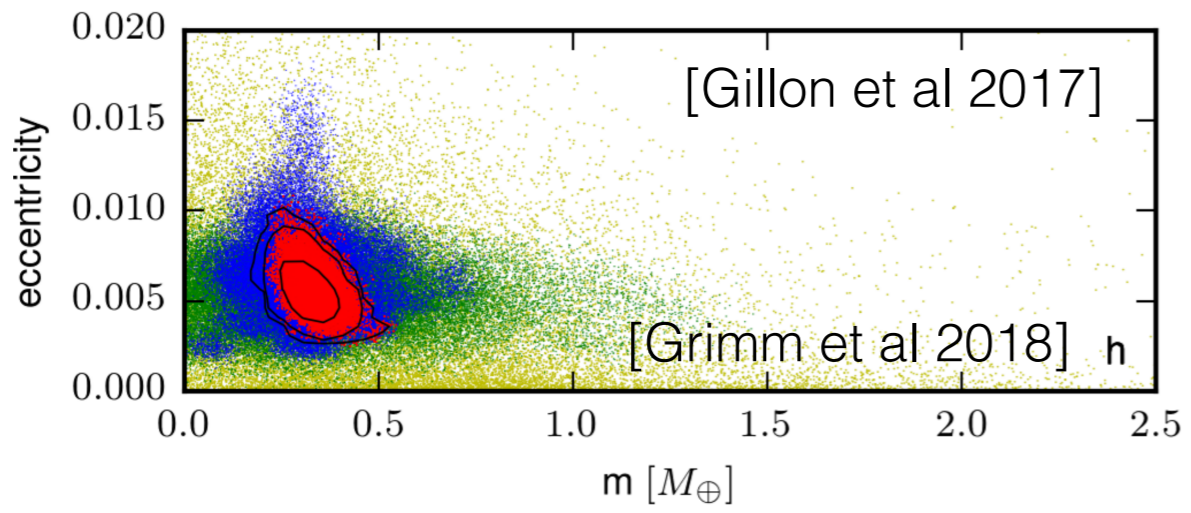


Variational Bayes and beyond: Foundations of scalable Bayesian inference

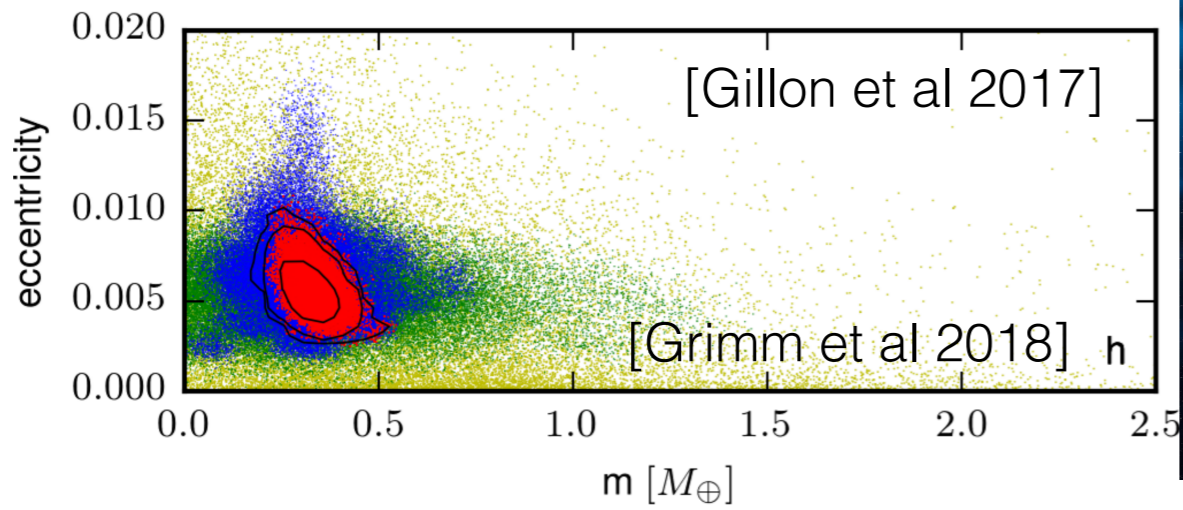
Tamara Broderick
Associate Professor
MIT

Bayesian inference

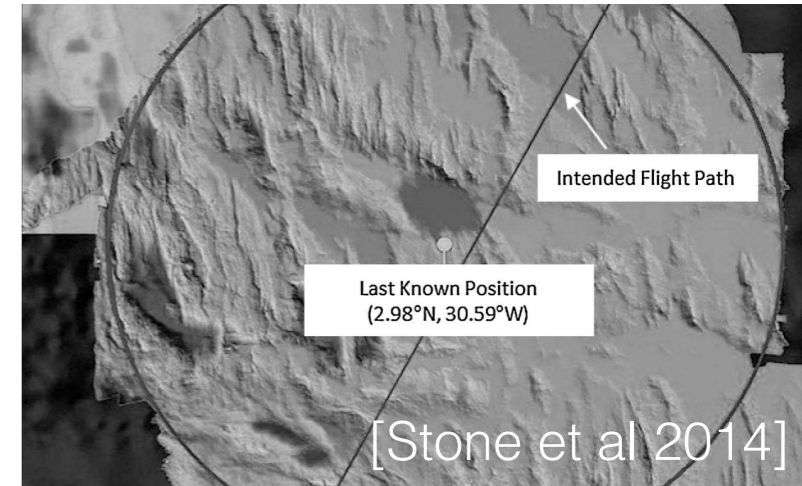
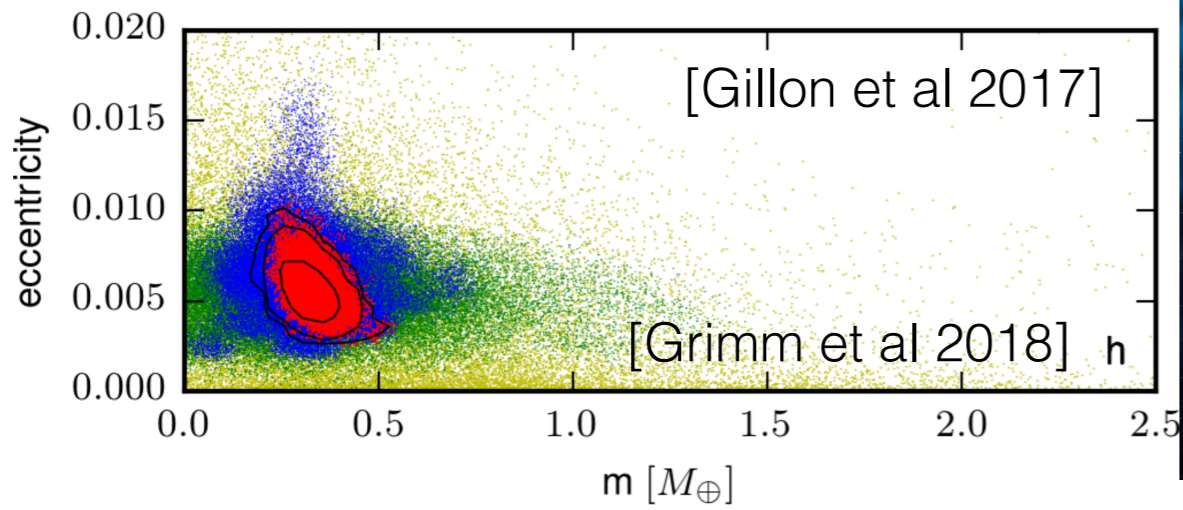
Bayesian inference



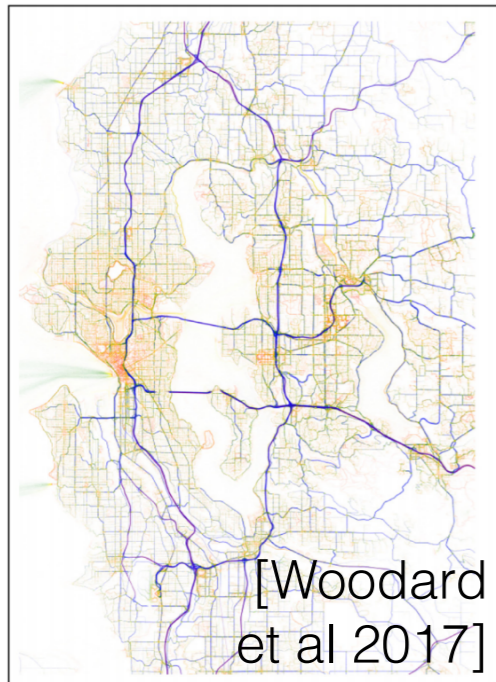
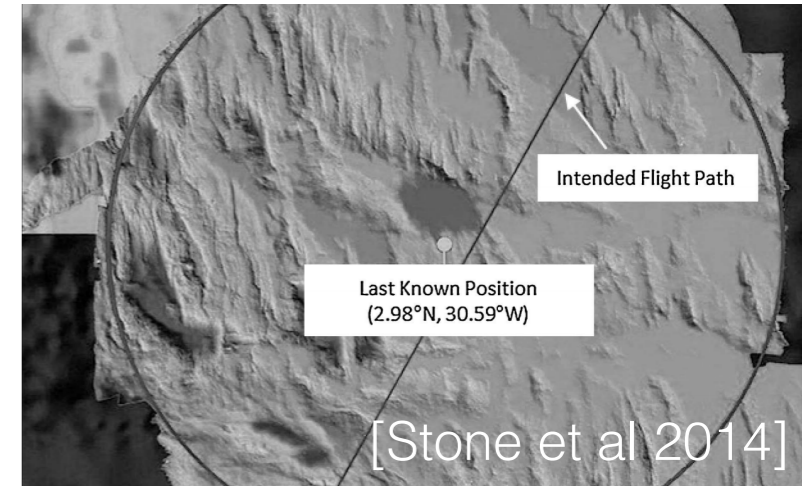
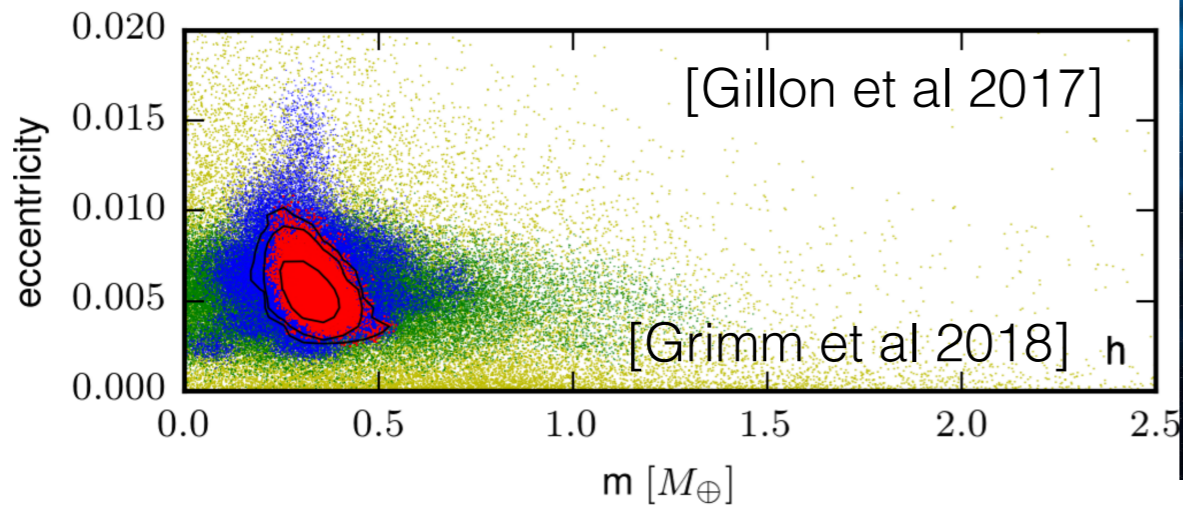
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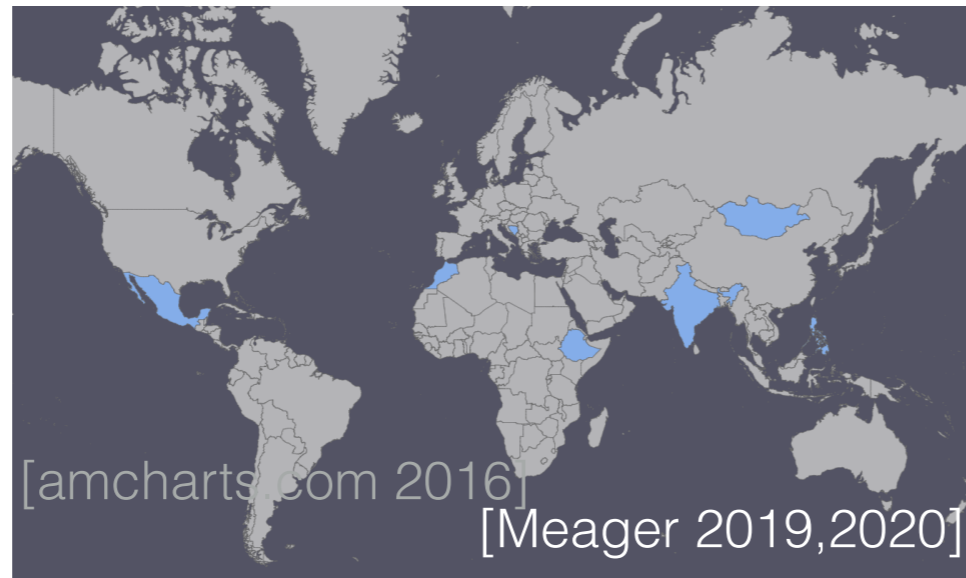
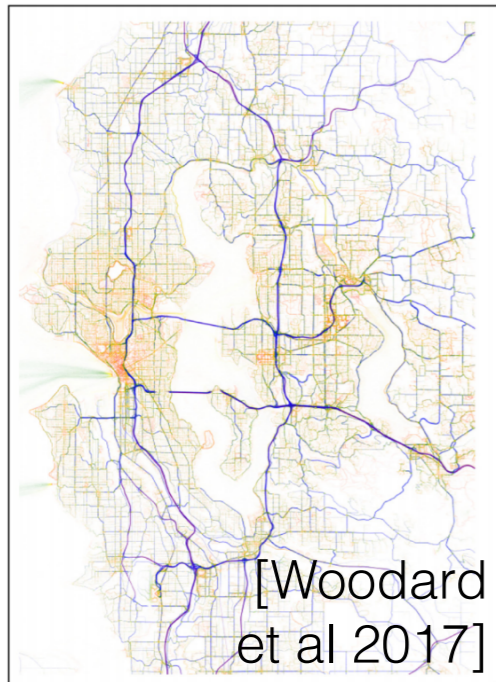
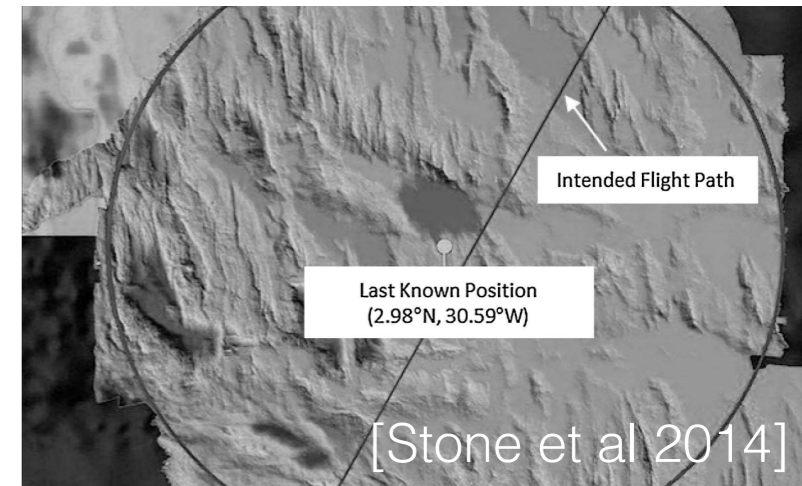
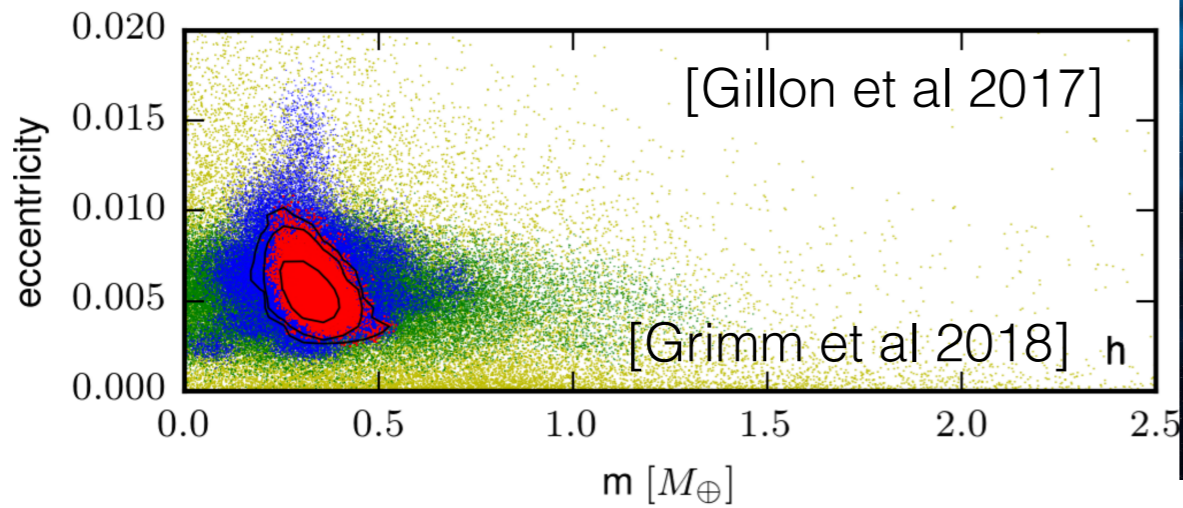
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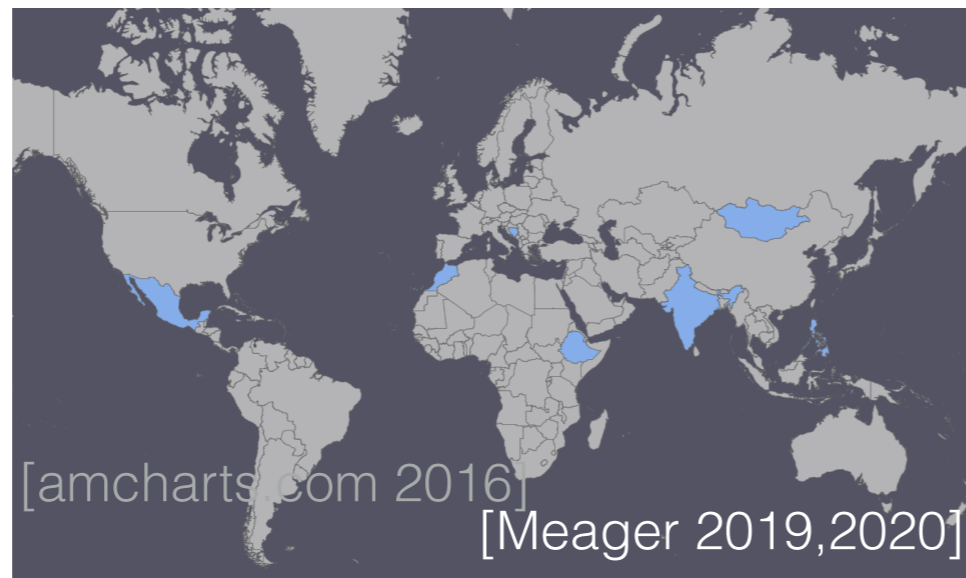
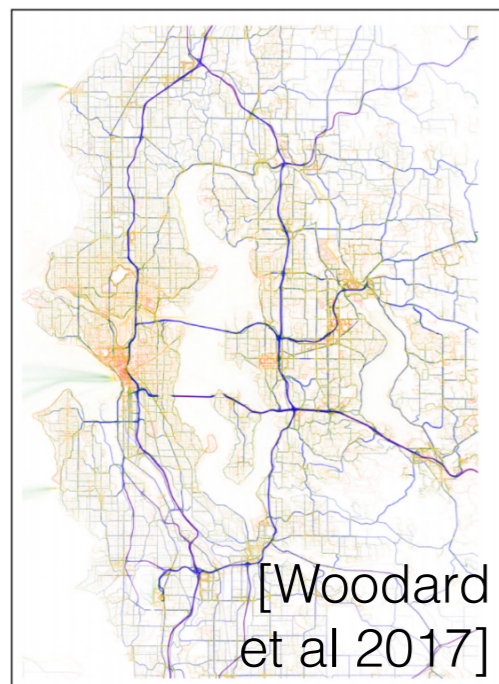
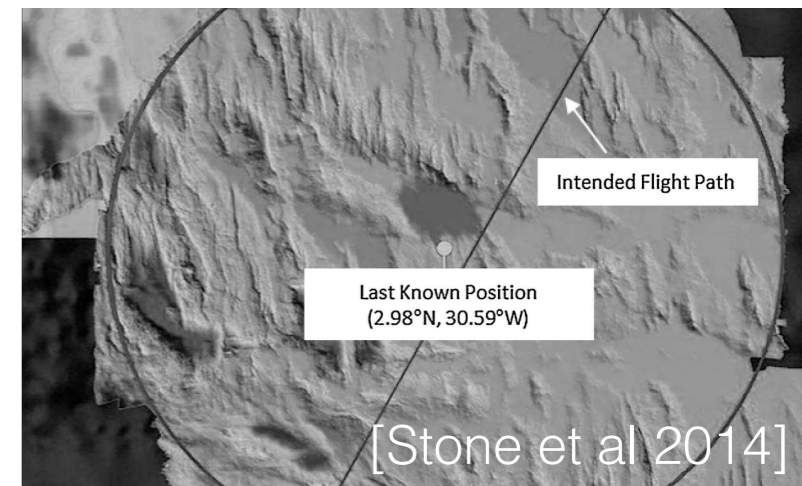
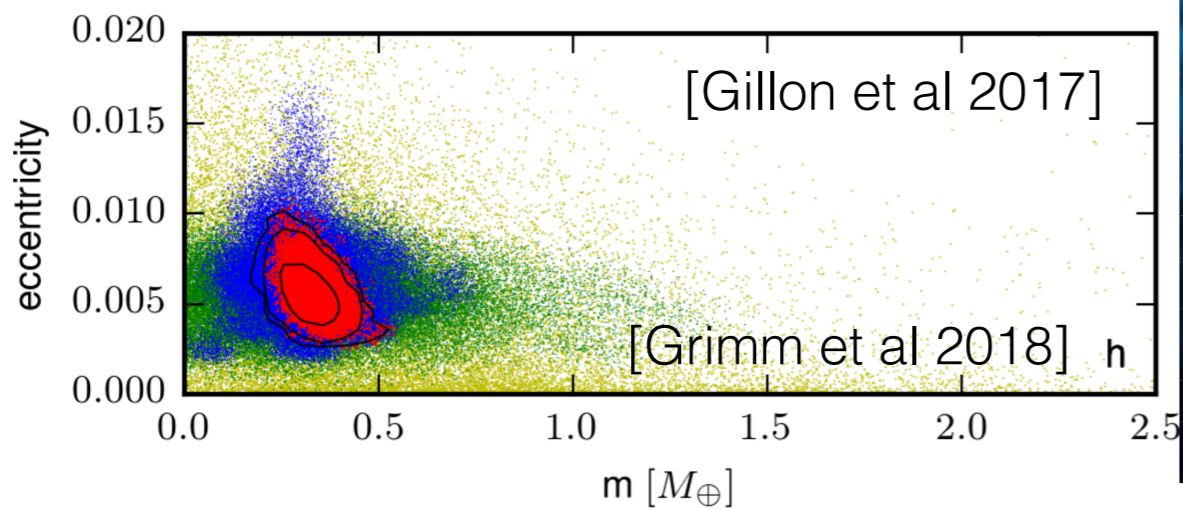
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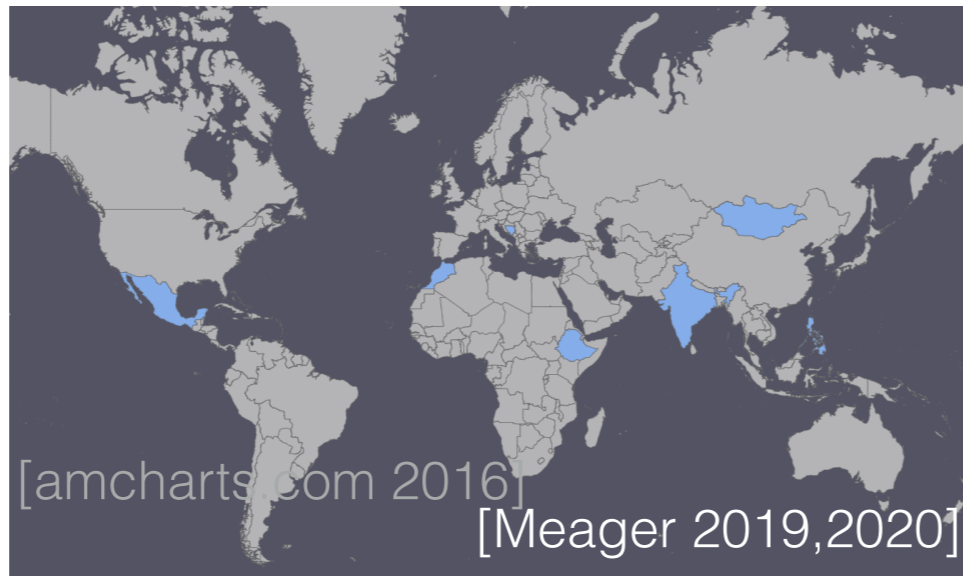
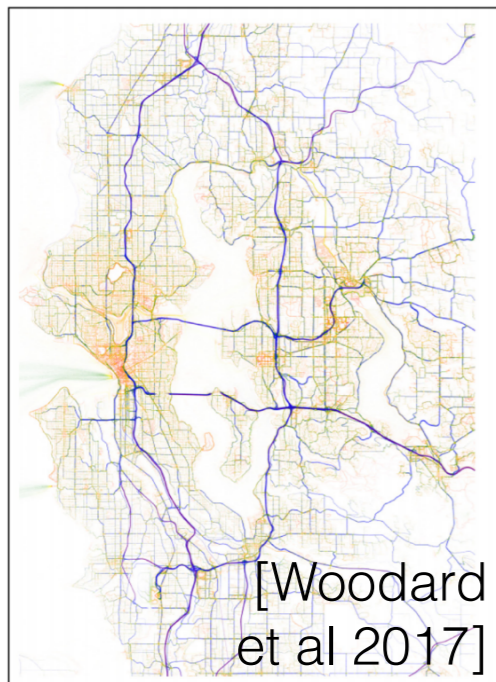
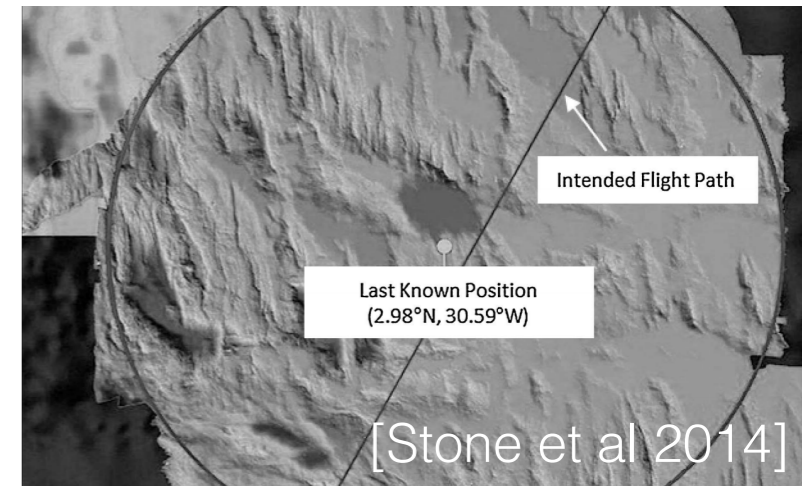
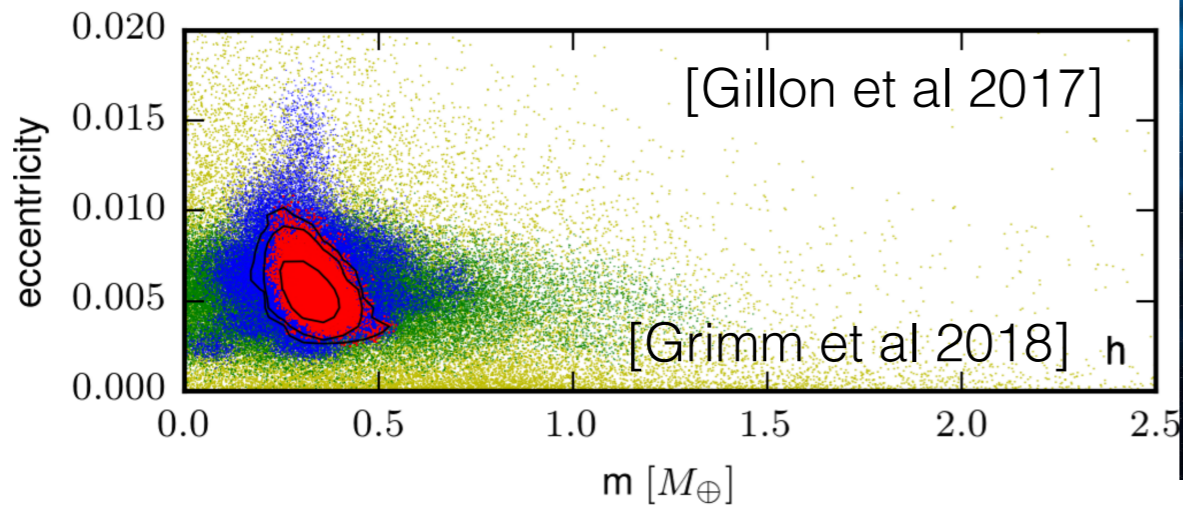
Bayesian inference



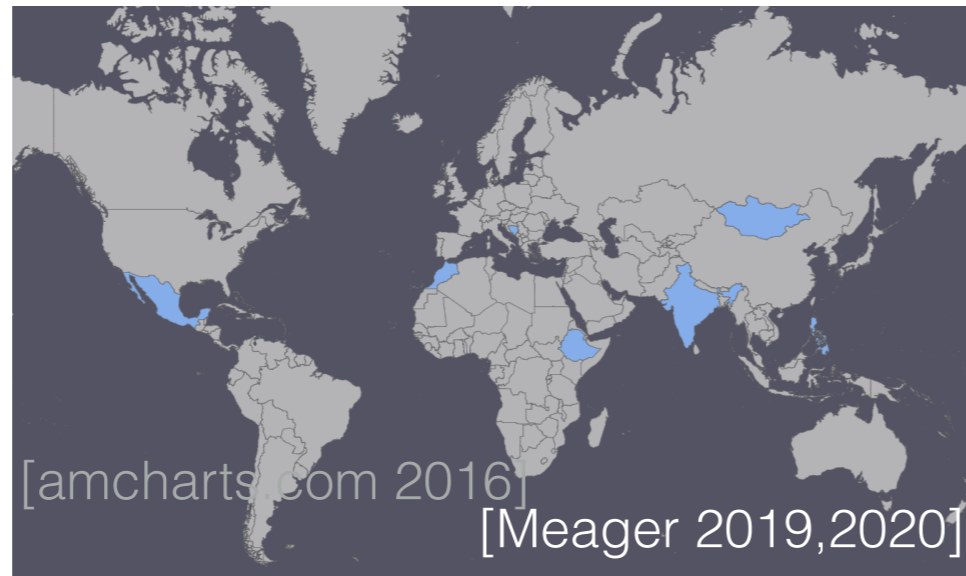
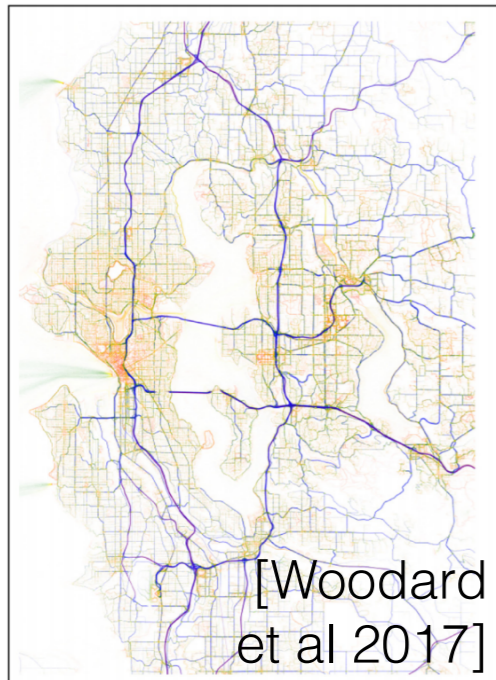
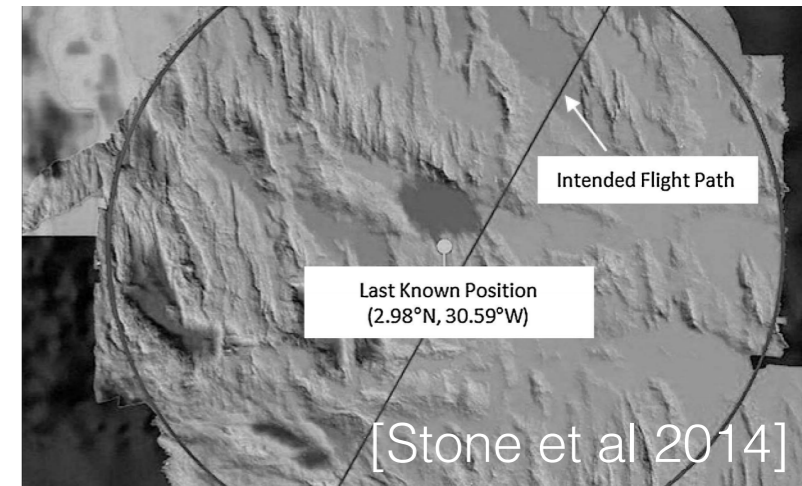
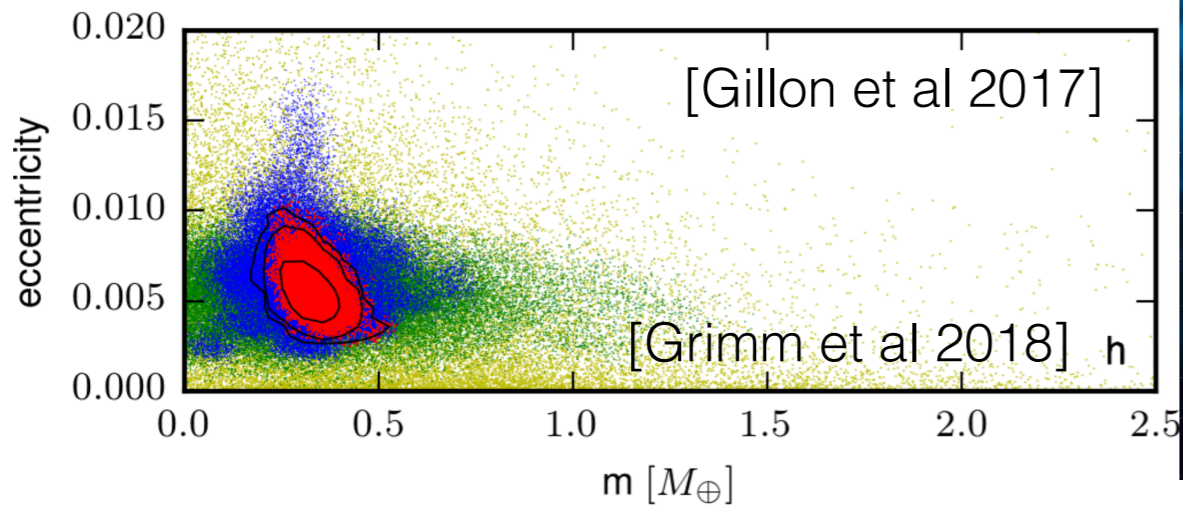
Bayesian inference



Bayesian inference

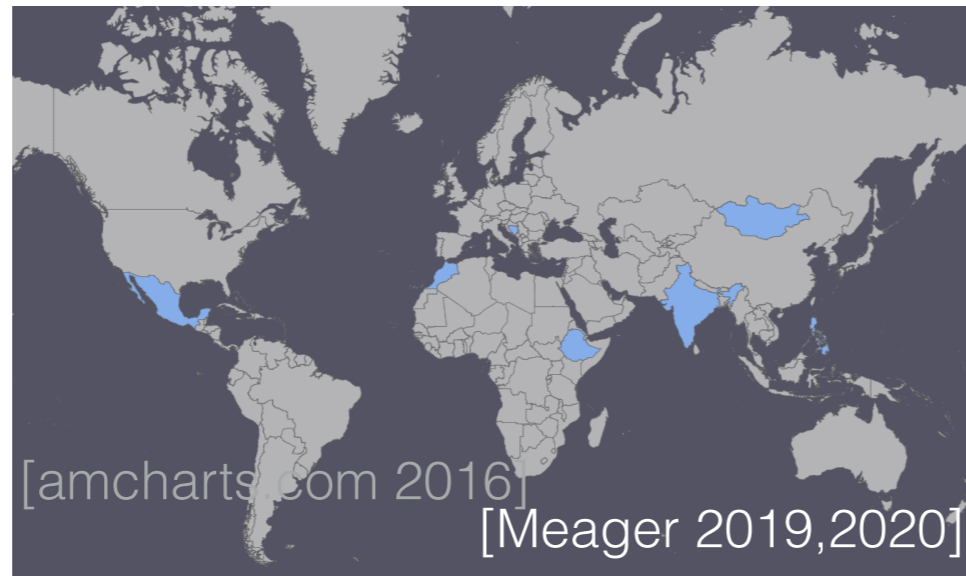
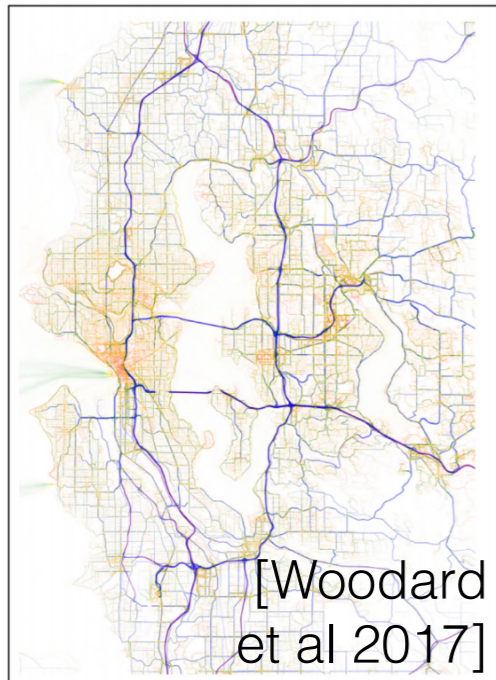
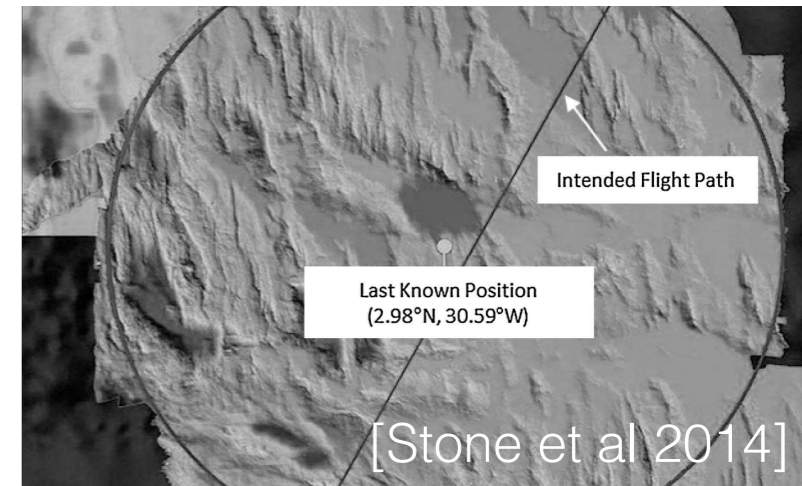
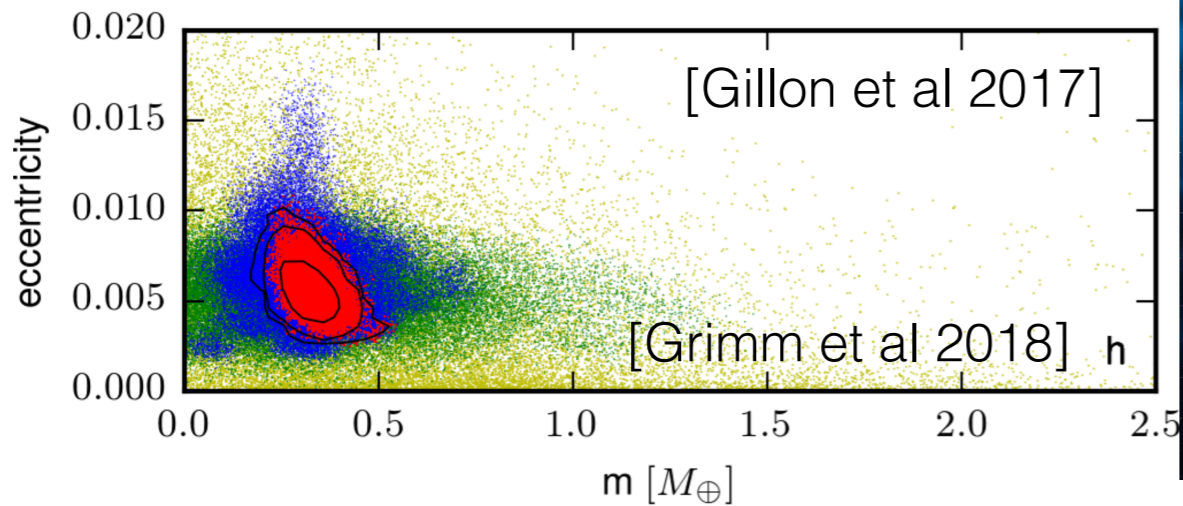


Bayesian inference



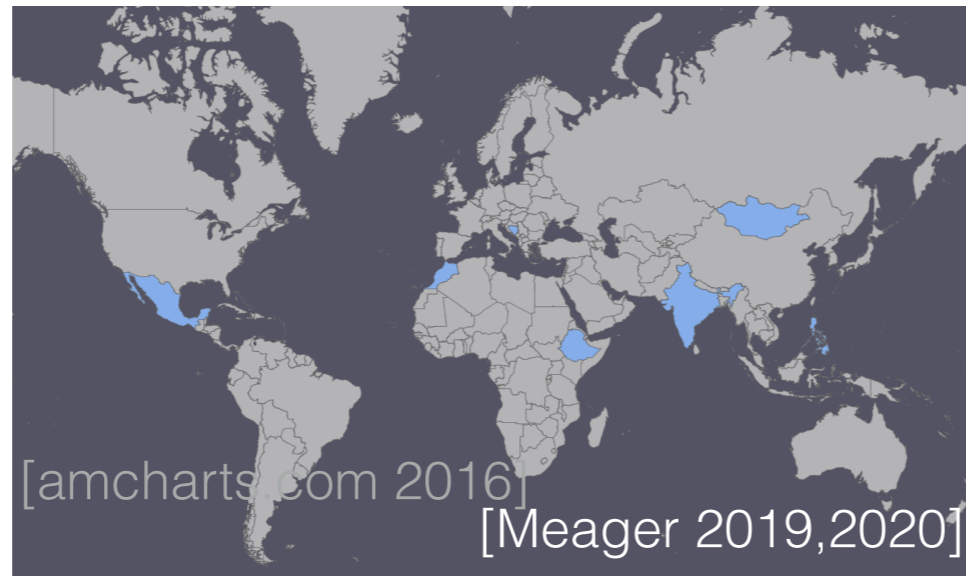
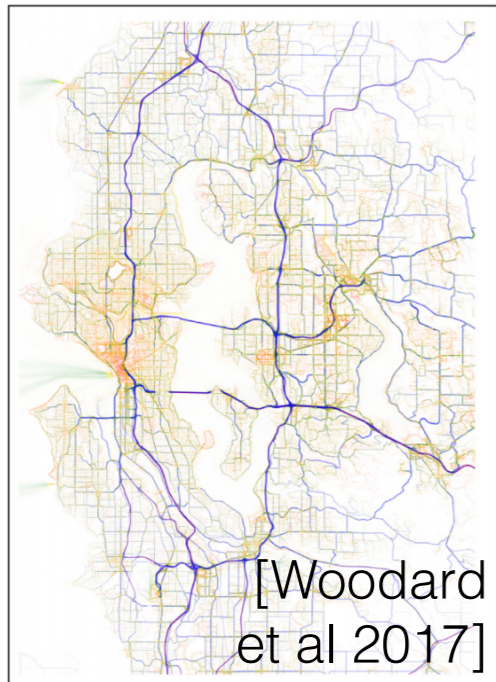
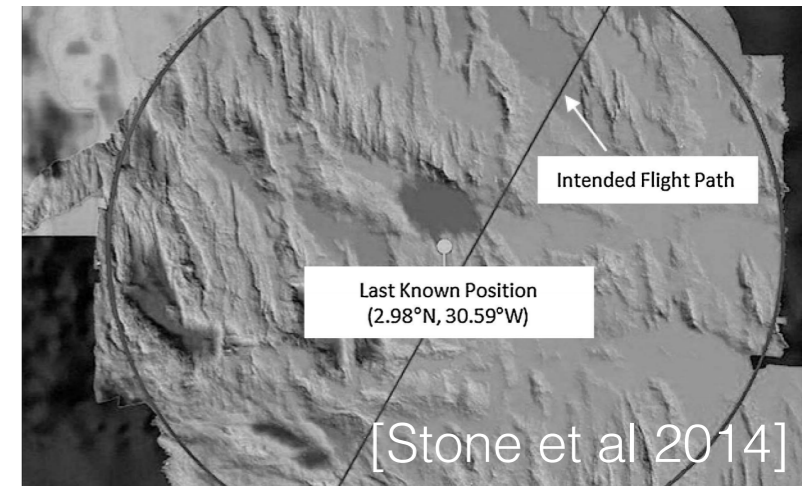
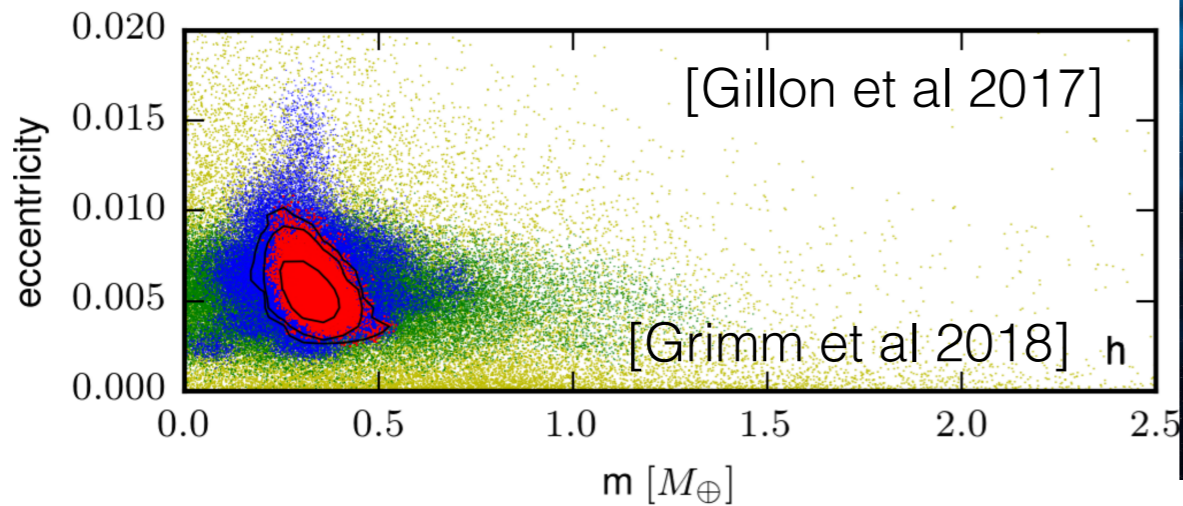
- Goals: good point estimates, uncertainty estimates

Bayesian inference



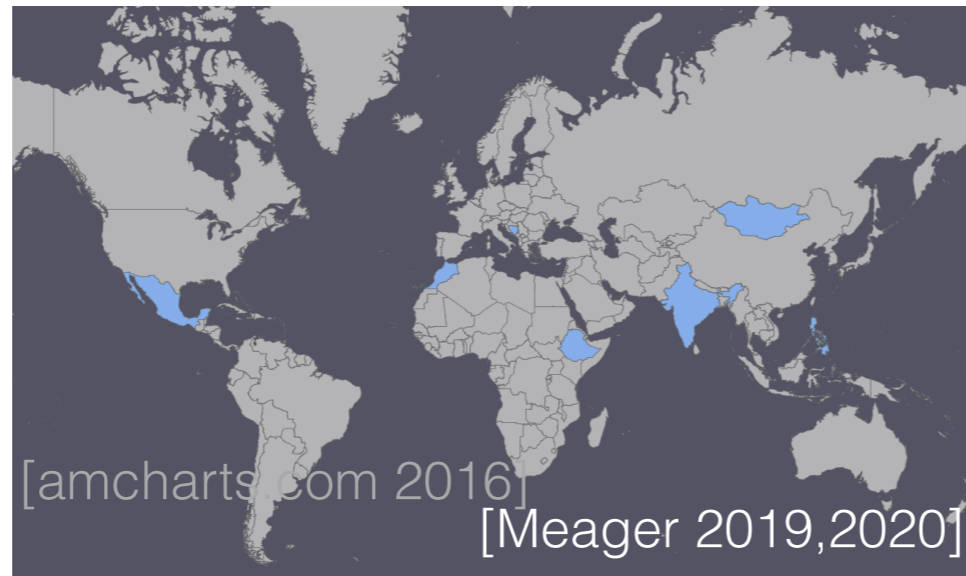
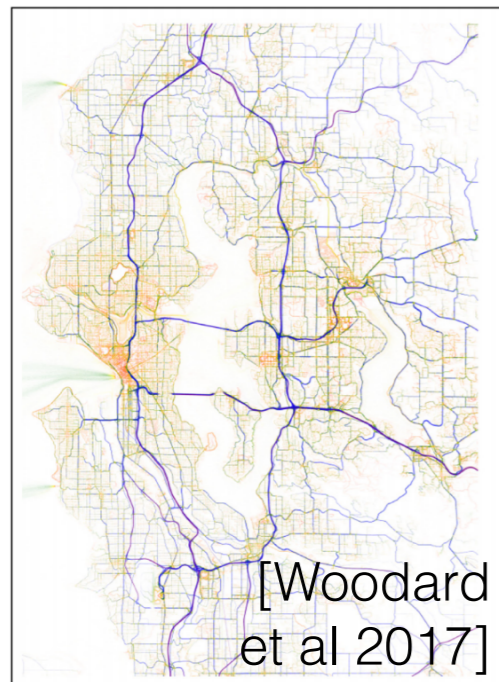
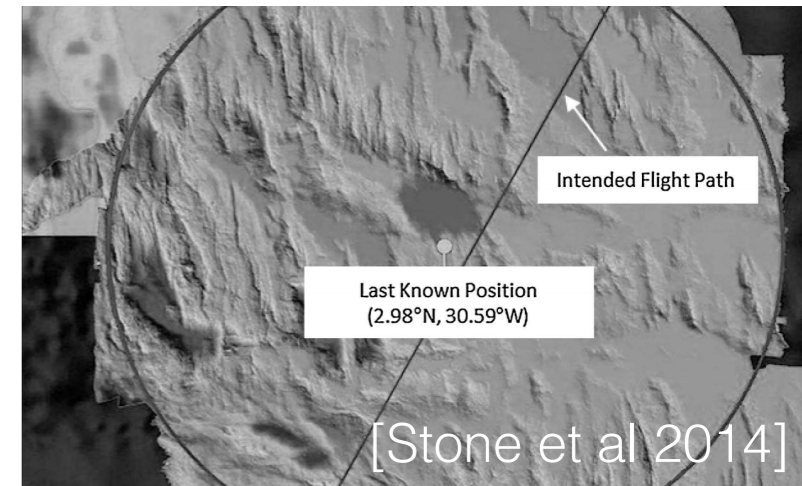
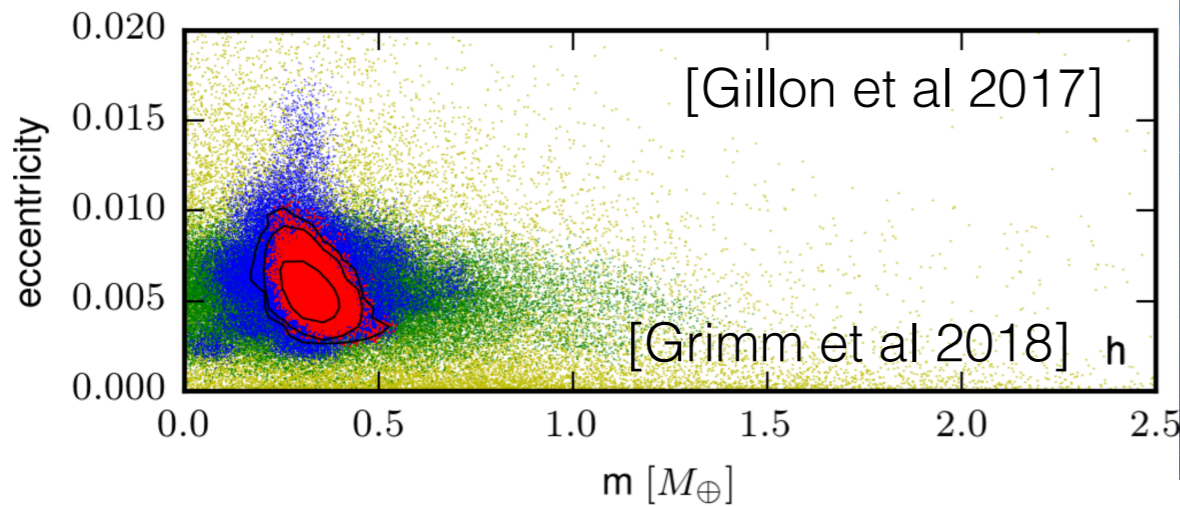
- Goals: good point estimates, uncertainty estimates
- More: interpretable, modular, expert info

Bayesian inference



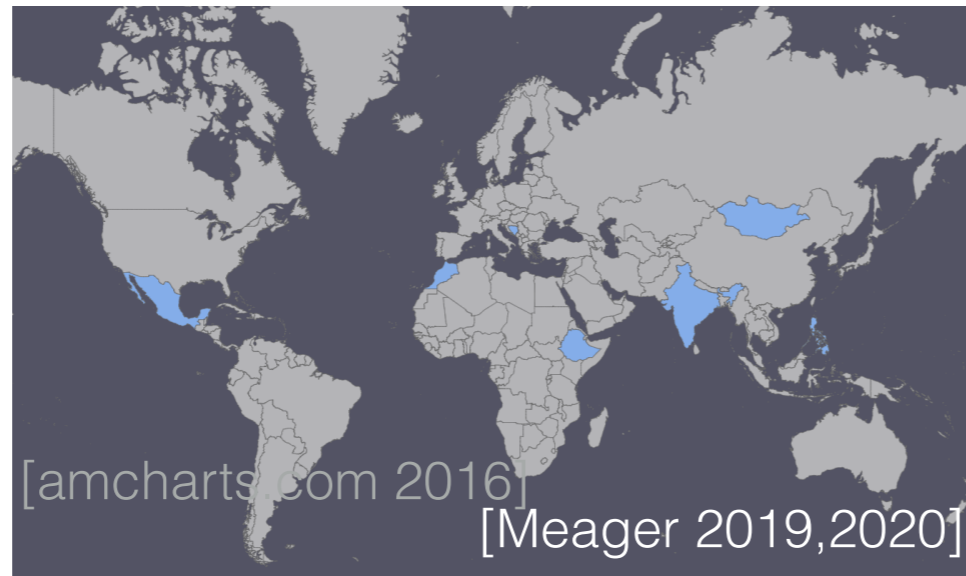
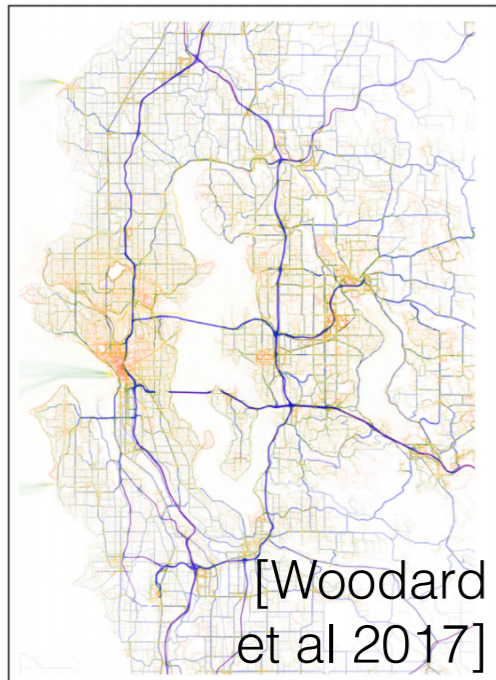
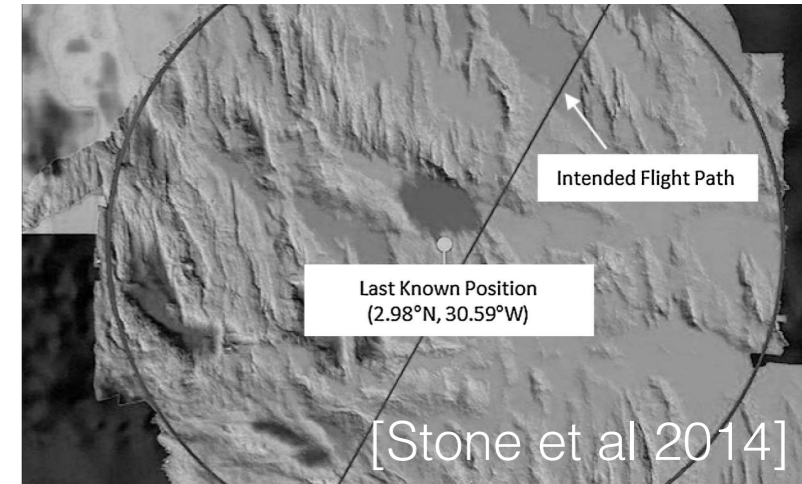
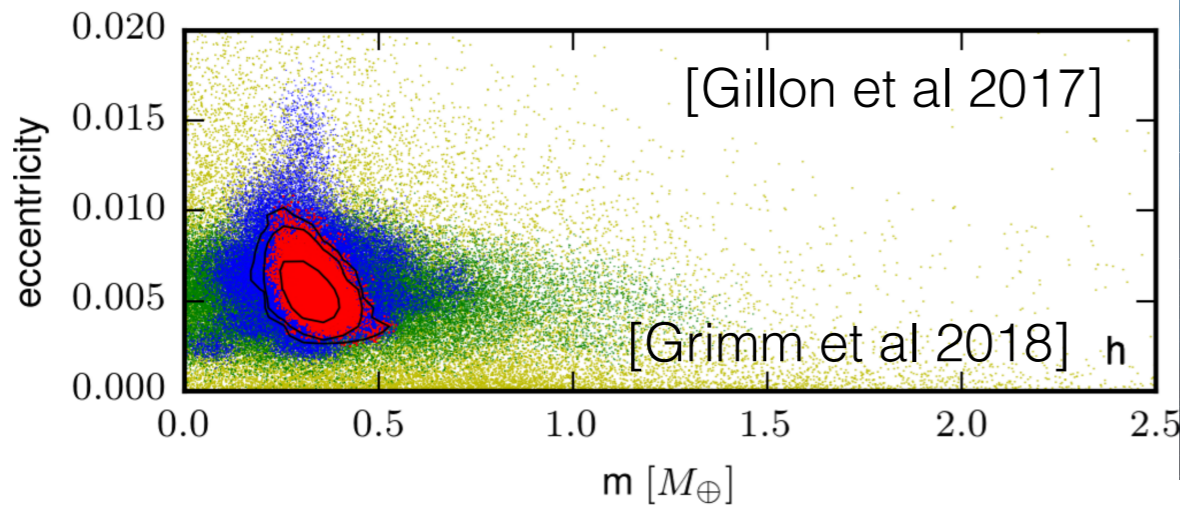
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Bayesian inference



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

Bayesian inference



- Goals: good point estimates, uncertainty estimates
 - More: interpretable, modular, expert info
- Challenge: speed (compute, user), reliable inference
- Uncertainty doesn't have to disappear in large data sets

Variational Bayes

Variational Bayes

- Modern problems: often large data, large dimensions

Variational Bayes

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- Variational Bayes can be very fast

