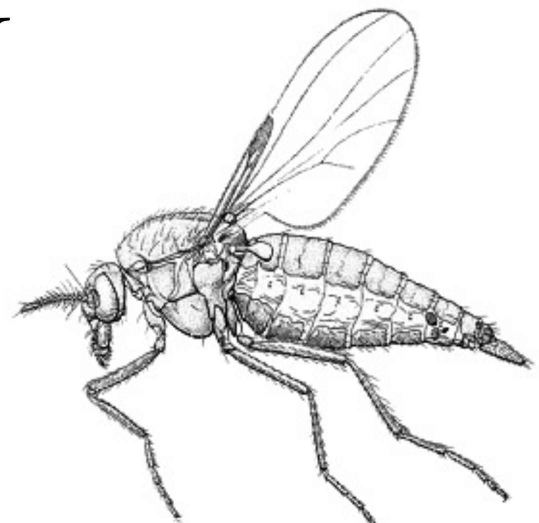

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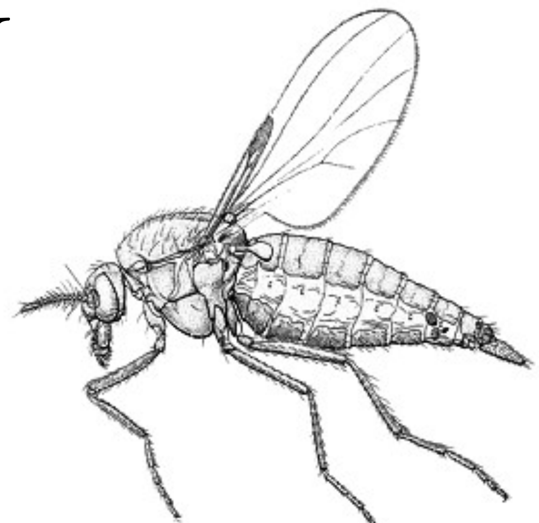

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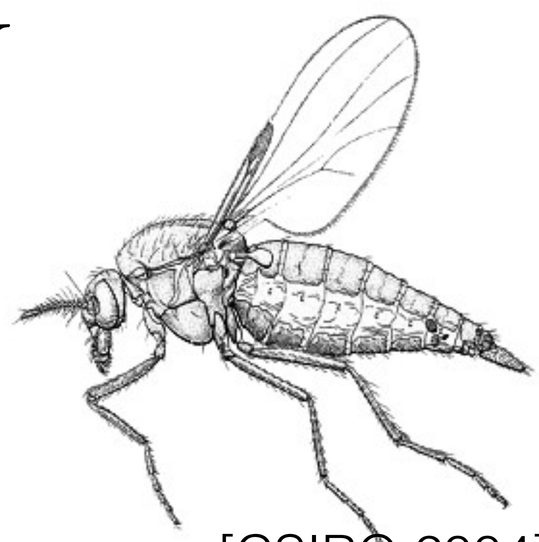

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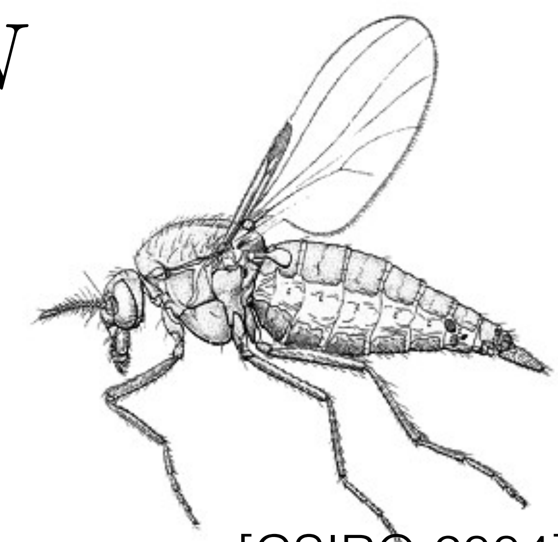

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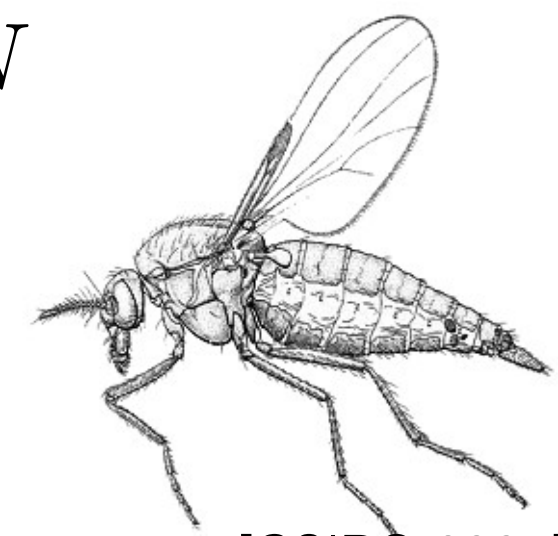

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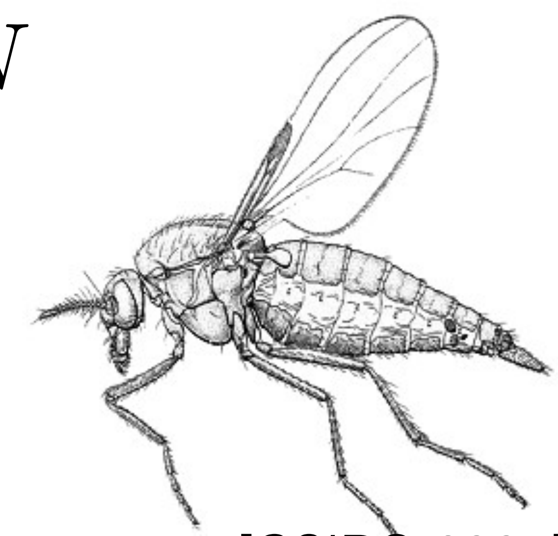

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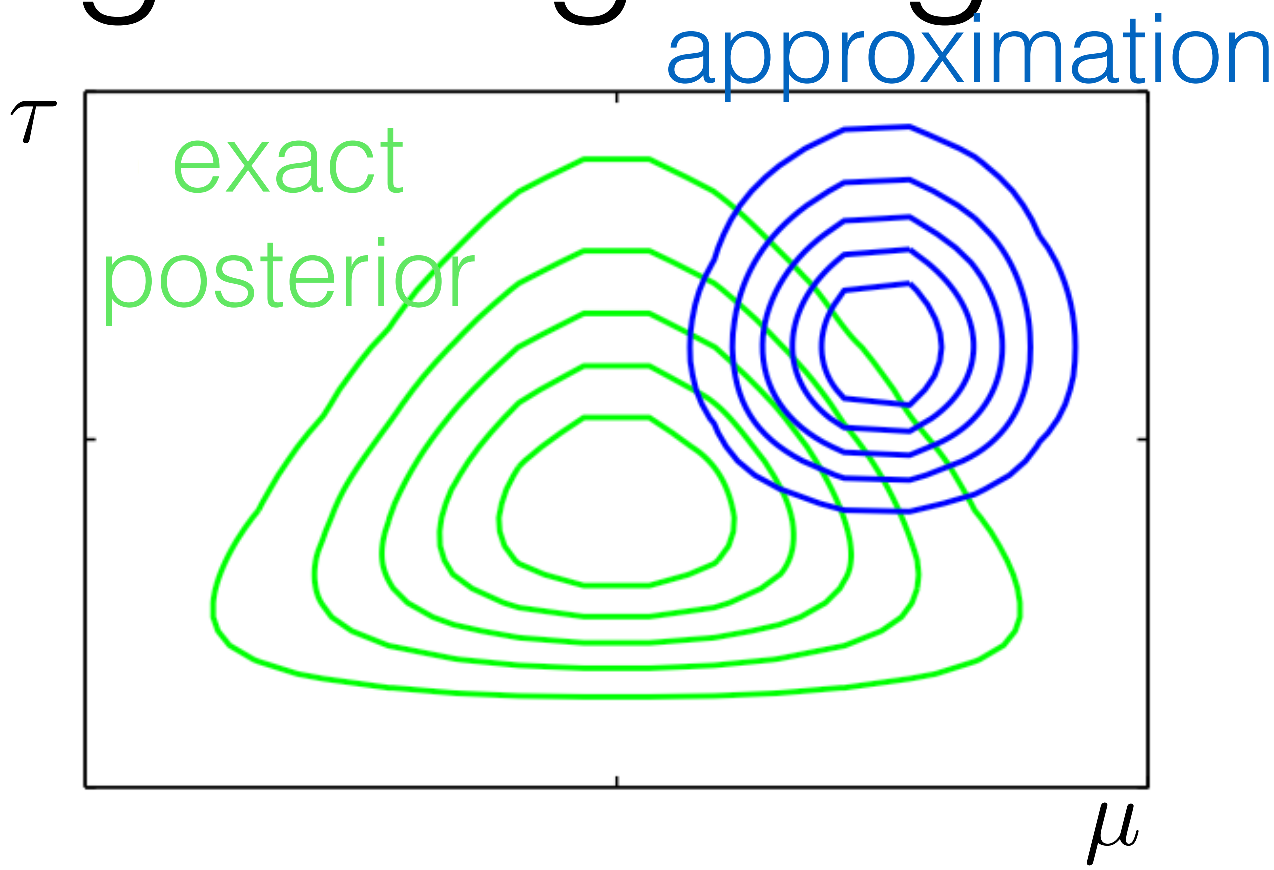

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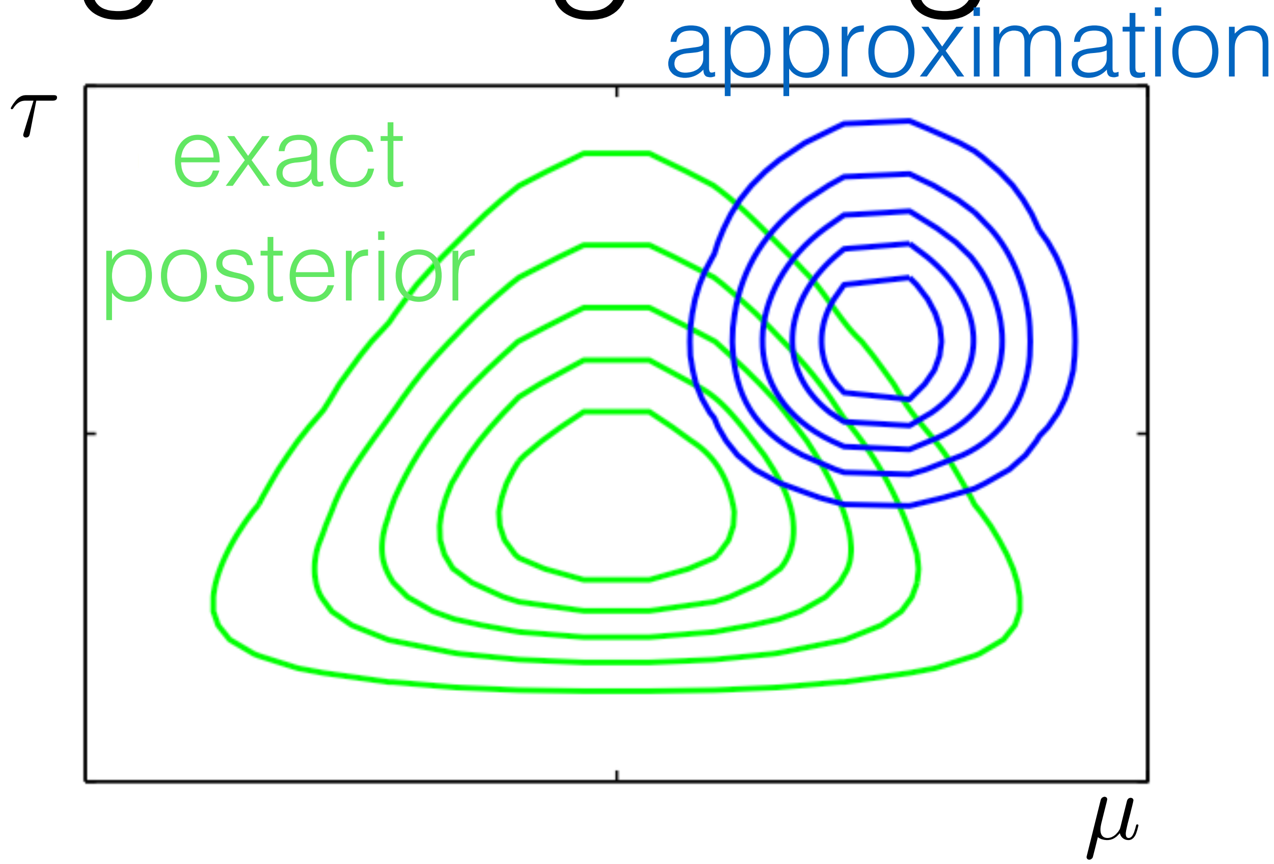

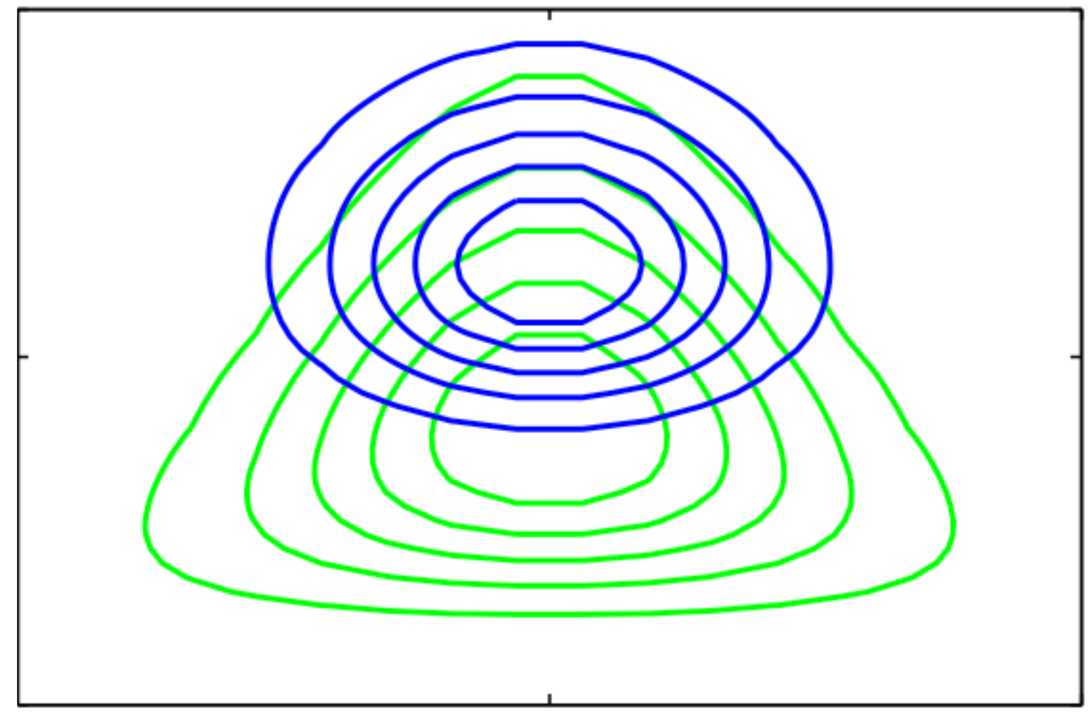

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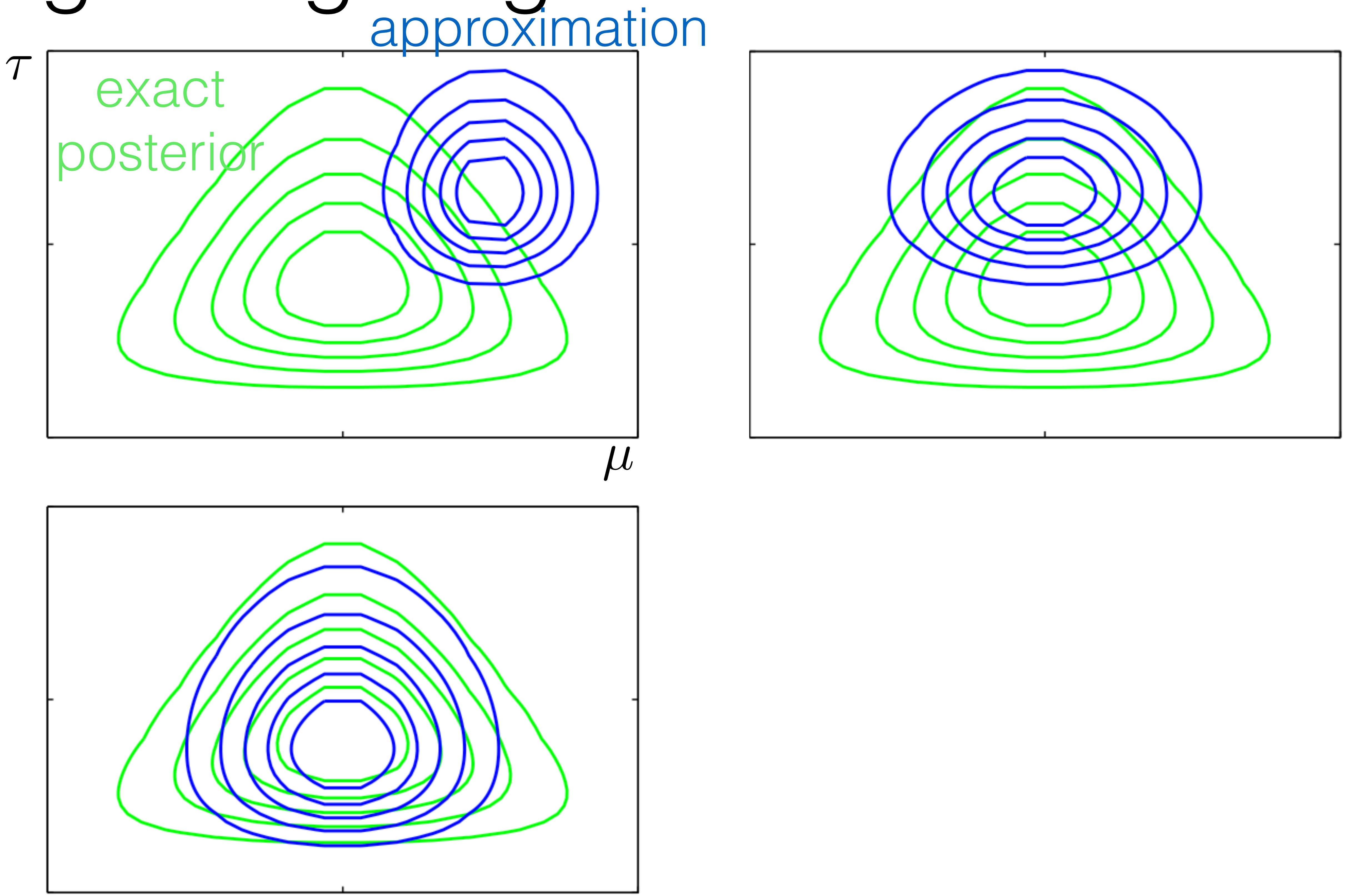

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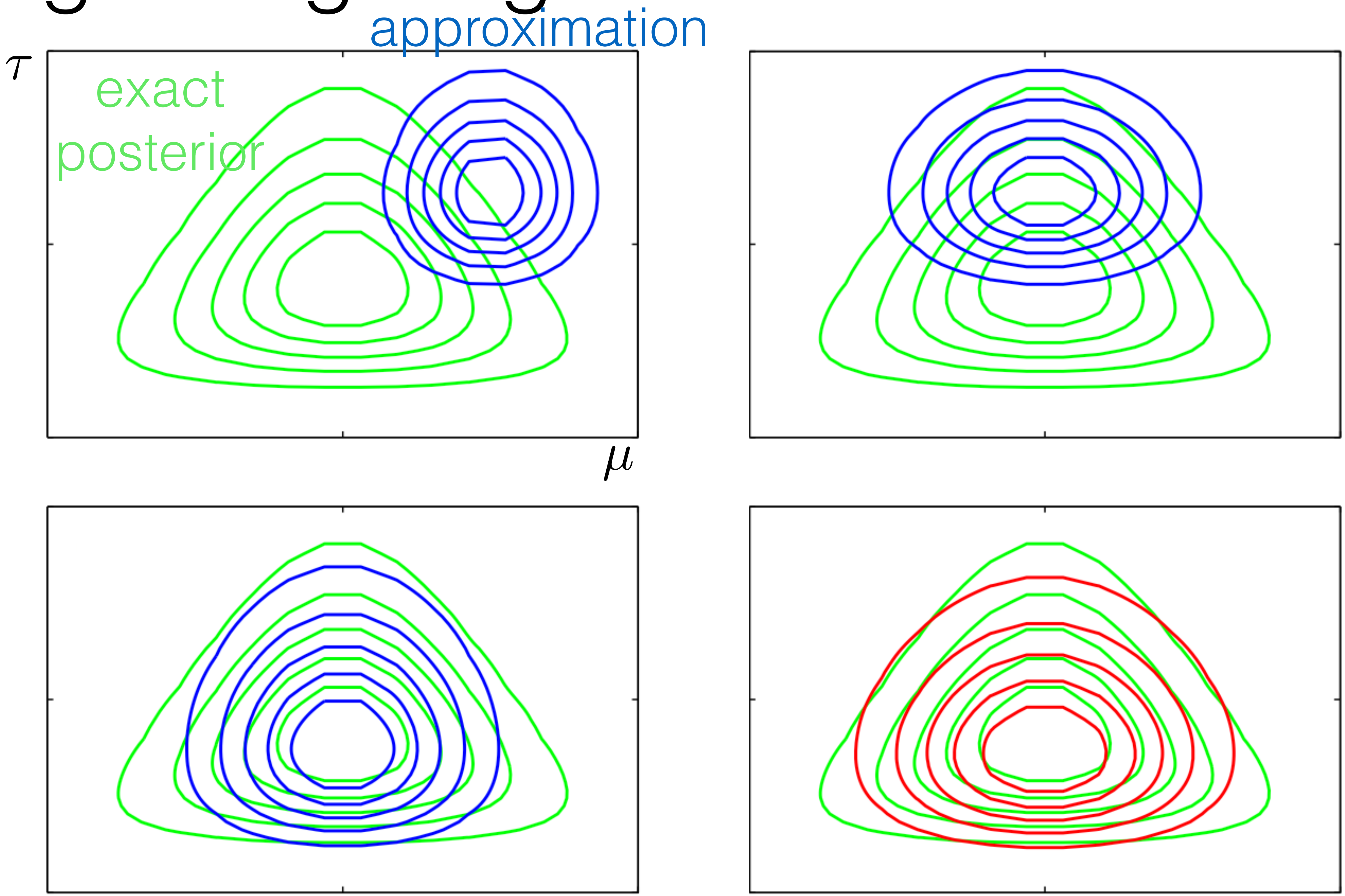

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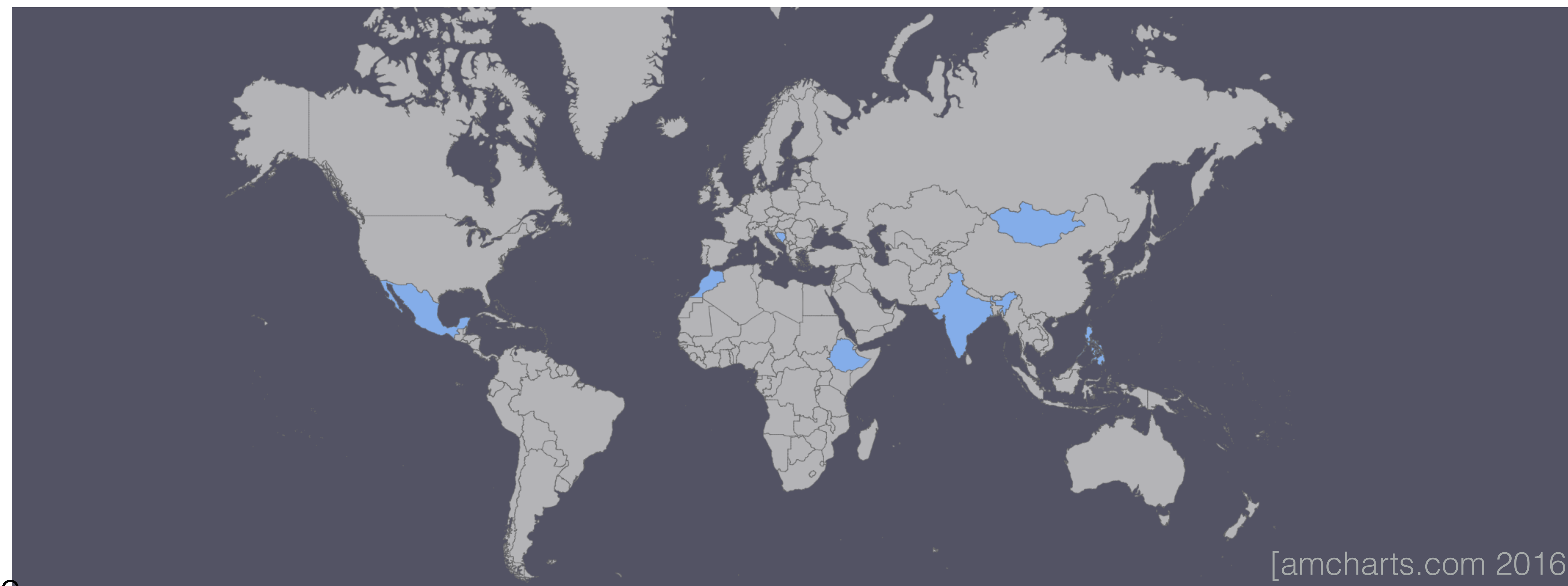
Microcredit Experiment



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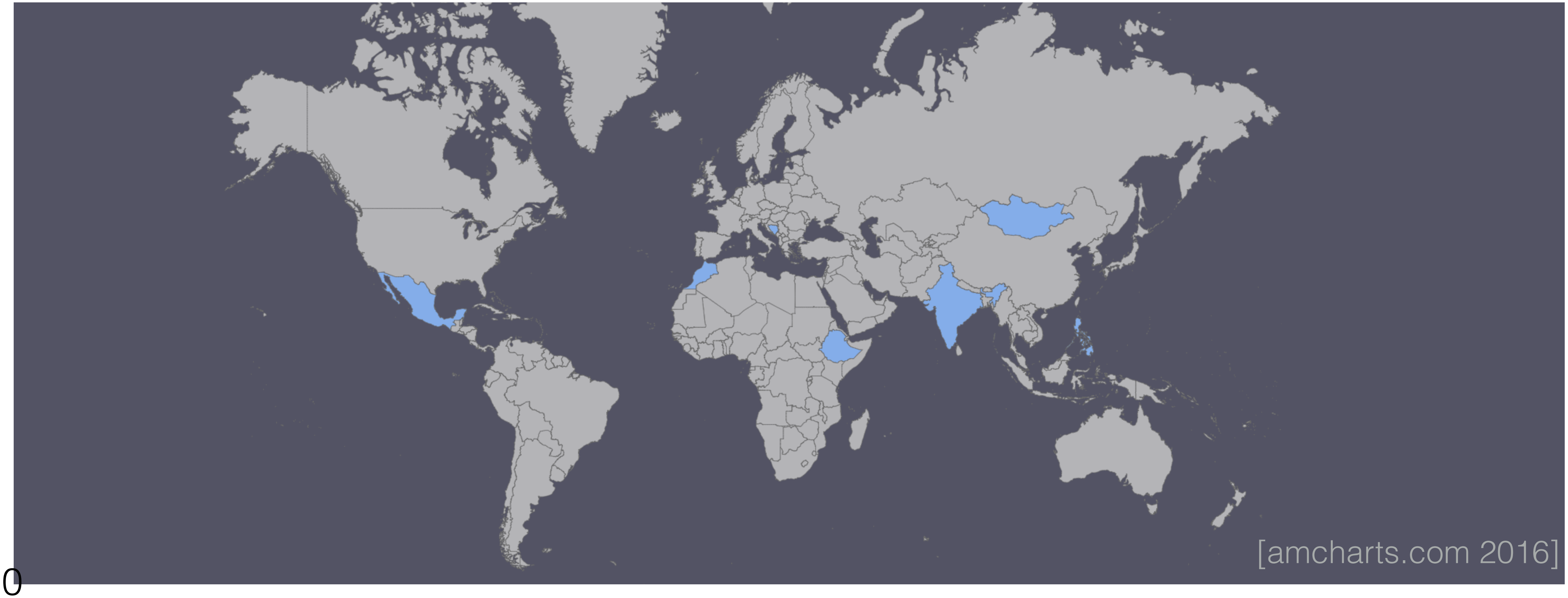

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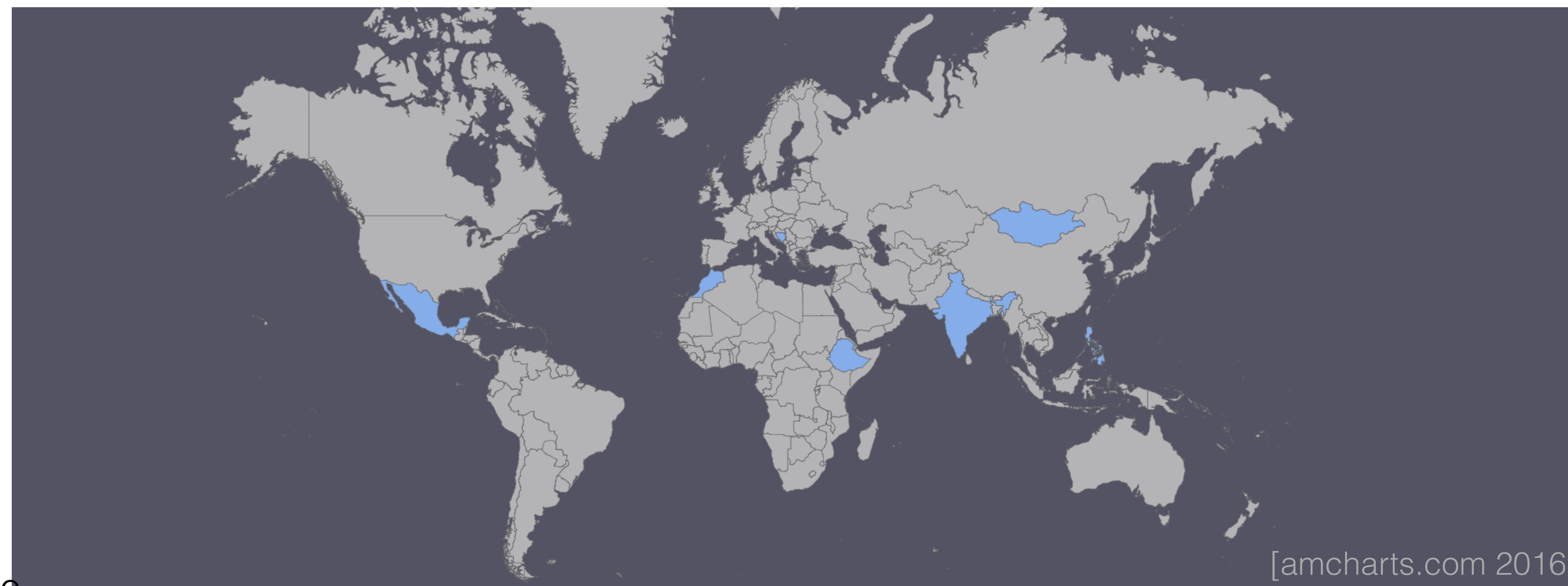

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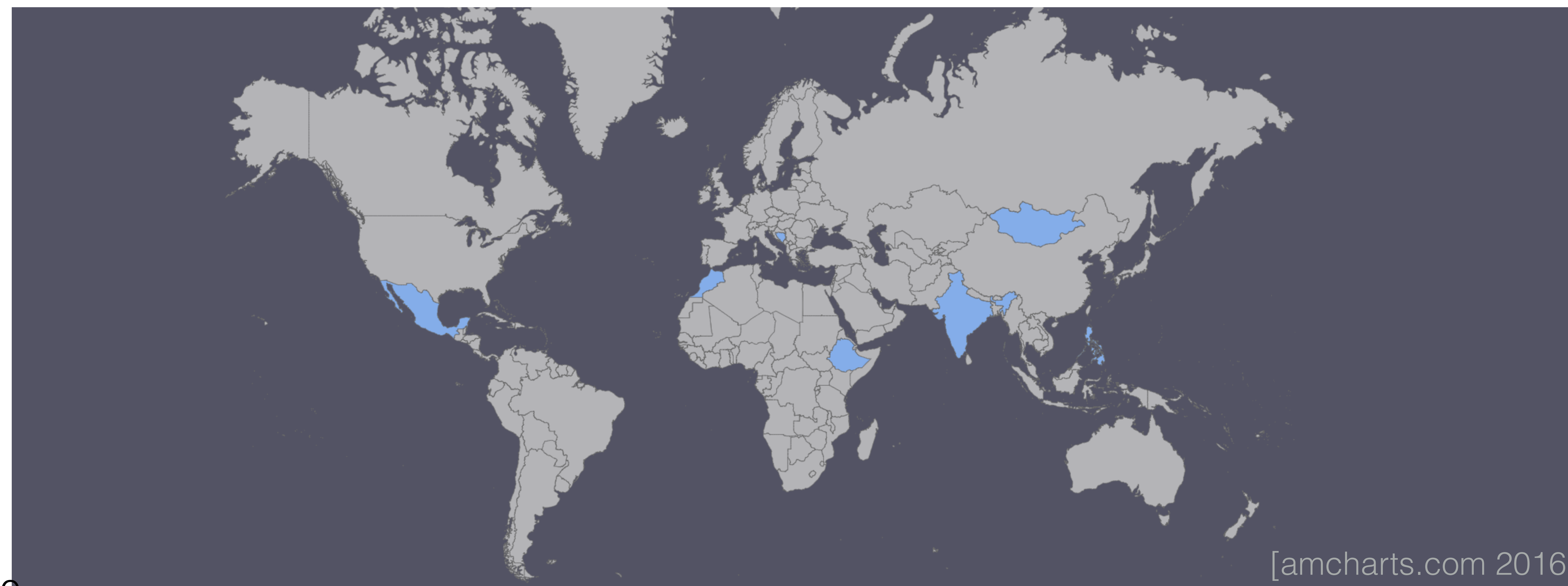

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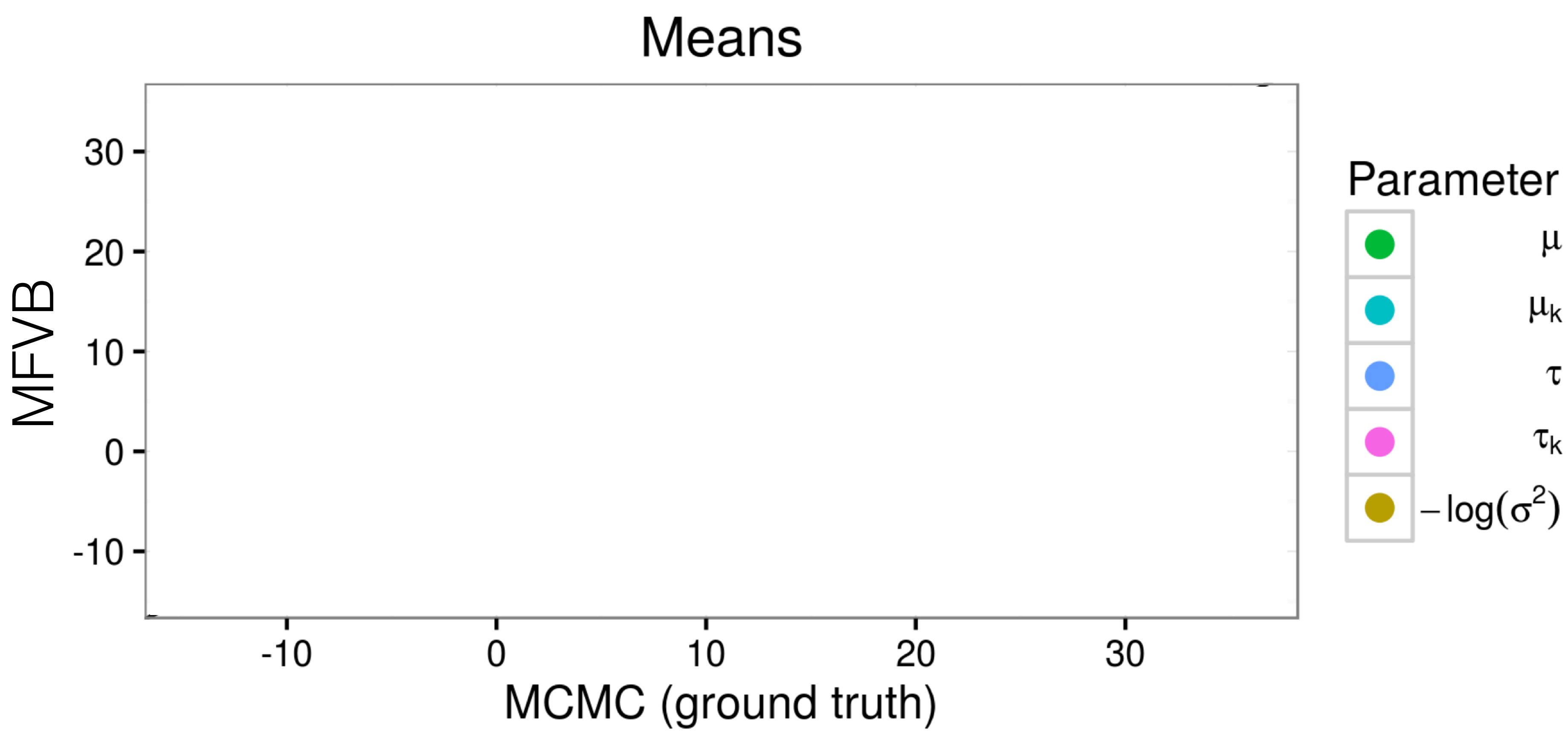
Microcredit

MFVB: Do we need to check the output?

Microcredit

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

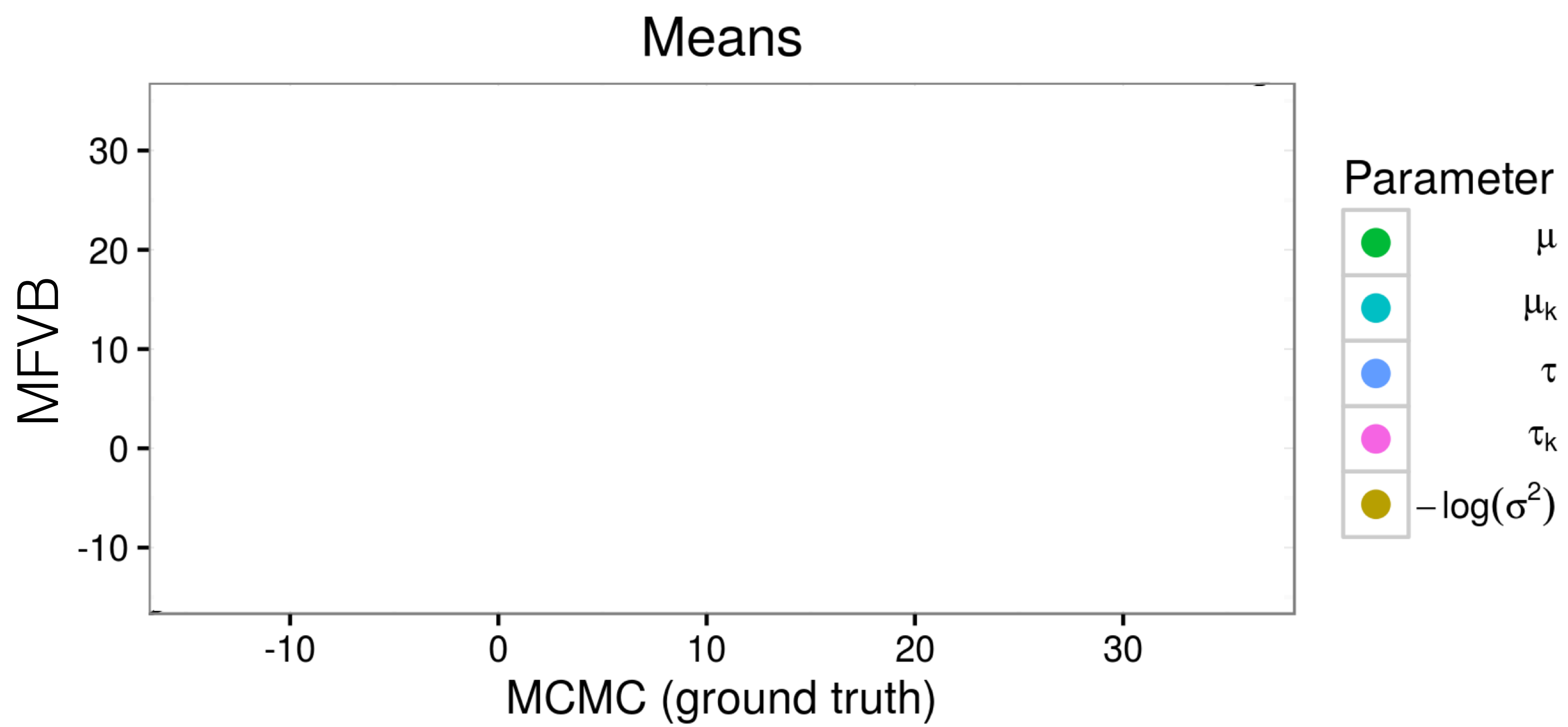
Microcredit



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

Microcredit

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



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Microcredit

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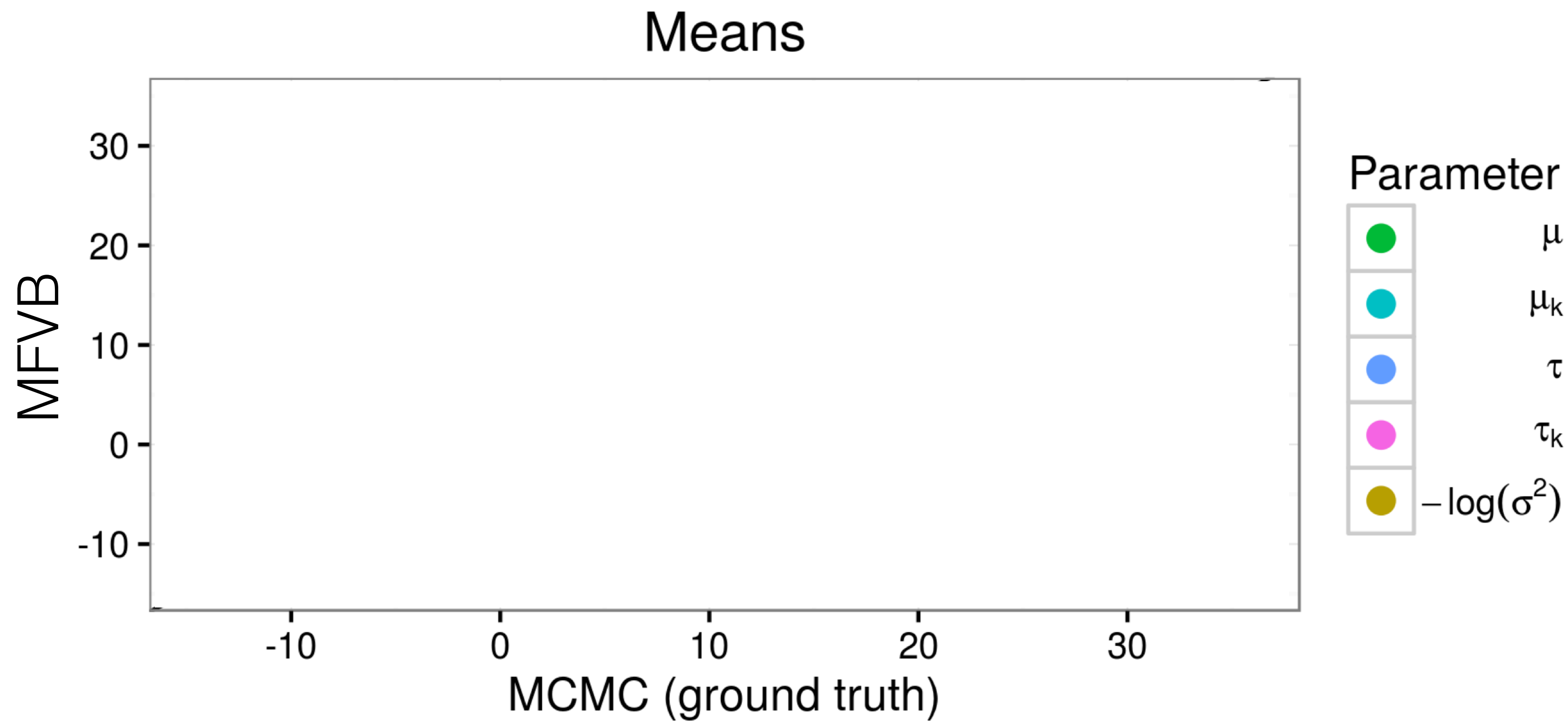

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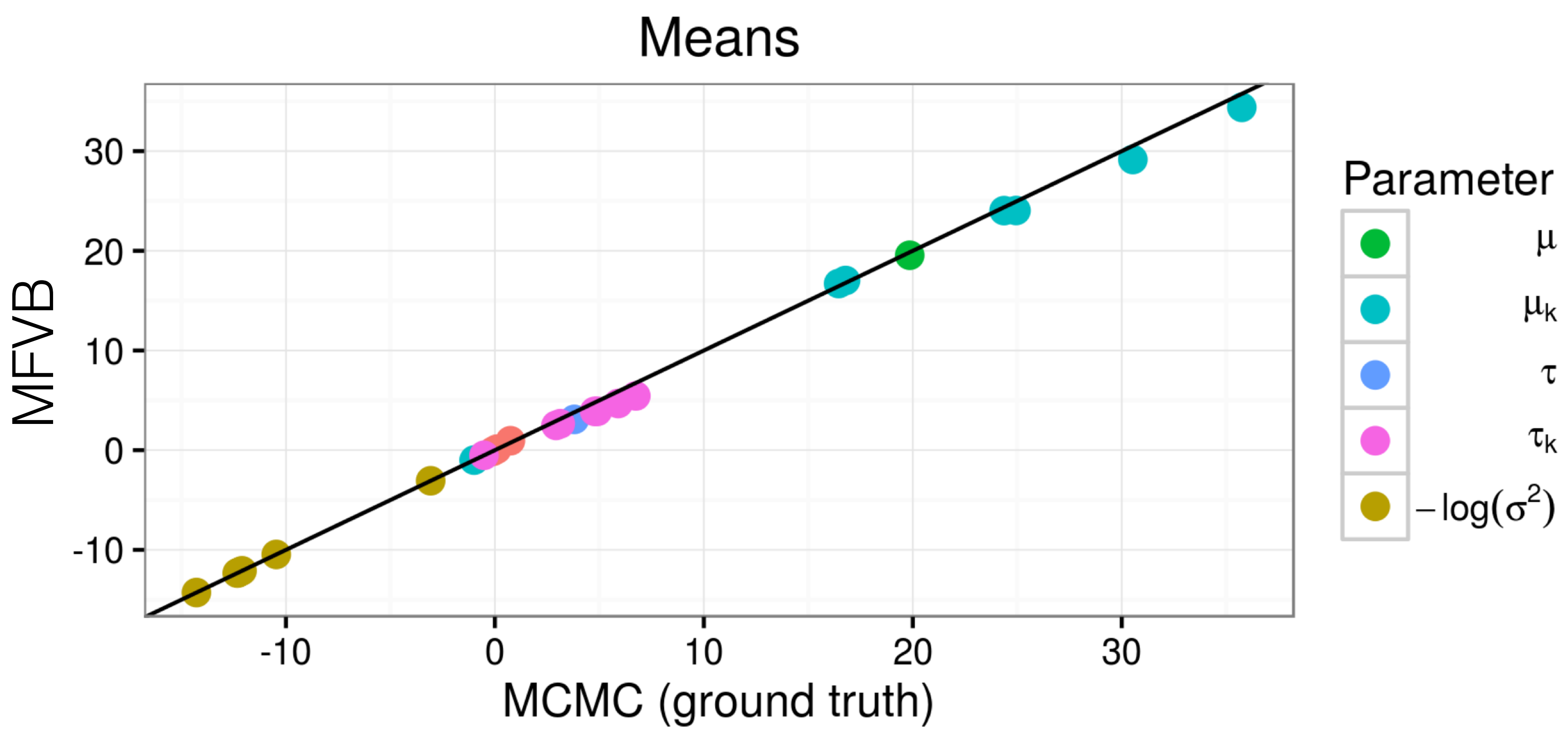

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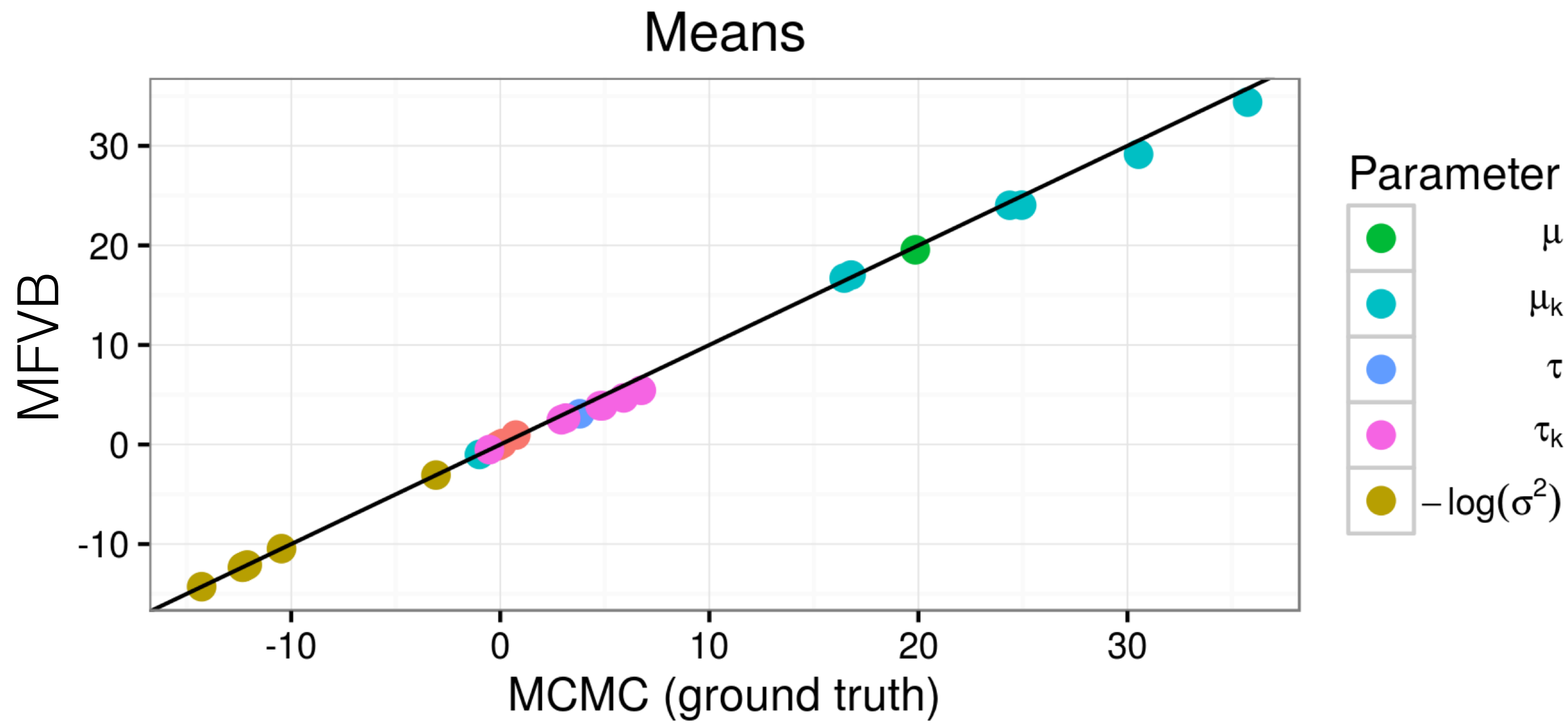

Criteo Online Ads Experiment

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

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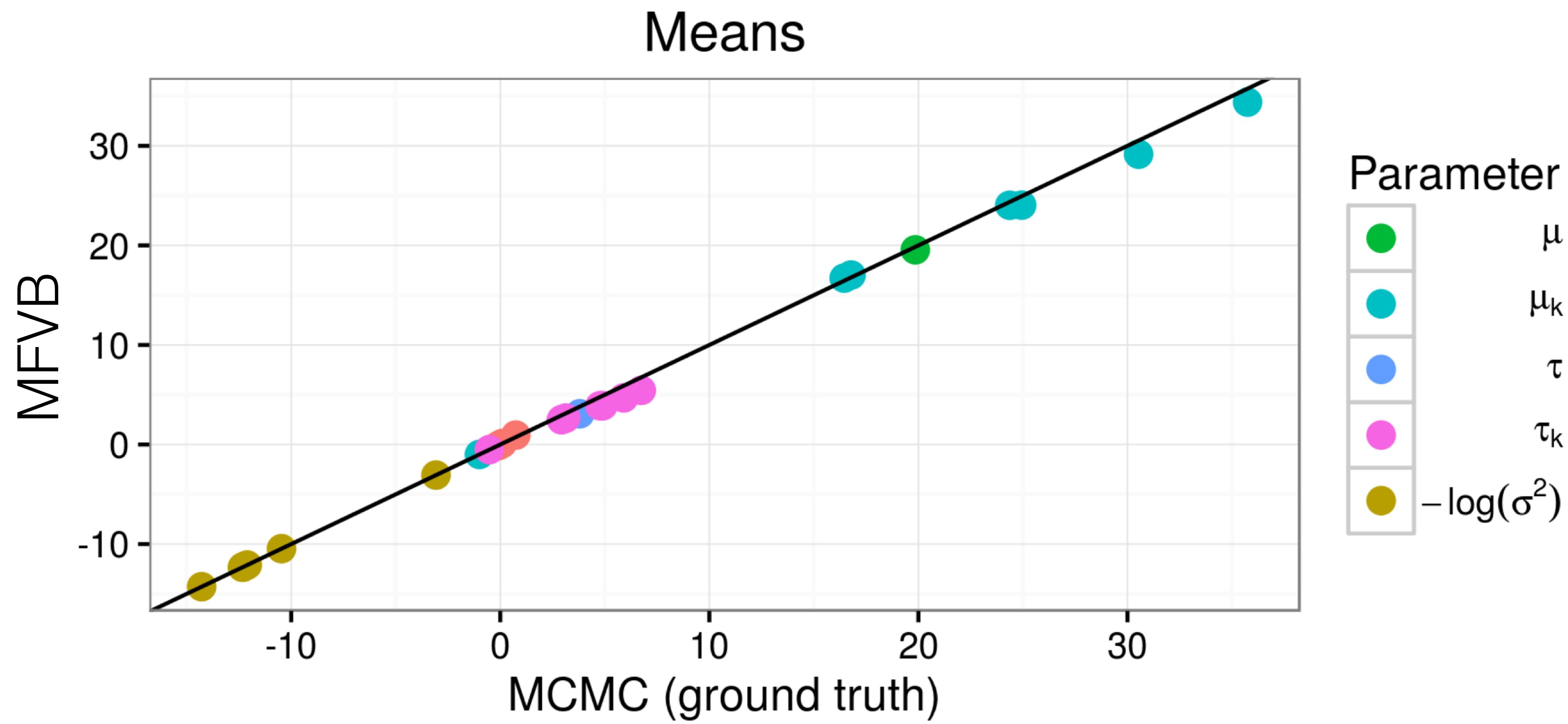

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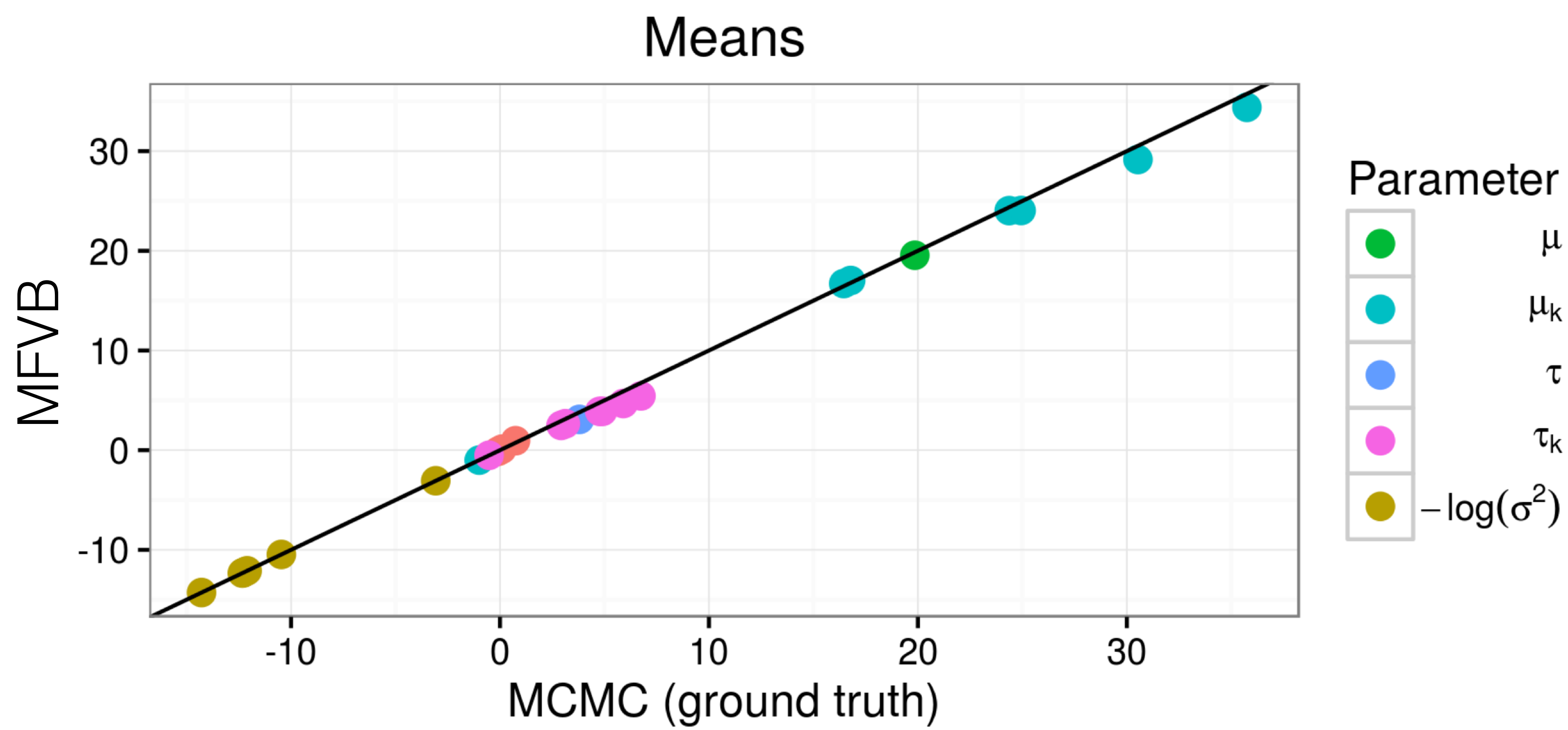

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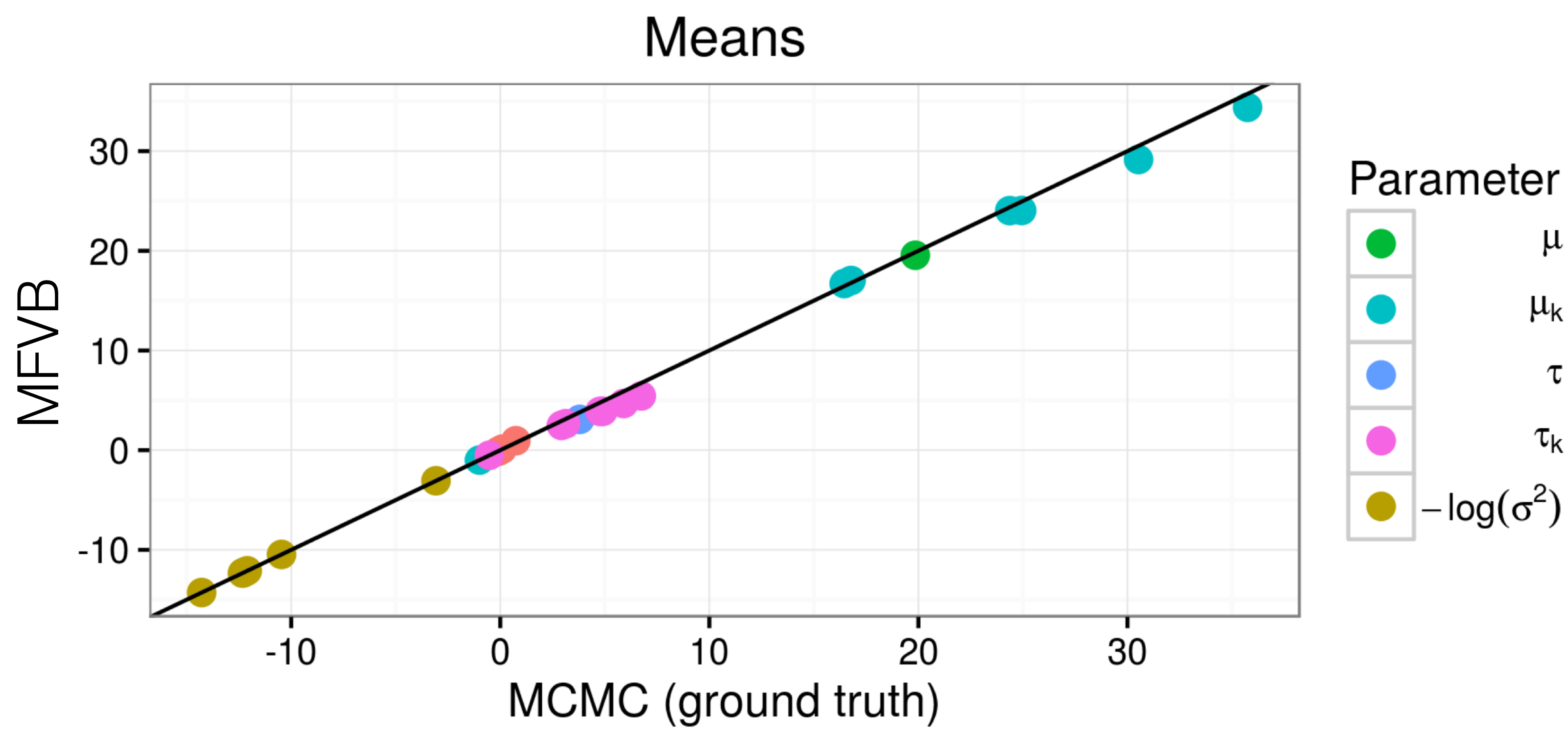

Criteo Online Ads Experiment

- Click-through conversion prediction
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- Q: How predictive of conversion are different features?
- 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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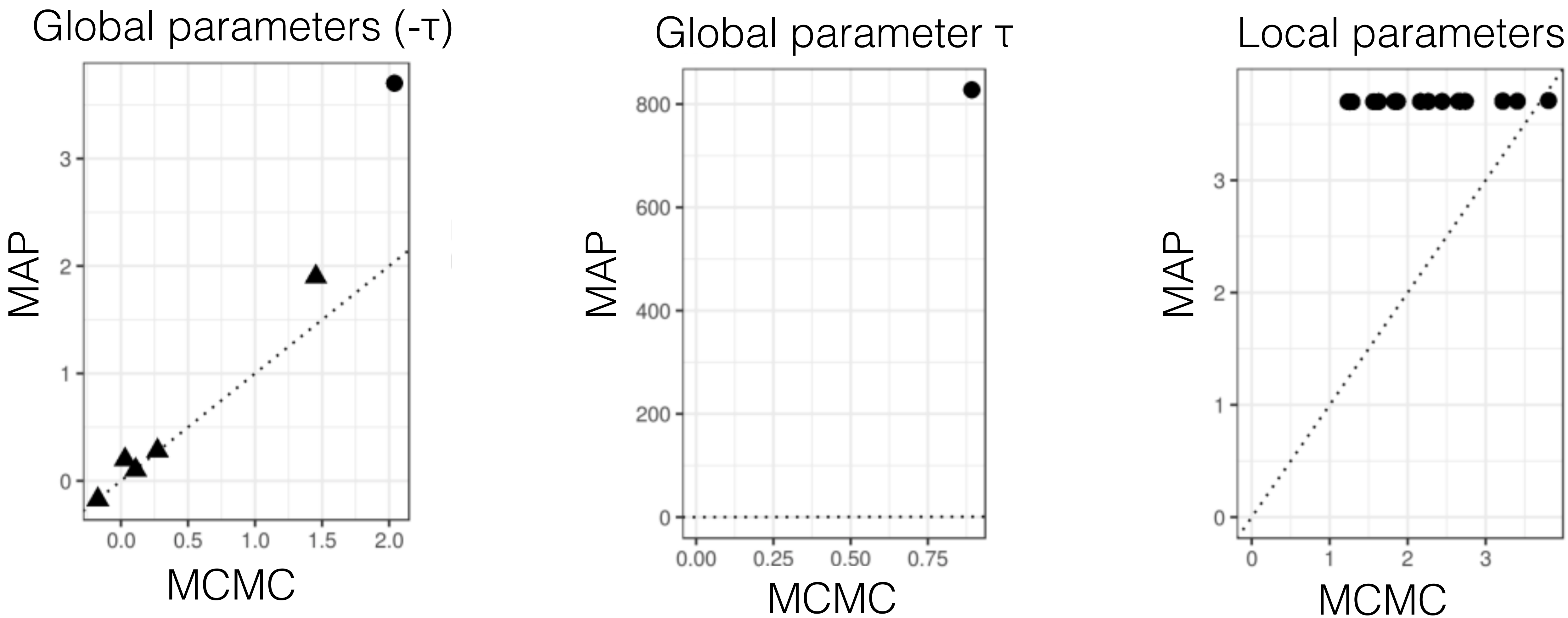

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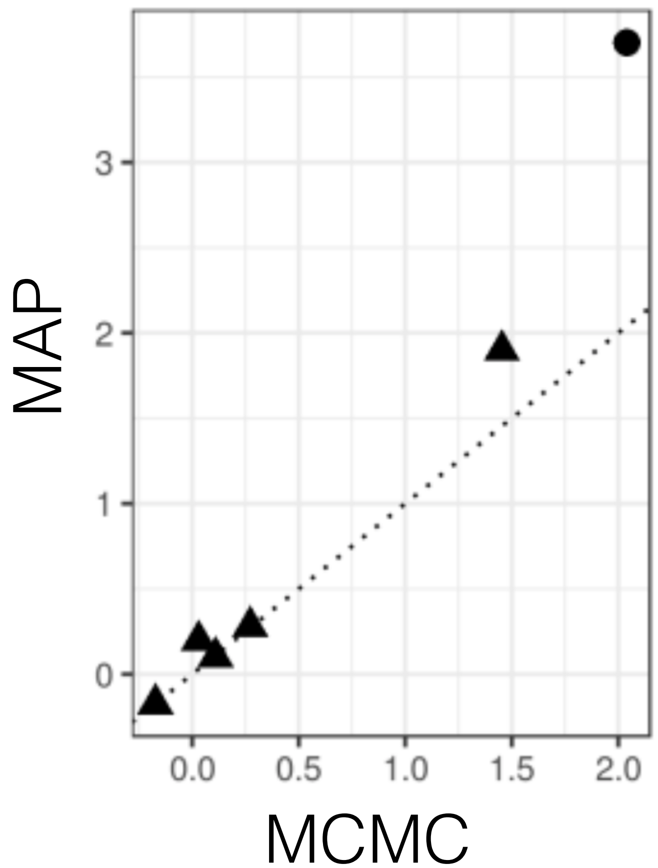
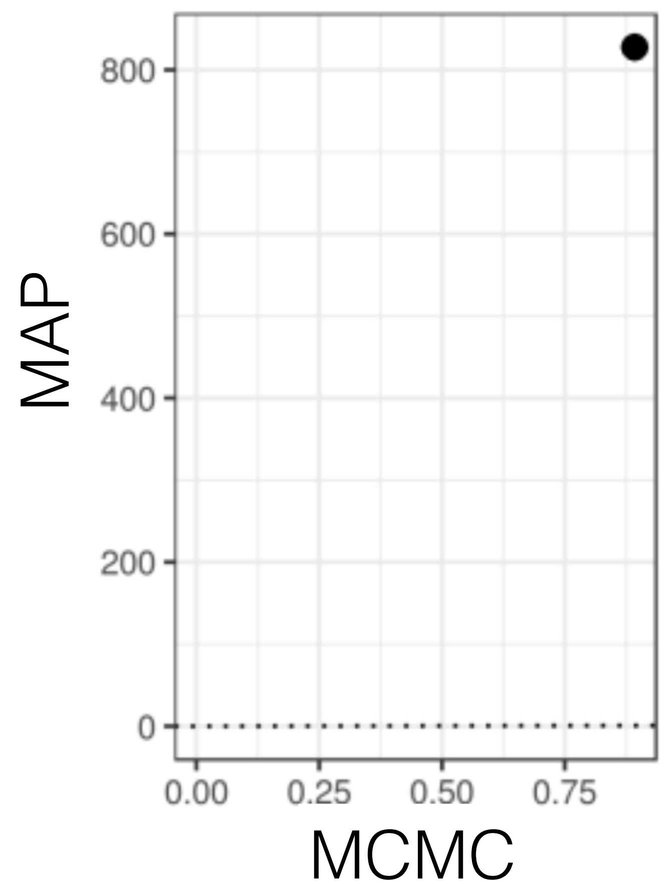
Criteo Online Ads Experiment

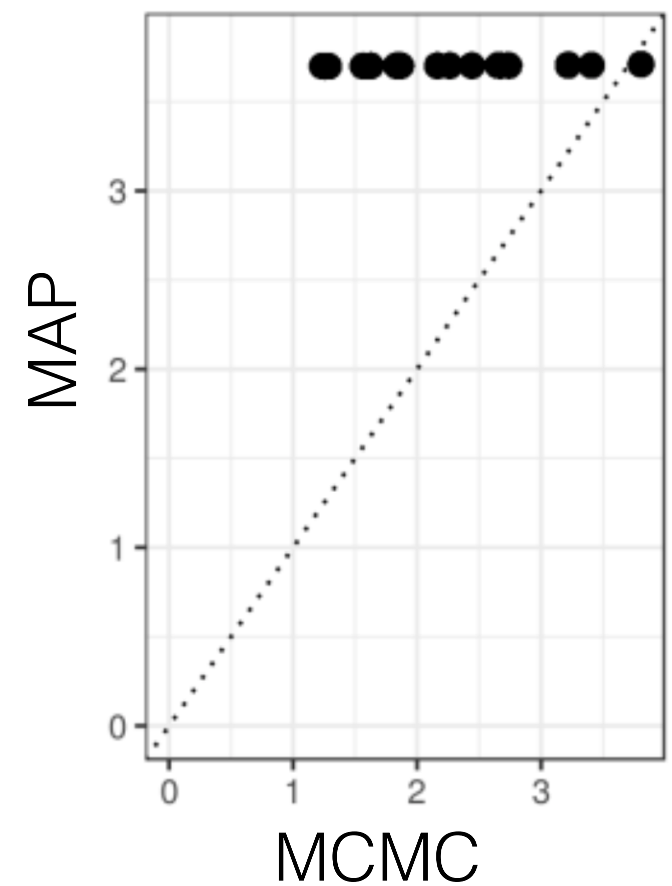
Global parameters (-τ)



Global parameter τ



Local parameters



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

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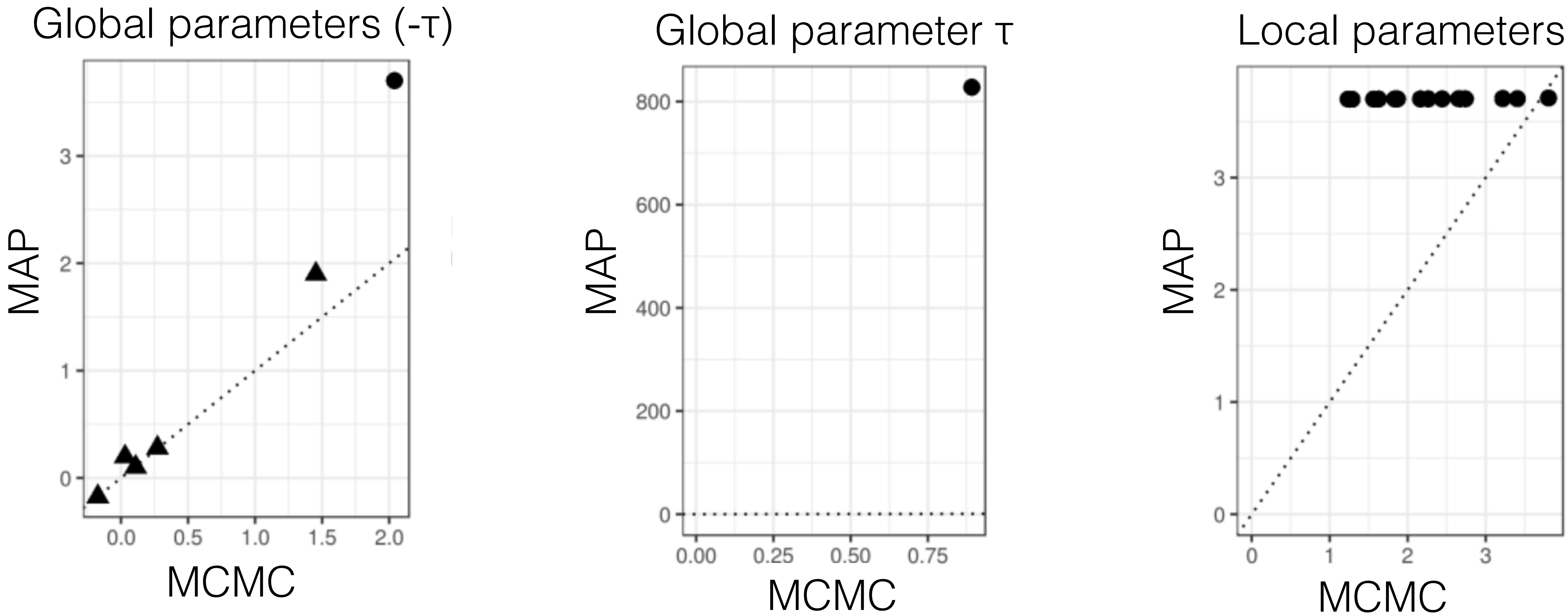

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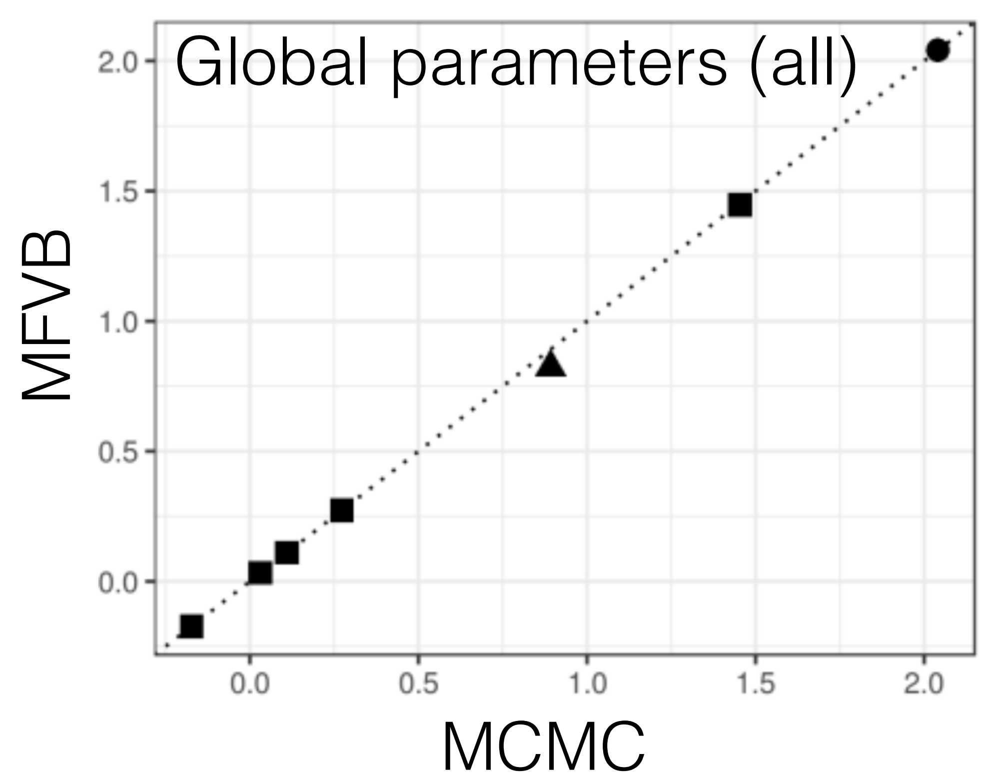

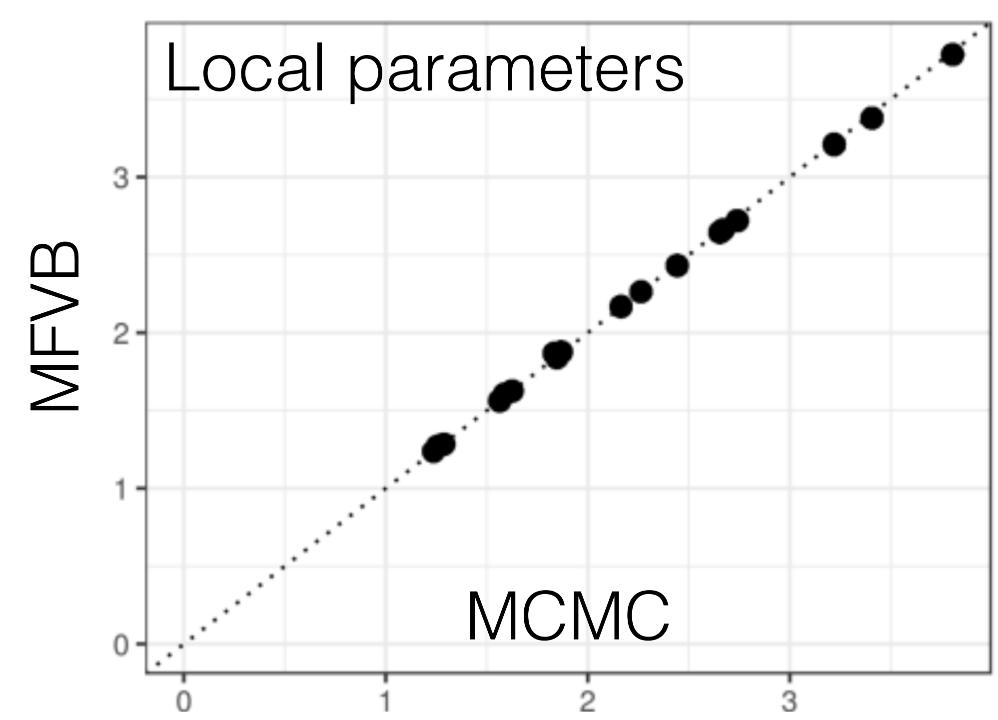

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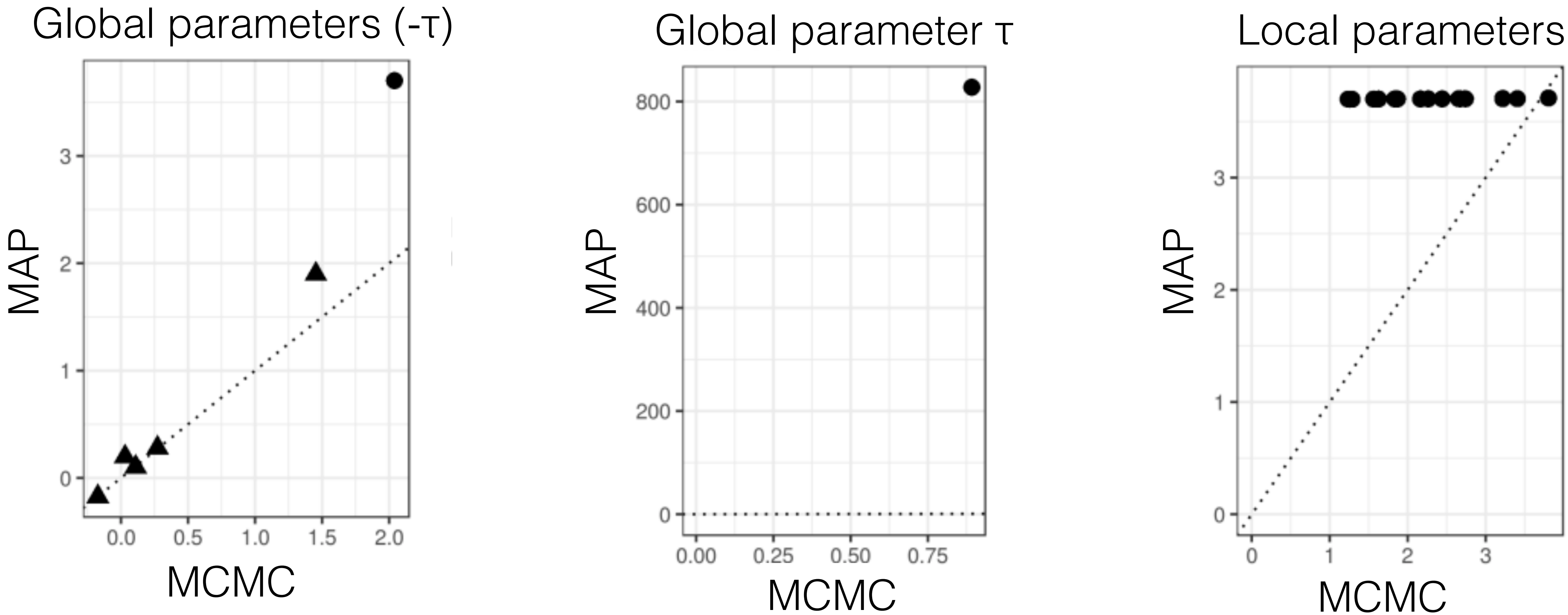
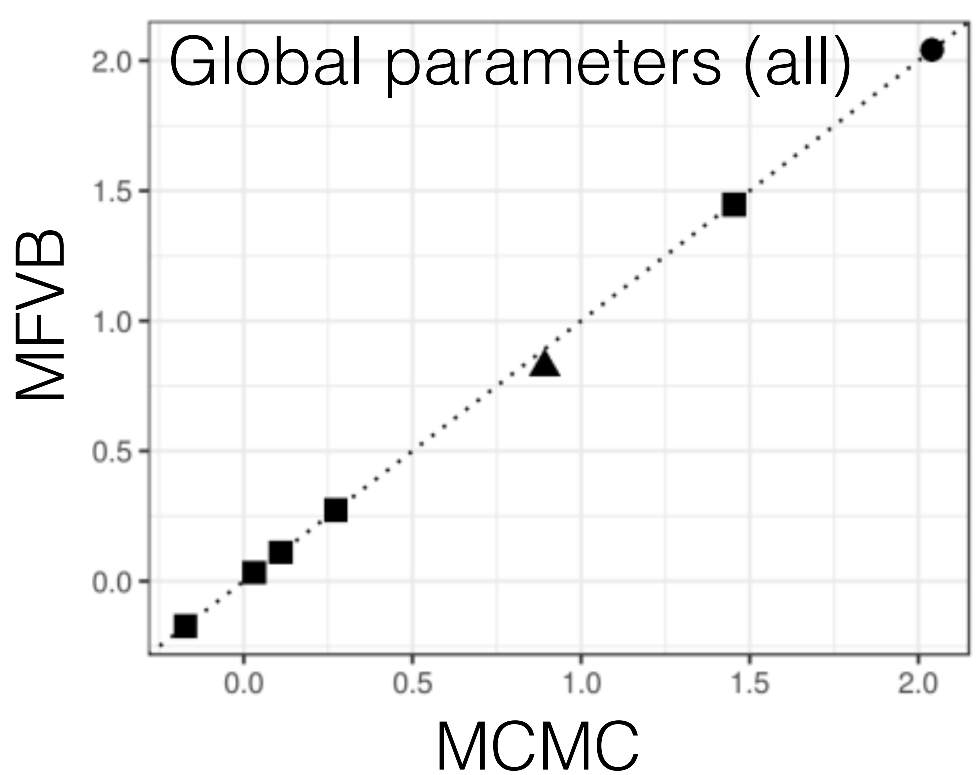
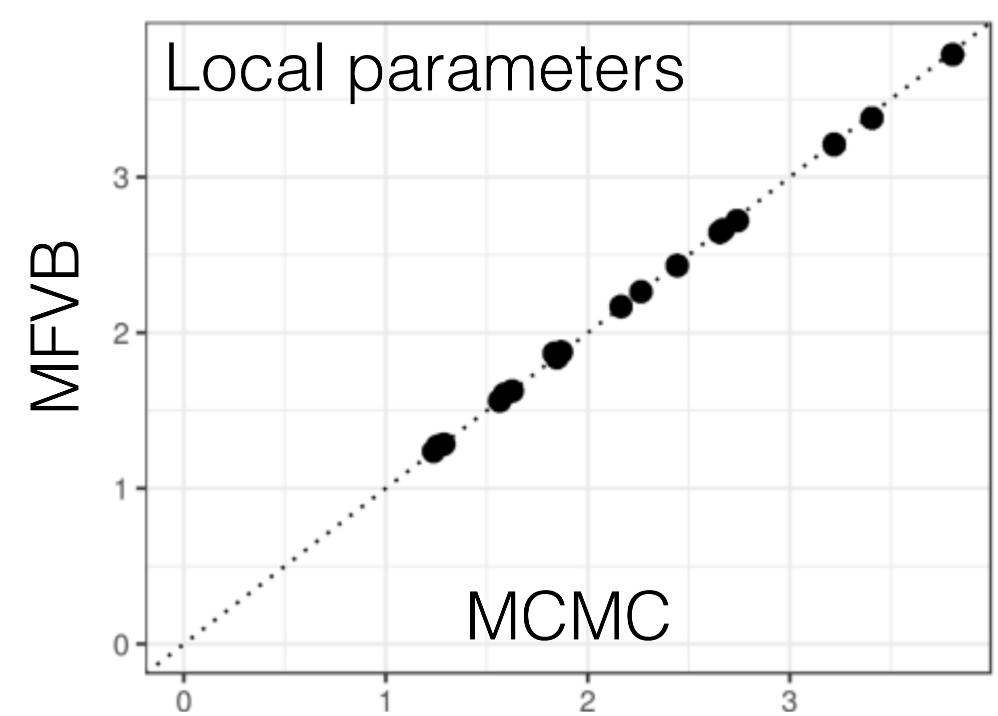


- MAP: **12 s**
- MFVB: **57 s**
- MCMC (5K samples): 21,066 s (**5.85 h**)





[Giordano, Broderick, Jordan 2018]

Why use MFVB?

- Topic discovery

"Arts"	"Budgets"	"Children"	"Education"
NEW	MILLION	CHILDREN	SCHOOL
FILM	TAX	WOMEN	STUDENTS
SHOW	PROGRAM	PEOPLE	SCHOOLS
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MOVIE	BILLION	YEARS	TEACHERS
PLAY	FEDERAL	FAMILIES	HIGH
MUSICAL	YEAR	WORK	PUBLIC
BEST	SPENDING	PARENTS	TEACHER
ACTOR	NEW	SAYS	BENNETT
FIRST	STATE	FAMILY	MANIGAT
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Roadmap

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

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What about uncertainty?

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

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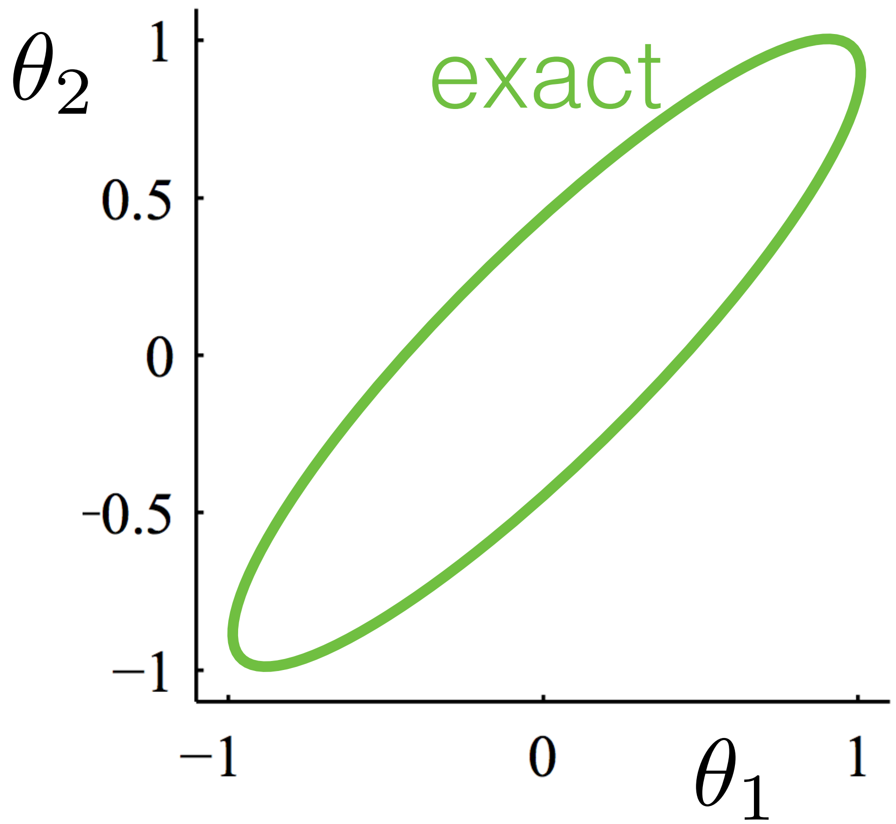

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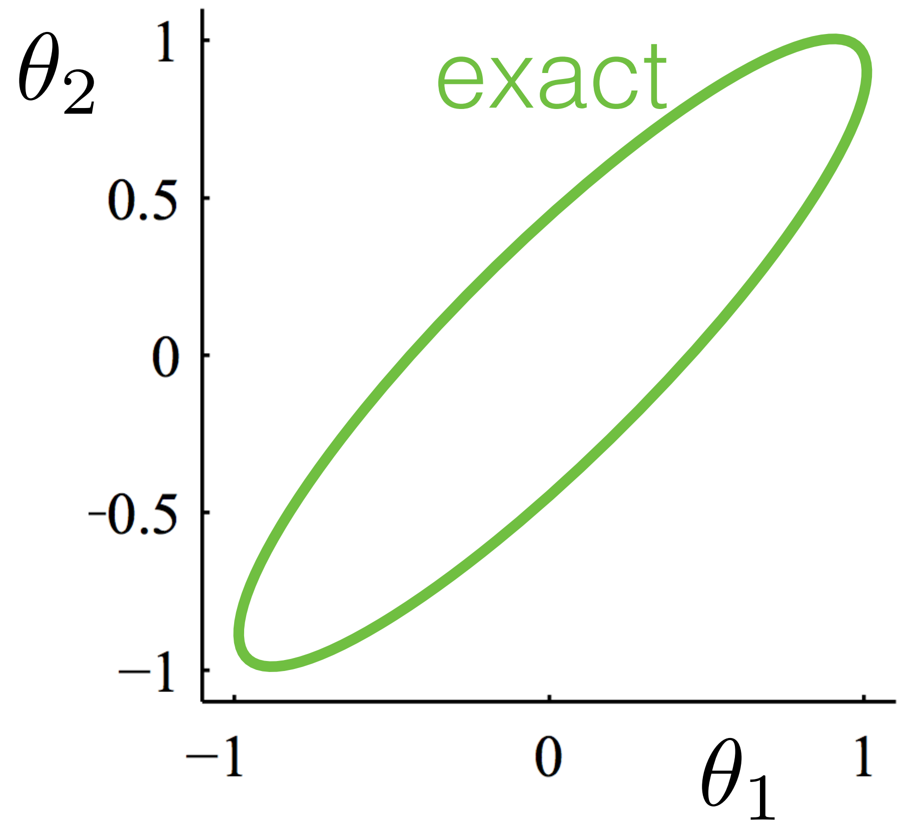

- Conjugate linear regression

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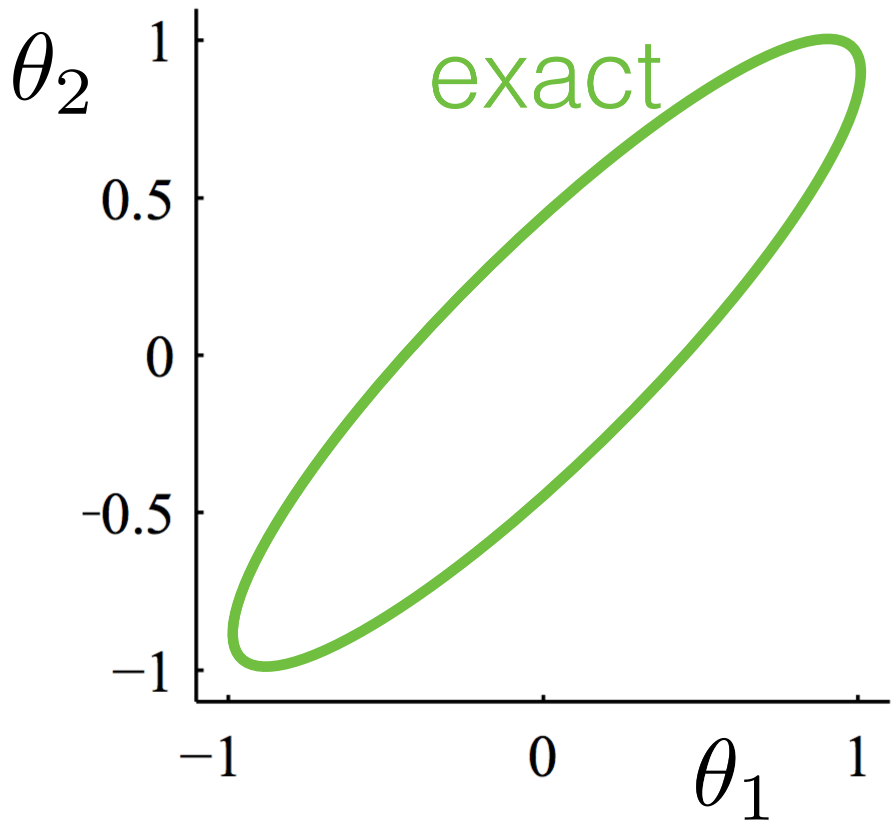

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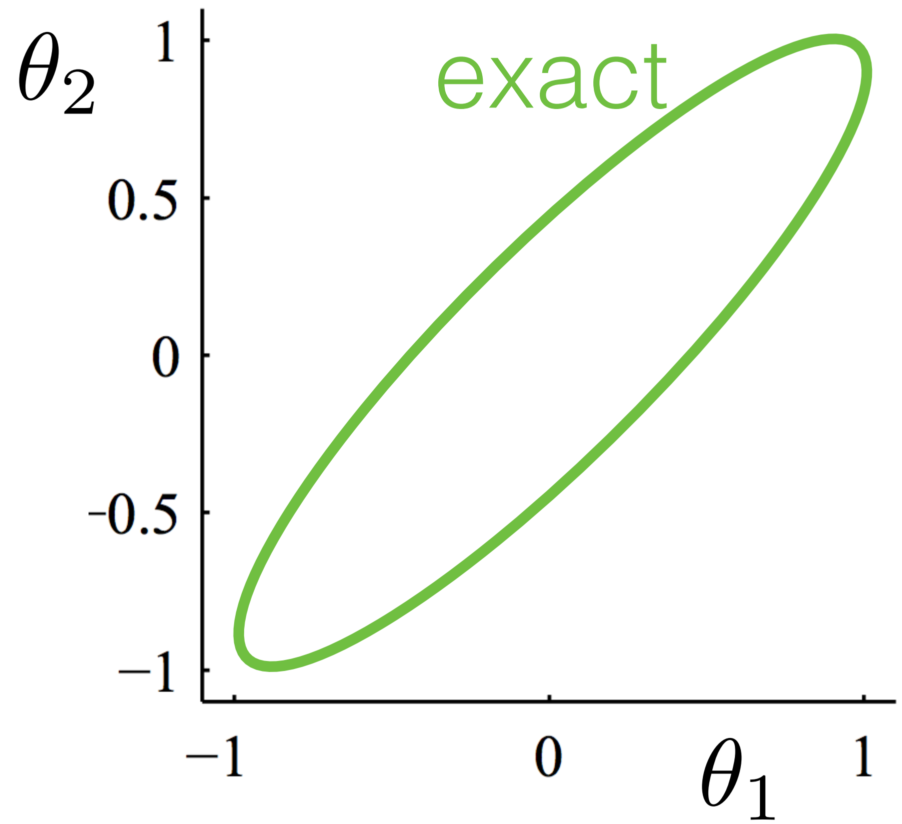

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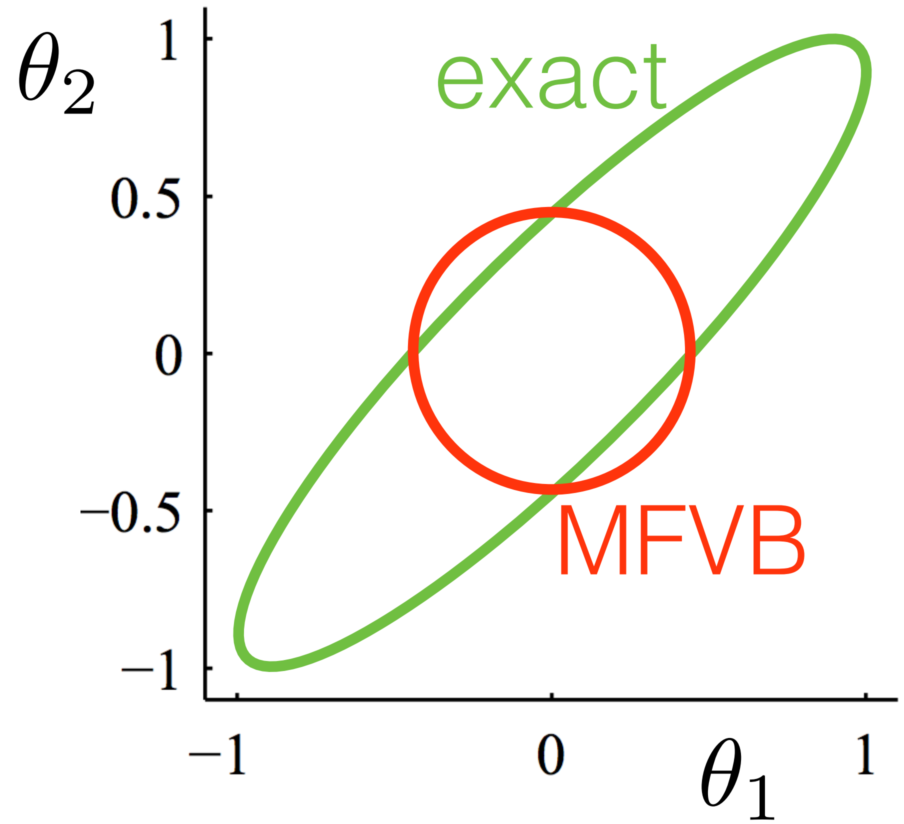