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“Arts”	“Budgets”	“Children”	“Education”	
NEW	MILLION	CHILDREN	SCHOOL	[Blei et al
FILM	TAX	WOMEN	STUDENTS	2003]
SHOW	PROGRAM	PEOPLE	SCHOOLS	
MUSIC	BUDGET	CHILD	EDUCATION	
MOVIE	BILLION	YEARS	TEACHERS	
PLAY	FEDERAL	FAMILIES	HIGH	
MUSICAL	YEAR	WORK	PUBLIC	
BEST	SPENDING	PARENTS	TEACHER	
ACTOR	NEW	SAYS	BENNETT	
FIRST	STATE	FAMILY	MANIGAT	
YORK	PLAN	WELFARE	NAMPHY	
OPERA	MONEY	MEN	STATE	
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LOVE	CONGRESS	LIFE	HAITI	

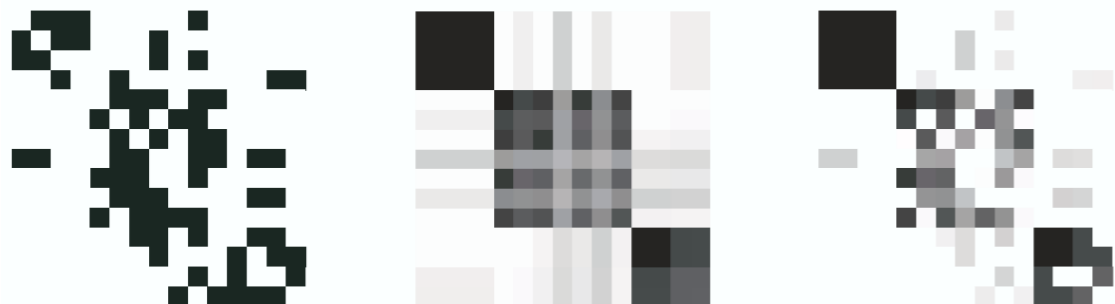
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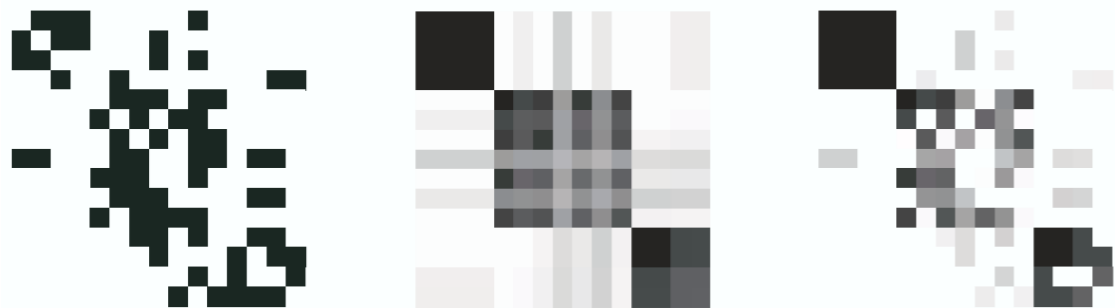
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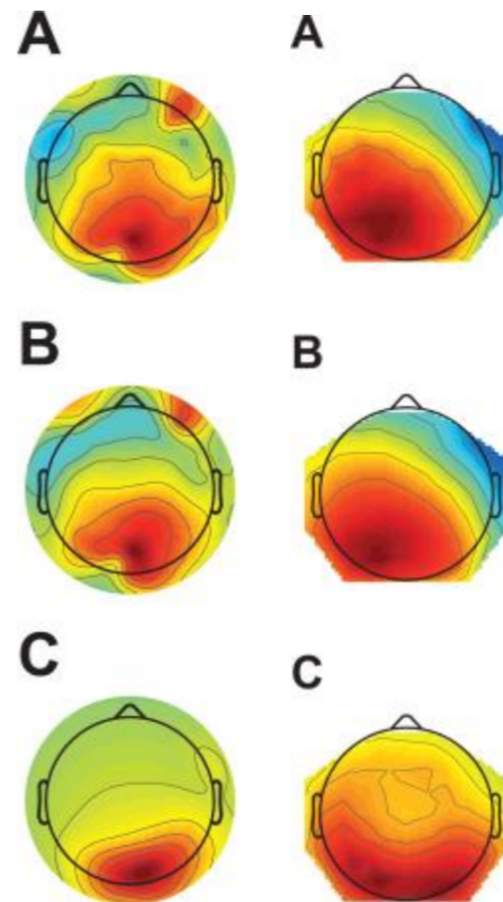
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[Blei et al 2003]

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[Airoldi et al 2008]



[Gershman et al 2014]

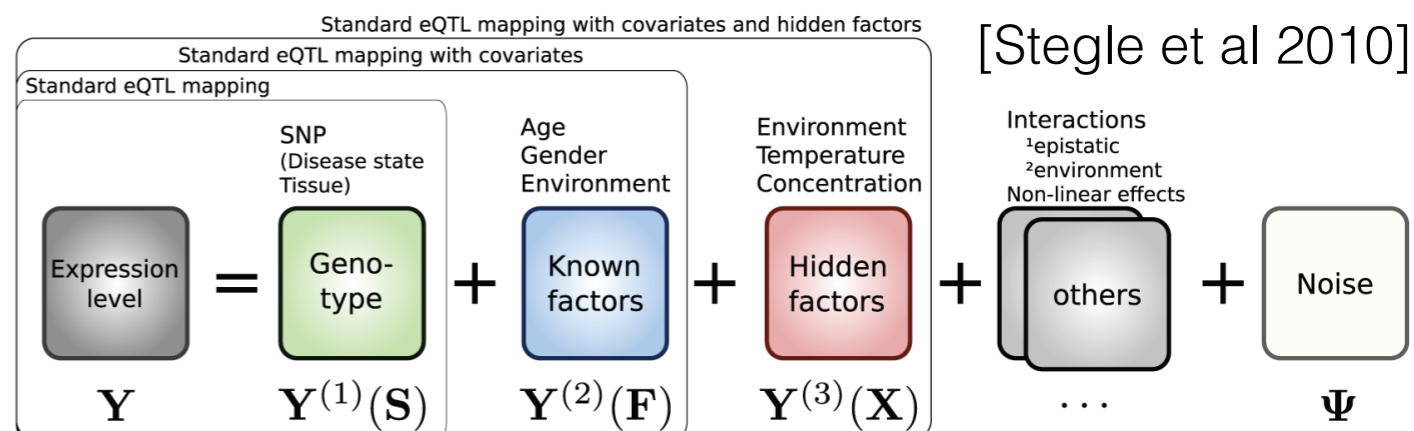
[Blei et al 2018]

Variational Bayes

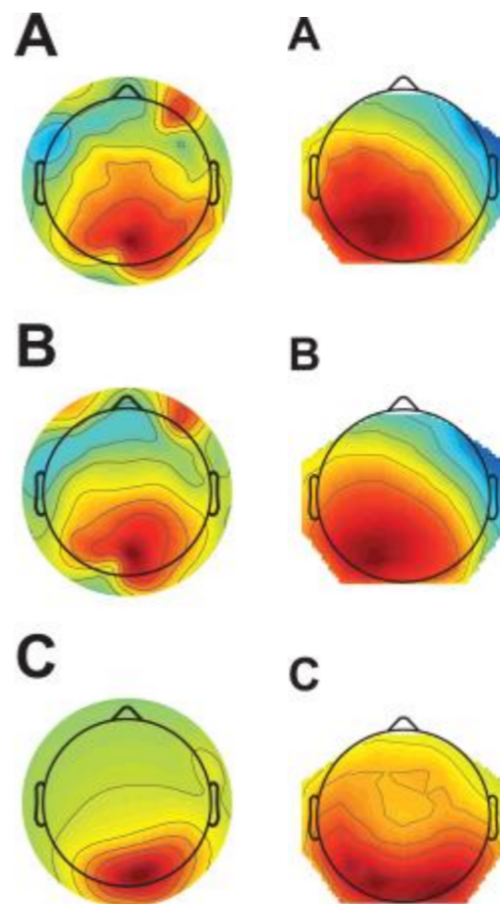
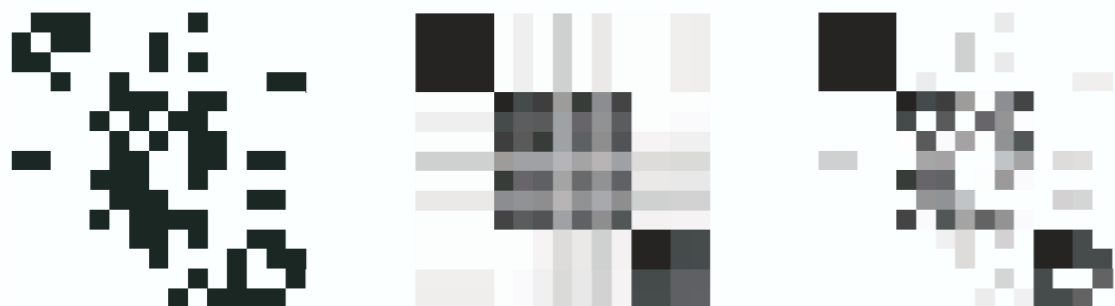
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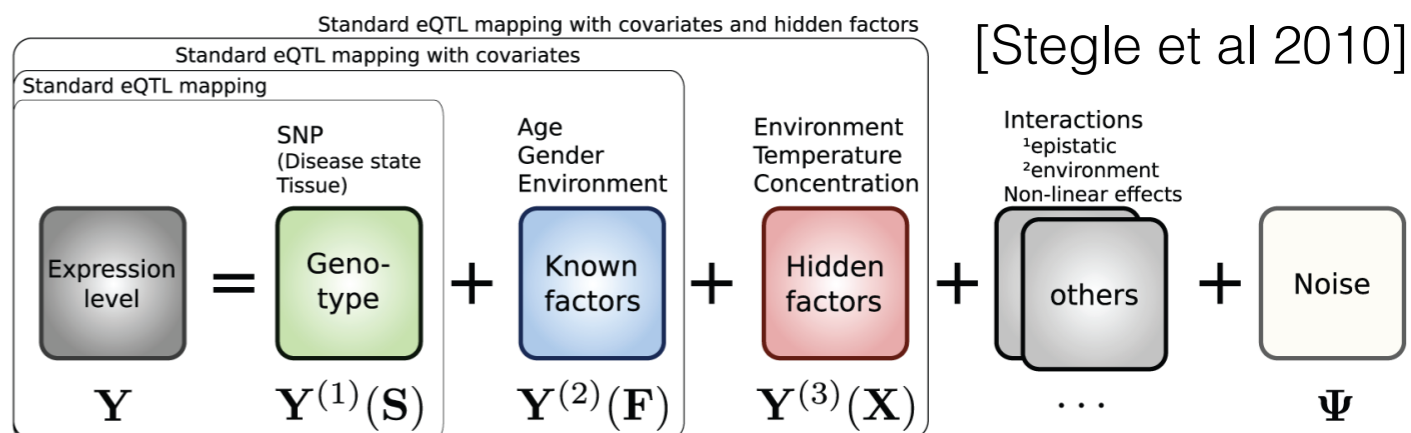


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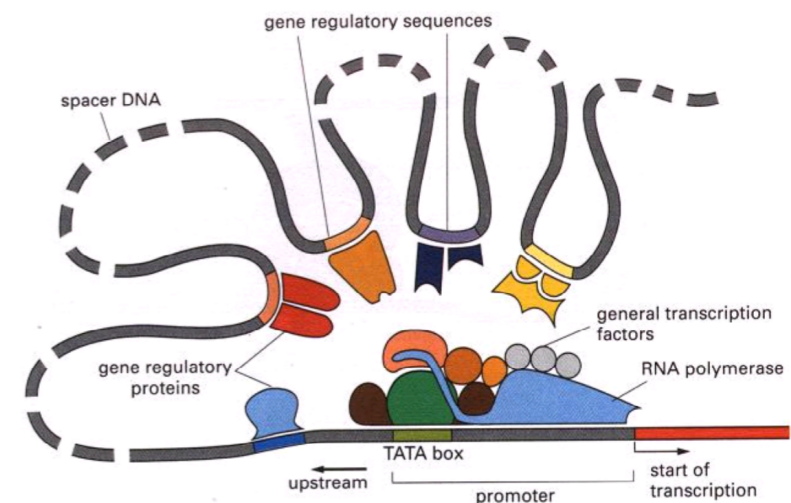
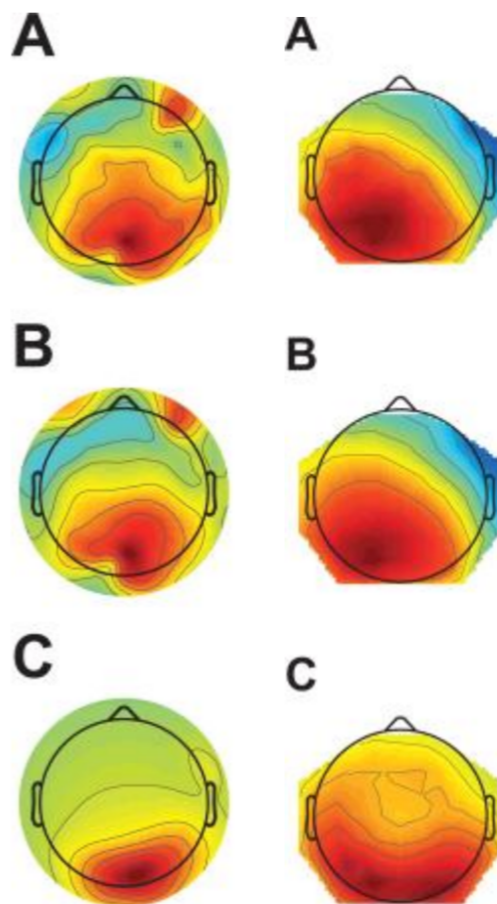
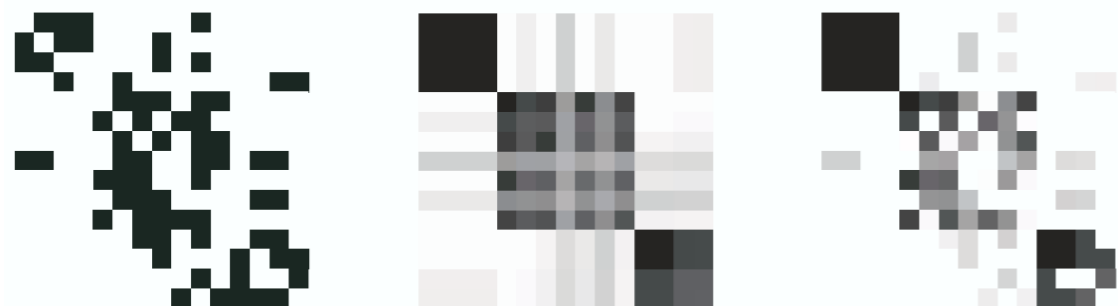
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Roadmap

- Bayes & Approximate Bayes review

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

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Bayesian inference

Bayesian inference

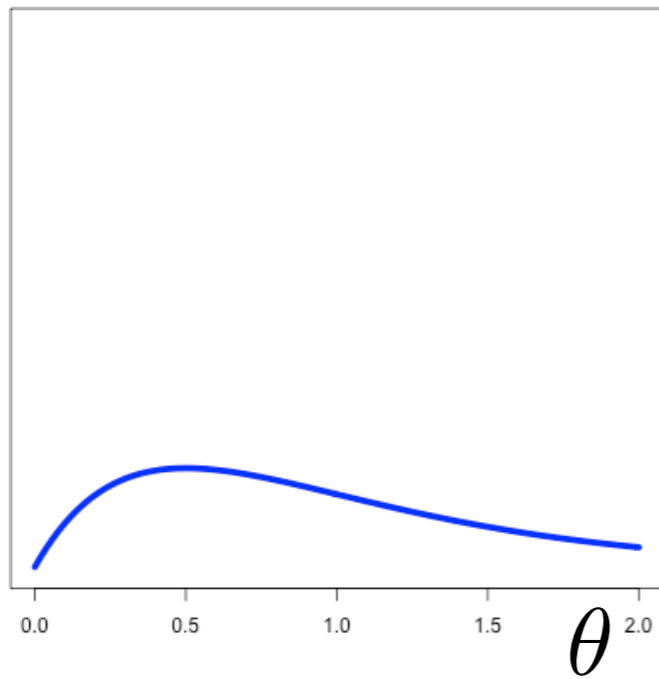
parameters

 θ

Bayesian inference

parameters

 $p(\theta)$
prior

Bayesian inference

parameters
↓
 $p(\theta)$
prior



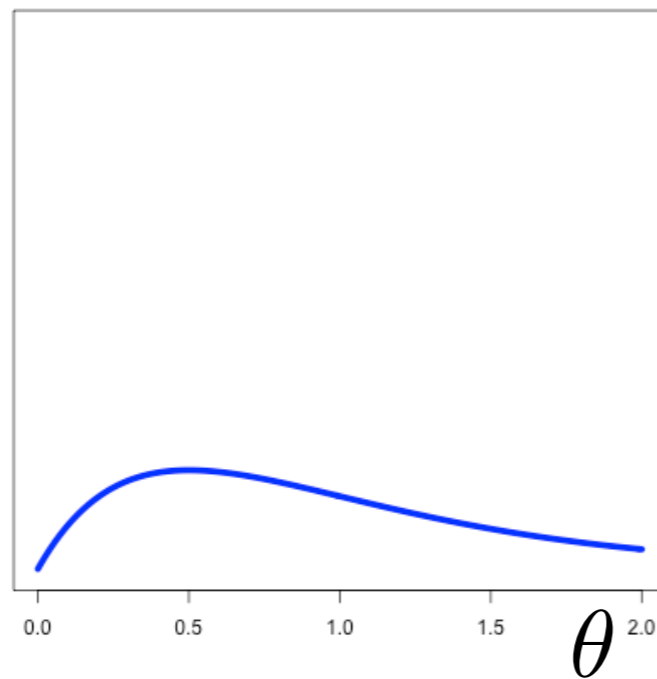
Bayesian inference

parameters



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

likelihood prior



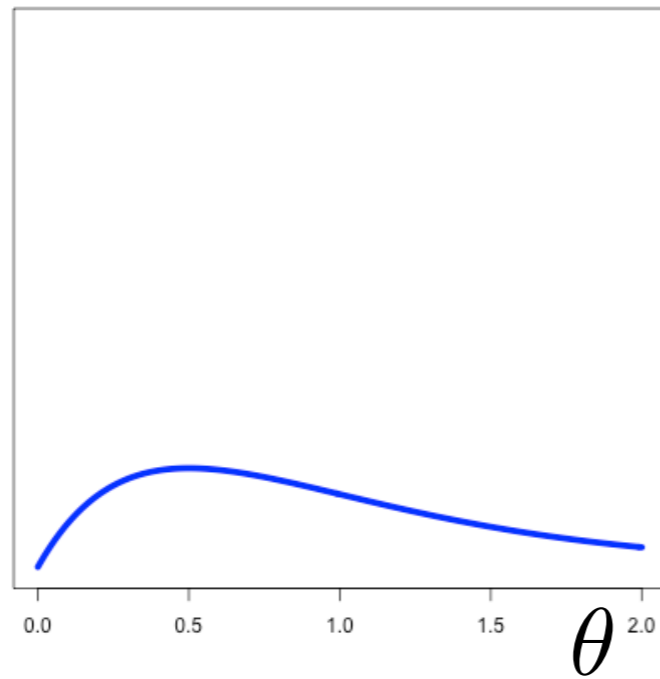
Bayesian inference

data

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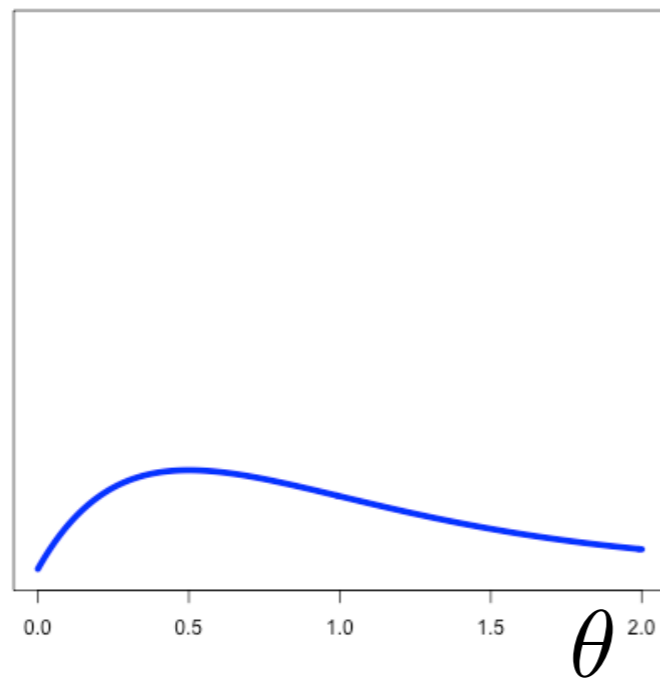
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posterior likelihood prior



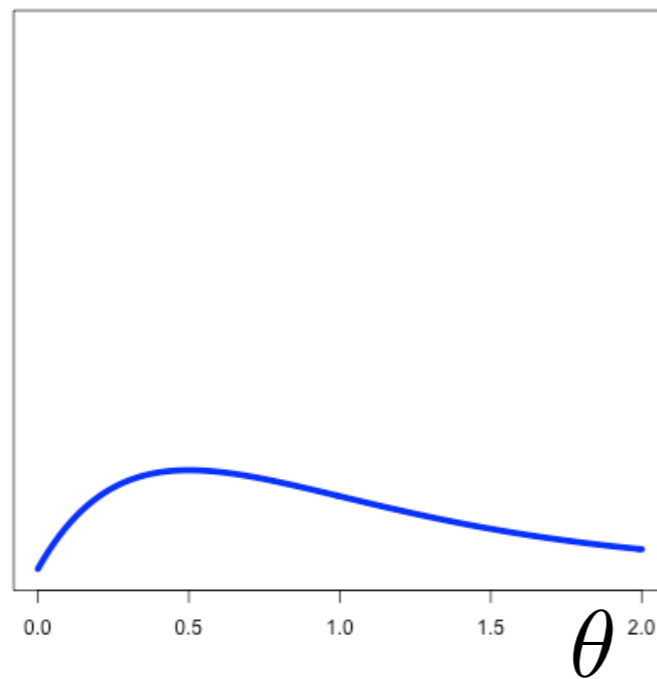
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**Bayes
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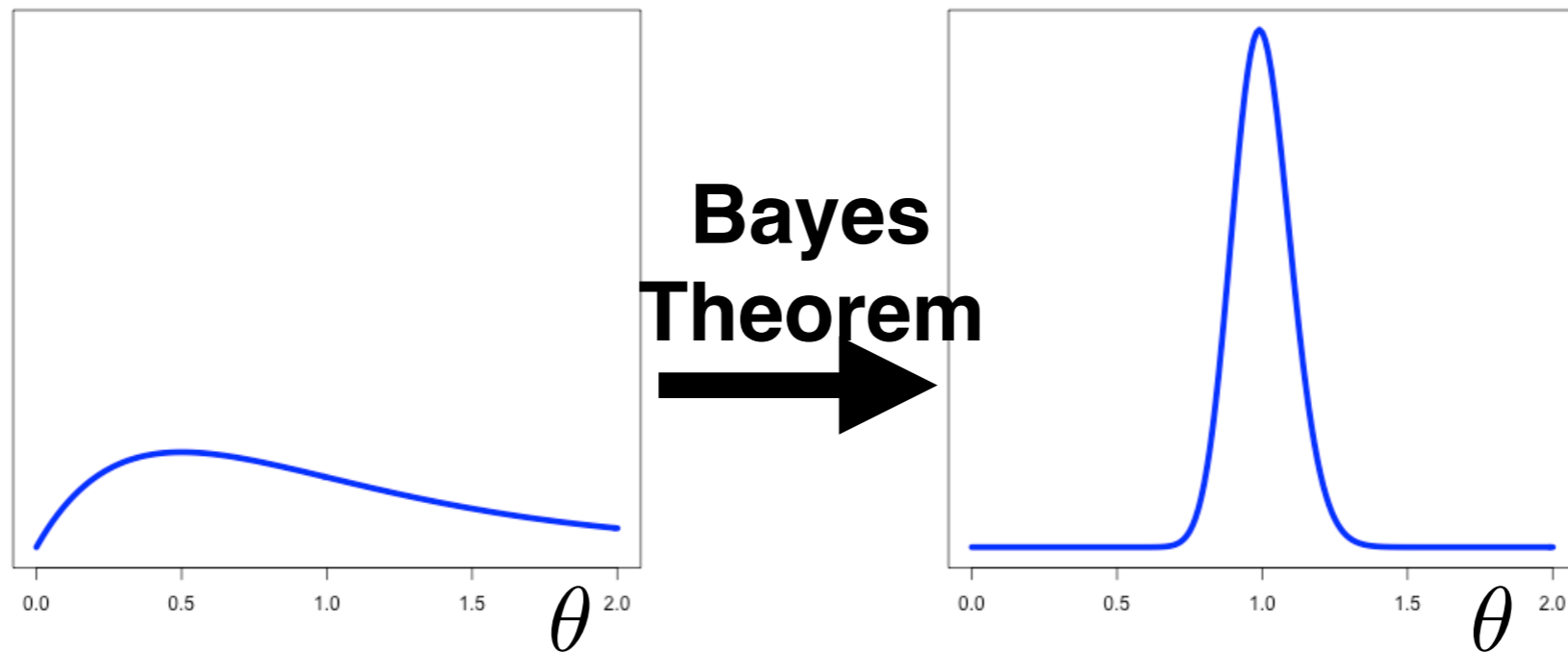
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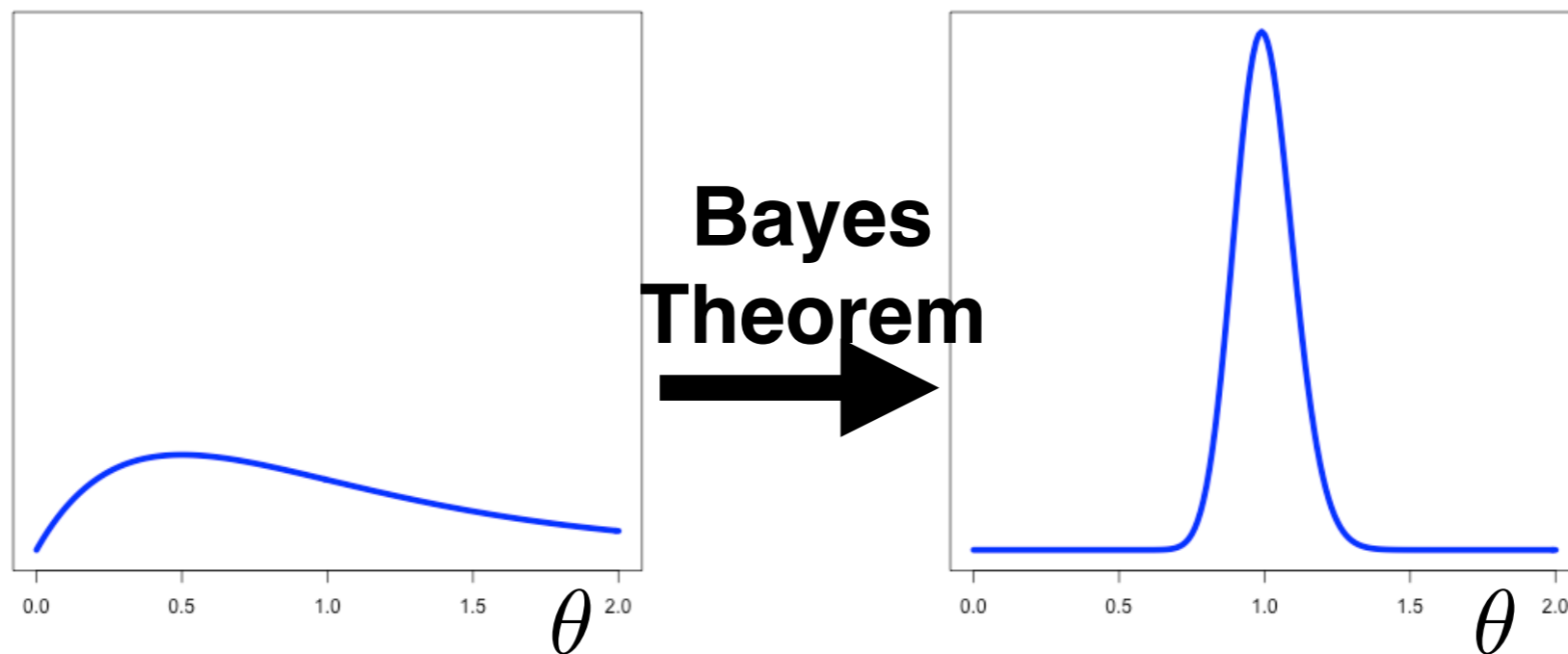
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1. Build a model: choose prior & choose likelihood

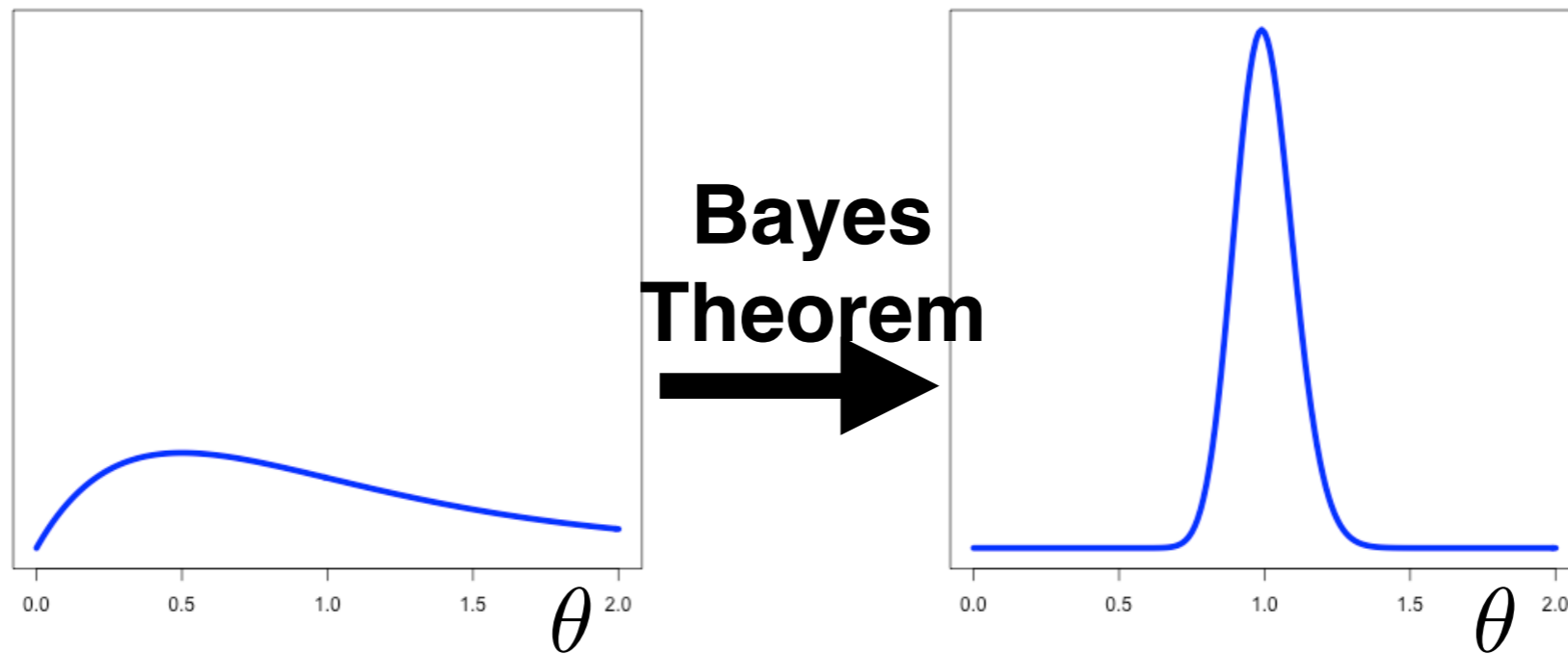
Bayesian inference

data

parameters

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posterior likelihood prior



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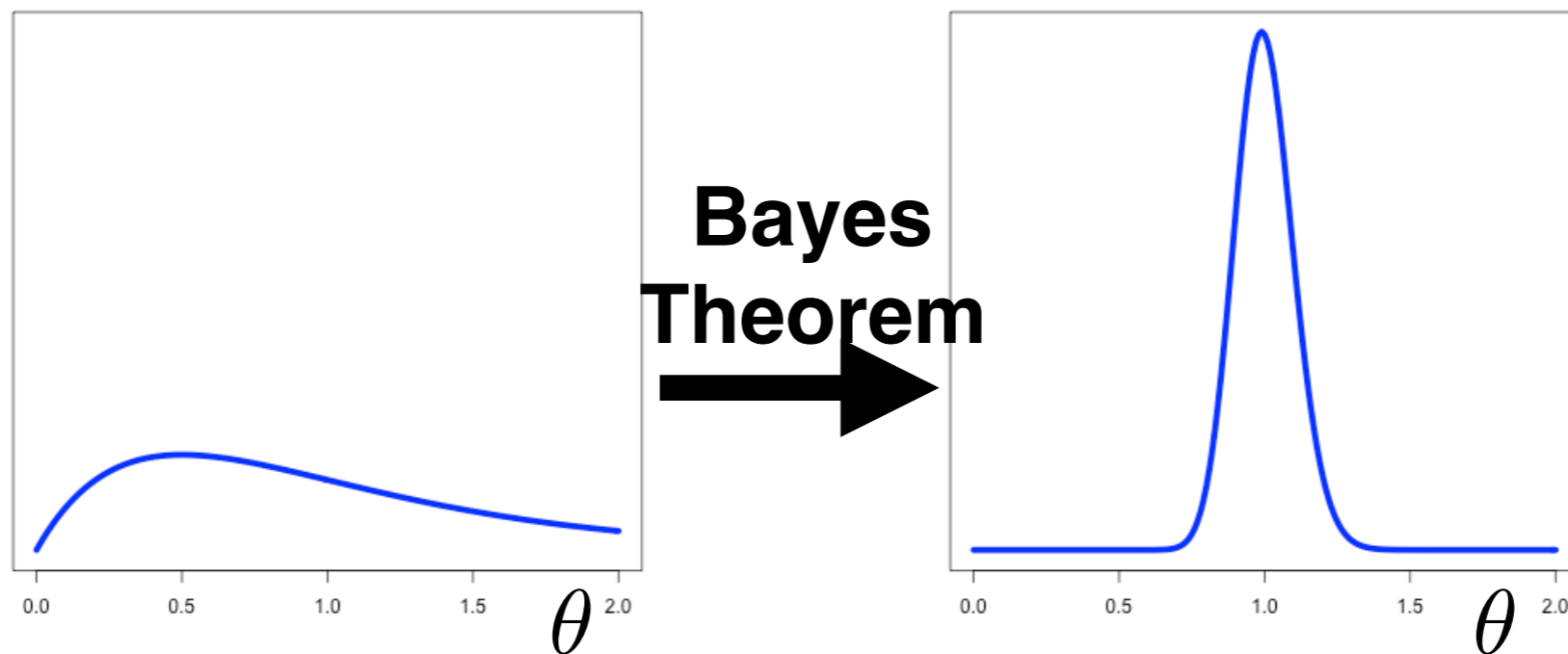
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1. Build a model: choose prior & choose likelihood
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3. Report a summary, e.g. posterior means and (co)variances

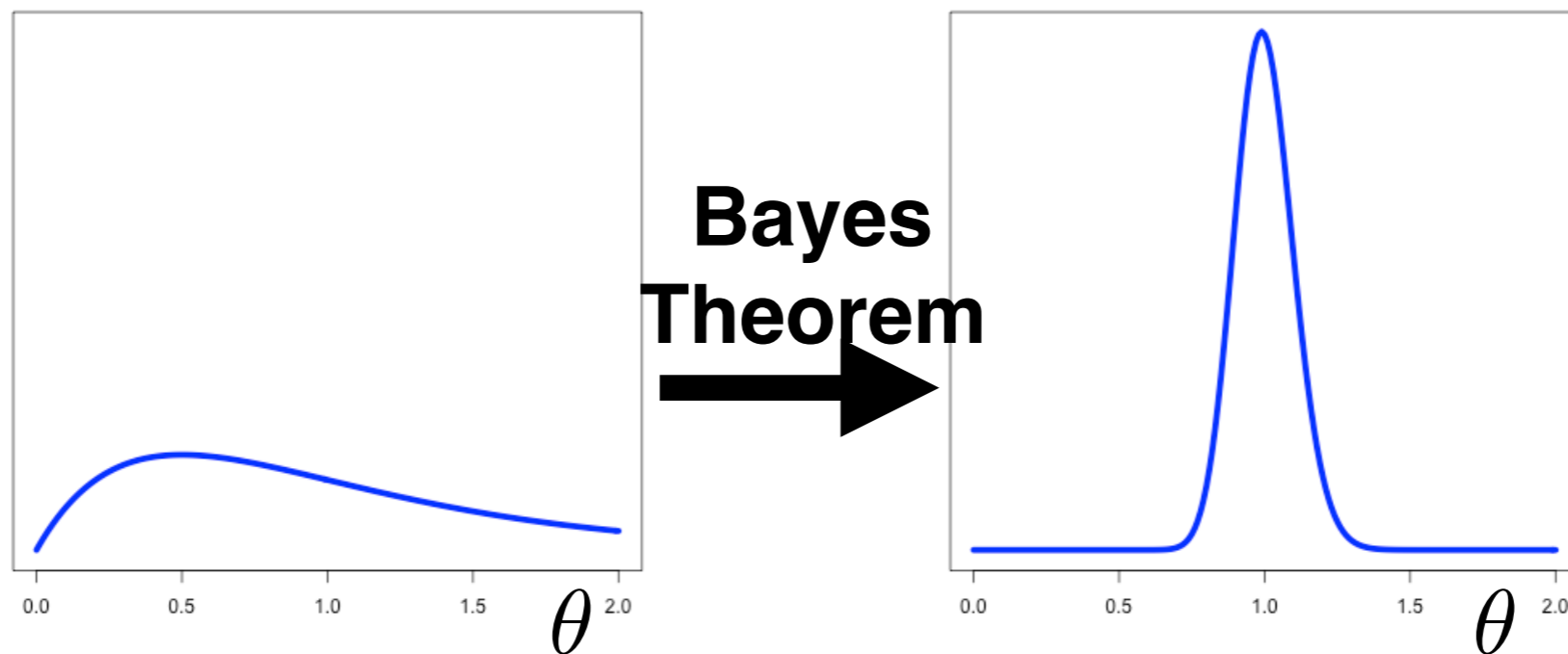
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- Why are steps 2 and 3 hard?

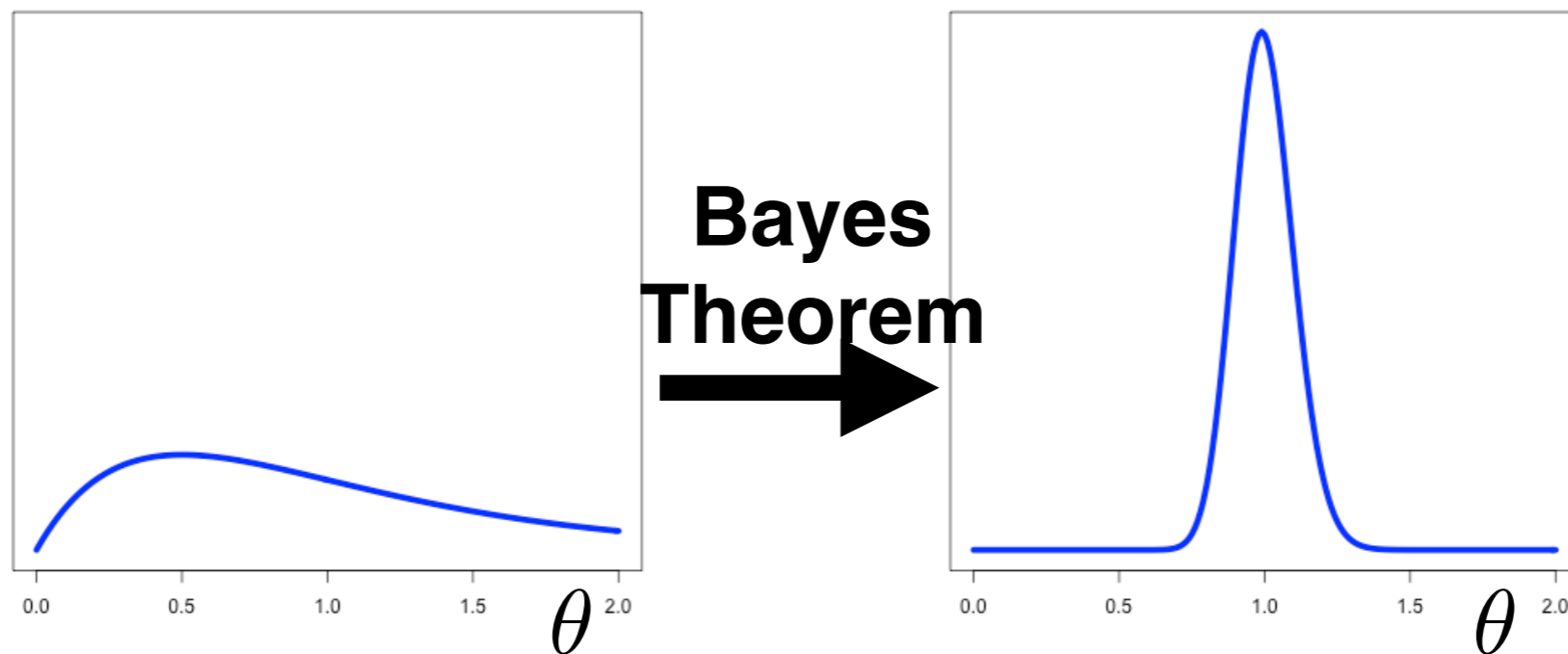
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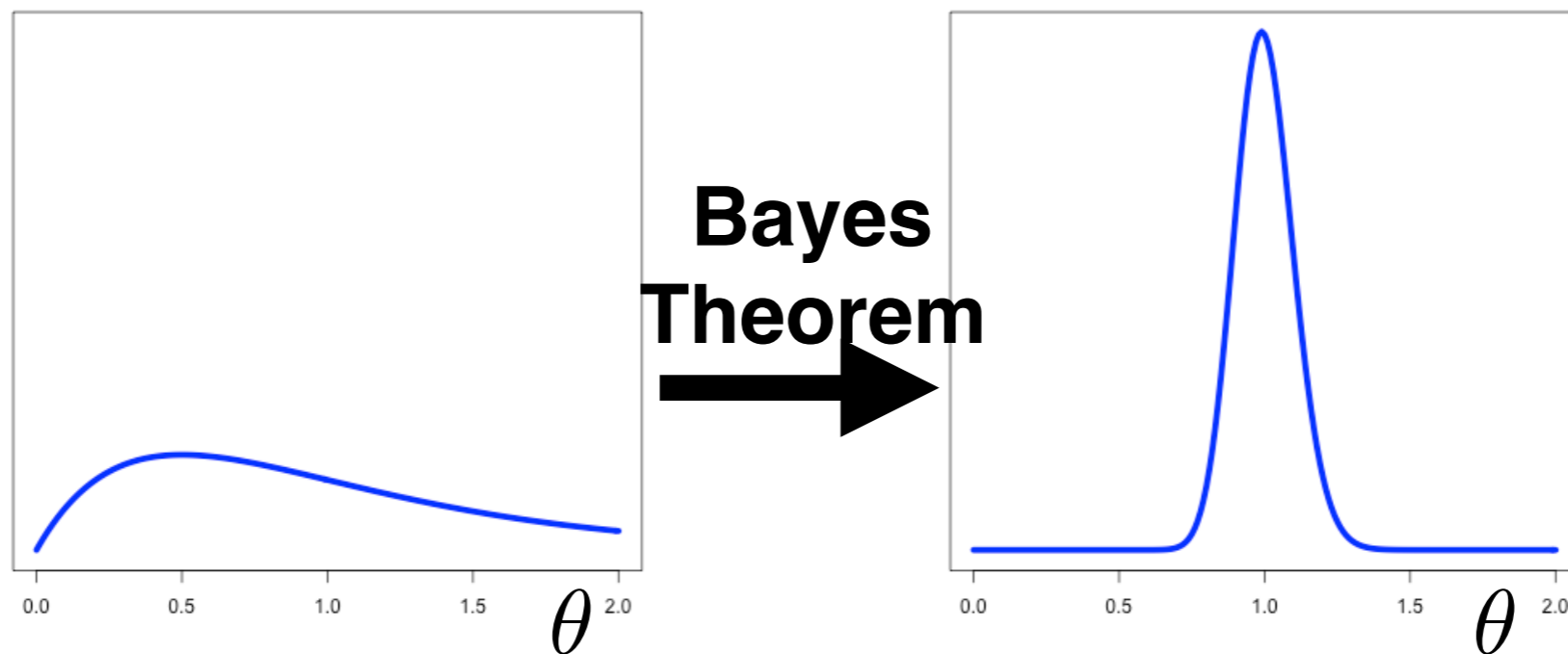
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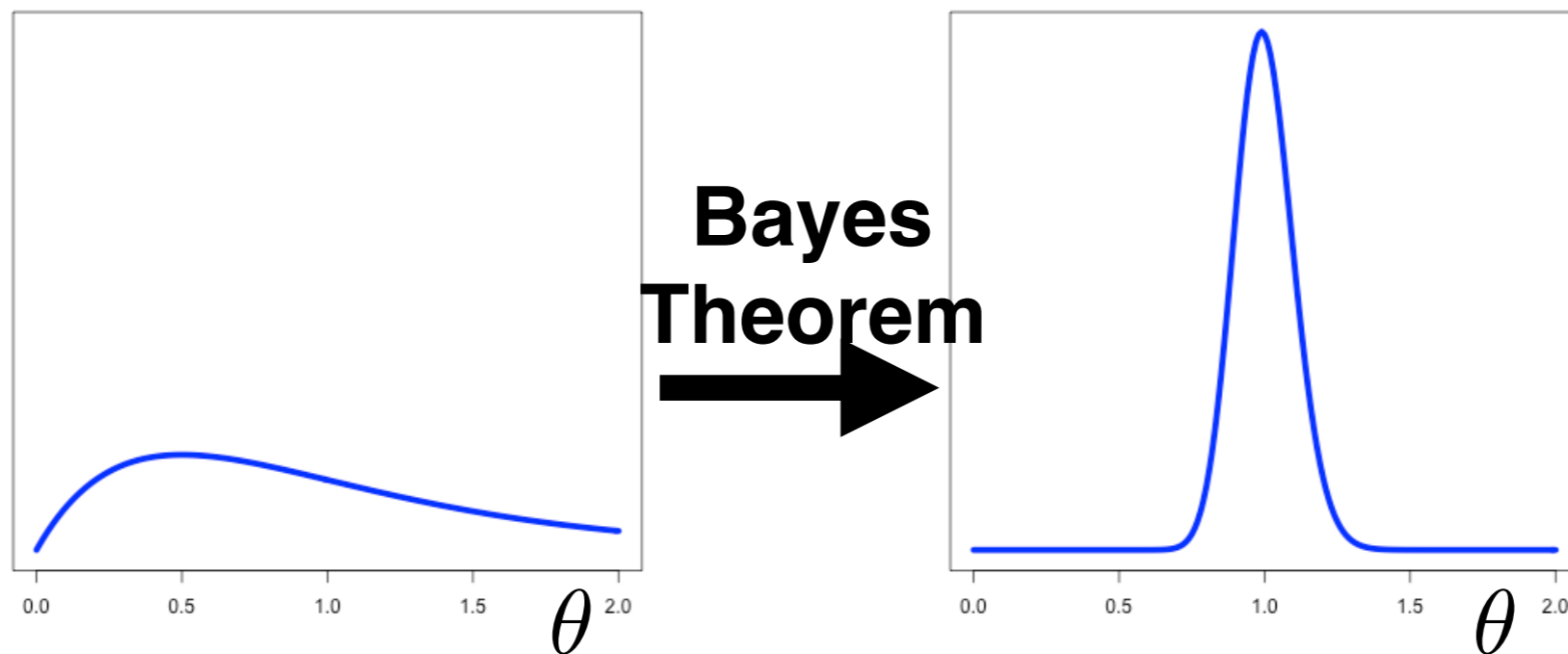
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$$p(\theta|y_{1:N}) = p(y_{1:N}|\theta)p(\theta)/p(y_{1:N})$$

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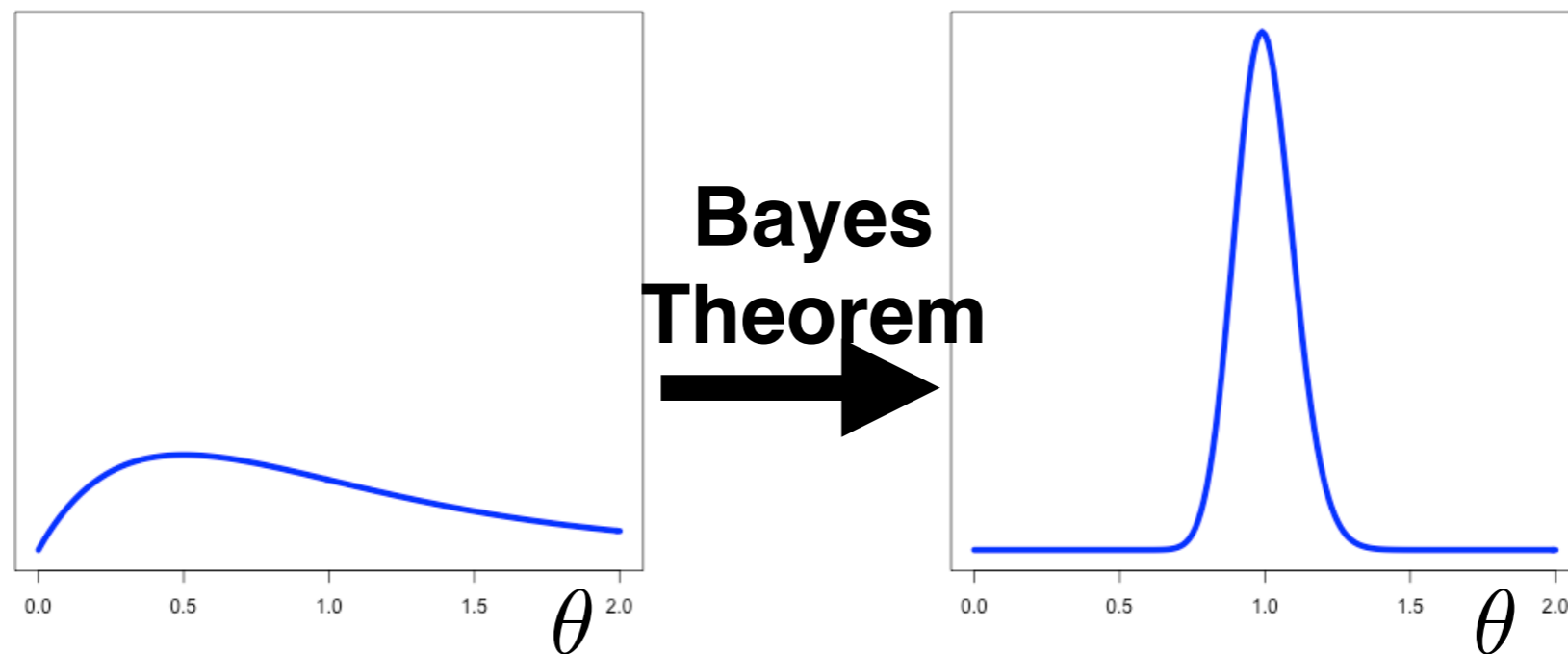
$$p(\theta|y_{1:N}) = p(y_{1:N}|\theta)p(\theta)/p(y_{1:N})$$

posterior

likelihood

prior

evidence



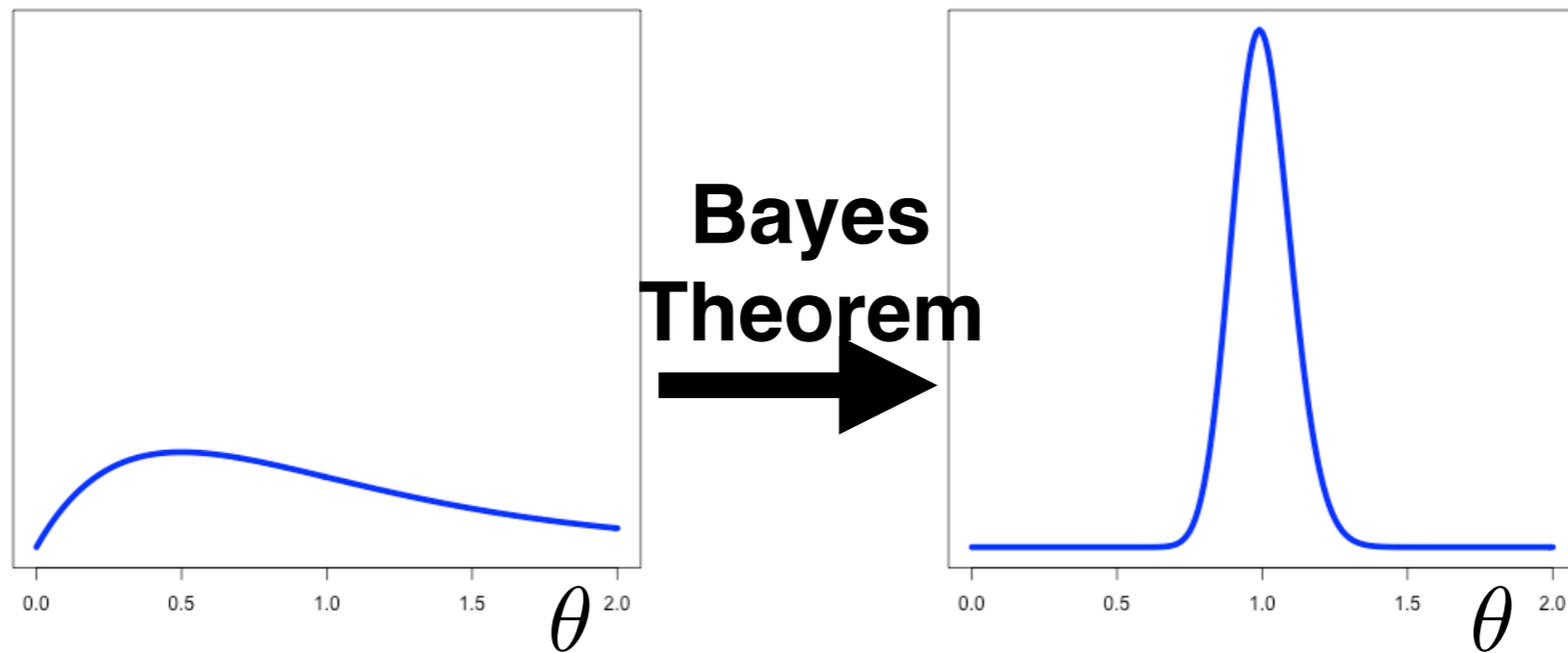
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$$p(\theta|y_{1:N}) = p(y_{1:N}|\theta)p(\theta) / \int p(y_{1:N}, \theta)d\theta$$

posterior likelihood prior evidence

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Approximate Bayesian Inference

Approximate Bayesian Inference

- Gold standard: Markov Chain Monte Carlo (MCMC)

[Bardenet,
Doucet,
Holmes
2017]

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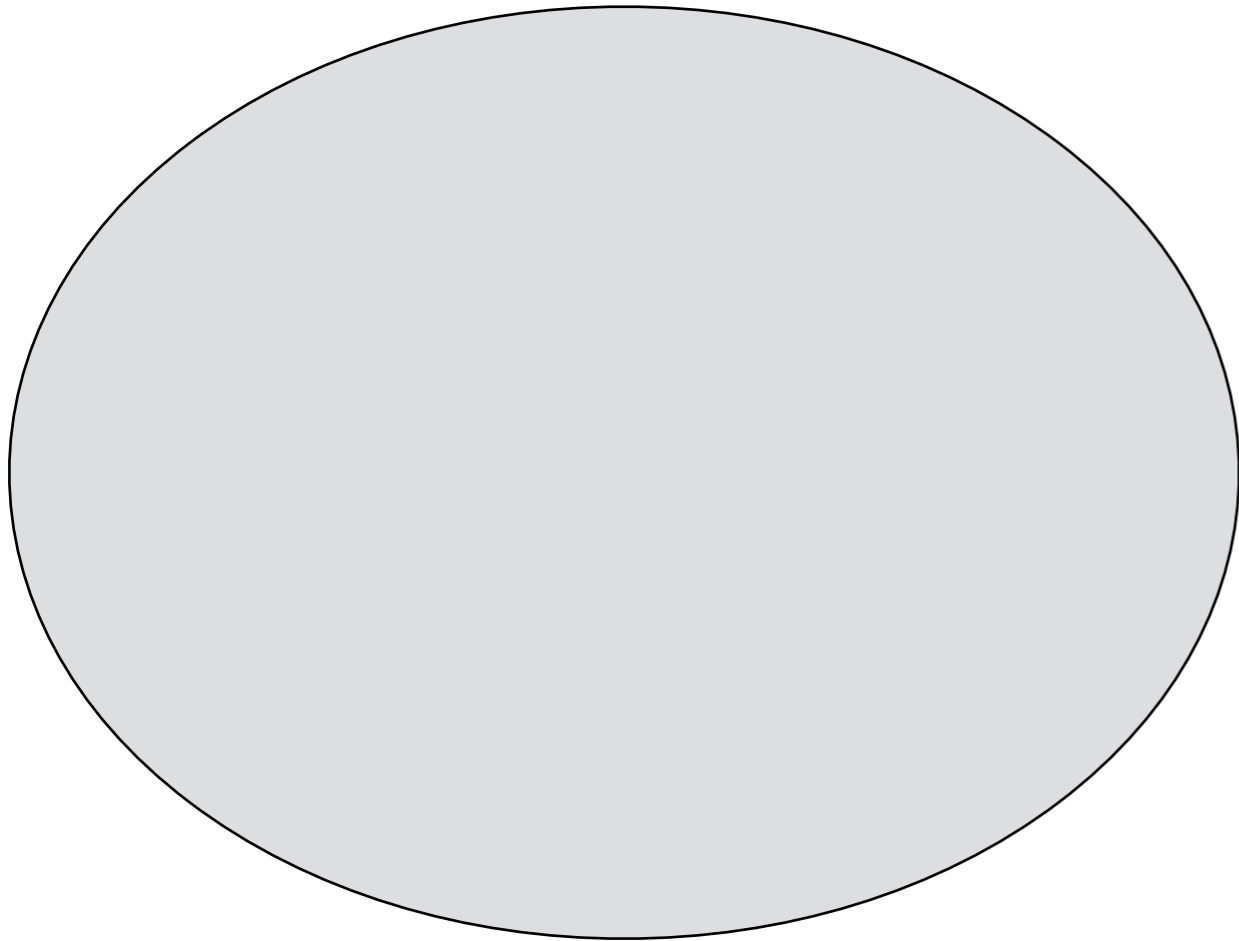
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- Approximate posterior with q^*