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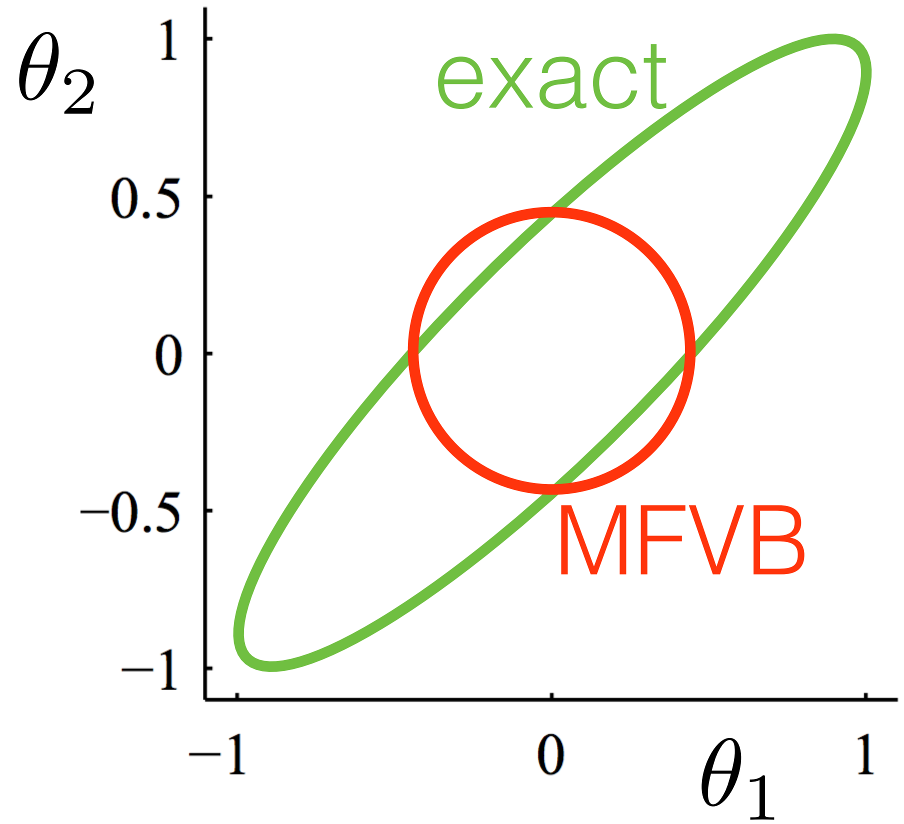

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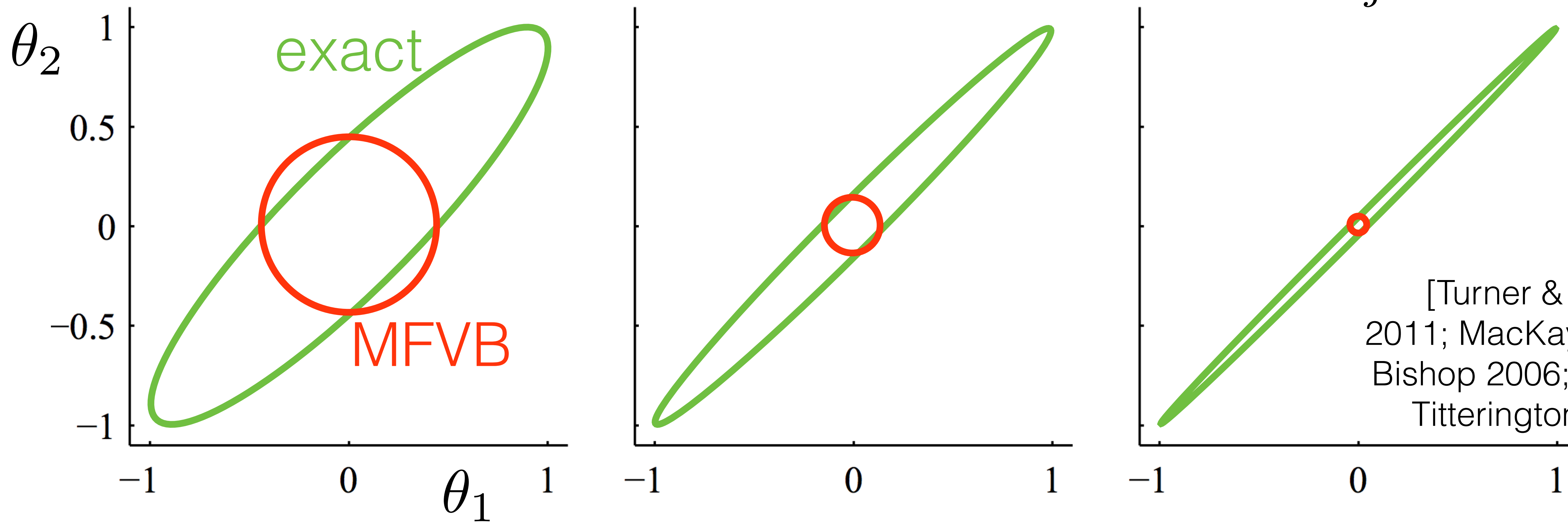

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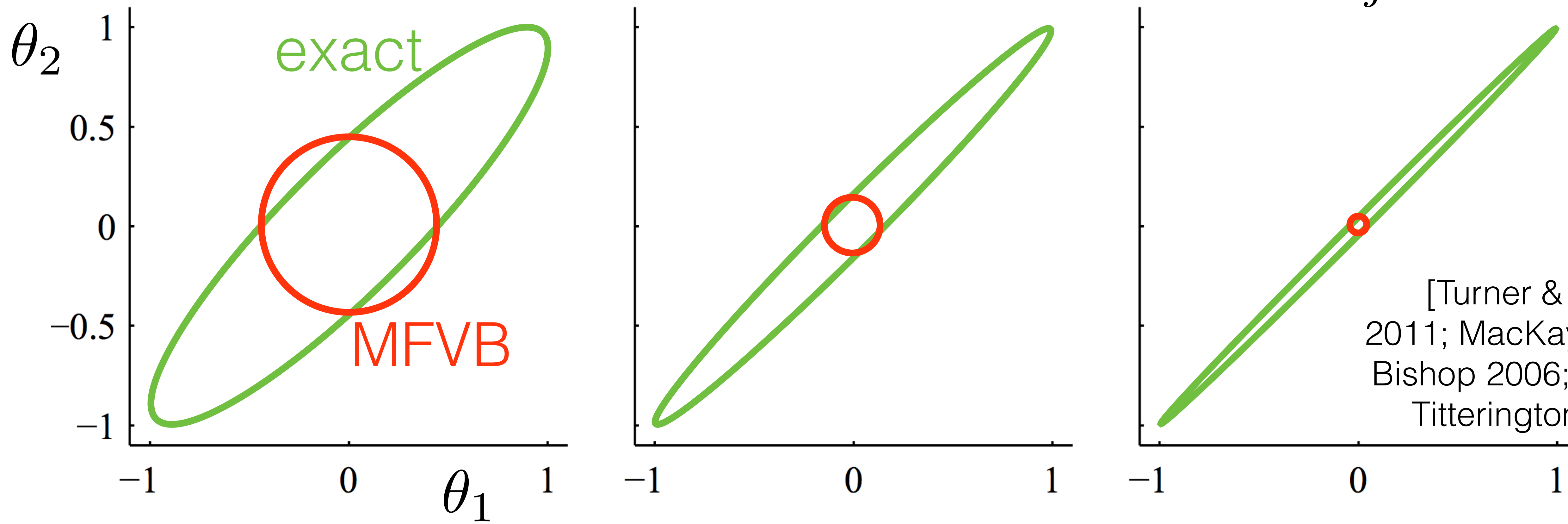

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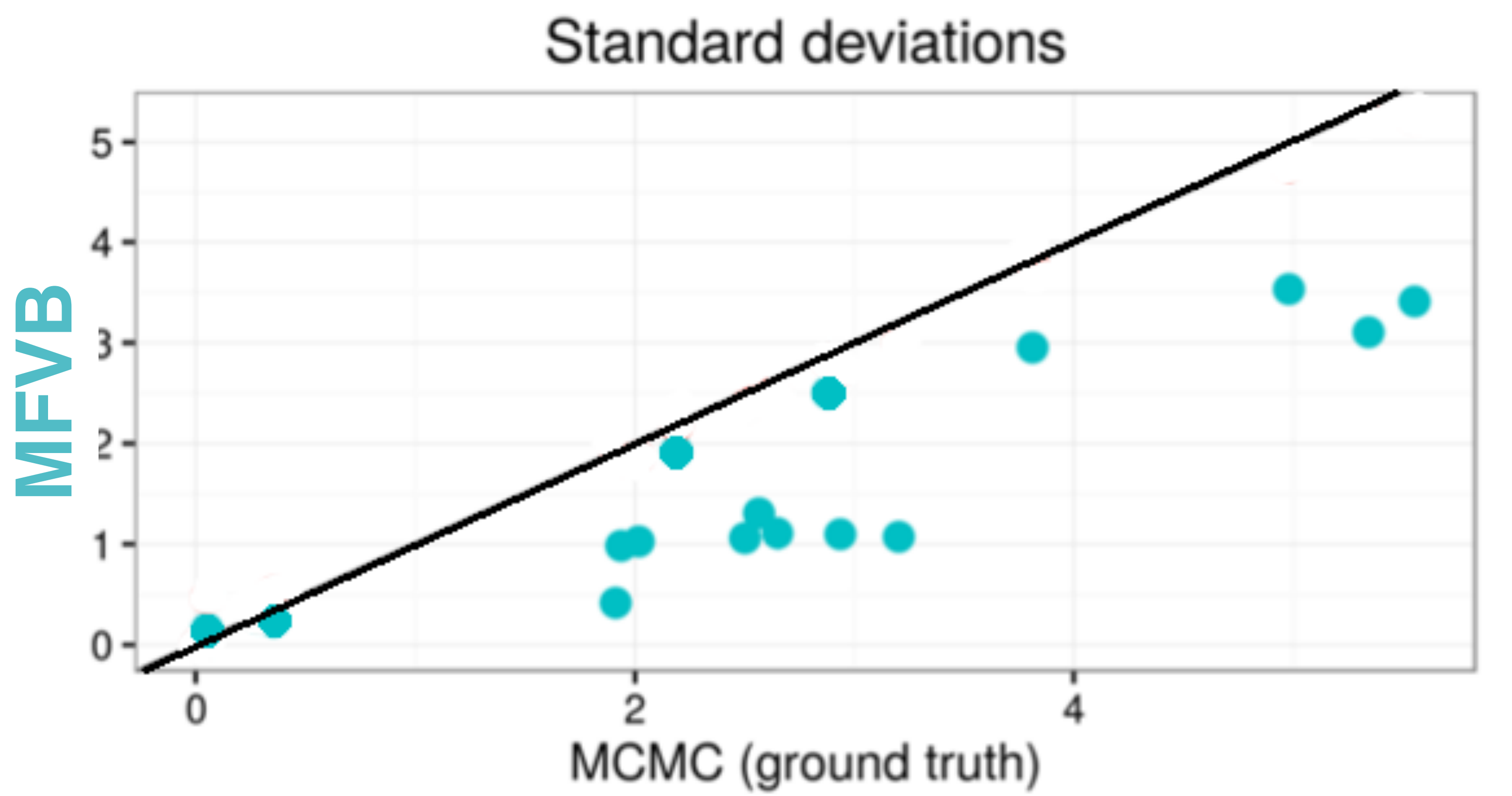

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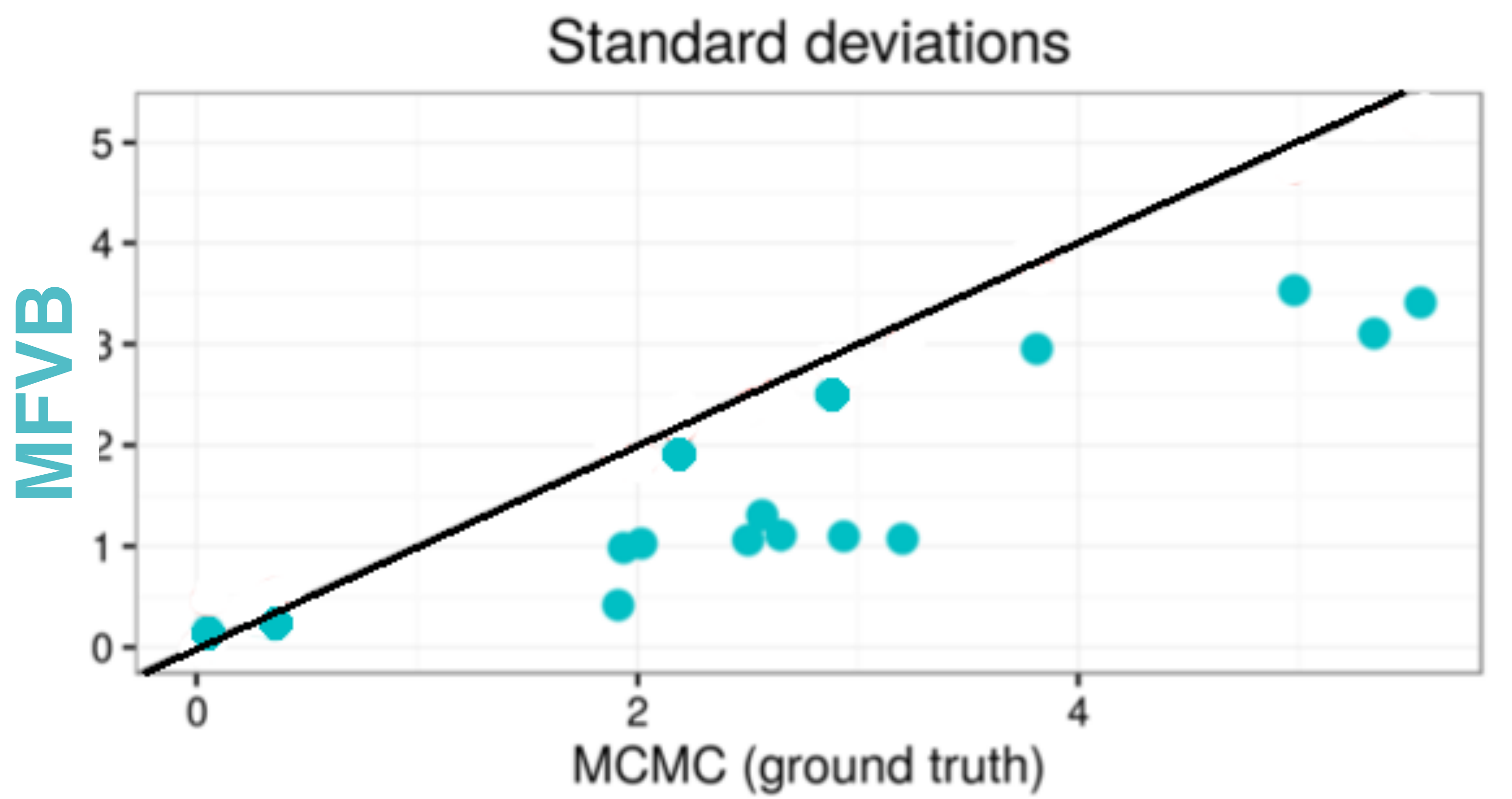

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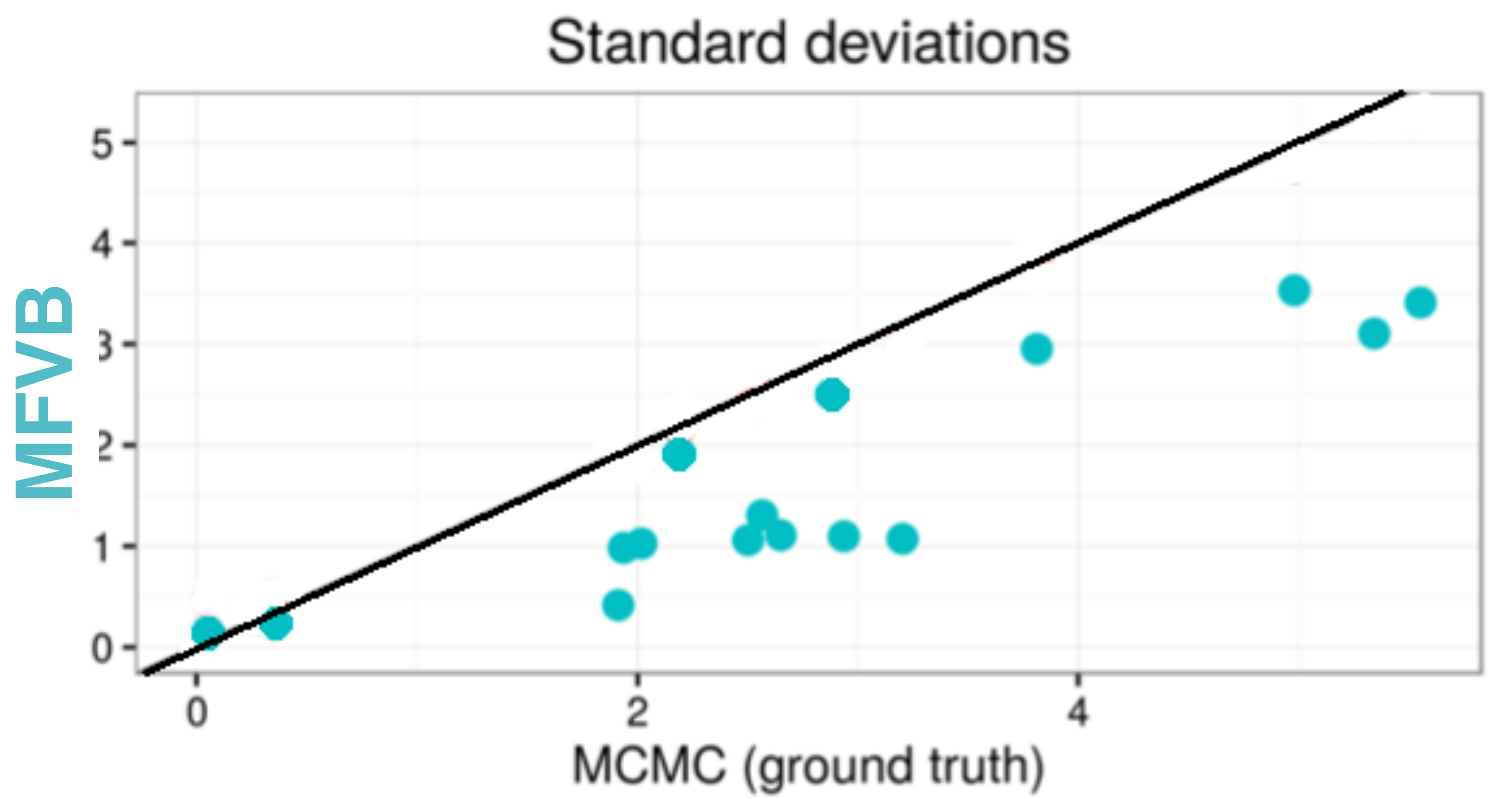

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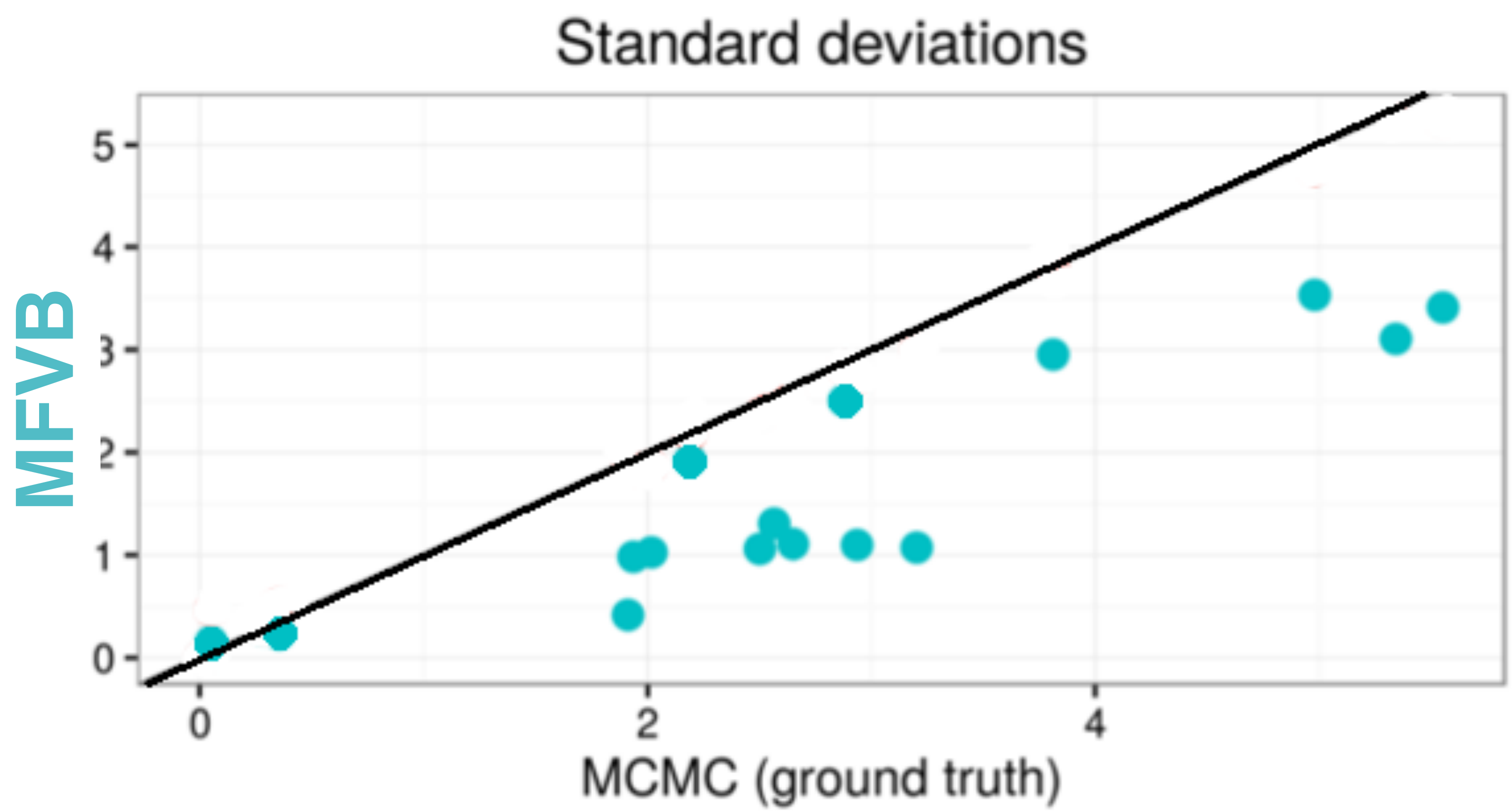

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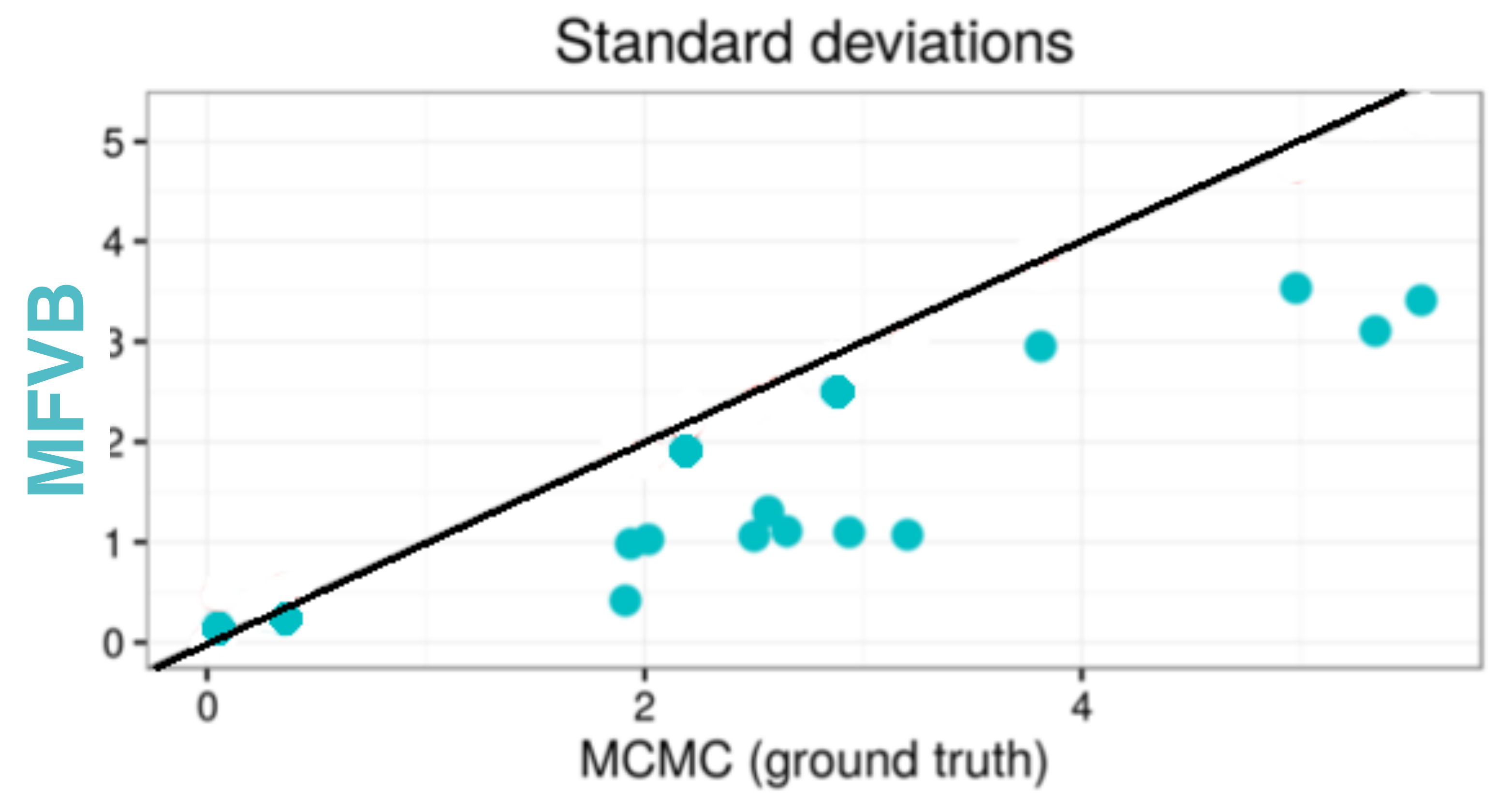
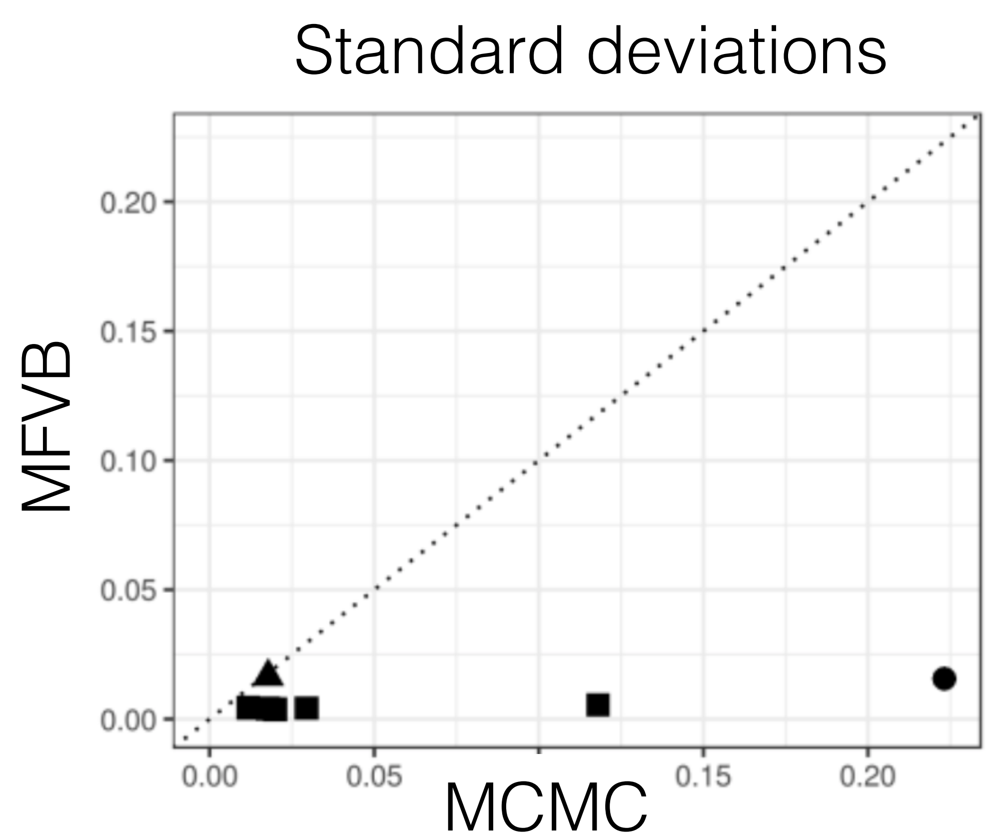


- Criteo online ads experiment



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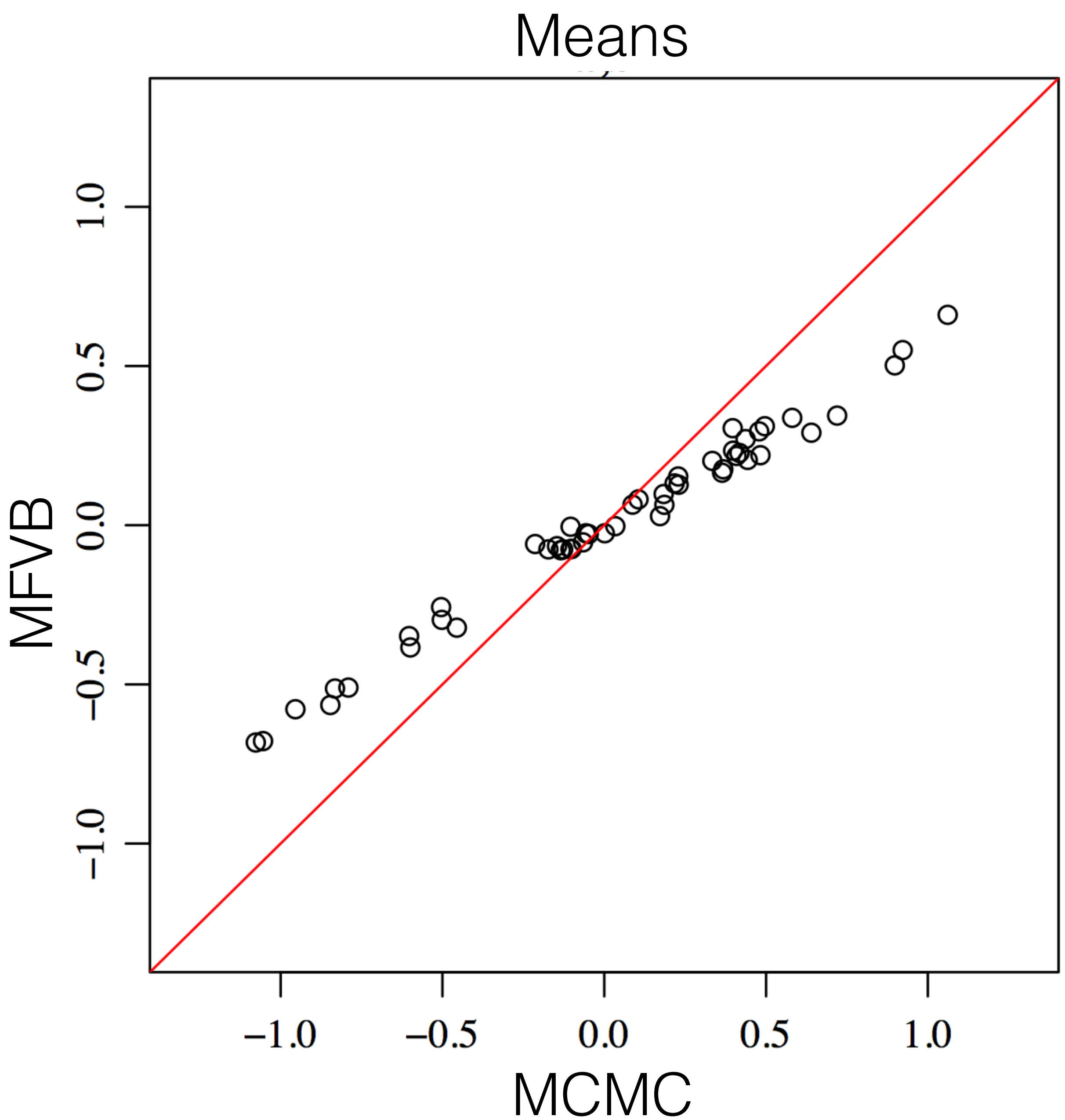

[Fosdick 2013, Ch 4, Fig 4.3]

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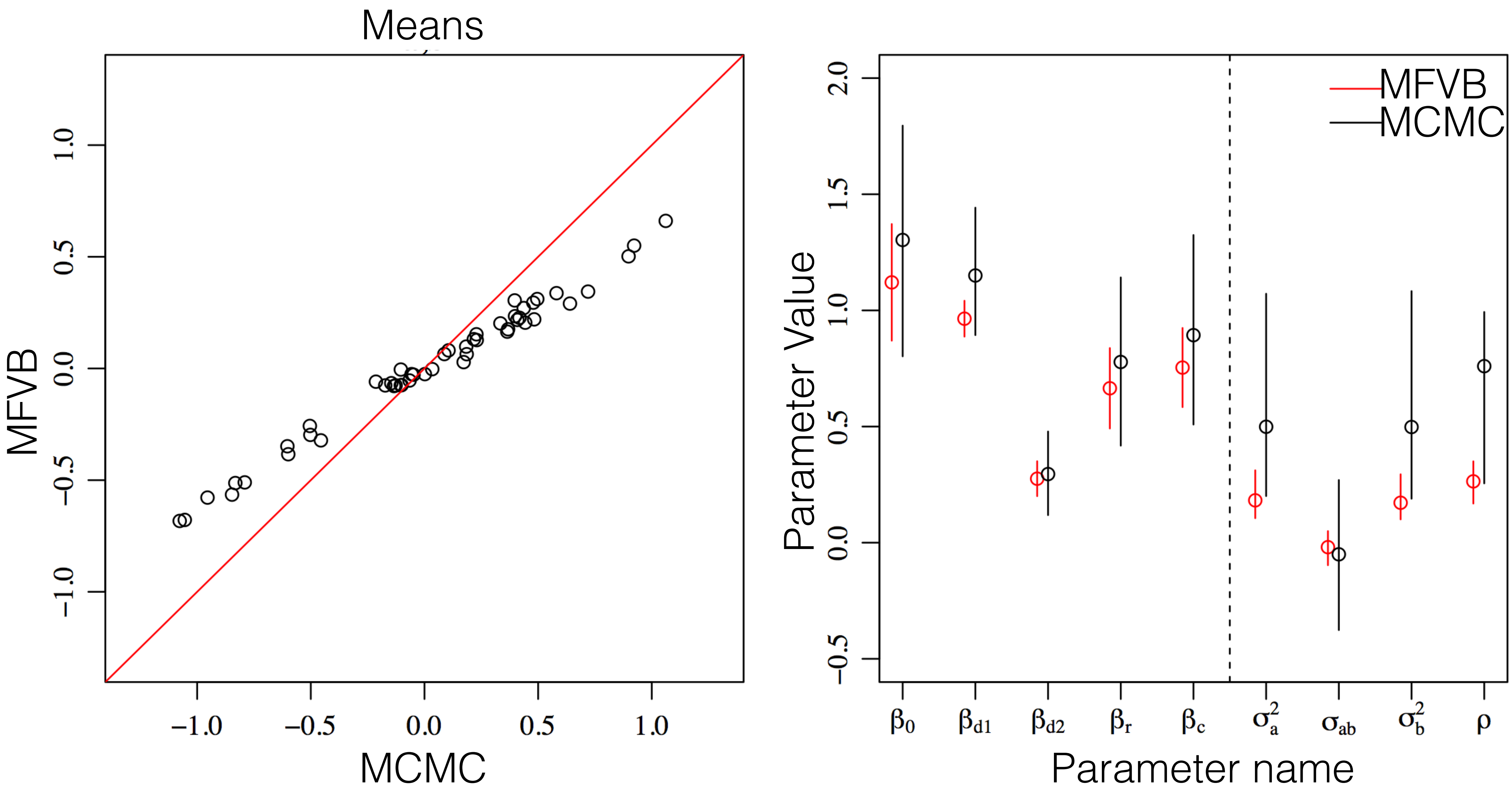

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Posterior means: revisited

- Want to predict college GPA y_n

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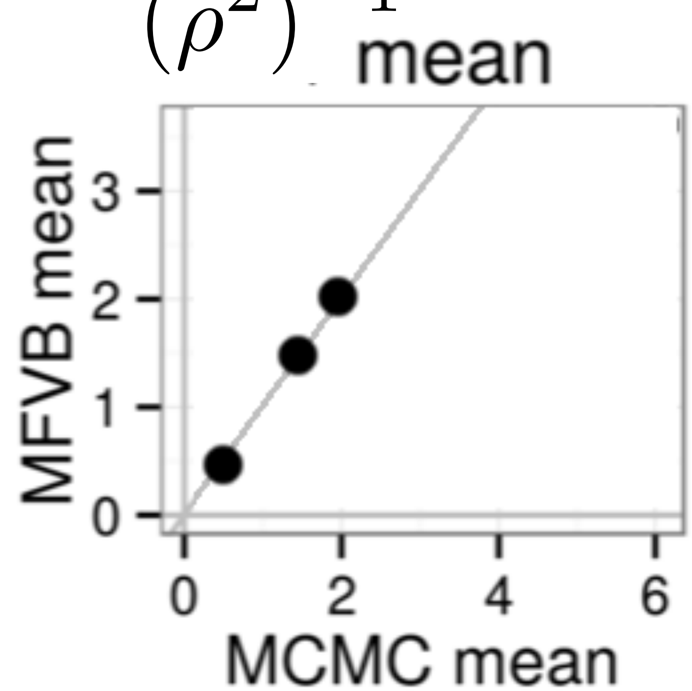
- Data simulated from model (3 data sets, 300 data points):

$(\rho^2)^{-1}$



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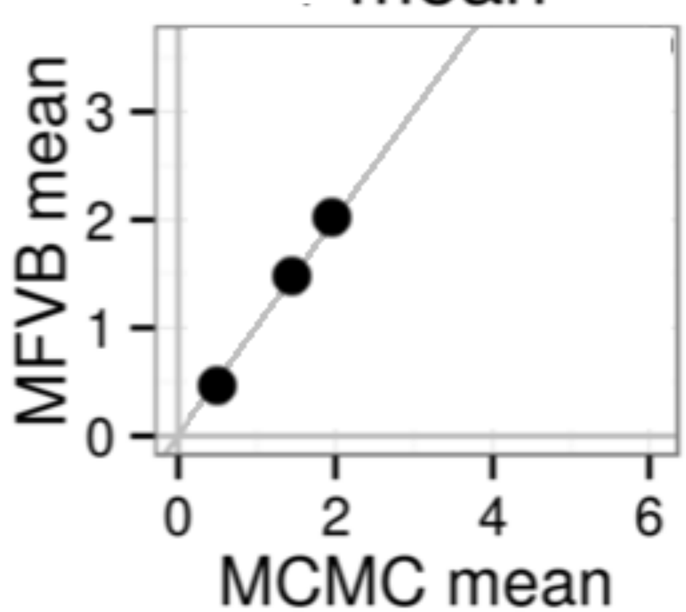
- Data simulated from model (3 data sets, 300 data points):

$(\rho^2)^{-1}$ mean



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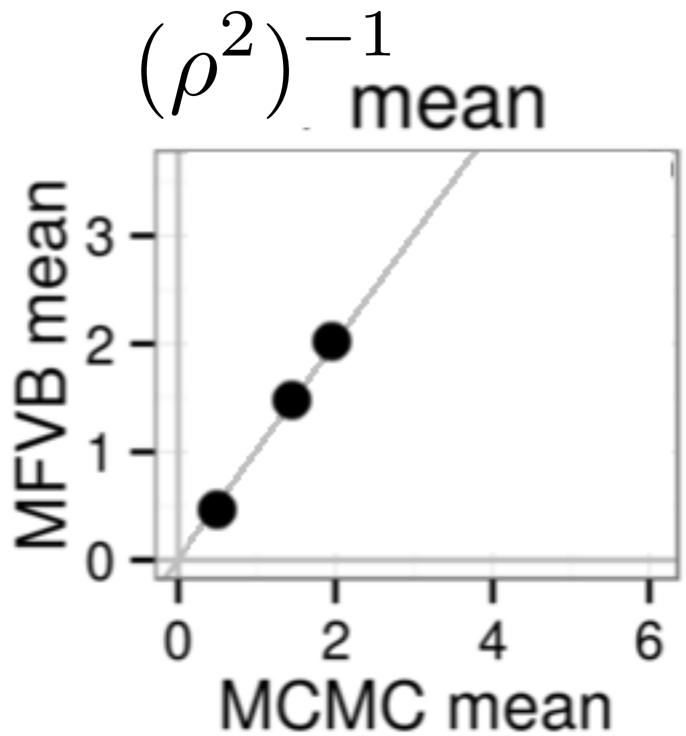

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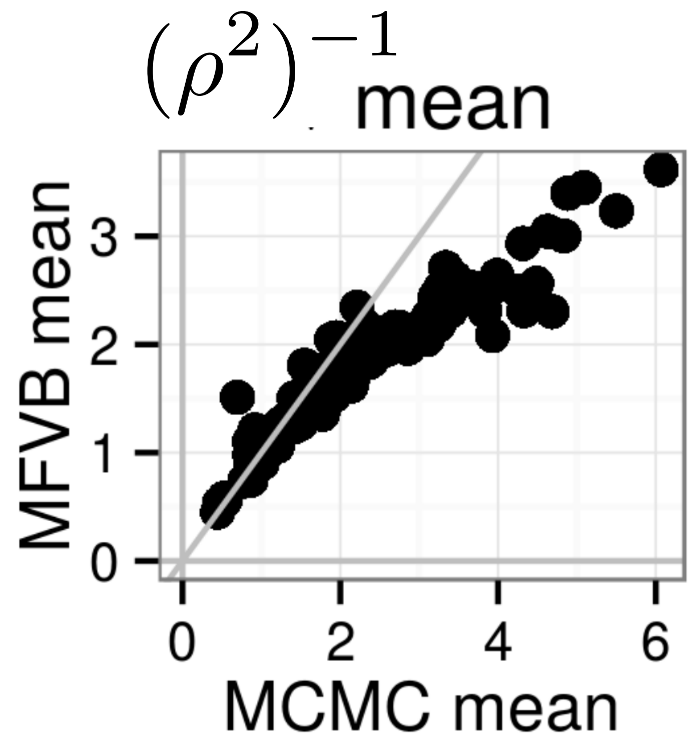

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Approximate Bayesian inference

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

Optimization

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Variational Bayes

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

How deep is the issue?

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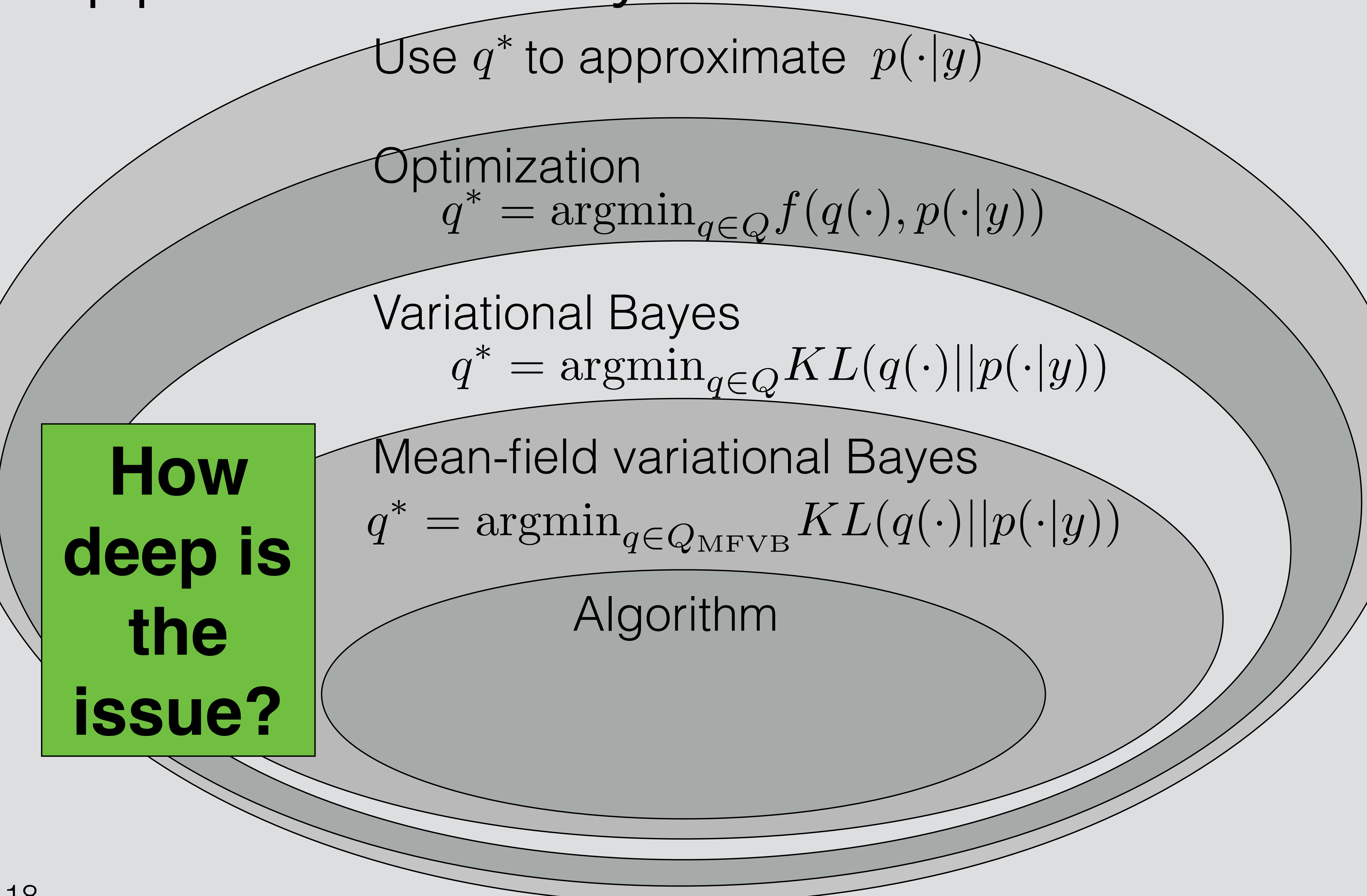

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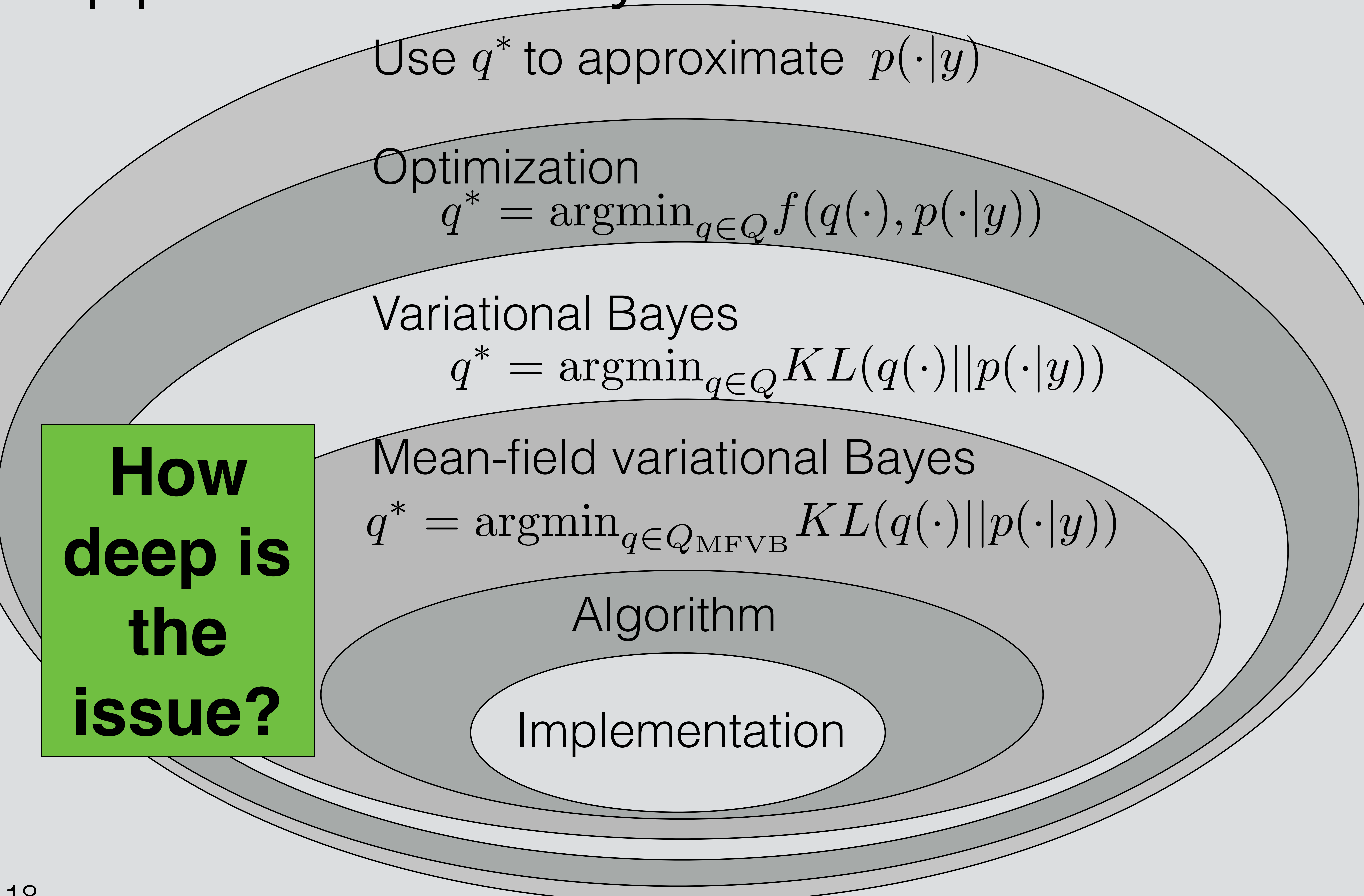

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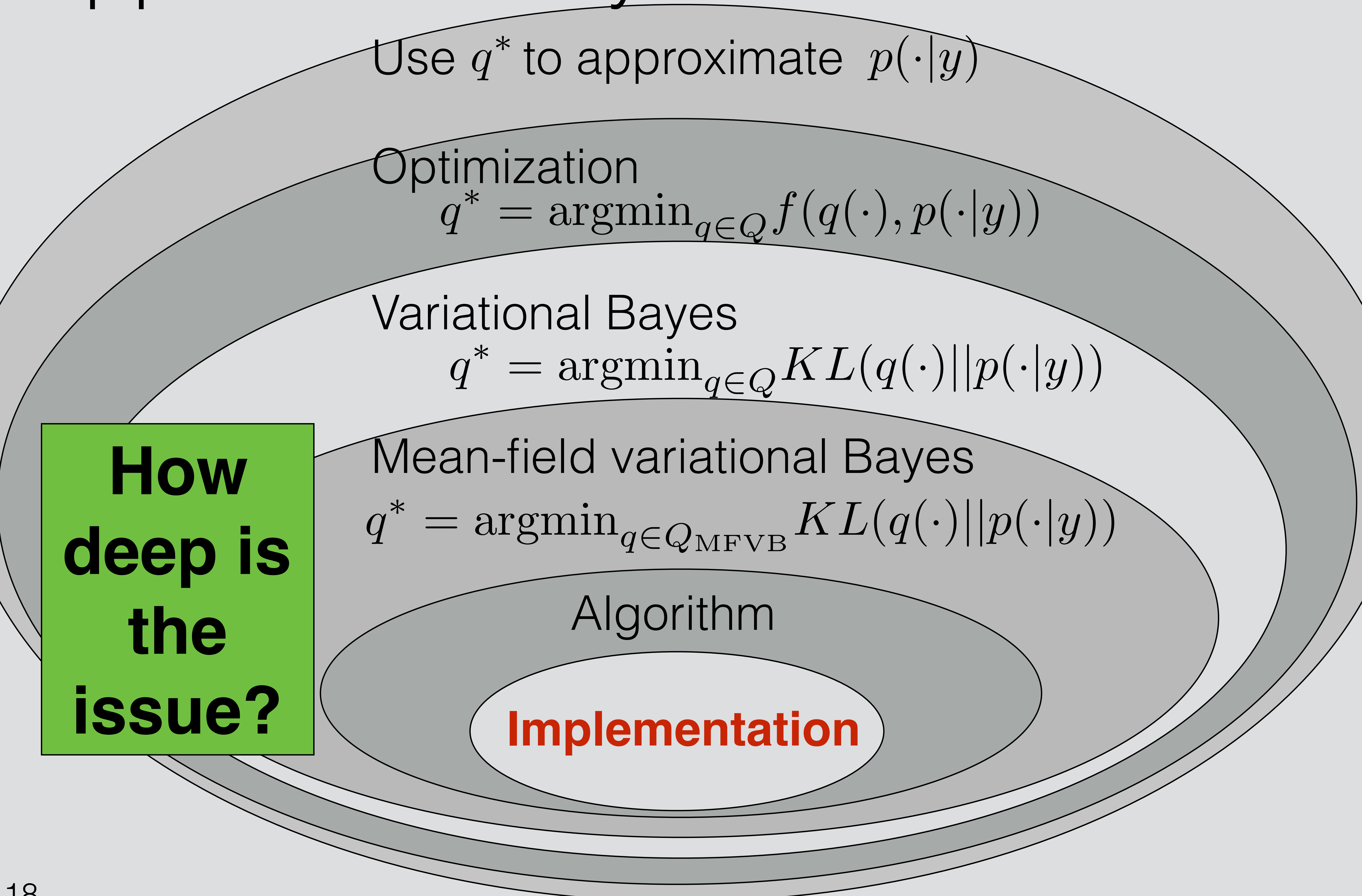

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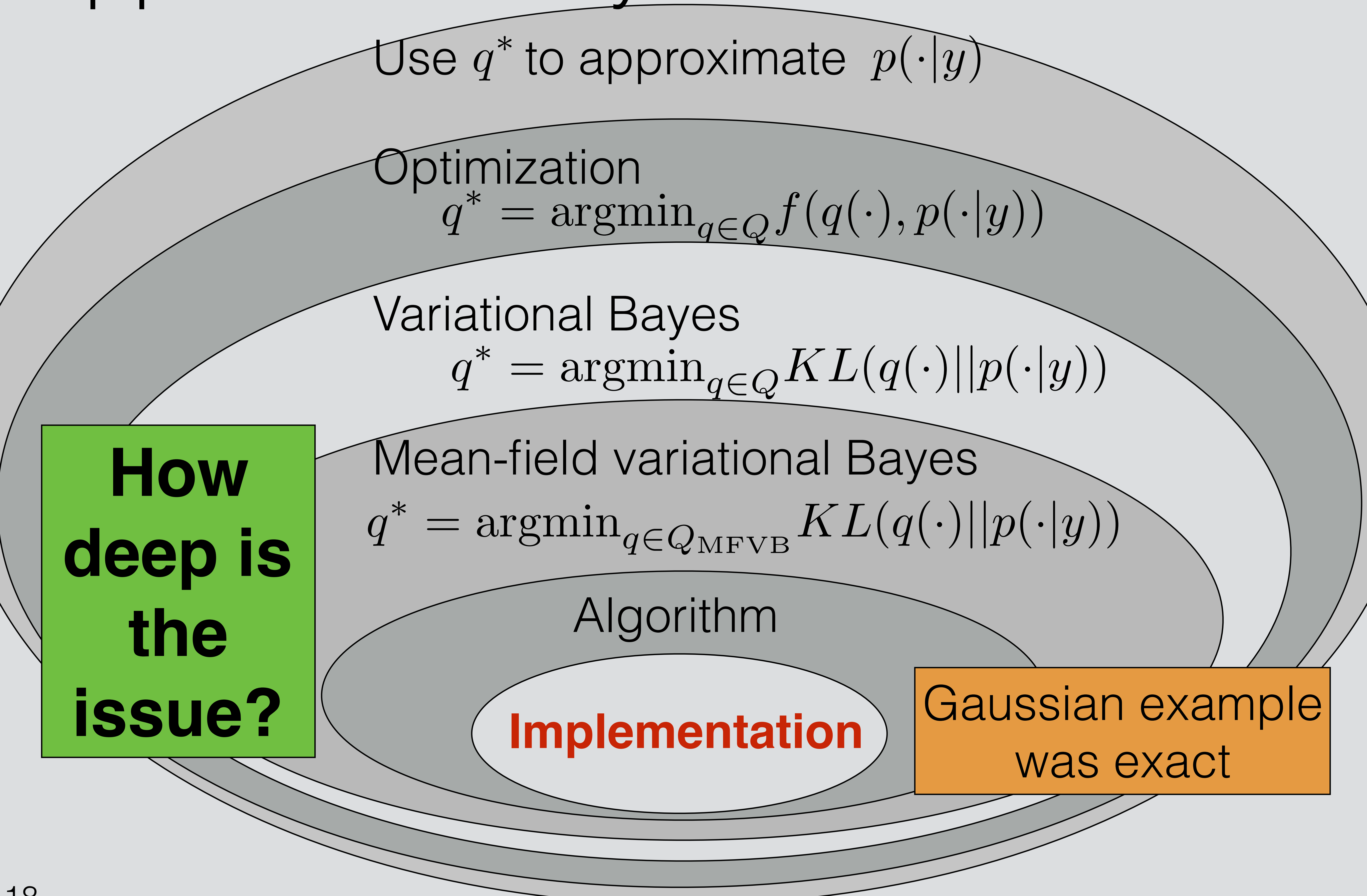

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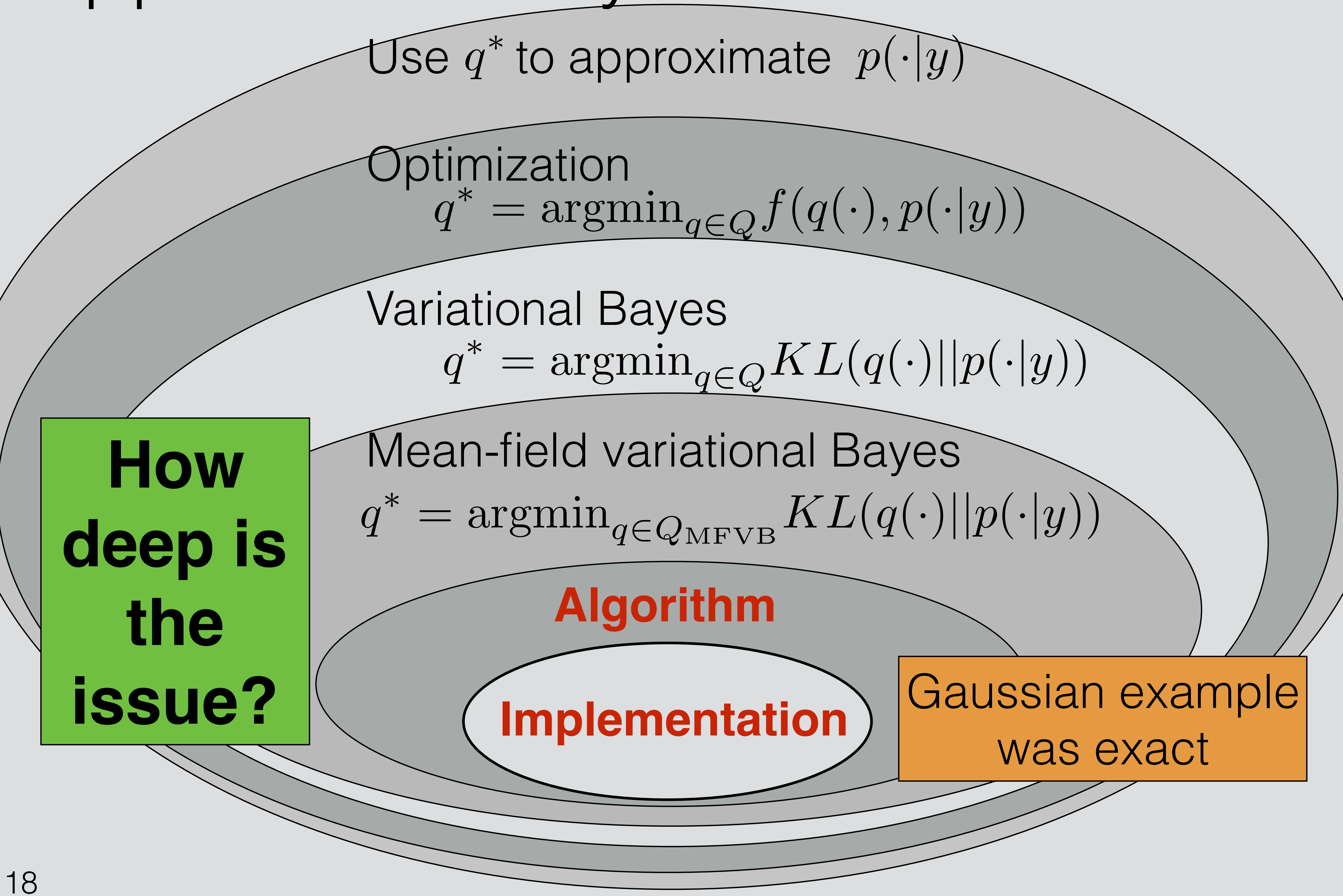

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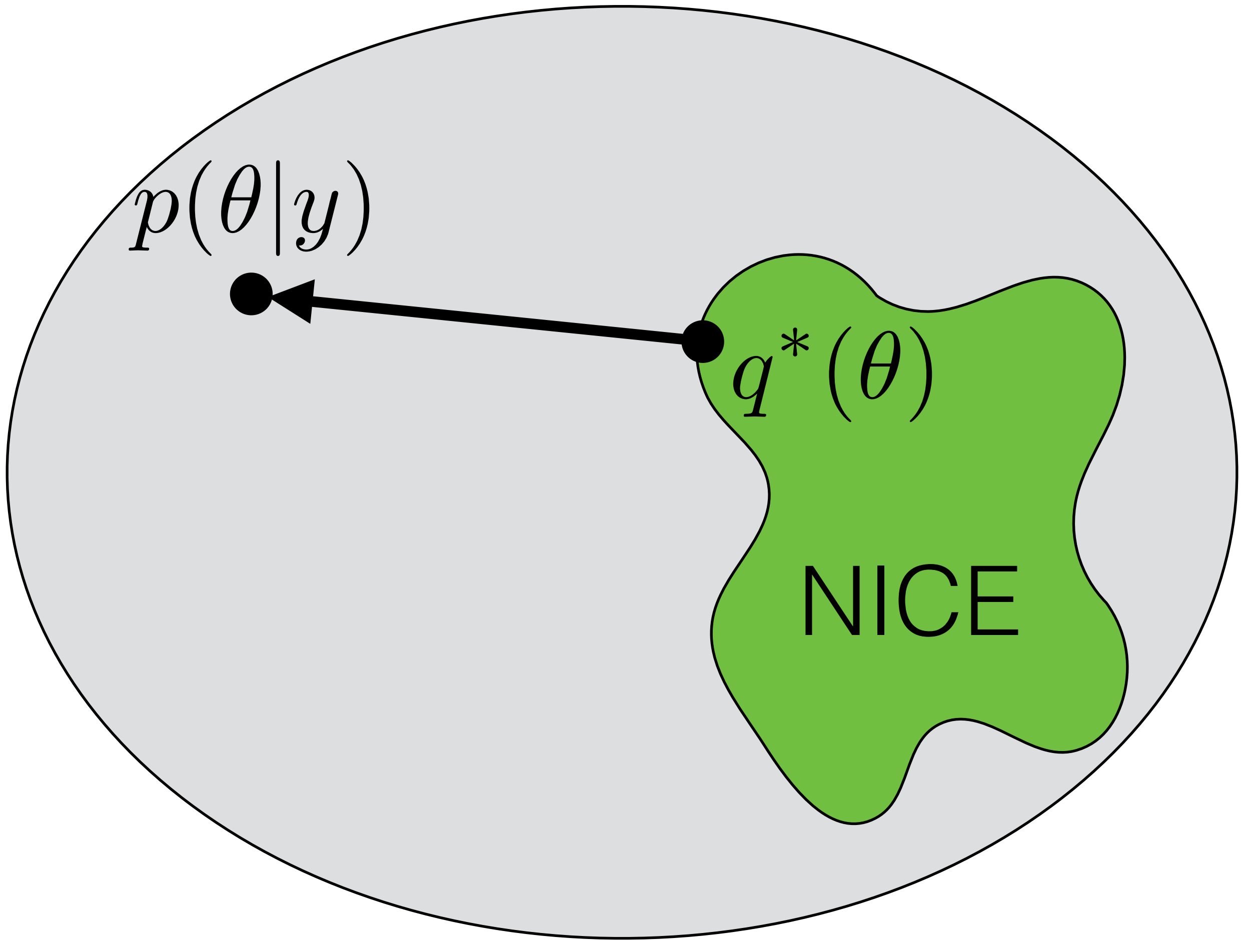

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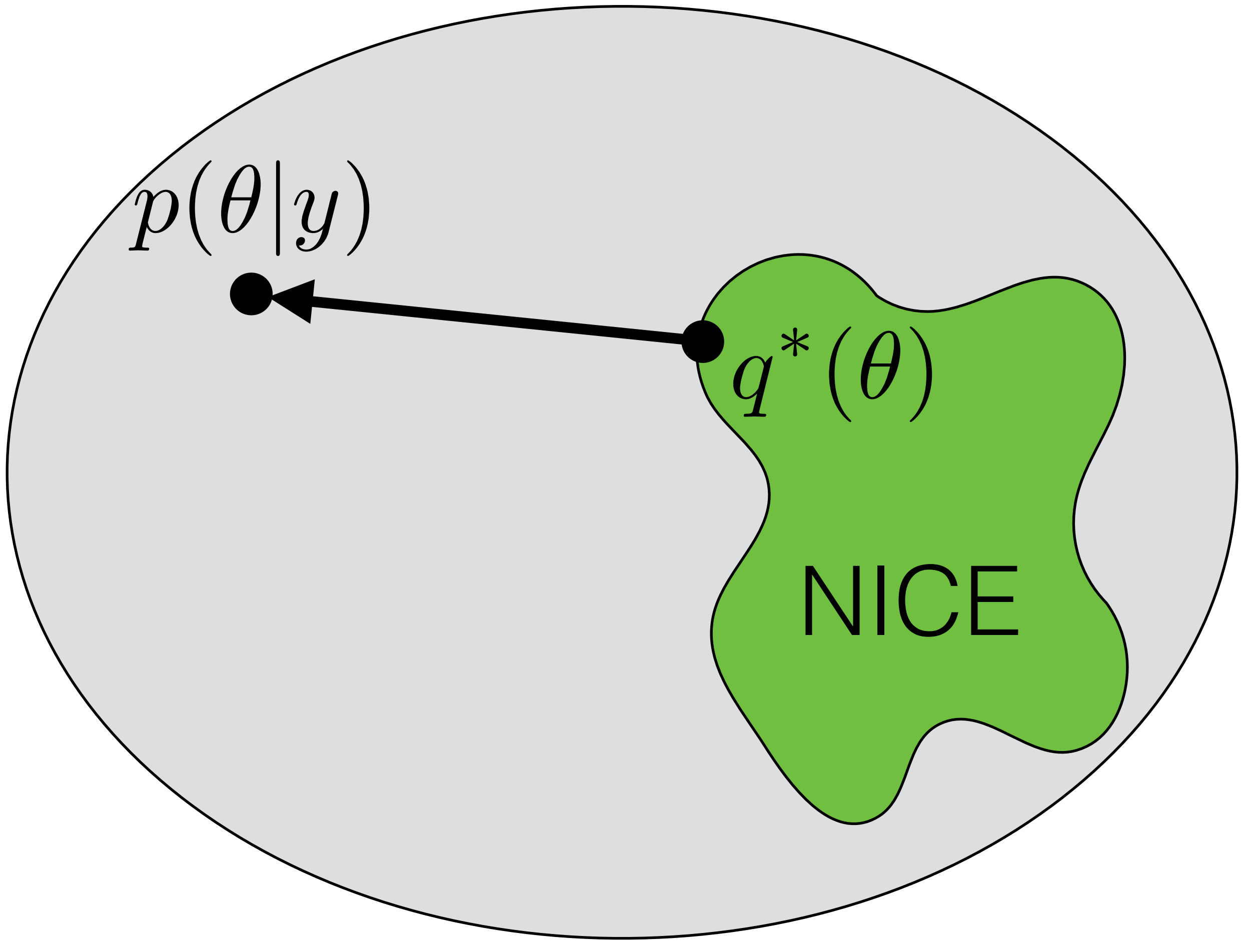

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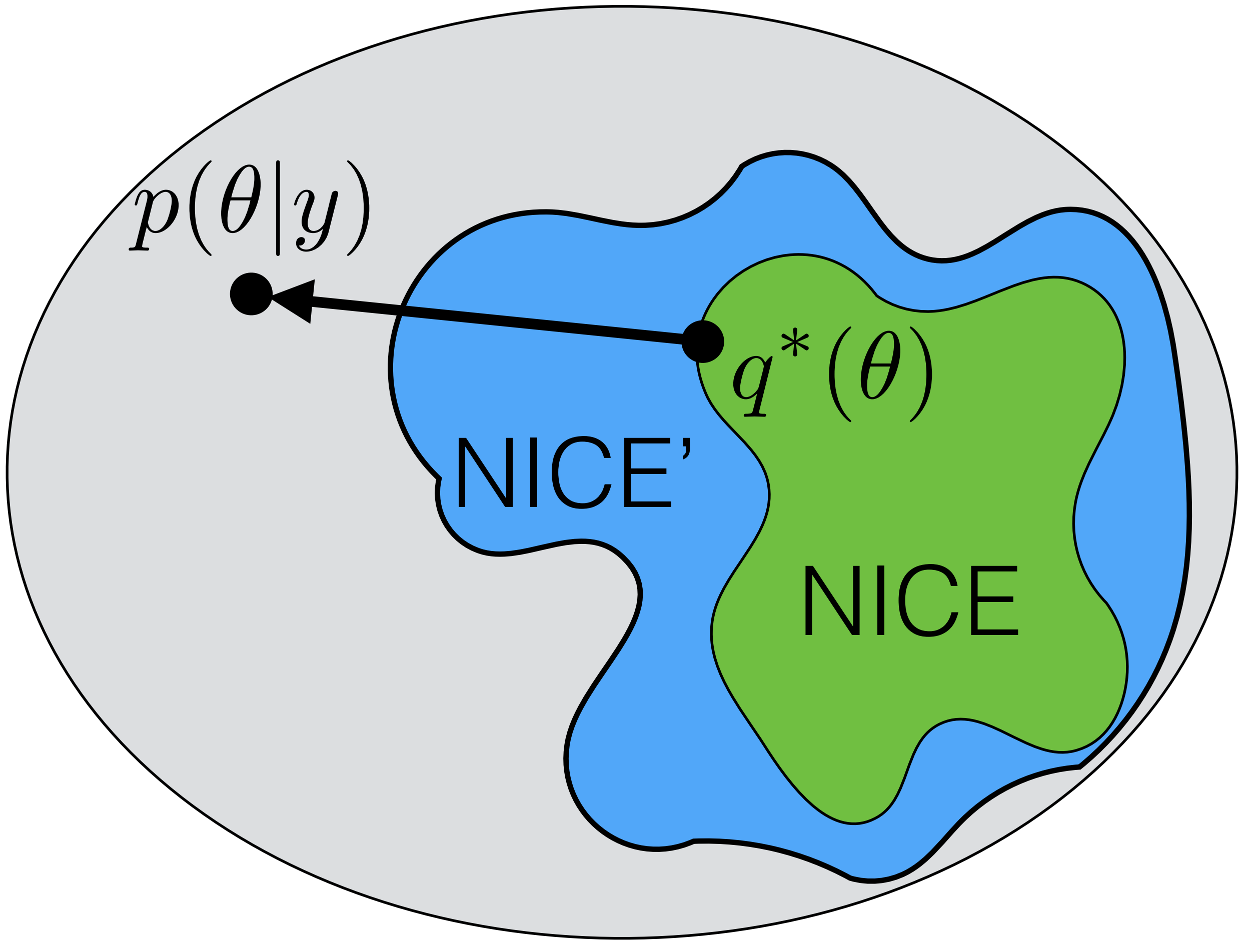

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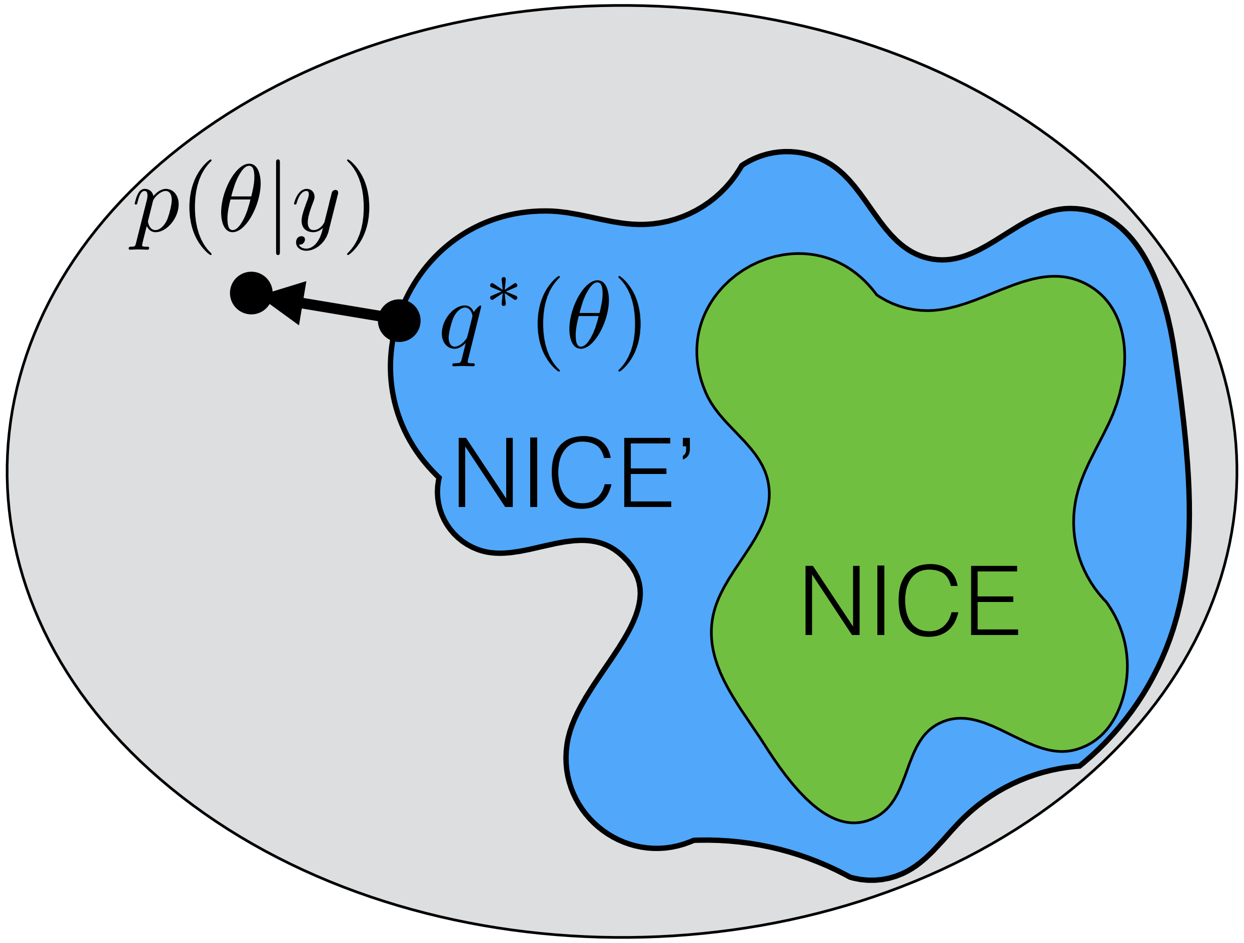

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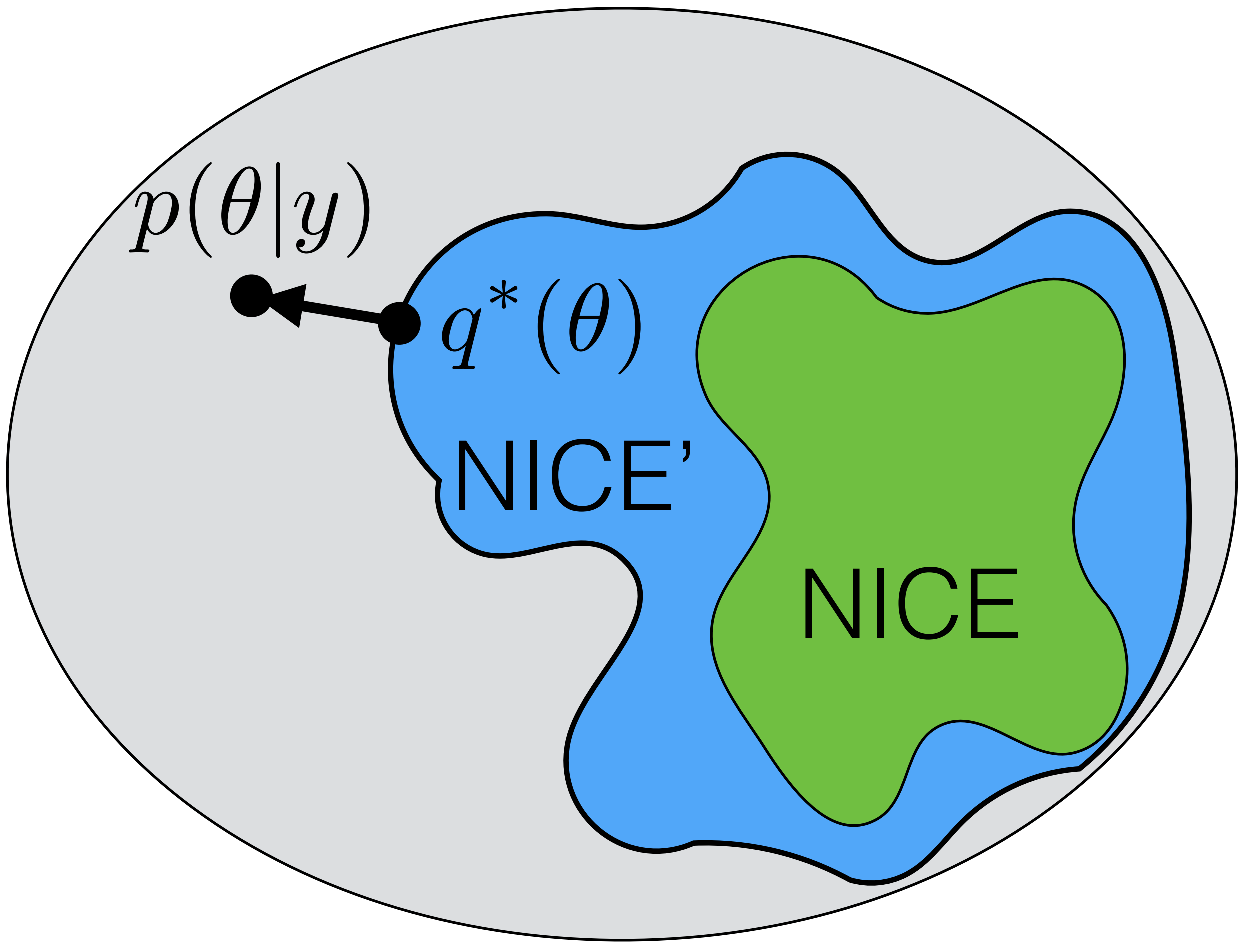

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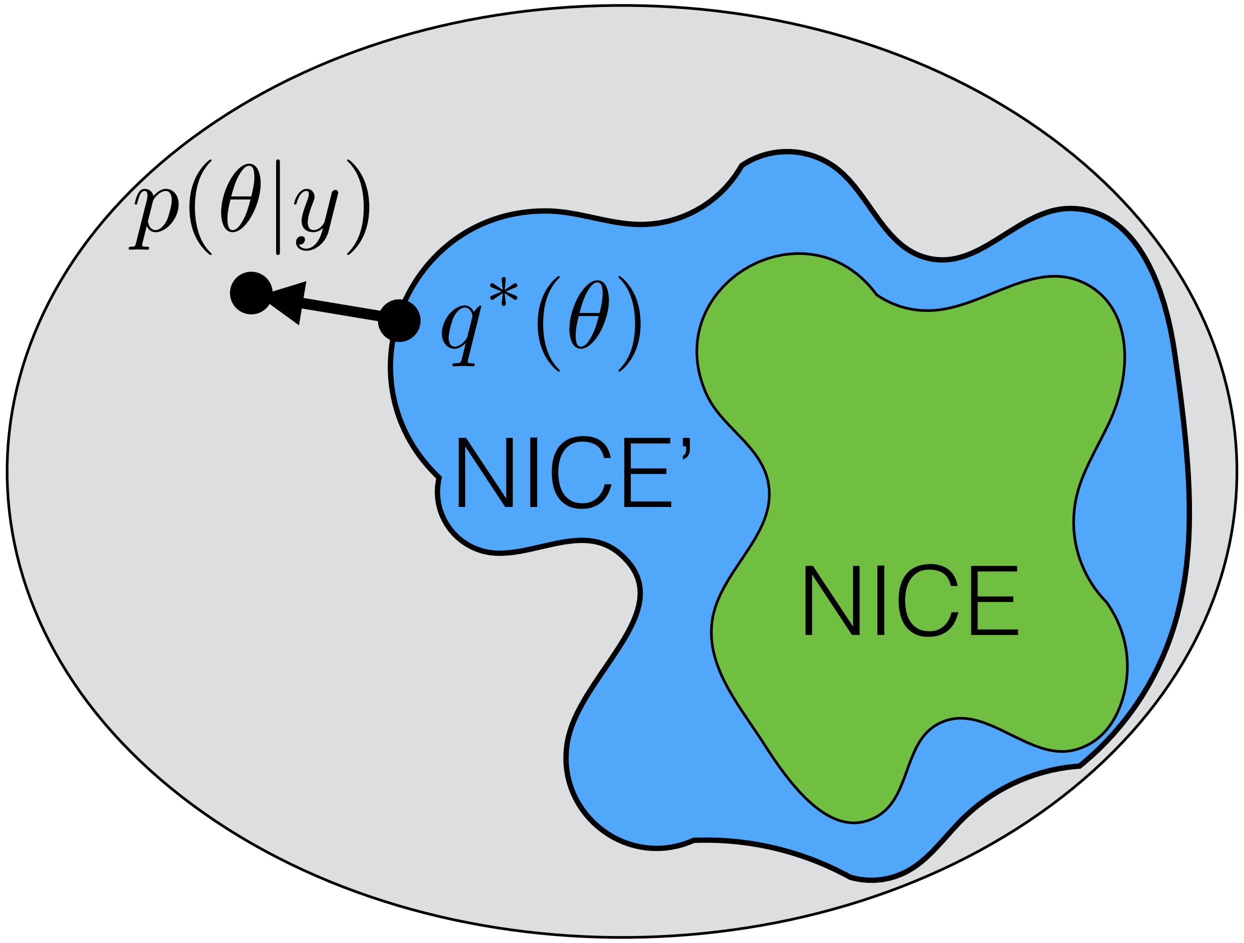

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- But how much worse can the estimates be? And could it have just been the implementation?

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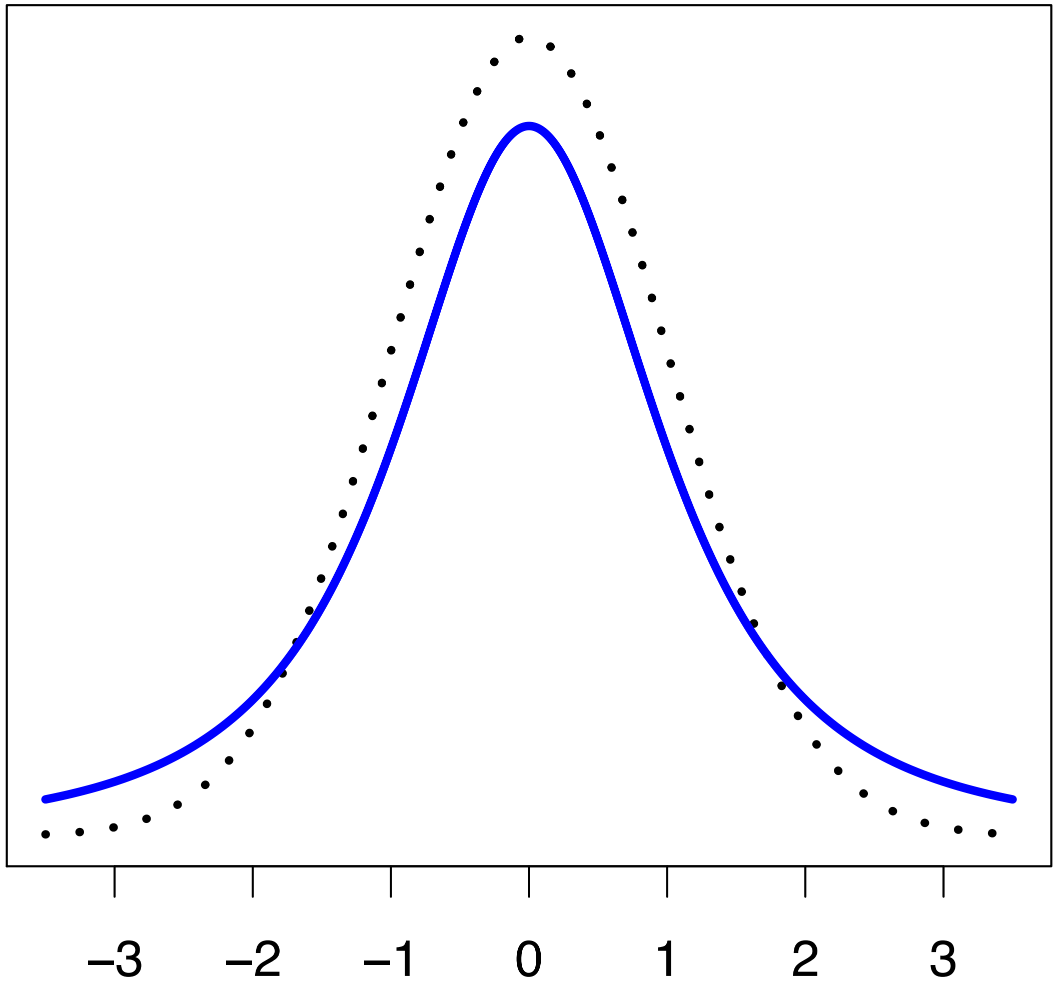

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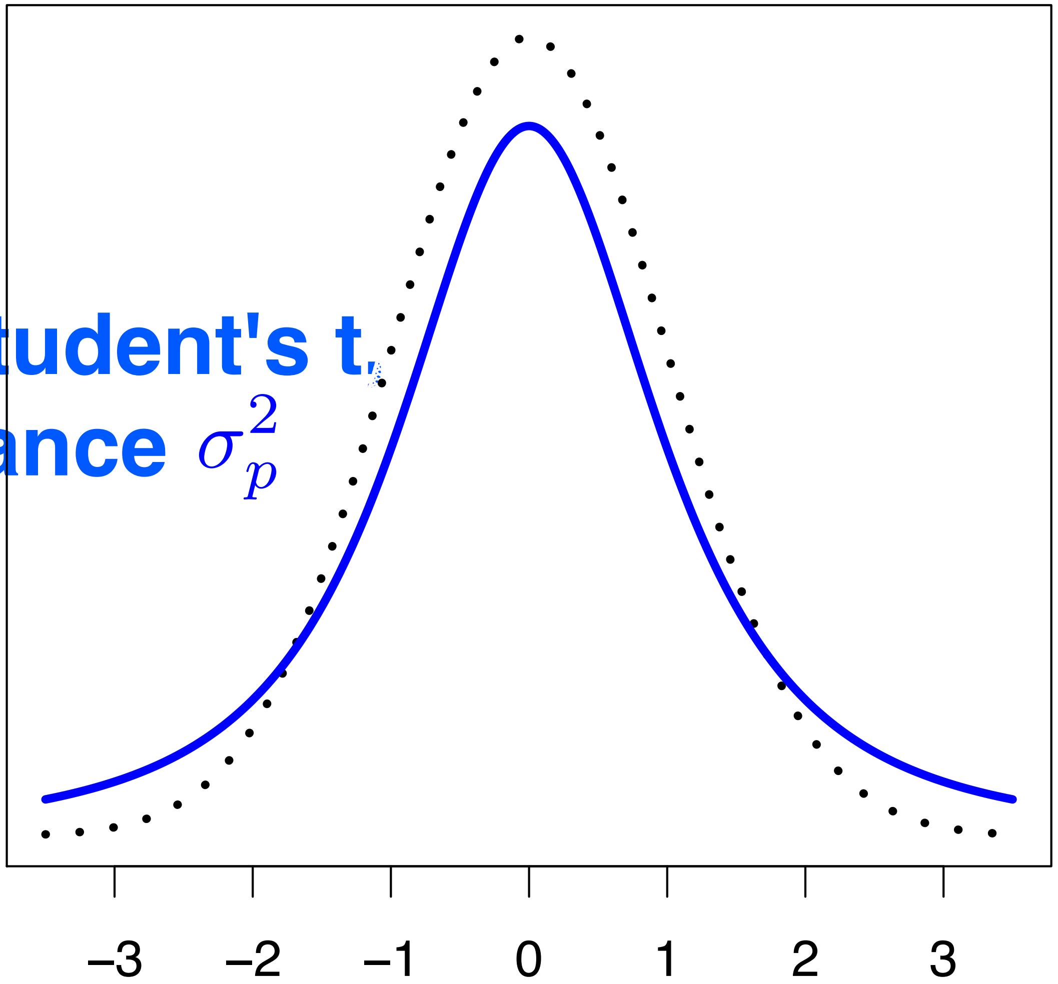

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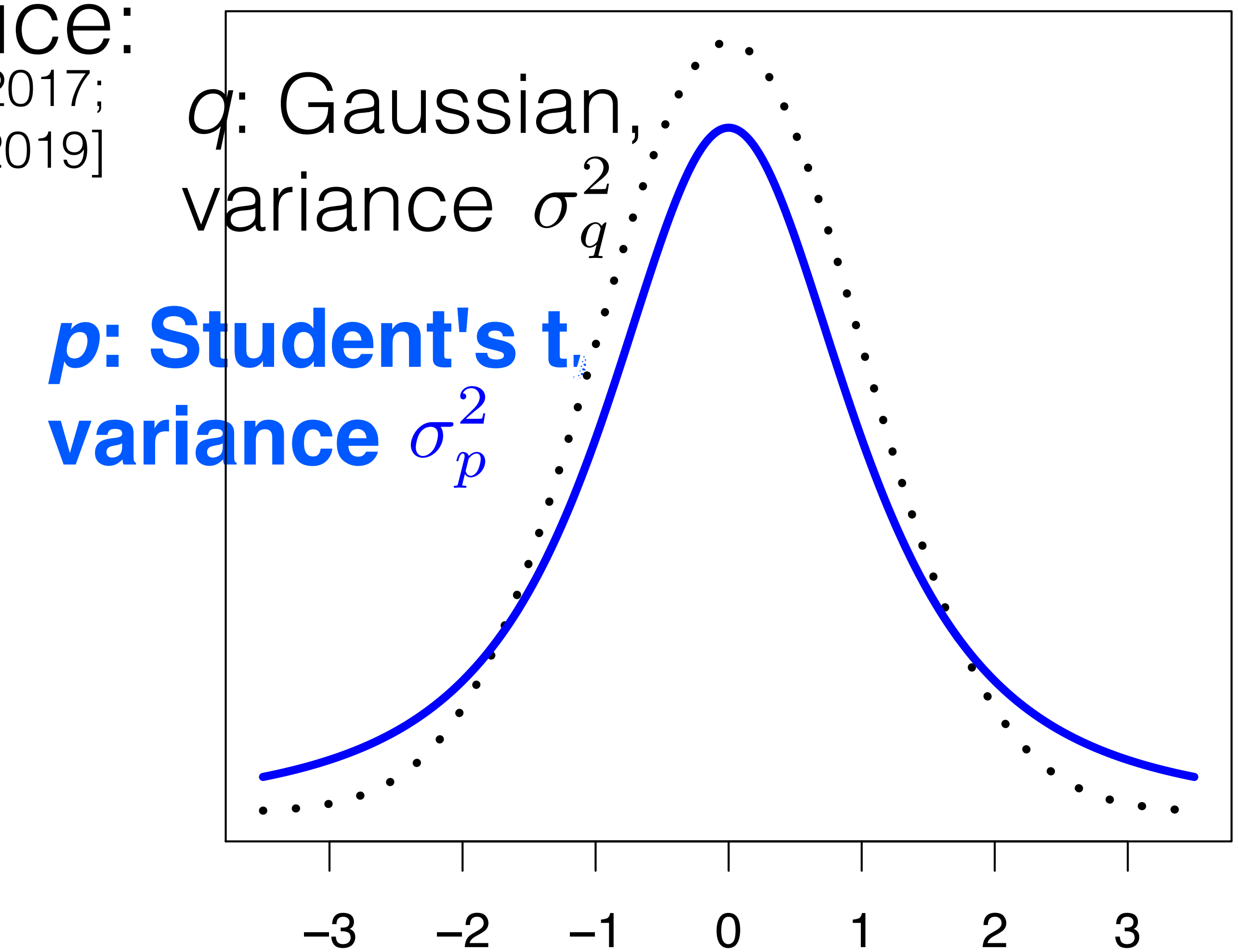

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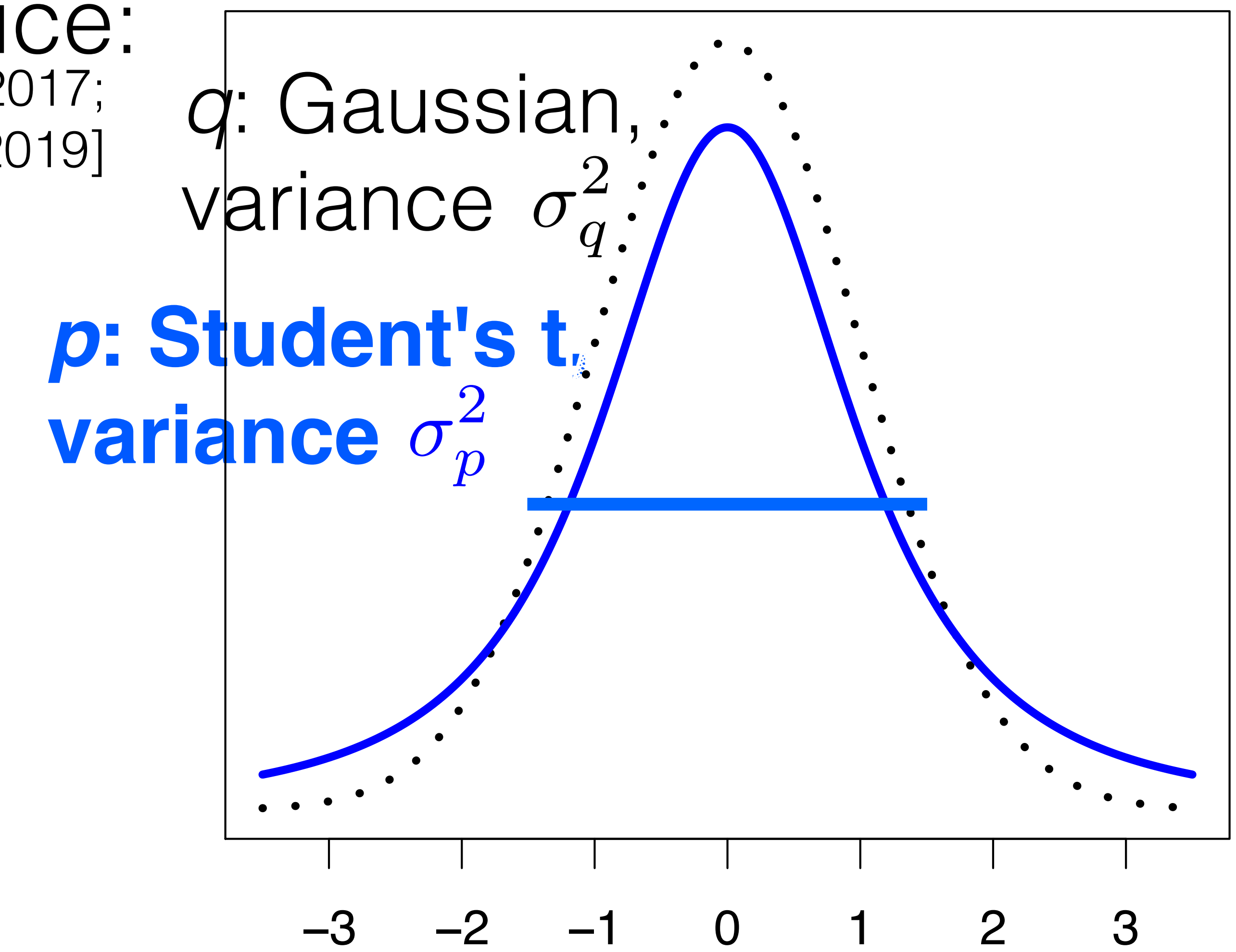

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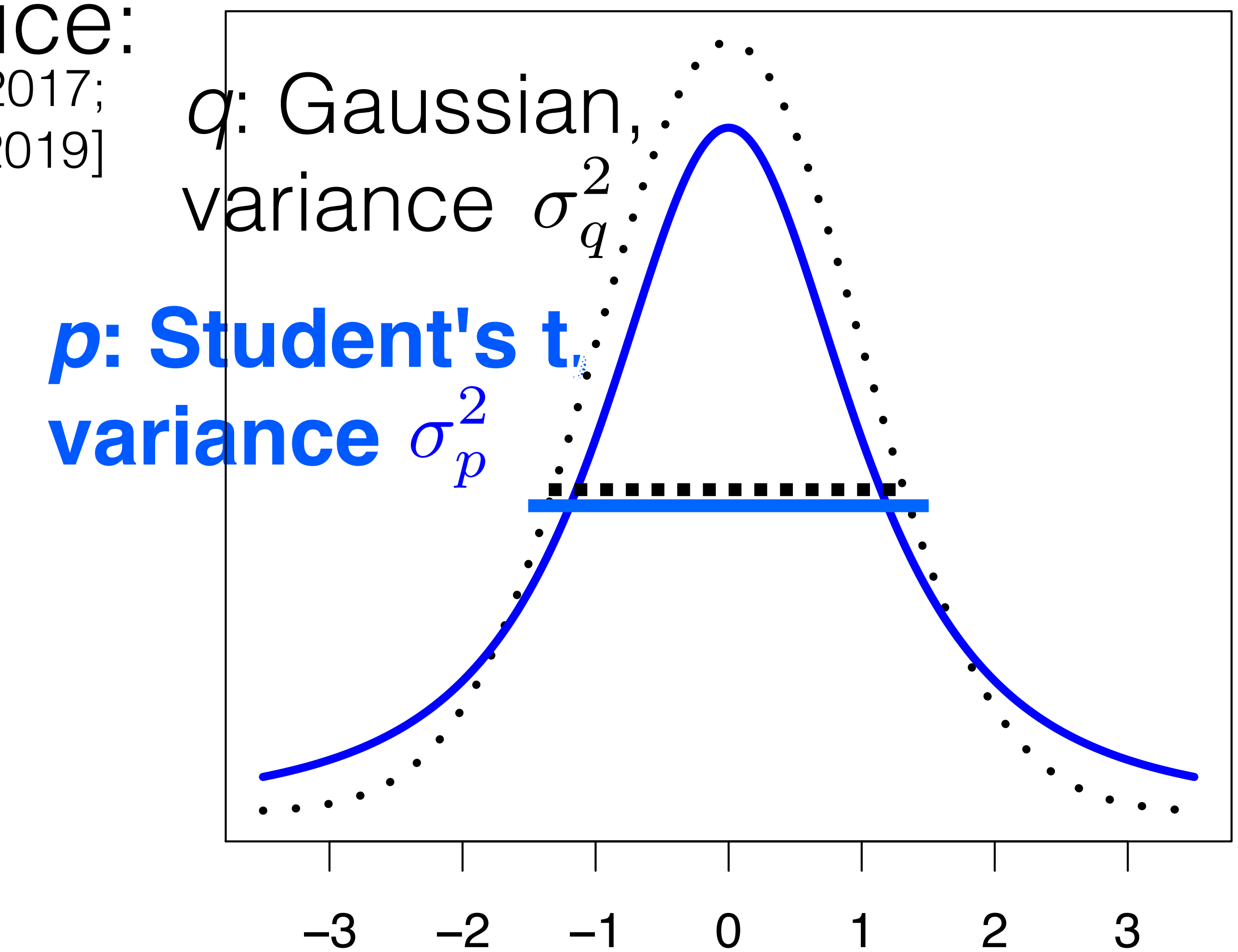