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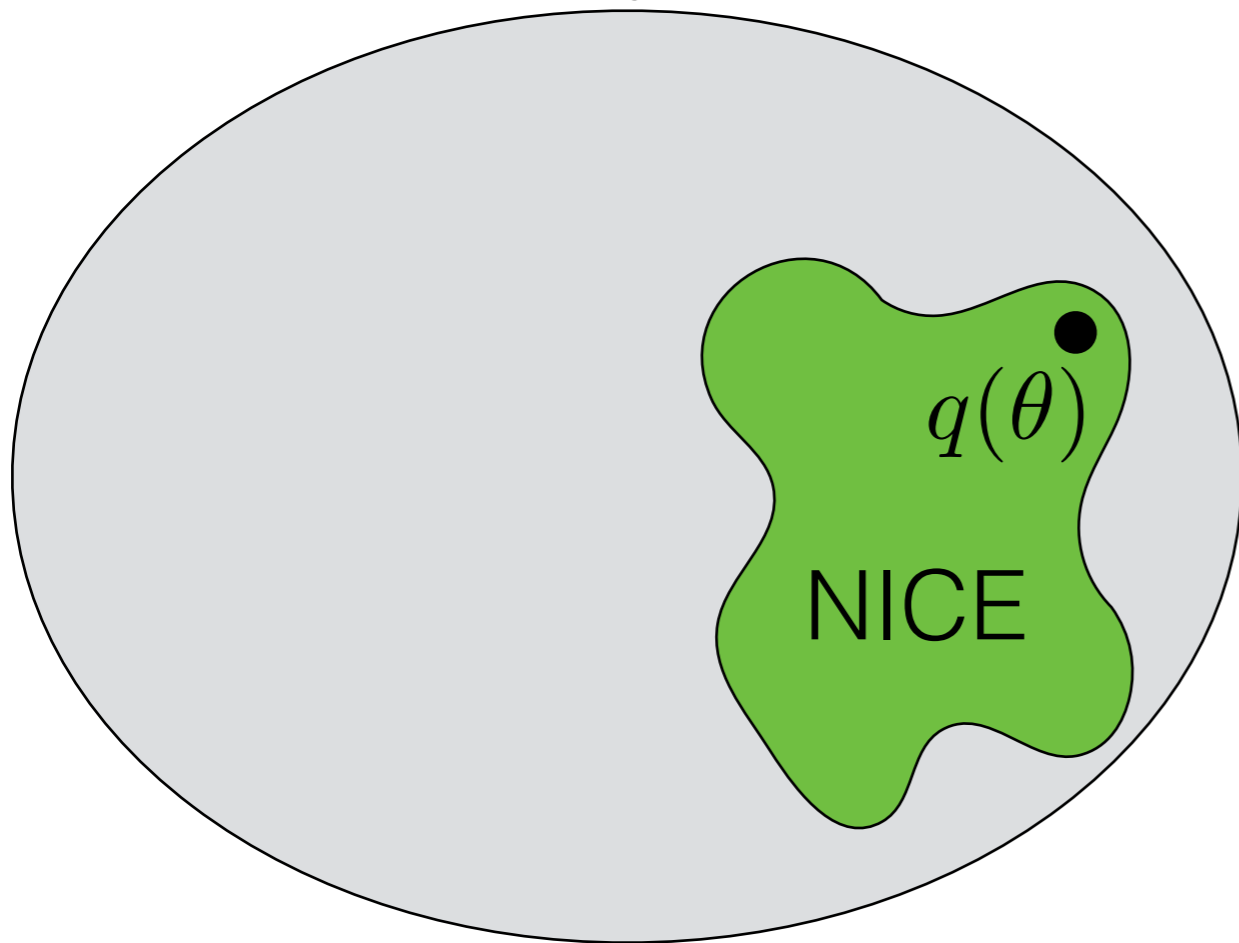
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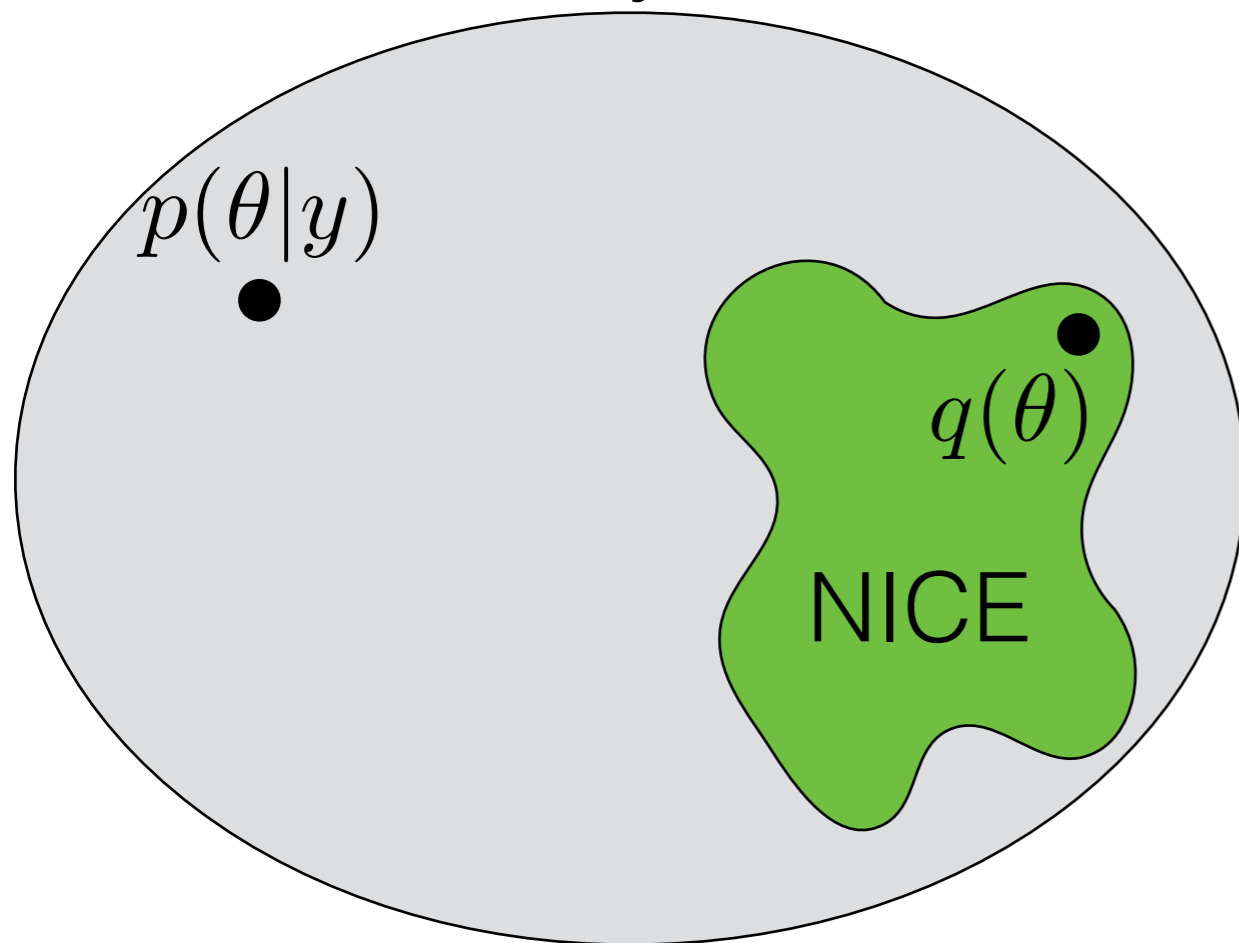
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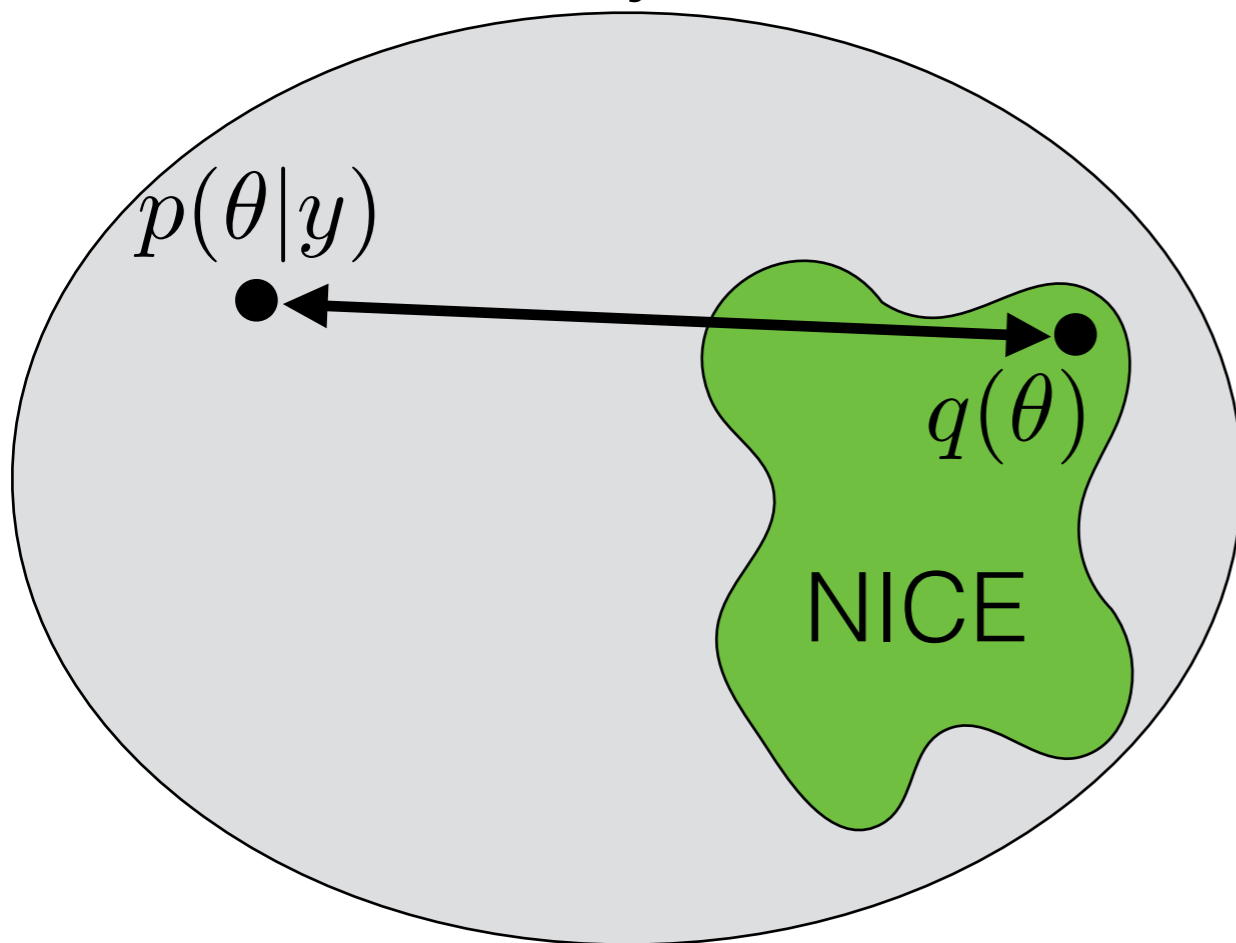
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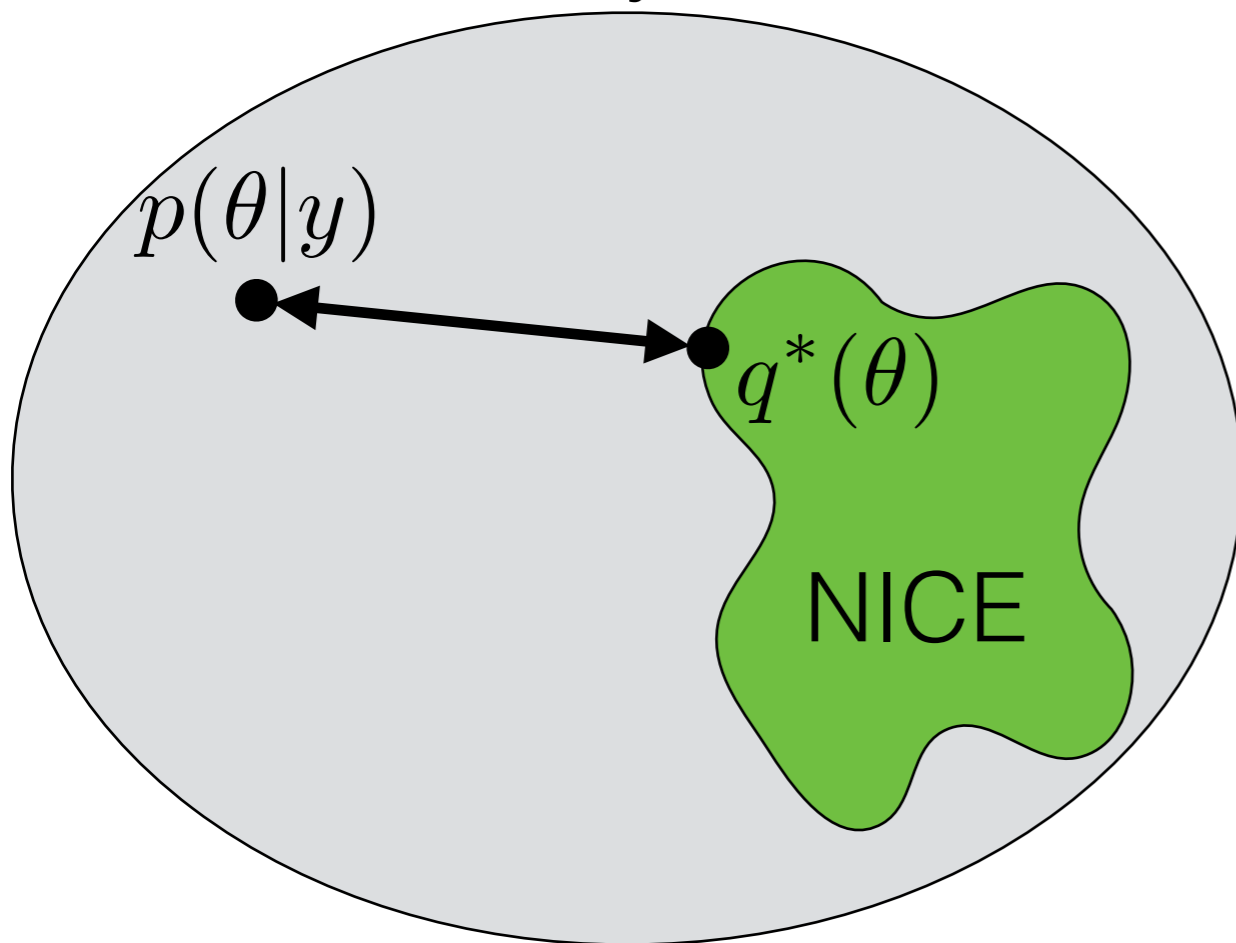
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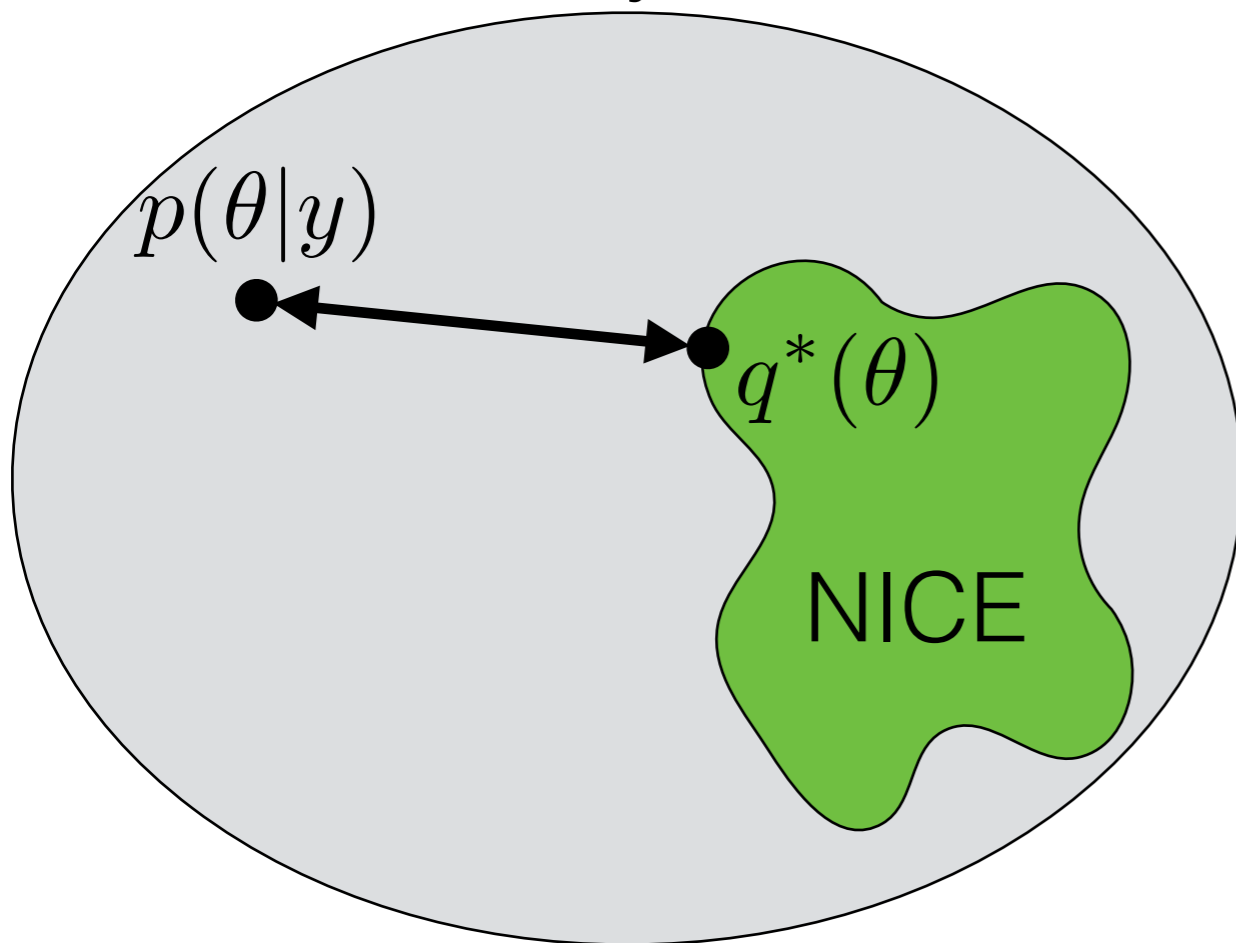
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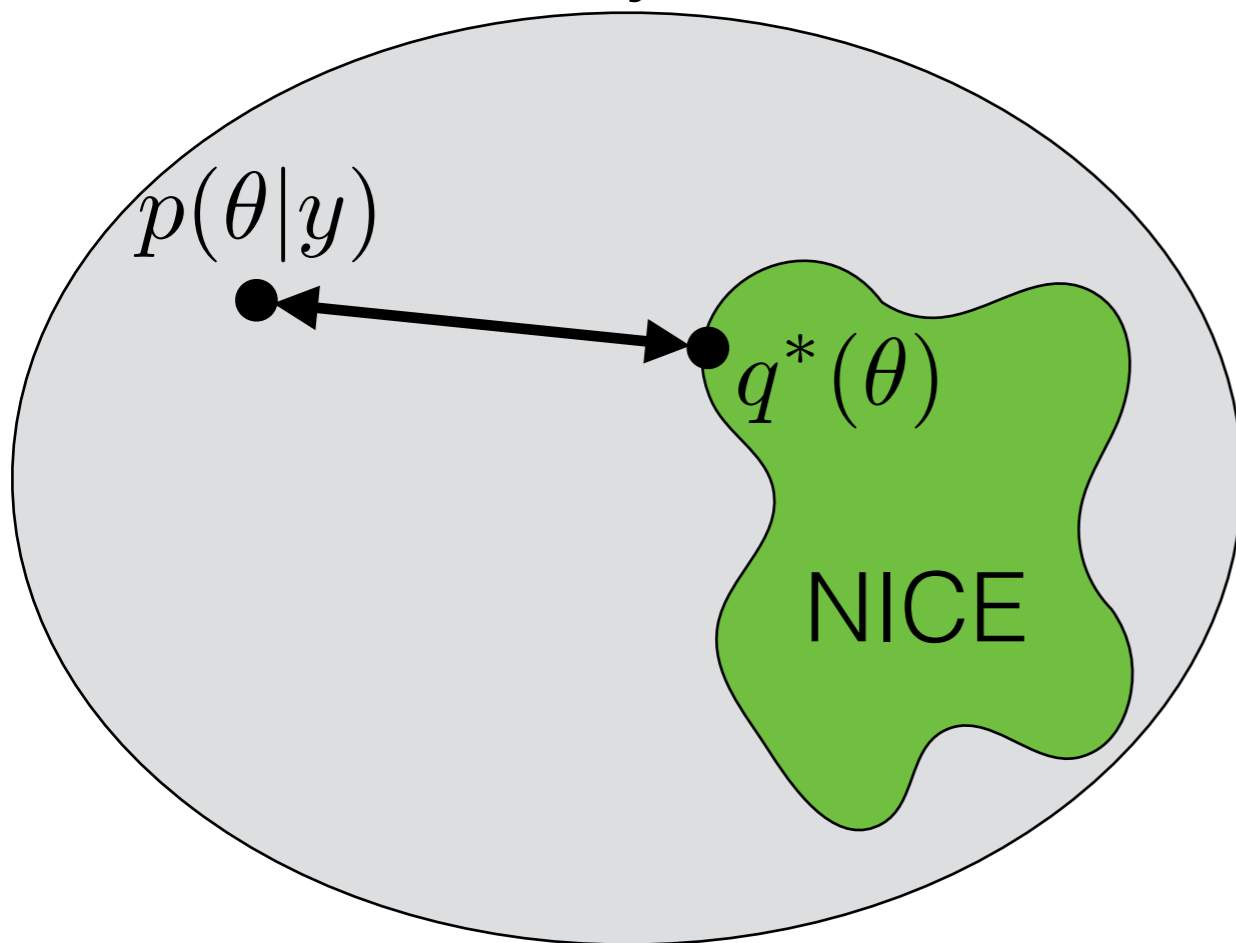
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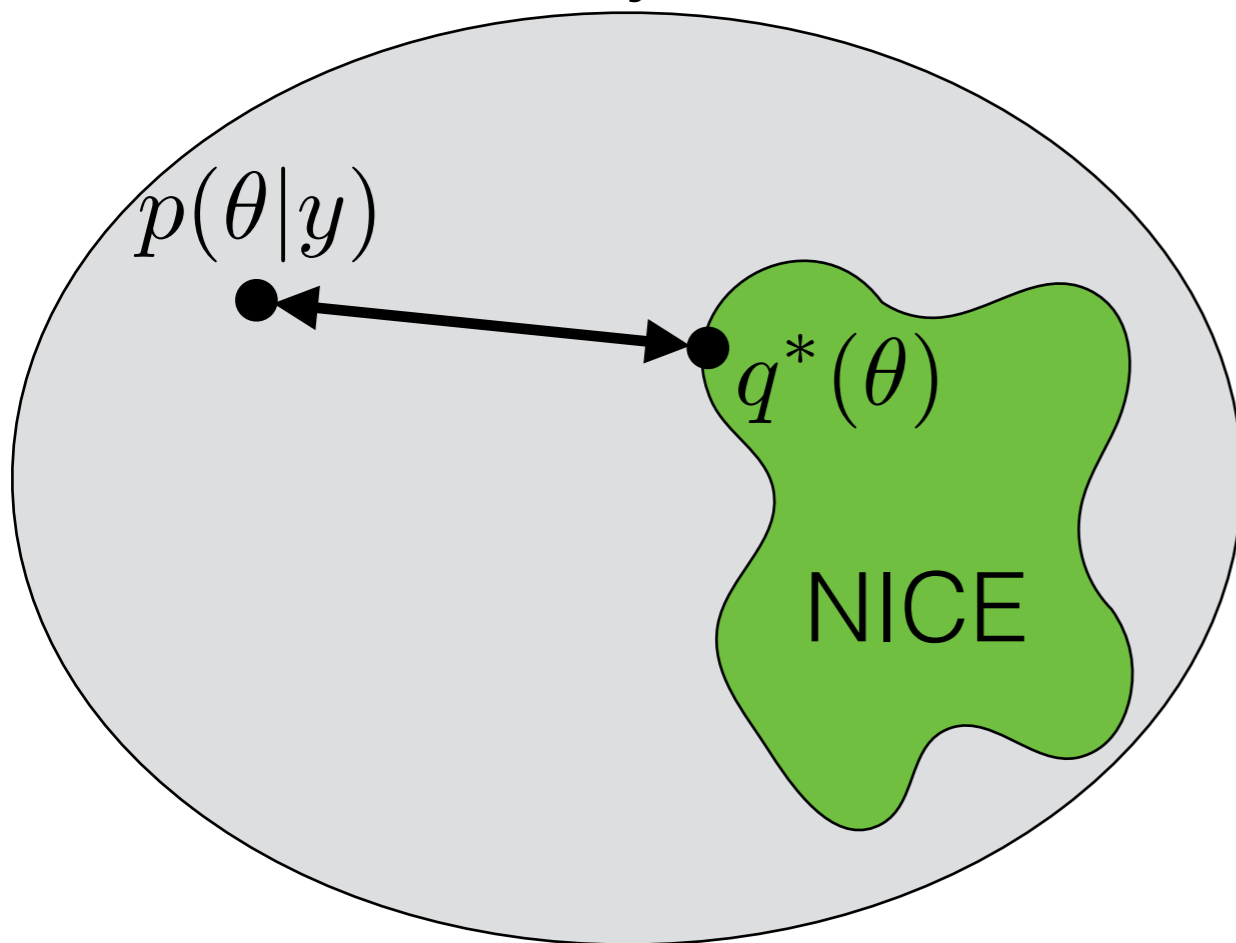
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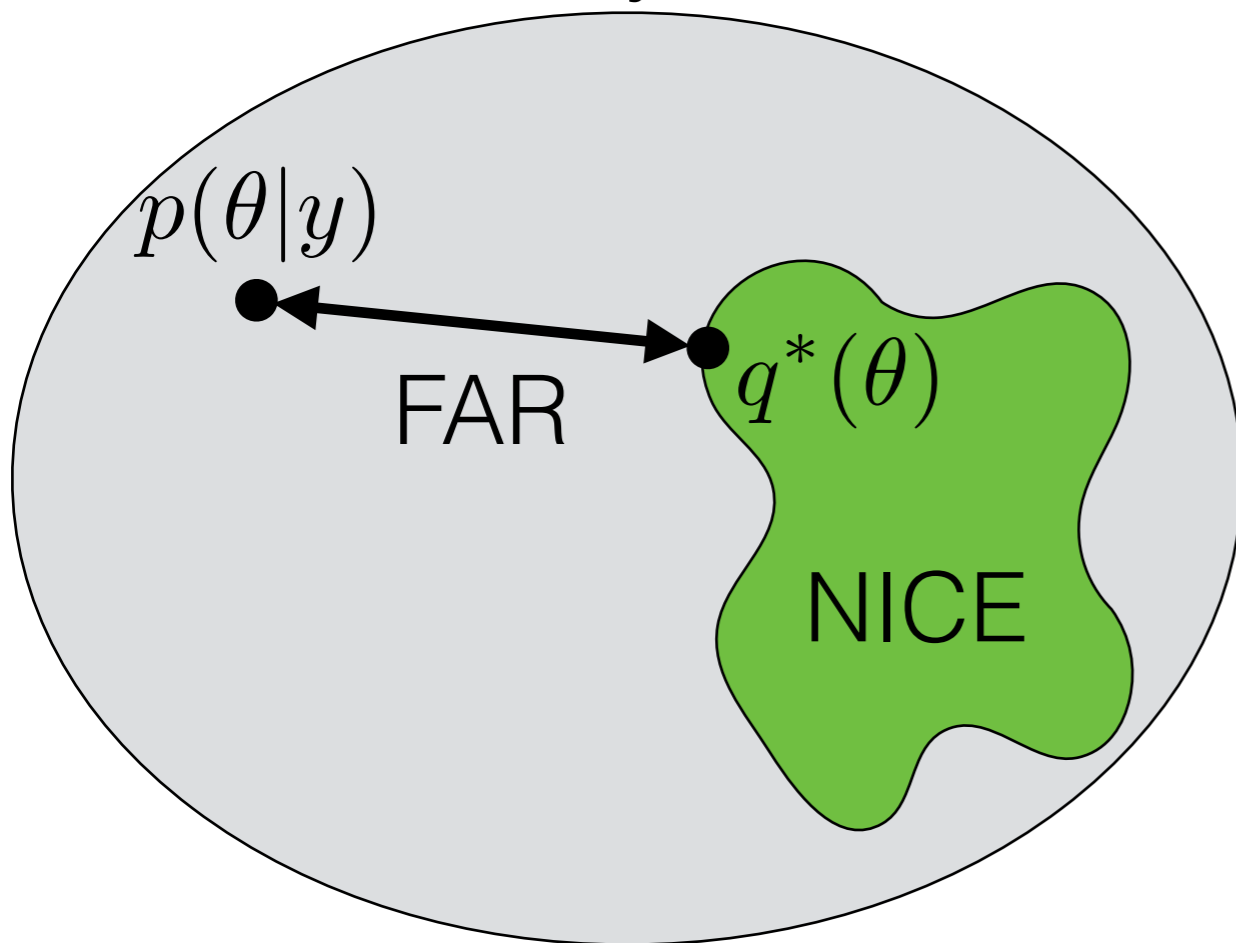
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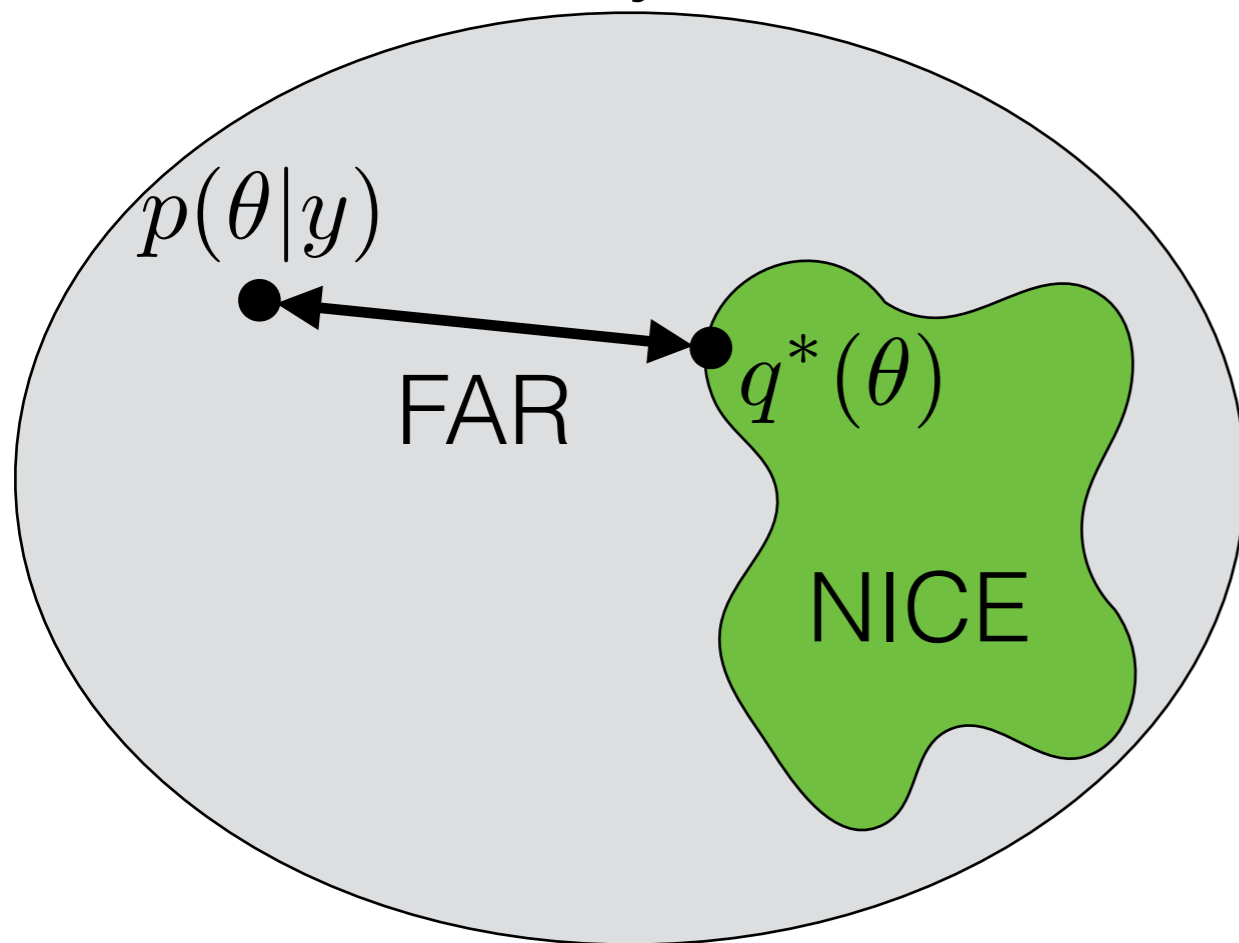
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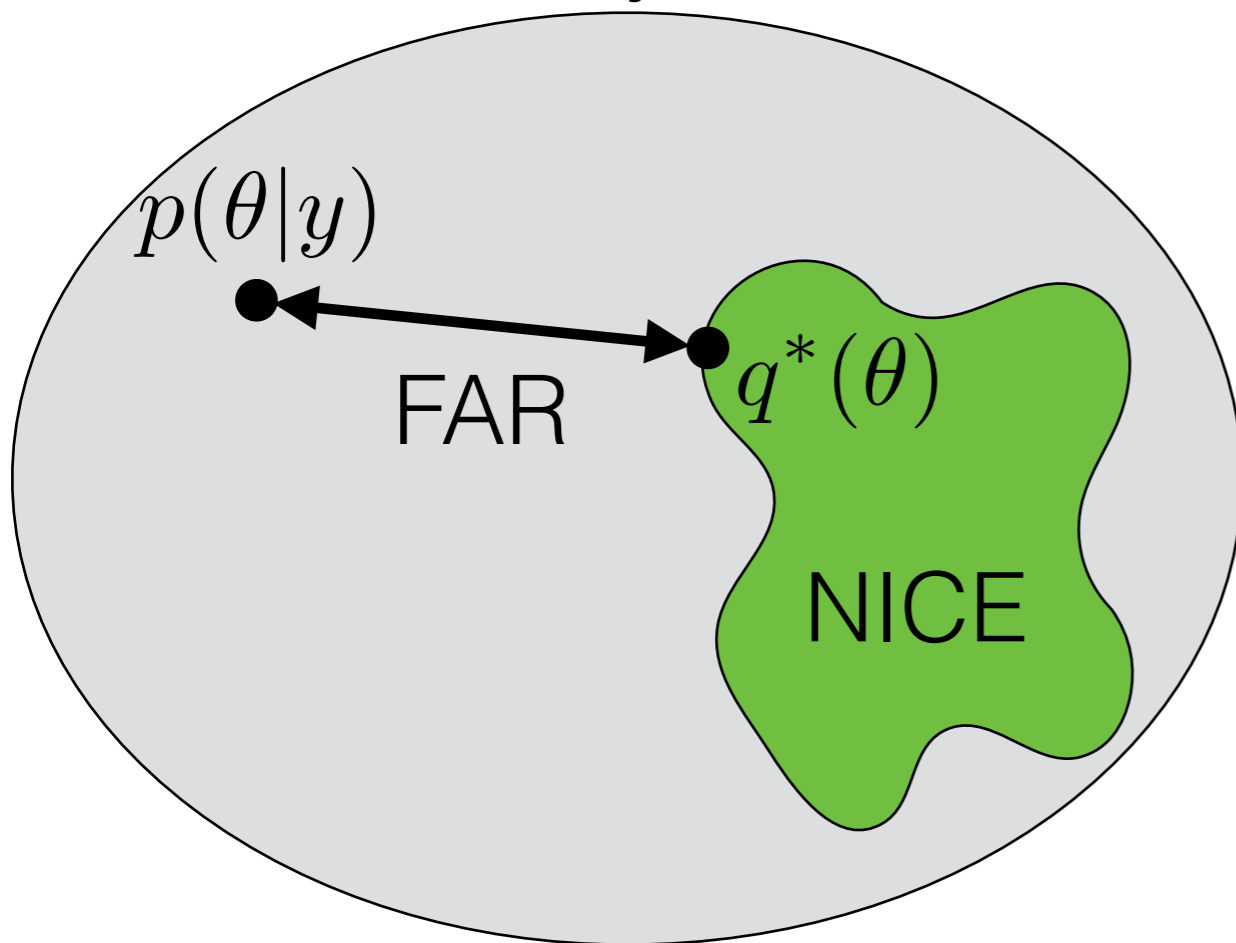
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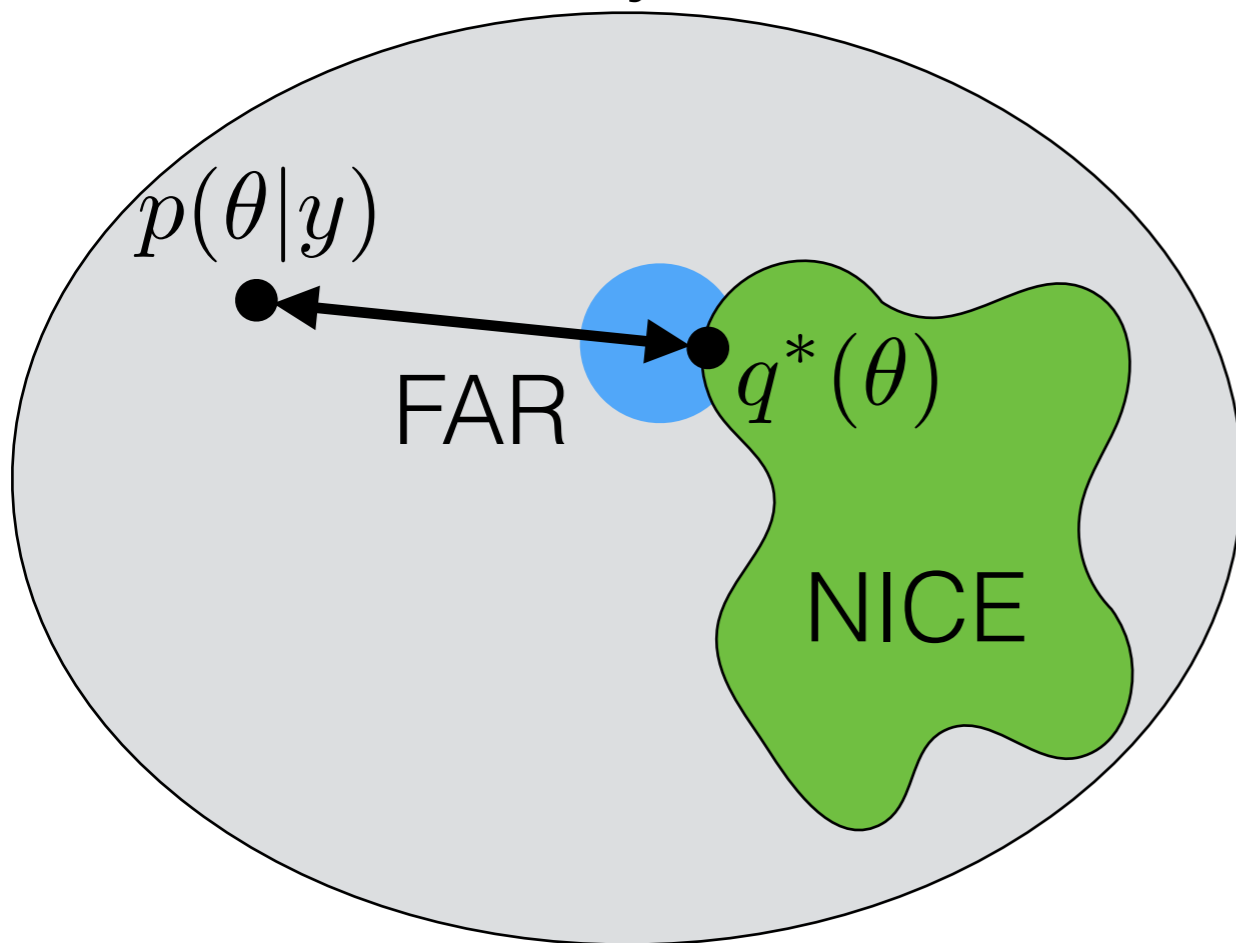
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$$KL(q(\cdot) || p(\cdot|y))$$

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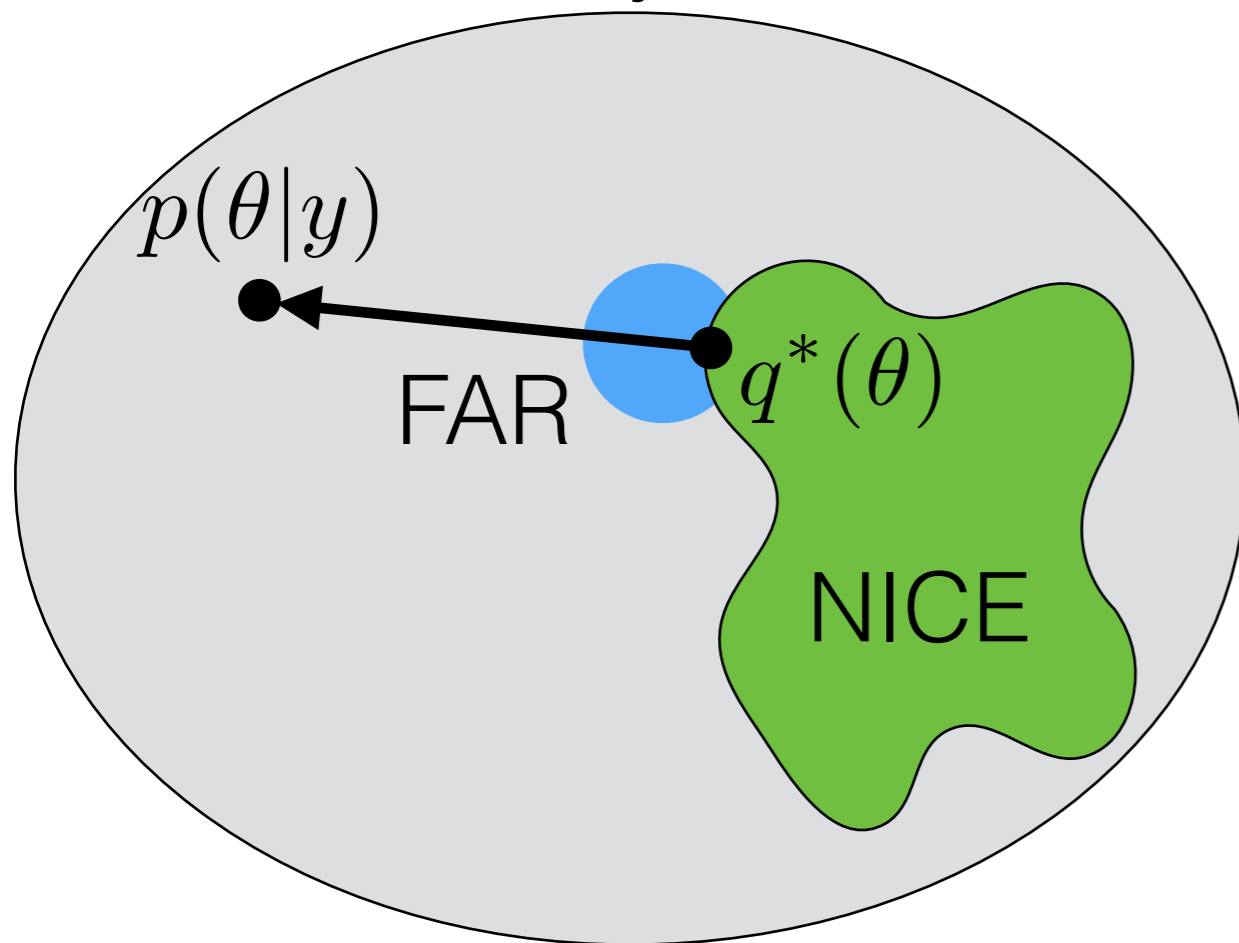
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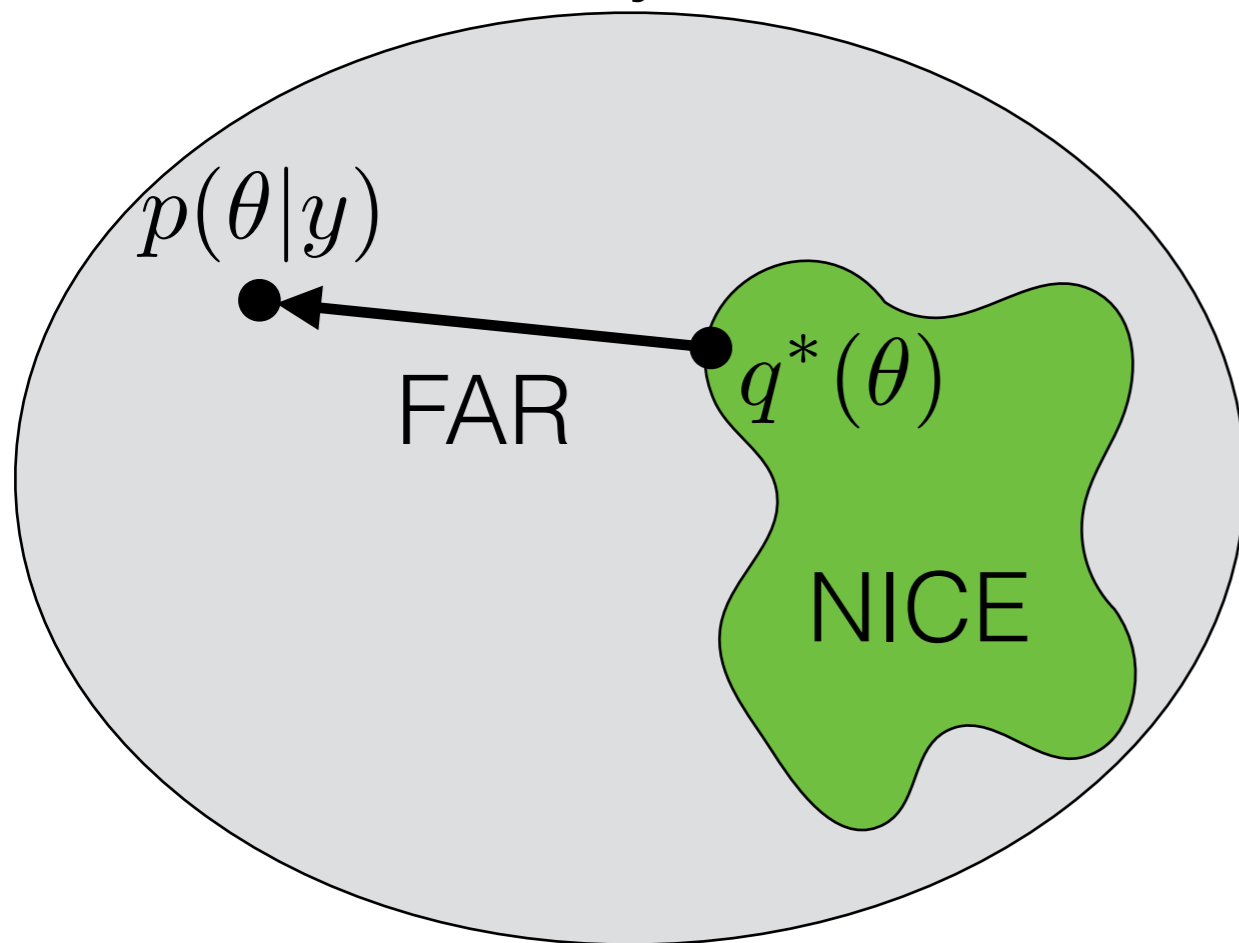
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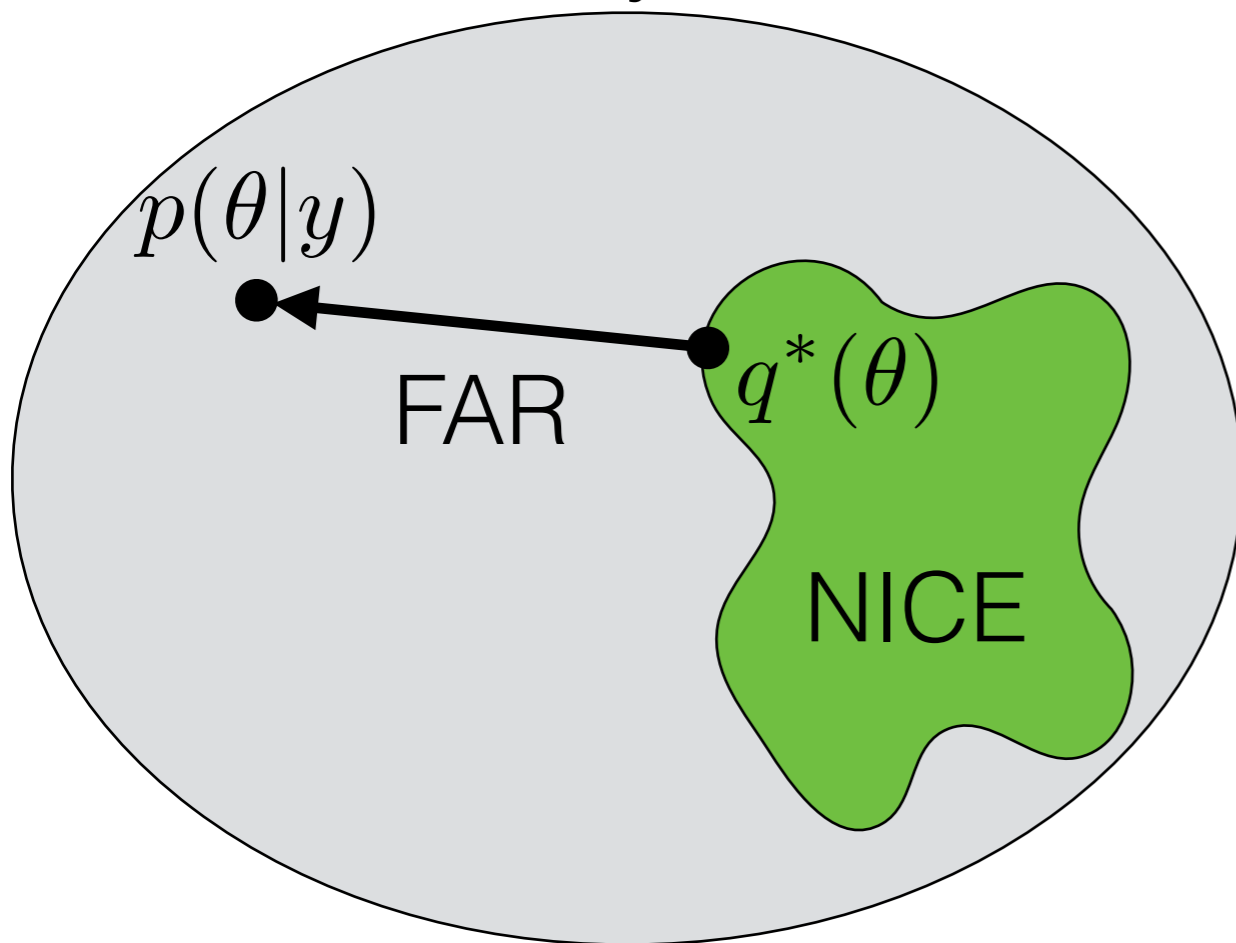
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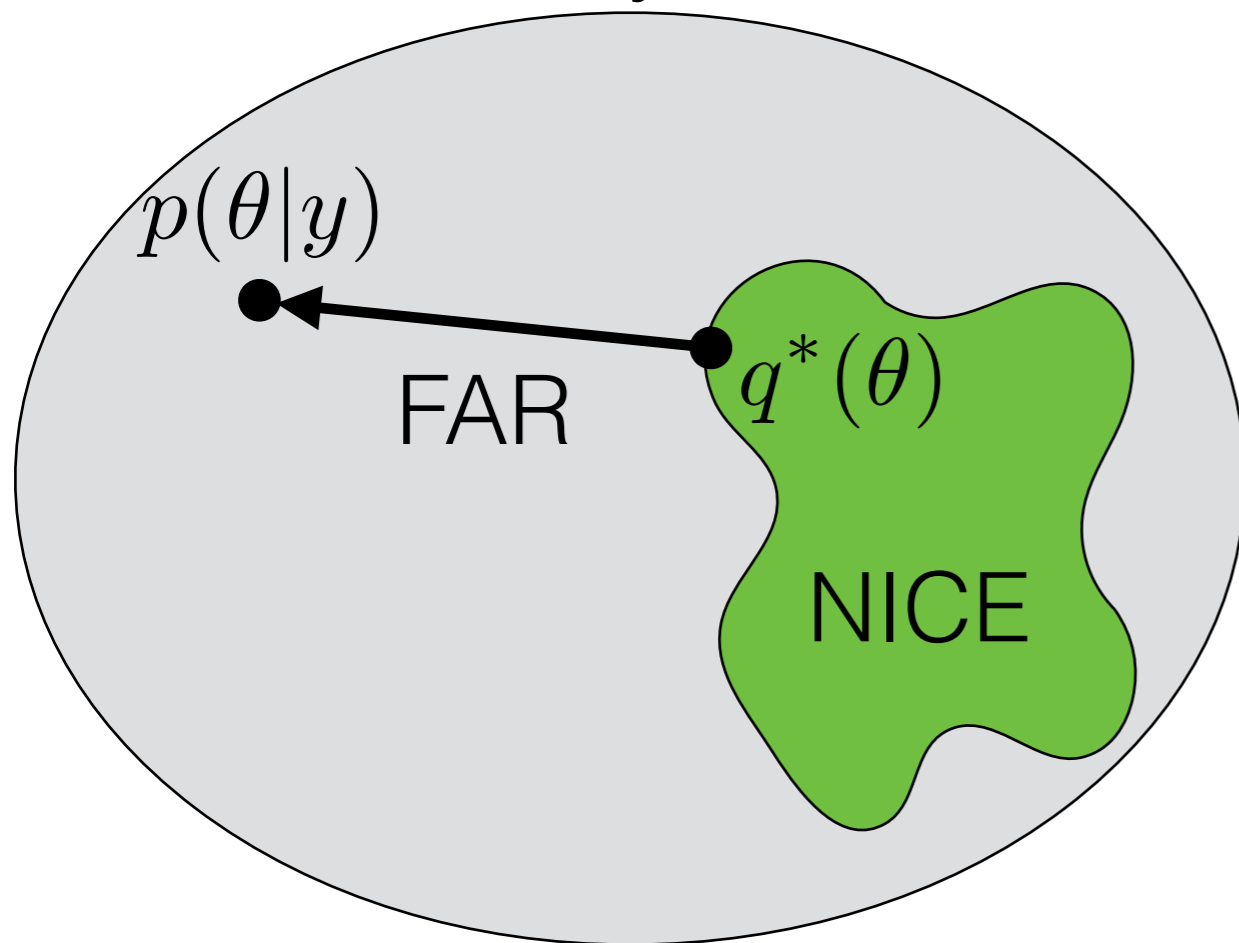
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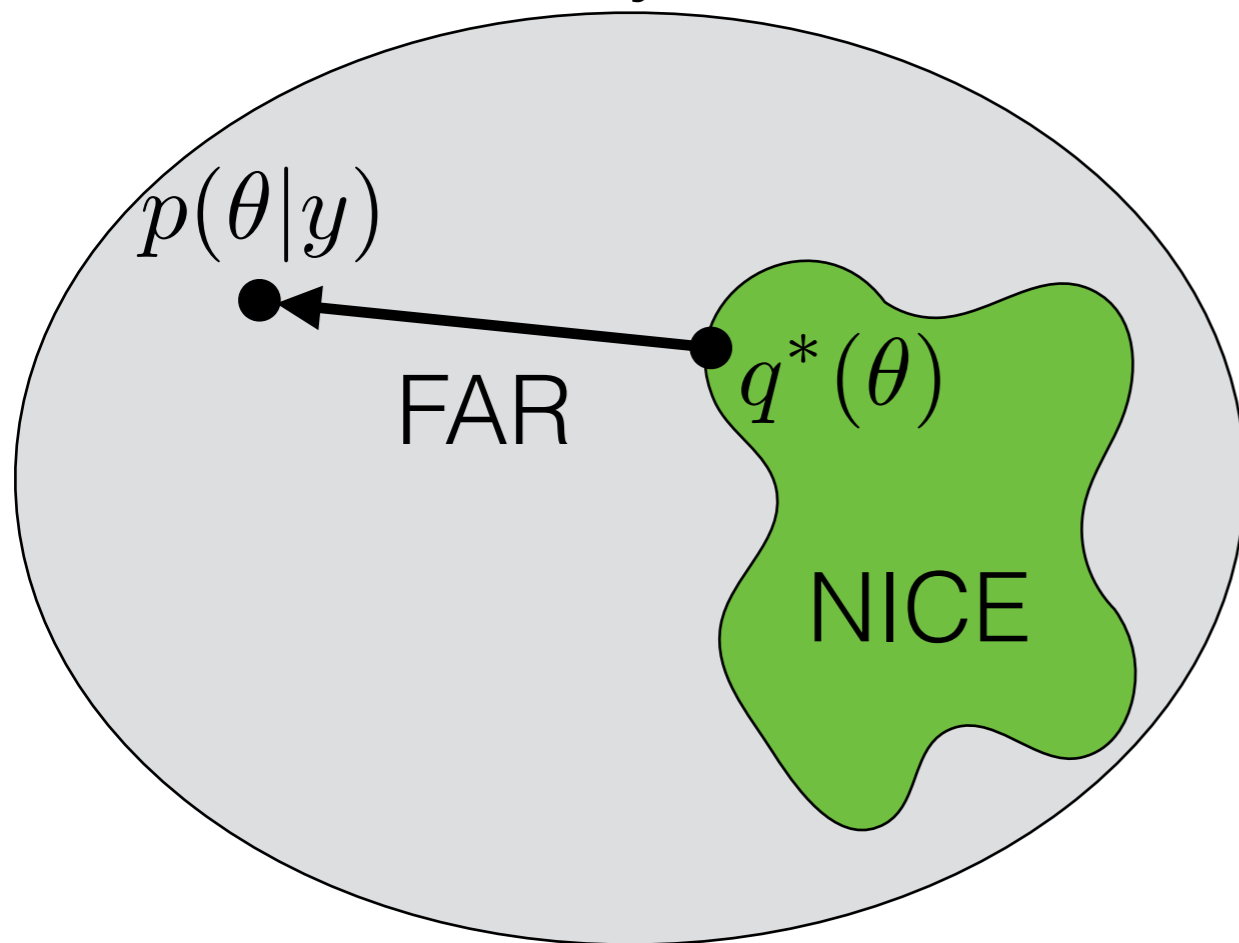
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Approximate Bayesian Inference

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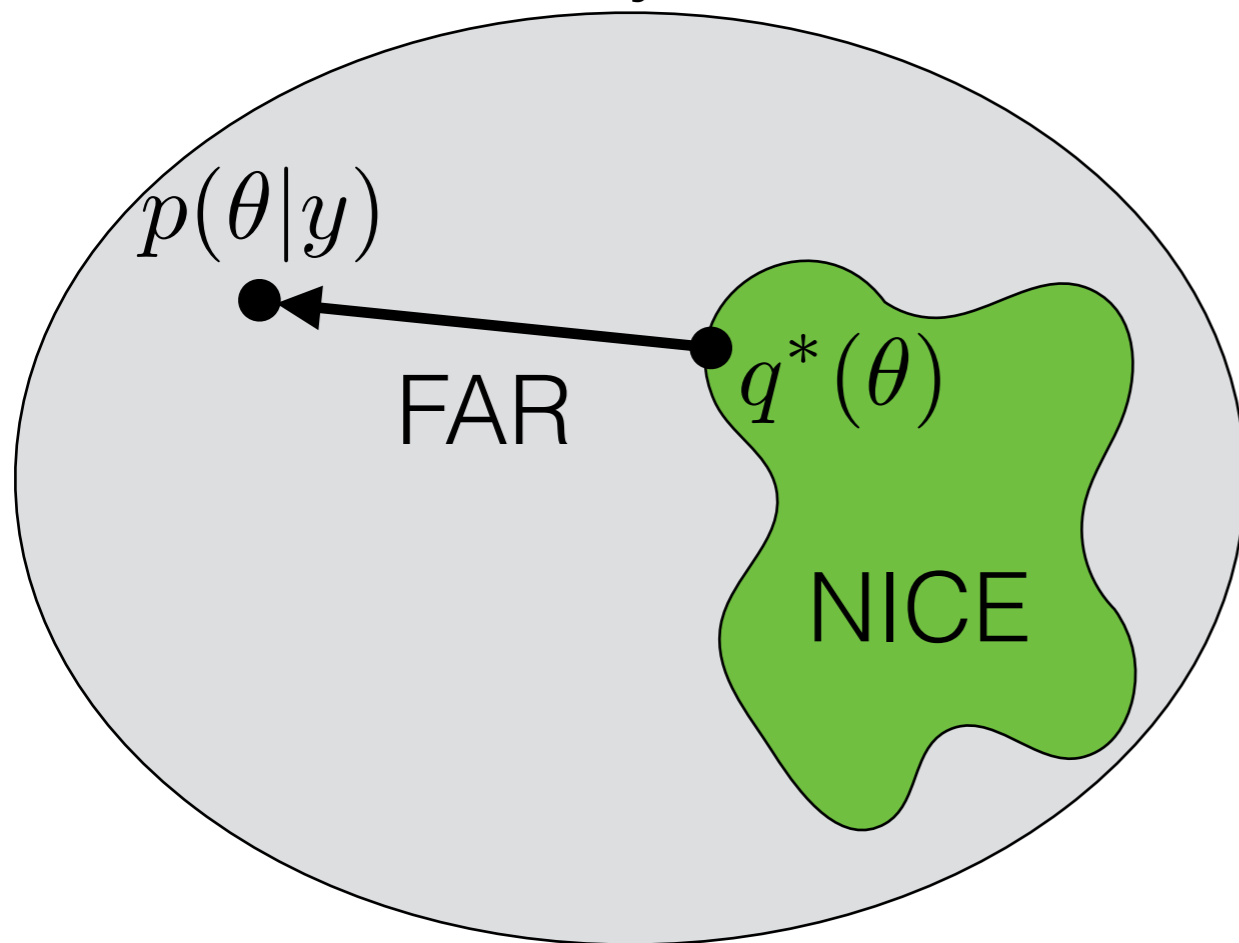
$$KL(q(\cdot) || p(\cdot|y))$$

- VB practical success: point estimates and prediction, fast

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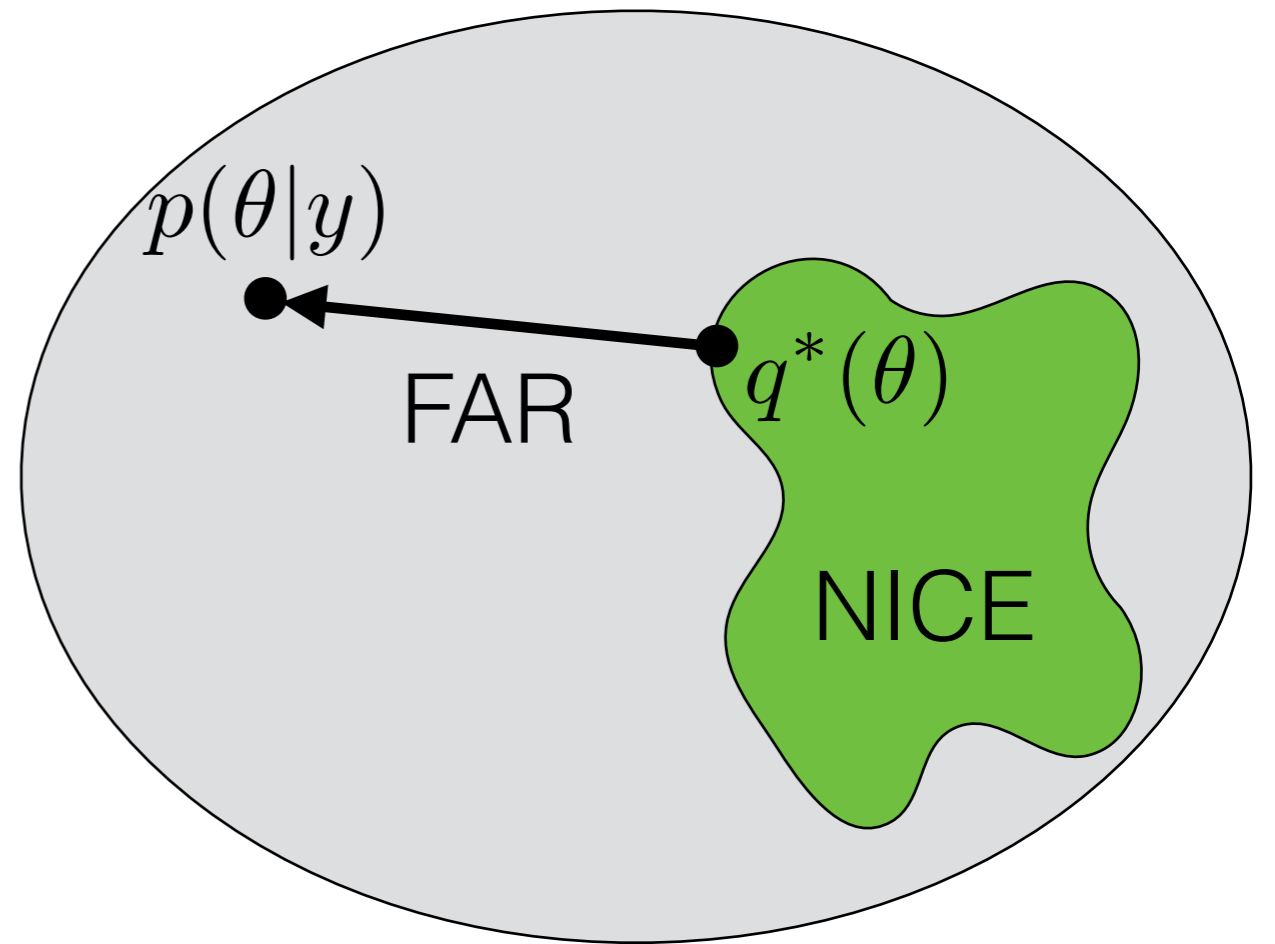
$$KL(q(\cdot) || p(\cdot|y))$$

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

Why KL?