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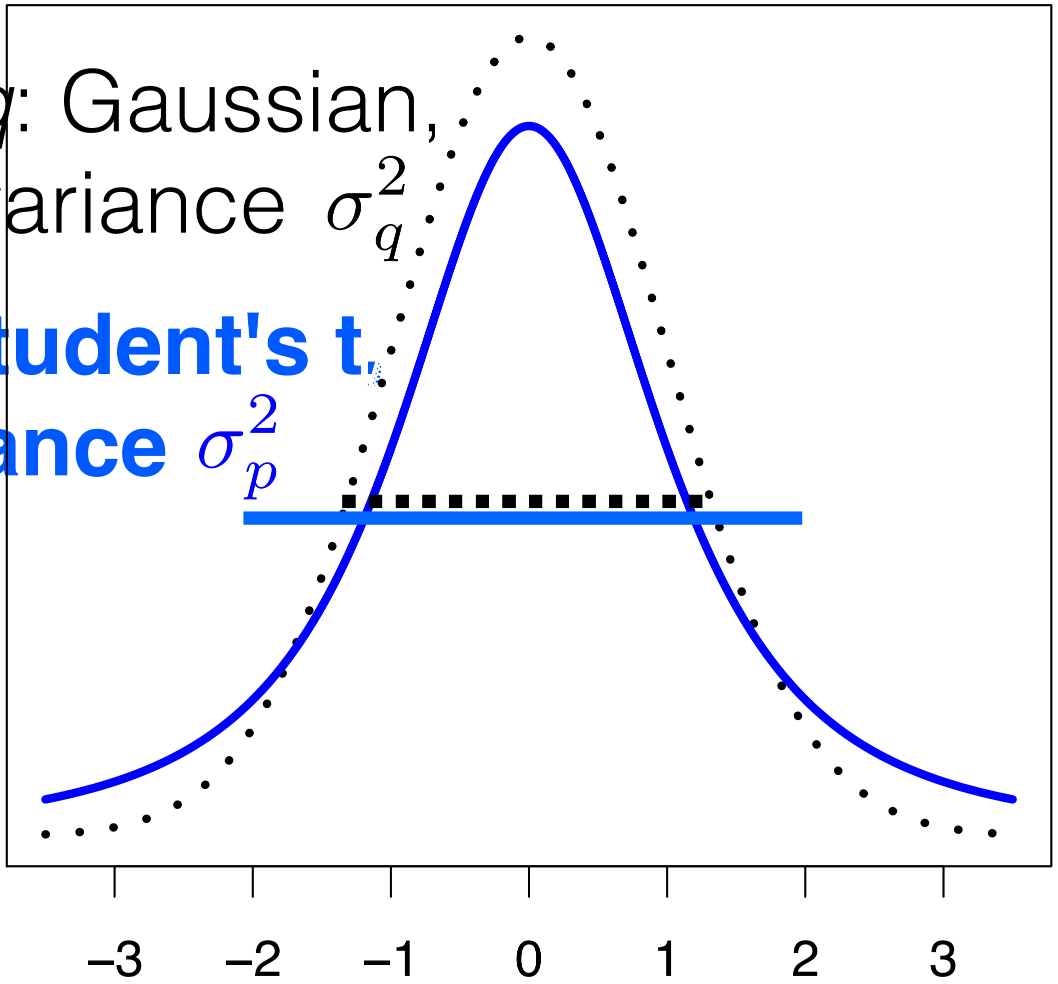

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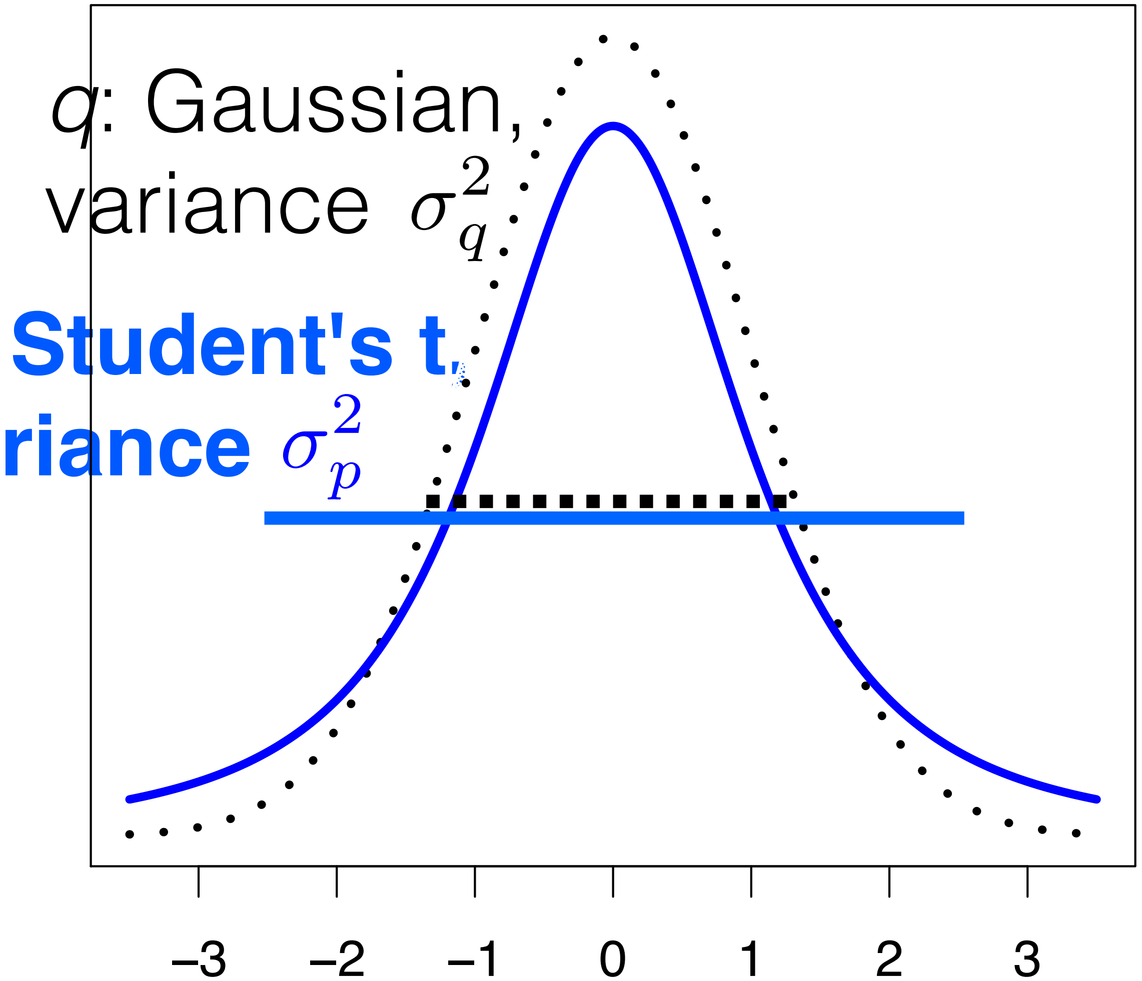

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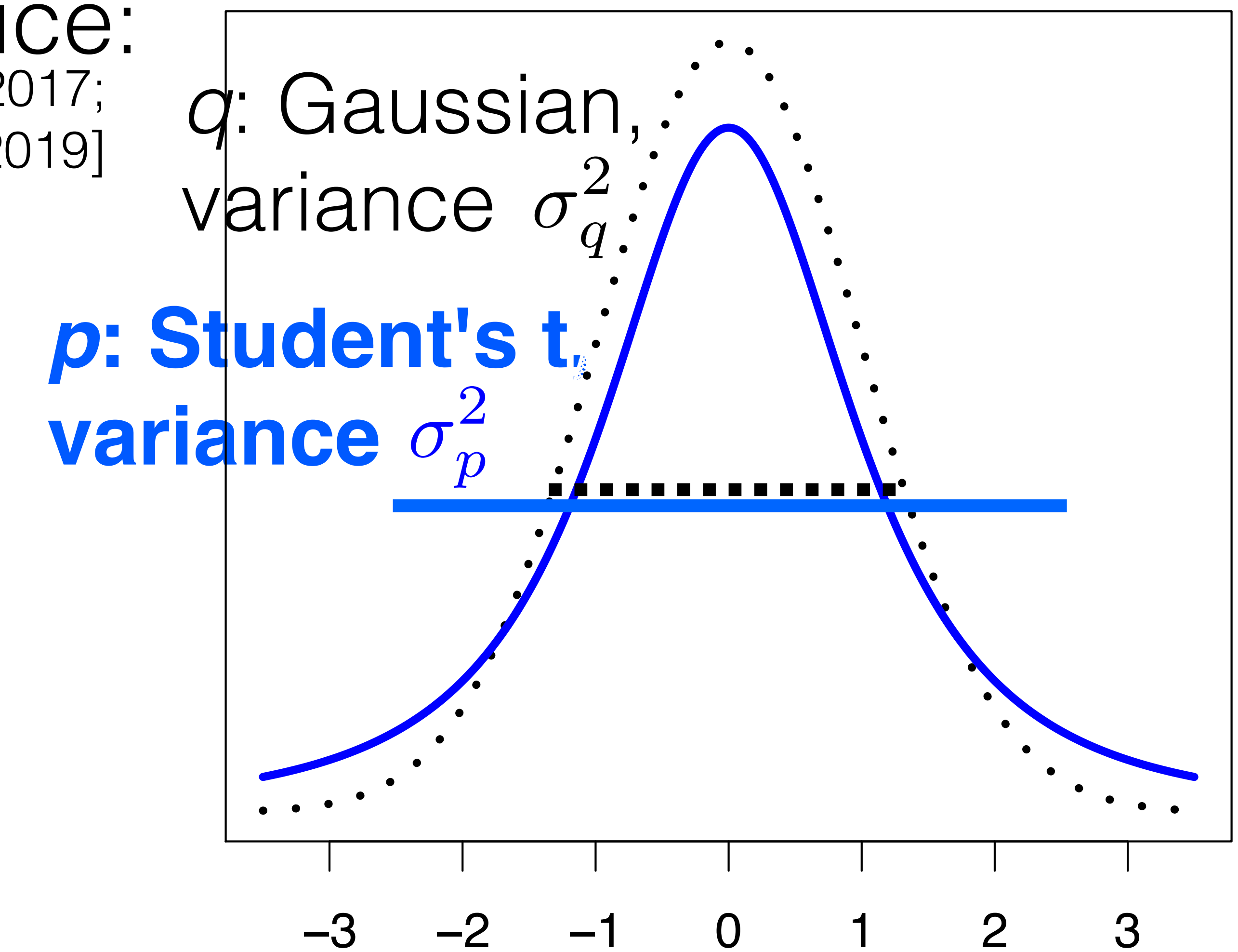

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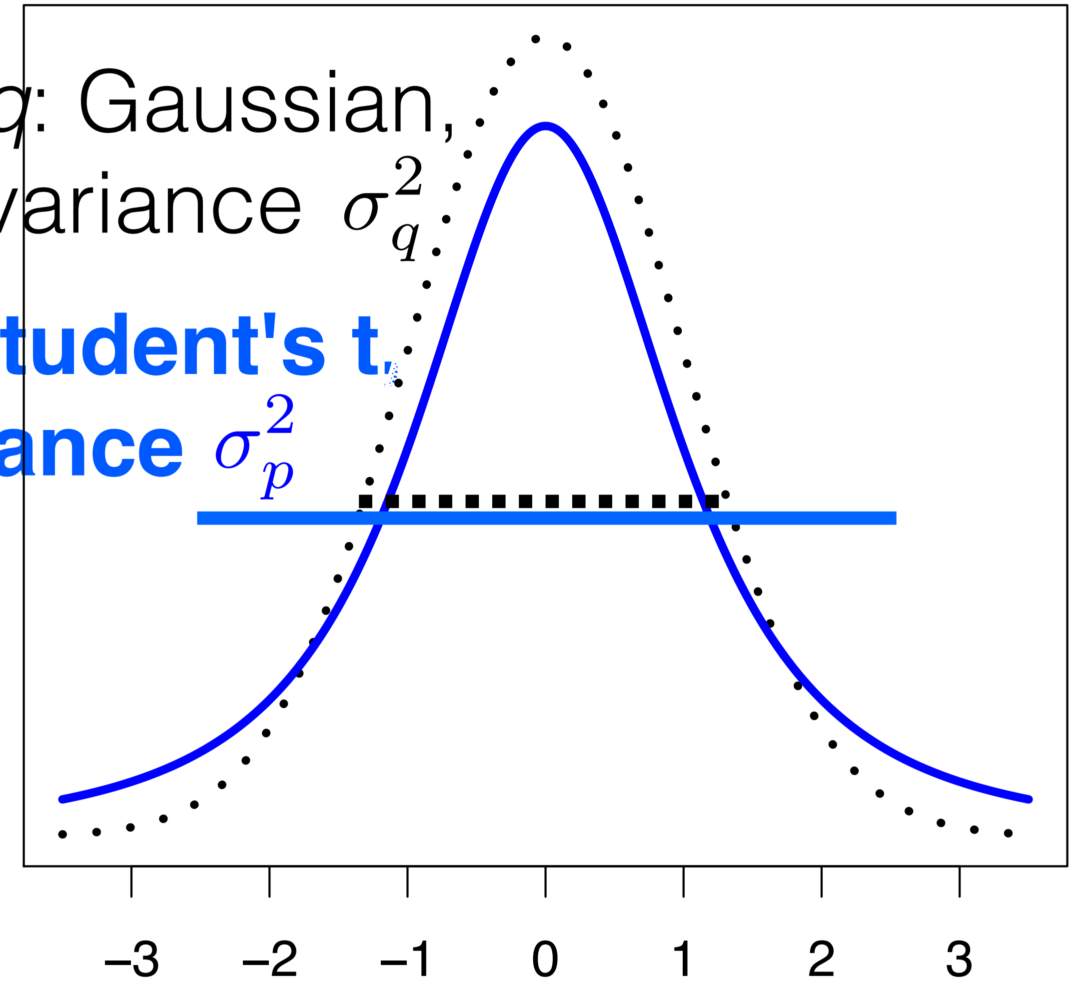

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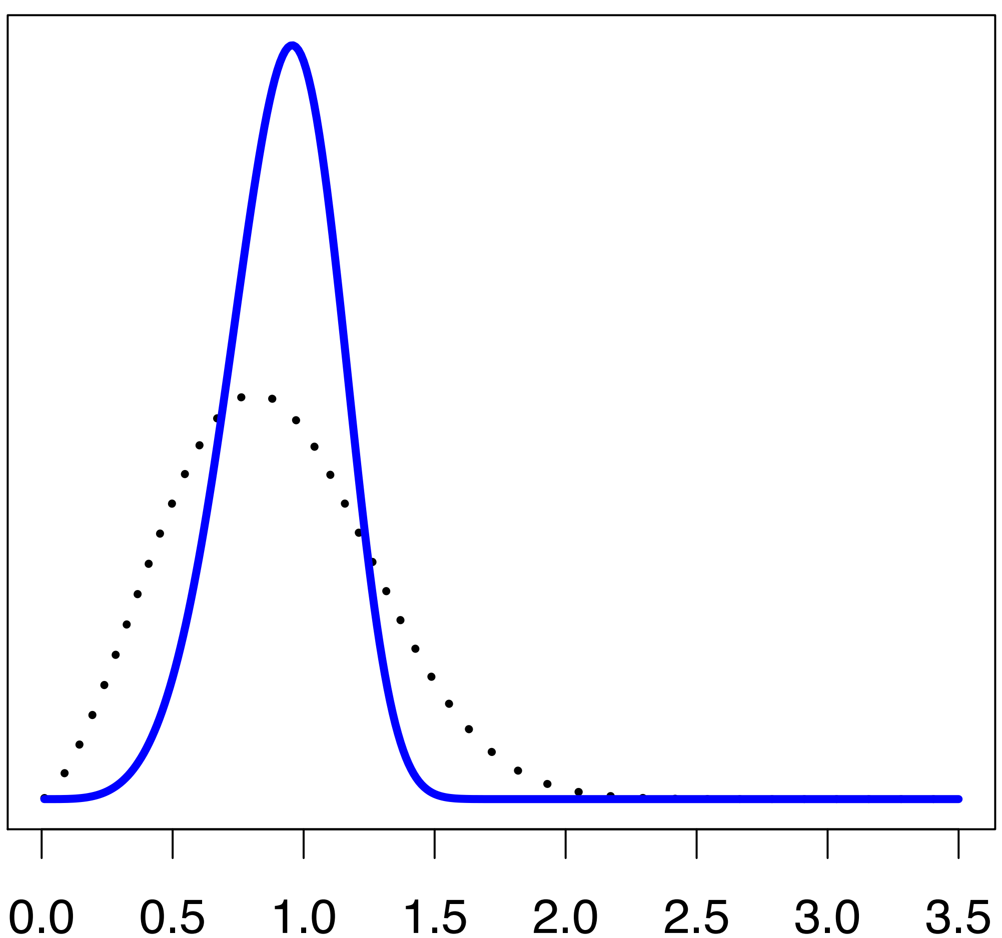

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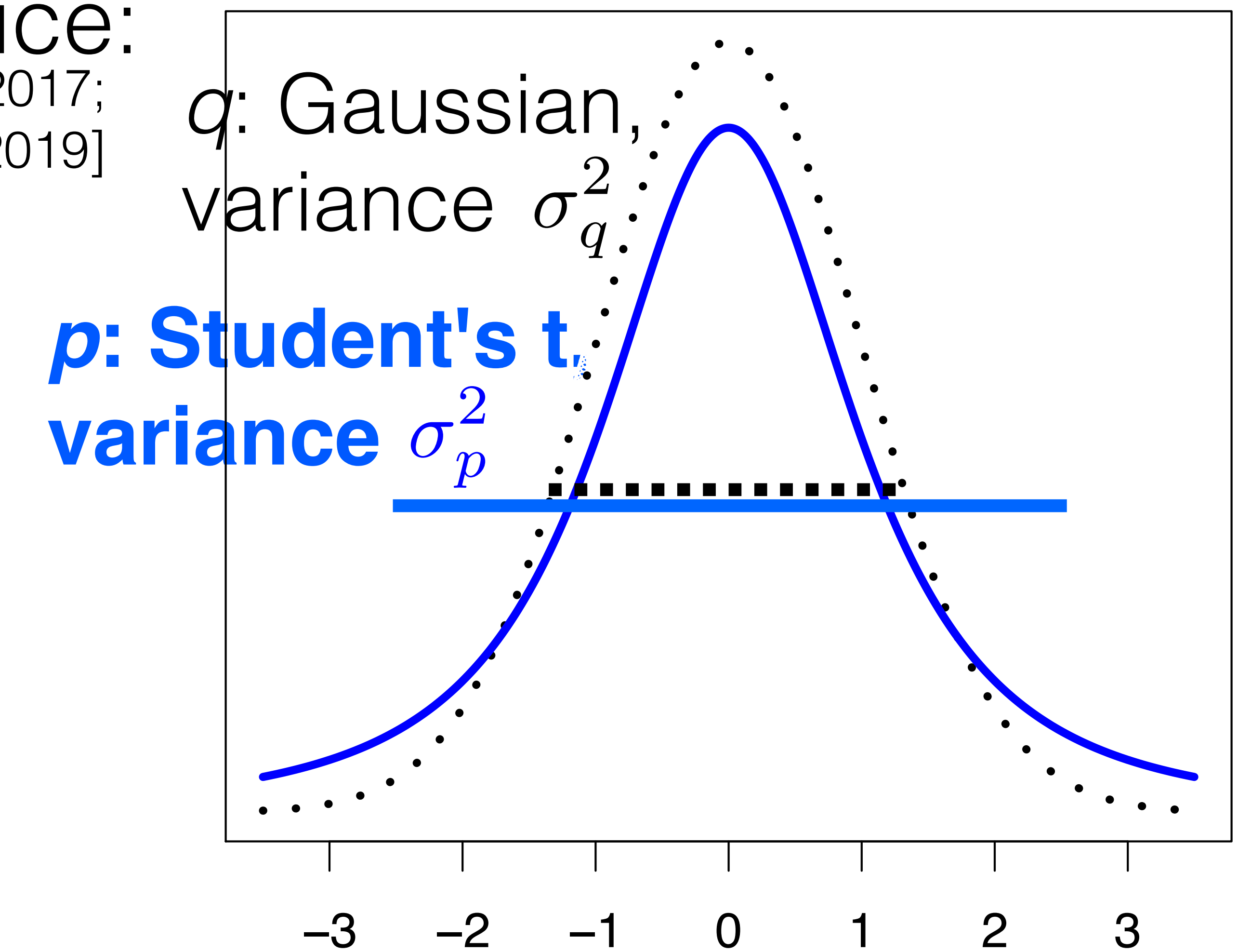

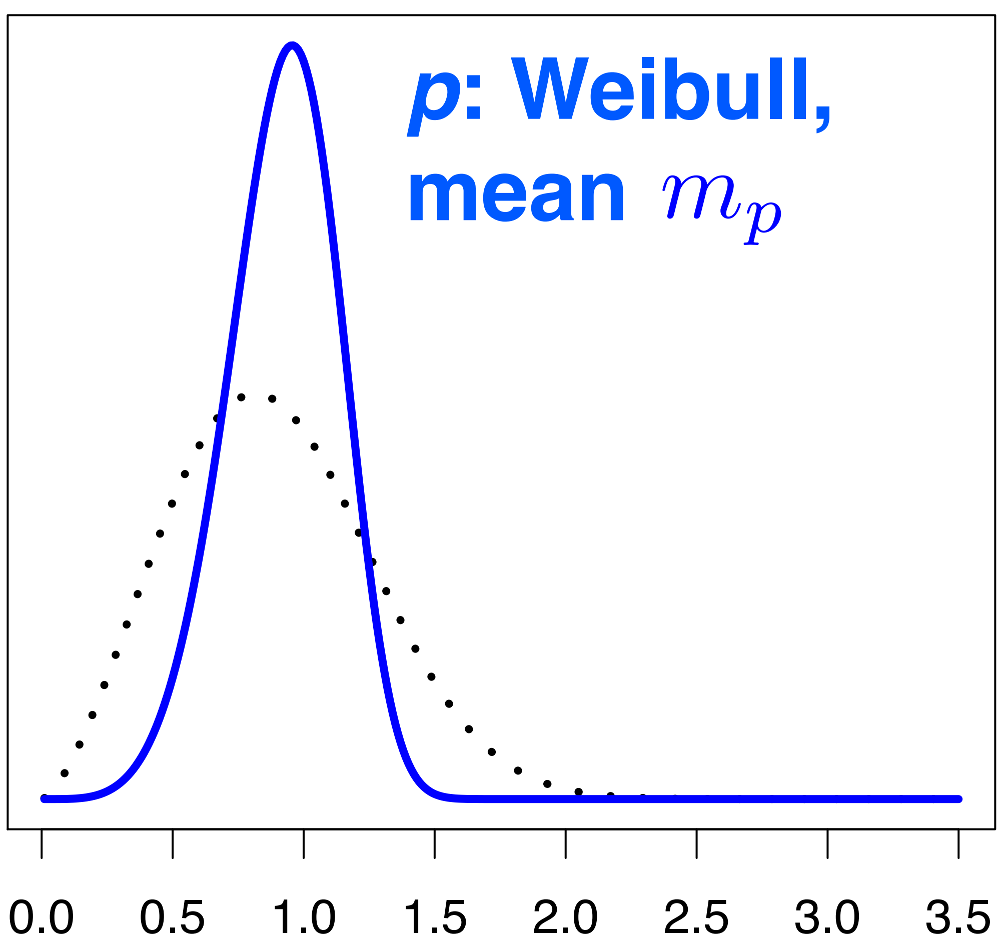

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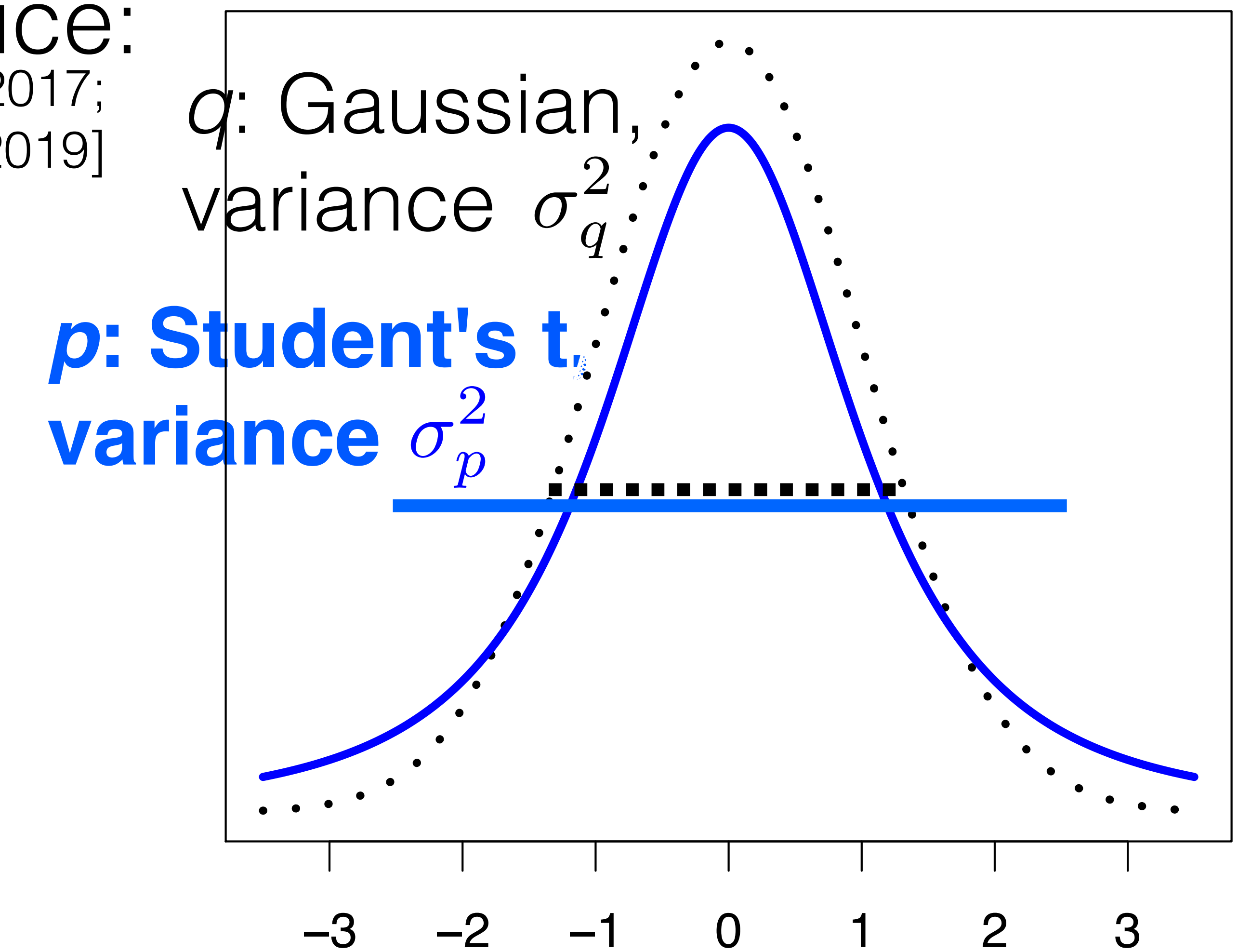

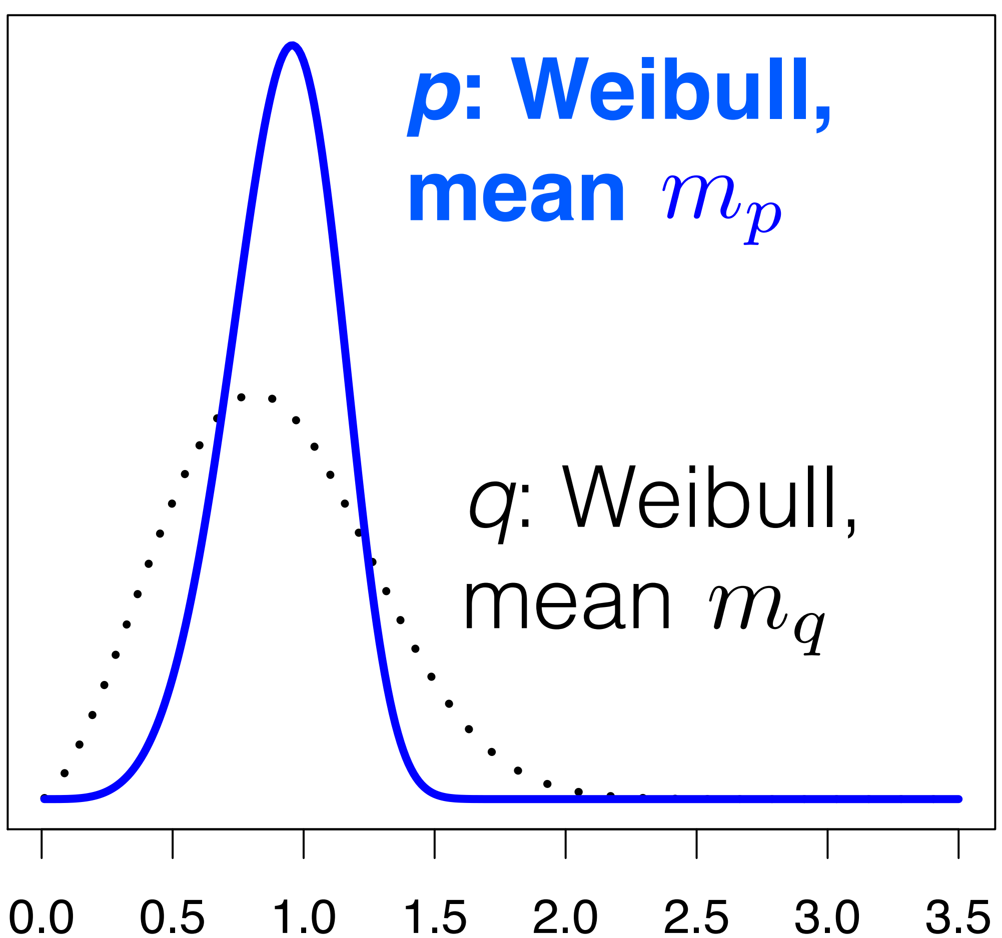

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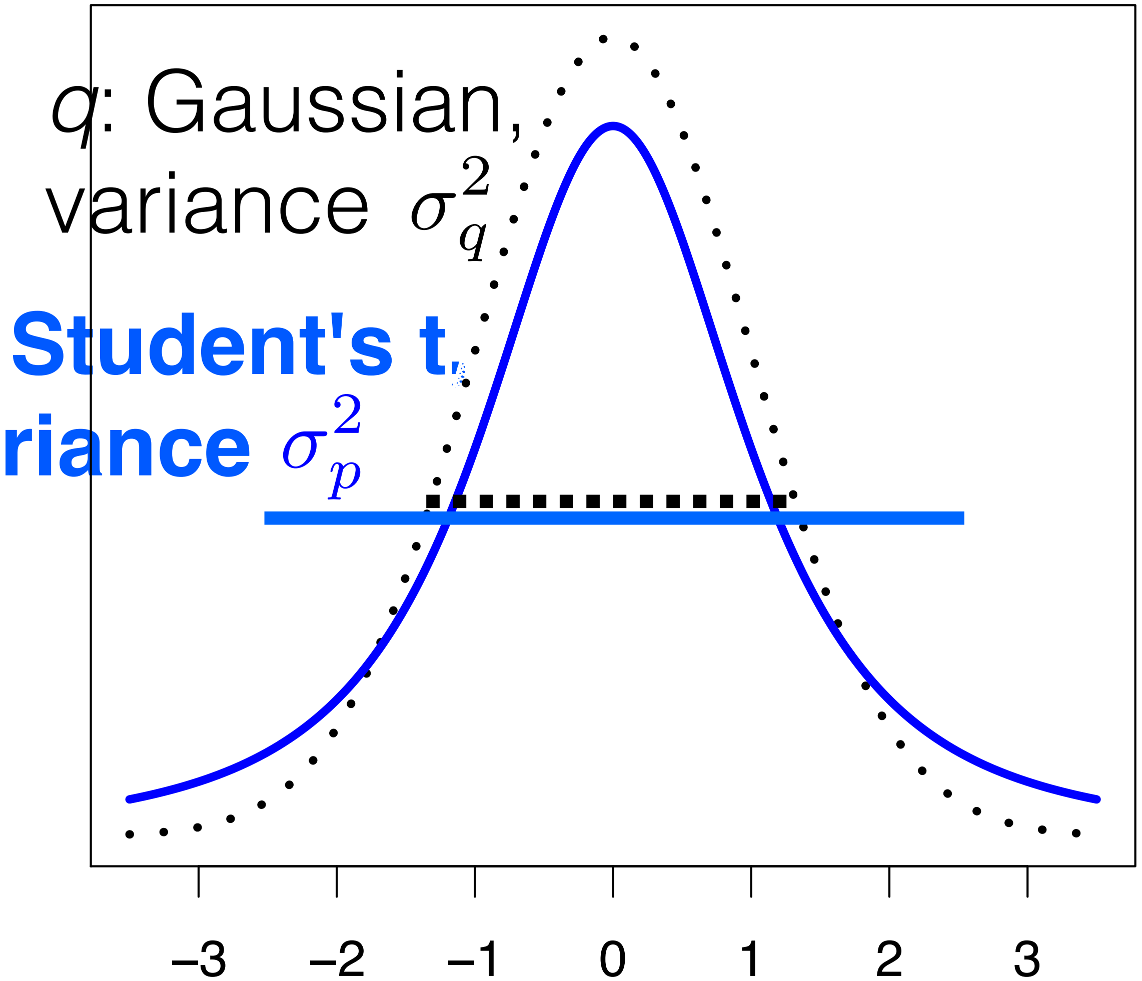

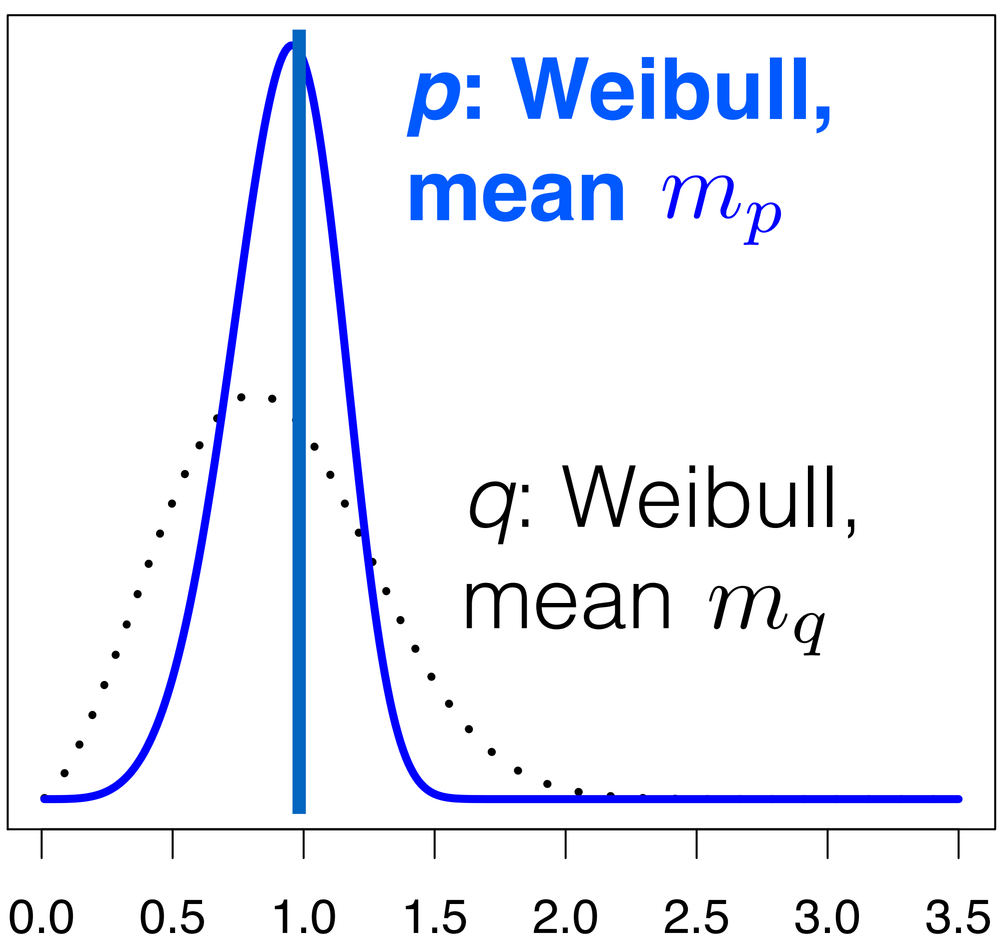

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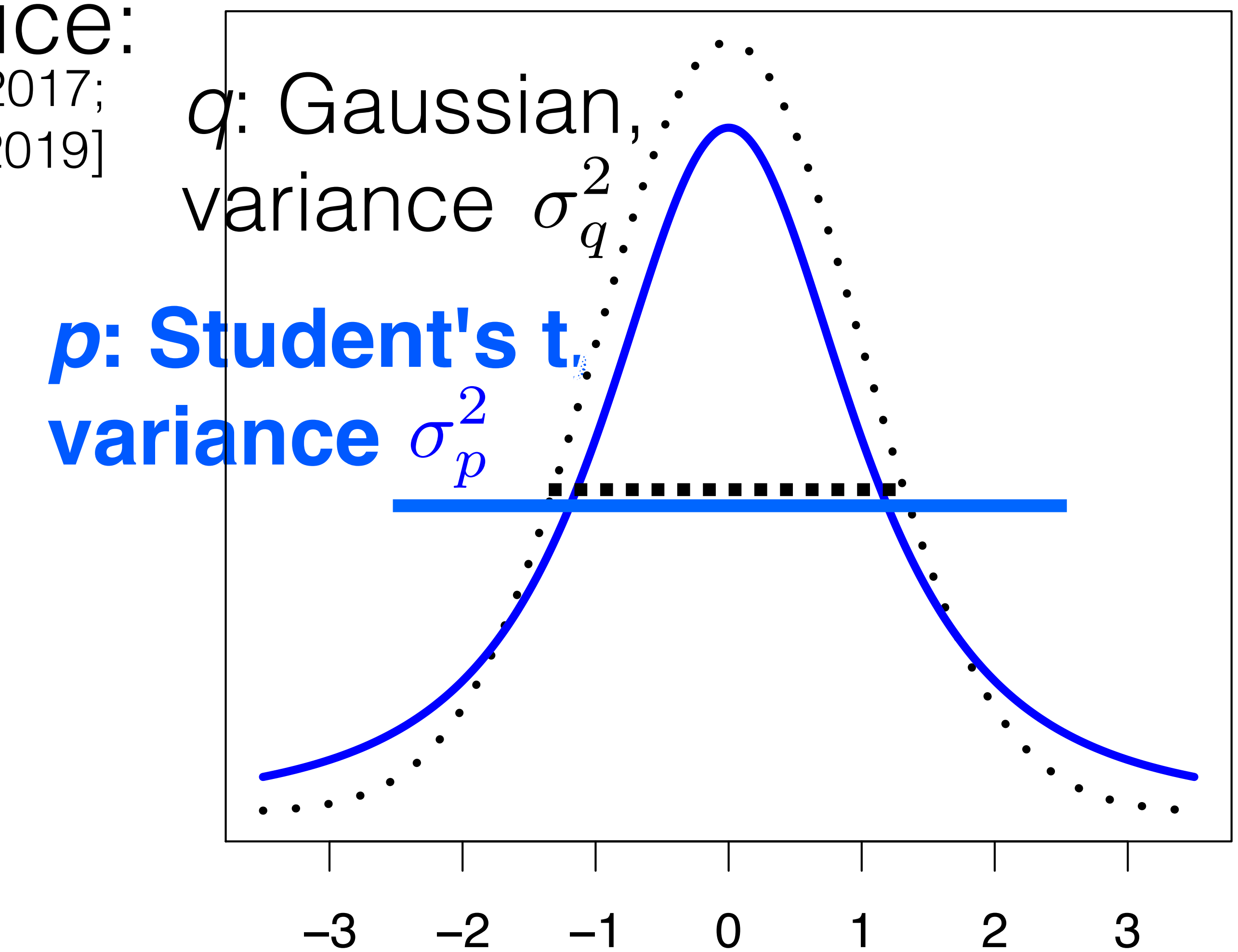

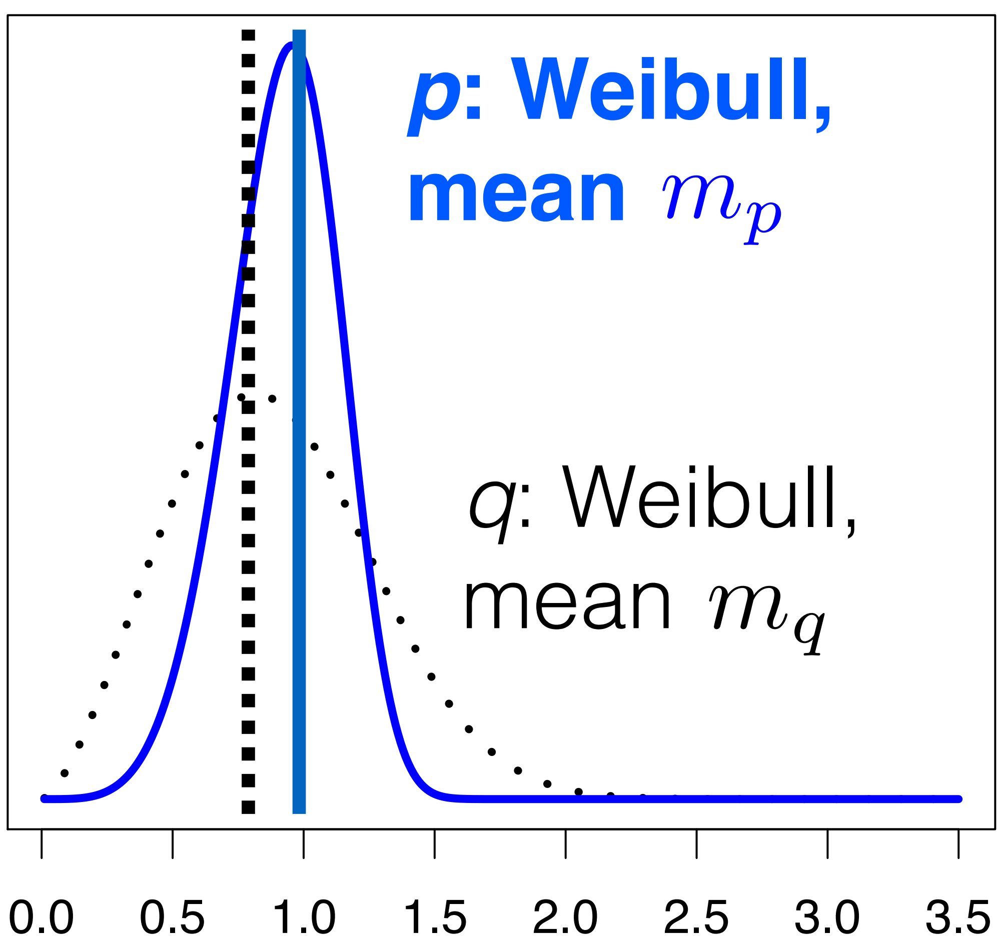

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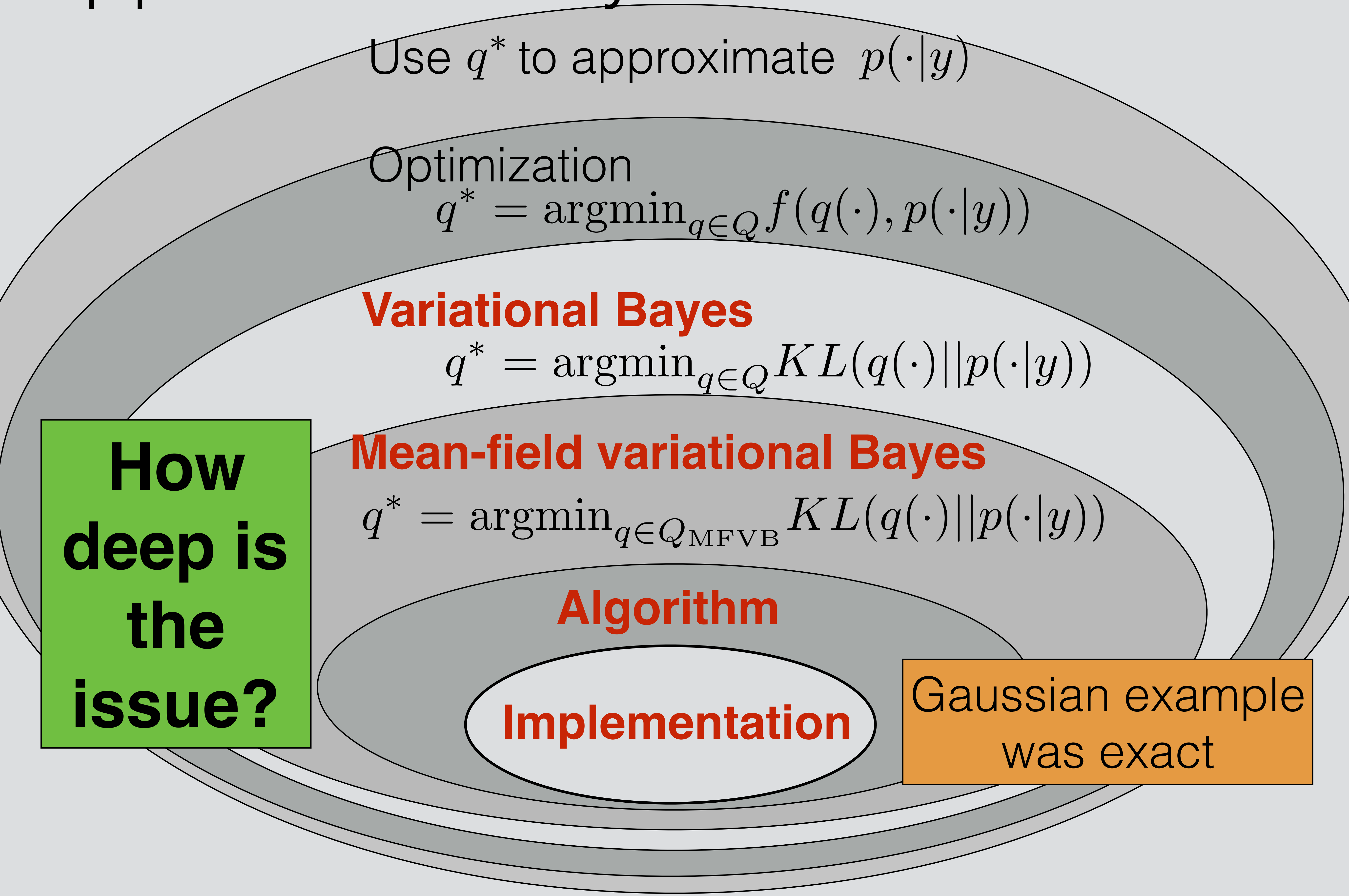

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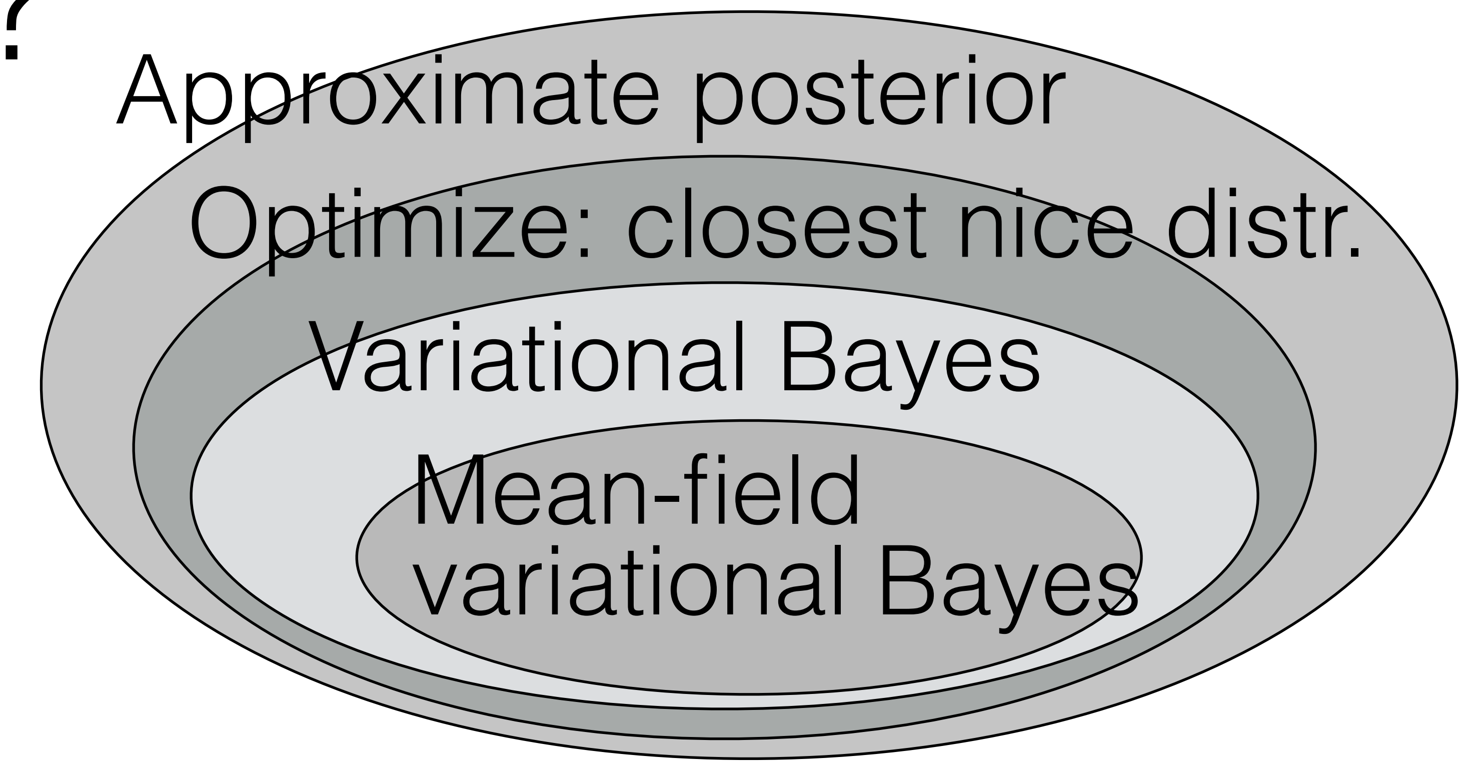