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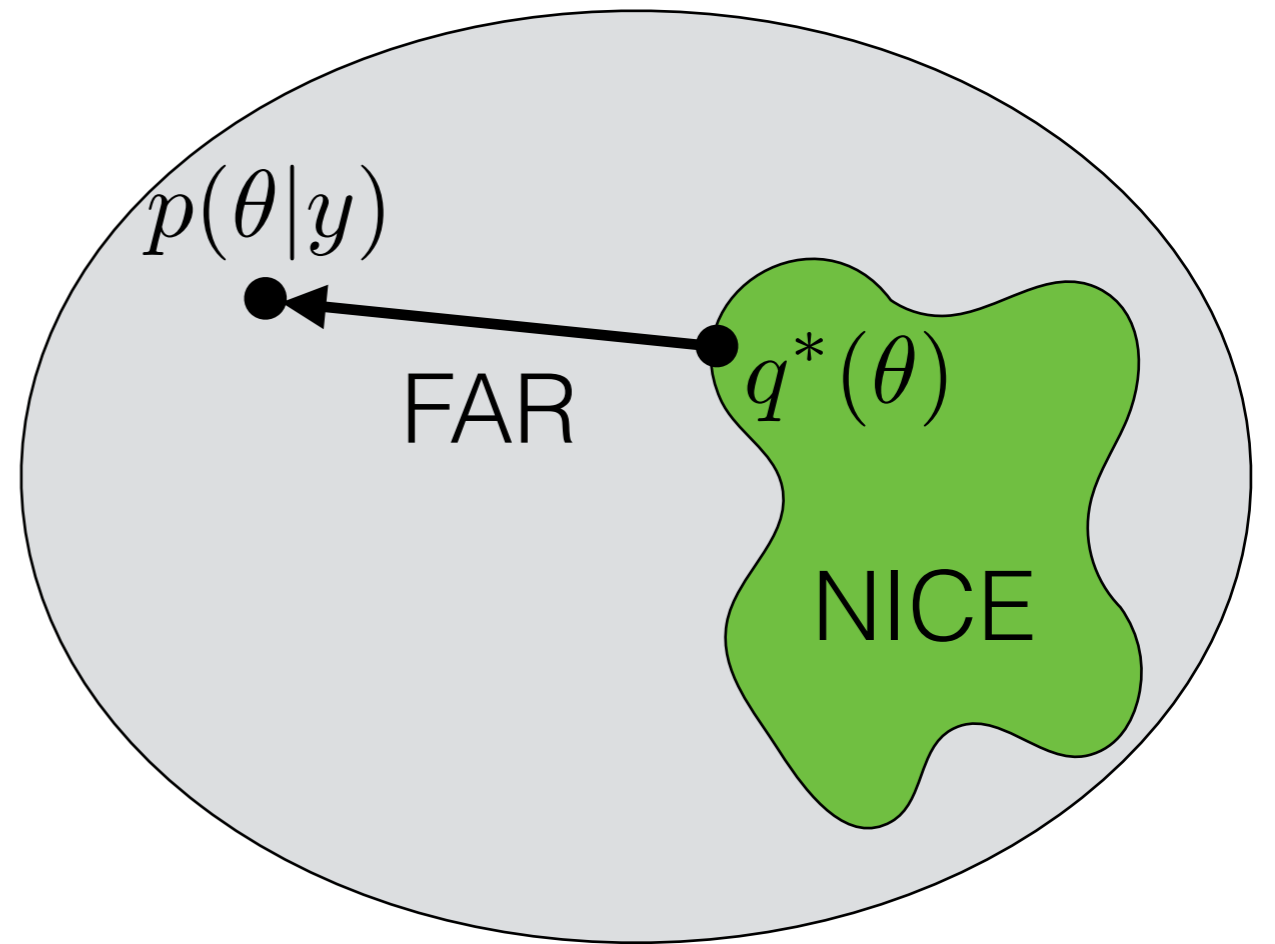
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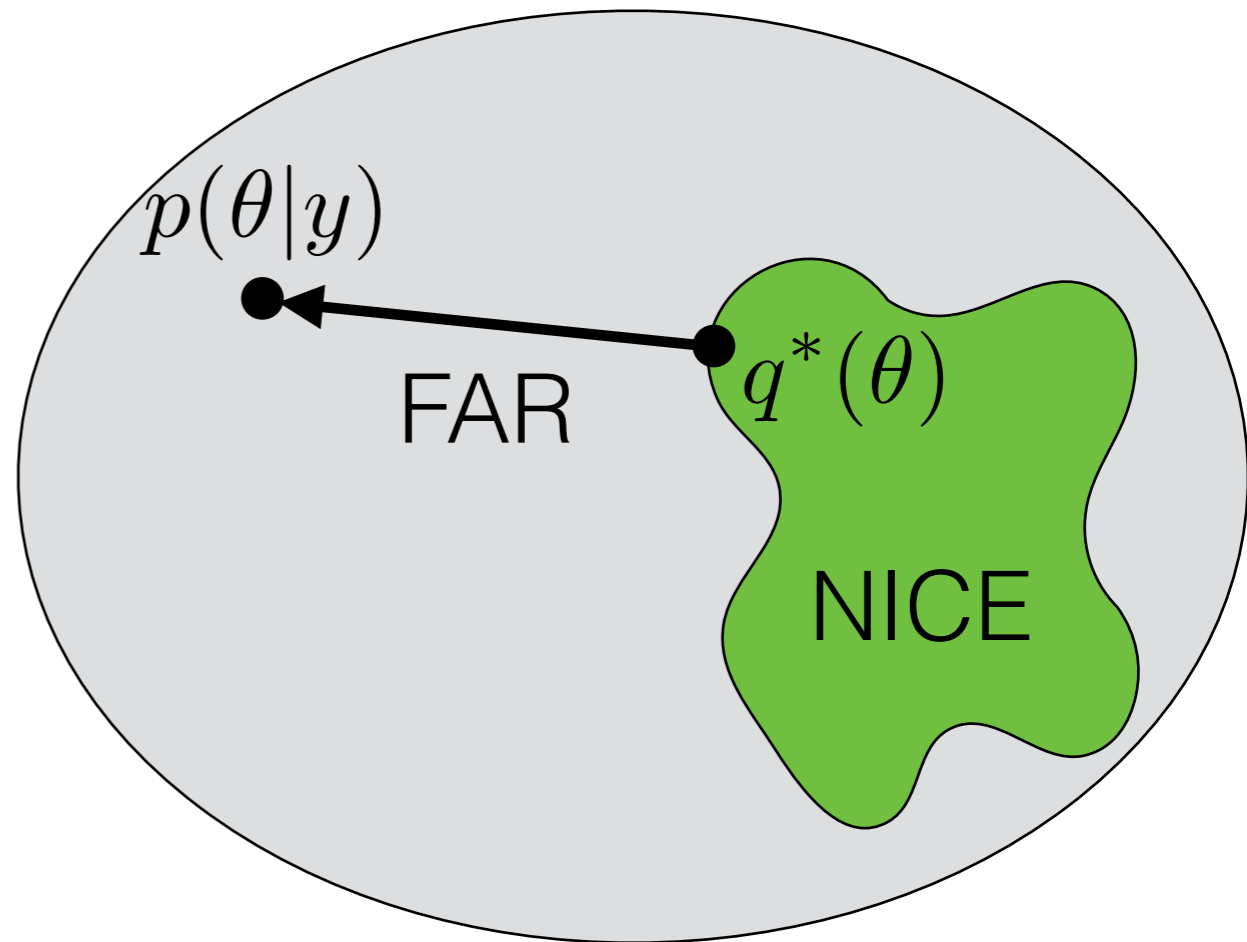
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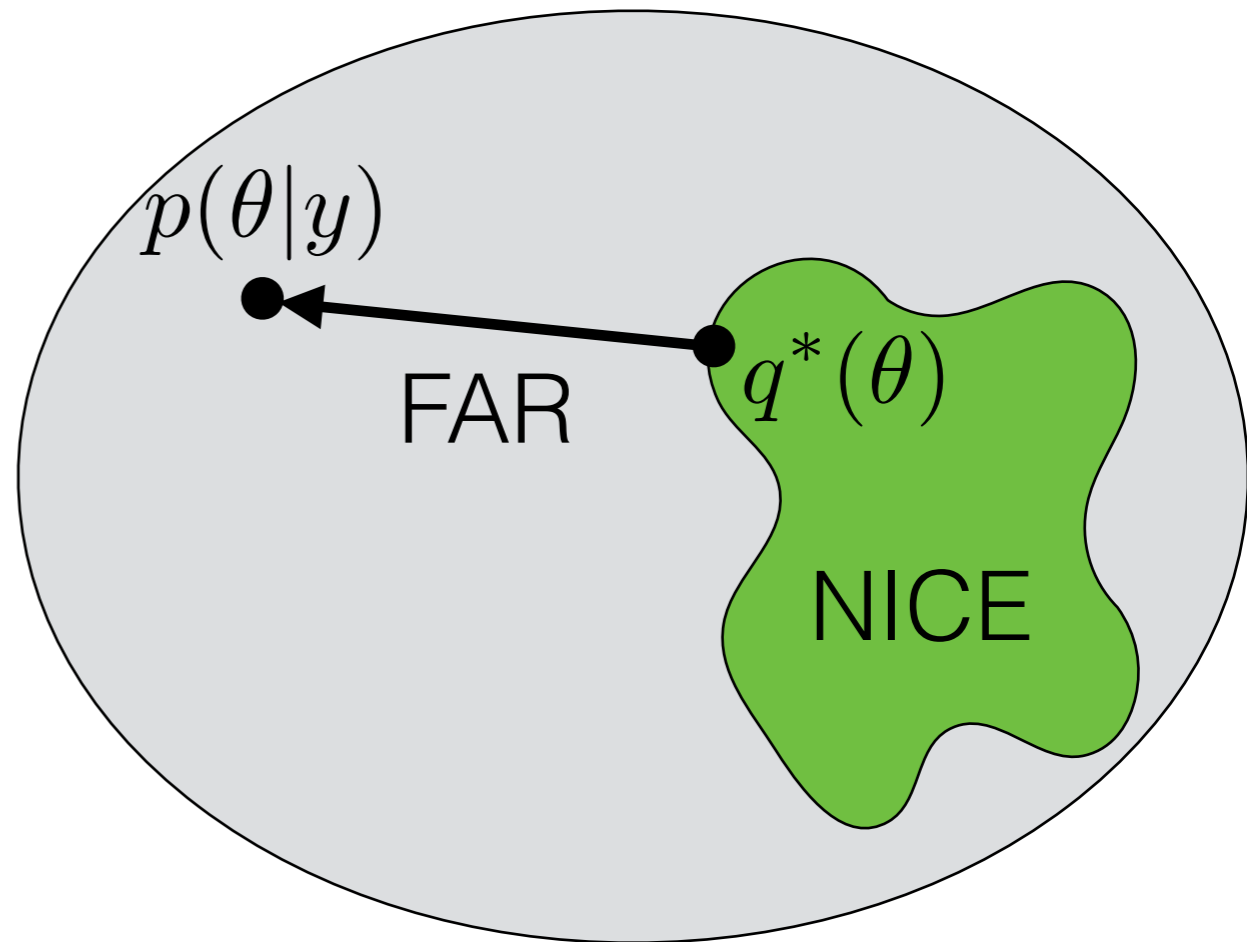
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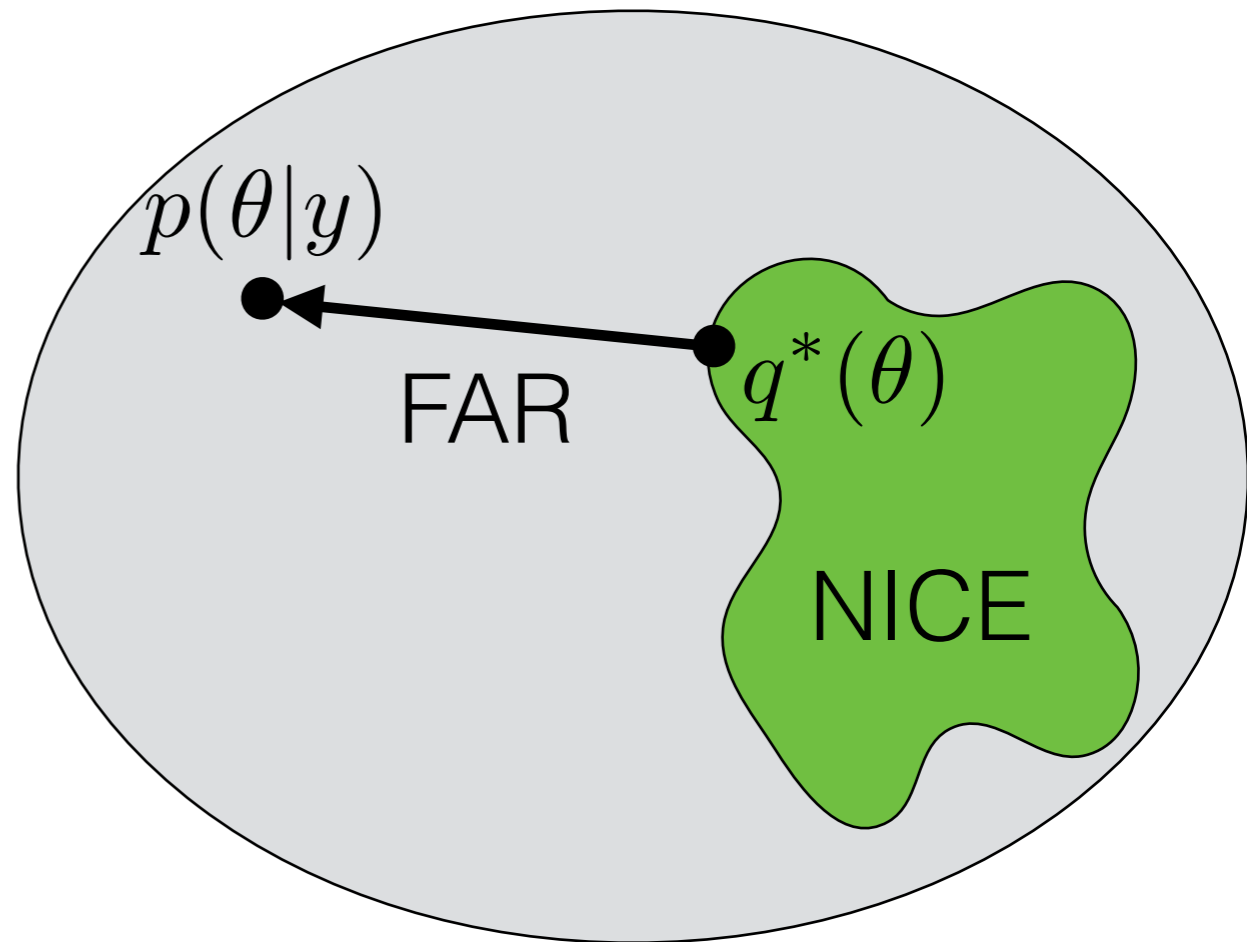
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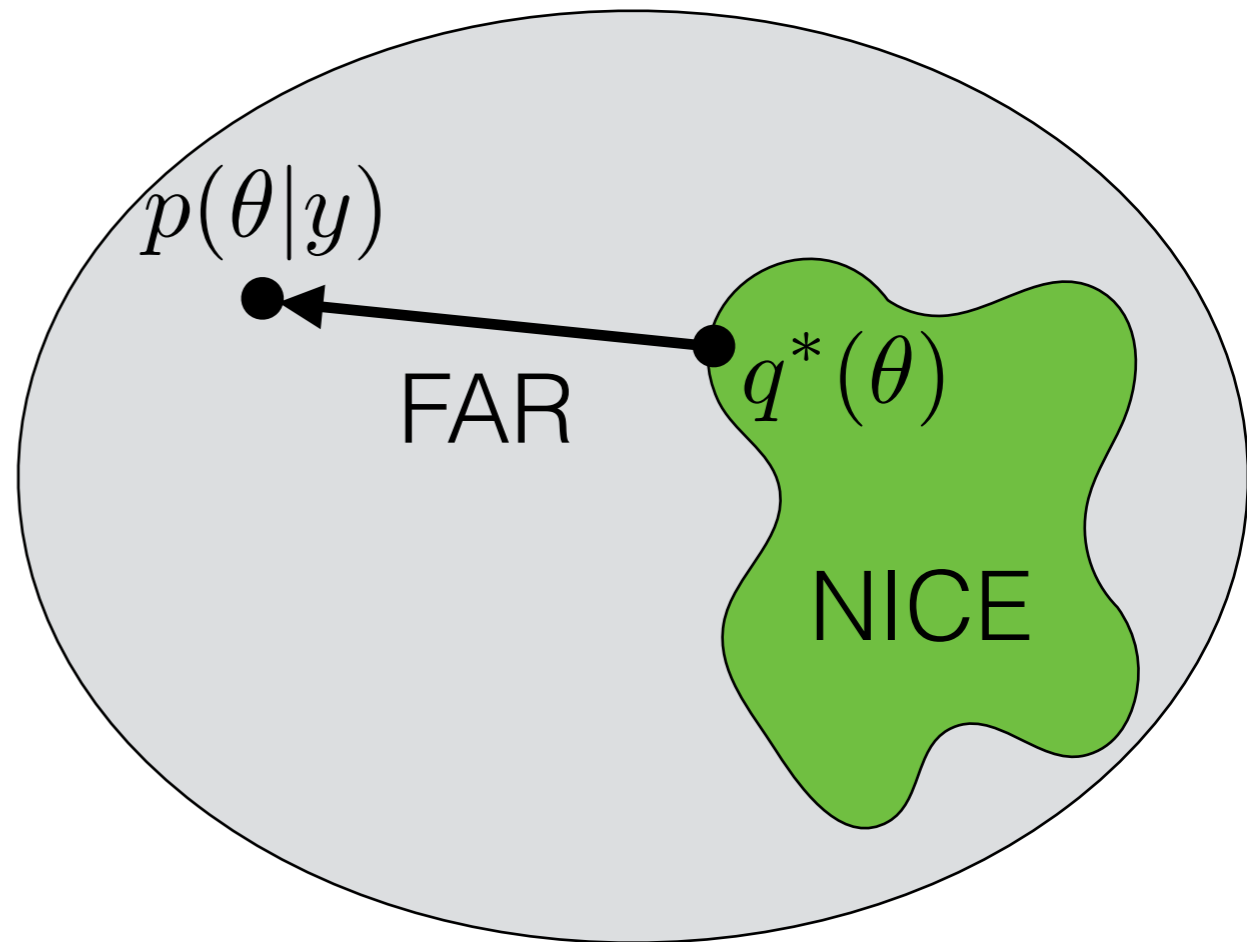
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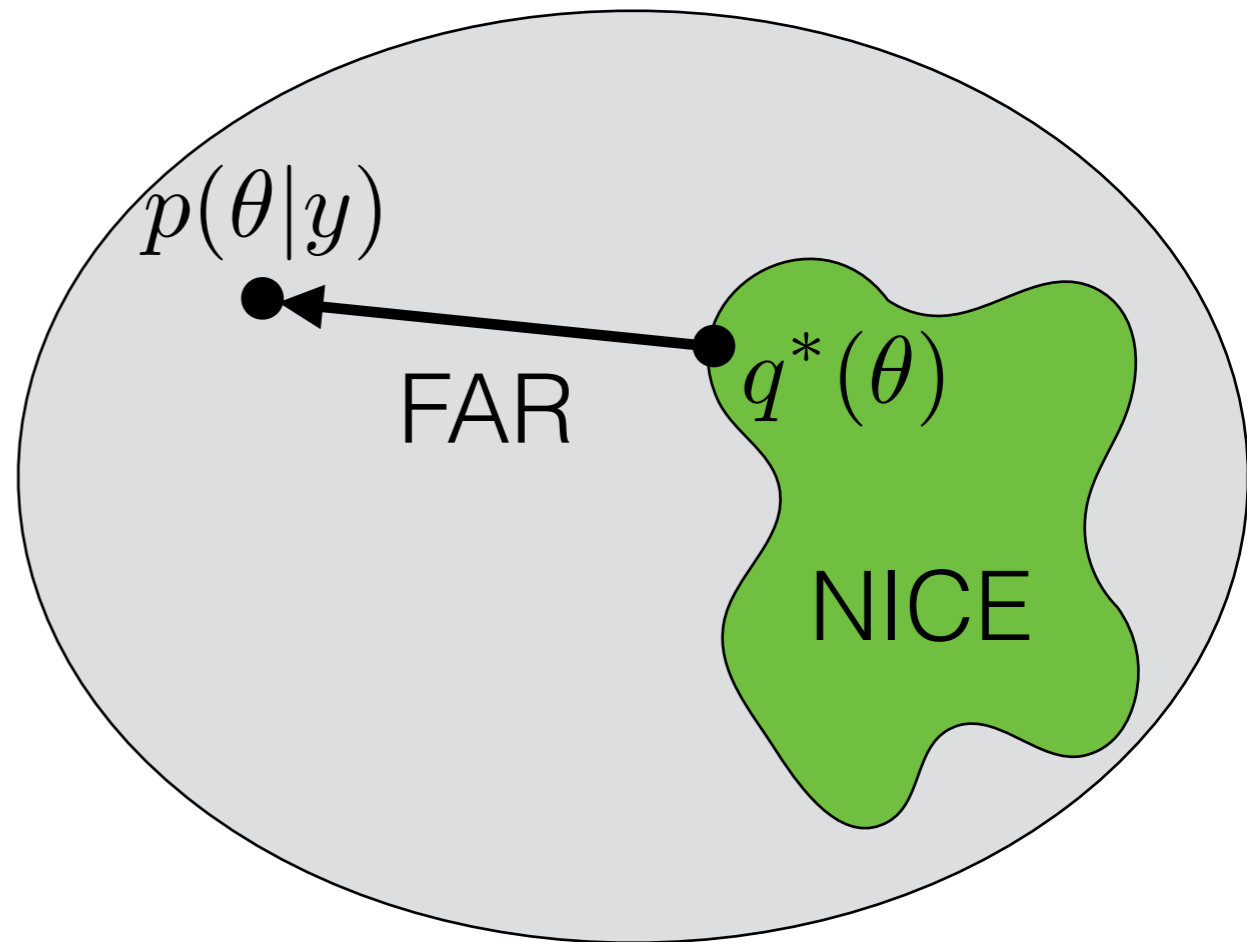
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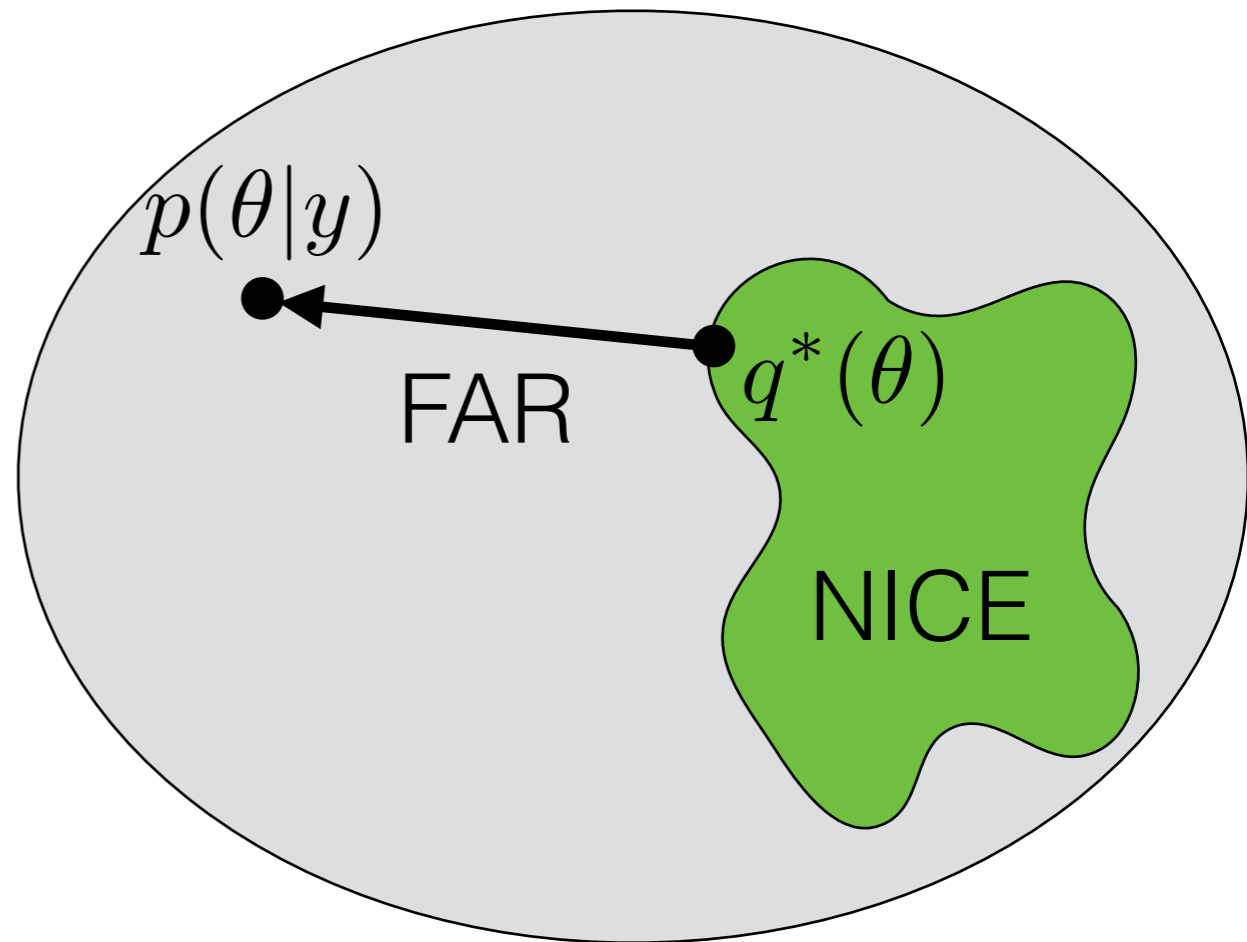
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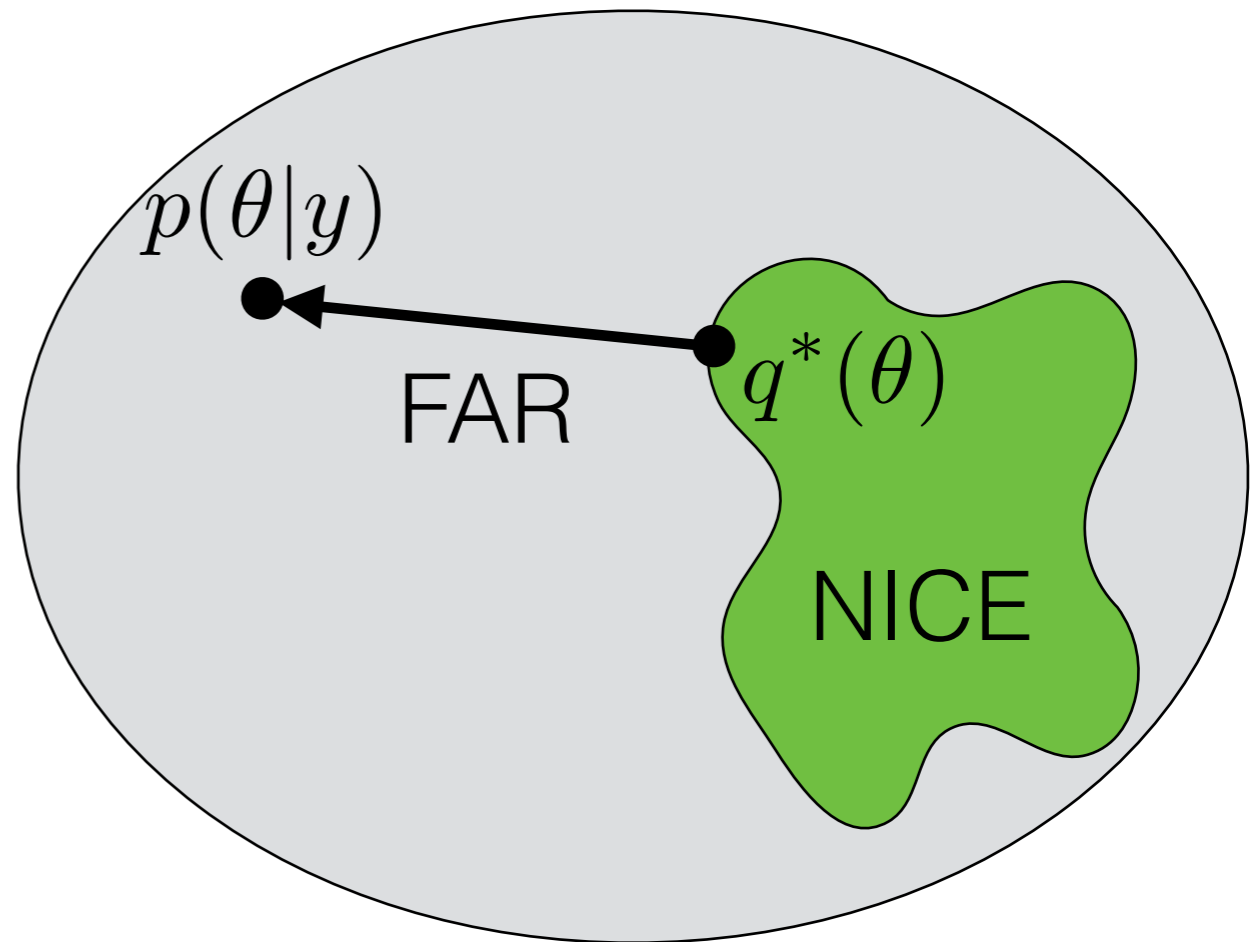
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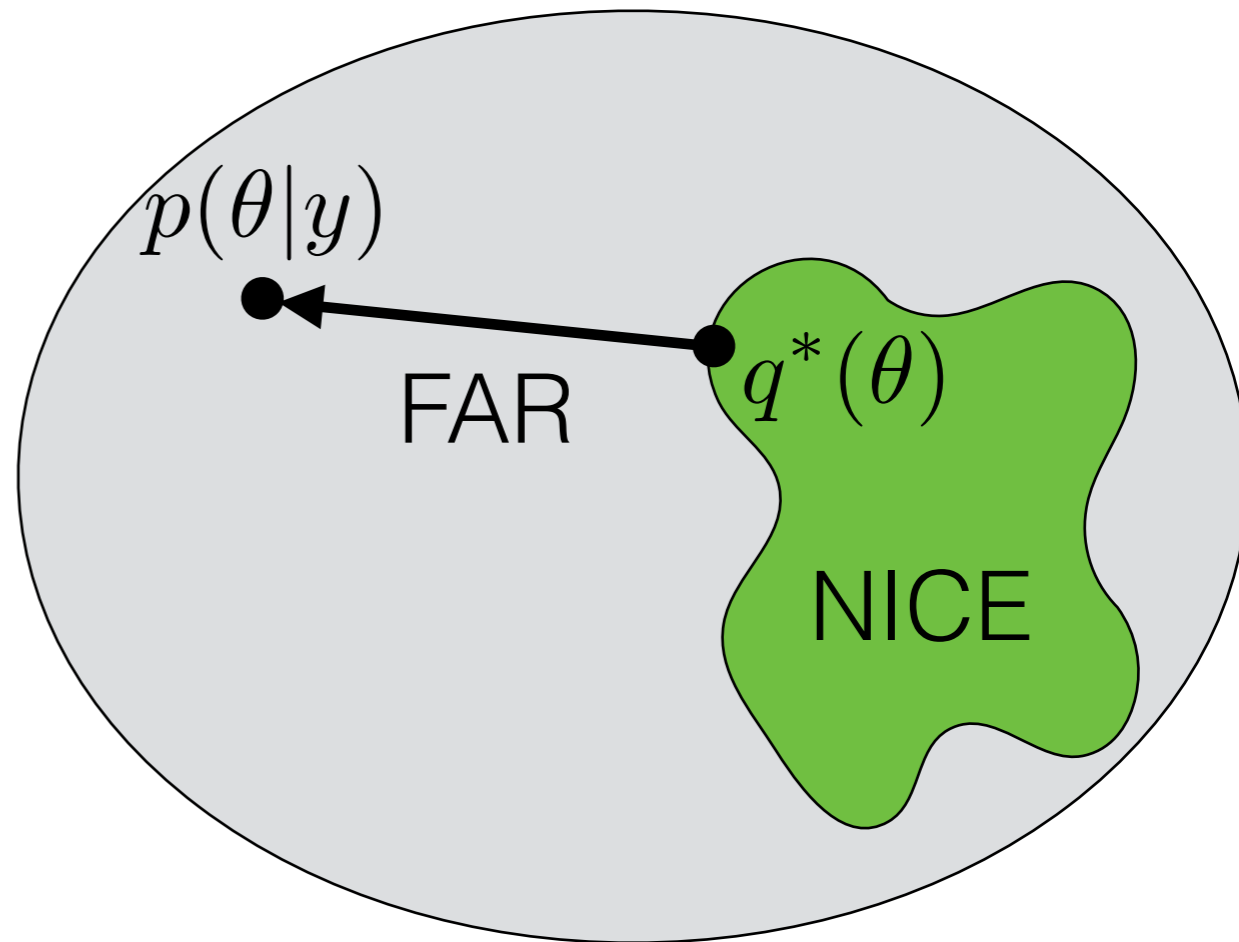
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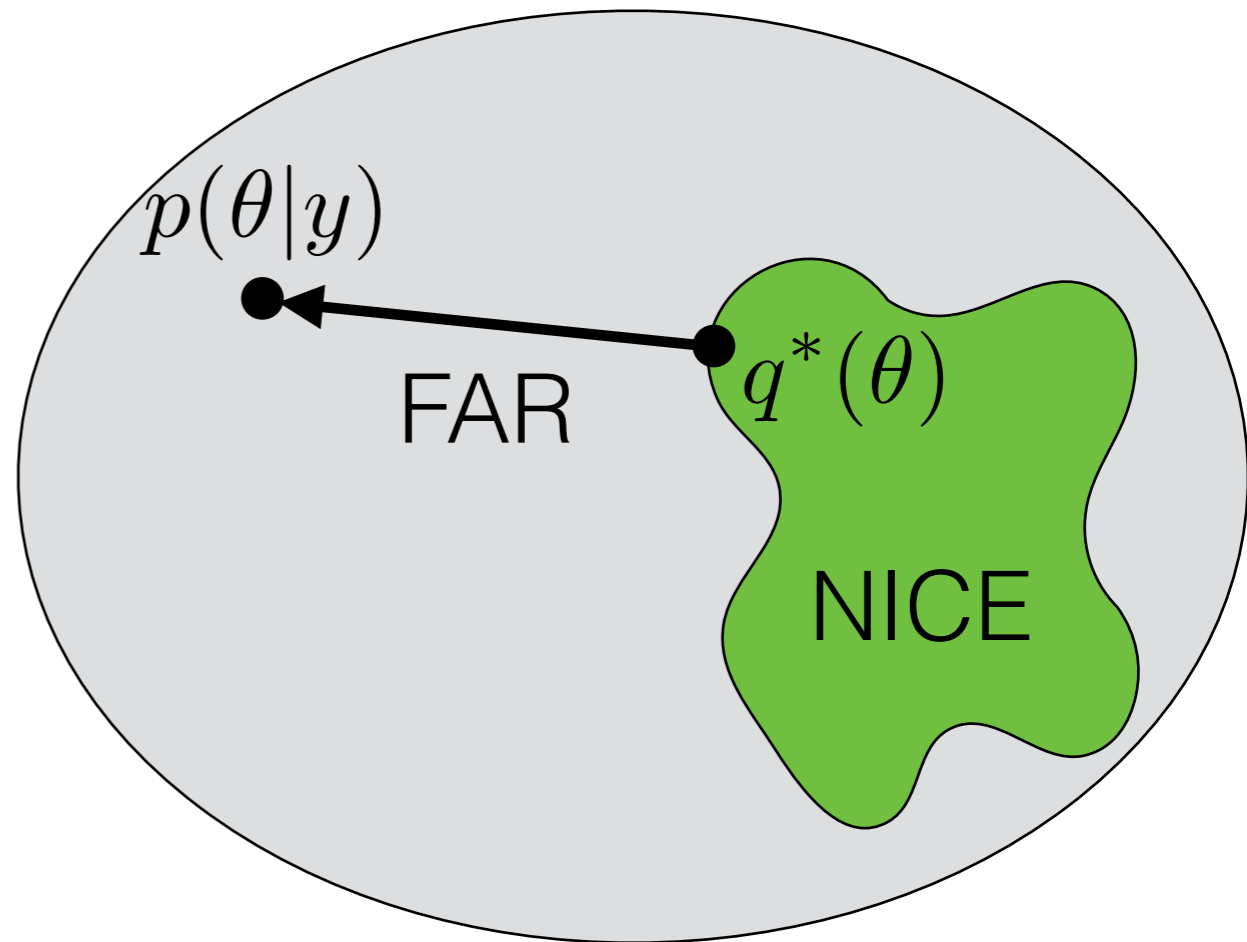
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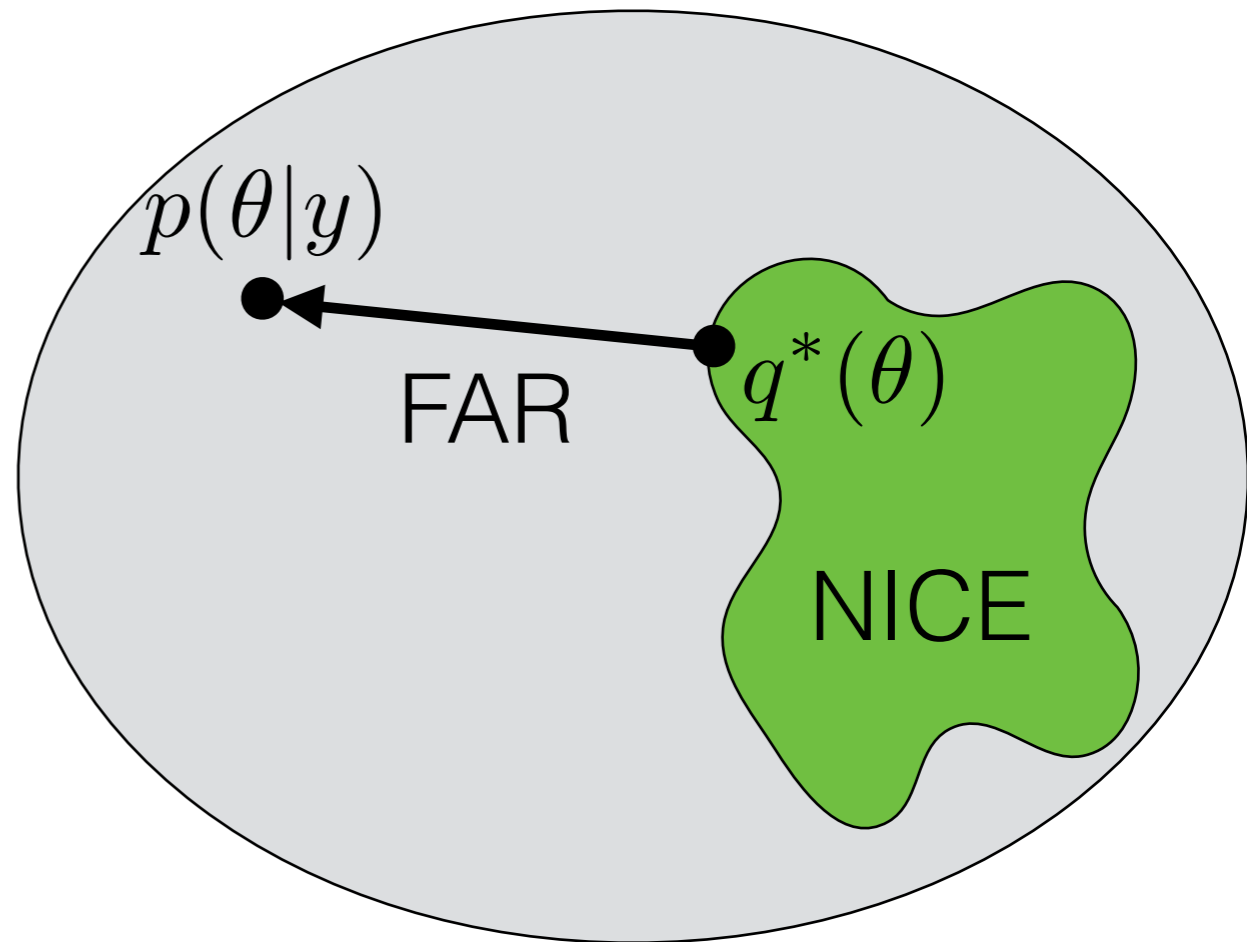
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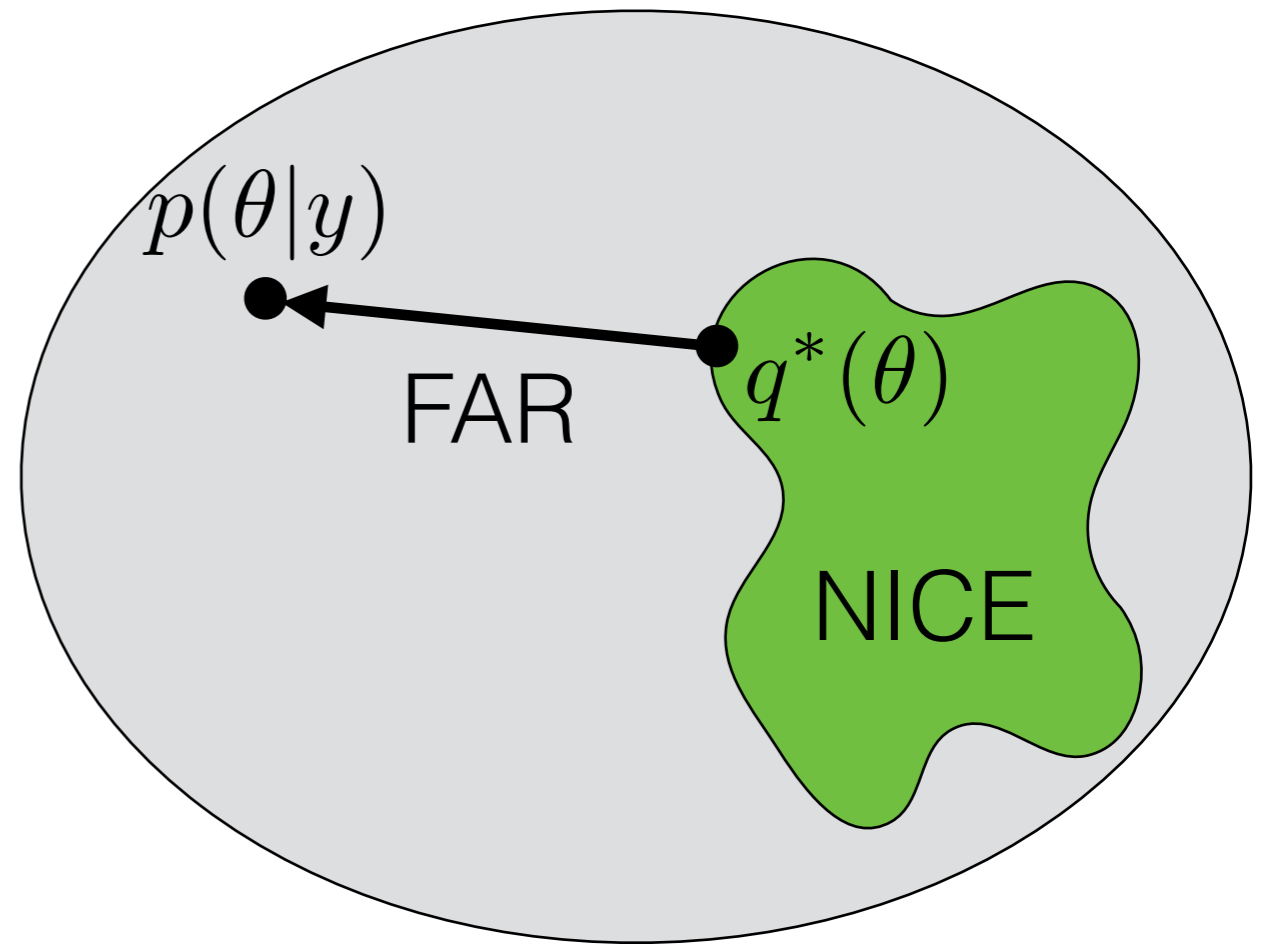
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- Variational Bayes

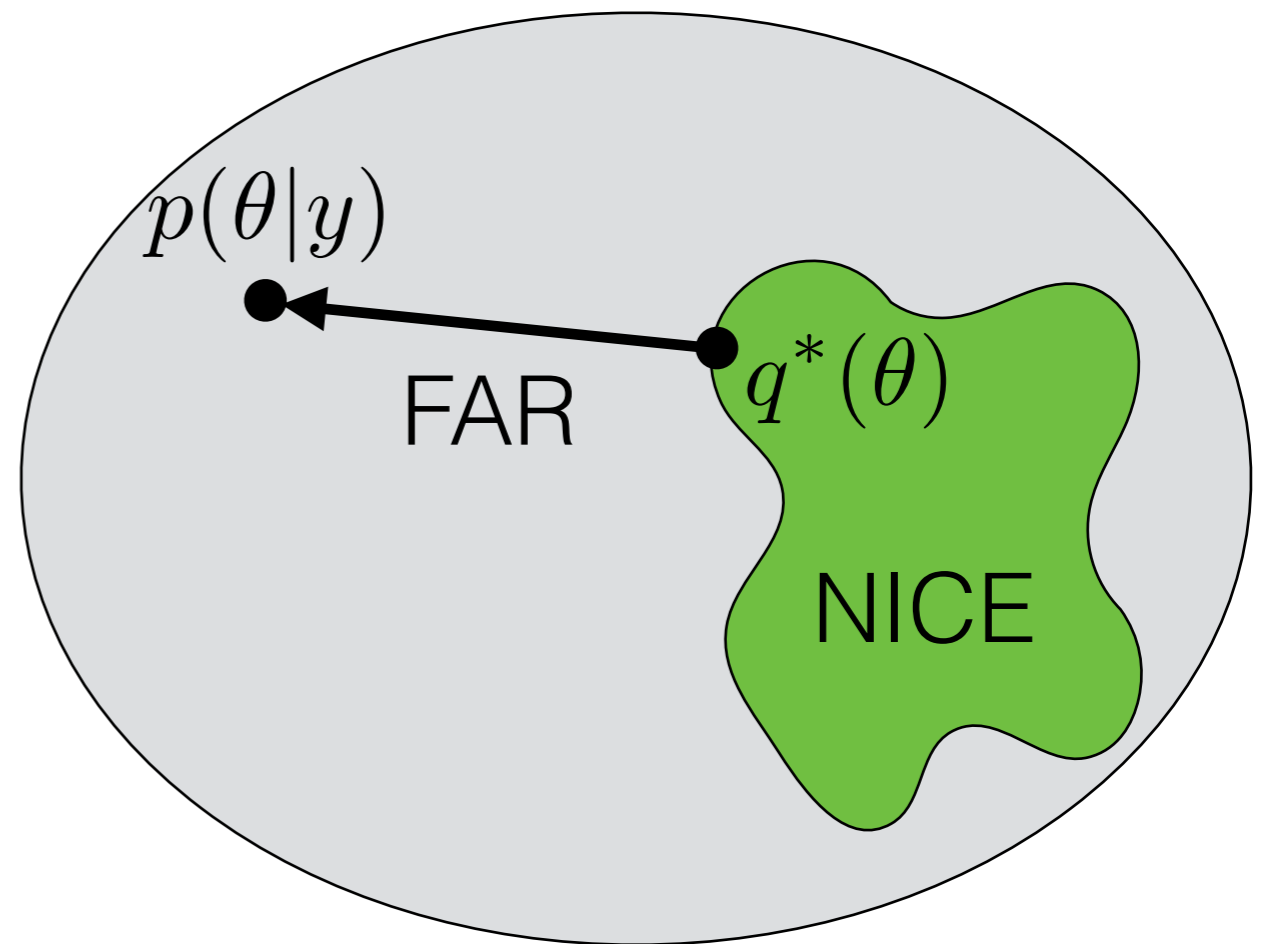
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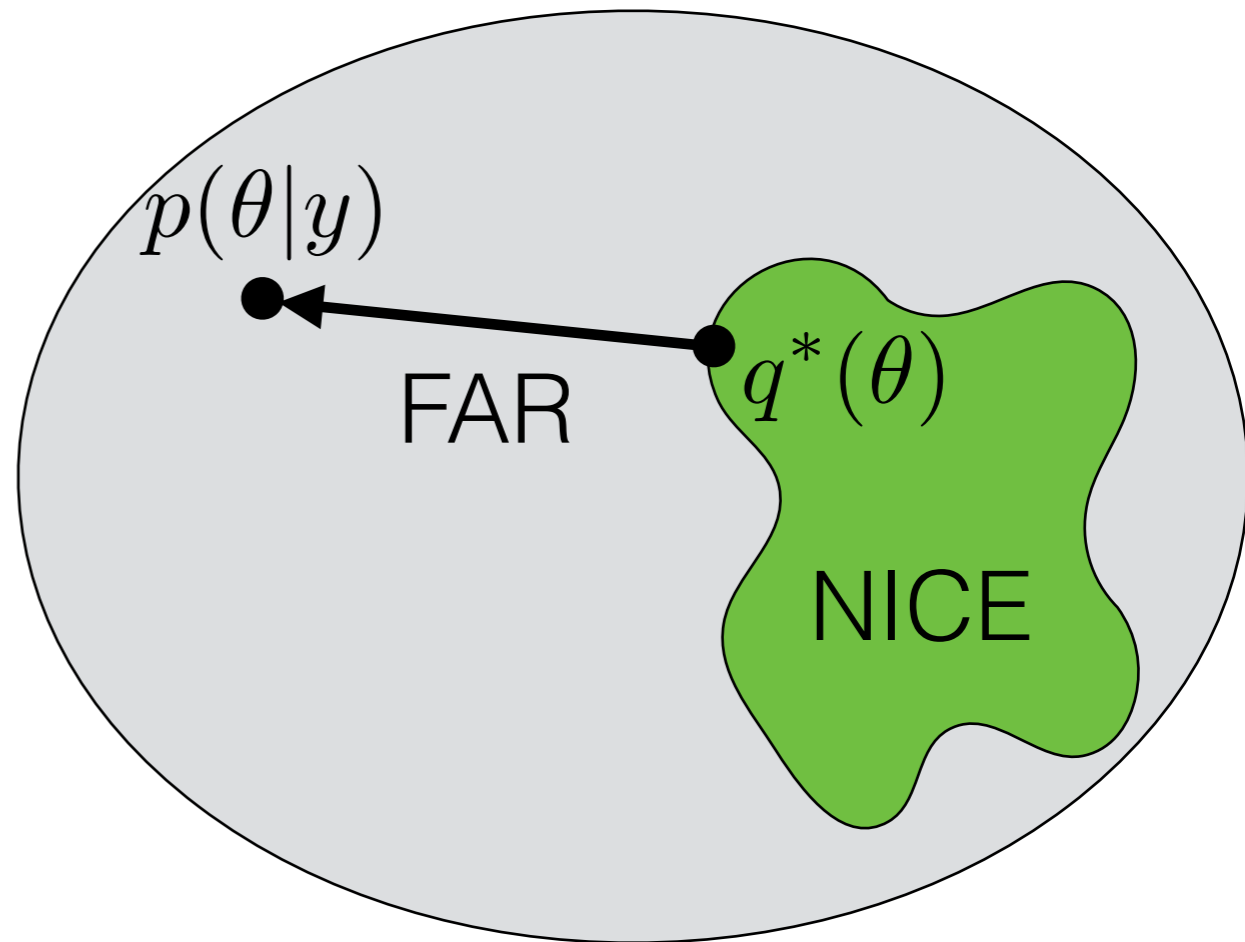
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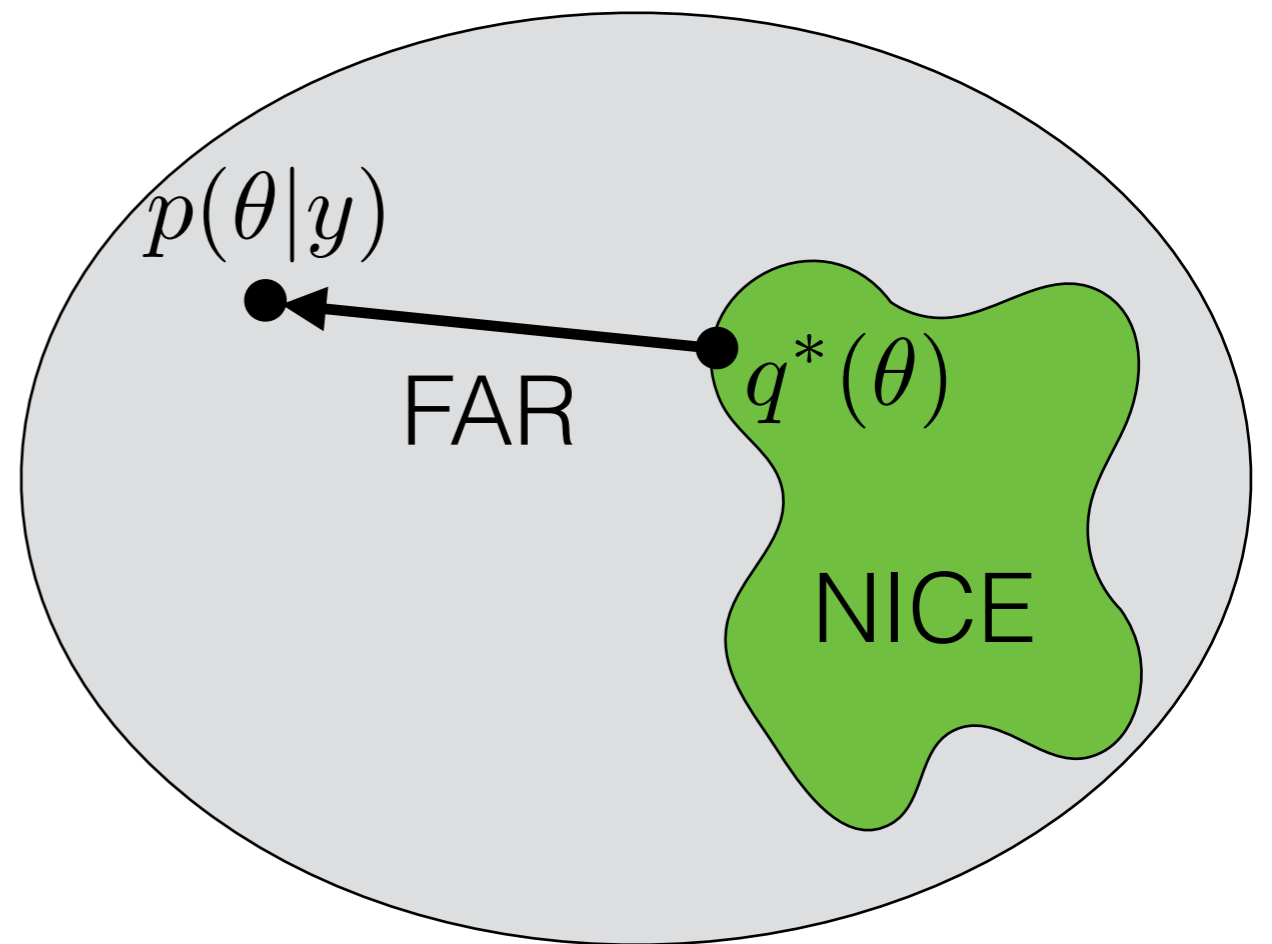
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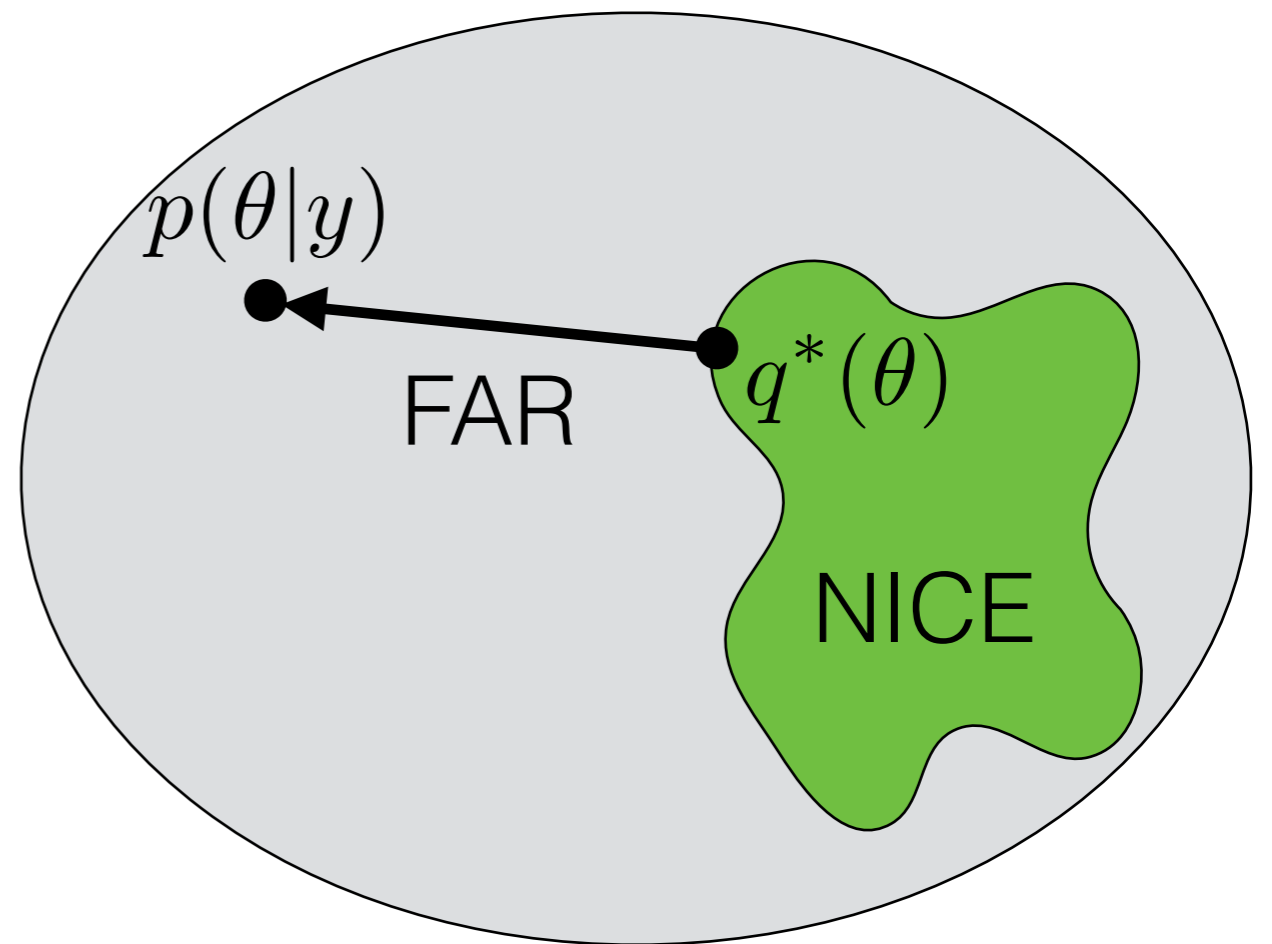
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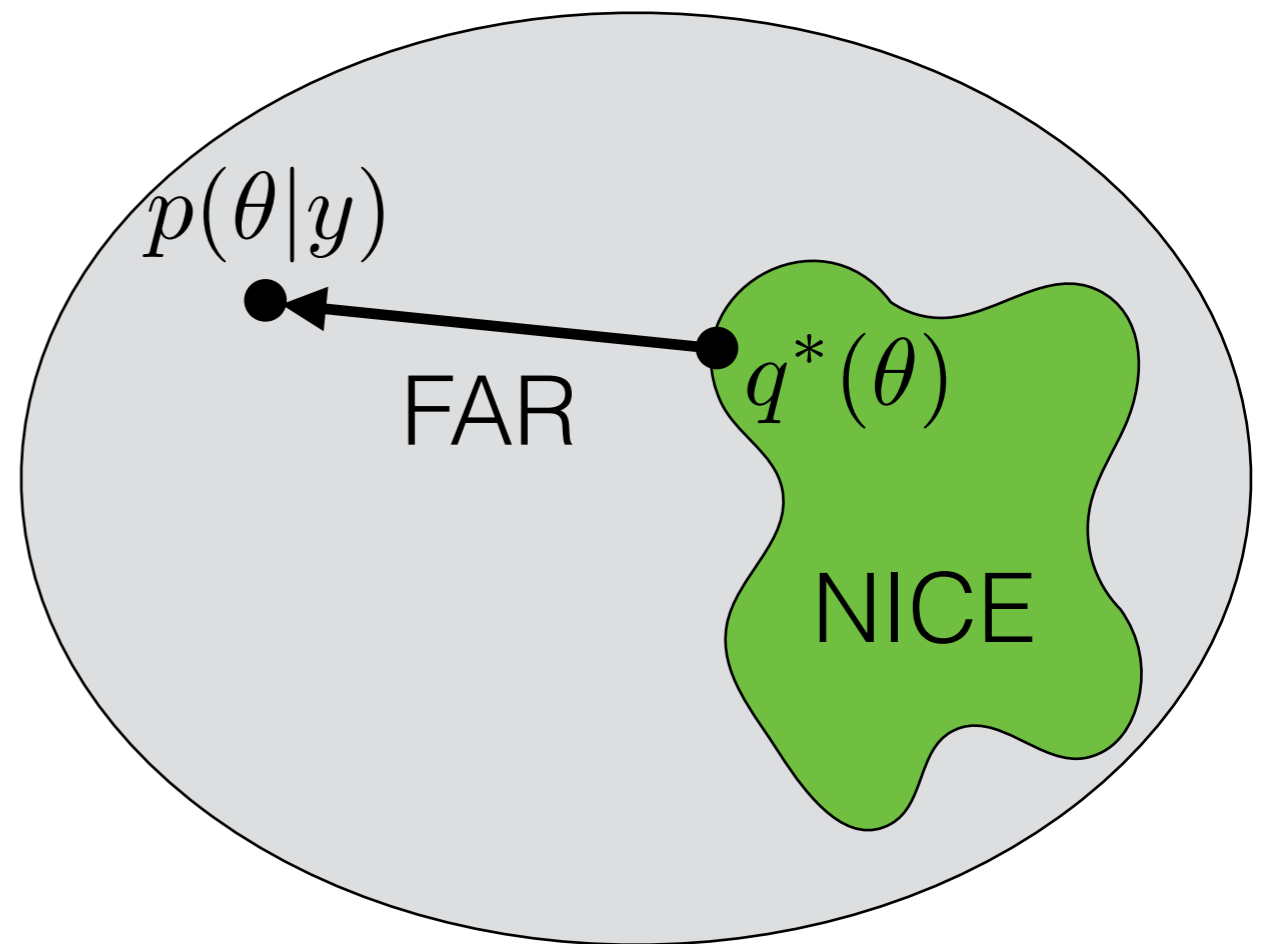
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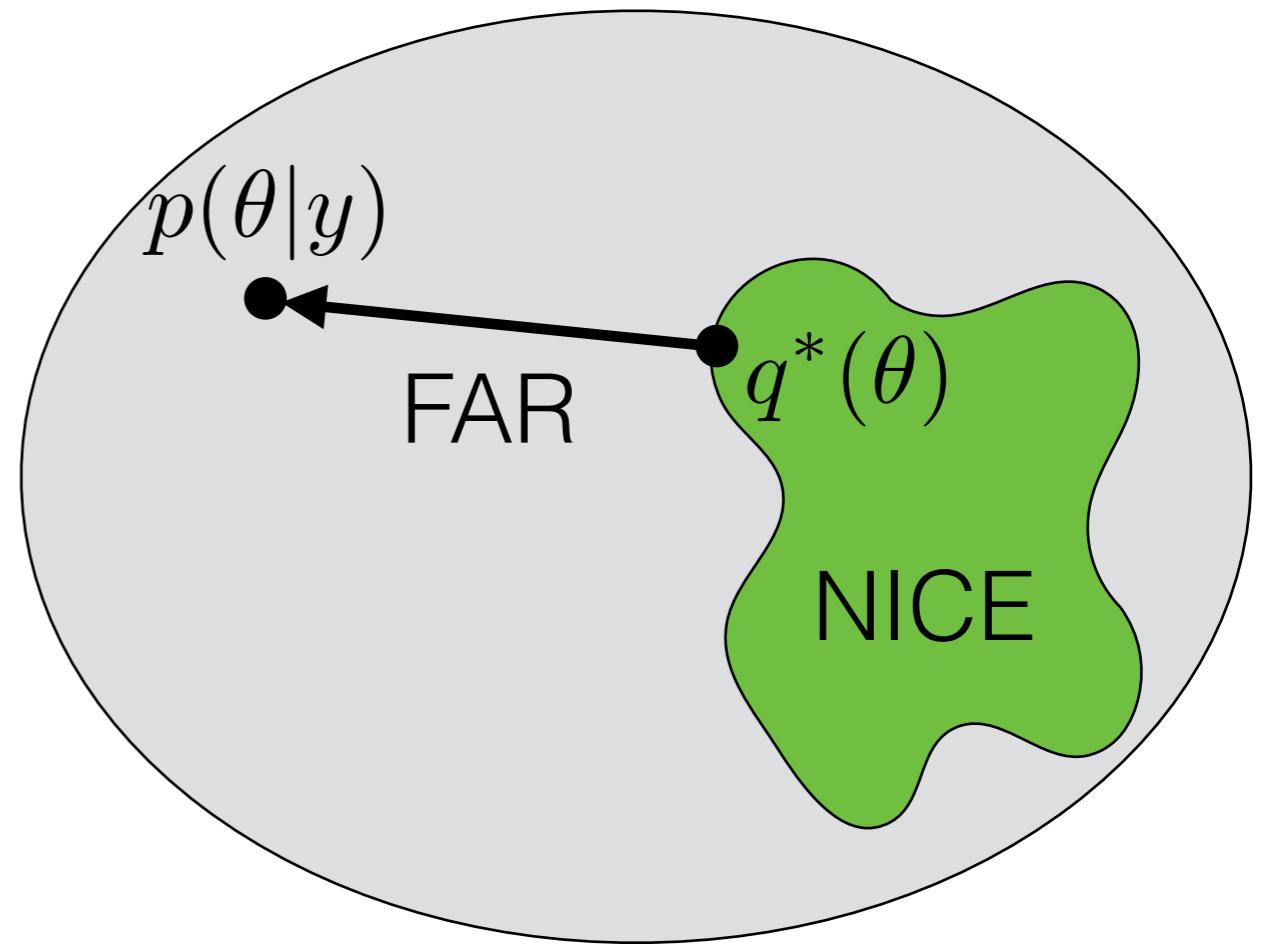
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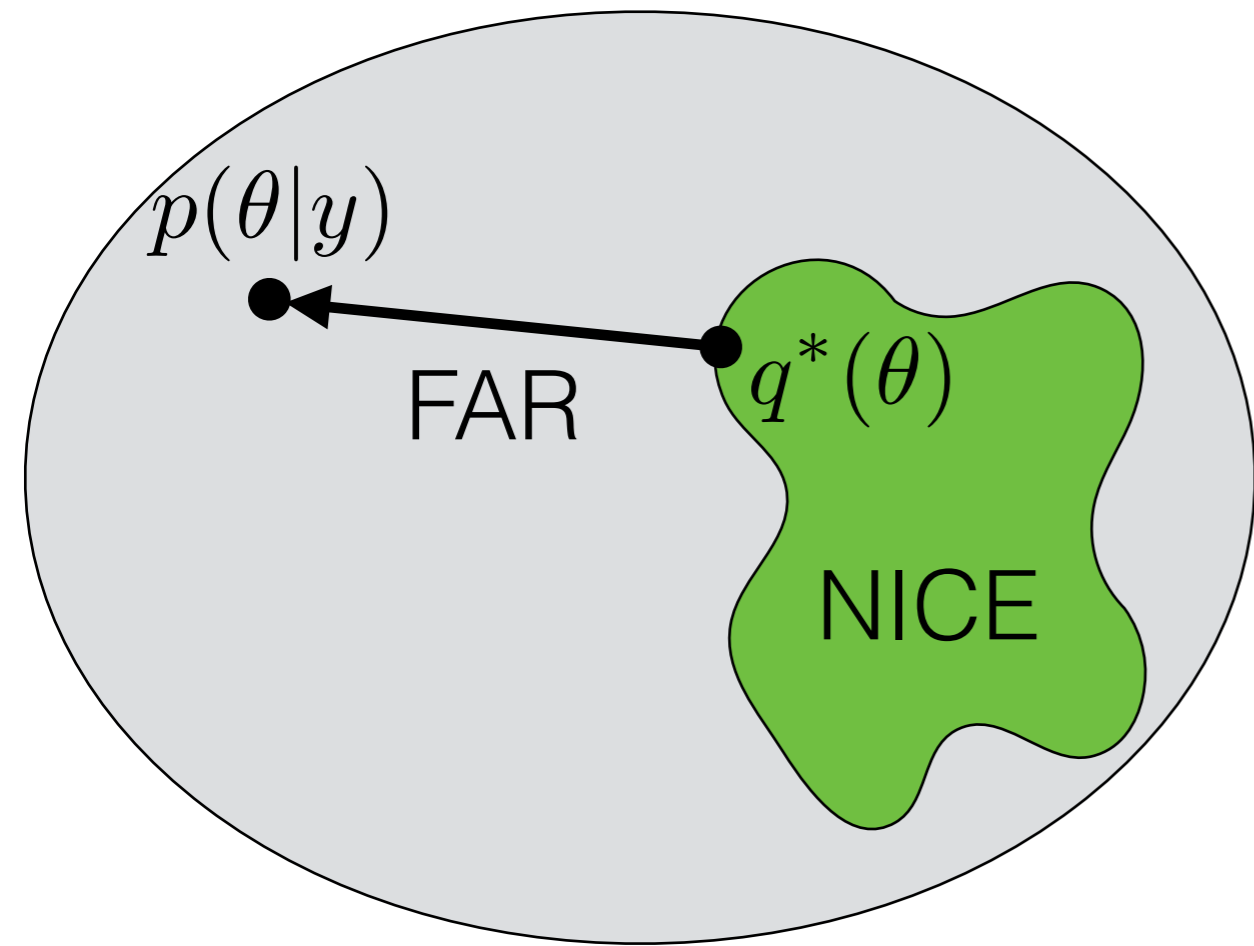
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“Evidence lower bound” (ELBO)