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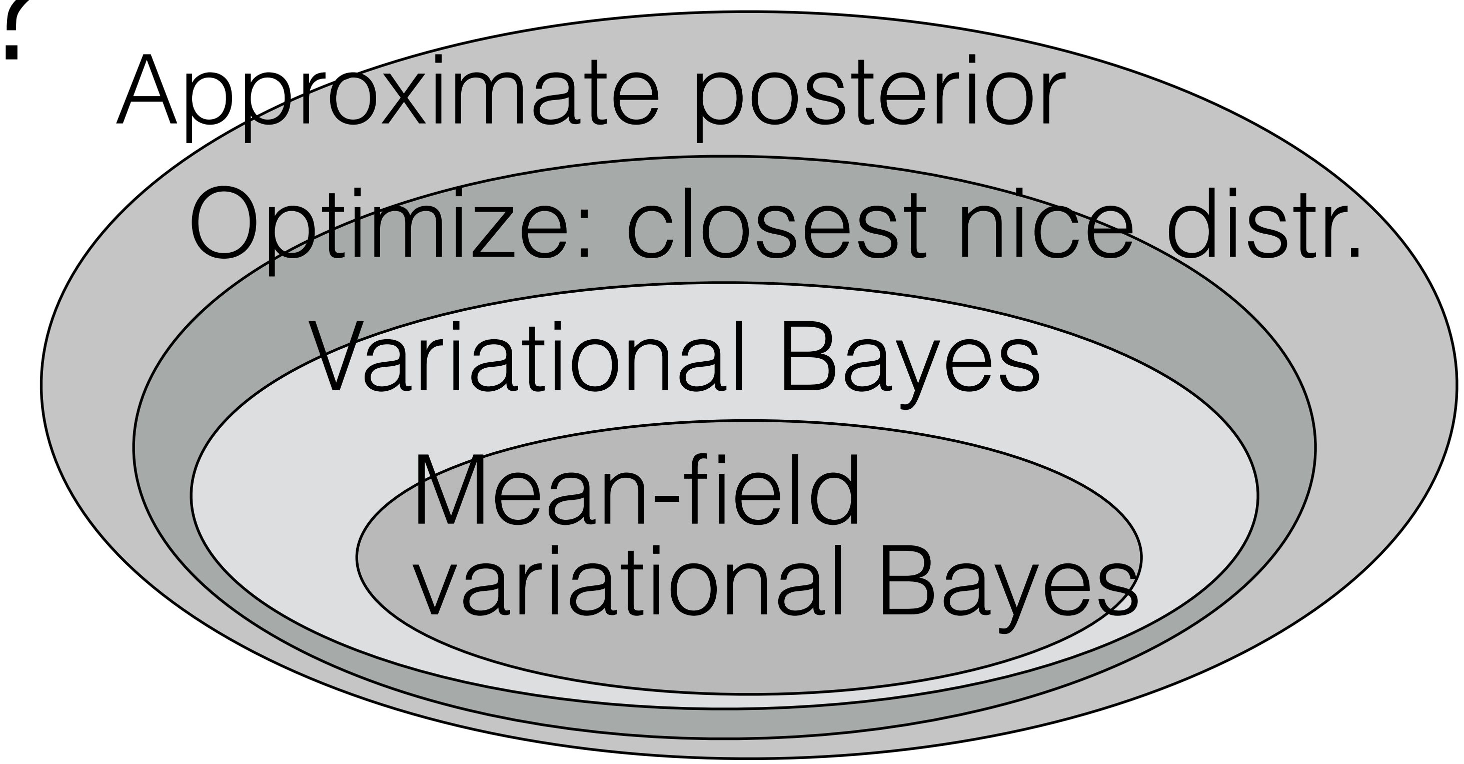

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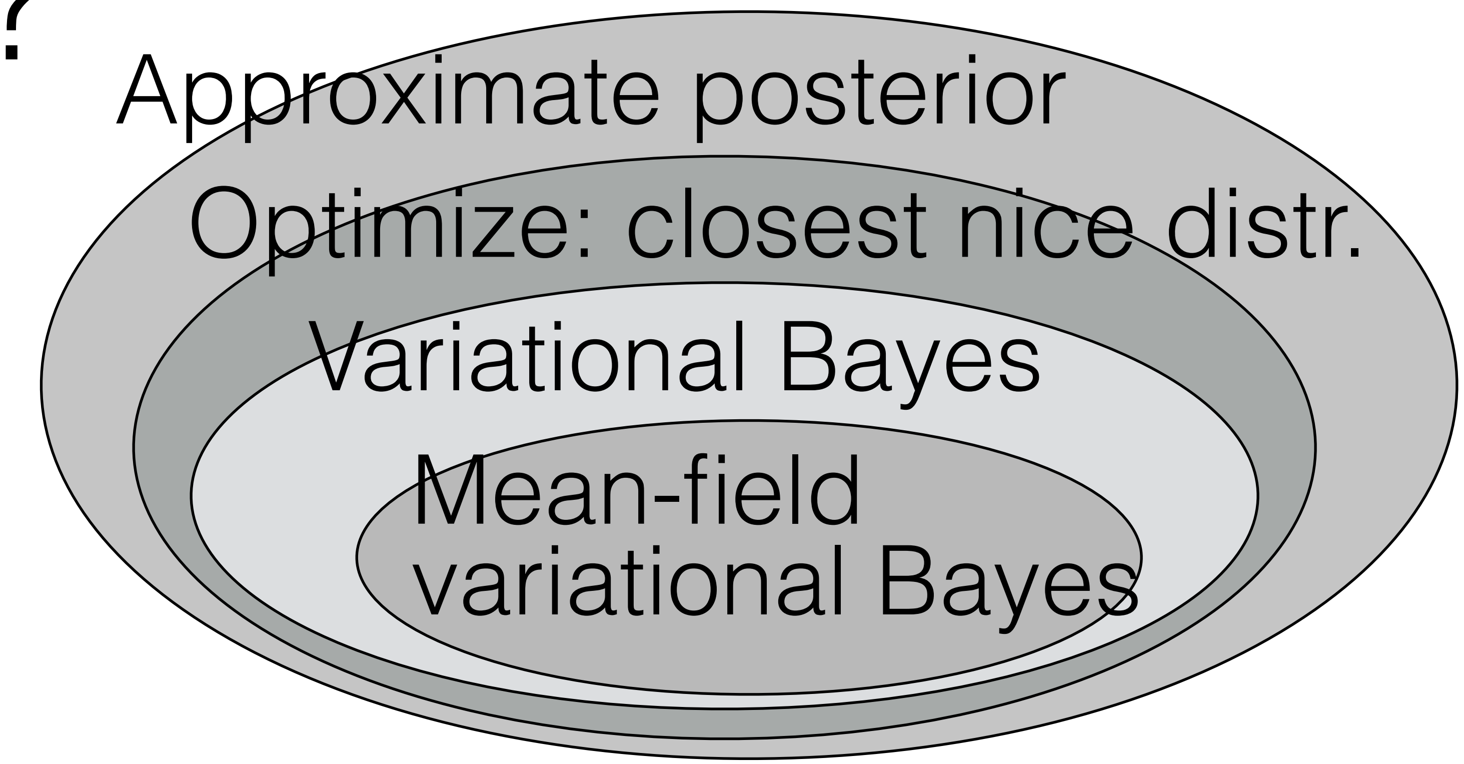

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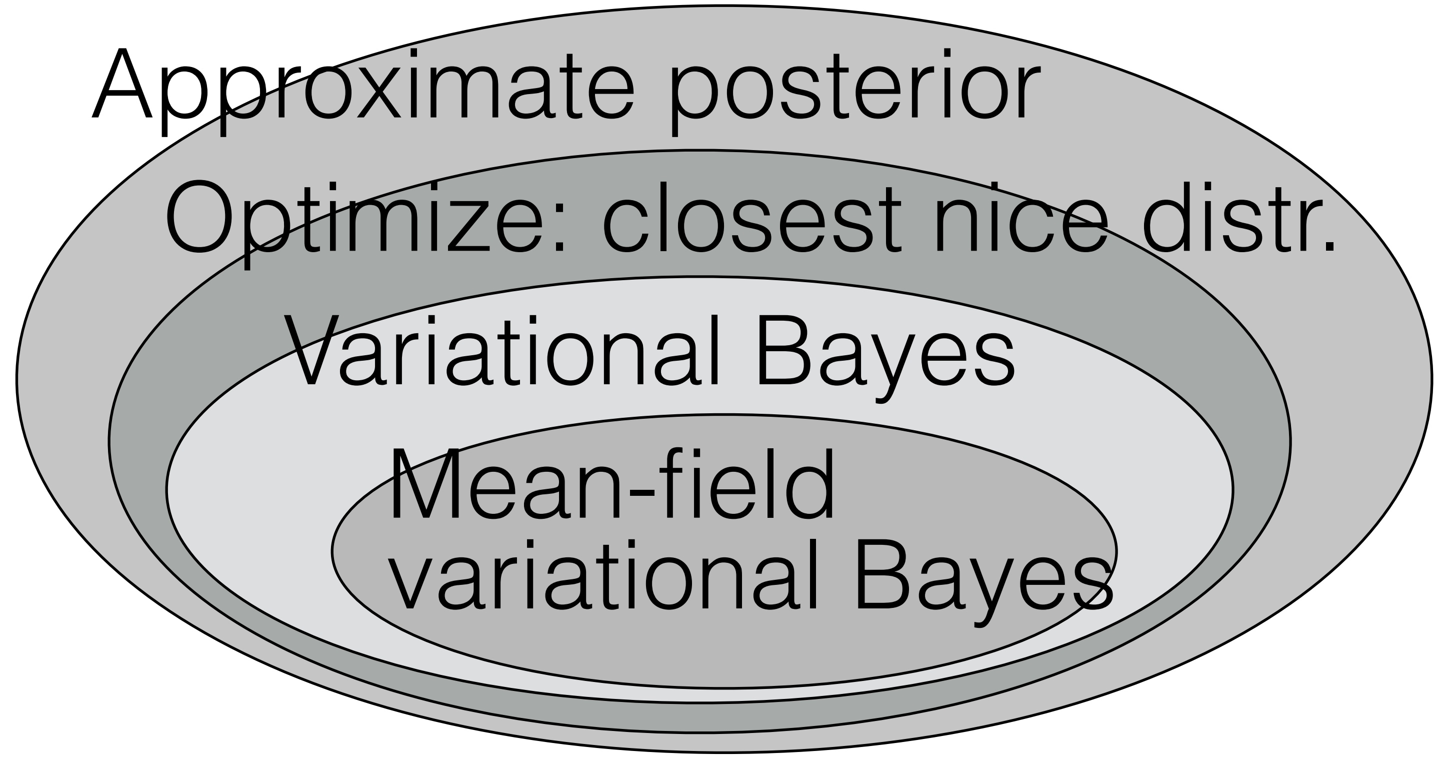

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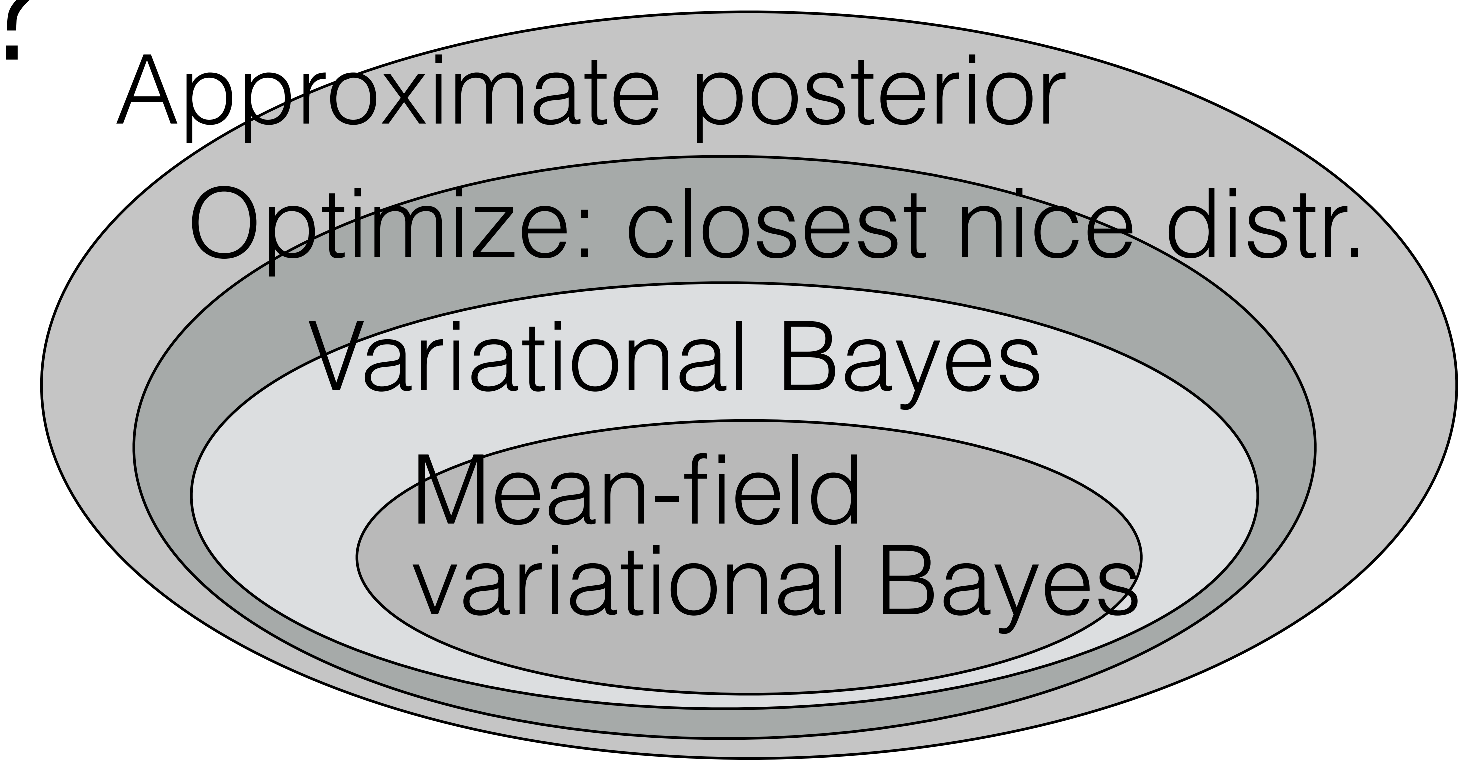

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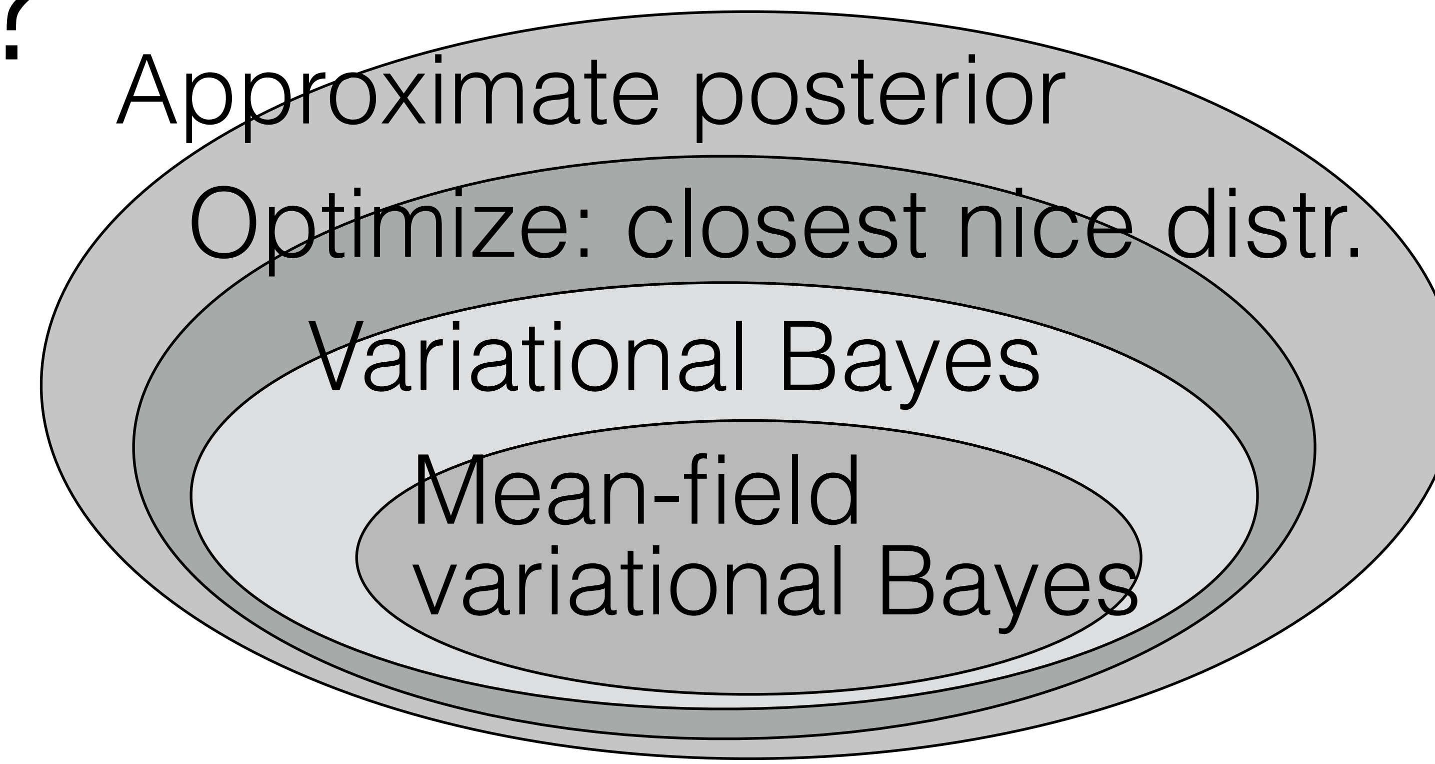

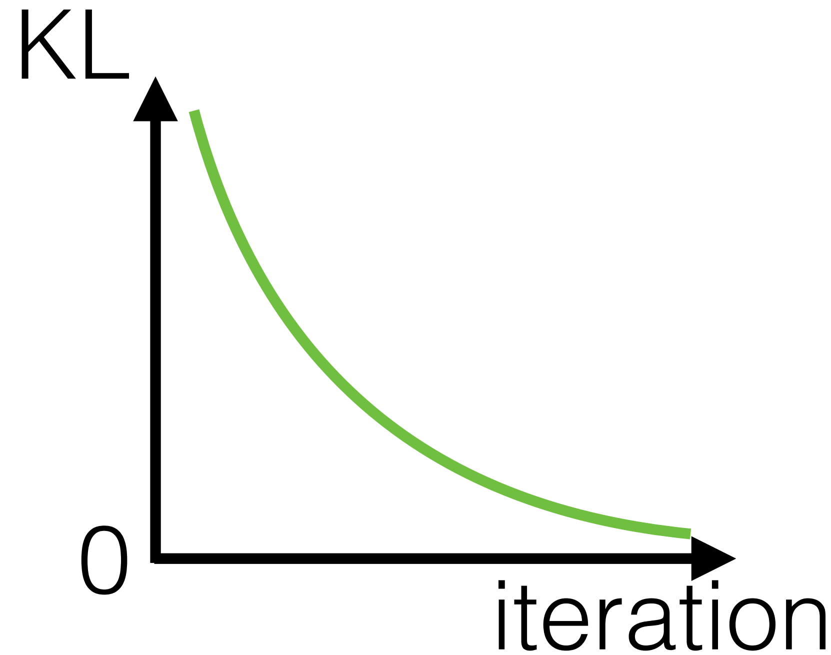

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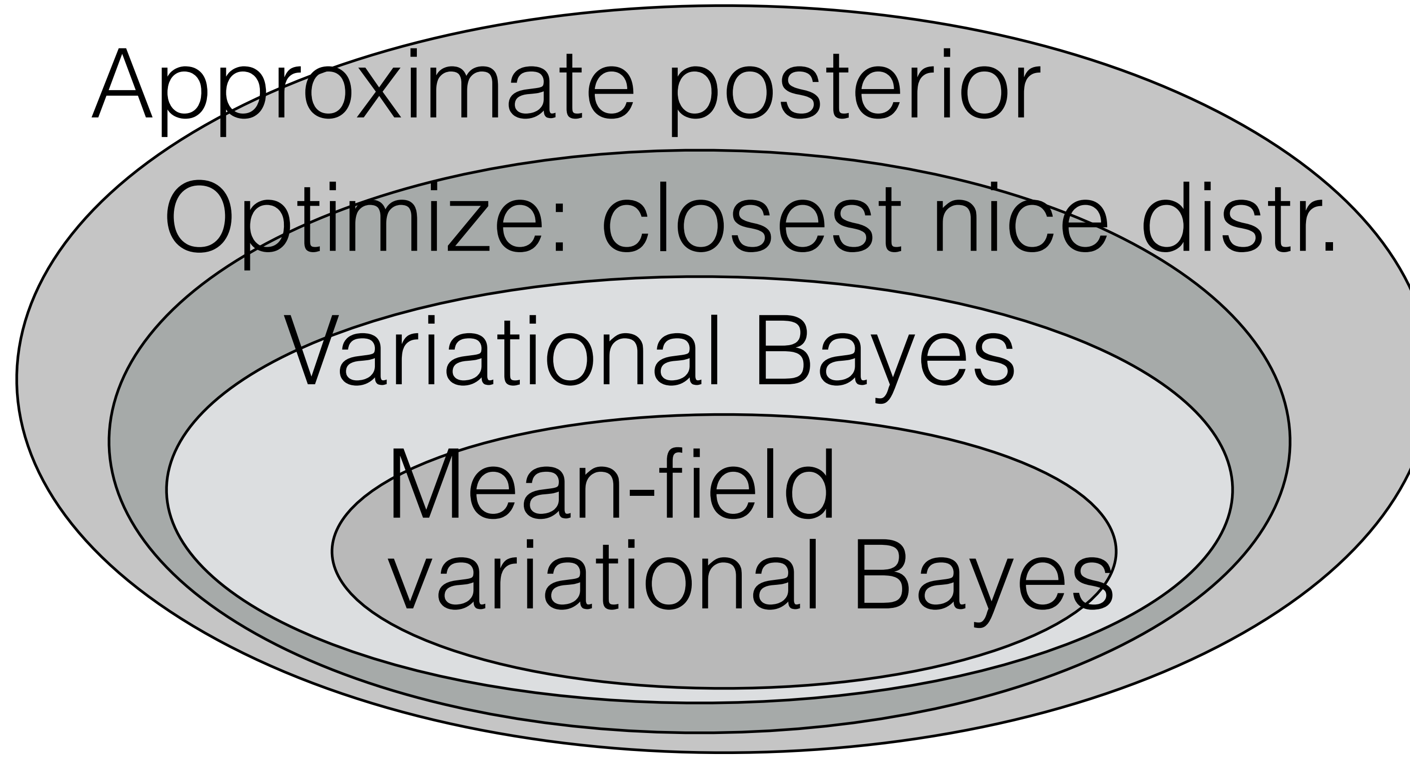

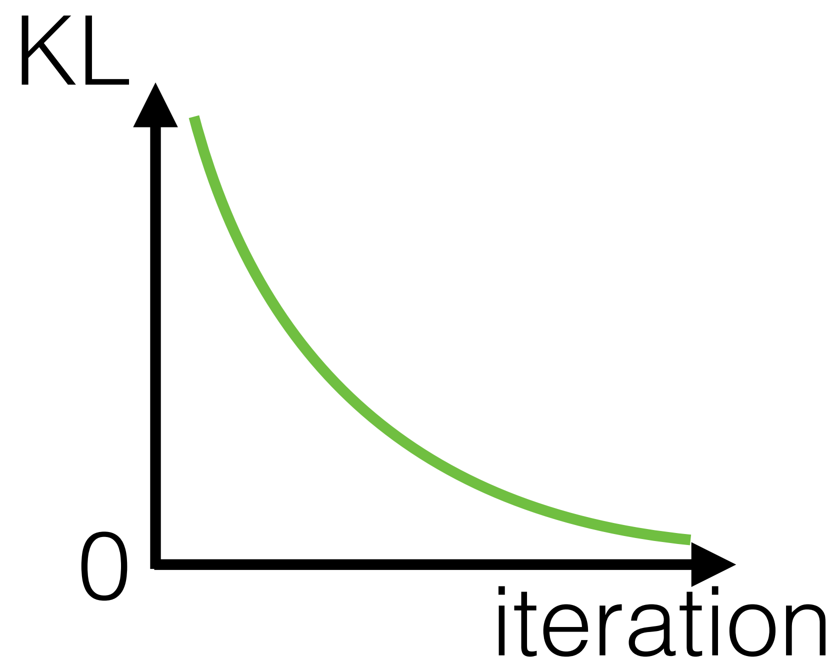

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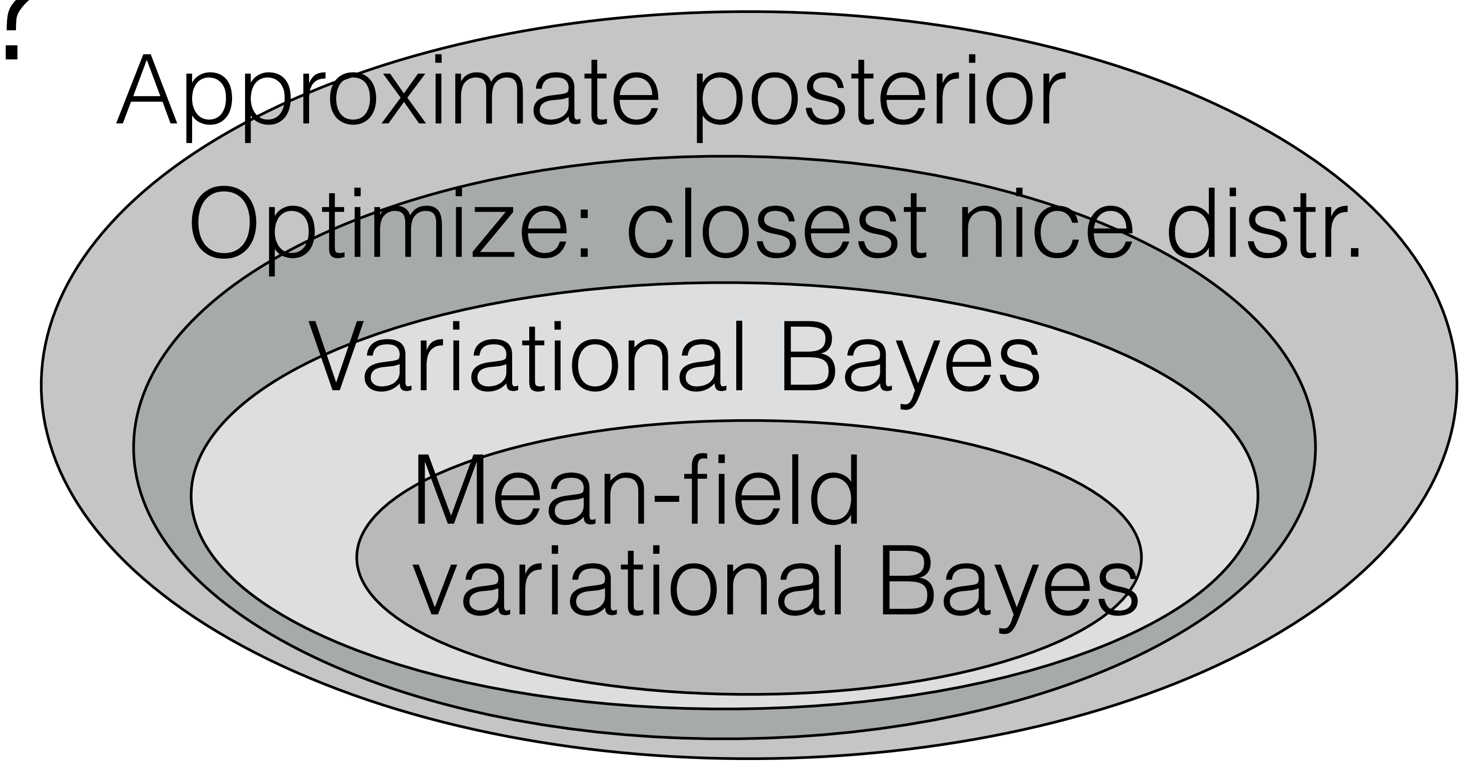

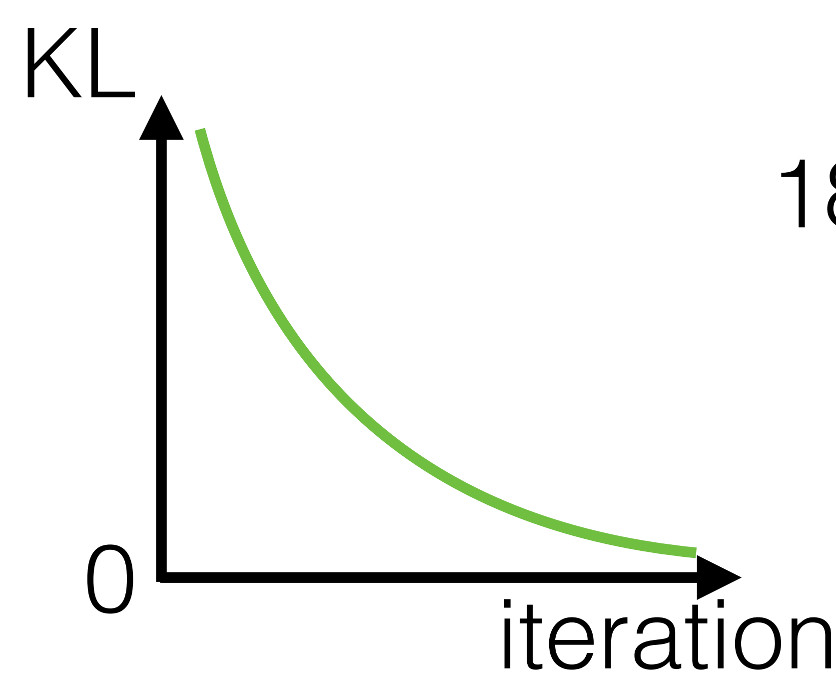

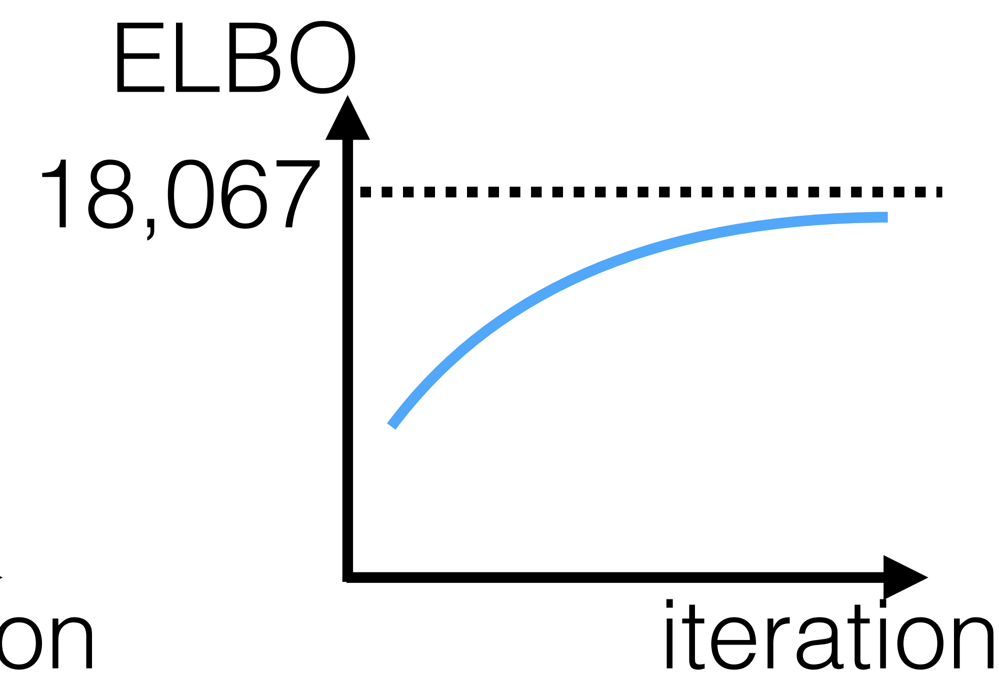

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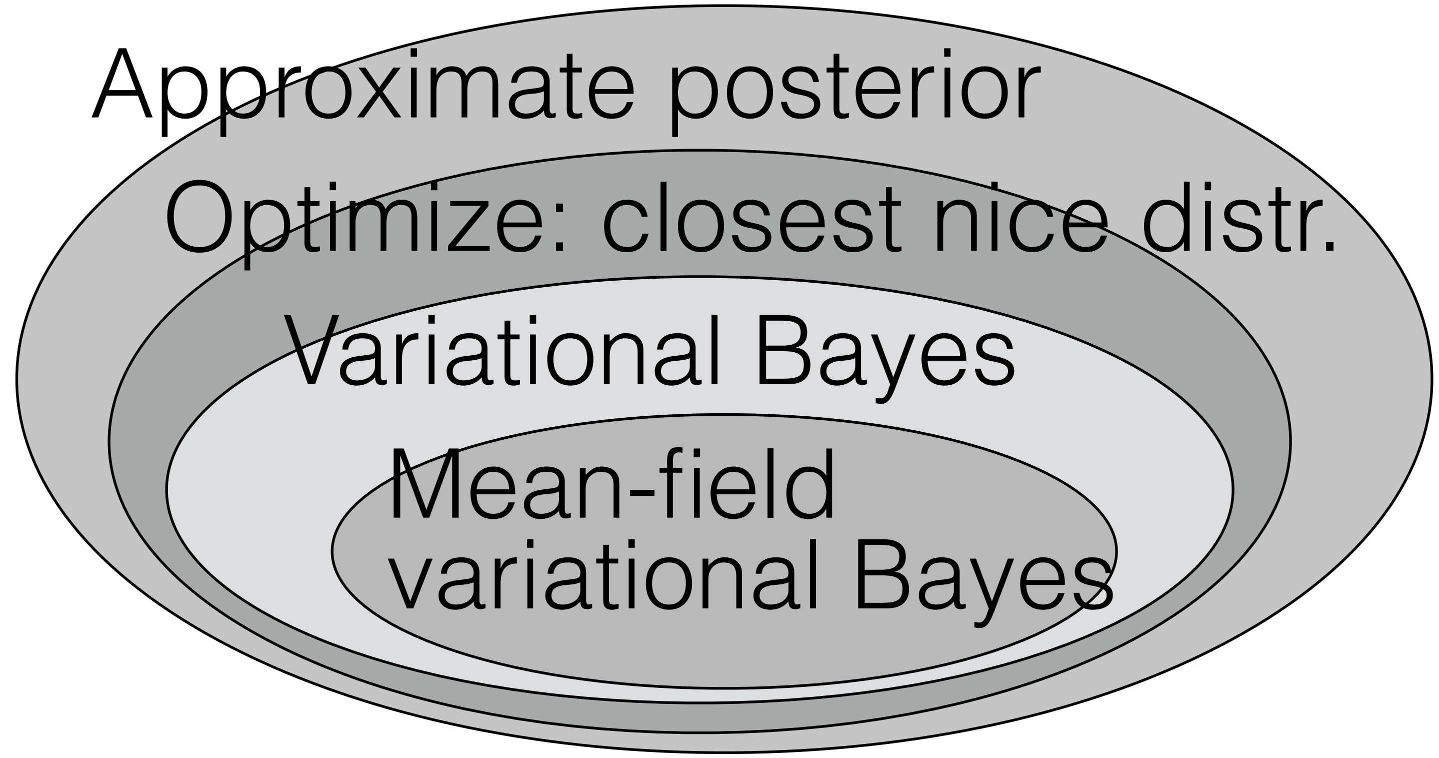

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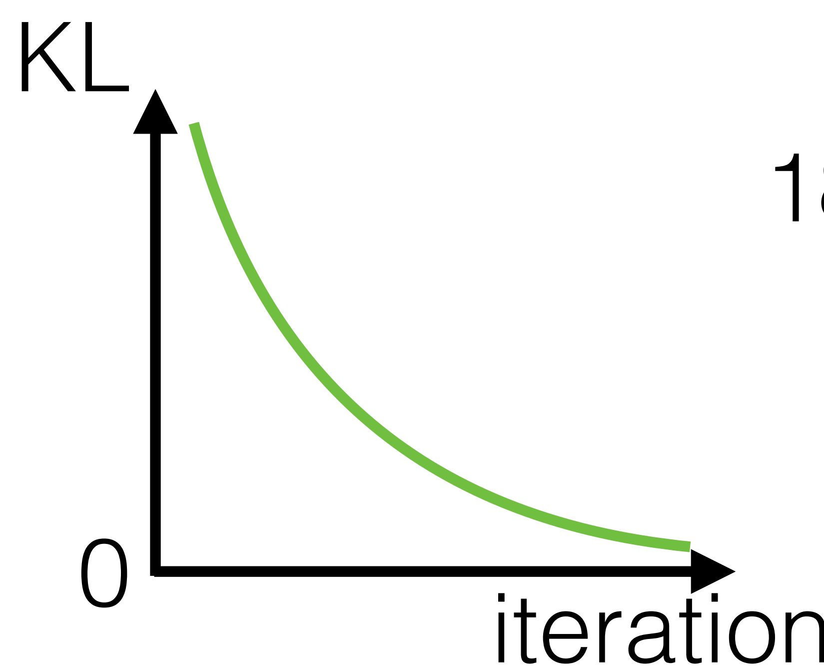

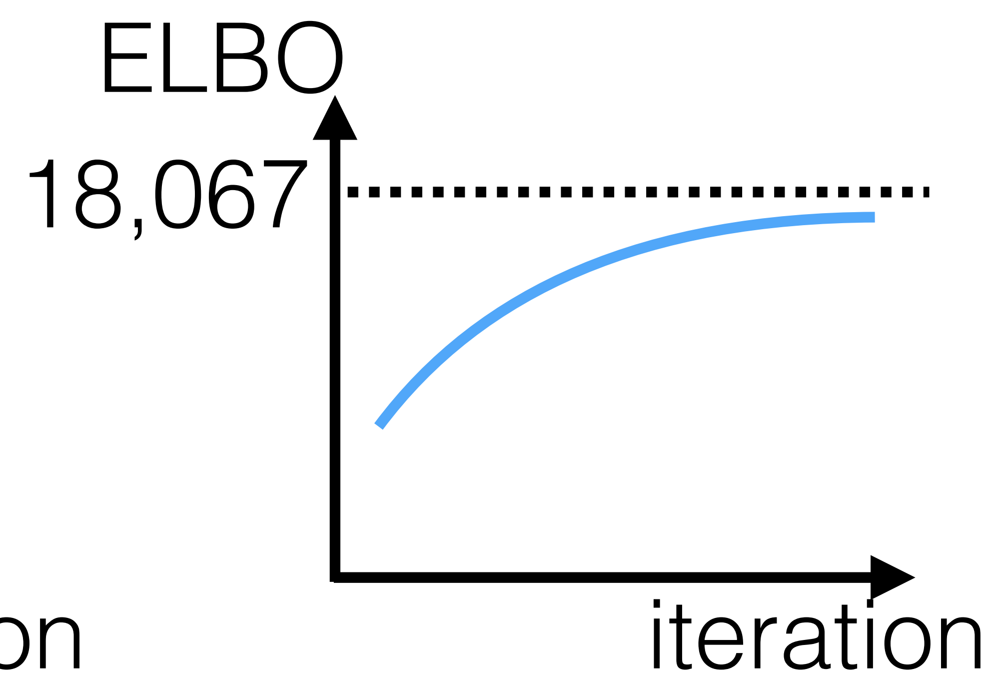

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"Yes, but did it work? Evaluating variational inference" ICML 2018

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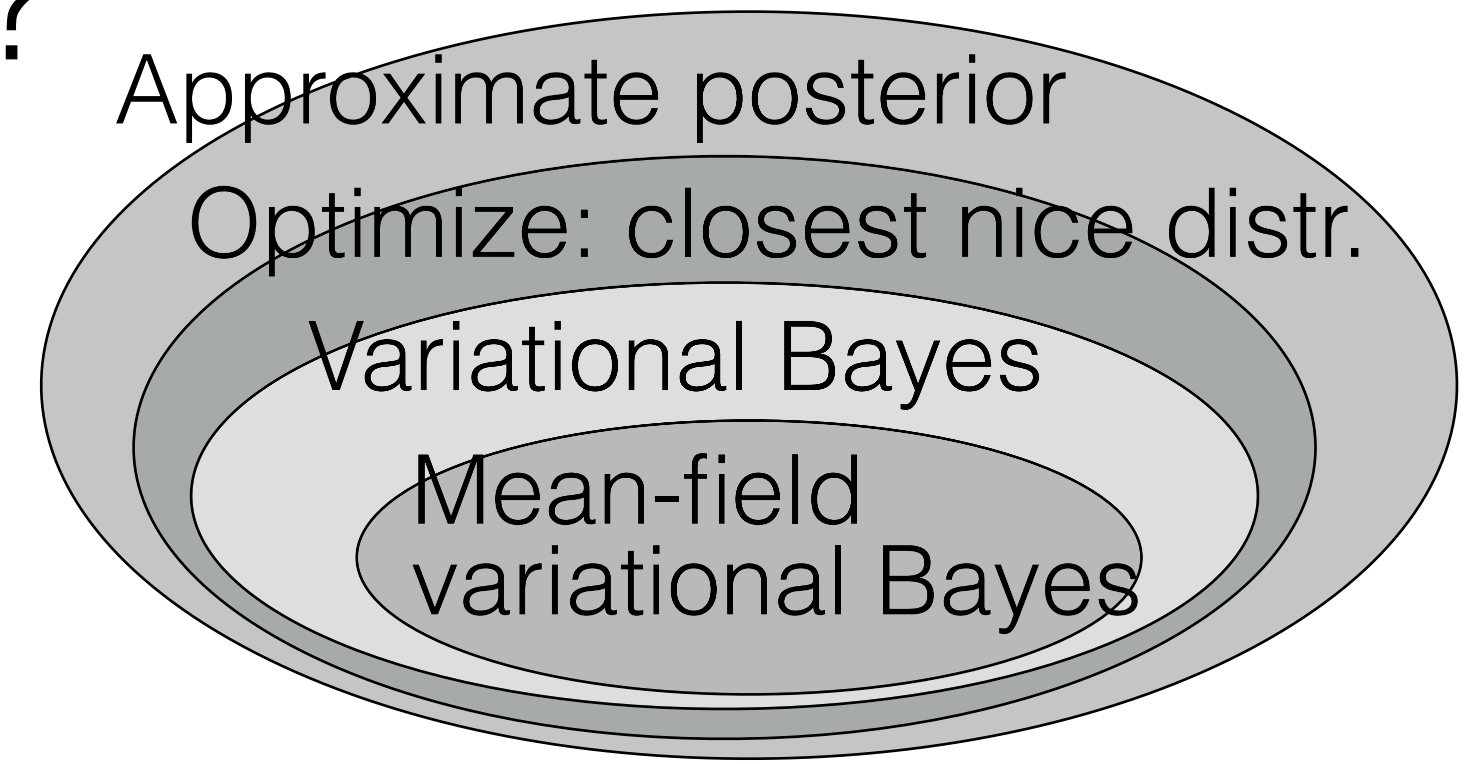

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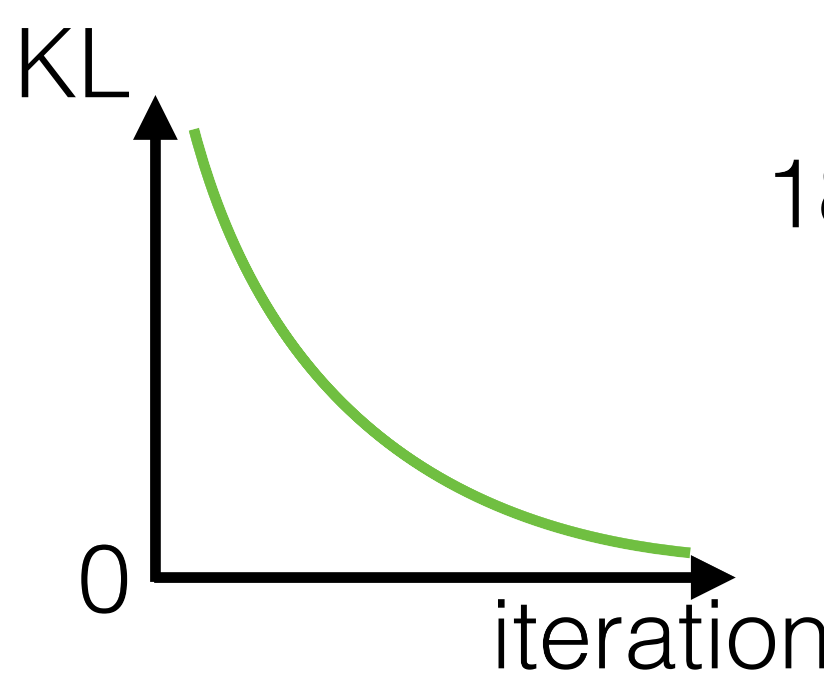

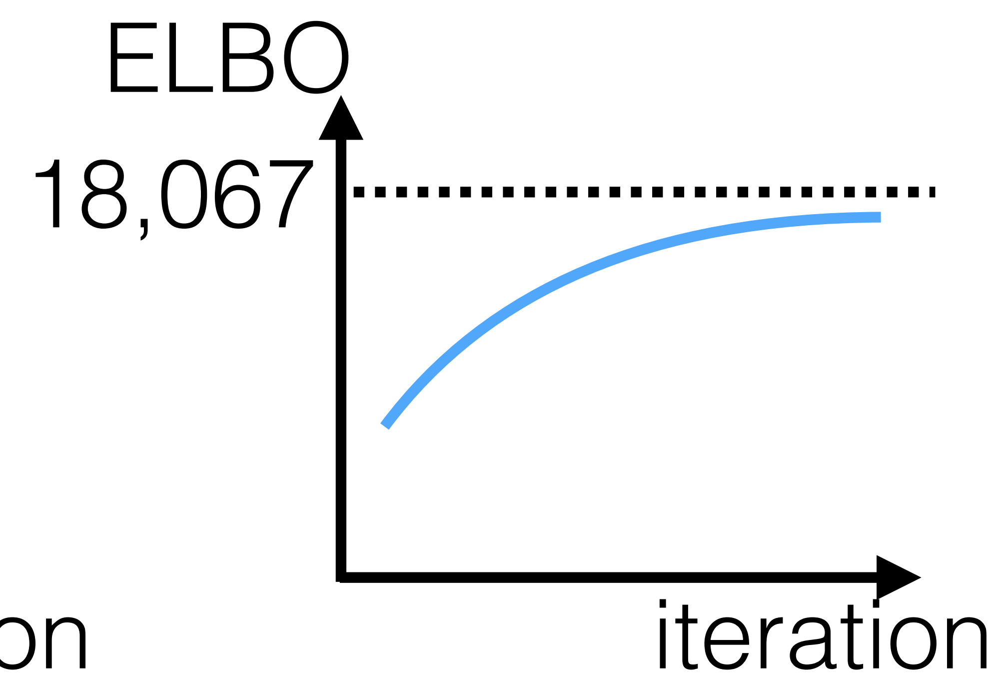

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→ "Practical posterior error bounds from variational objectives" AISTATS 2020, to appear.