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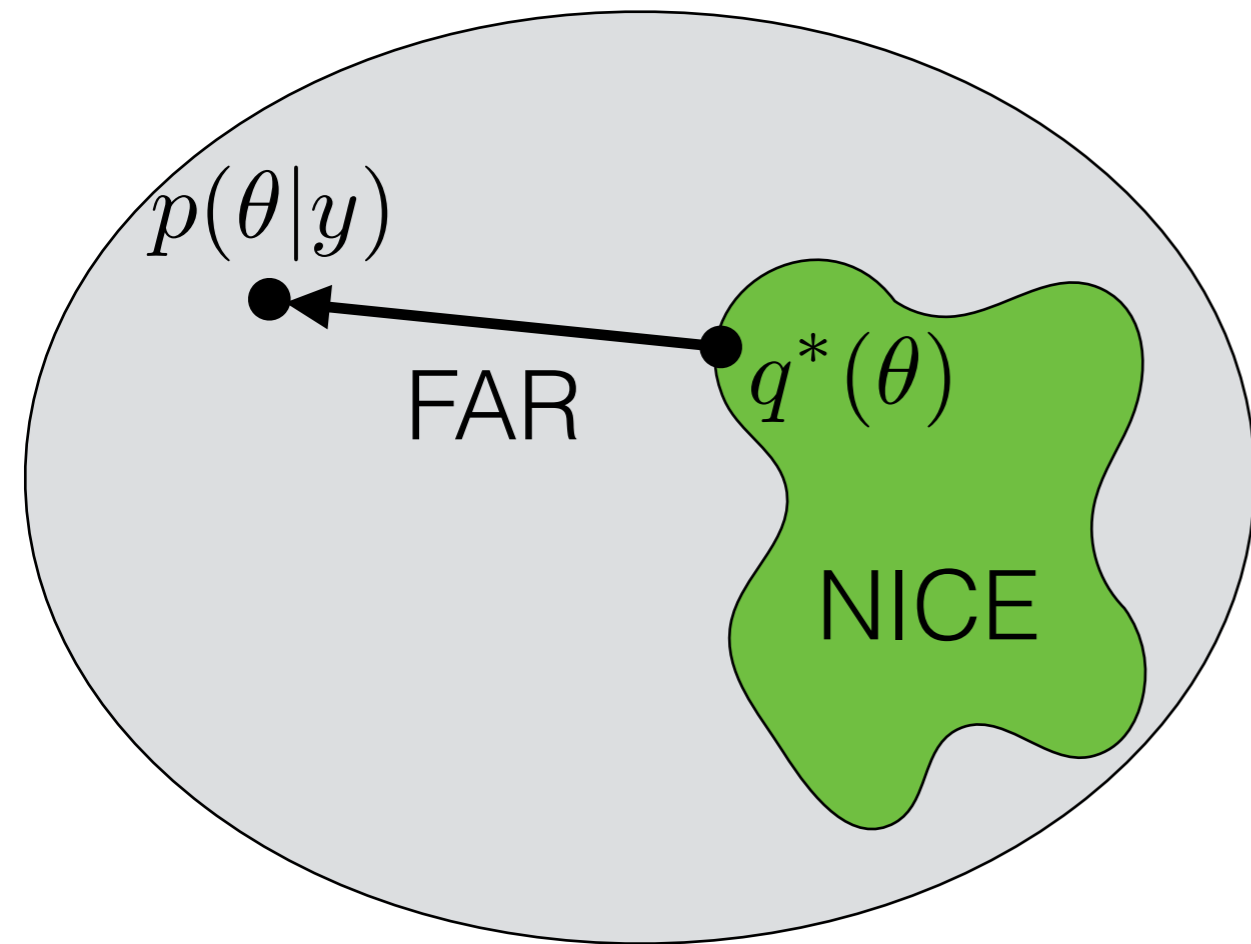
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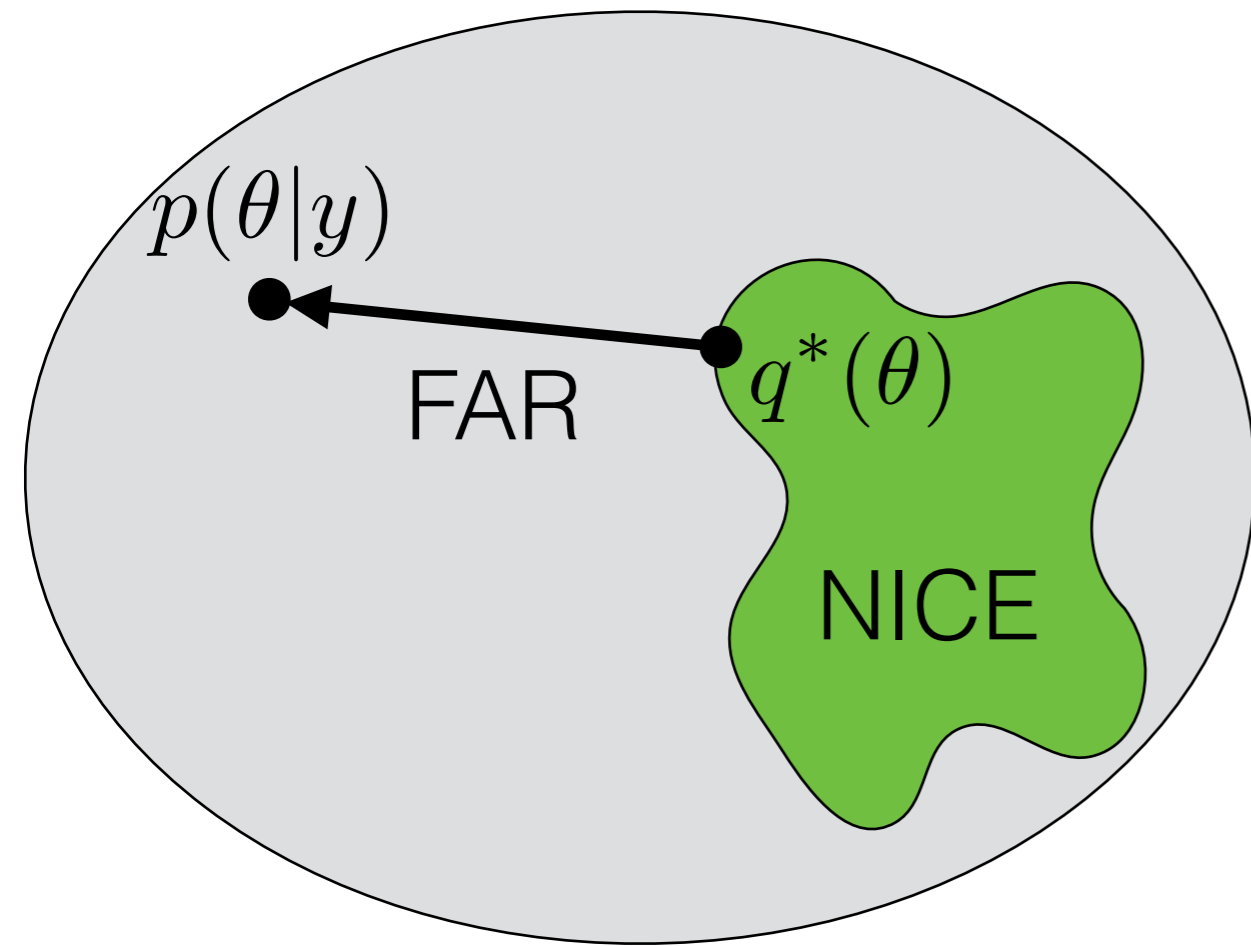
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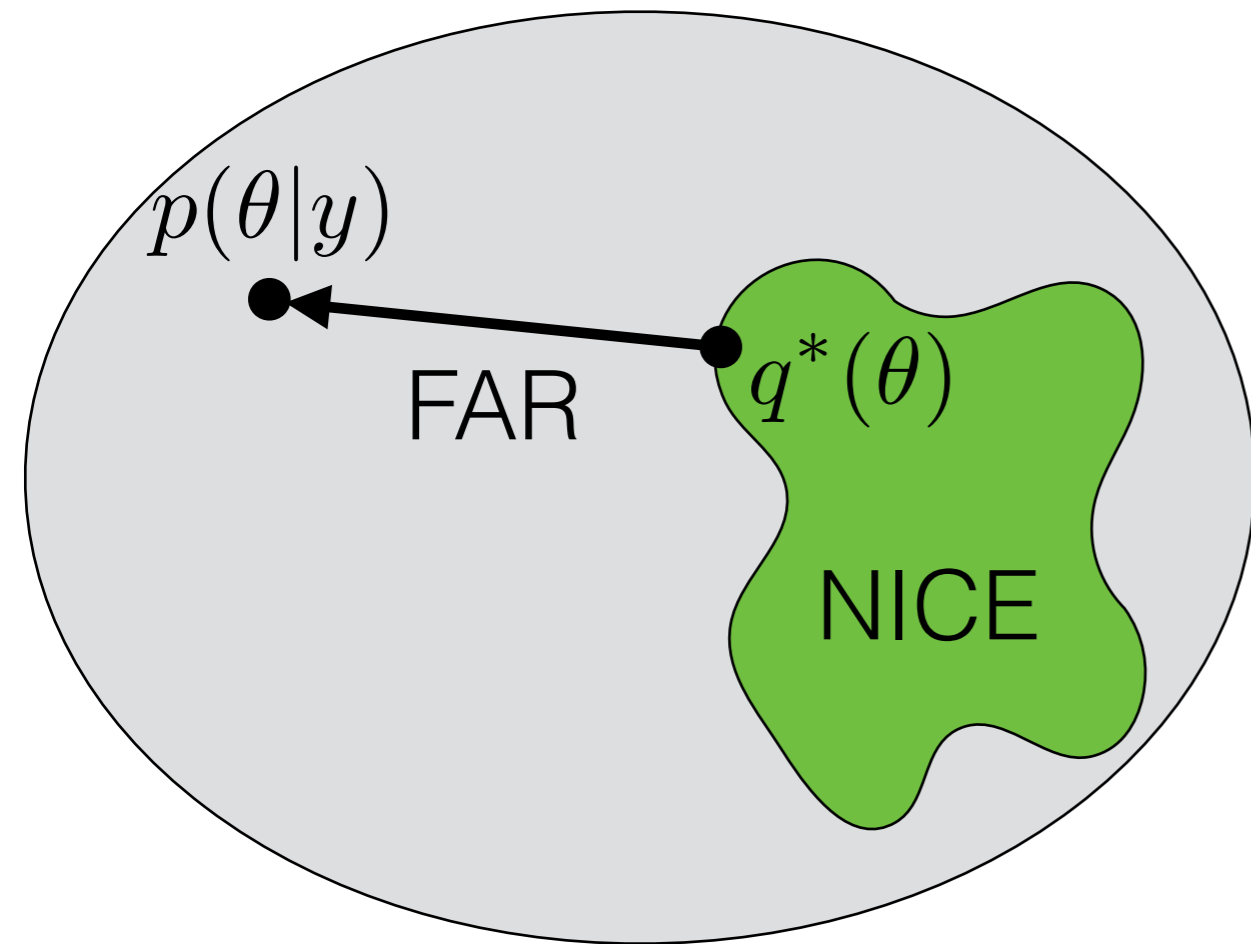
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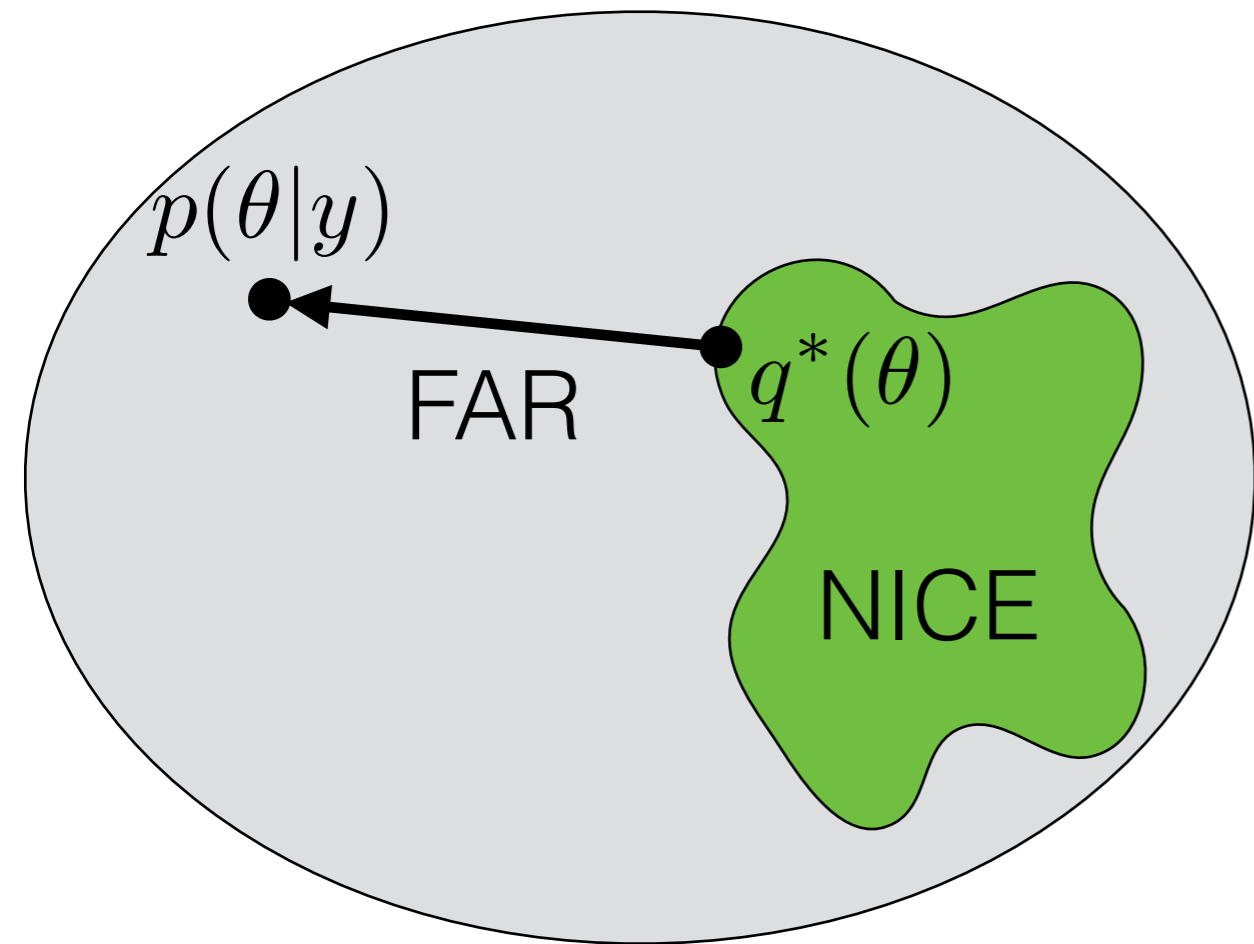
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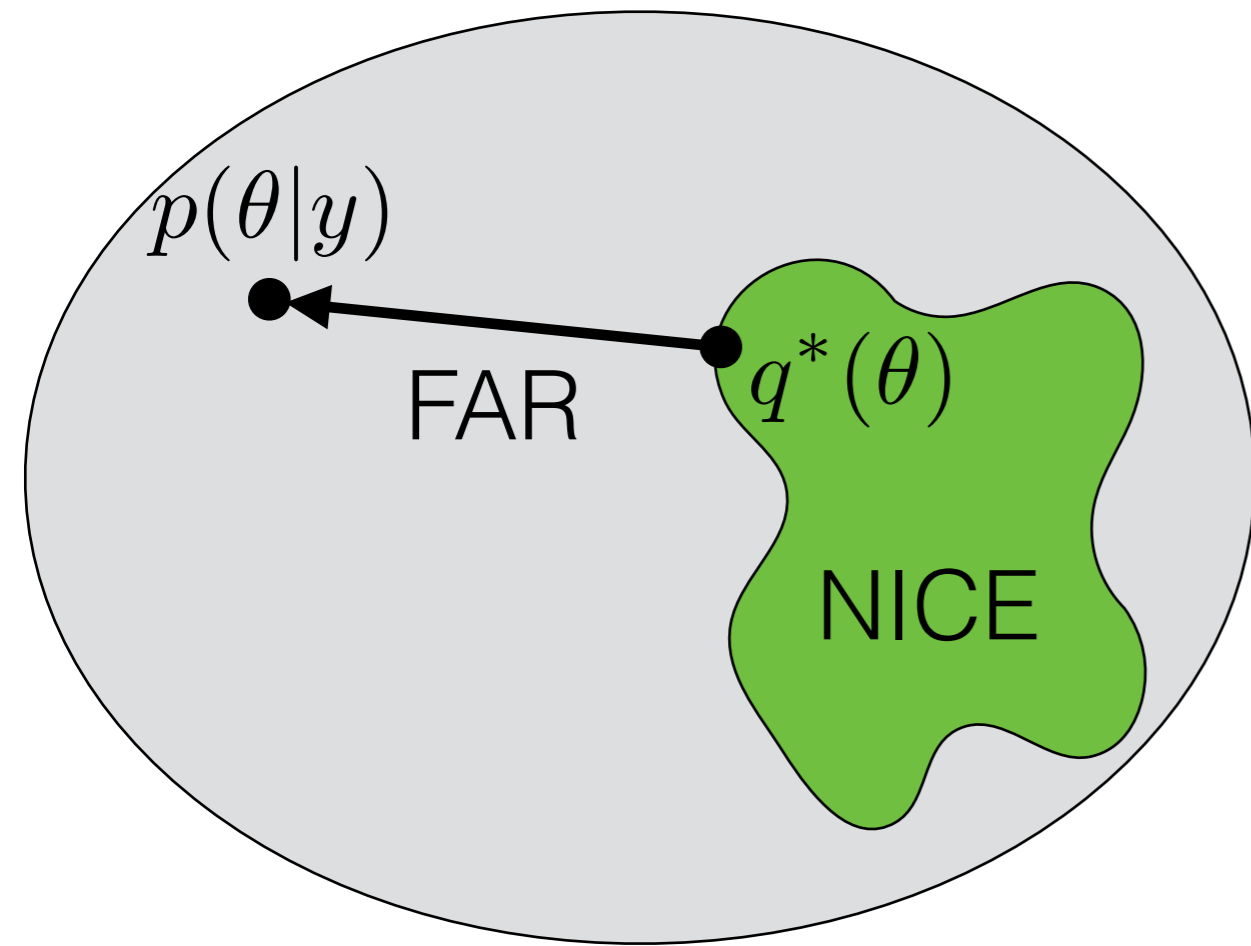
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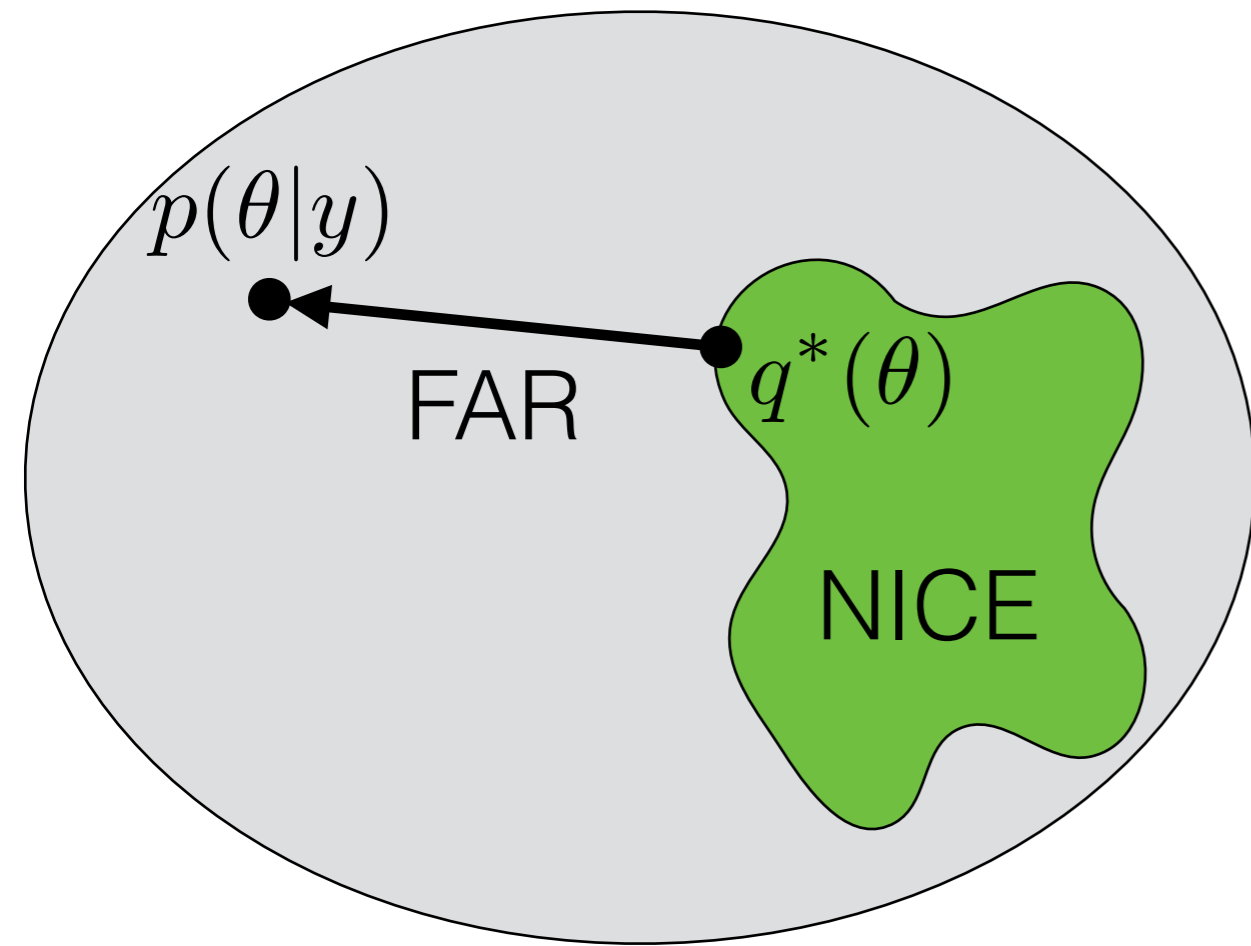
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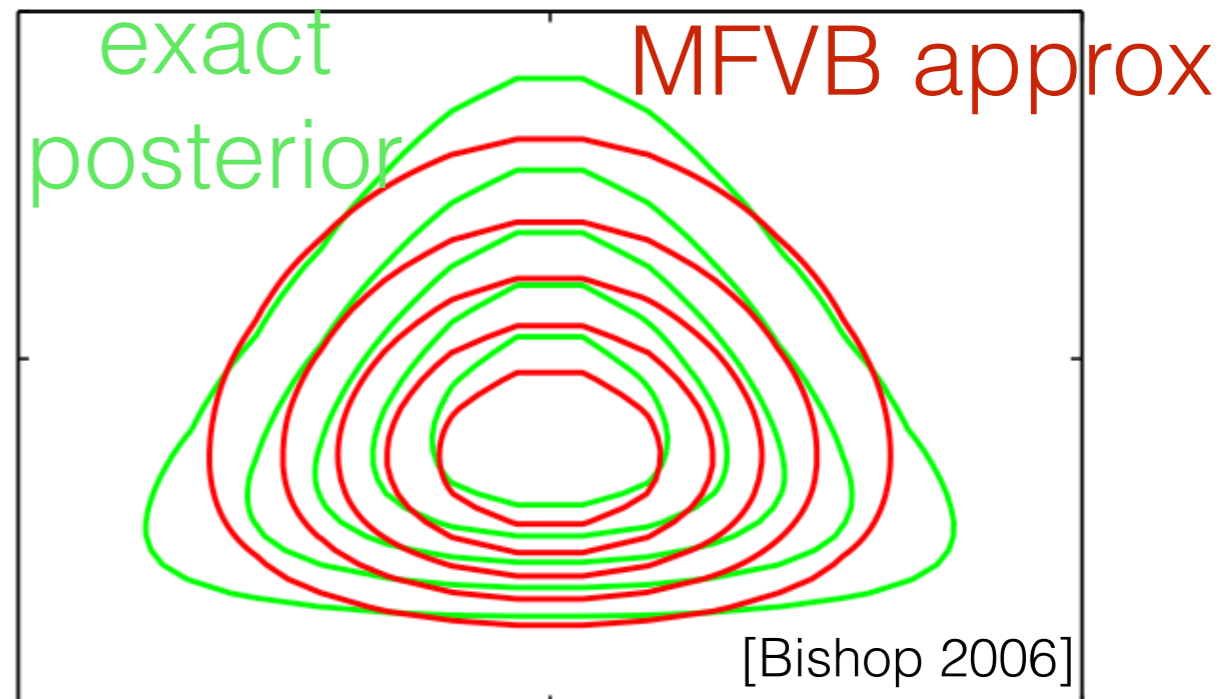
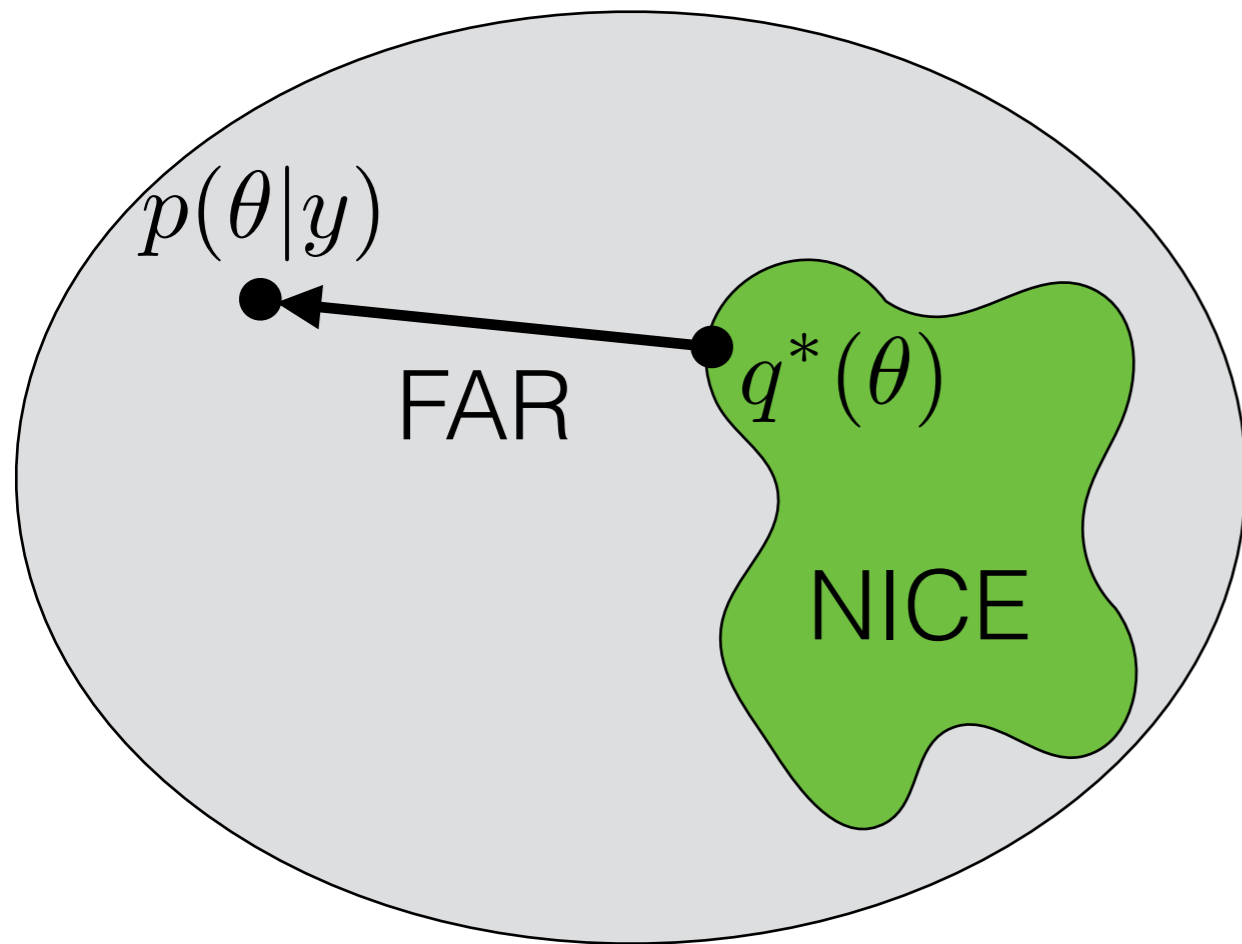
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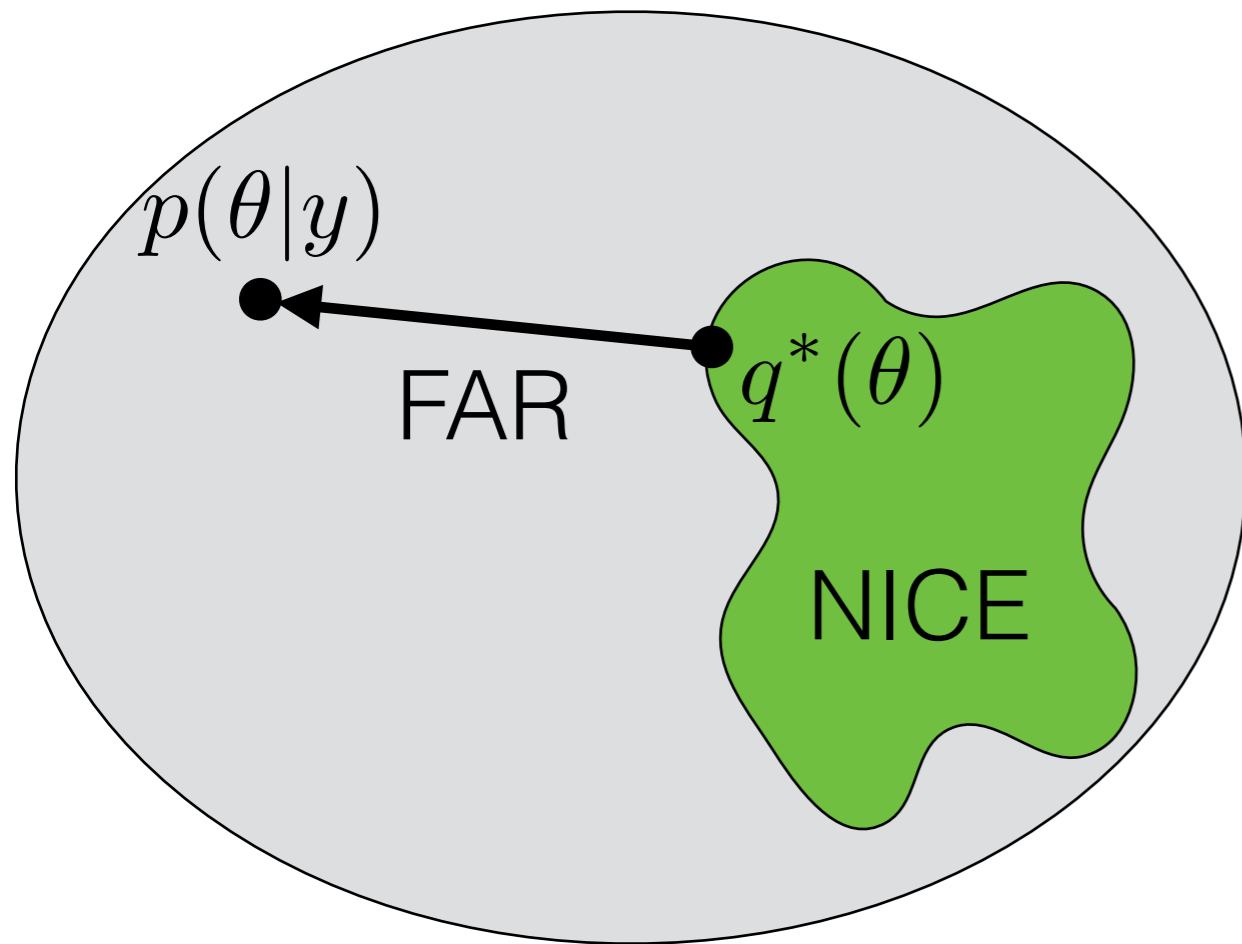
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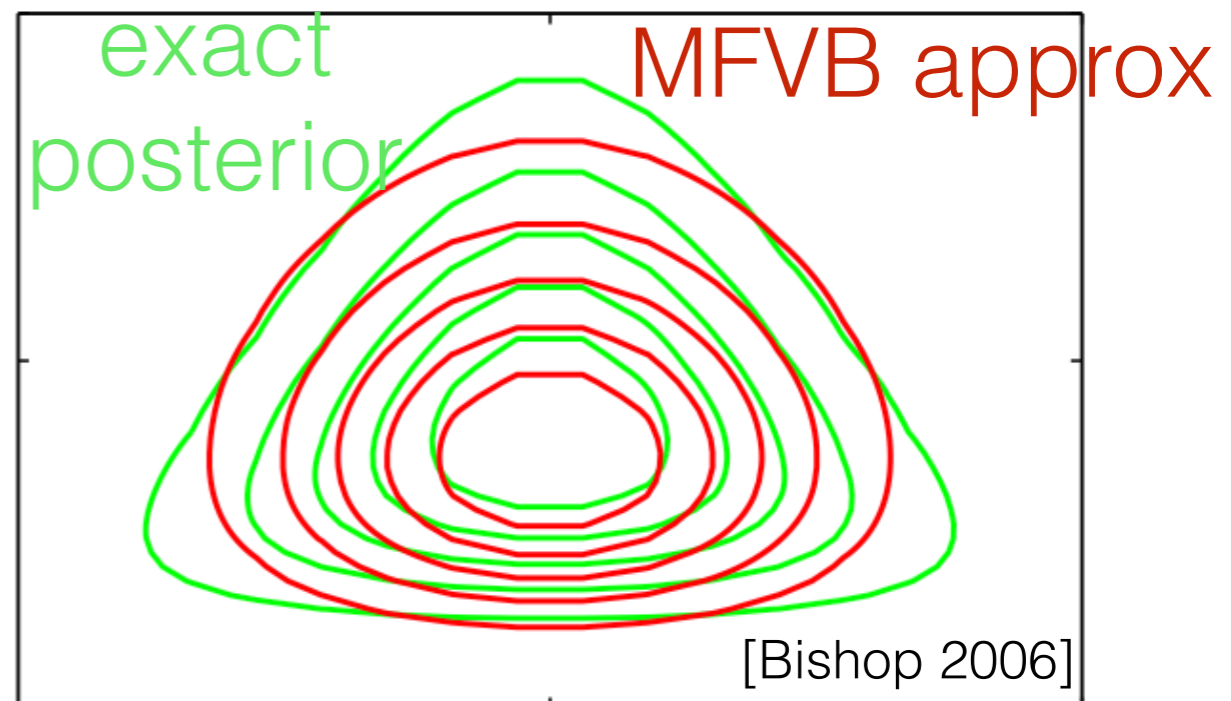
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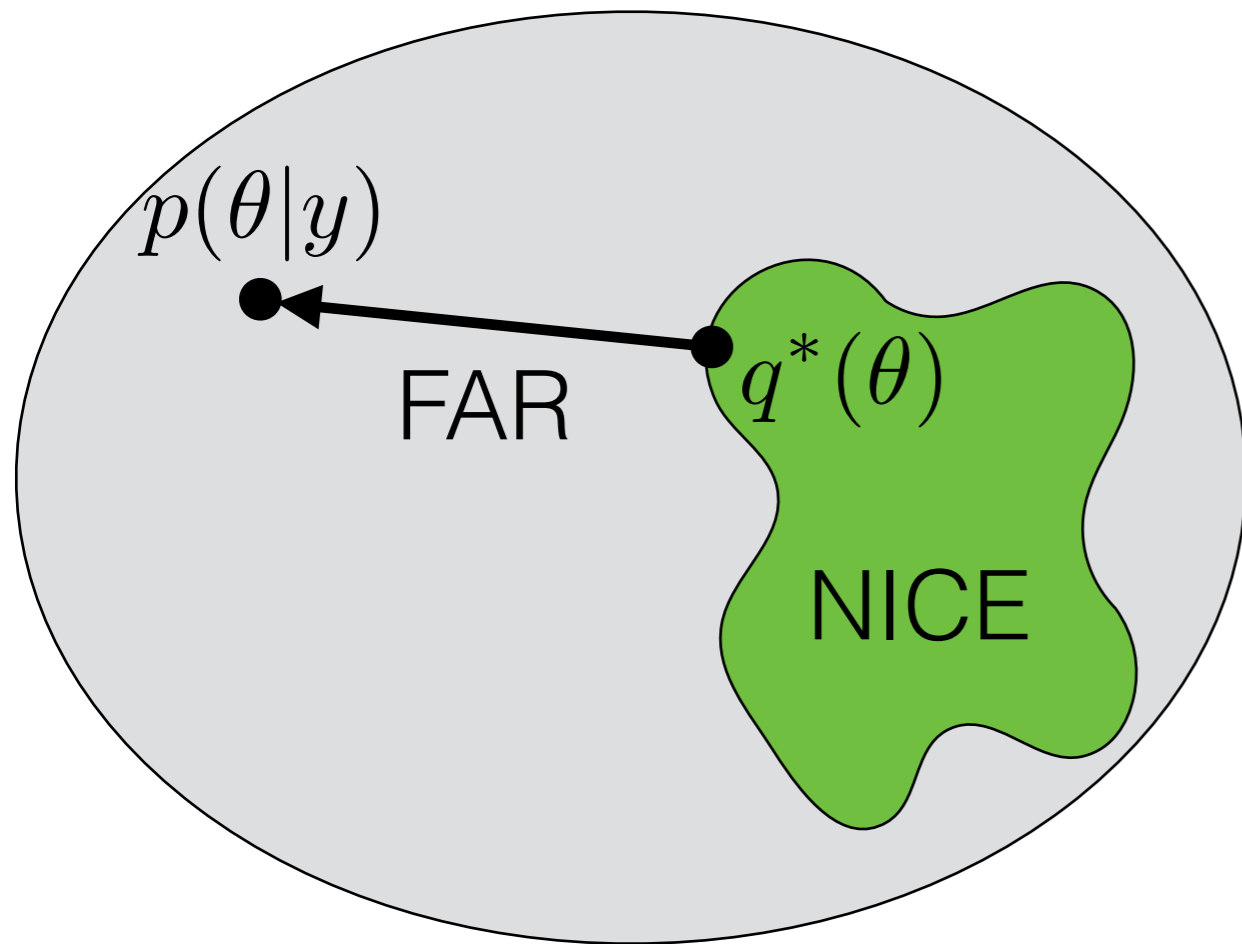
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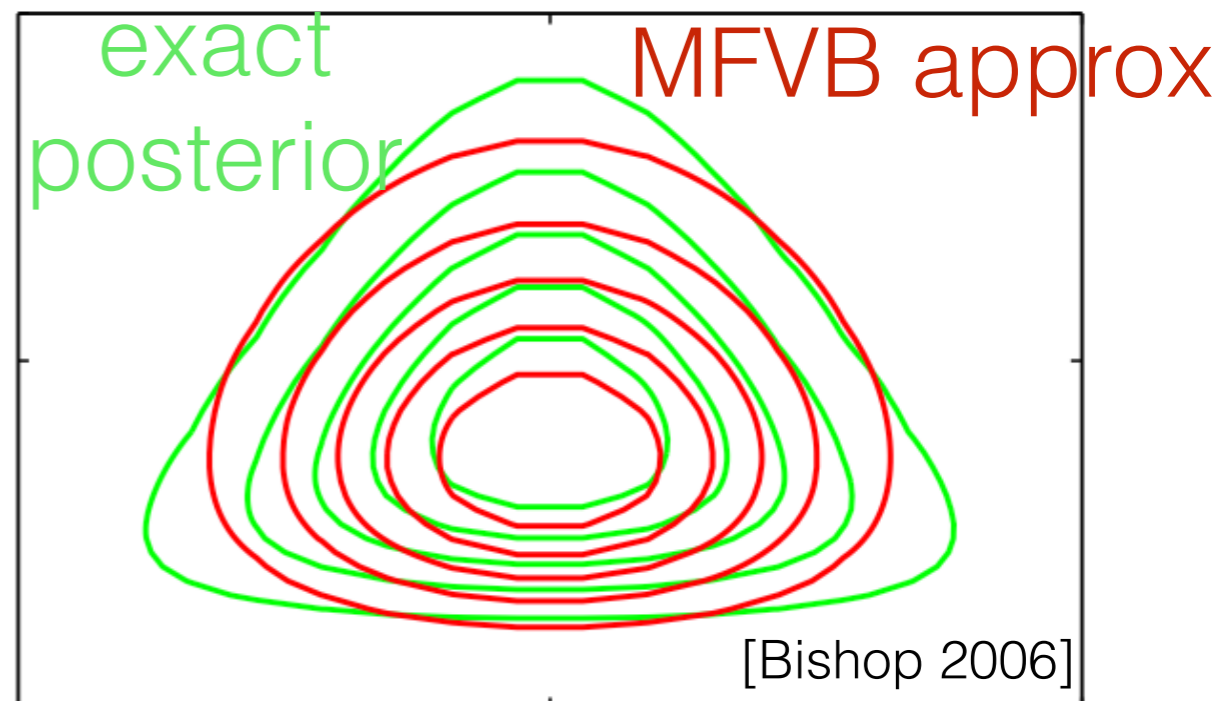
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- One option: Coordinate descent in q_1, \dots, q_J



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[Krongut 2020]

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[Krongut 2020]

Air pollution: Particulate matter

- Sensor readings of log PM2.5 $y = (y_1, \dots, y_N)$
- Parameters of interest: PM2.5 mean and precision $\theta = (\mu, \tau)$
- Model (conjugate prior): [Exercise: find the posterior]

$$p(y|\theta) : y_n \stackrel{iid}{\sim} \mathcal{N}(\mu, \tau^{-1}),$$

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

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

- Exercise: check

$$p(\mu, \tau|y) \neq f_1(\mu, y)f_2(\tau, y)$$

- MFVB approximation:

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

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

$$q_\mu^*(\mu) = \mathcal{N}(\mu|\mu_N, \rho_N^{-1})$$

$$q_\tau^*(\tau) = \text{Gamma}(\tau|a_N, b_N)$$

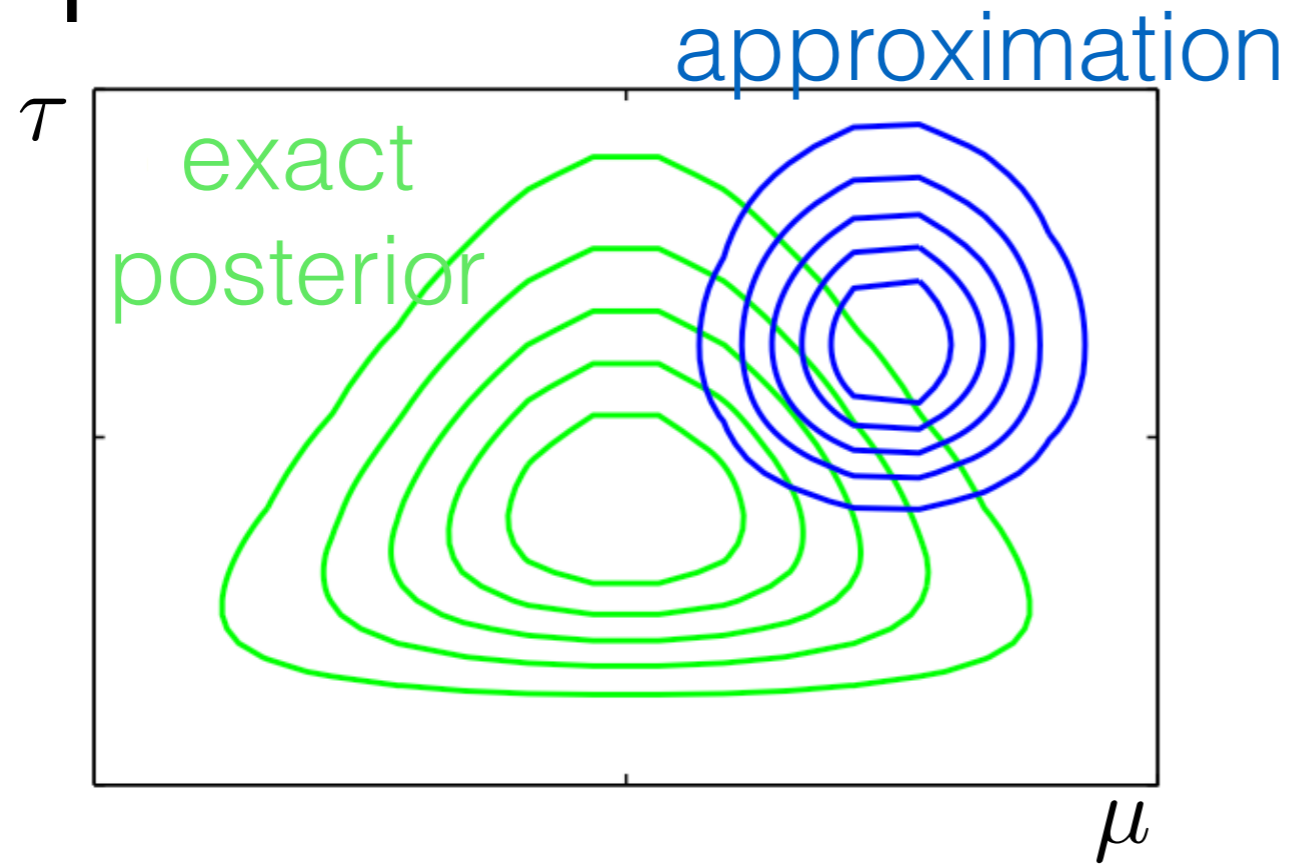
“variational
parameters”

[MacKay 2003; Bishop 2006]



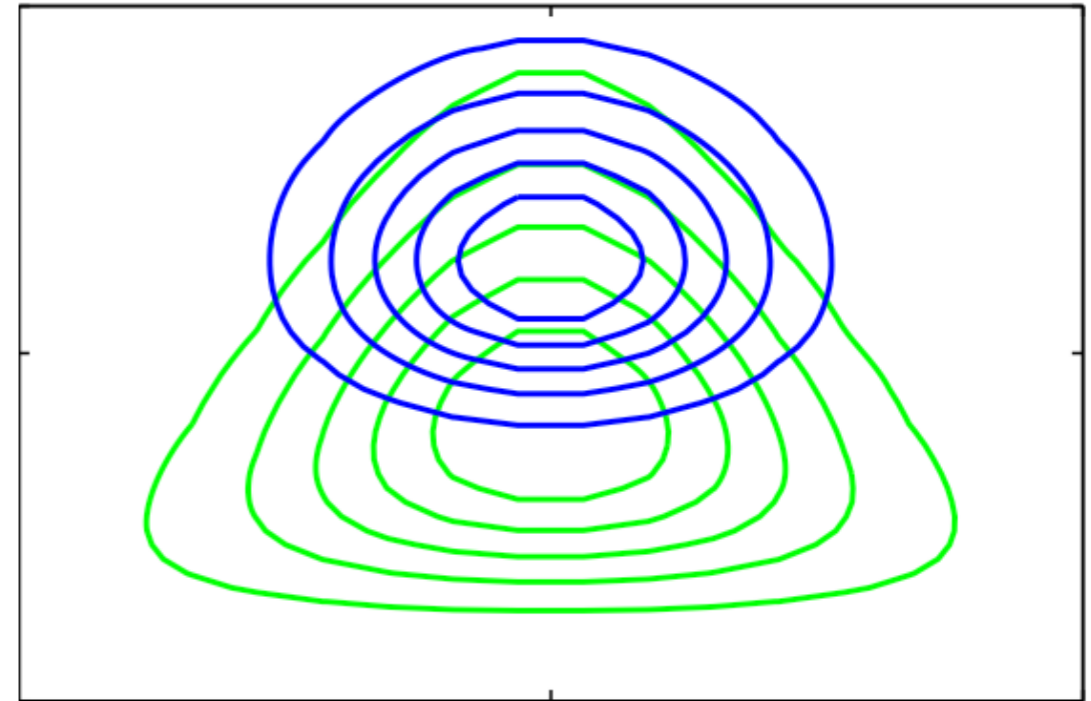
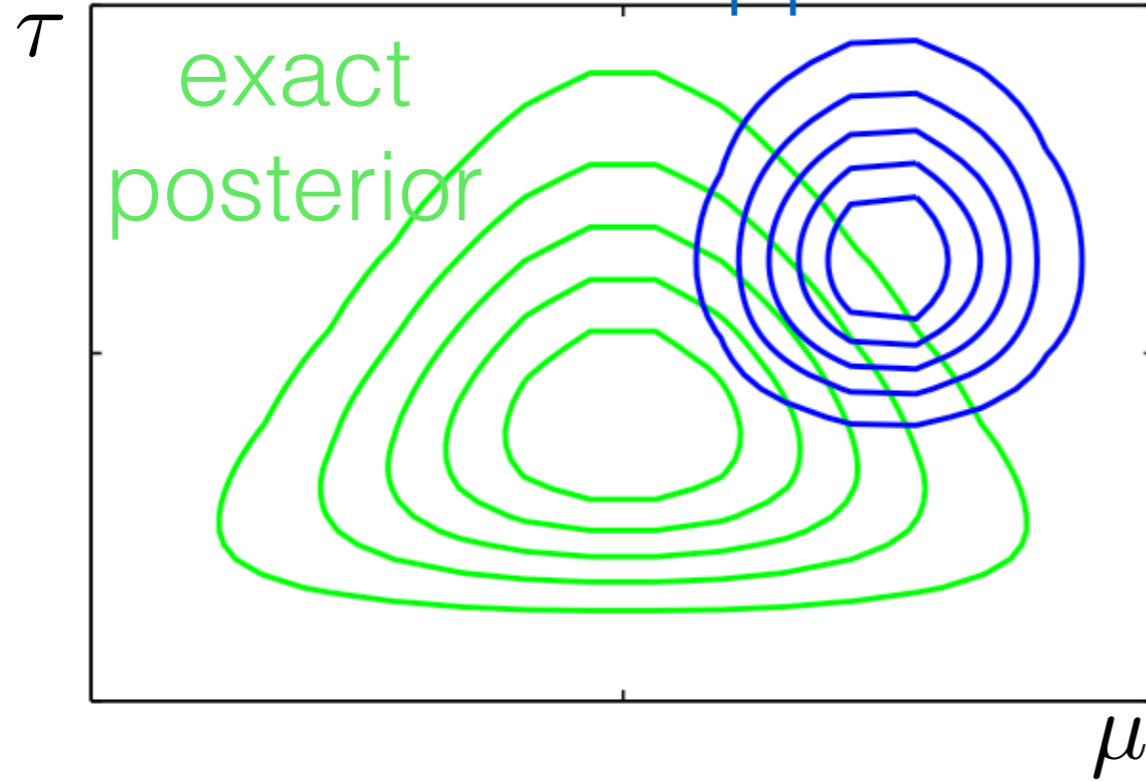
[Krongut 2020]

Air pollution: Particulate matter



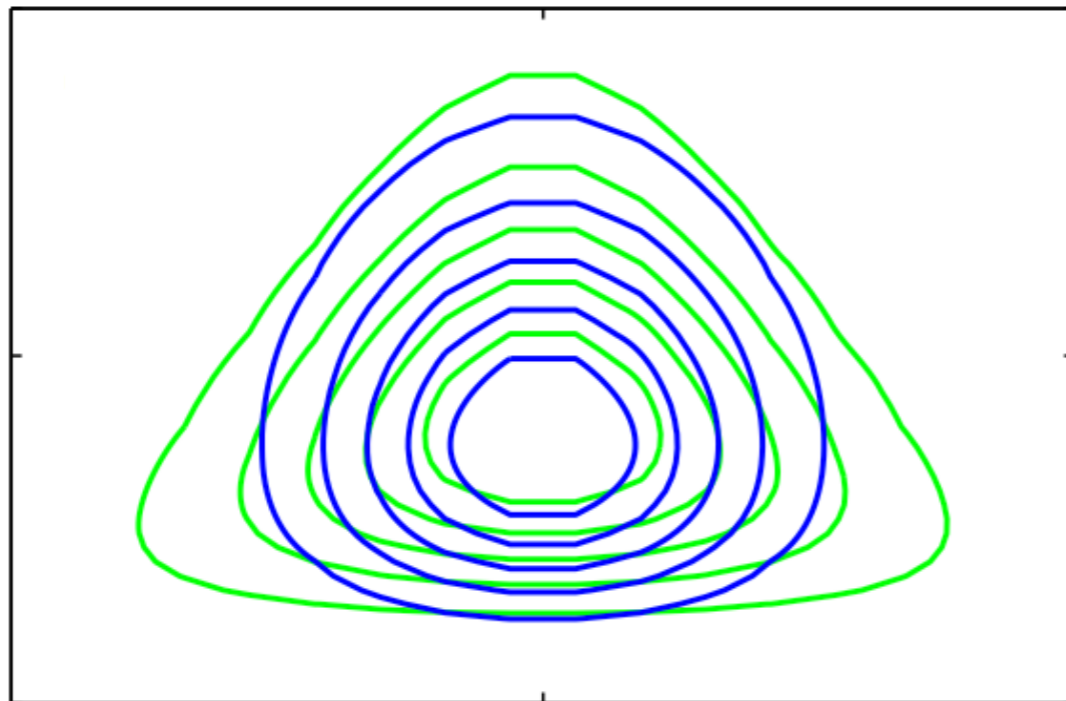
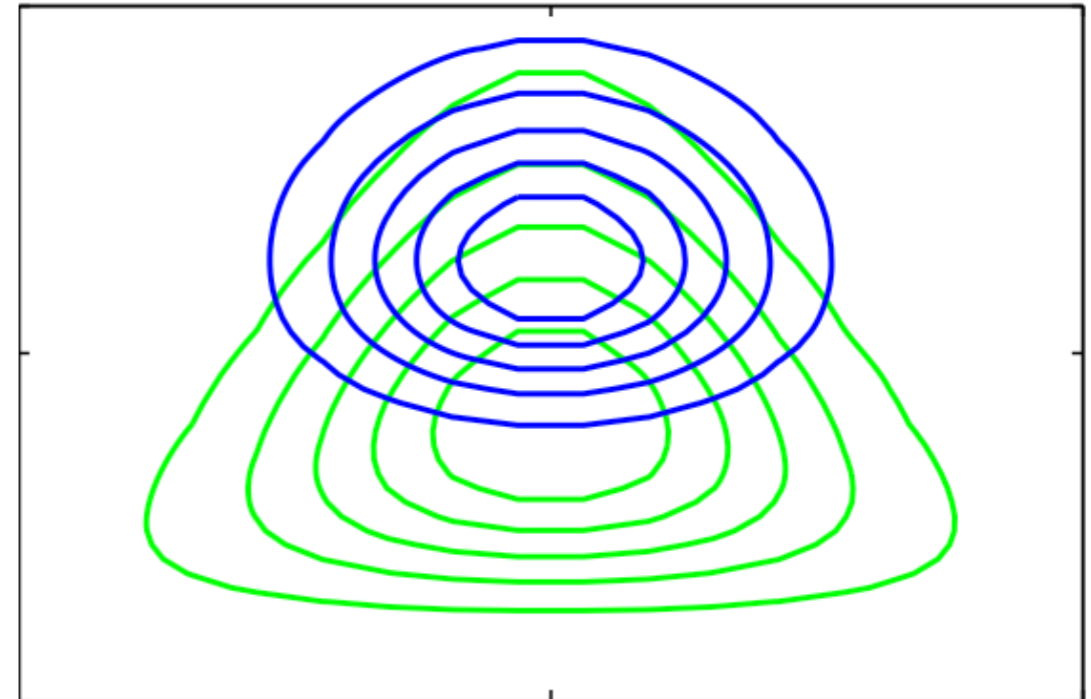
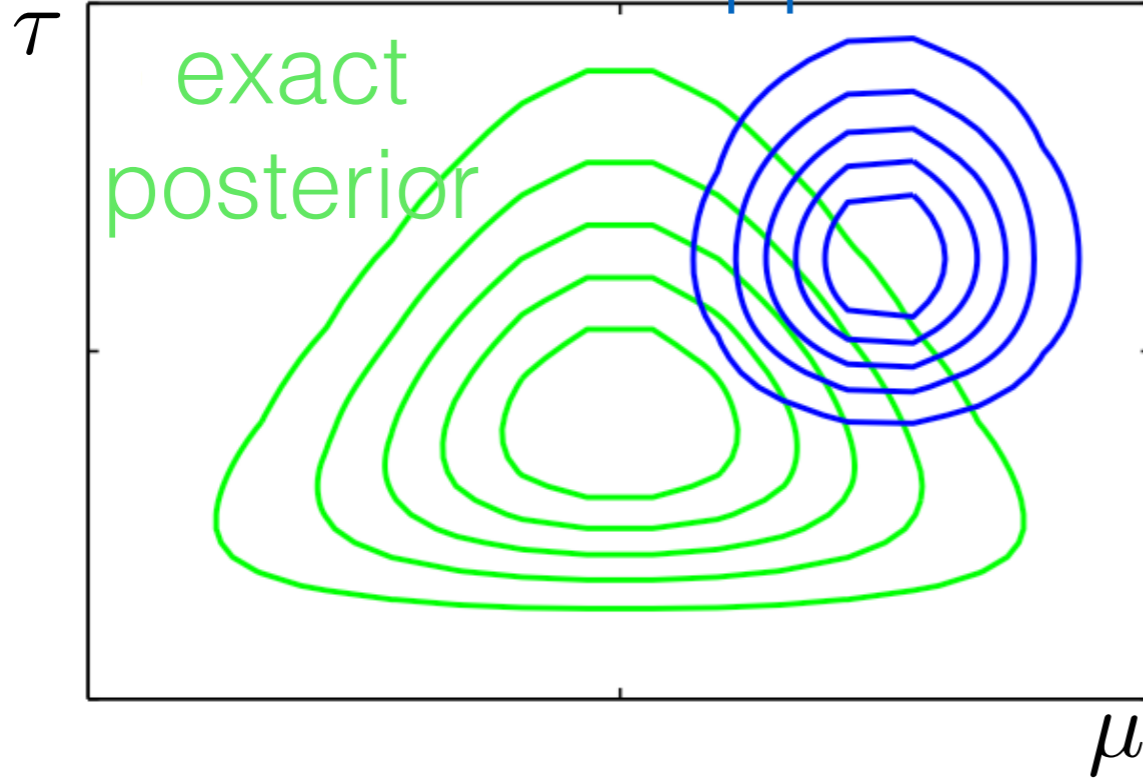
Air pollution: Particulate matter

approximation



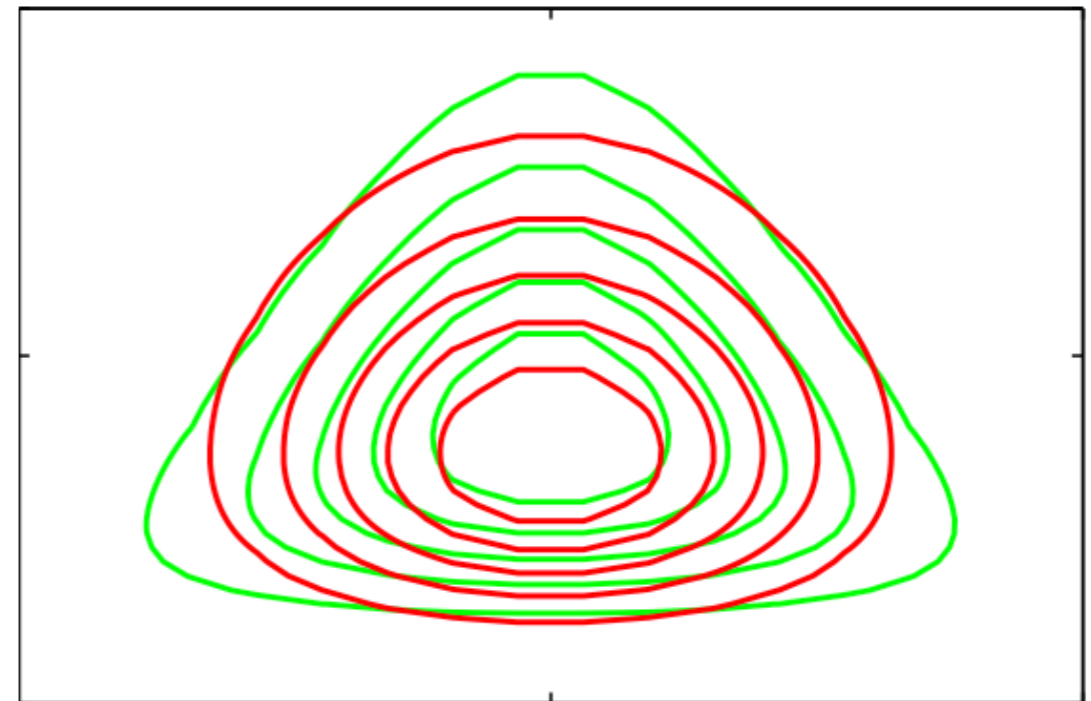
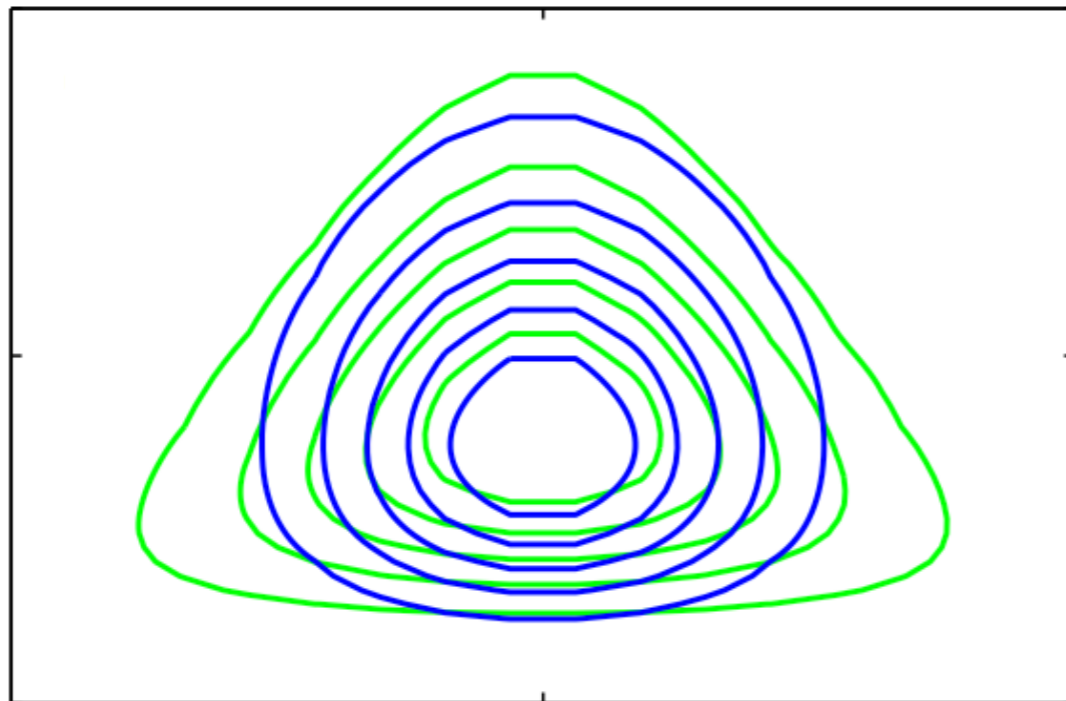
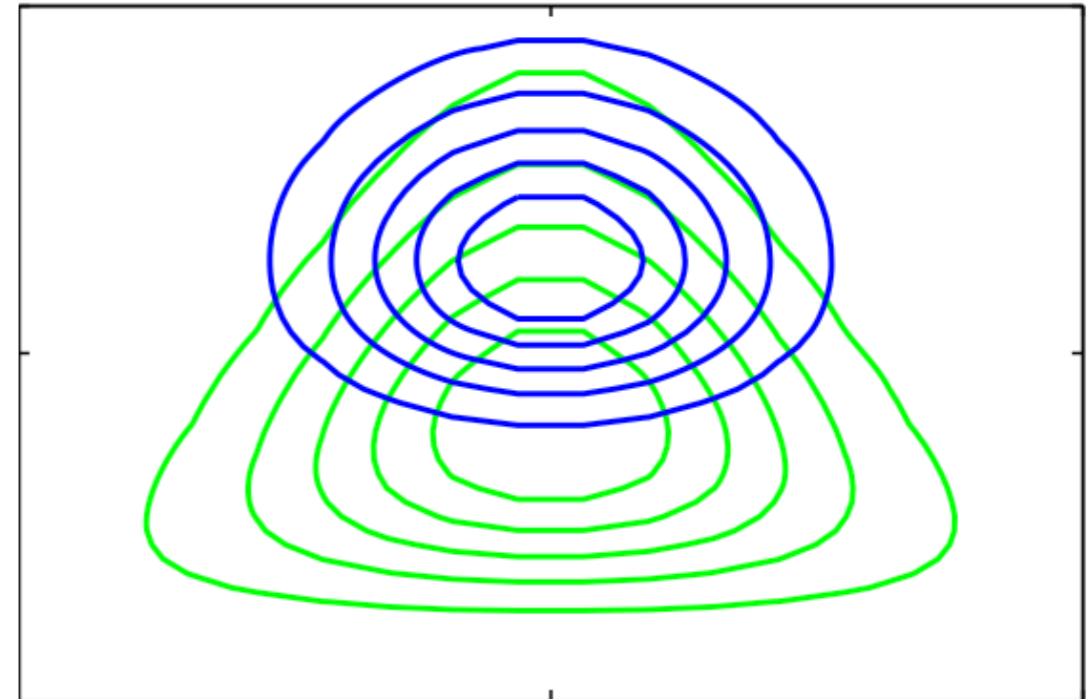
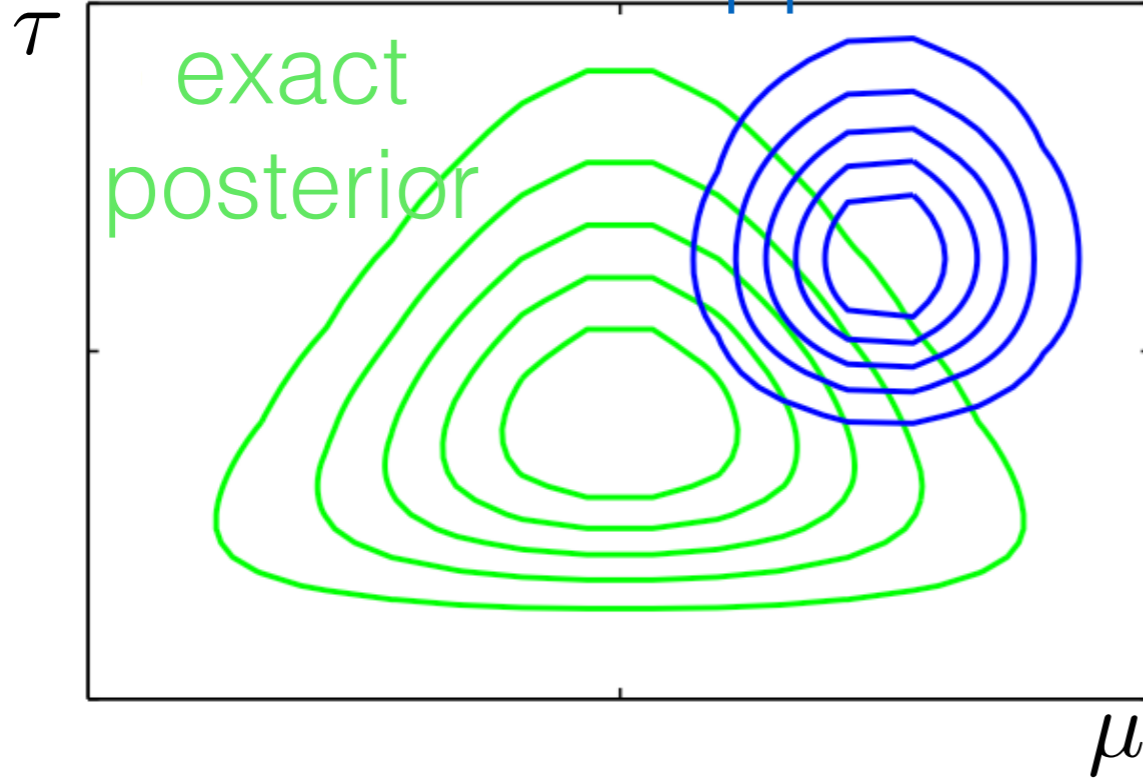
Air pollution: Particulate matter

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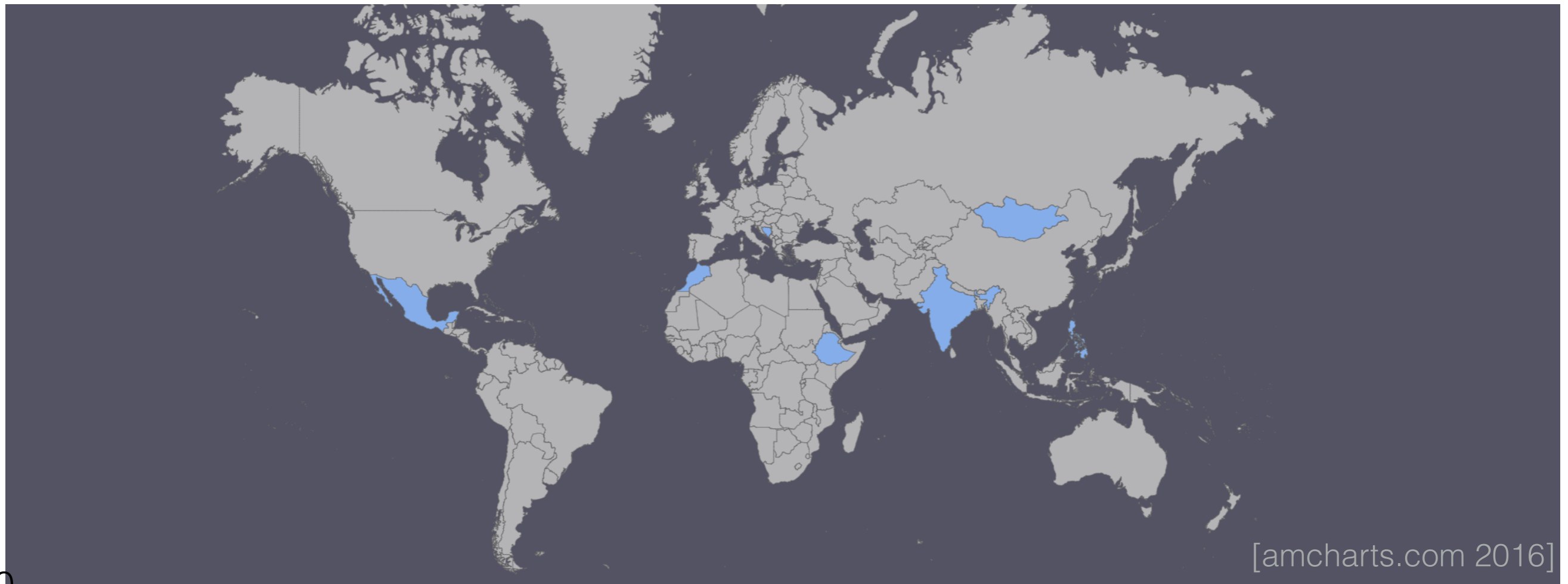


Air pollution: Particulate matter

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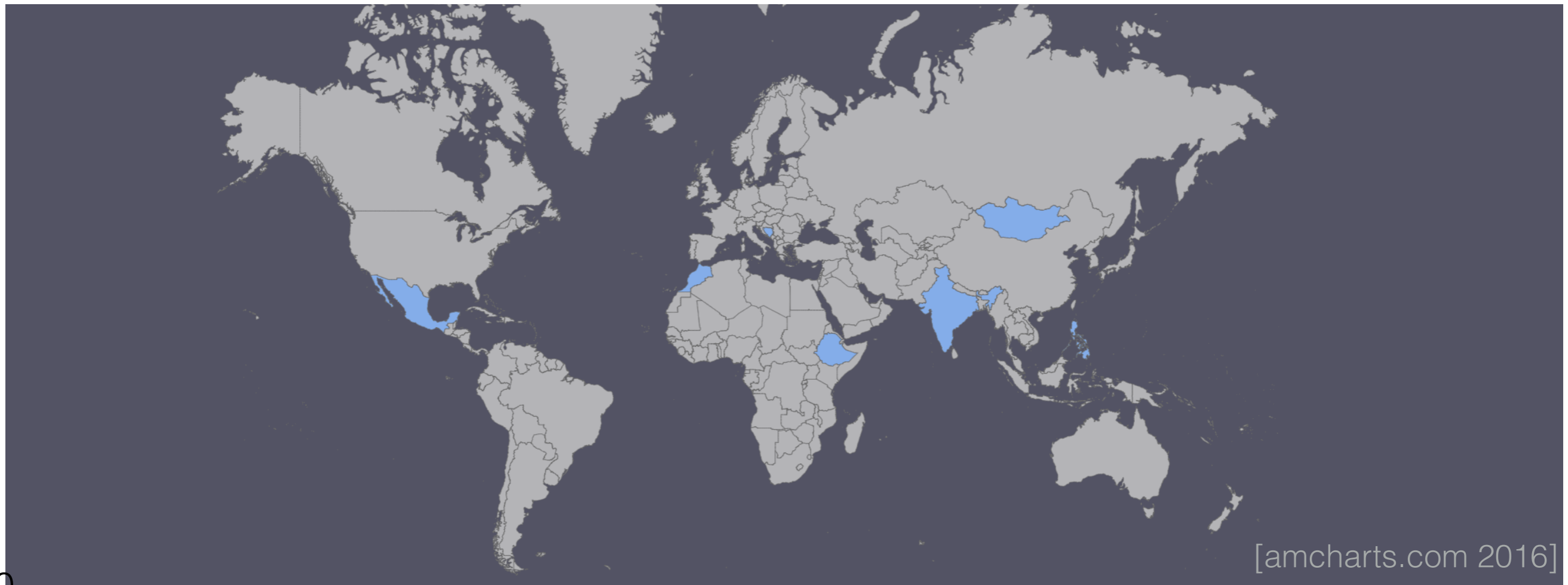
Microcredit Experiment



[amcharts.com 2016]

Microcredit Experiment

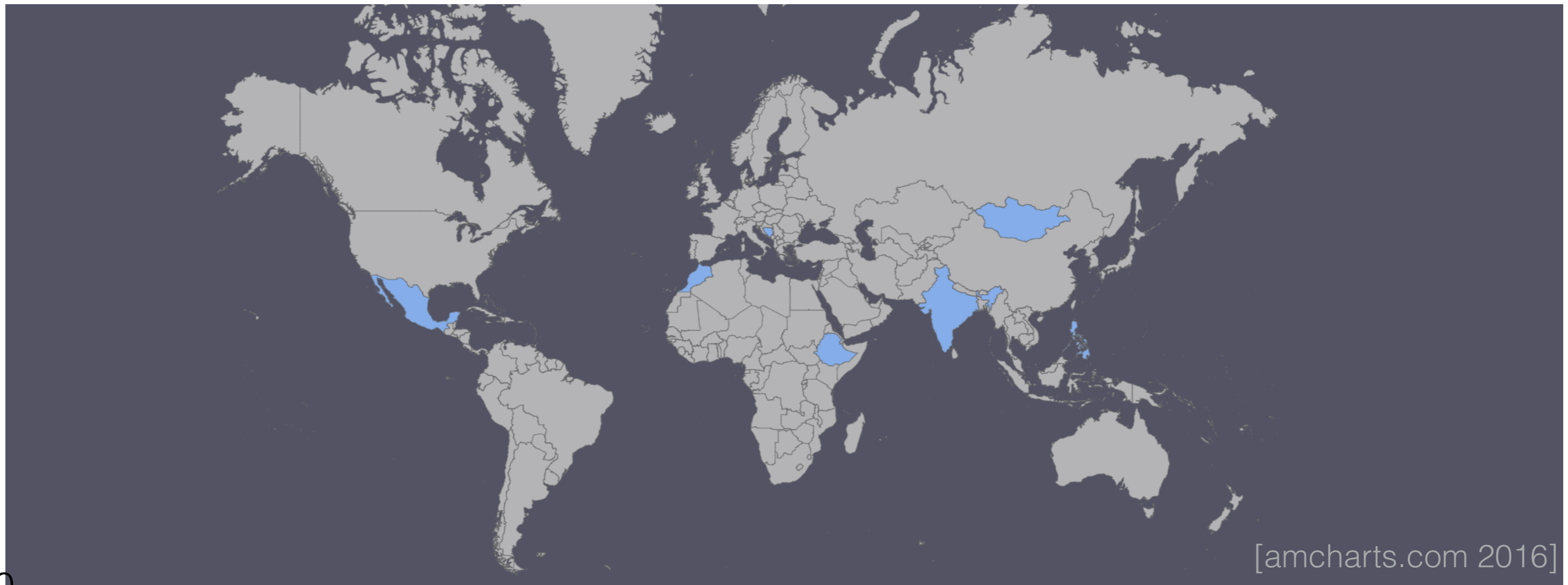
- Simplified from Meager (2019)



[amcharts.com 2016]

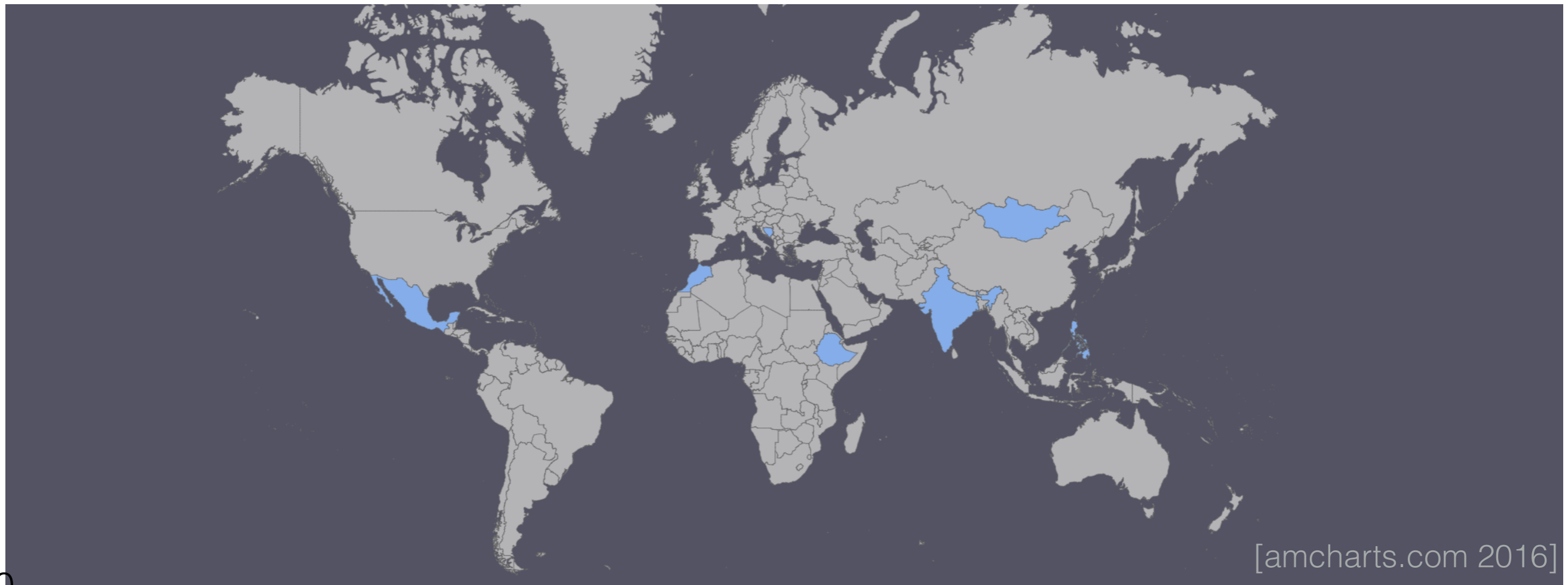
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profit  y_{kn}

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- Priors and hyperpriors:

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

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

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

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

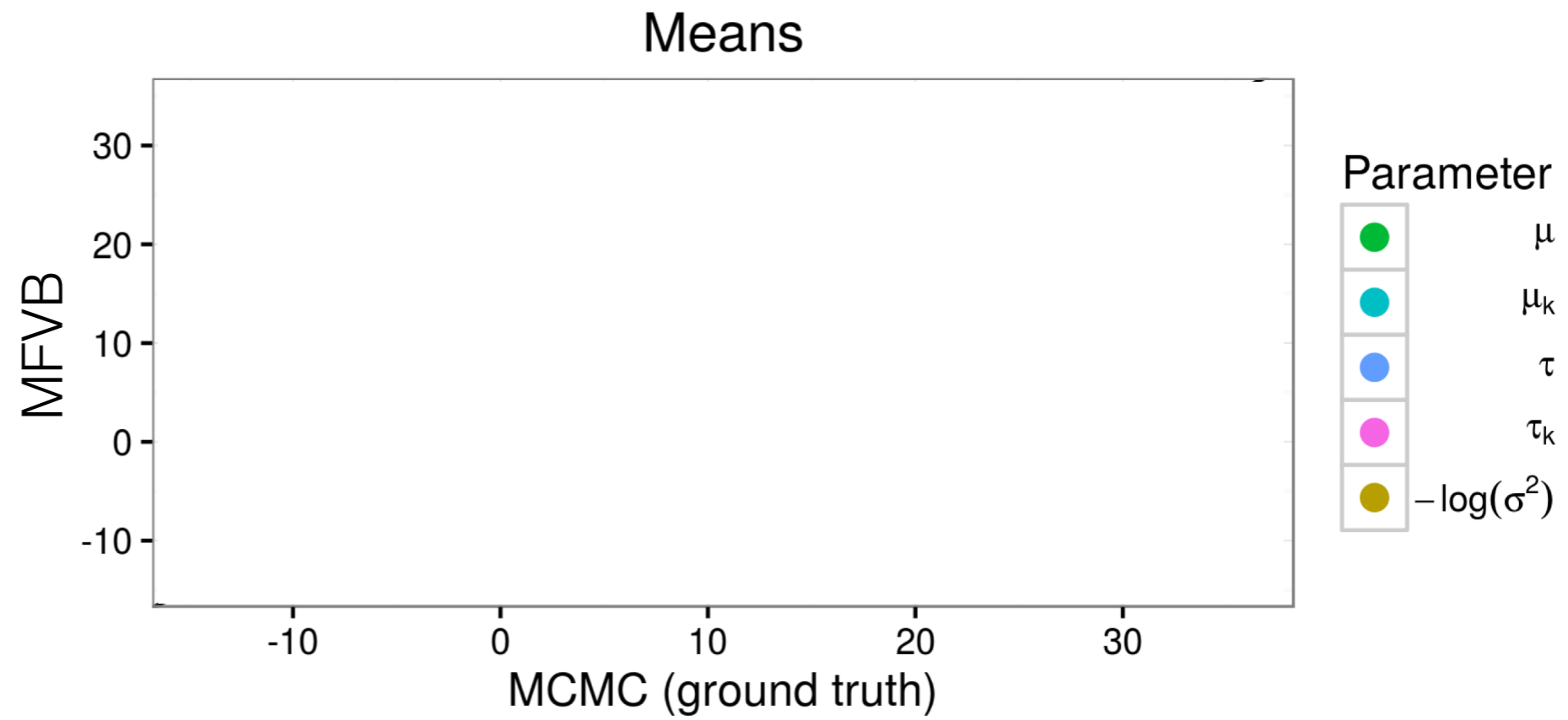
Microcredit

MFVB: Do we need to check the output?

Microcredit

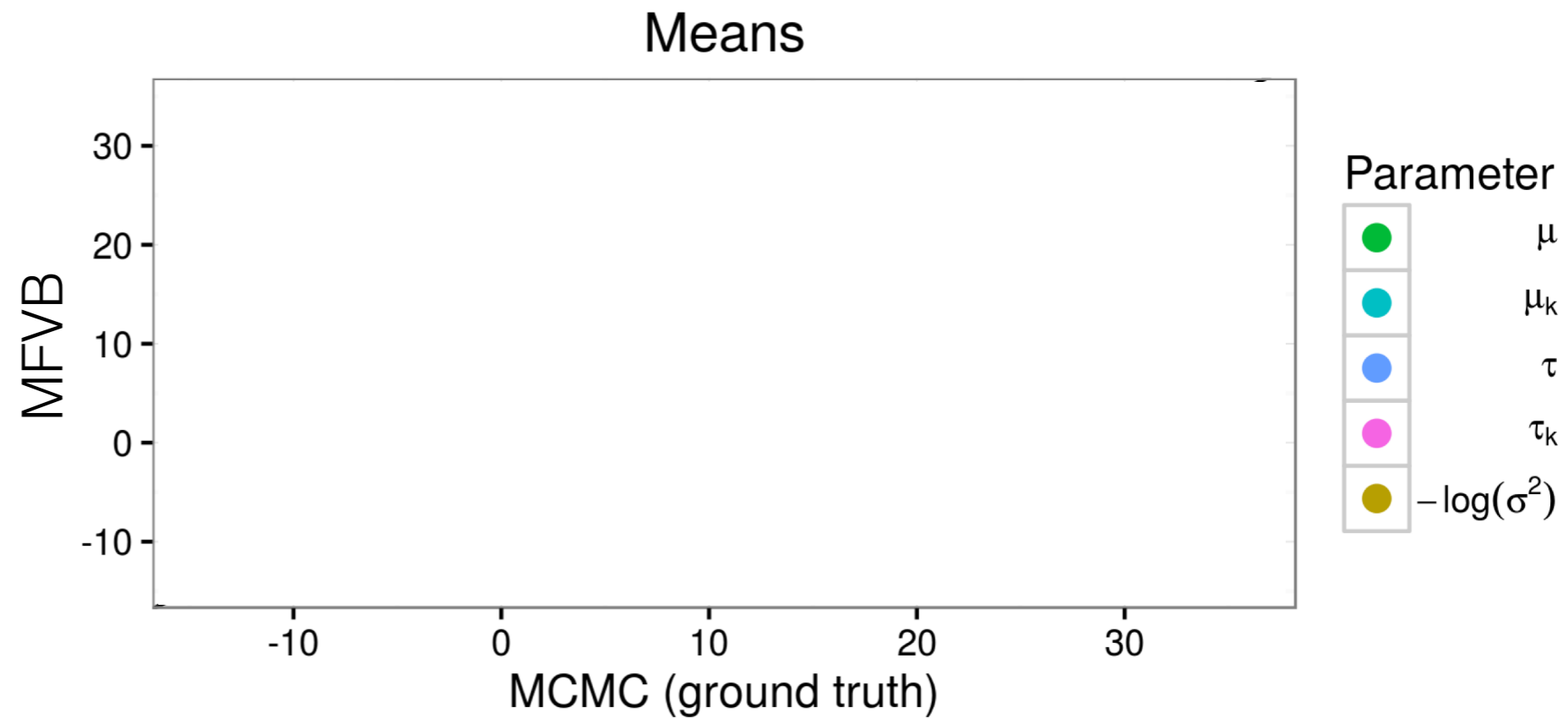
MFVB: How will we know if it's working?

Microcredit



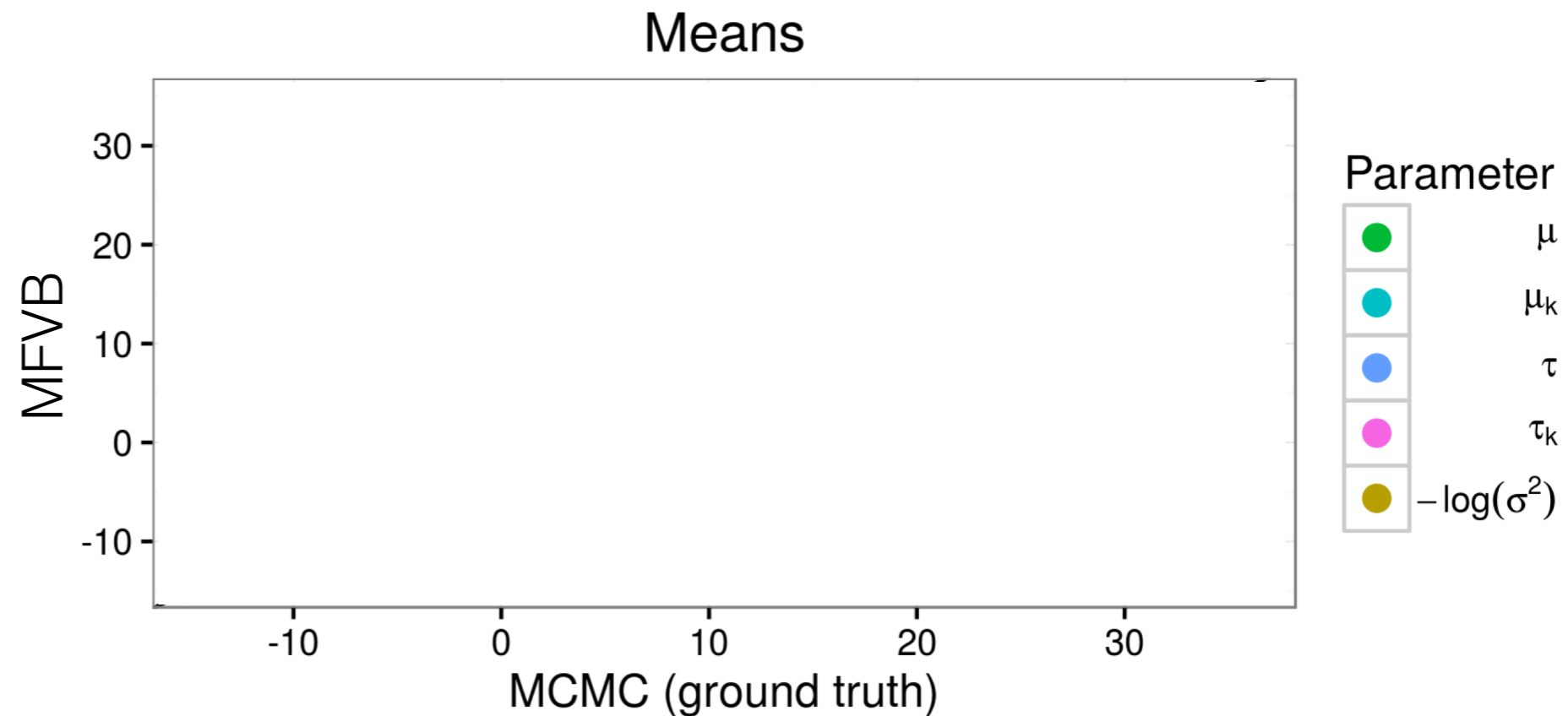
Microcredit

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



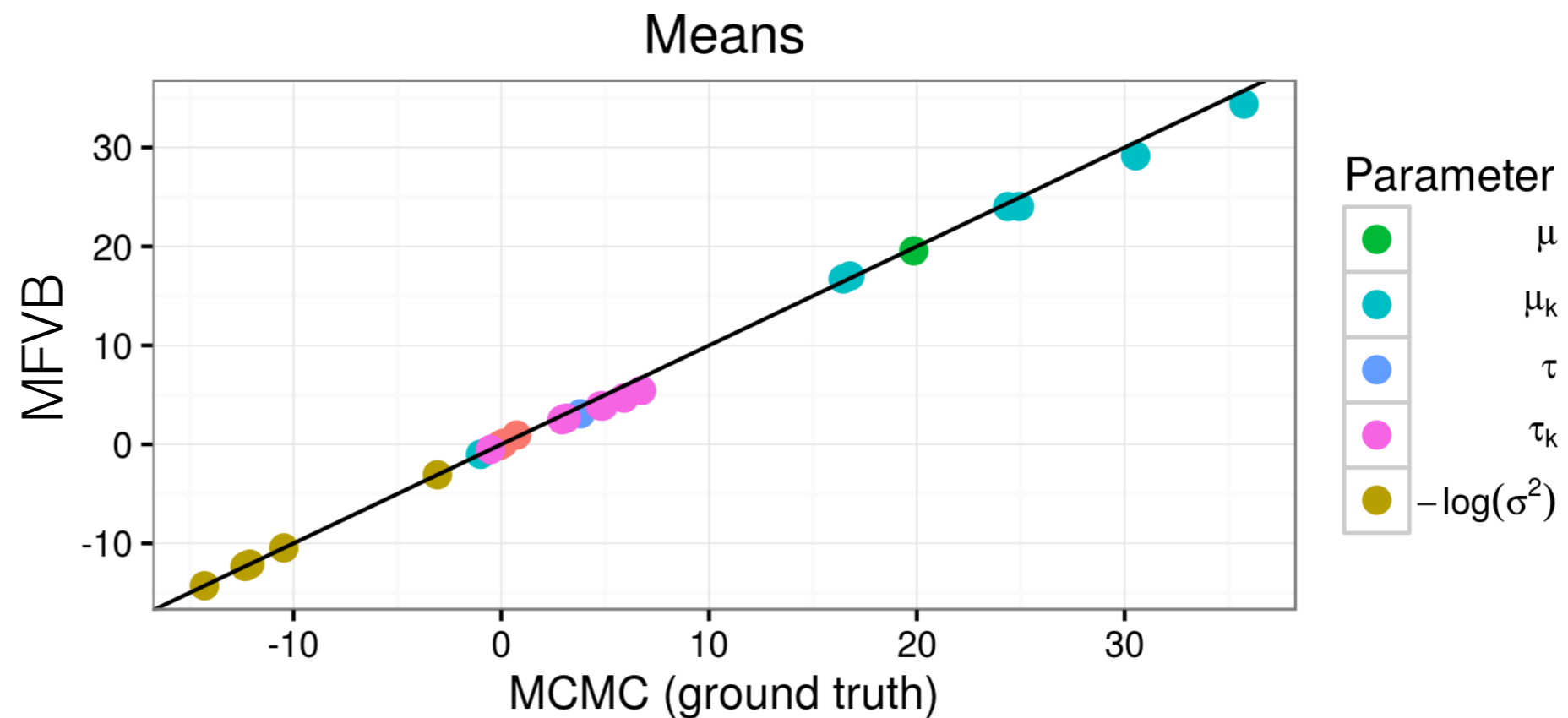
Microcredit

- *One set of 2500* MCMC draws:
45 minutes
- MFVB optimization:
<1 min



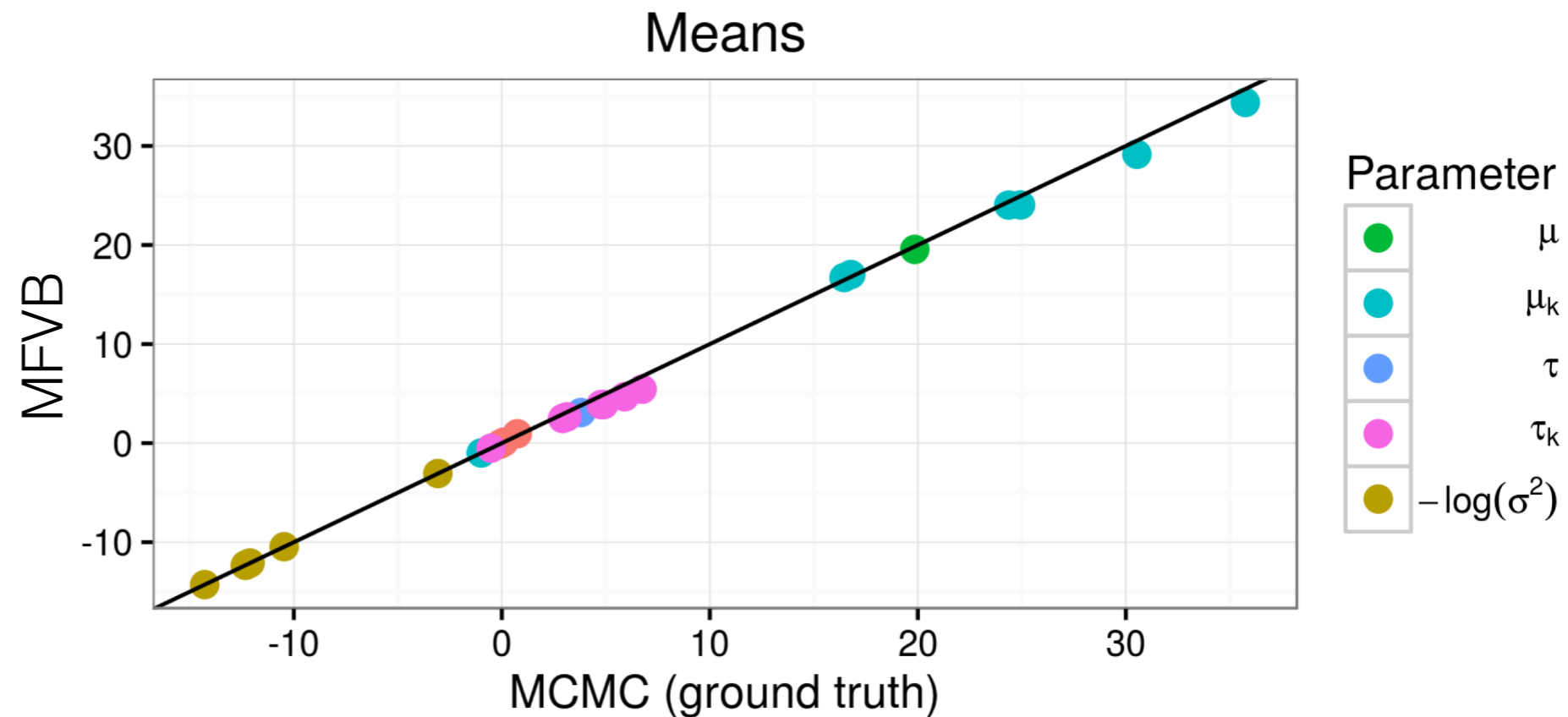
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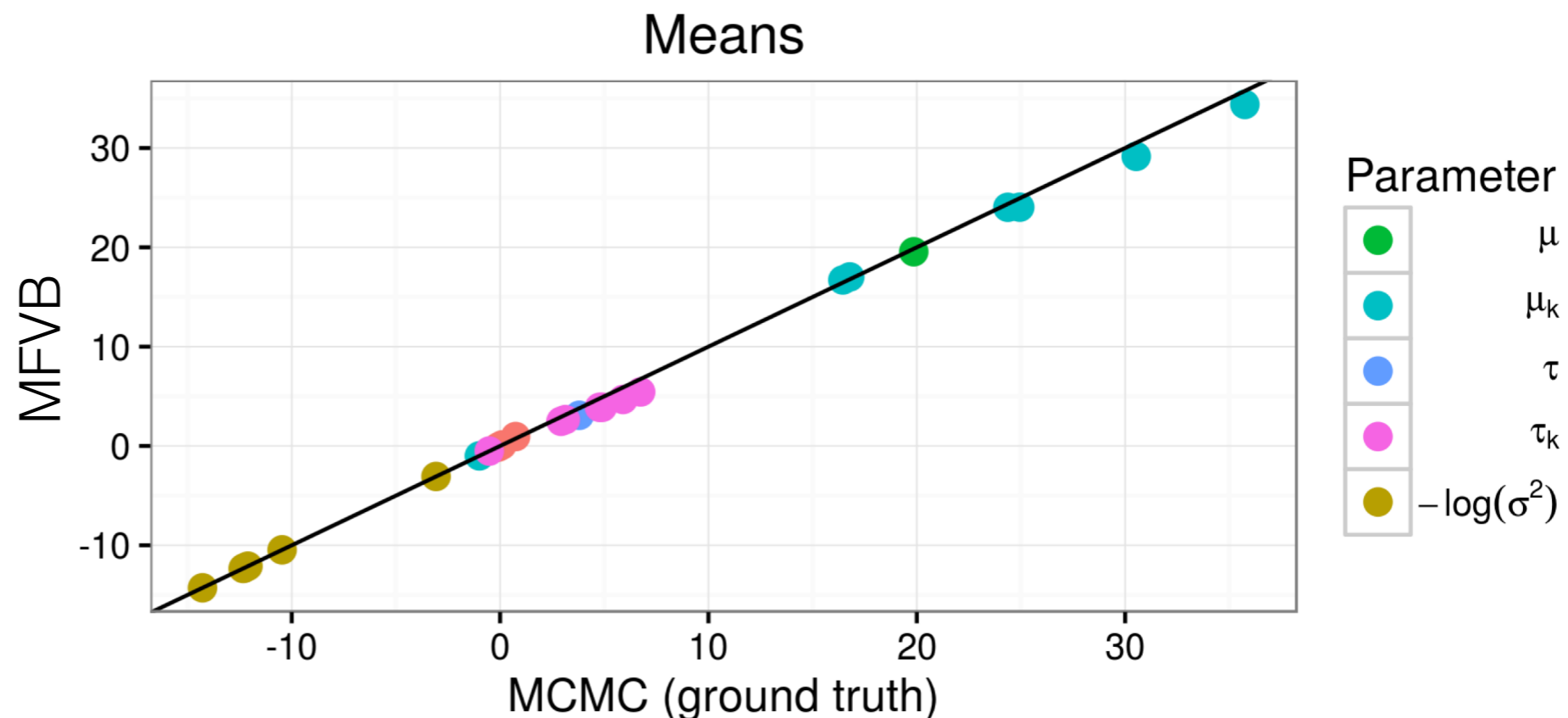


Criteo Online Ads Experiment

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

Microcredit

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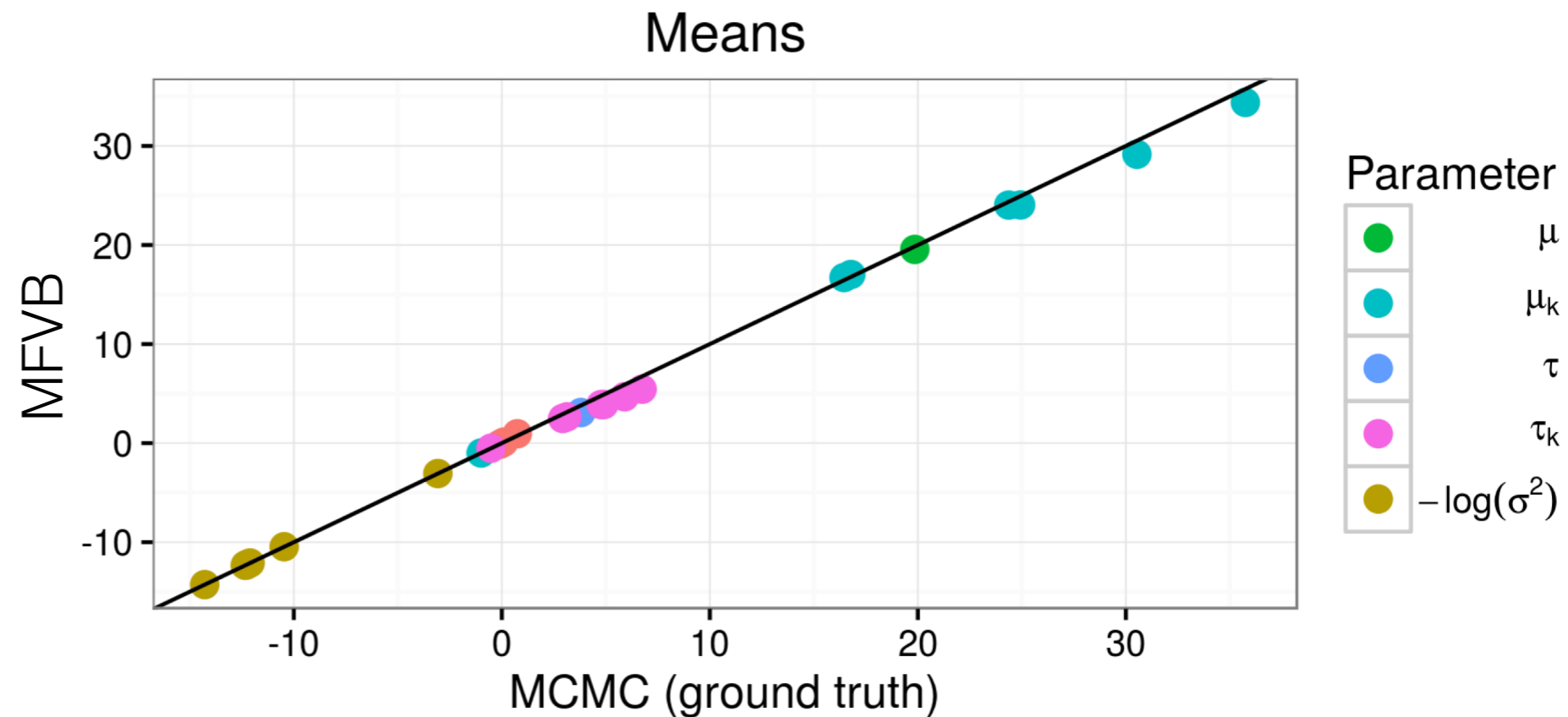


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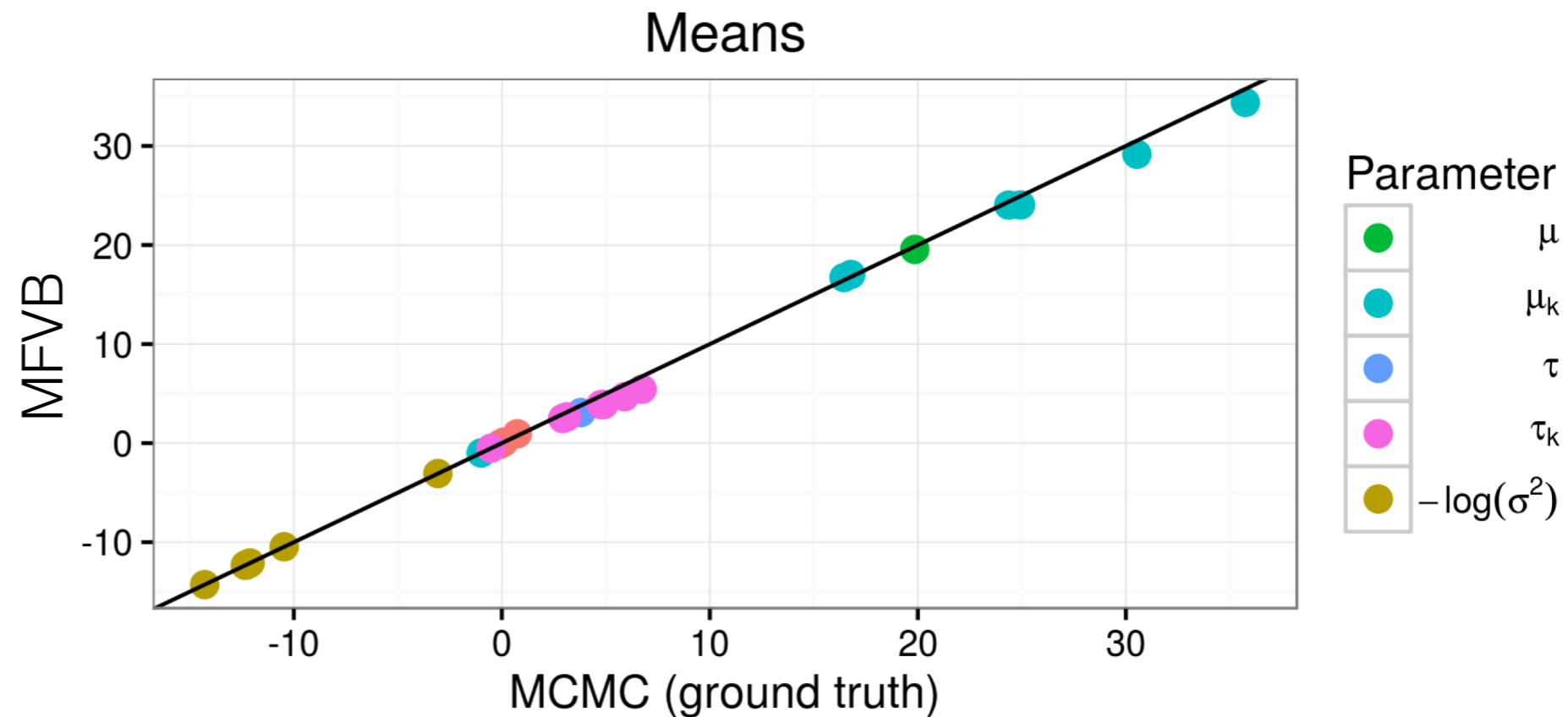


Criteo Online Ads Experiment

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- Logistic GLMM

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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