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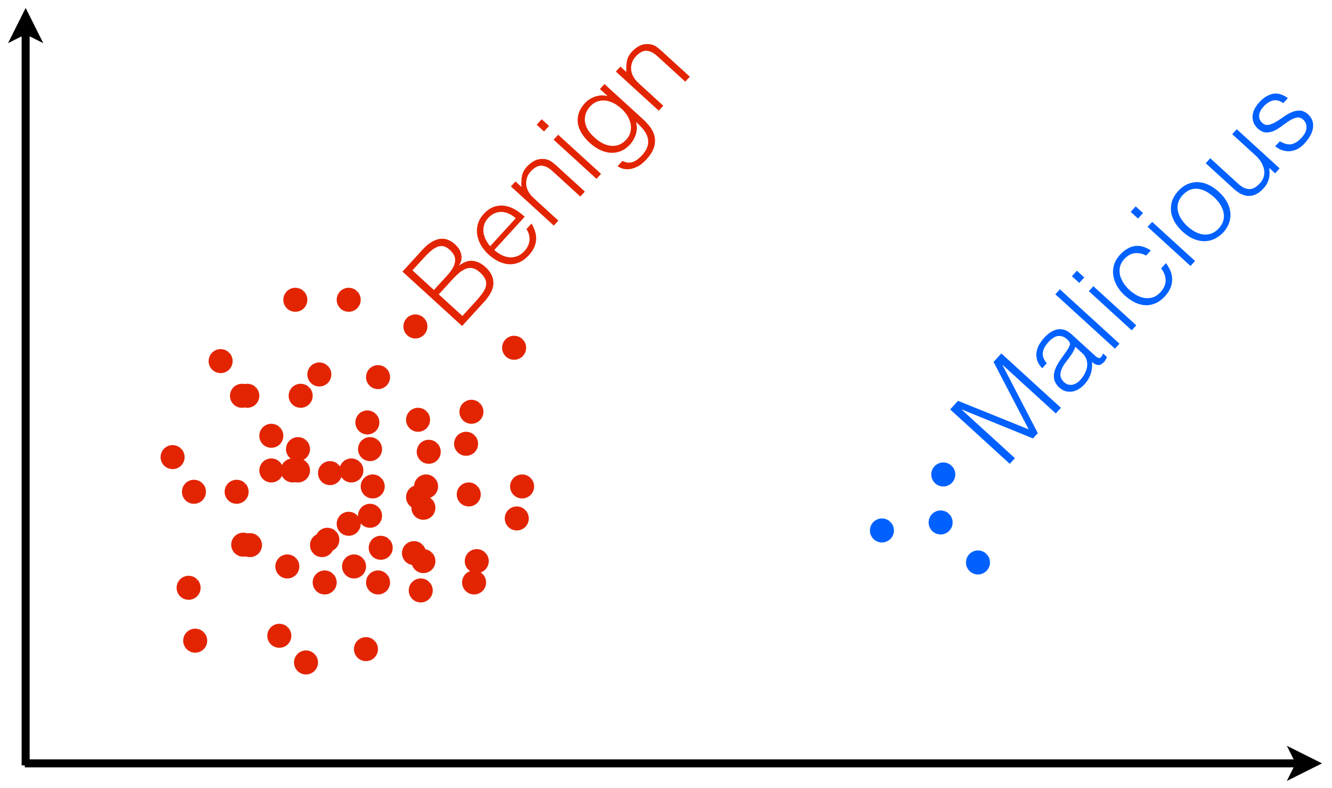

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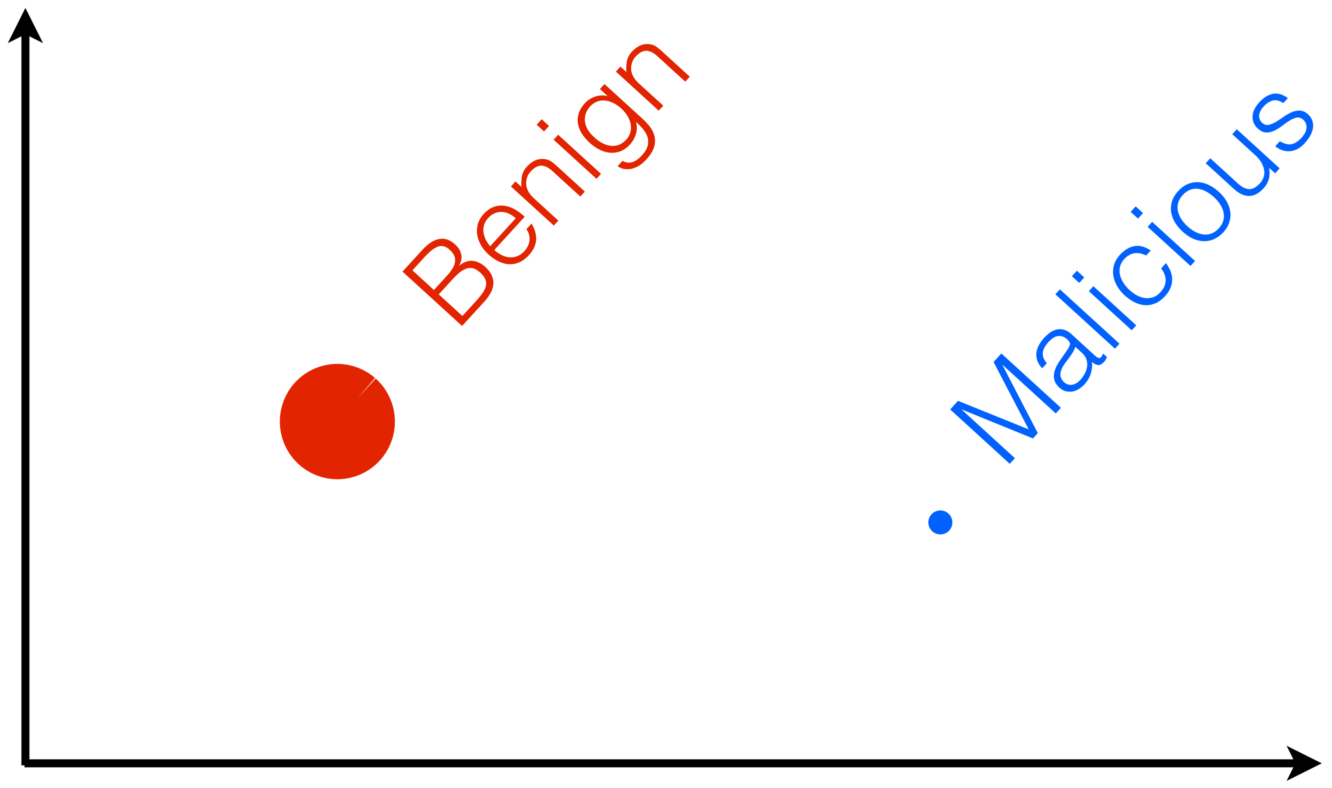

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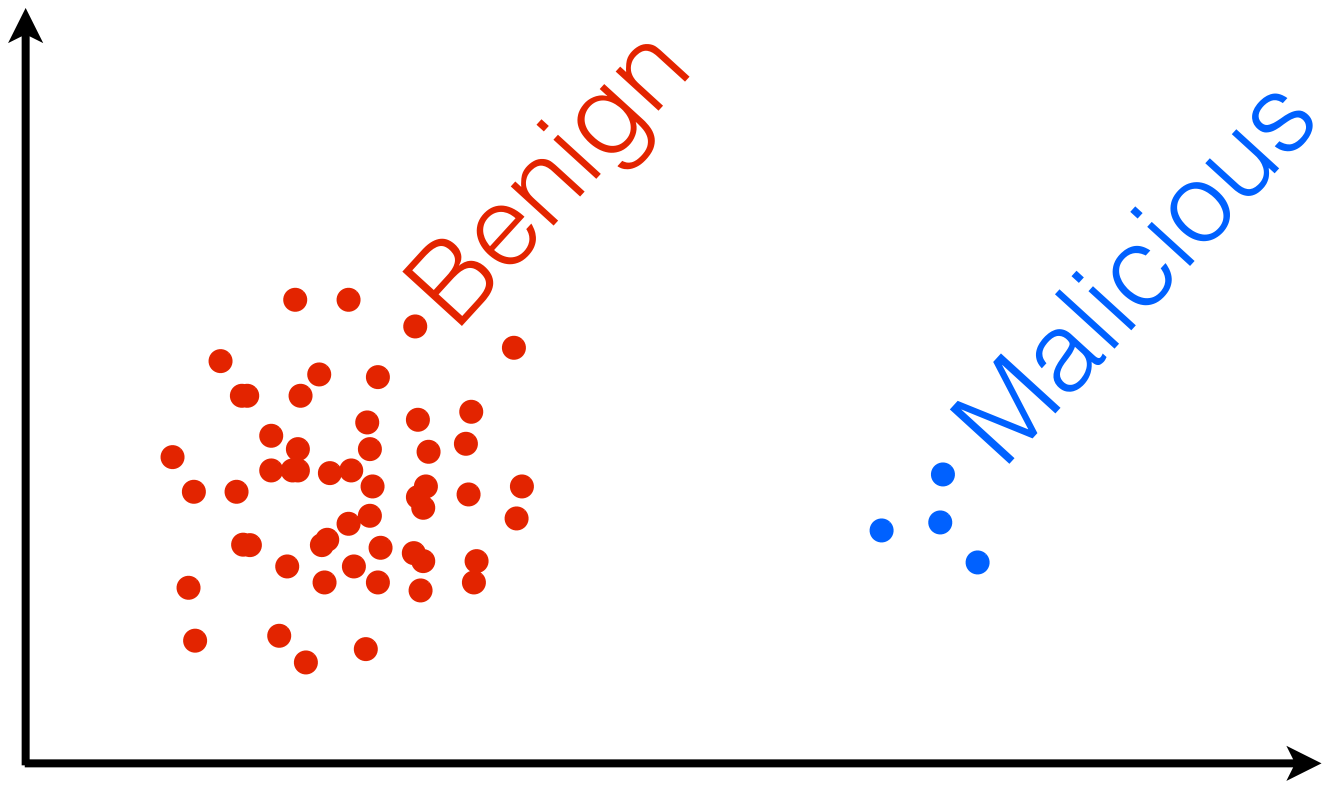

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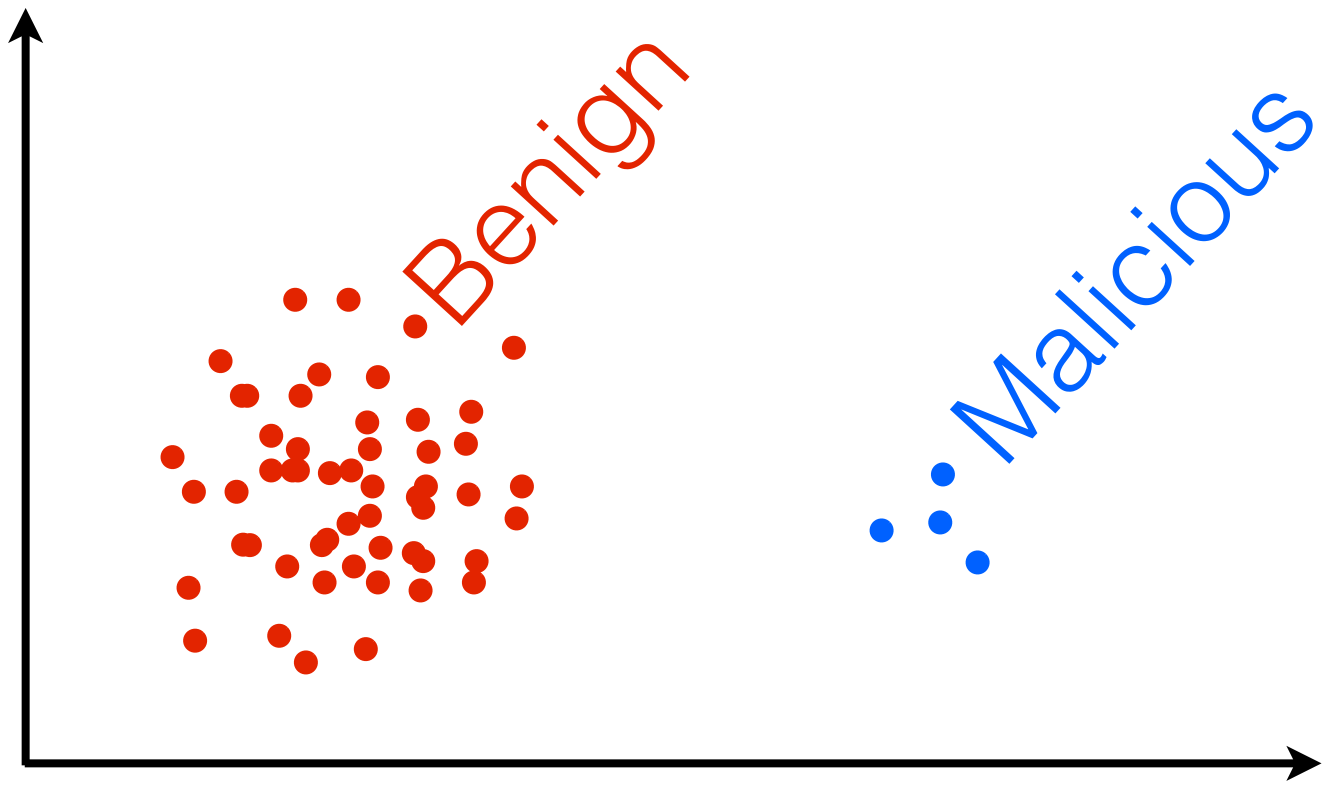

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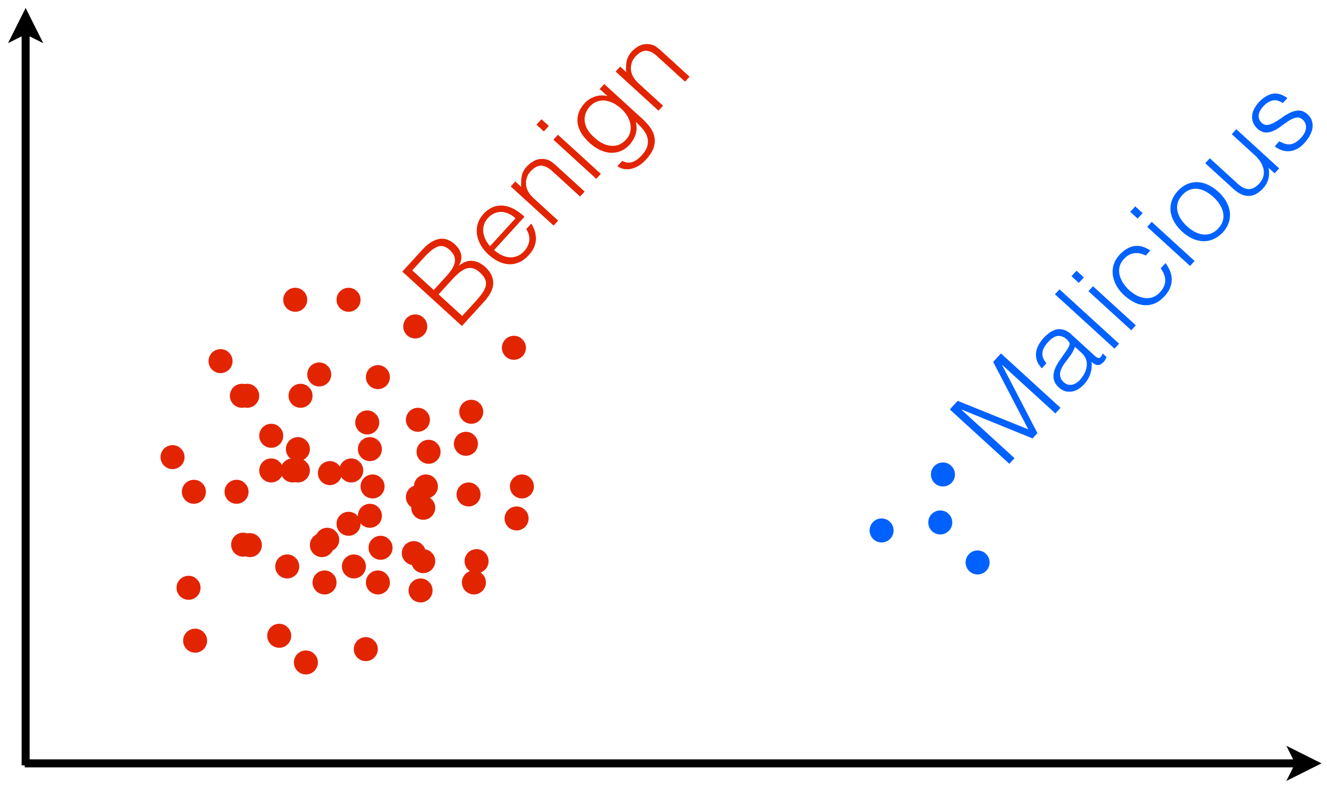

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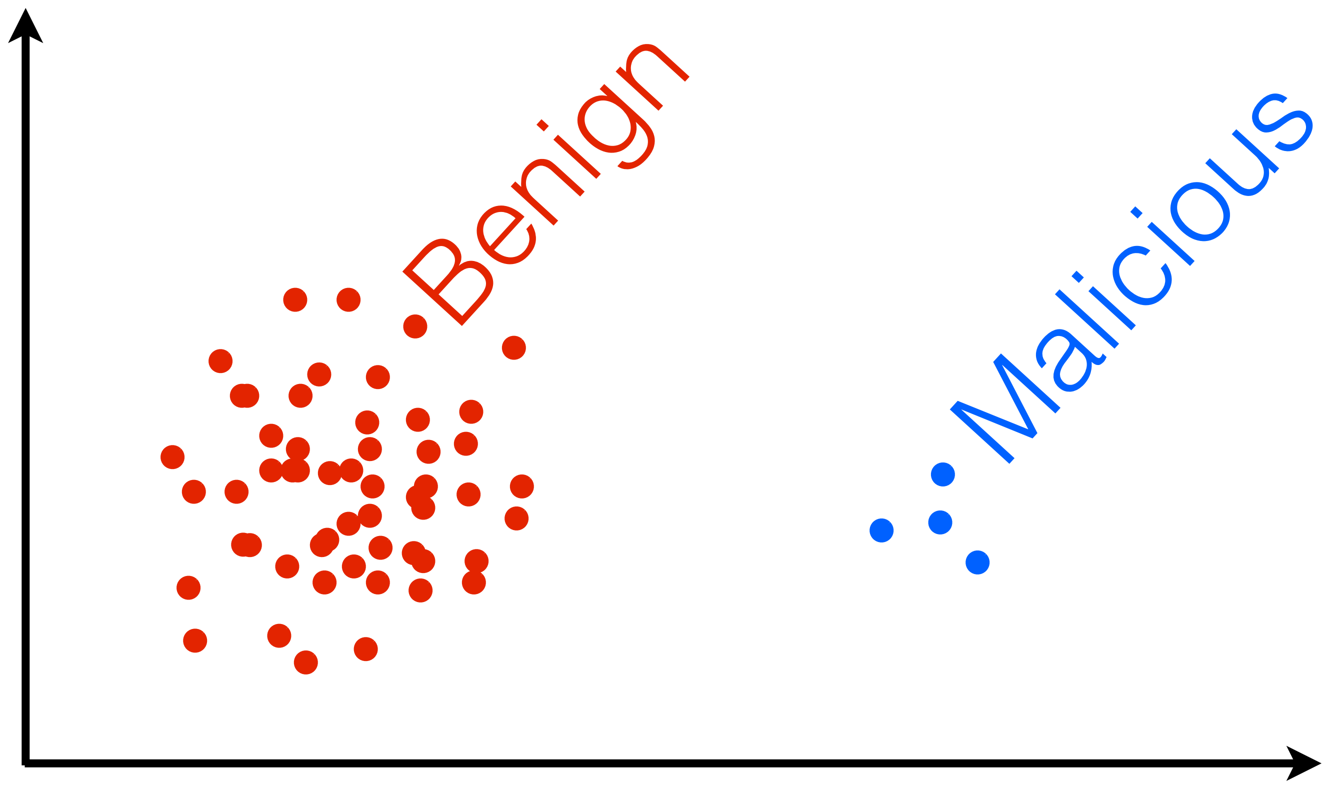

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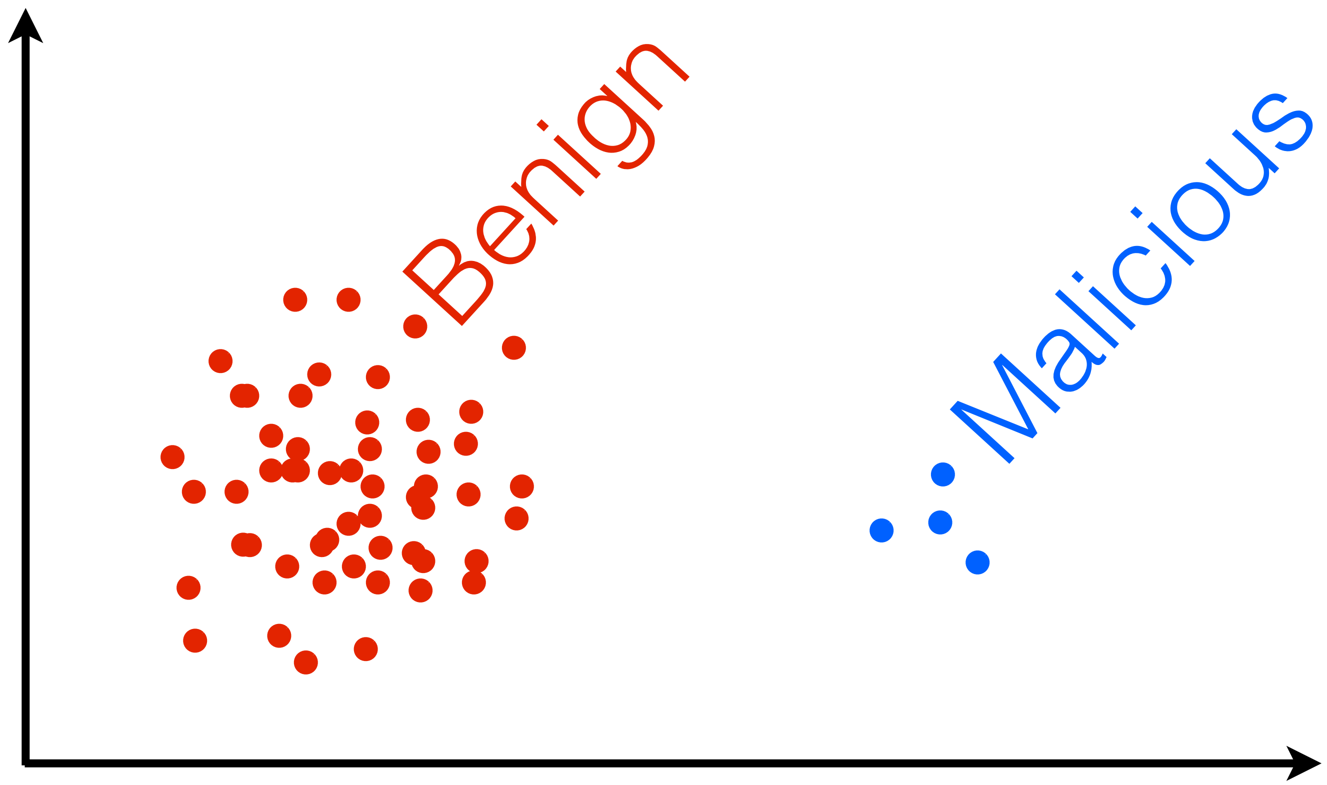

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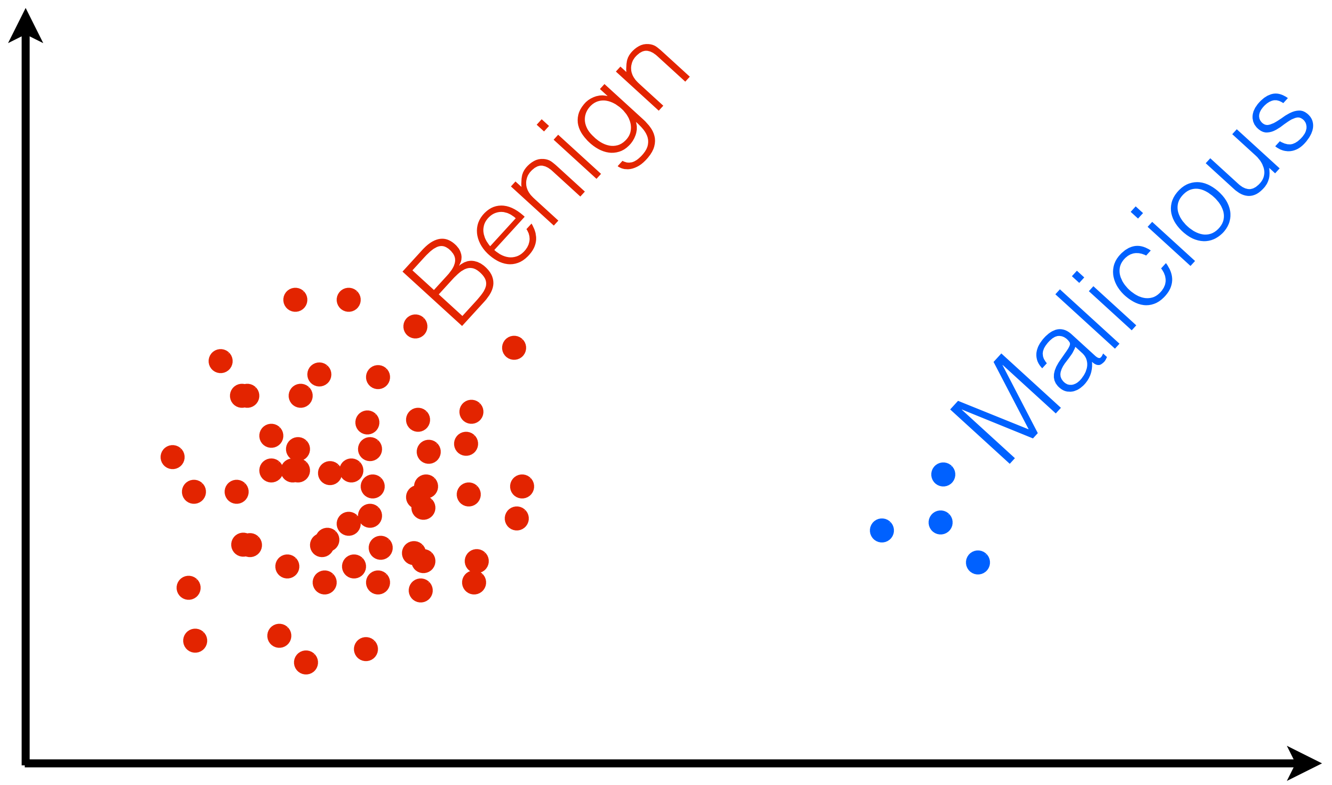

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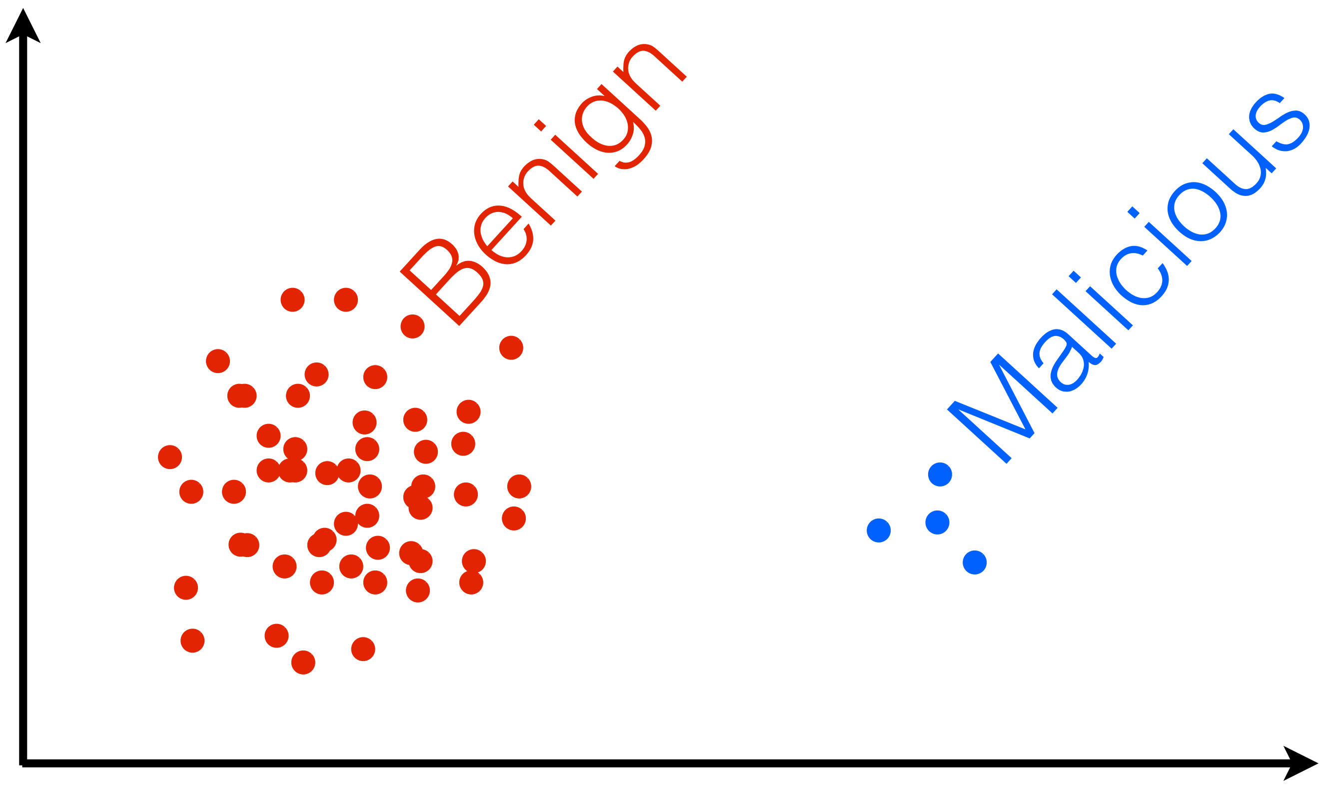

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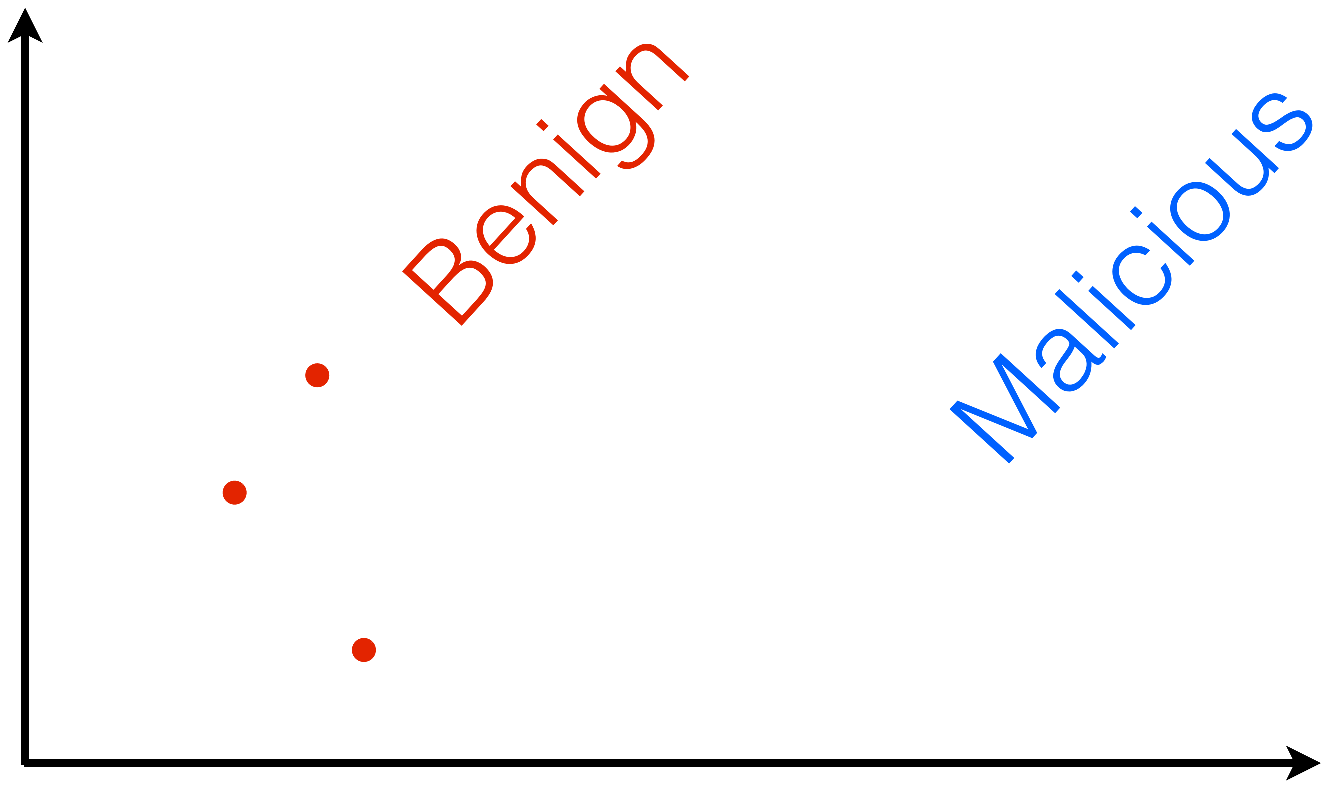

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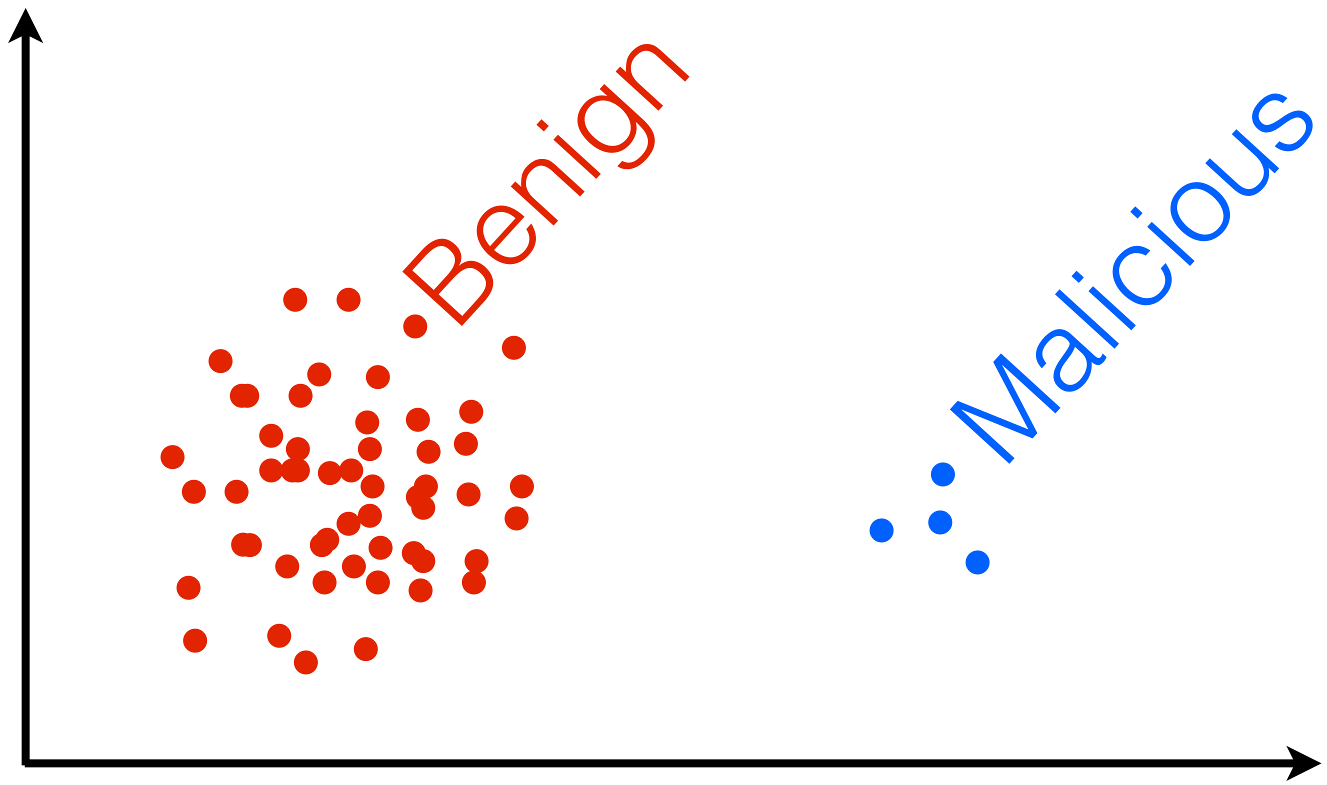

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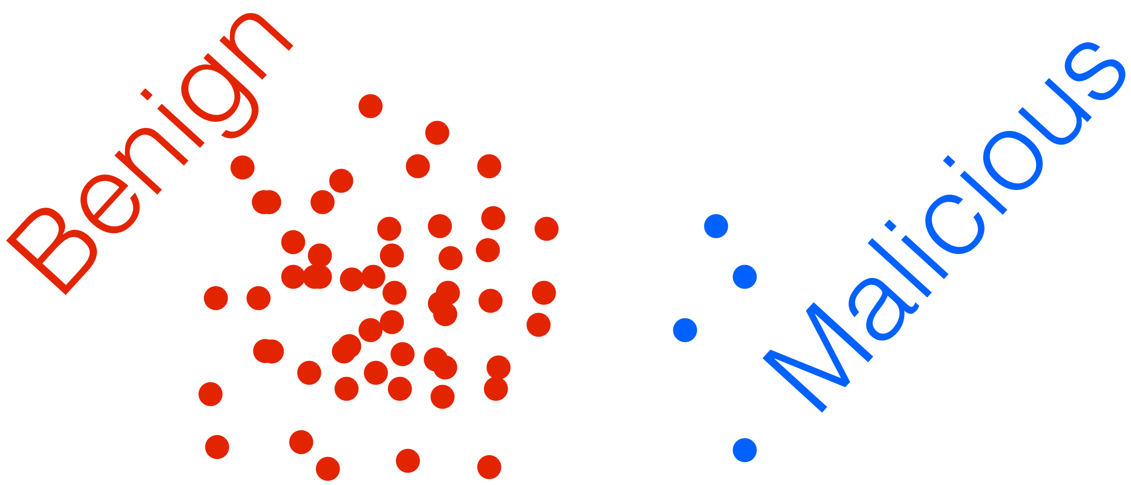

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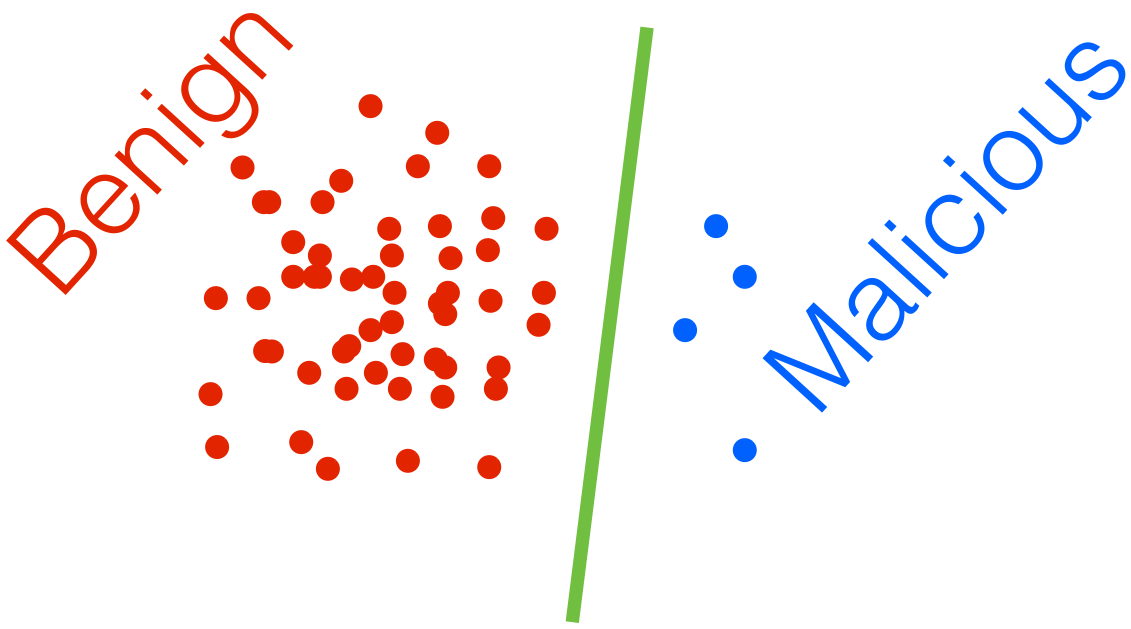

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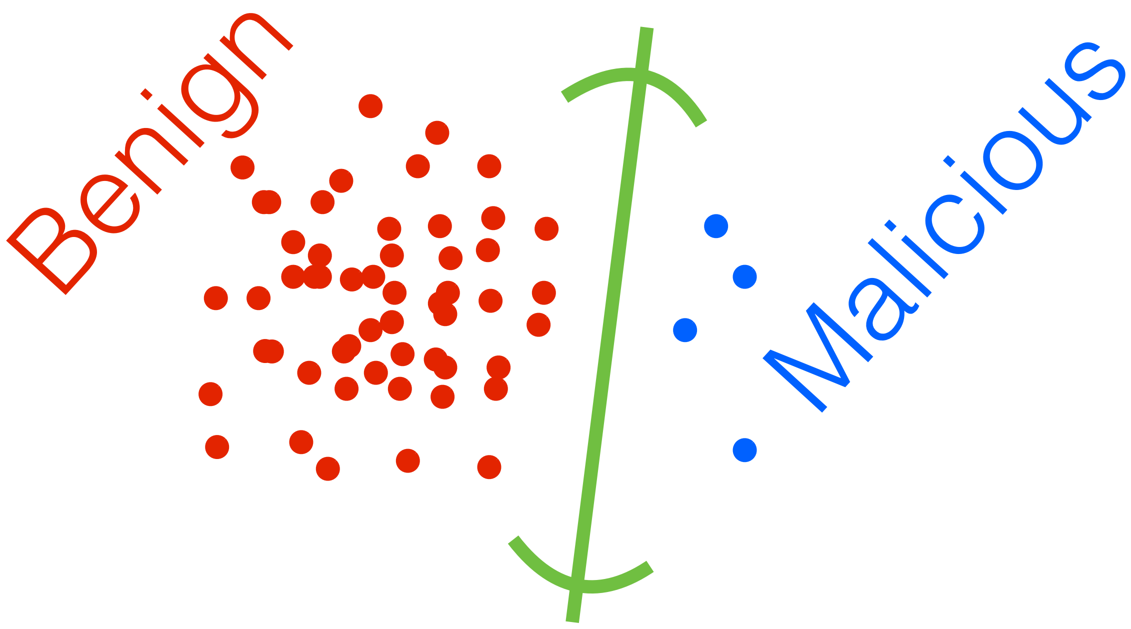

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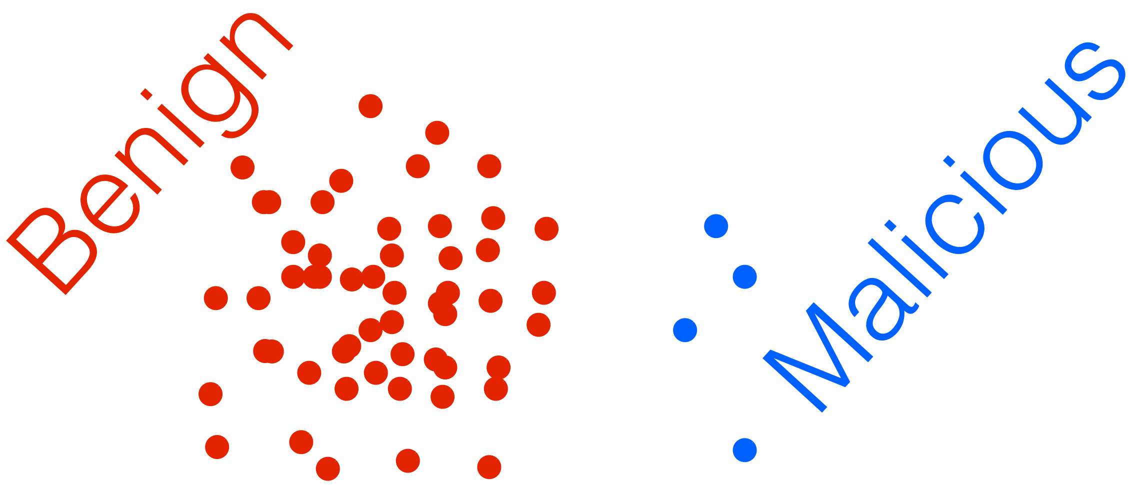

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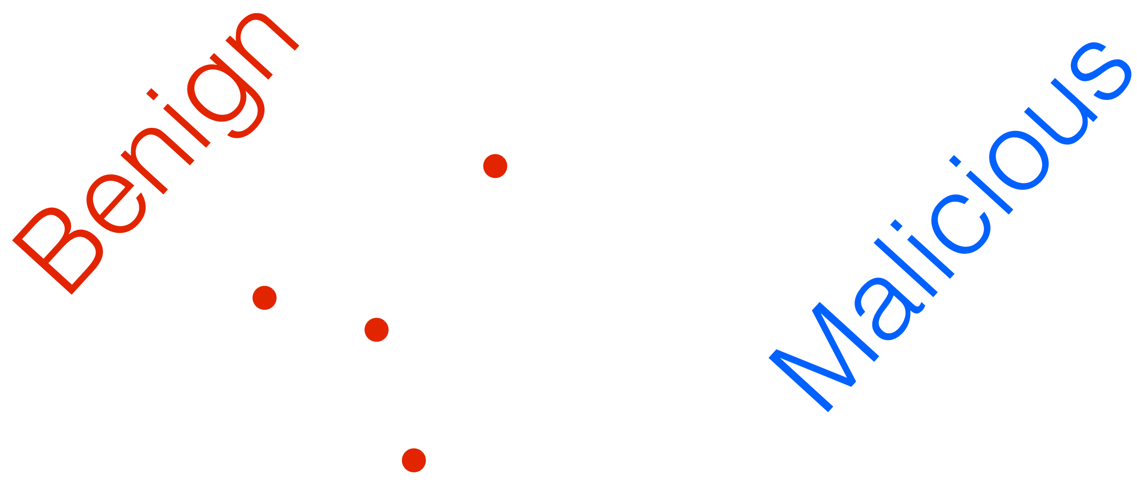

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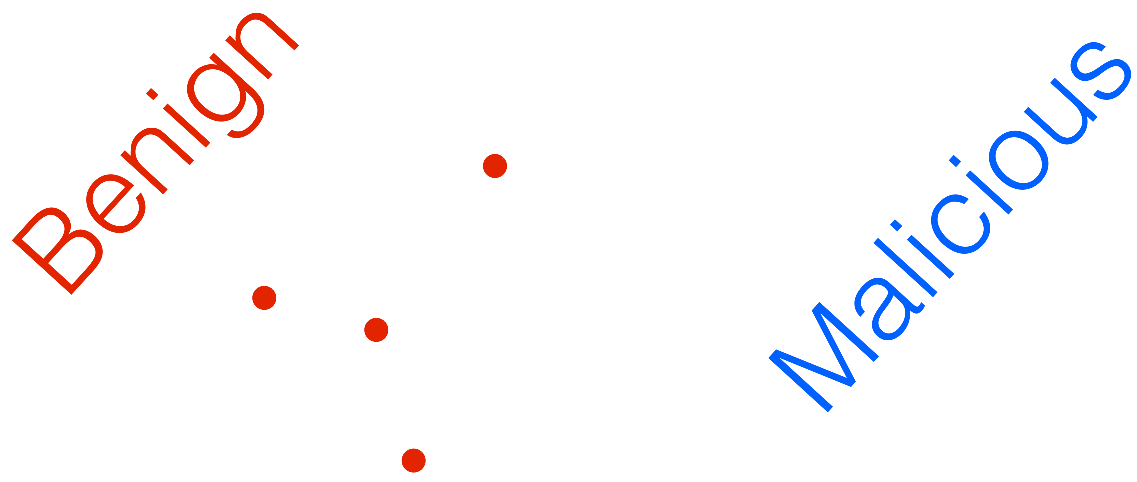

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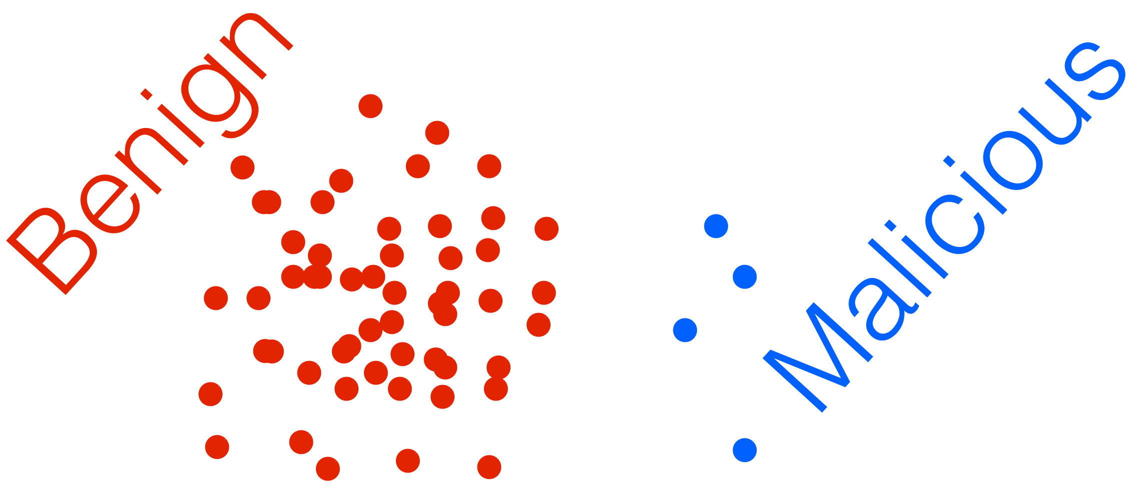

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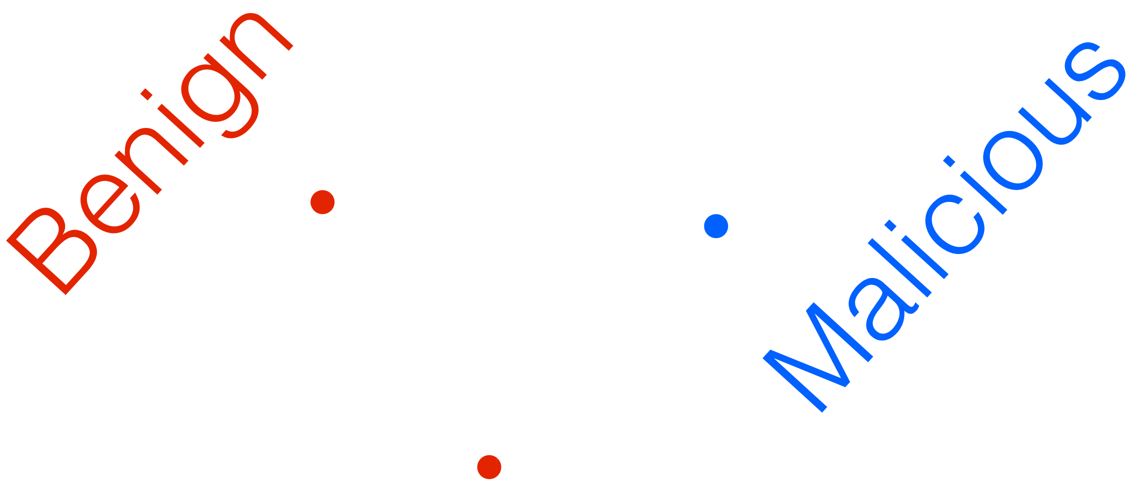