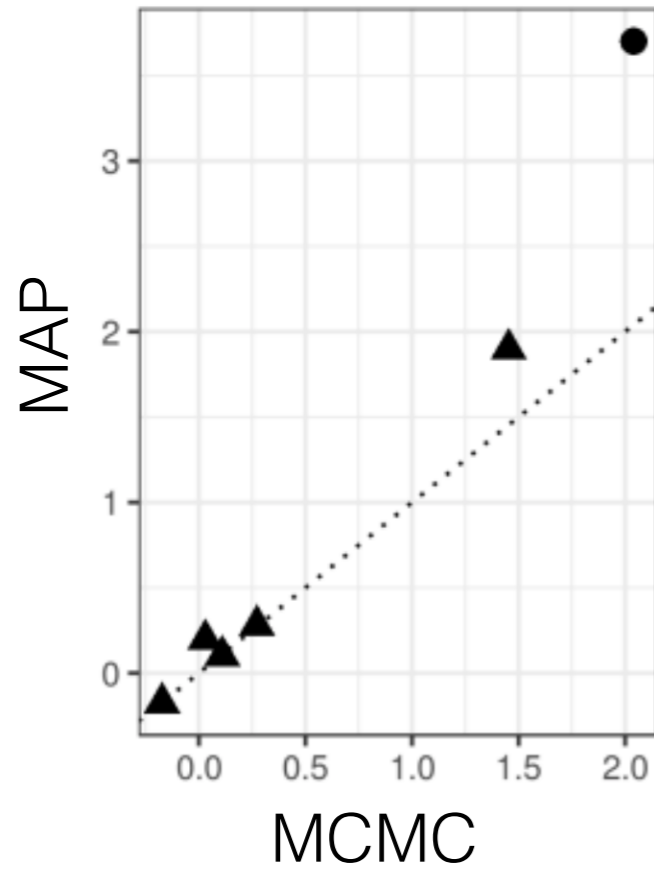
Criteo Online Ads Experiment

Criteo Online Ads Experiment

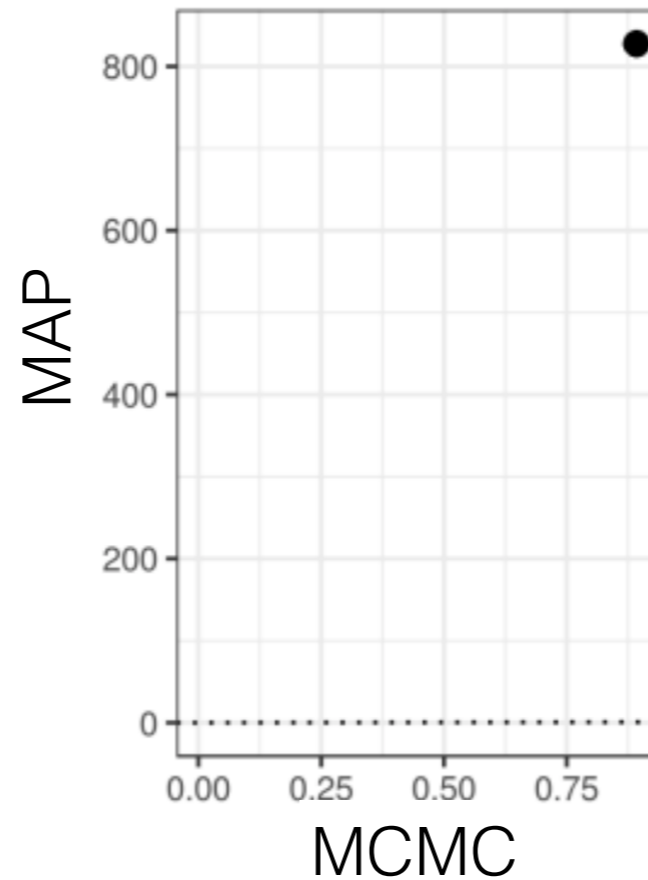
- MAP: **12 s**

Criteo Online Ads Experiment

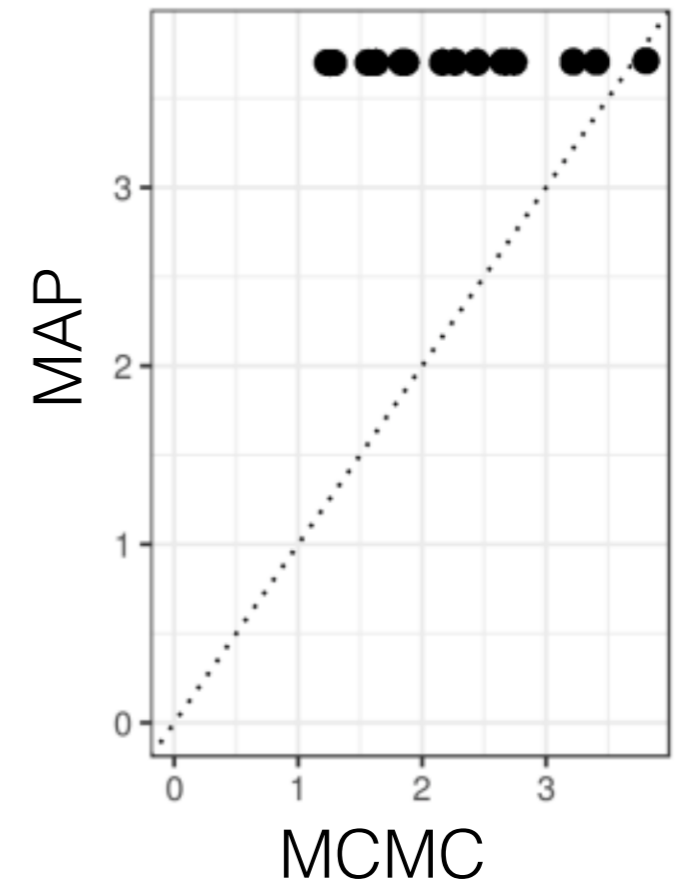
Global parameters ($-\tau$)



Global parameter τ



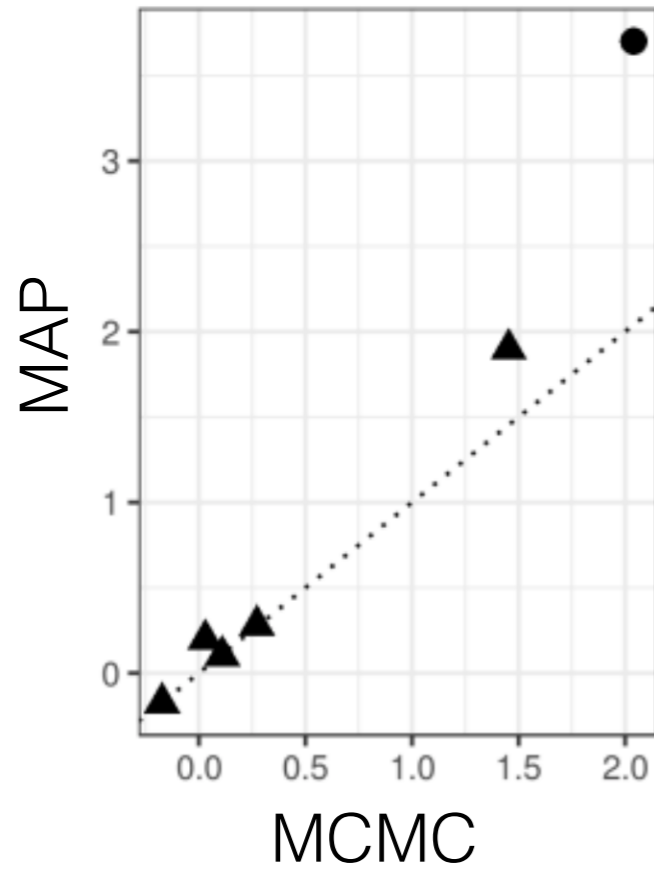
Local parameters



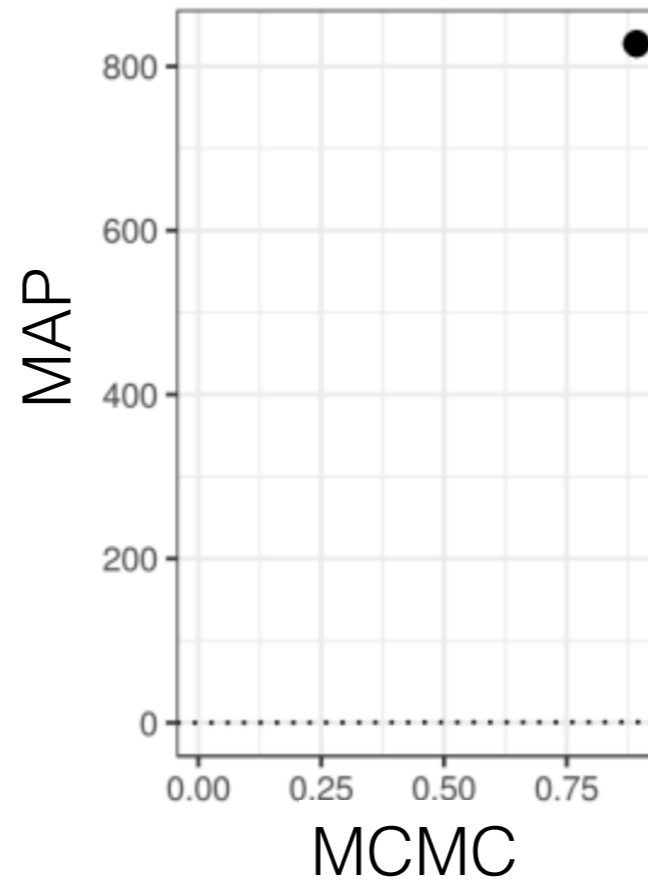
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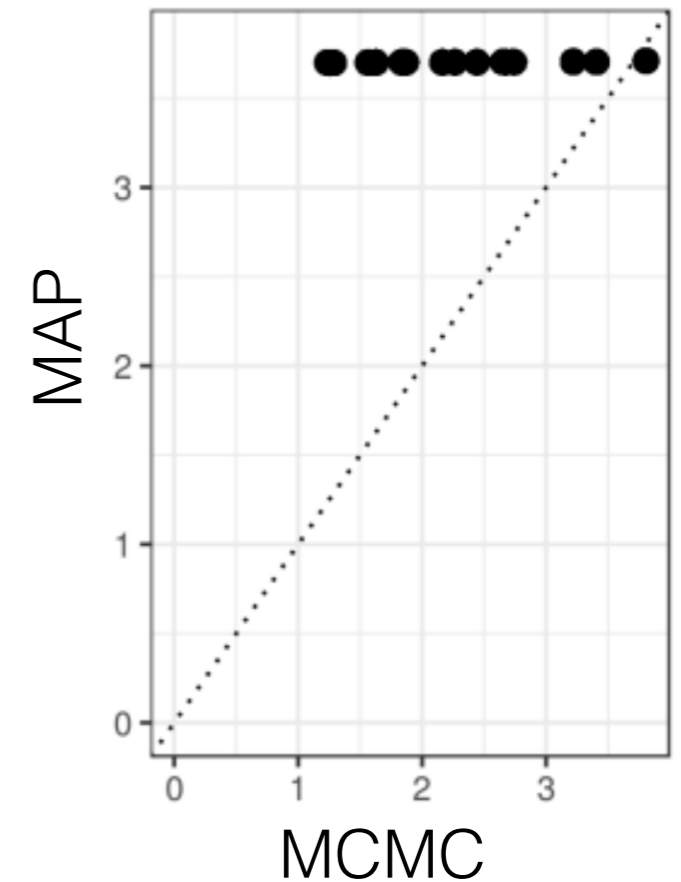
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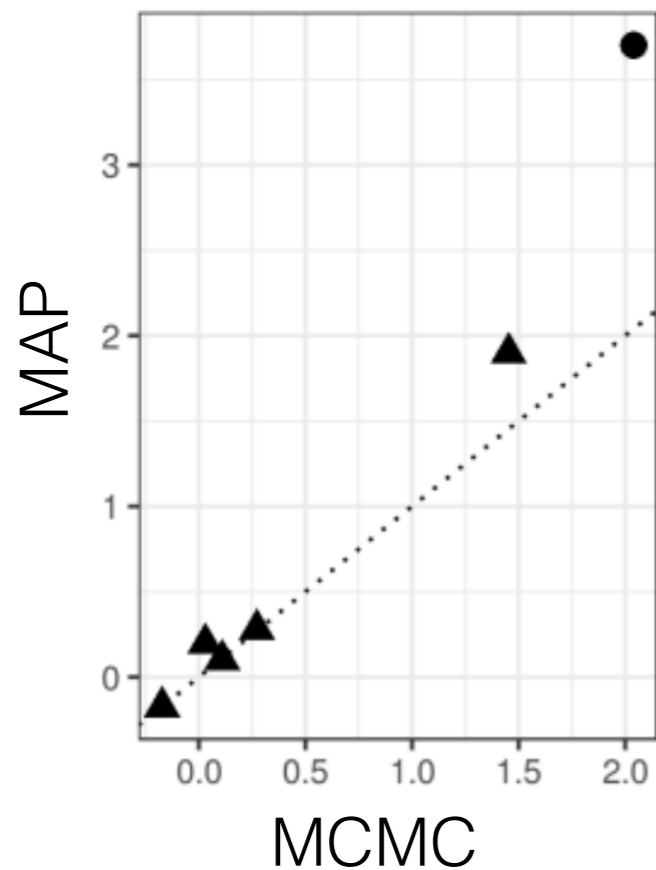
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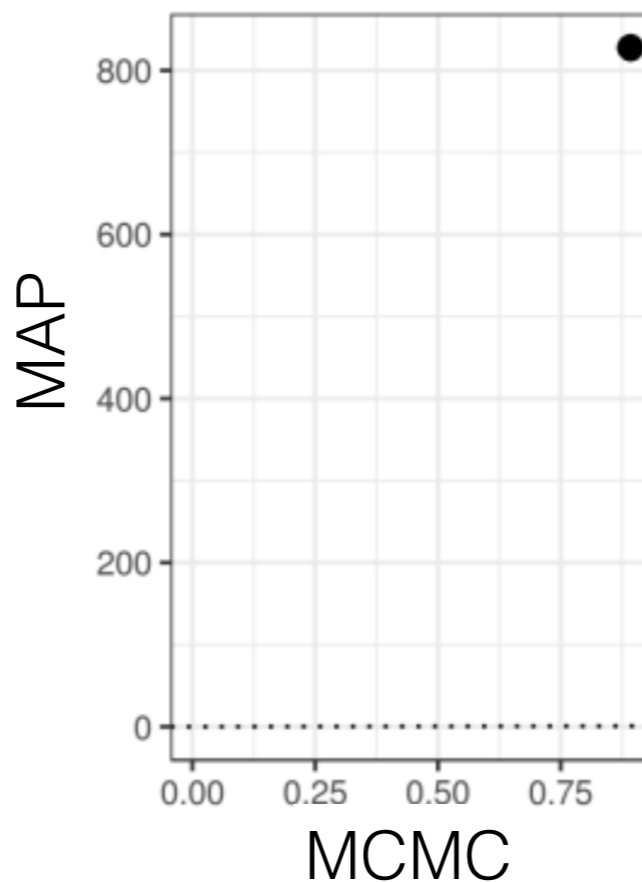
- MAP: **12 s**
- MFVB: **57 s**

Criteo Online Ads Experiment

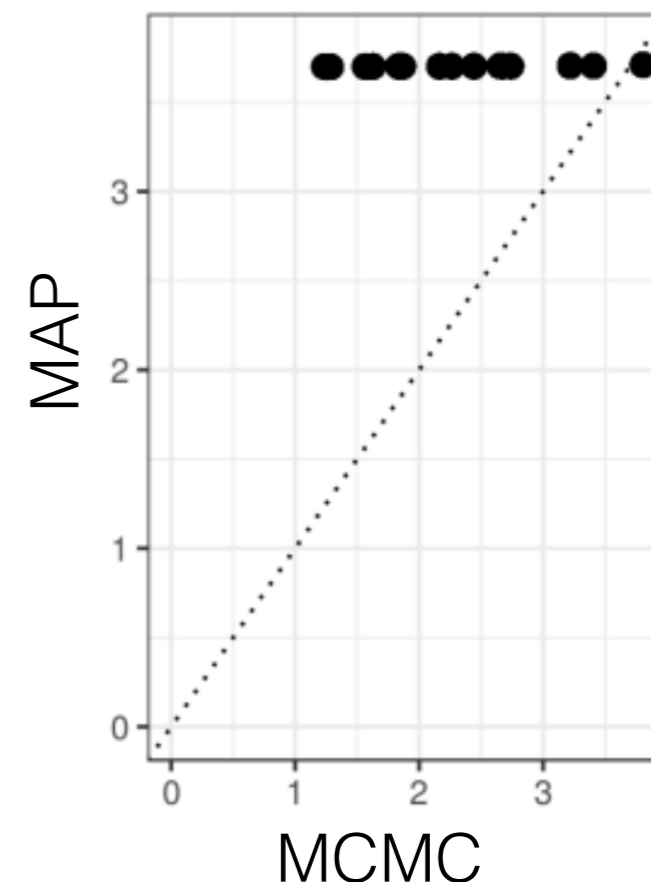
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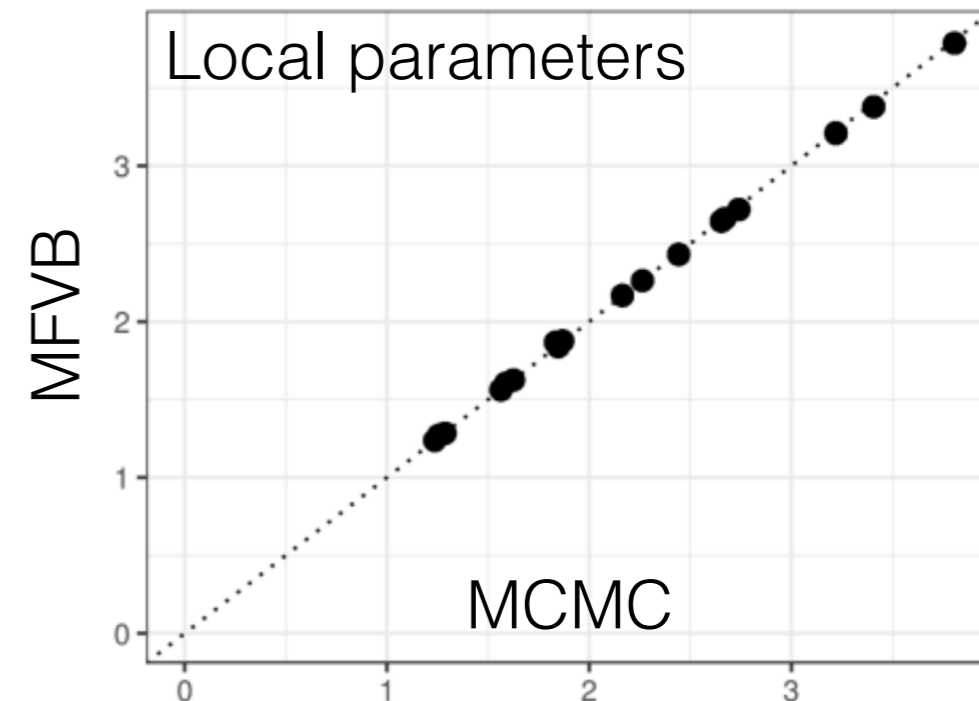
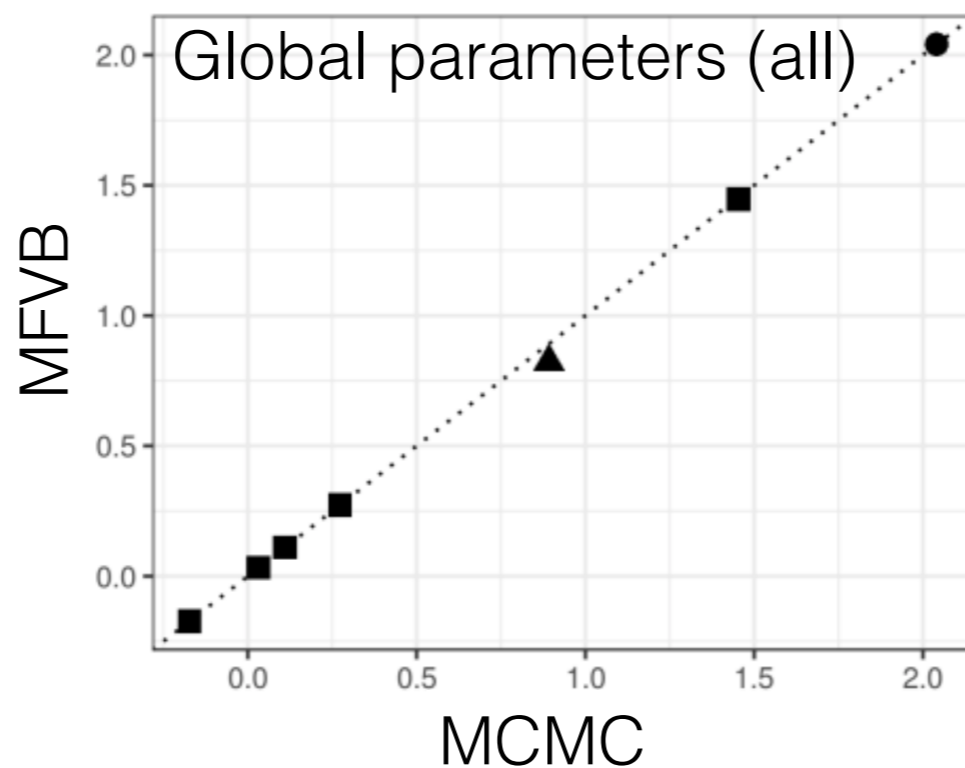
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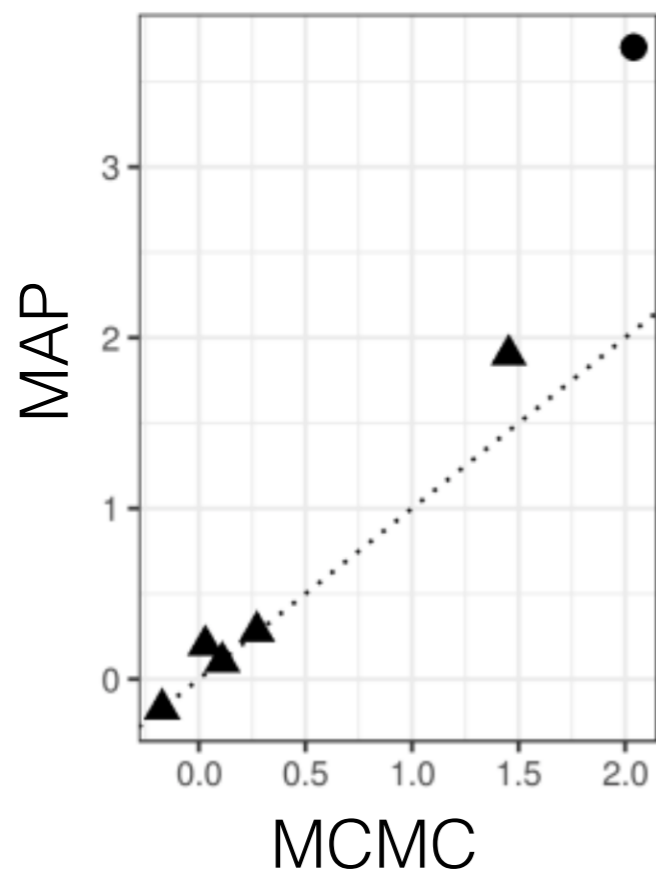
- MAP: **12 s**
- MFVB: **57 s**



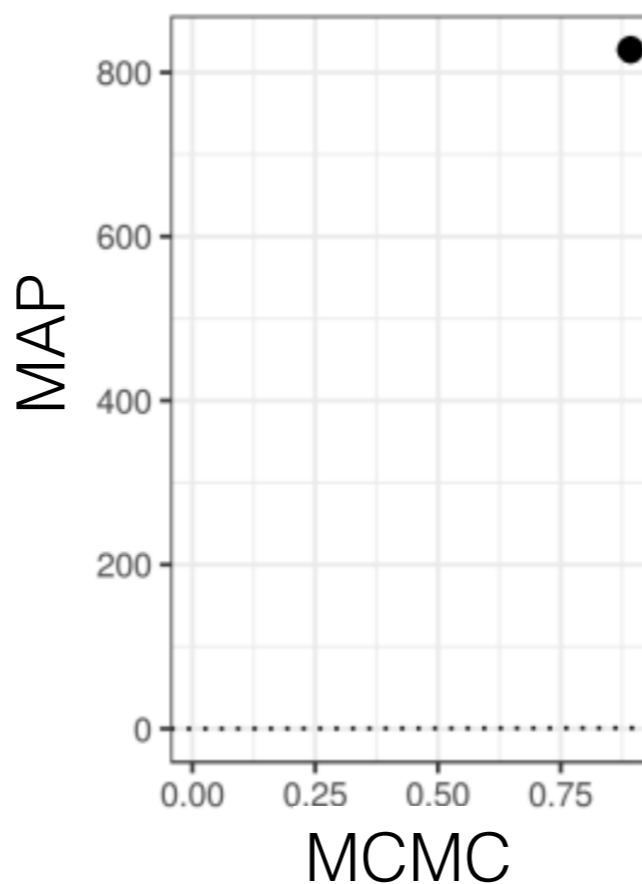
[Giordano, Broderick, Jordan 2018]

Criteo Online Ads Experiment

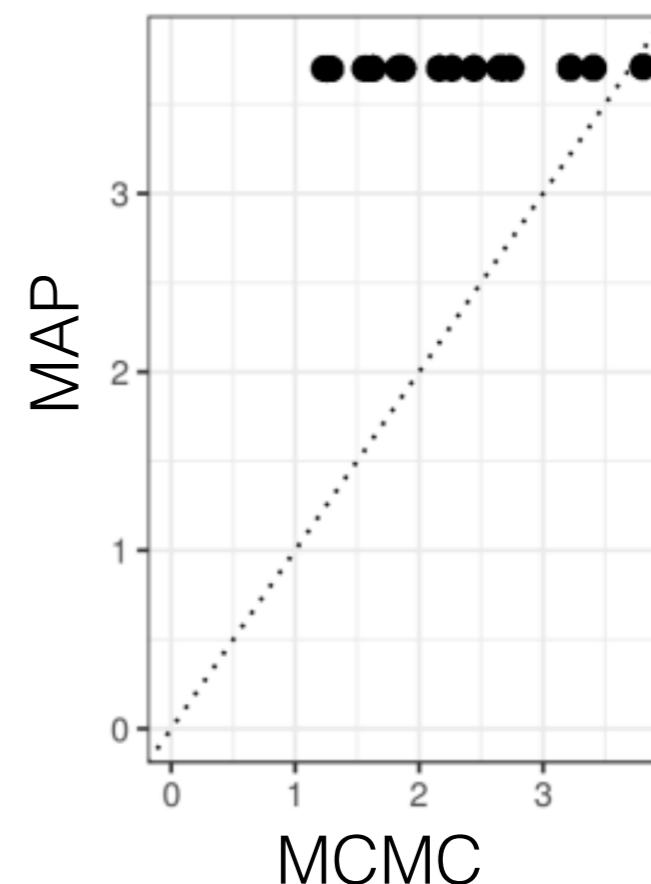
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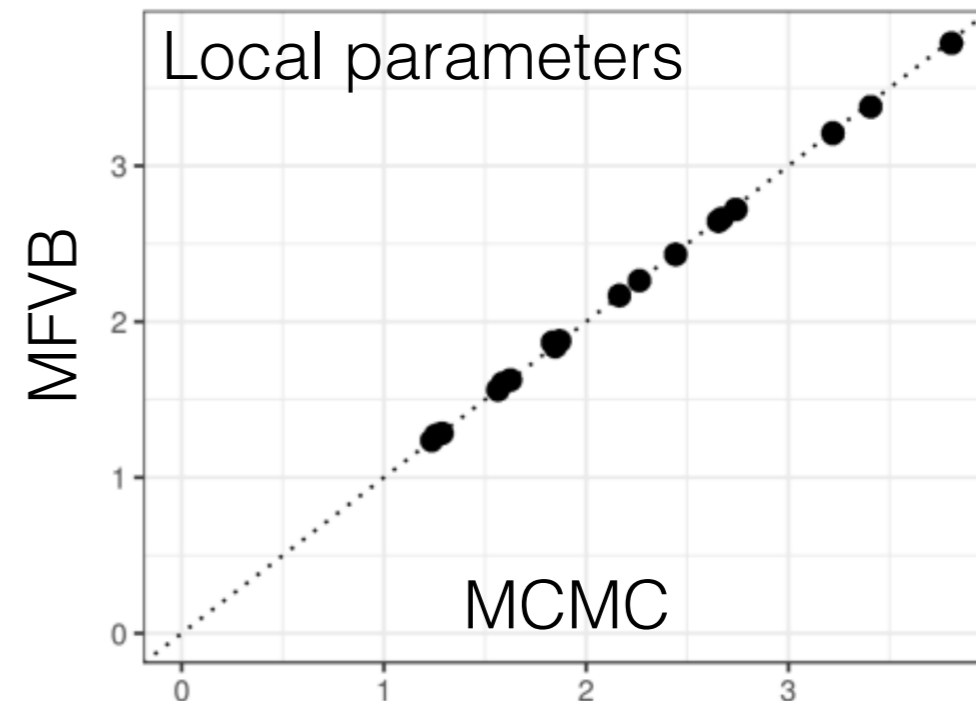
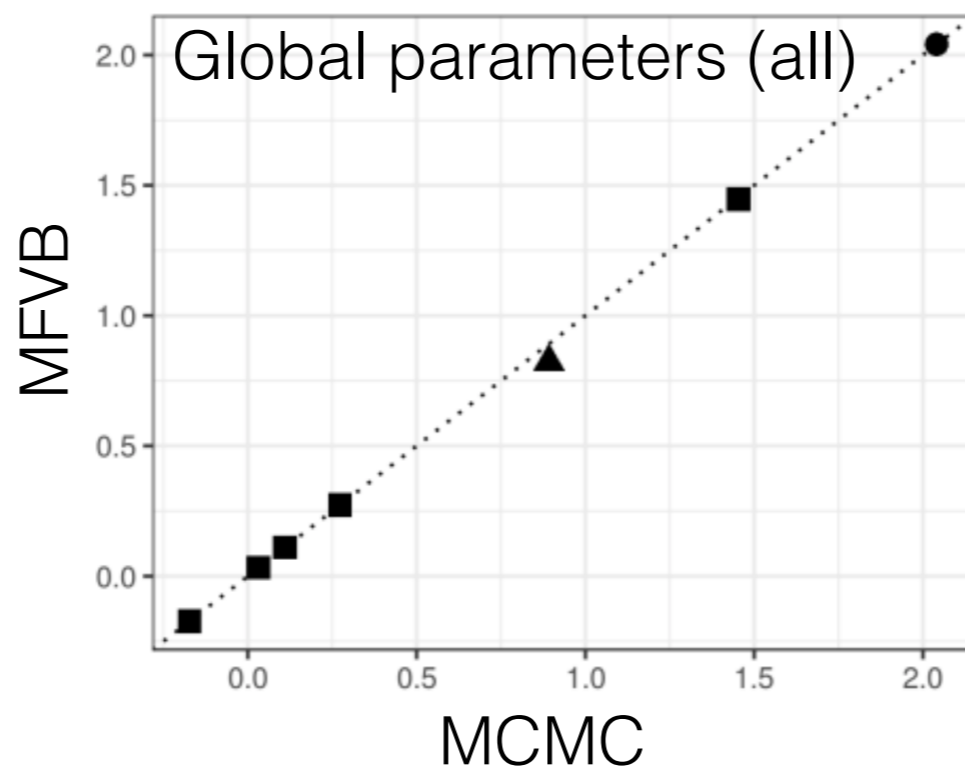
Global parameter τ



Local parameters



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



Why use MFVB?

- Topic discovery

“Arts”	“Budgets”	“Children”	“Education”
NEW	MILLION	CHILDREN	SCHOOL
FILM	TAX	WOMEN	STUDENTS
SHOW	PROGRAM	PEOPLE	SCHOOLS
MUSIC	BUDGET	CHILD	EDUCATION
MOVIE	BILLION	YEARS	TEACHERS
PLAY	FEDERAL	FAMILIES	HIGH
MUSICAL	YEAR	WORK	PUBLIC
BEST	SPENDING	PARENTS	TEACHER
ACTOR	NEW	SAYS	BENNETT
FIRST	STATE	FAMILY	MANIGAT
YORK	PLAN	WELFARE	NAMPHY
OPERA	MONEY	MEN	STATE
THEATER	PROGRAMS	PERCENT	PRESIDENT
ACTRESS	GOVERNMENT	CARE	ELEMENTARY
LOVE	CONGRESS	LIFE	HAITI

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.

Why use MFVB?

- Topic discovery
- Latent Dirichlet allocation (LDA)

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- Topic discovery
- Latent Dirichlet allocation (LDA): 31,000+ citations

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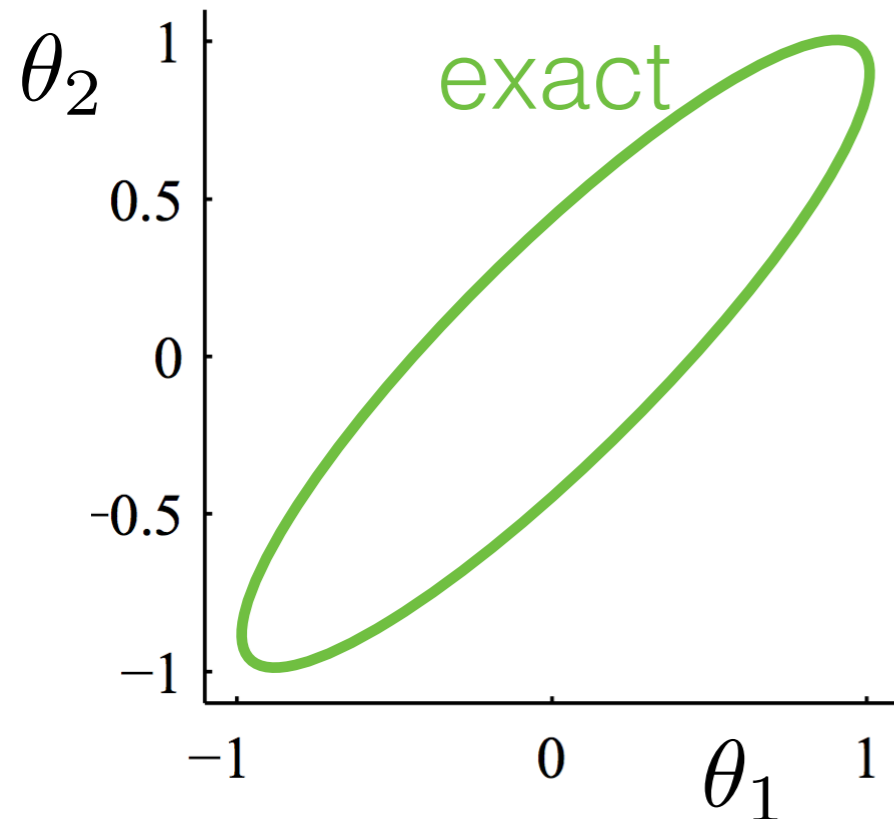
$$KL(q||p(\cdot|y)) = \int_{\theta} q(\theta) \log \frac{q(\theta)}{p(\theta|y)} d\theta$$

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

What about uncertainty?

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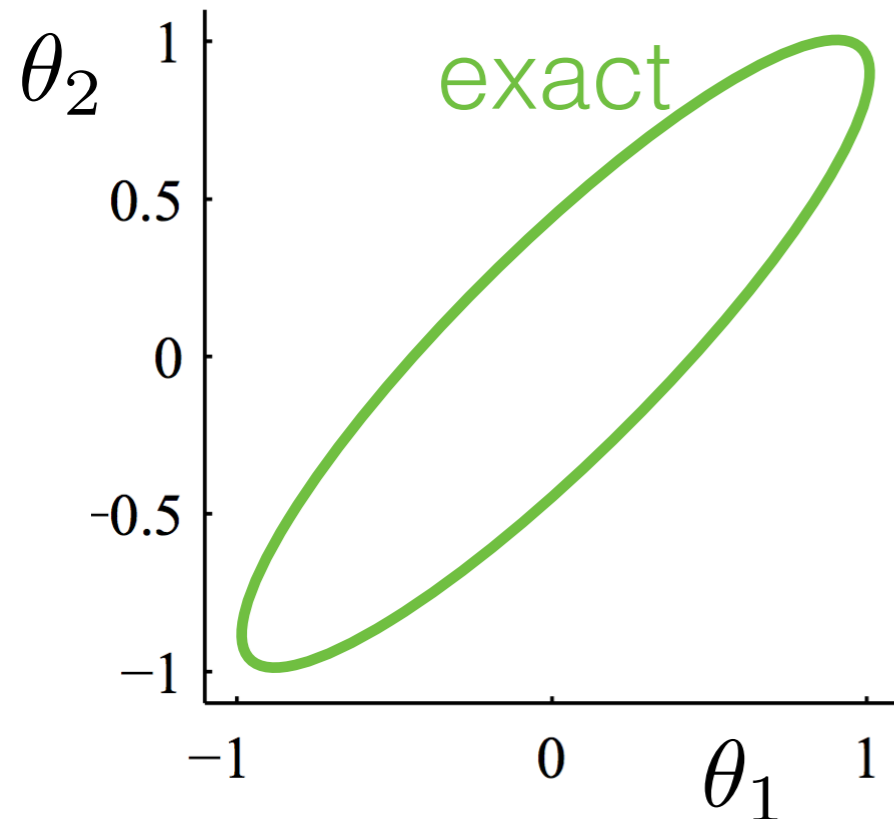


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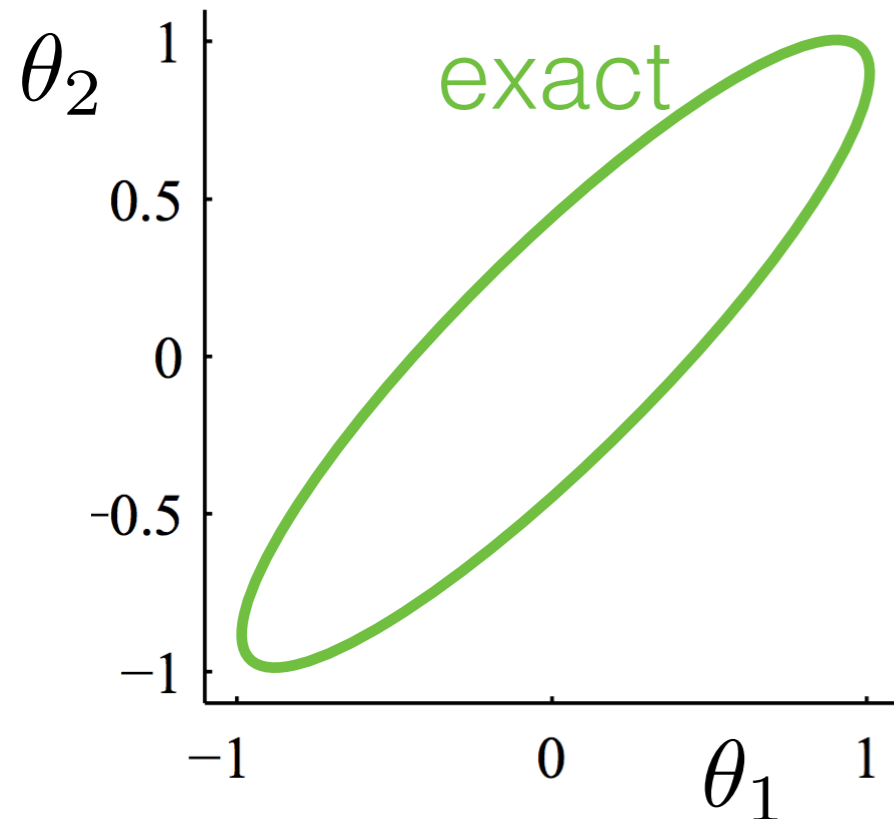
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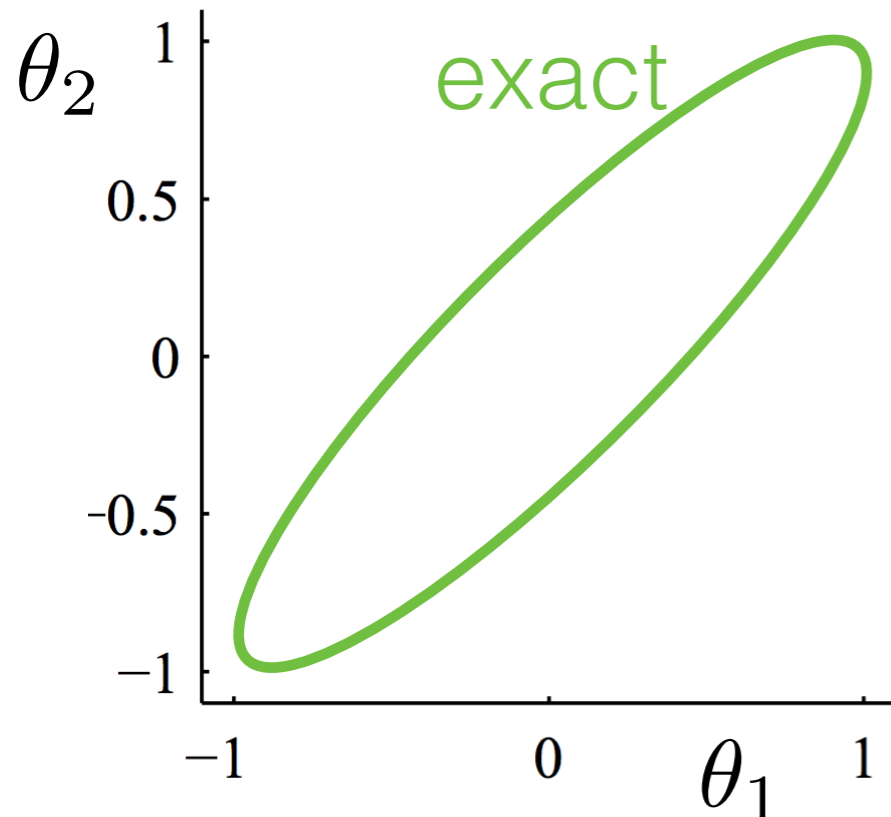
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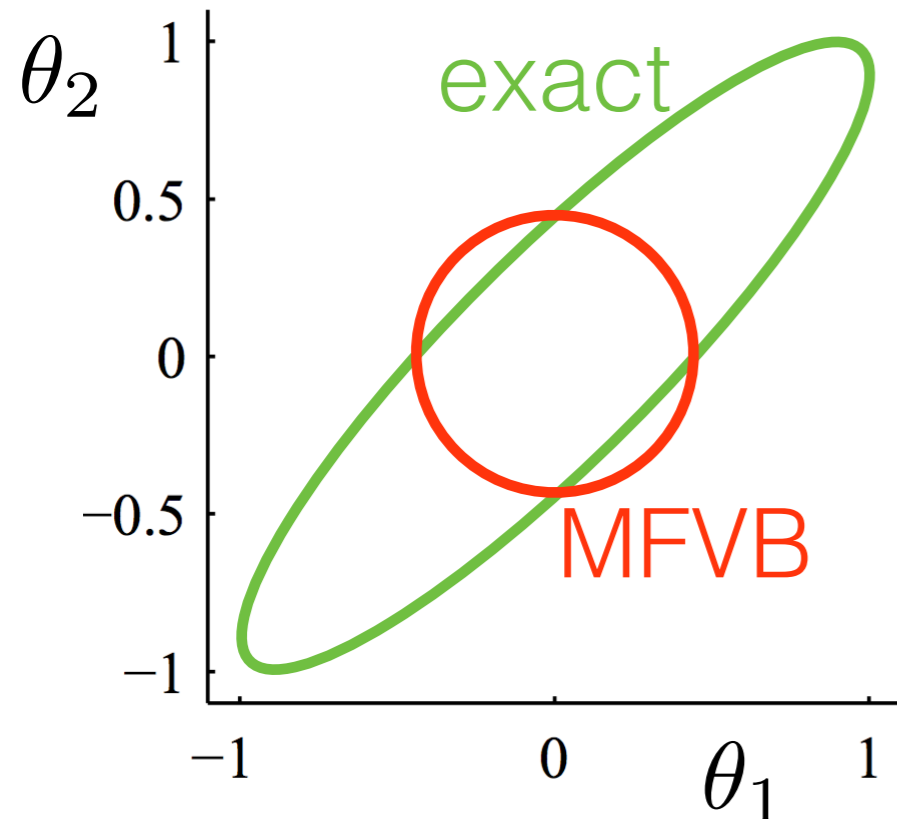
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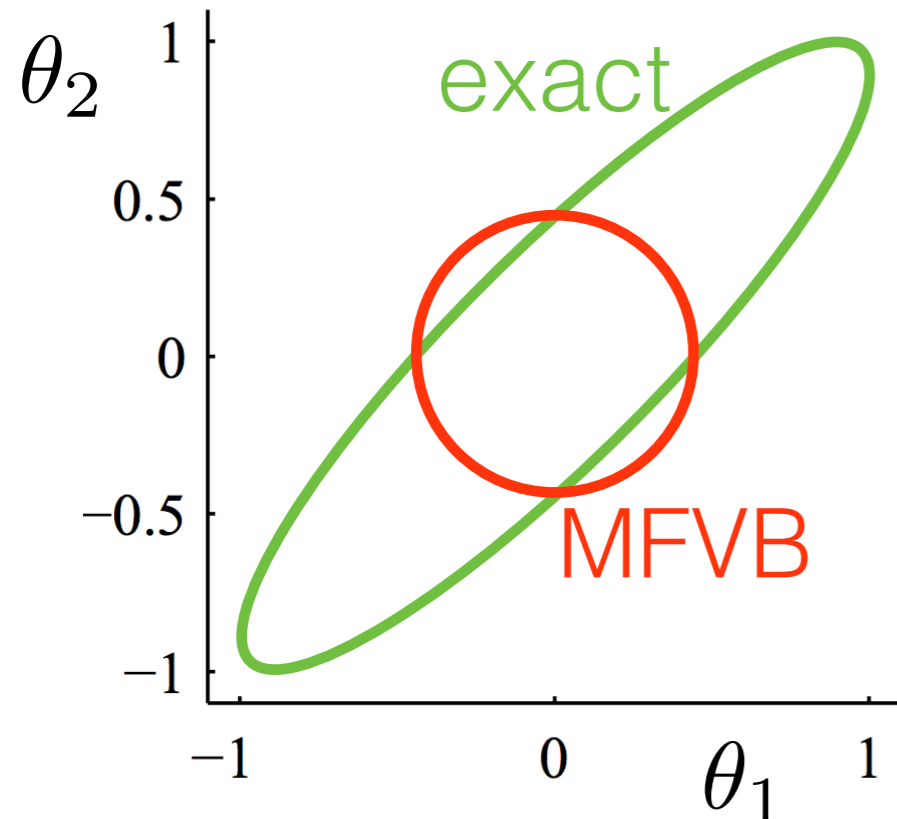
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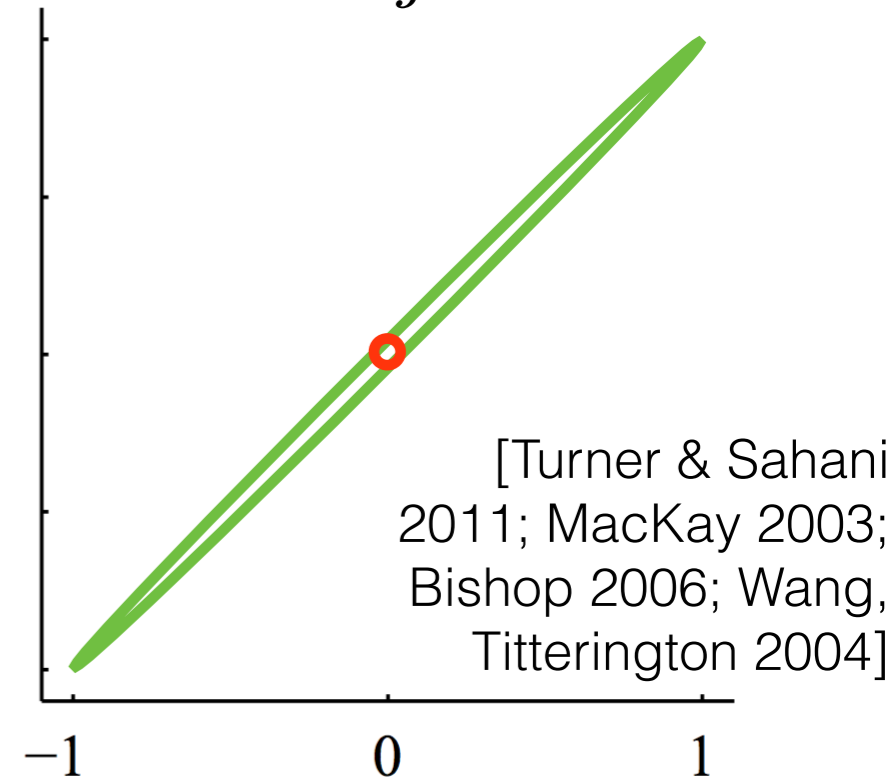
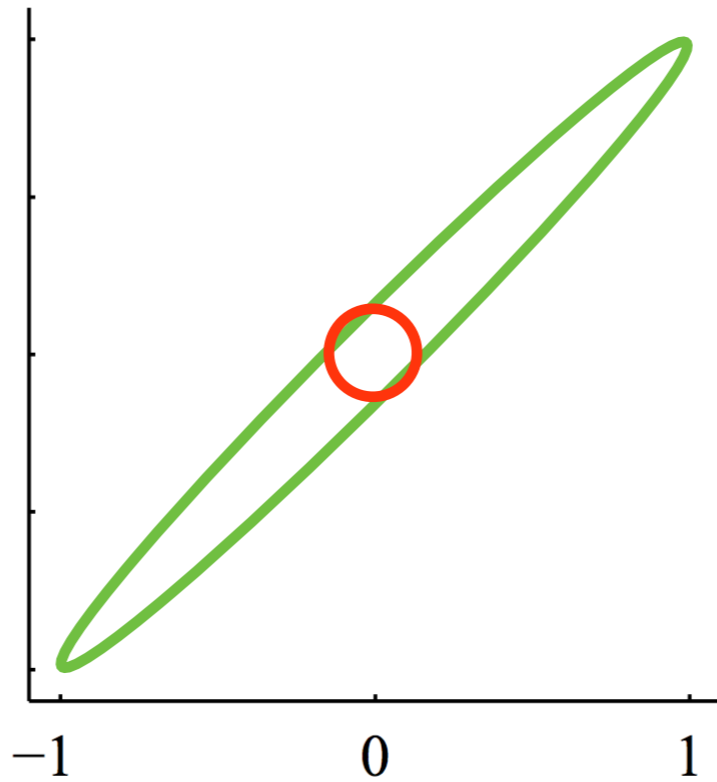
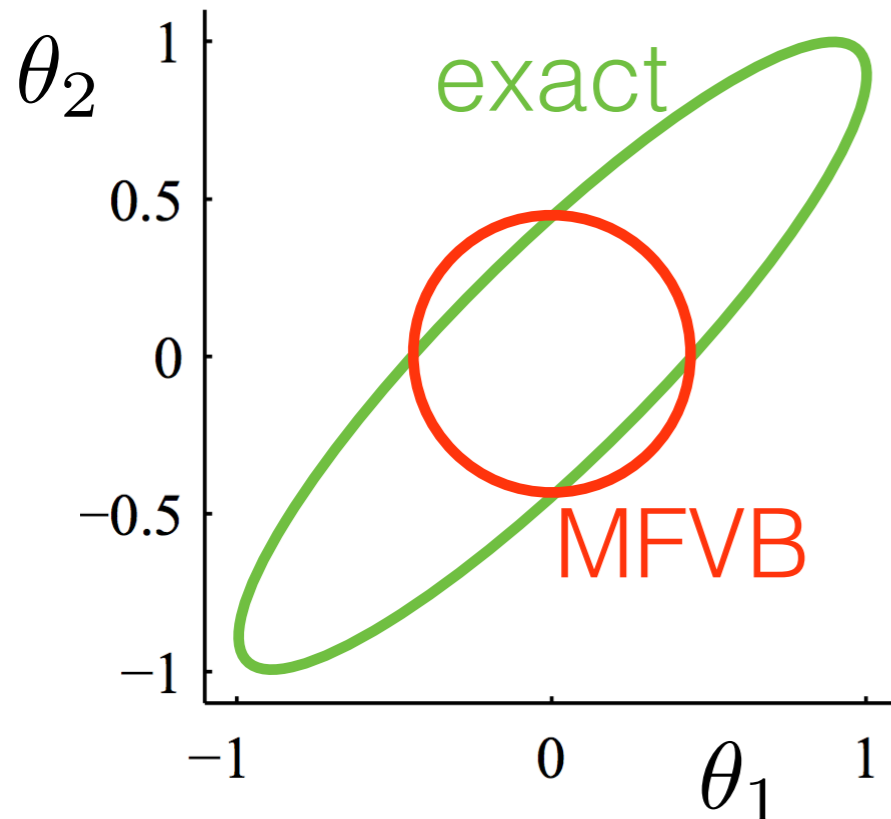
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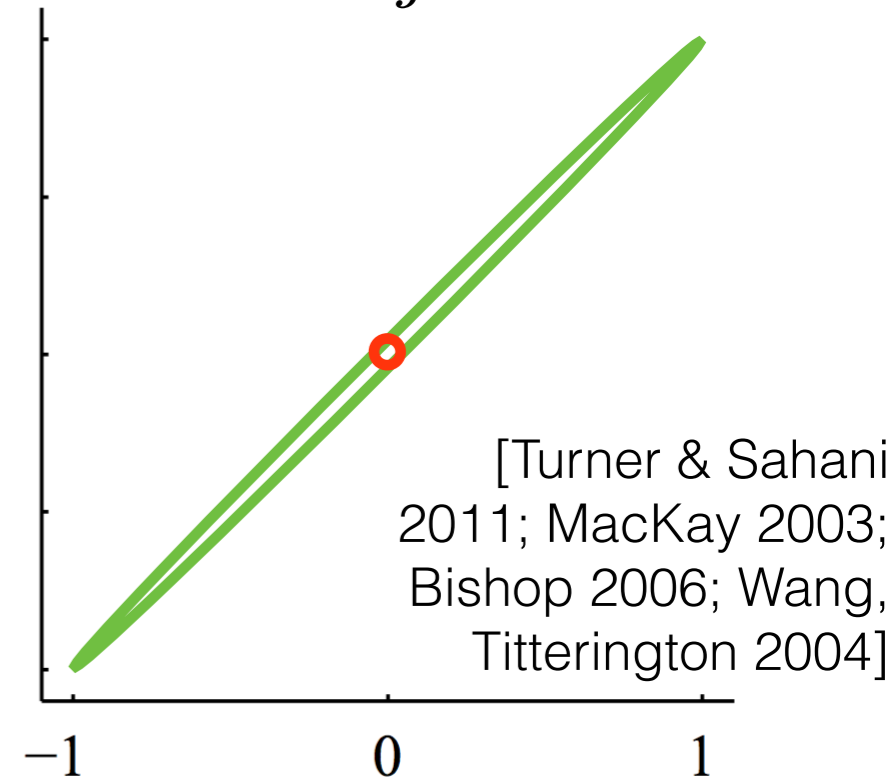
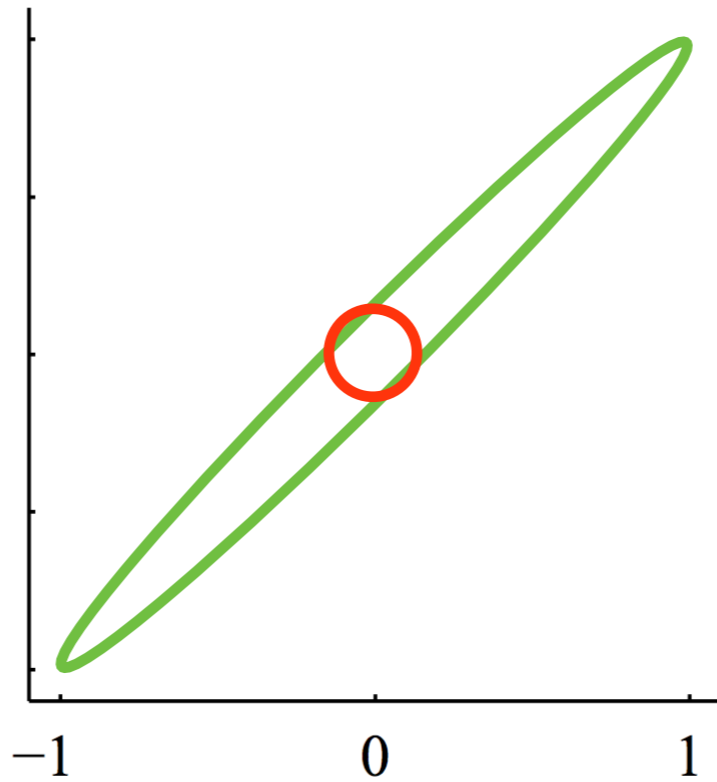
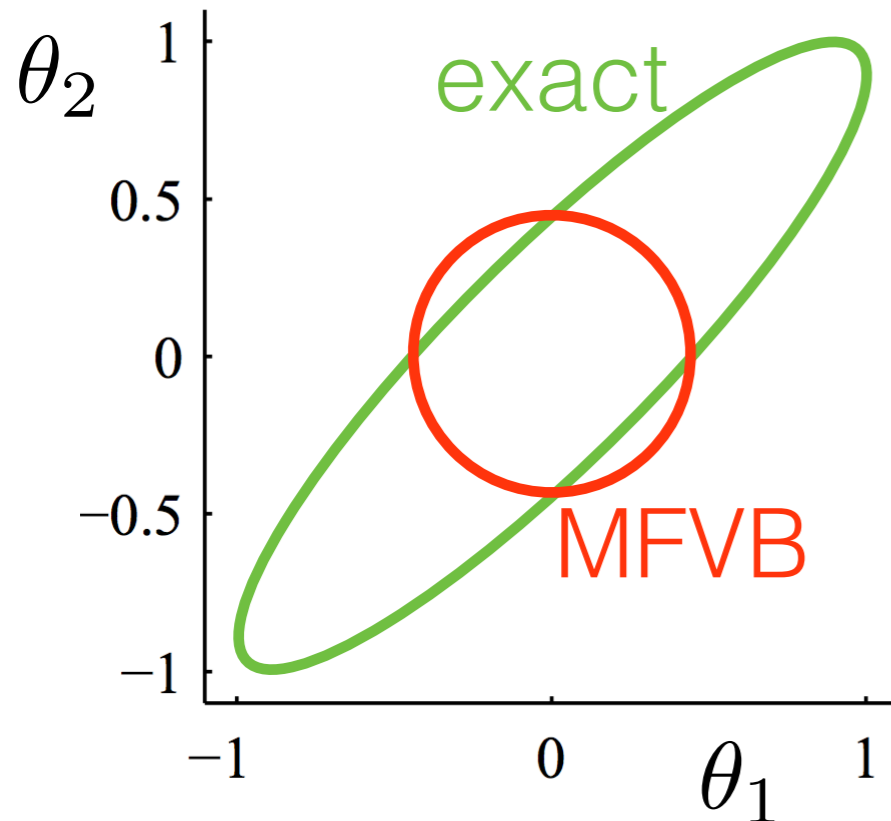
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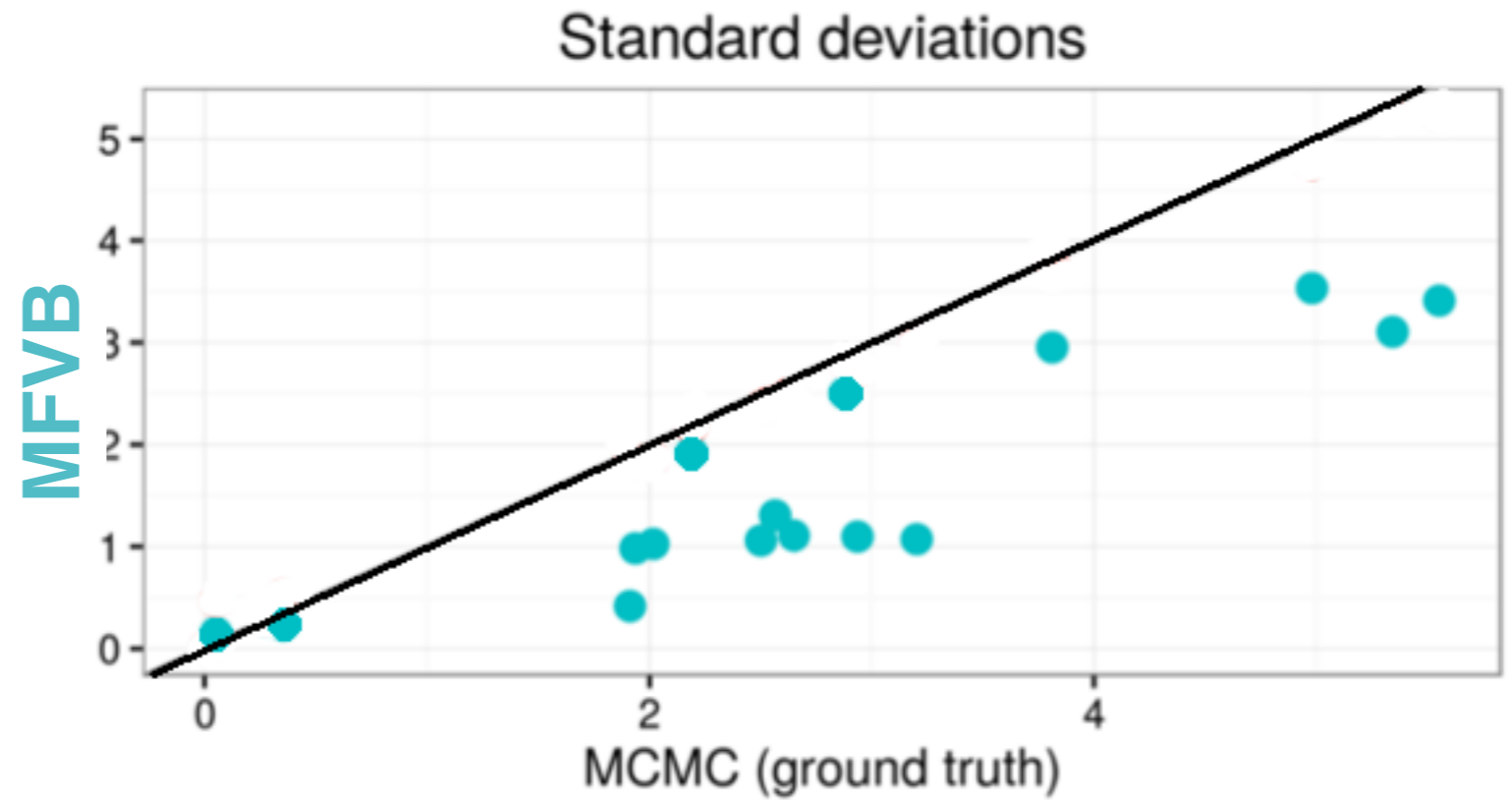
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What about uncertainty?