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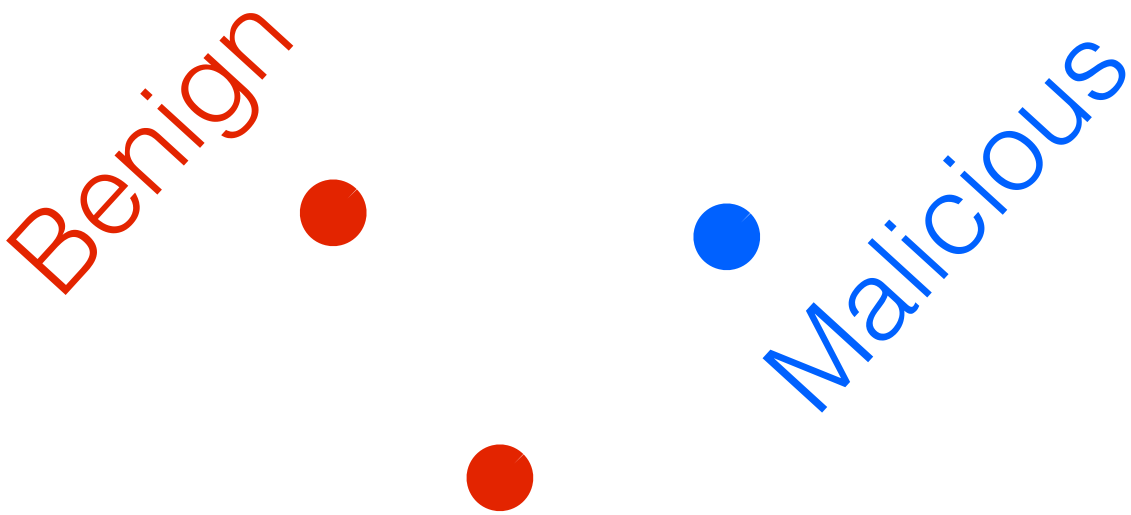

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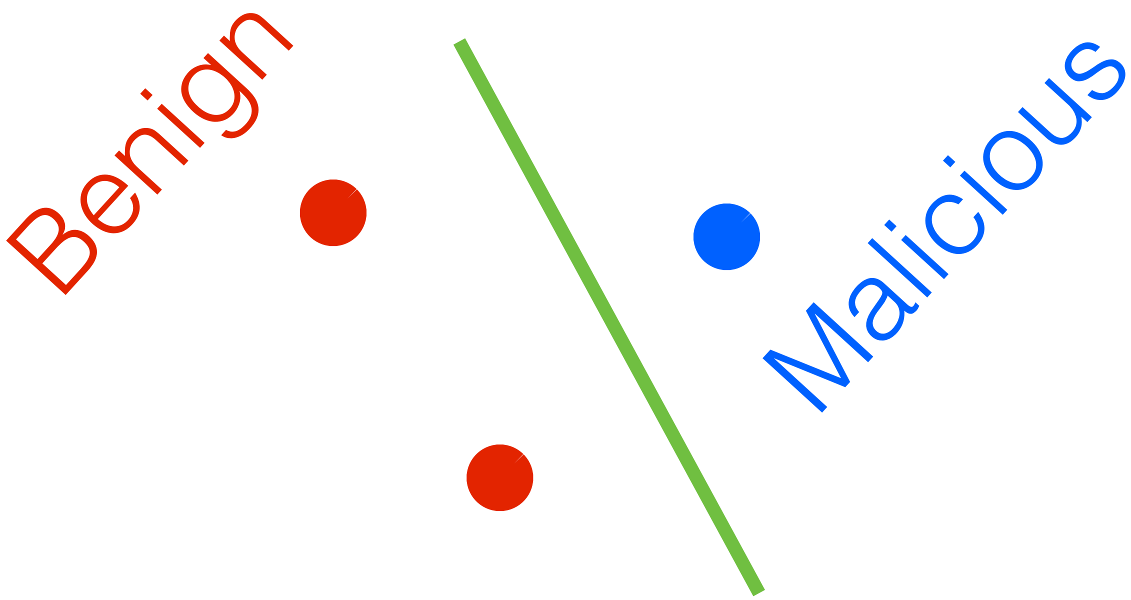

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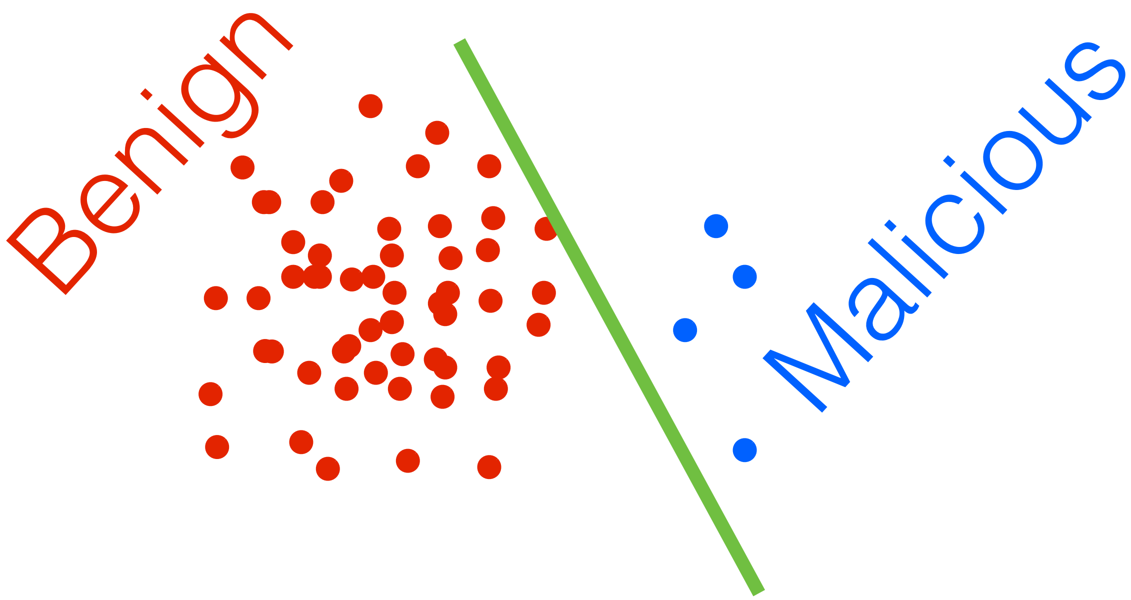

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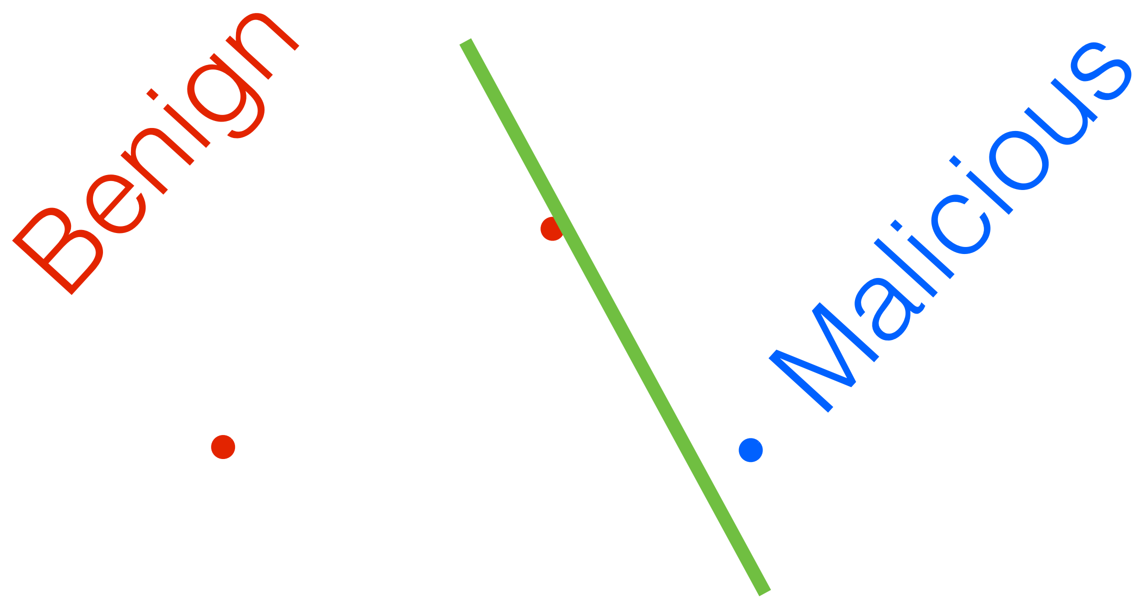

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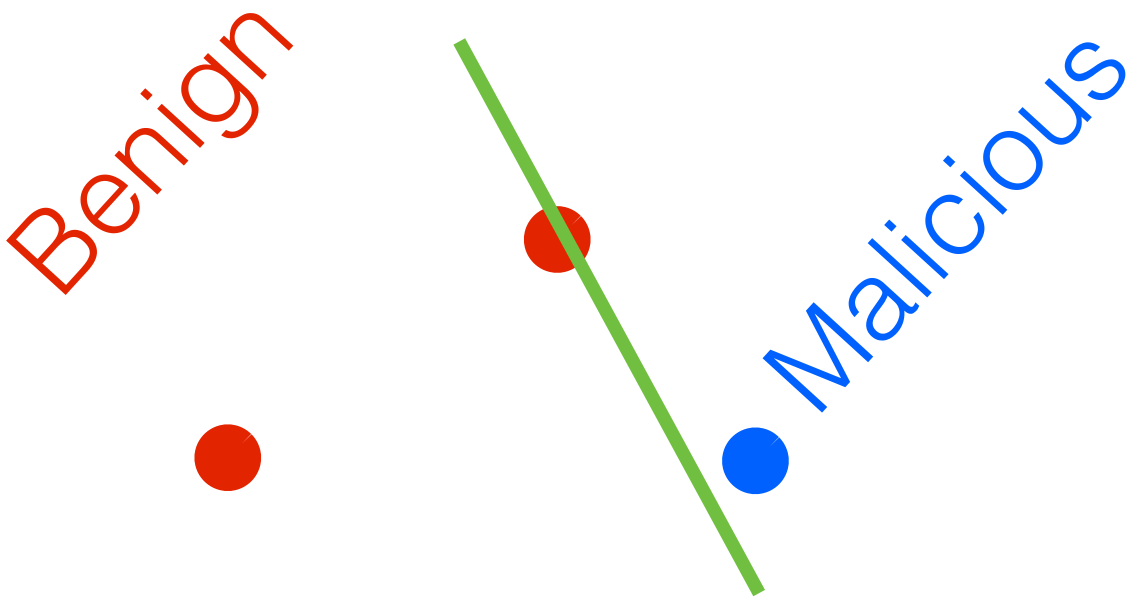

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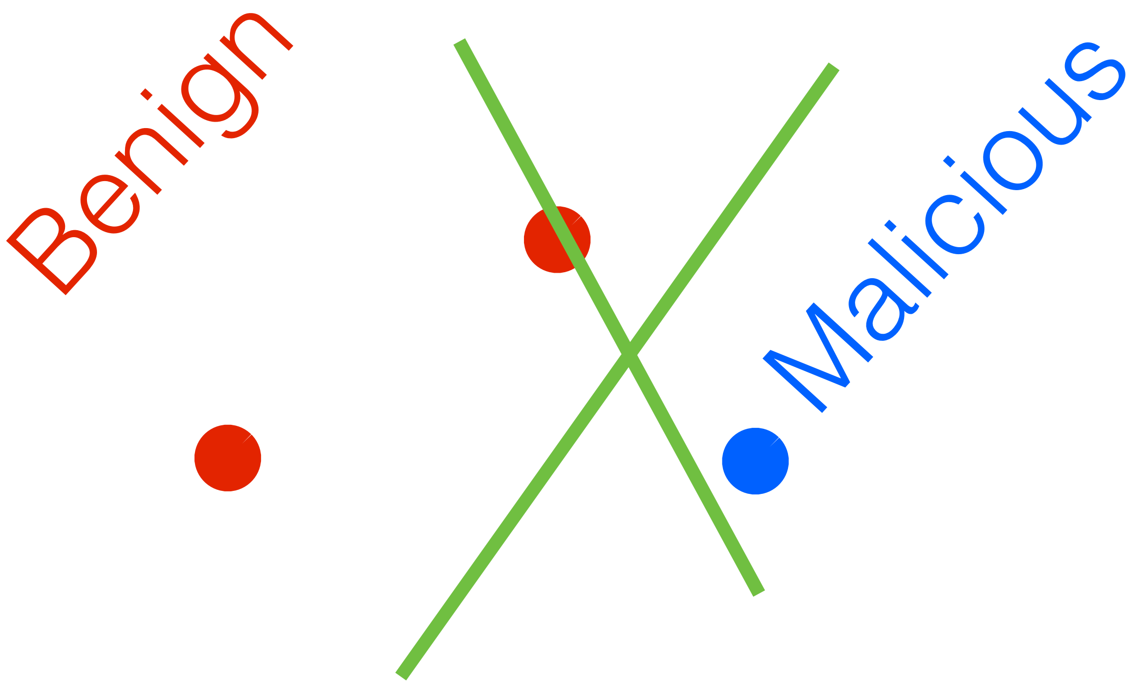

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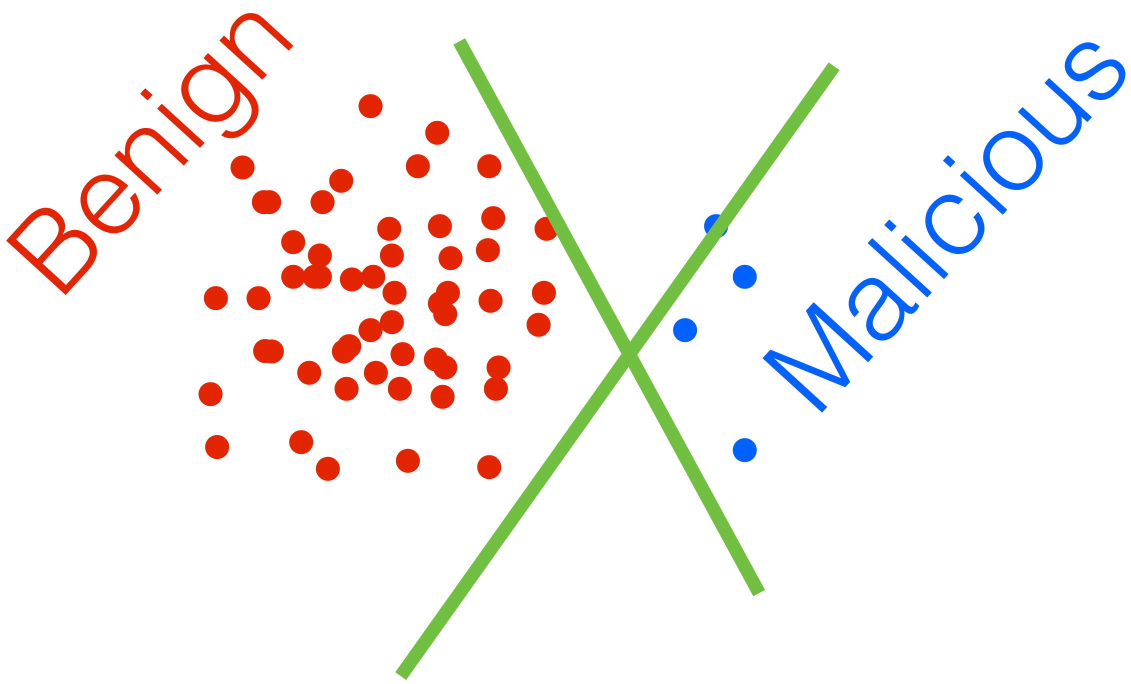

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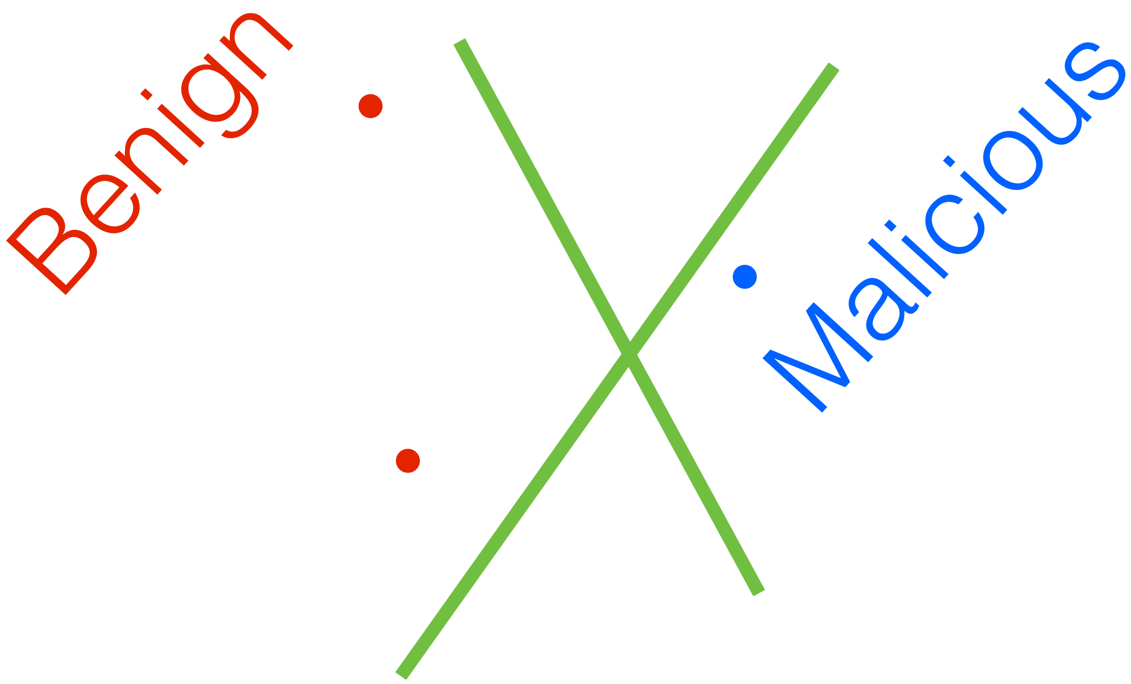

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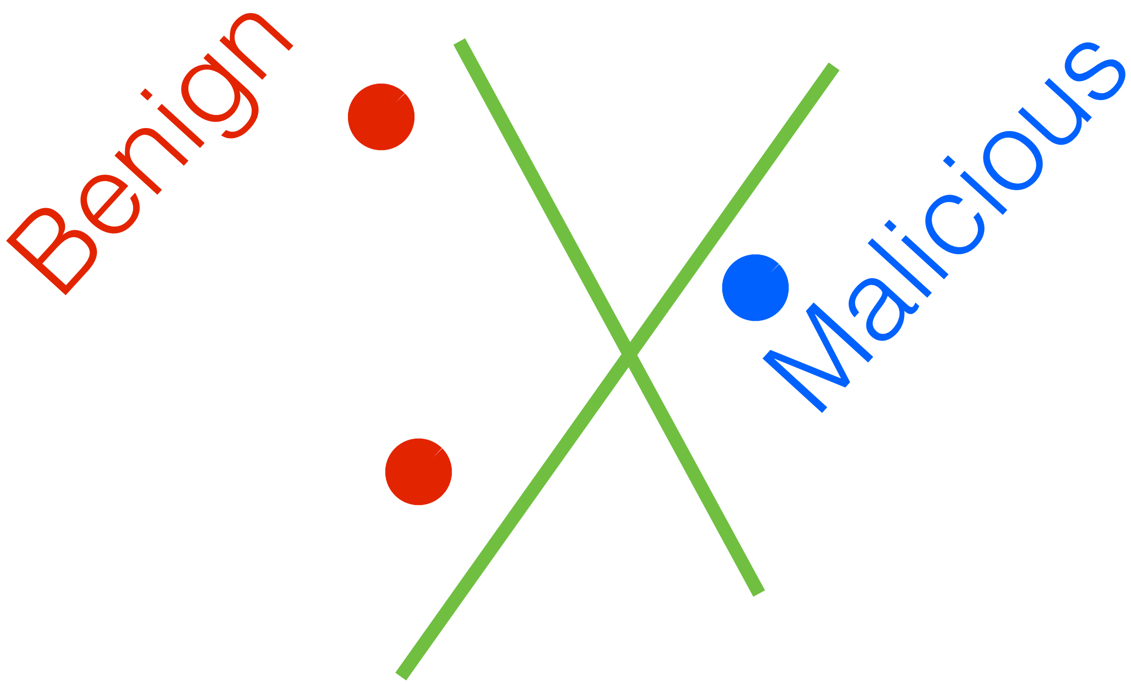

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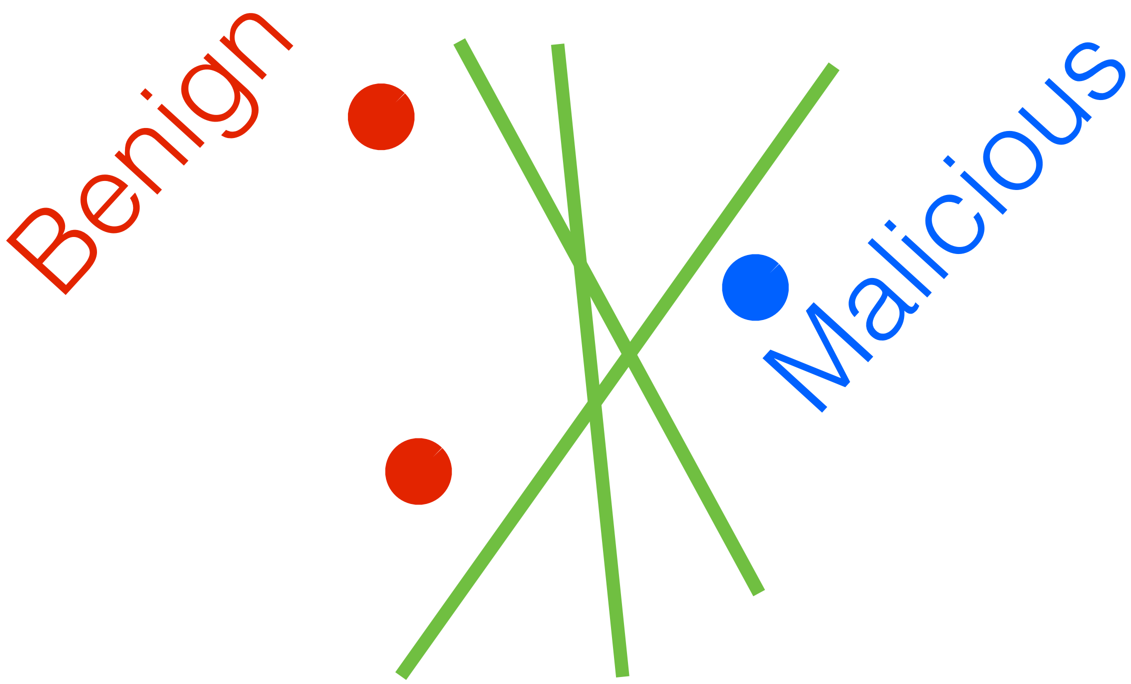

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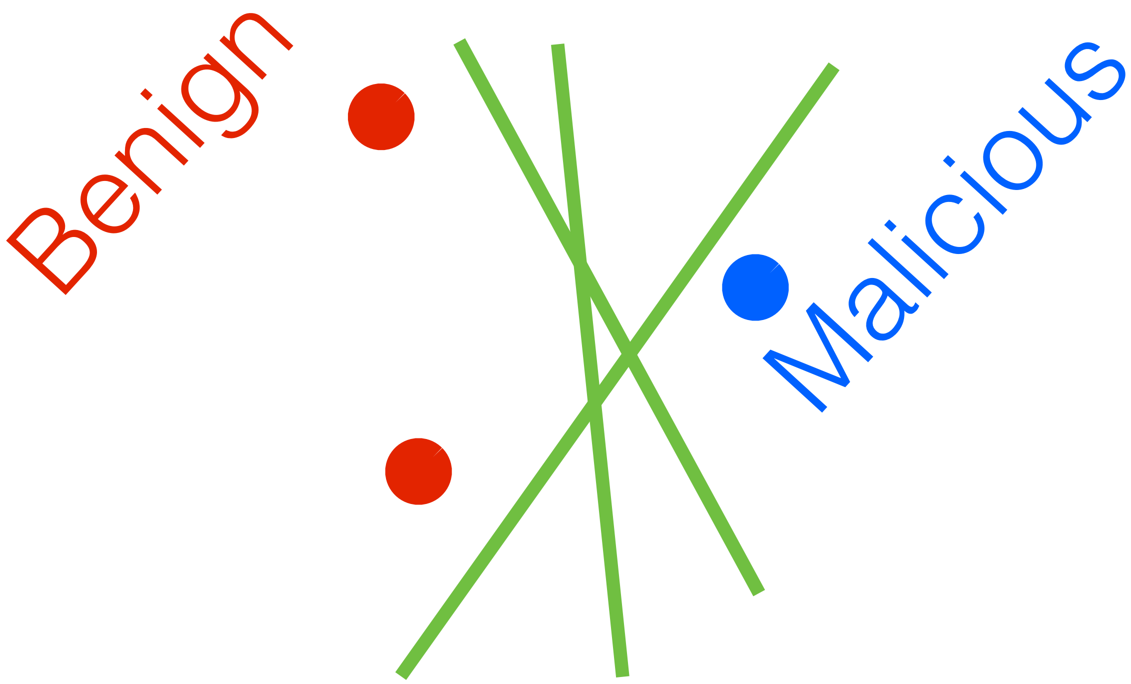
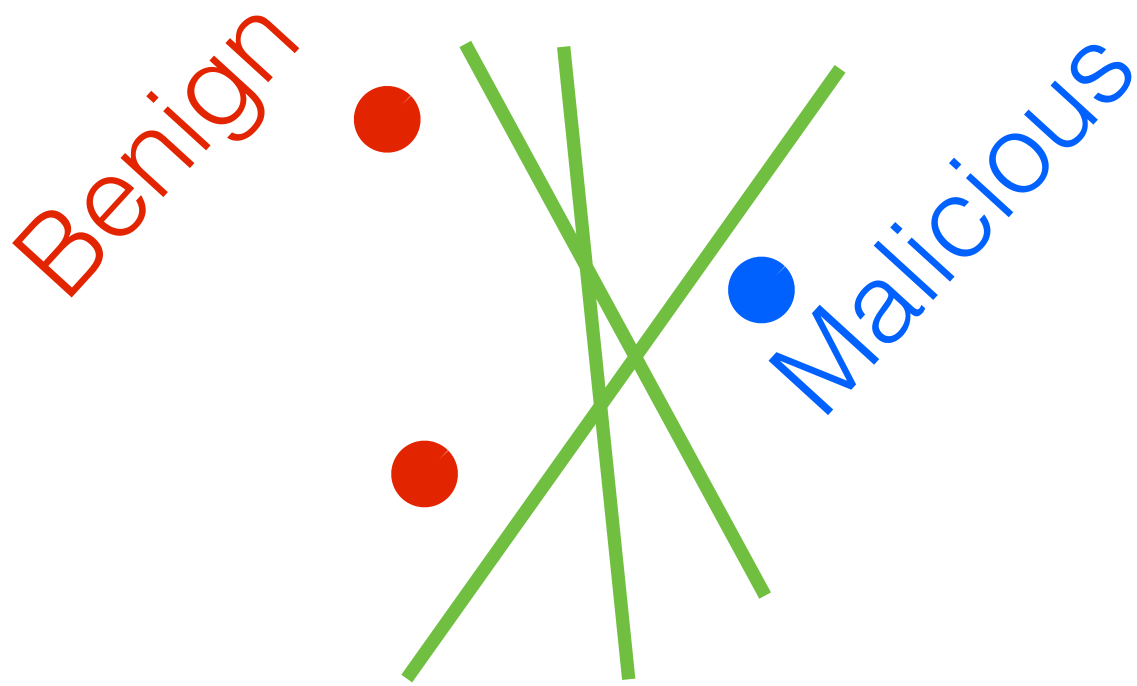


- Might miss important data
- Noisy estimates

Uniform subsampling



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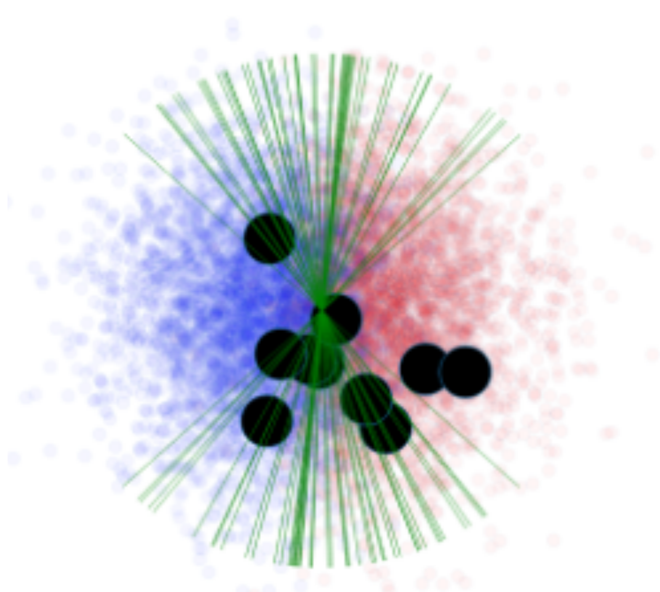
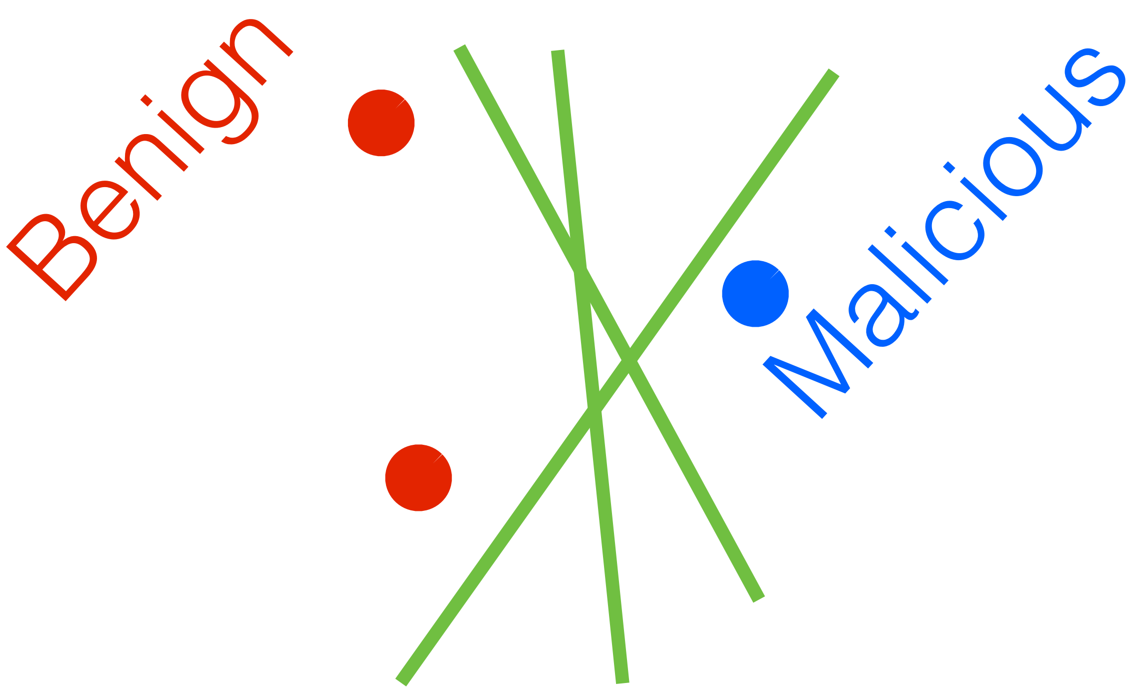


$M = 10$

Uniform subsampling



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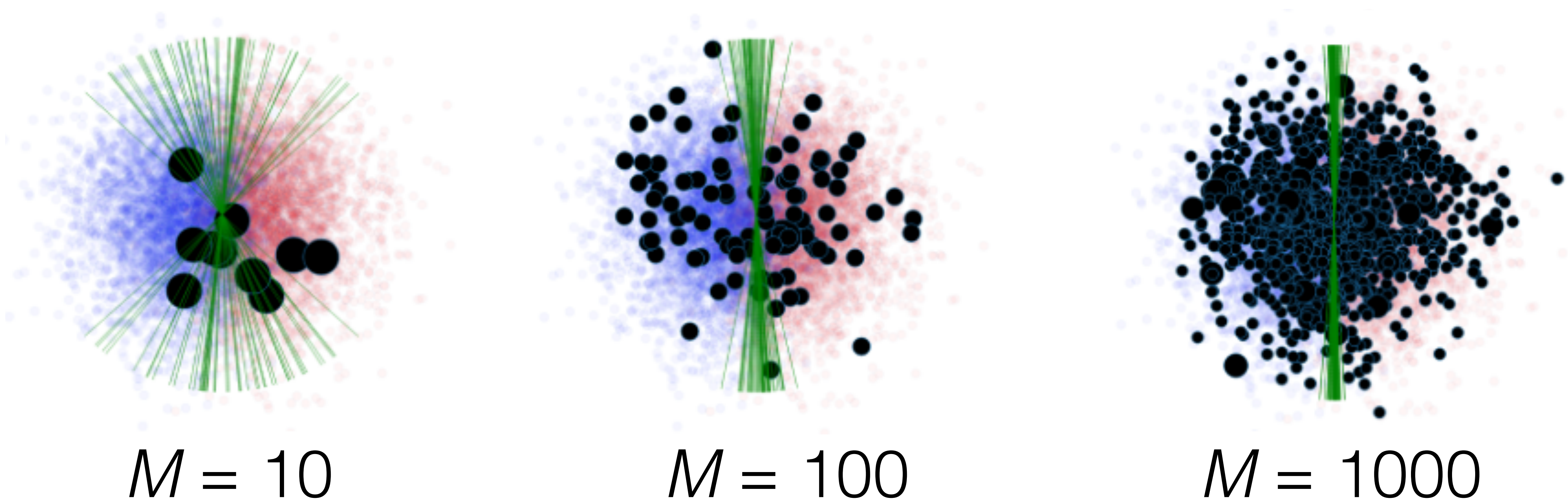
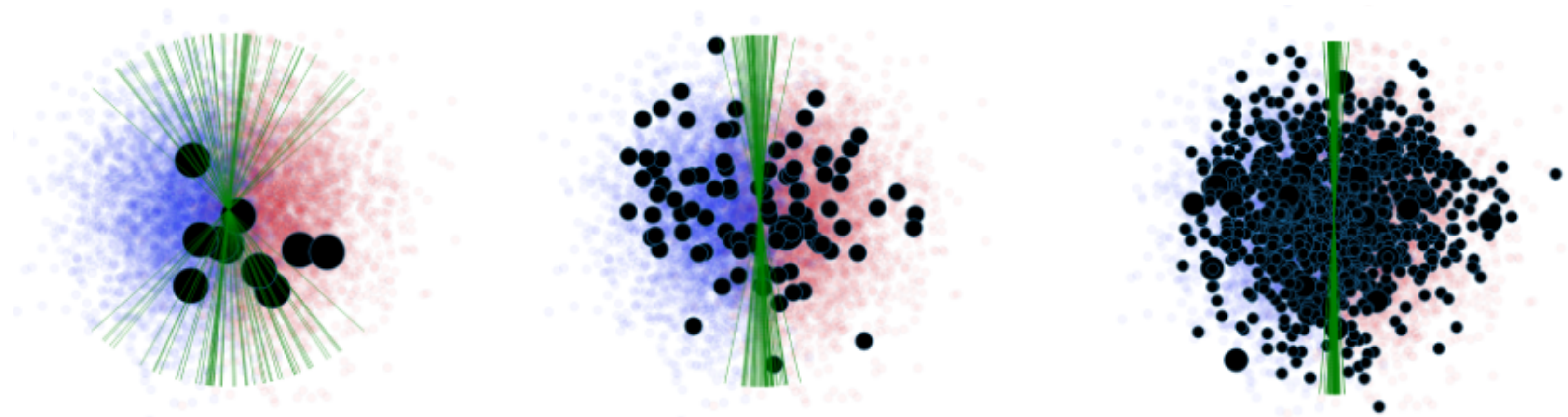


Data summarization alternatives

Uniform subsampling

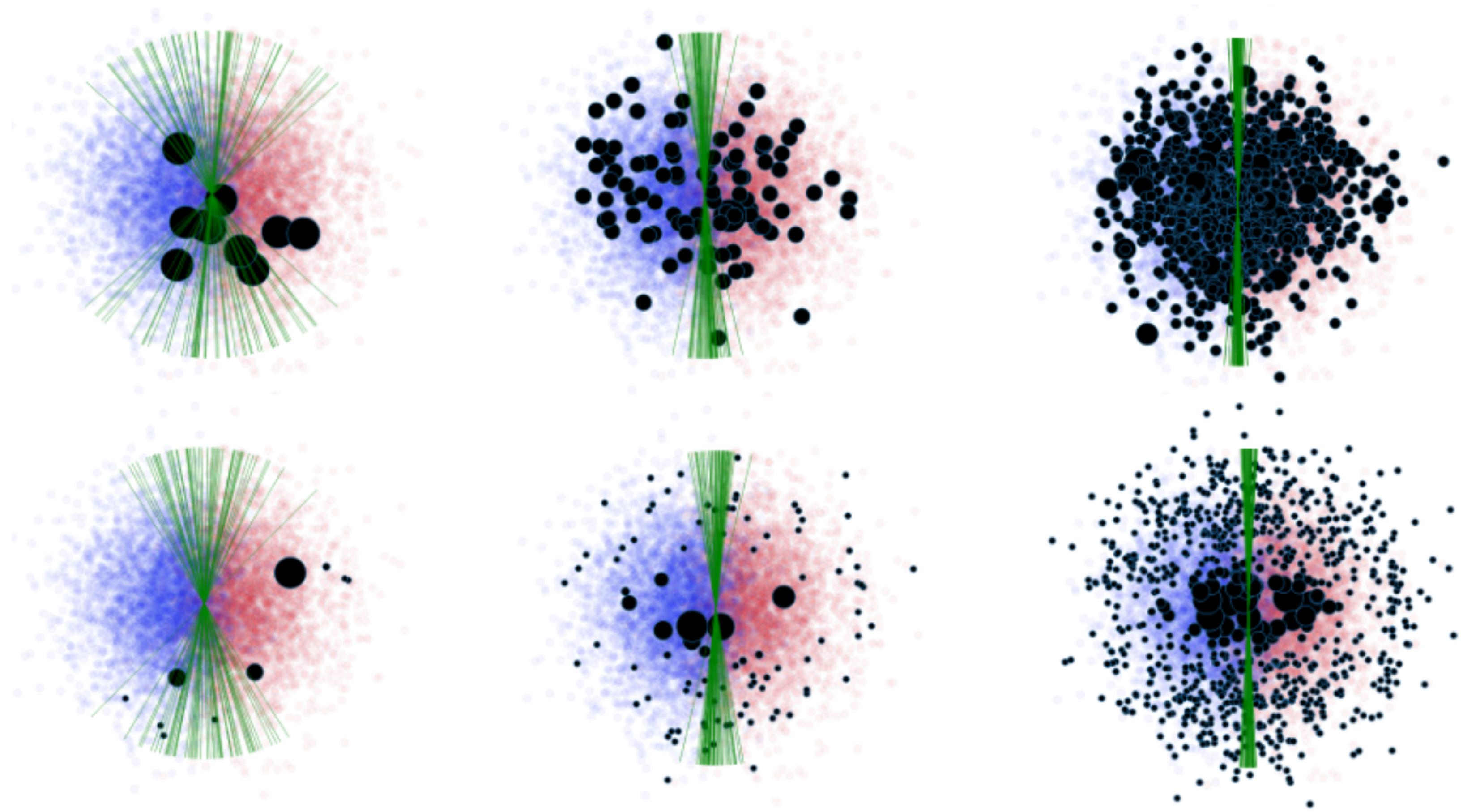


$M = 10$ $M = 100$ $M = 1000$

Data summarization alternatives

Uniform subsampling

Importance sampling



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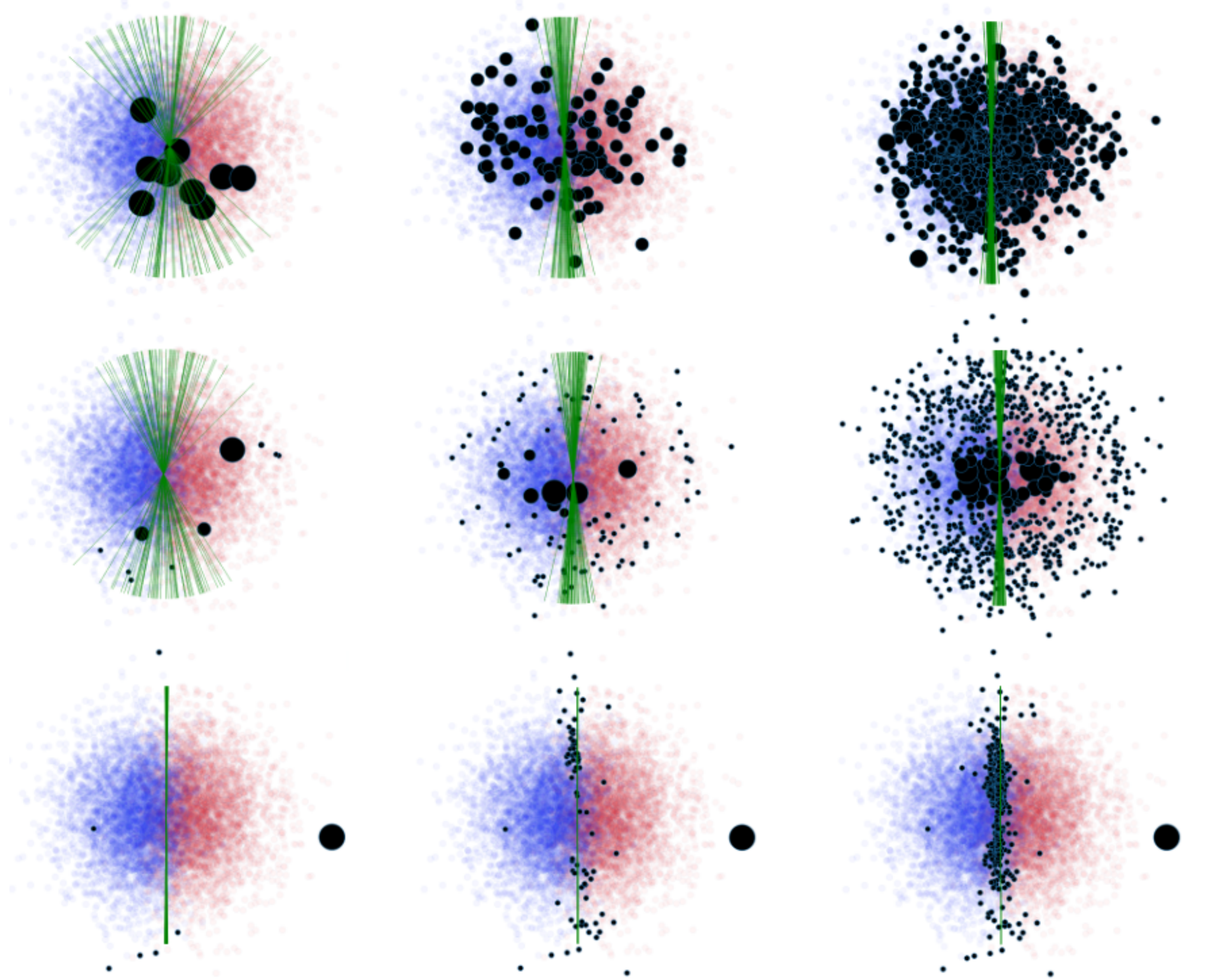
Data summarization alternatives

Uniform subsampling

Importance sampling

Bayesian/Hilbert coresets



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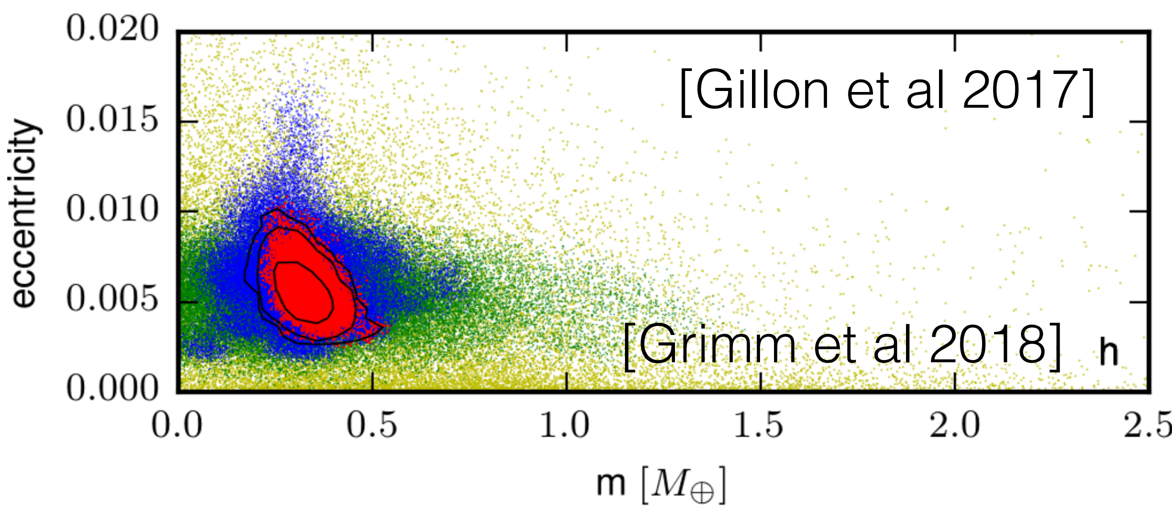
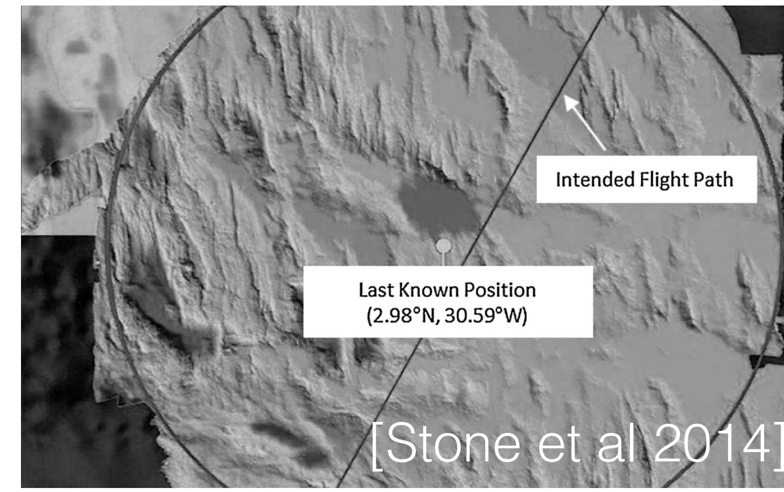
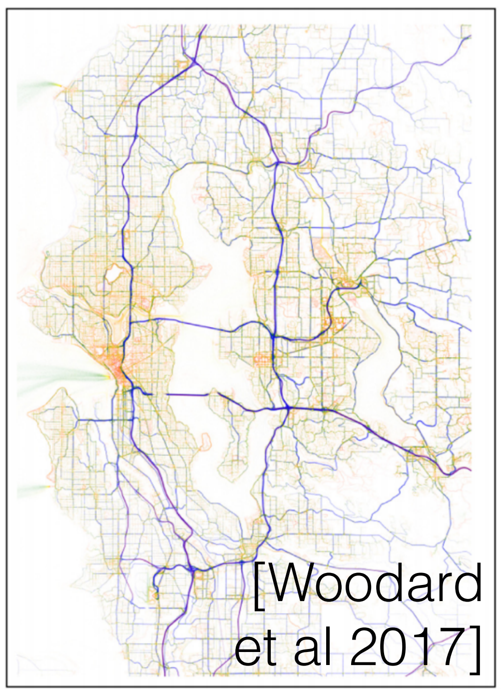
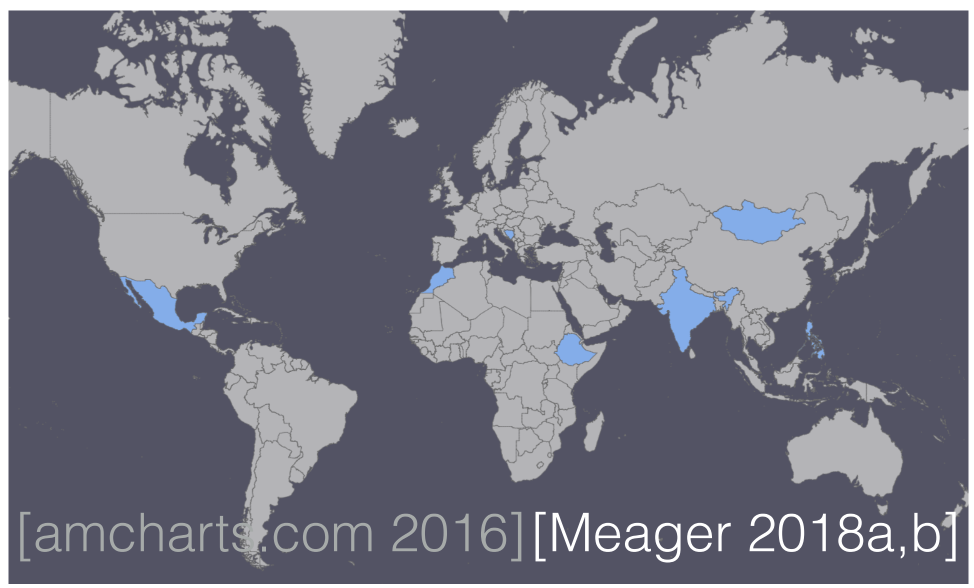
Bayesian inference









[mc-stan.org]

- Goals: good point estimates, uncertainty estimates

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

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.

Our 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, JH 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. *JMLR* 2018.
- J Huggins, M Kasprzak, T Campbell, T Broderick. Practical posterior error bounds from variational objectives, 2019. ArXiv: 1910.04102. *AISTATS* 2020, to appear.
- T Campbell and T Broderick. Automated scalable Bayesian inference via Hilbert coresets. *JMLR* 2019.
- T Campbell and T Broderick. Bayesian Coreset Construction via Greedy Iterative Geodesic Ascent. *ICML* 2018.

References (1/6)

R Agrawal, T Campbell, JH Huggins, and T Broderick. Data-dependent compression of random features for large-scale kernel approximation. *AISTATS* 2019.

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