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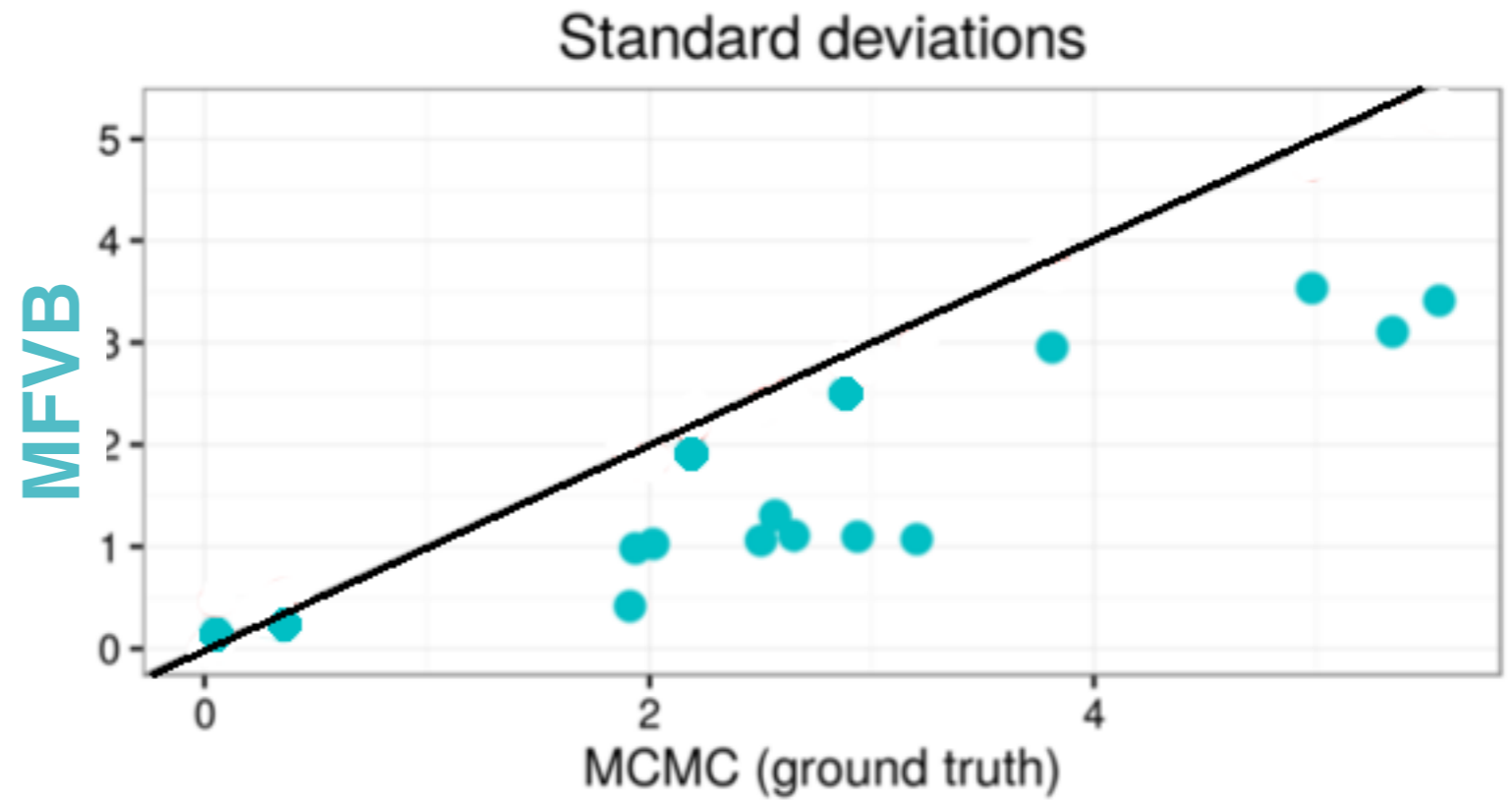
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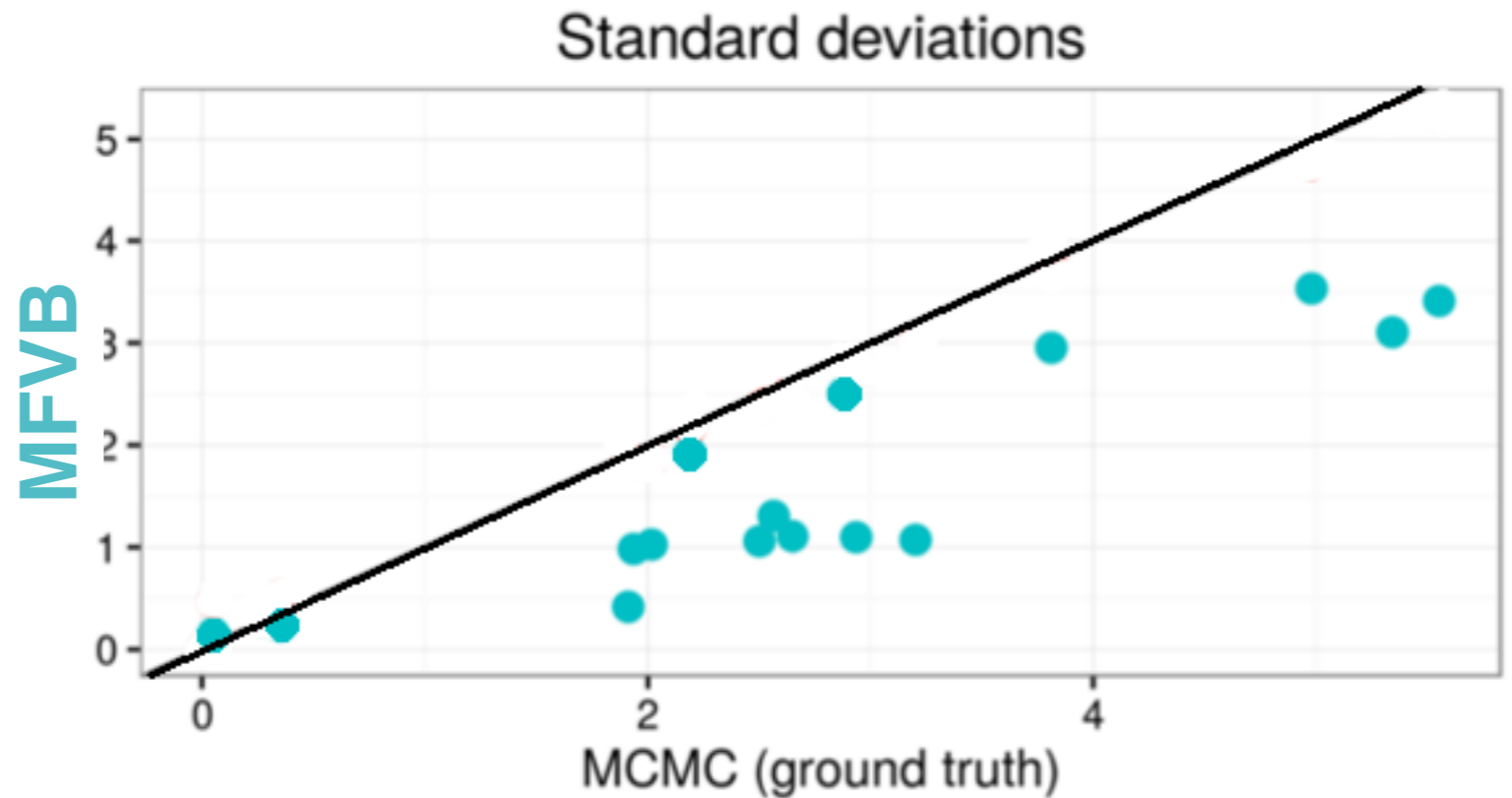
What about uncertainty?

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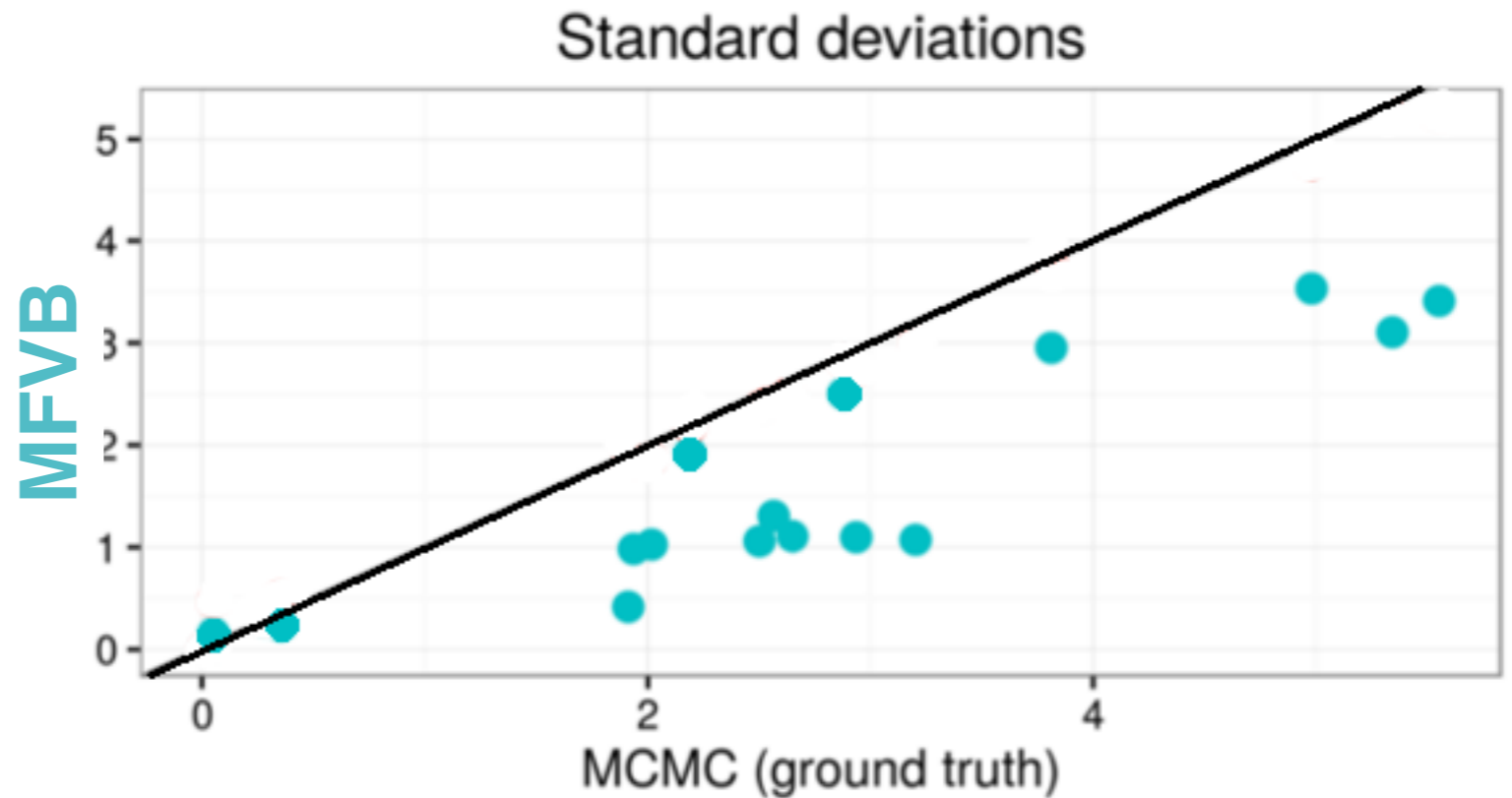
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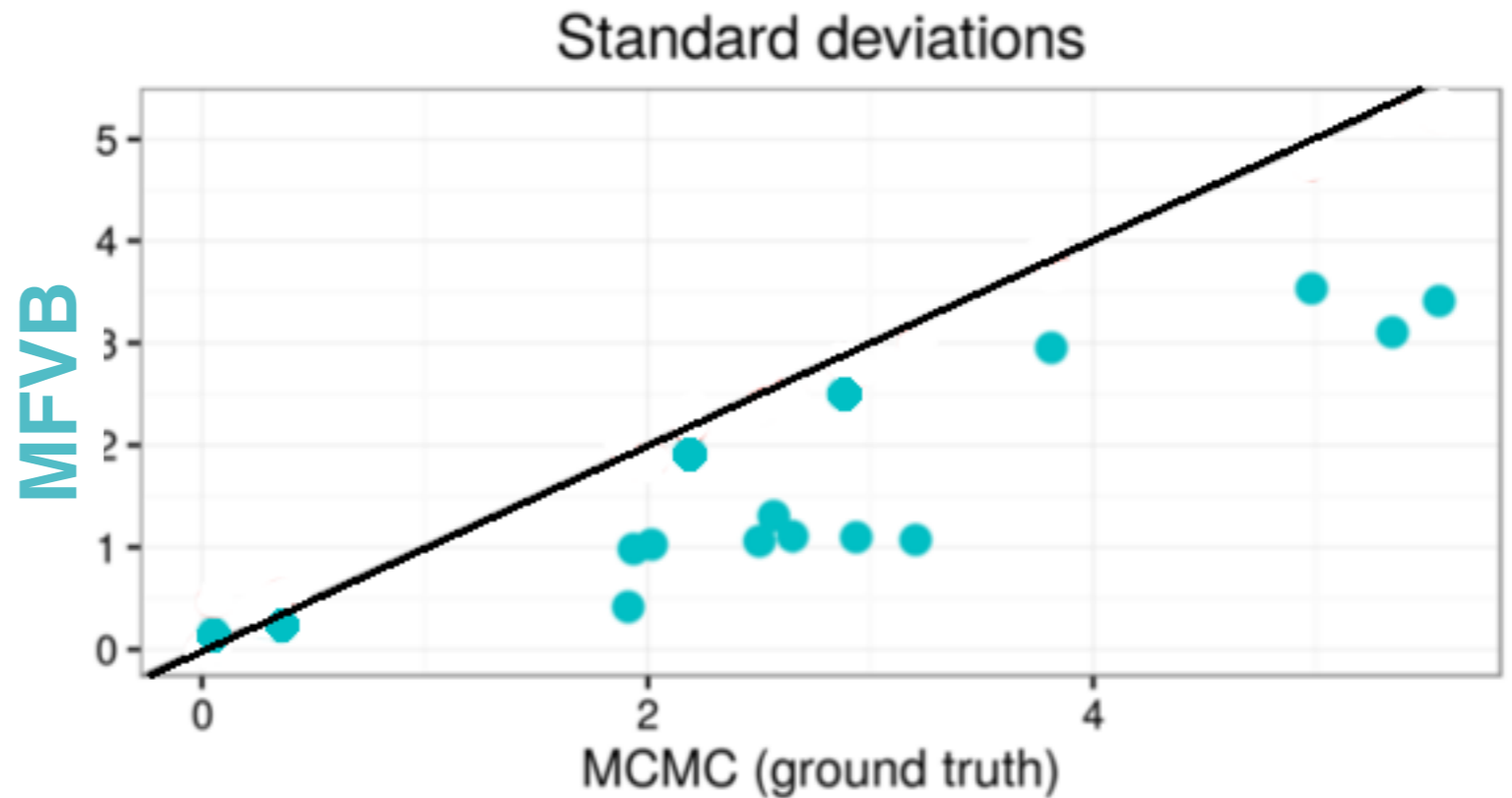
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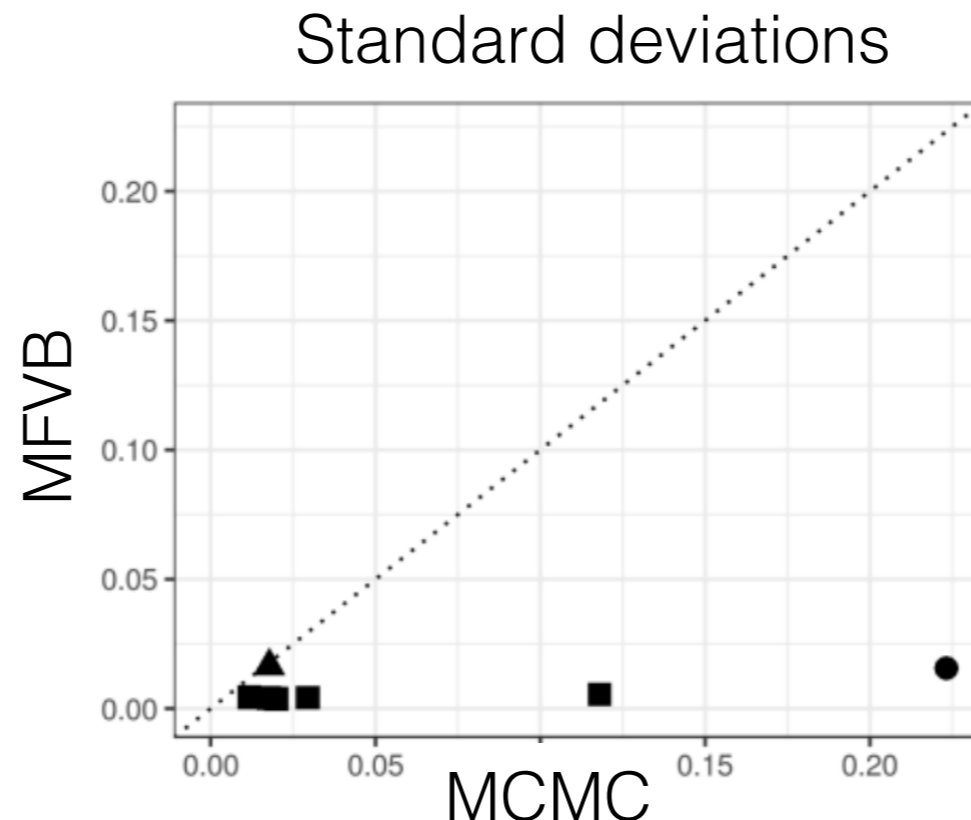


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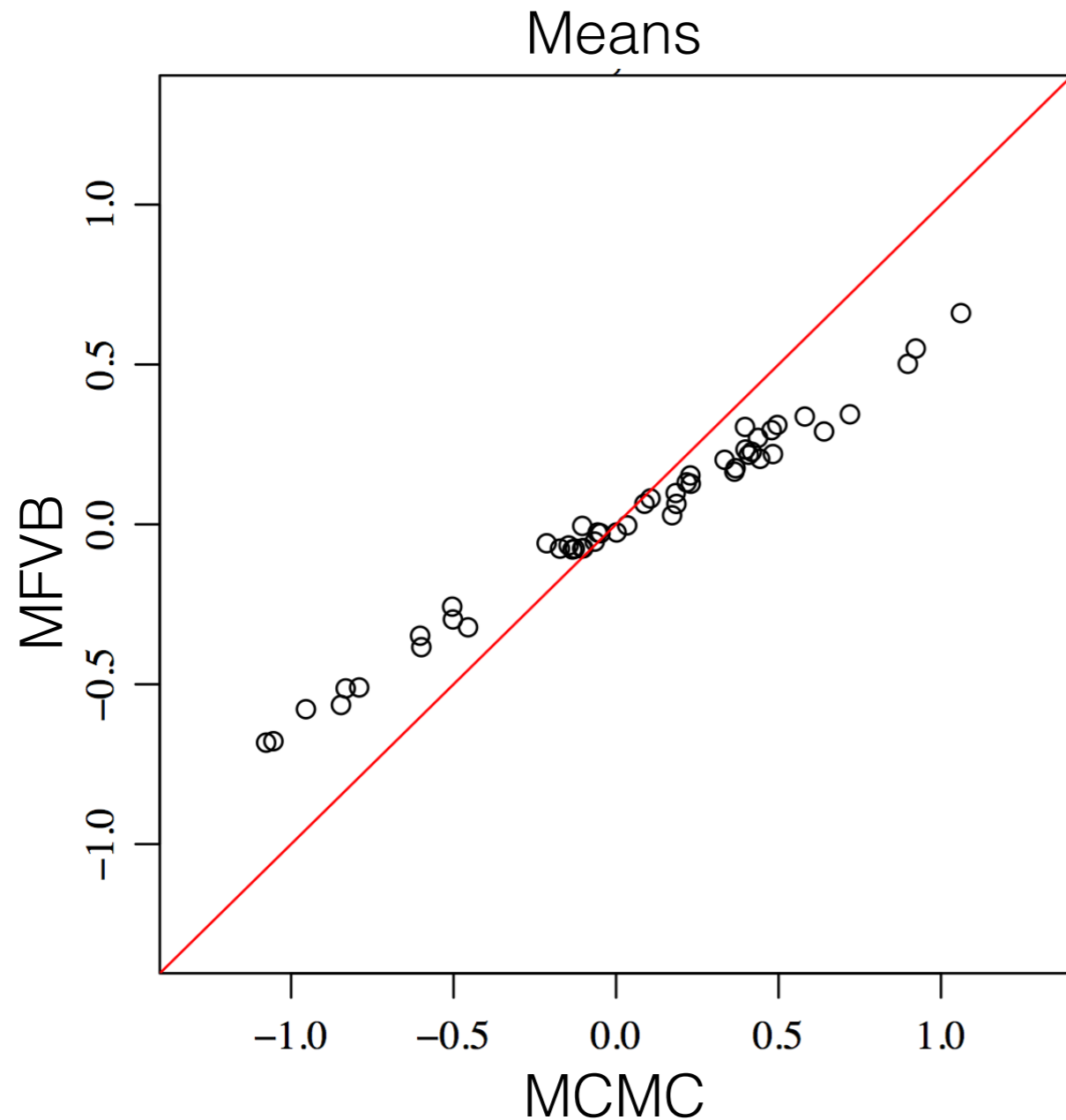


- Criteo
online ads
experiment



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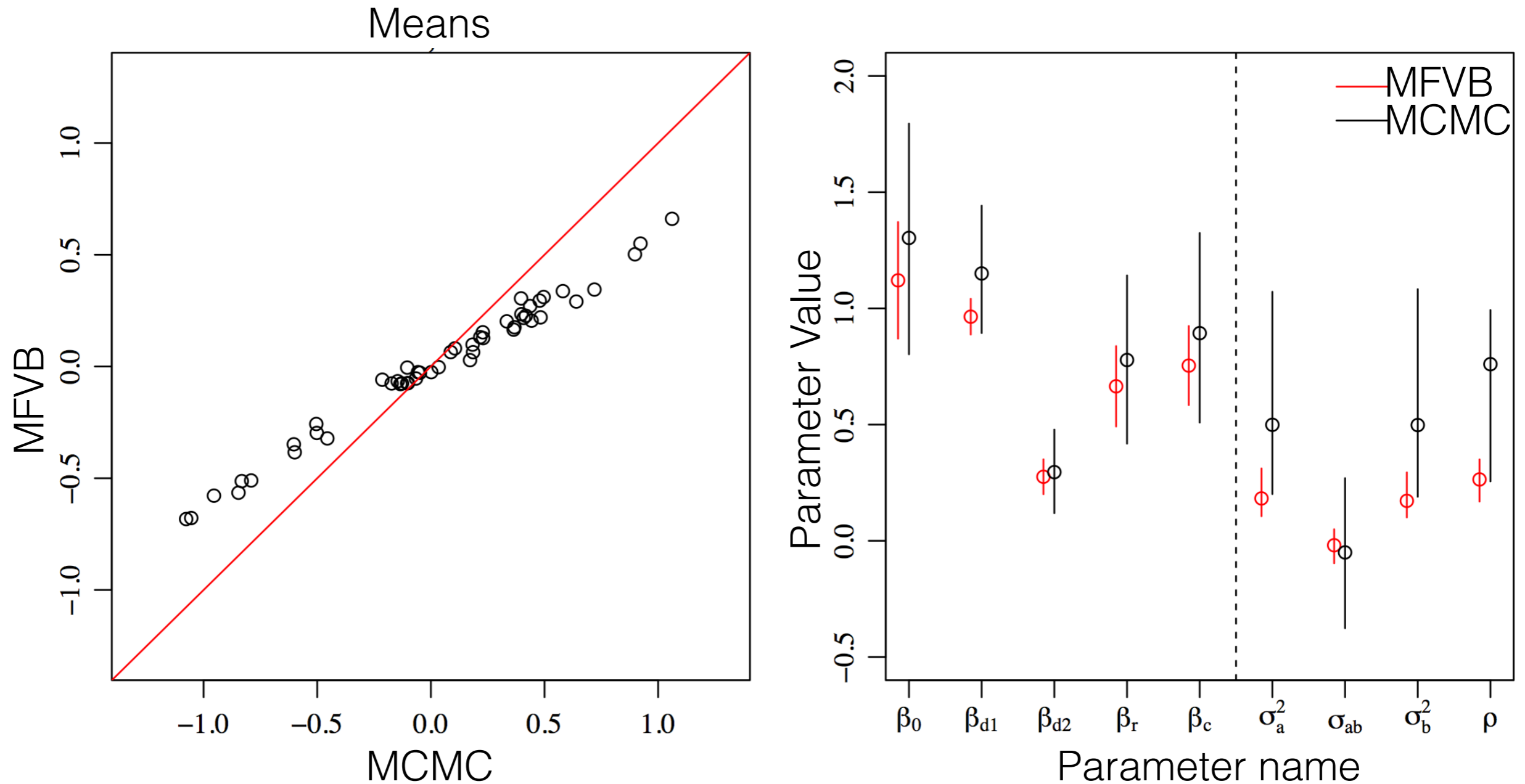
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[Fosdick 2013, Ch 4, Fig 4.3]

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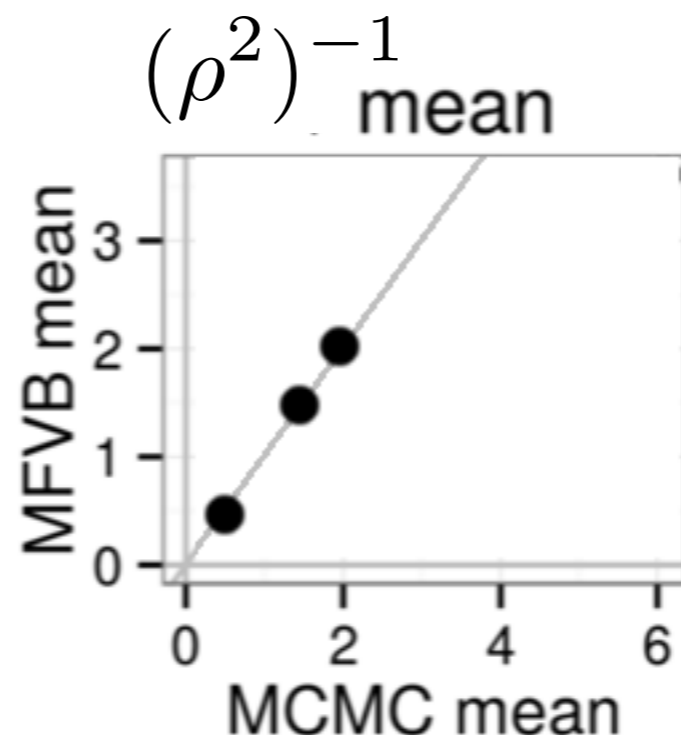
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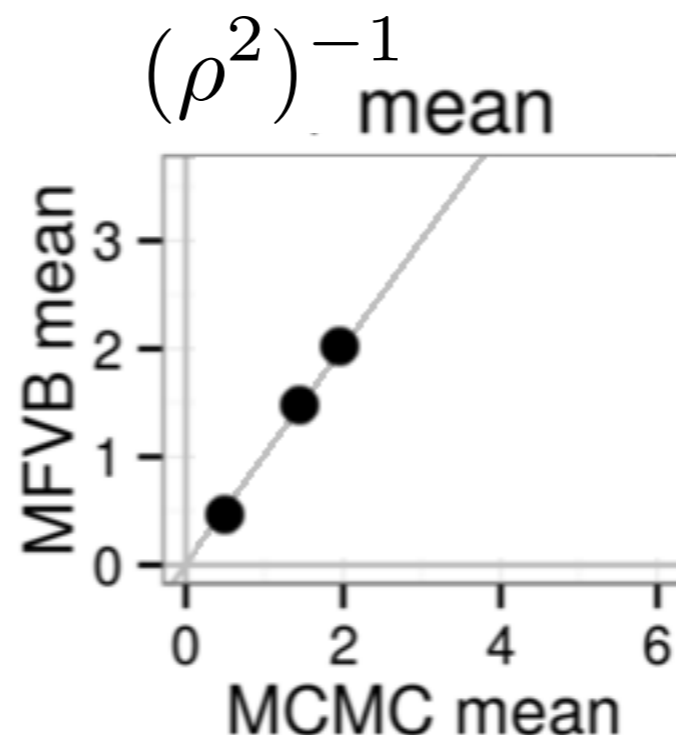
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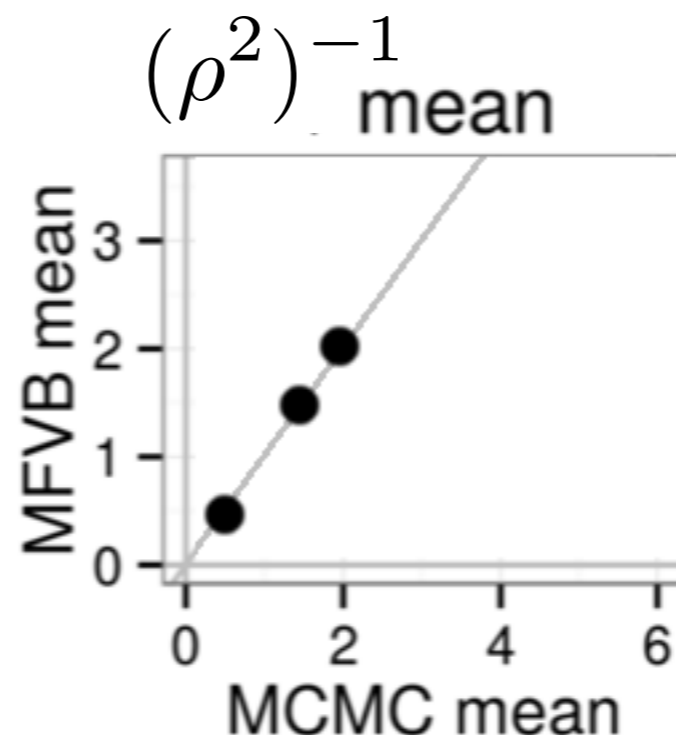
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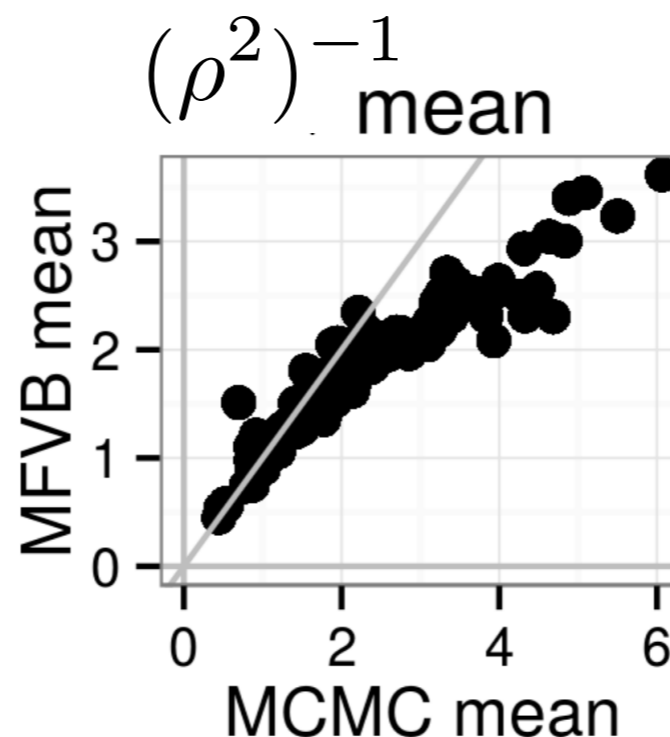
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Use q^* to approximate $p(\cdot|y)$

Optimization

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

Variational Bayes

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

Mean-field variational Bayes

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

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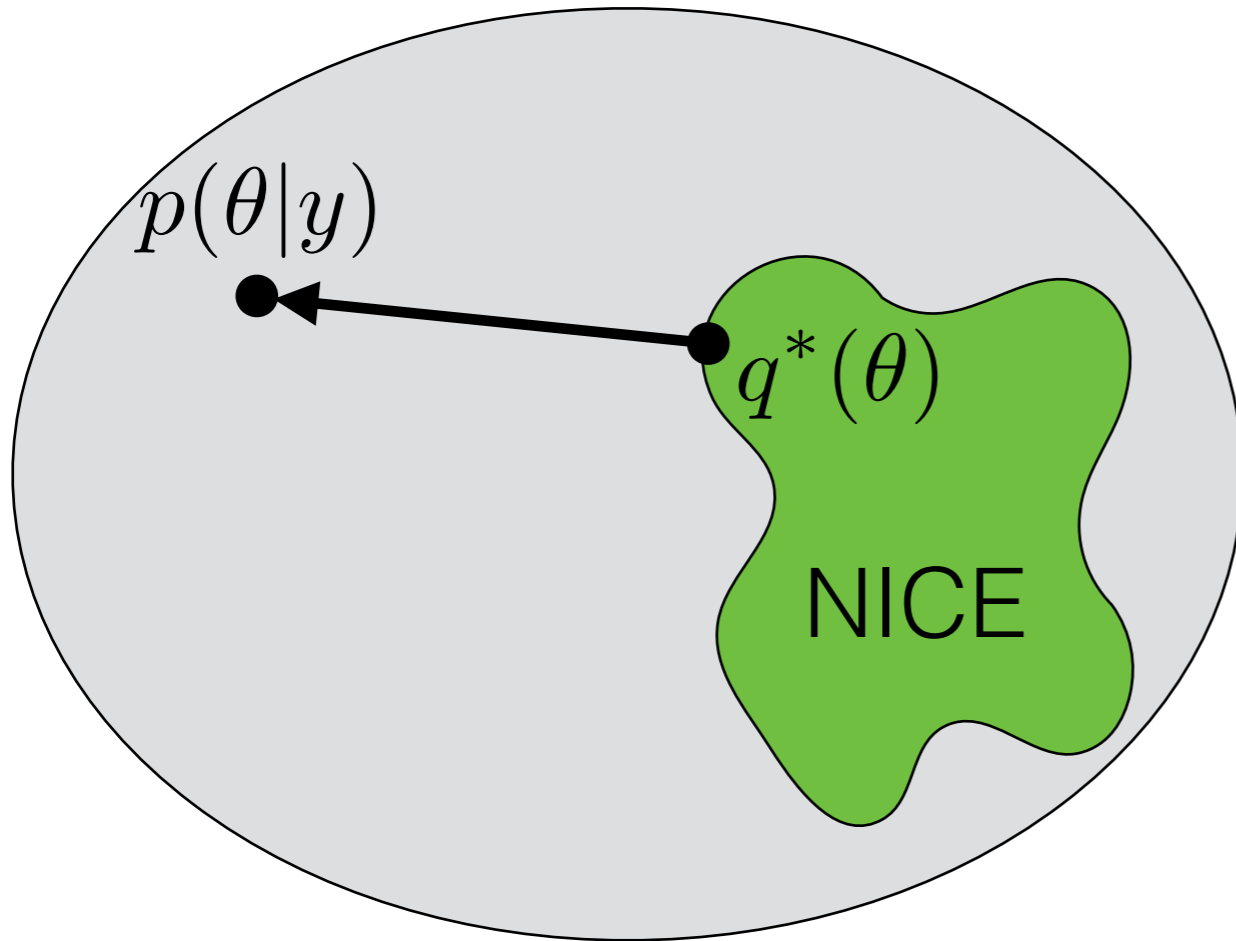
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Is it just MFVB?

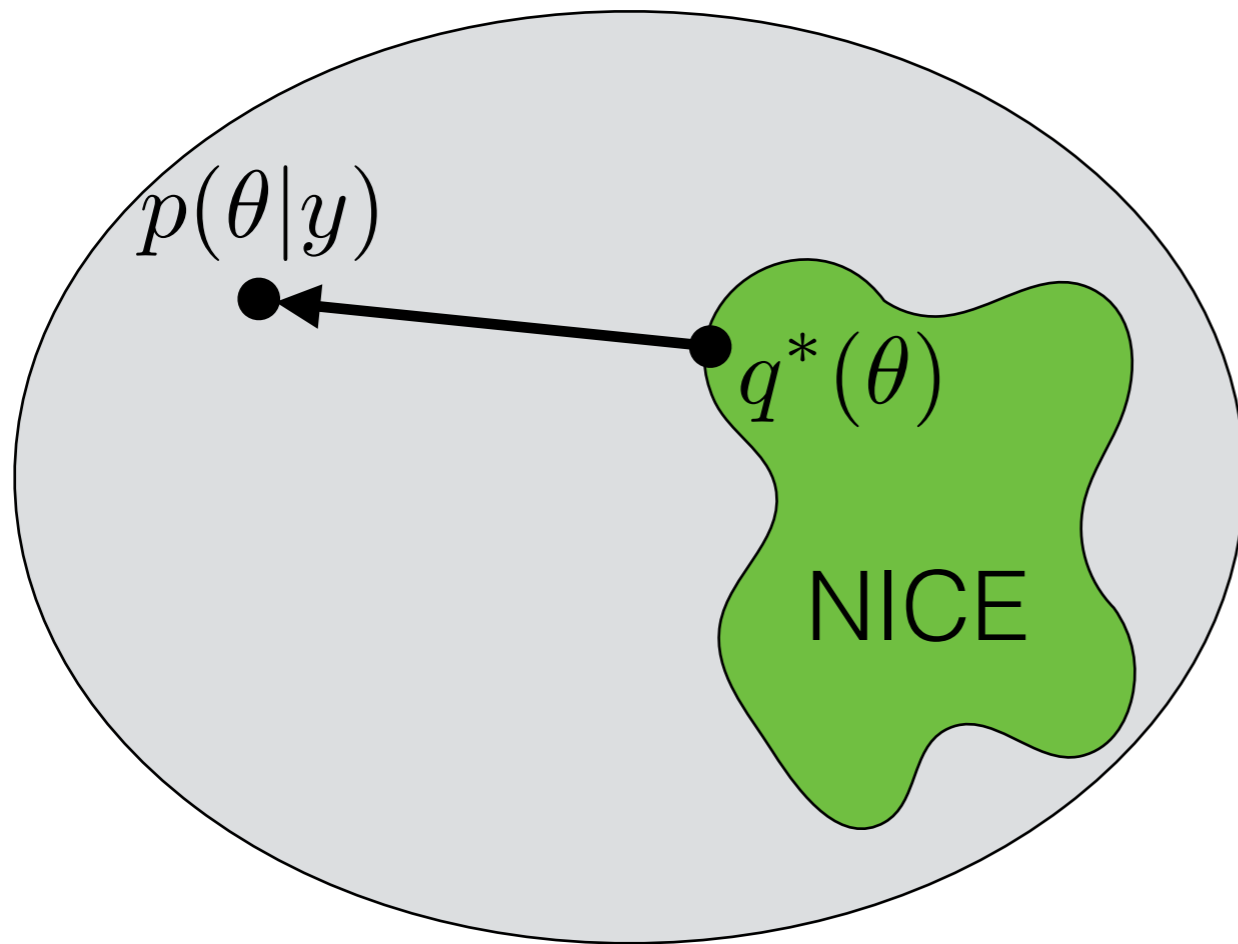
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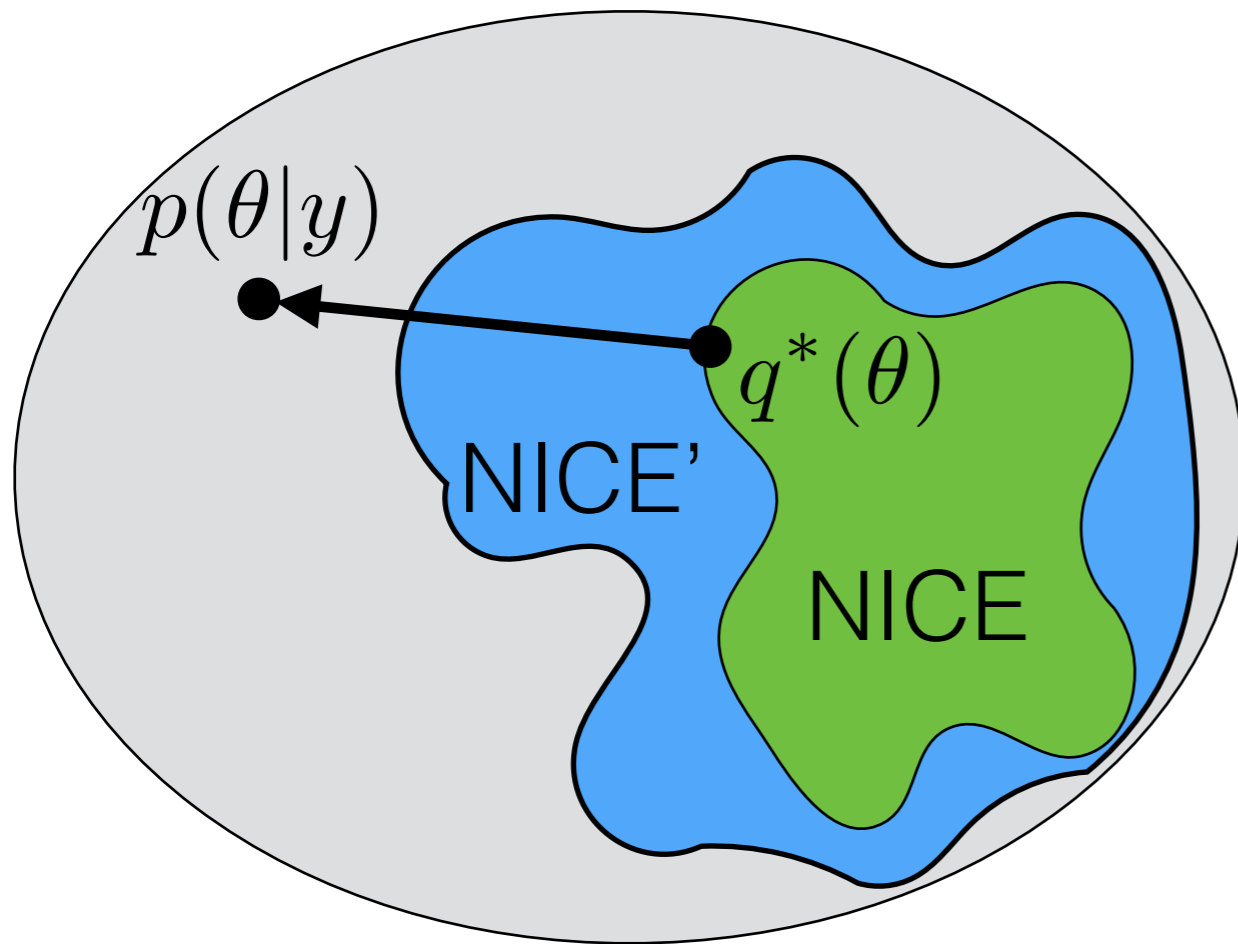


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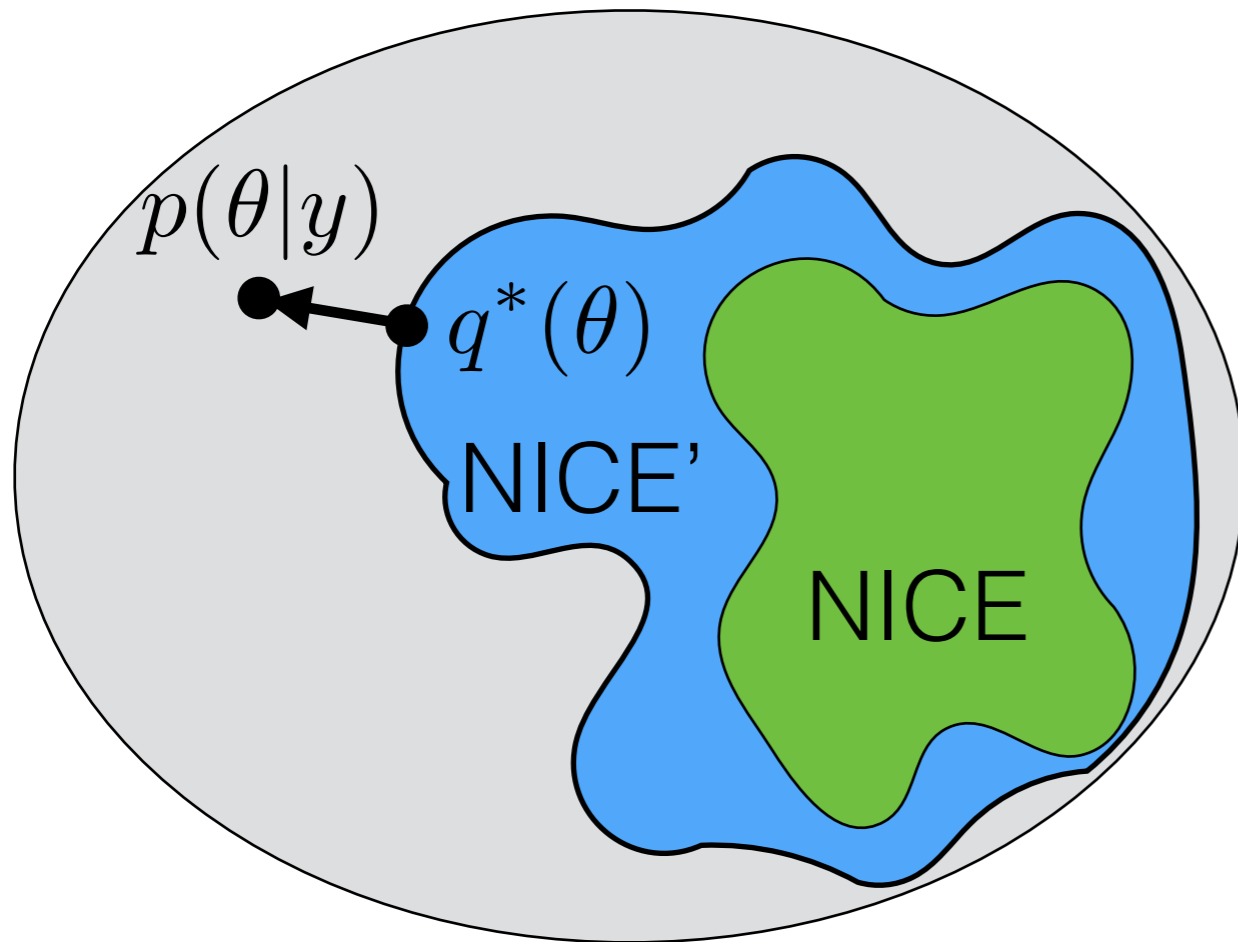
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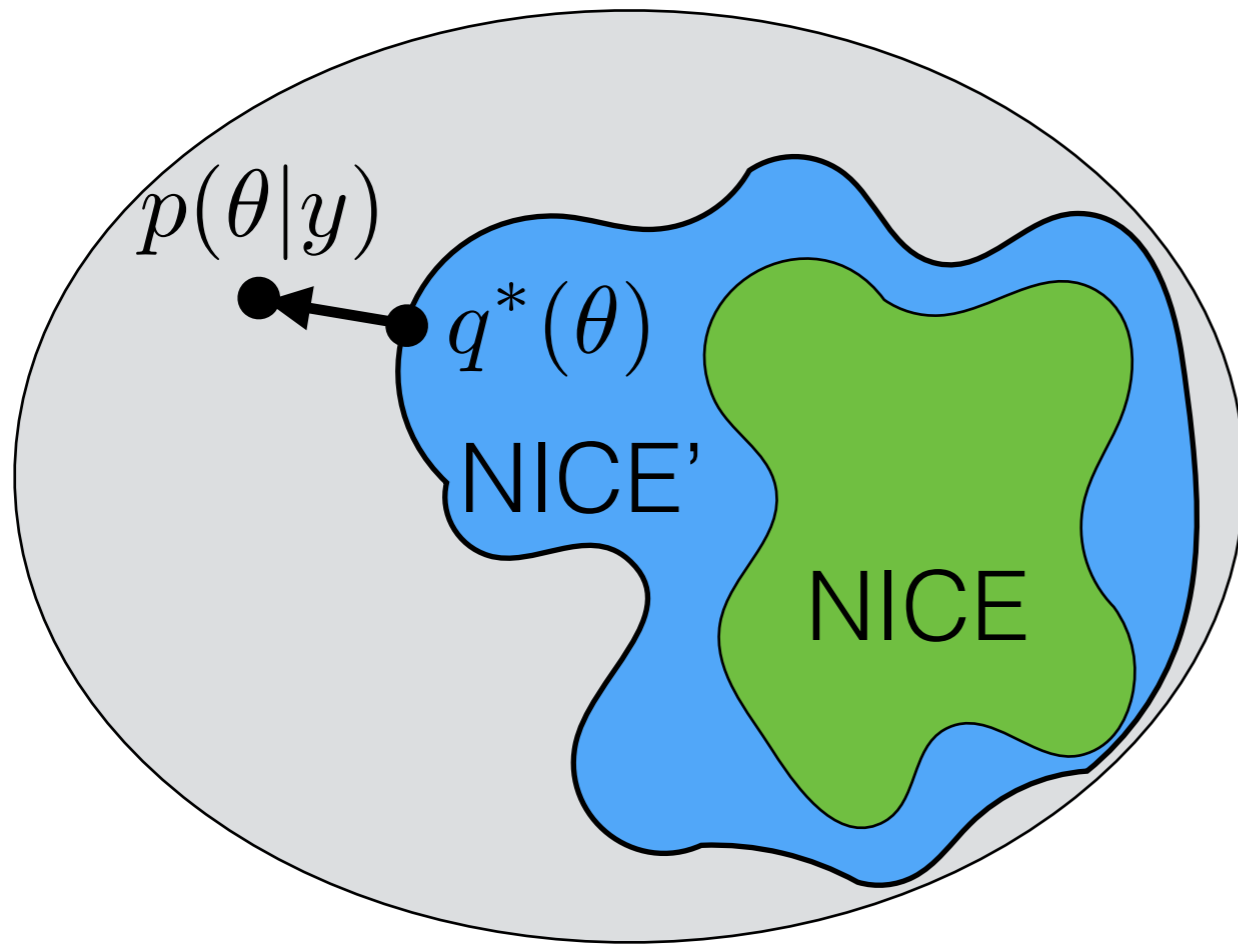
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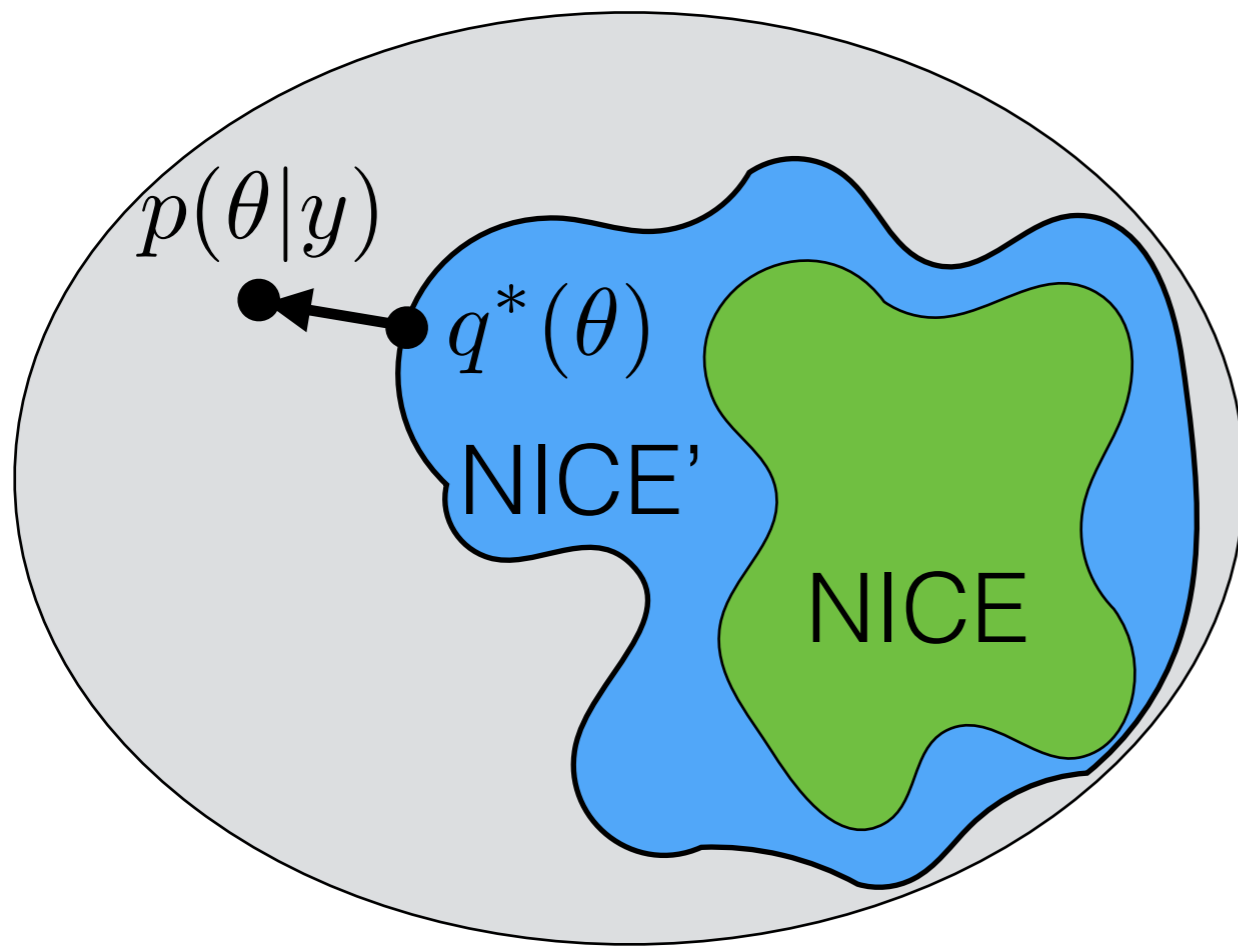
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- Exercise: Show, with a simple example, that a smaller KL does not imply better mean and variance estimates
- But how much worse can the estimates be? And could it have just been the implementation?

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Proposition. Can have small KL (<0.23) & arbitrarily bad variance estimate

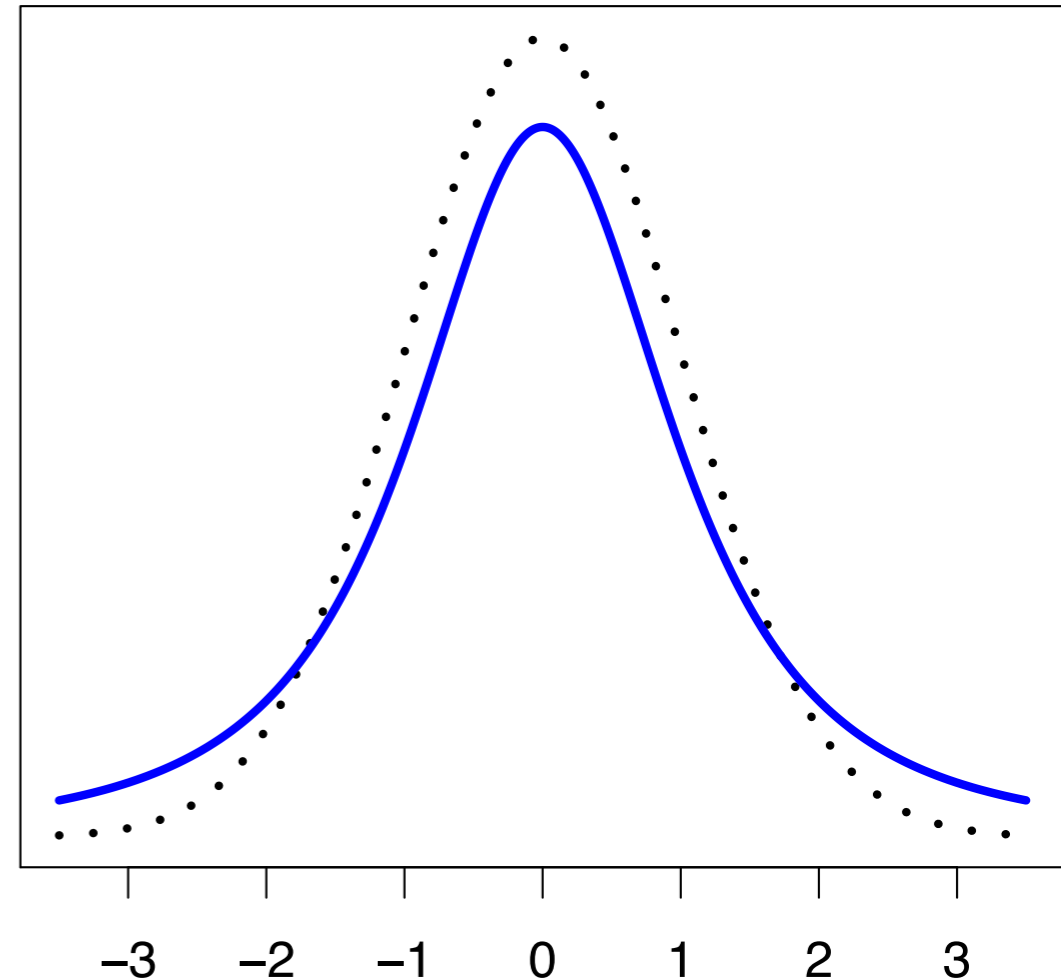
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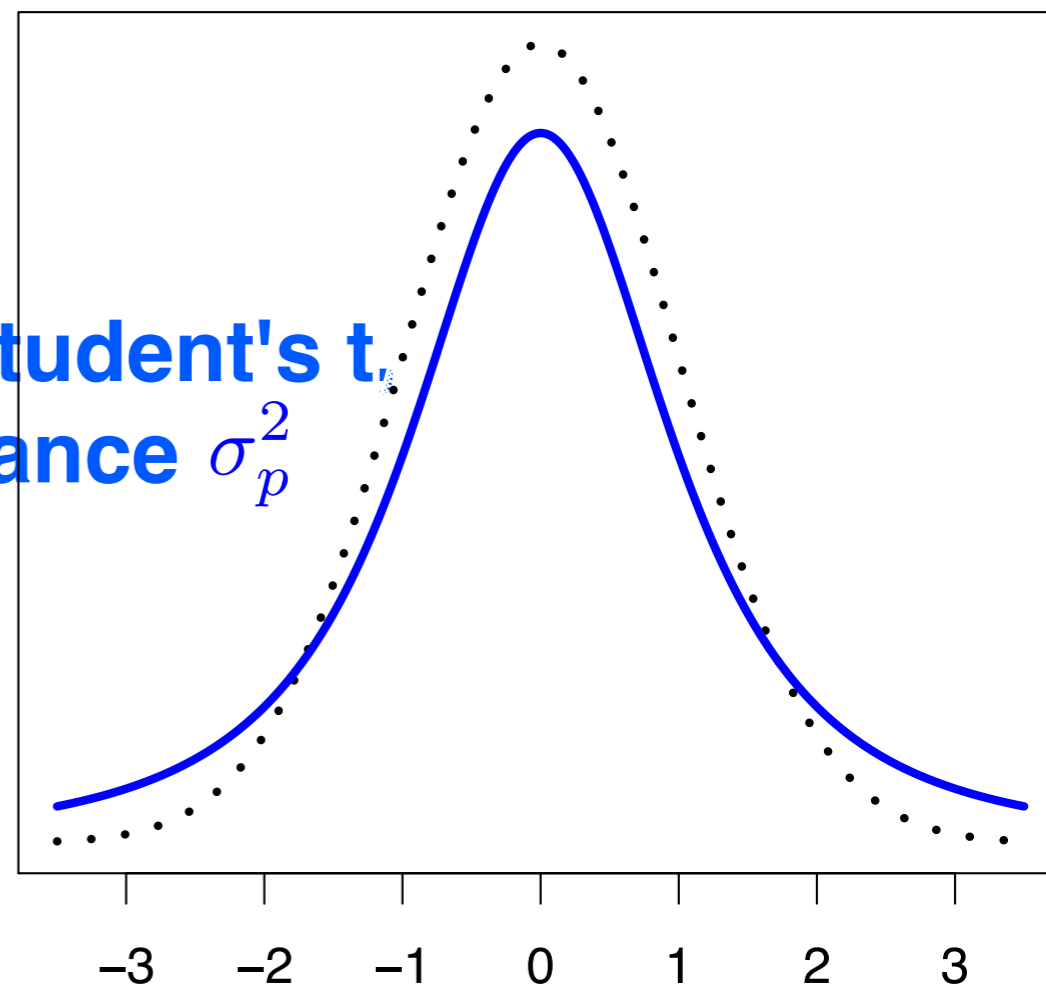
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p : Student's t ,
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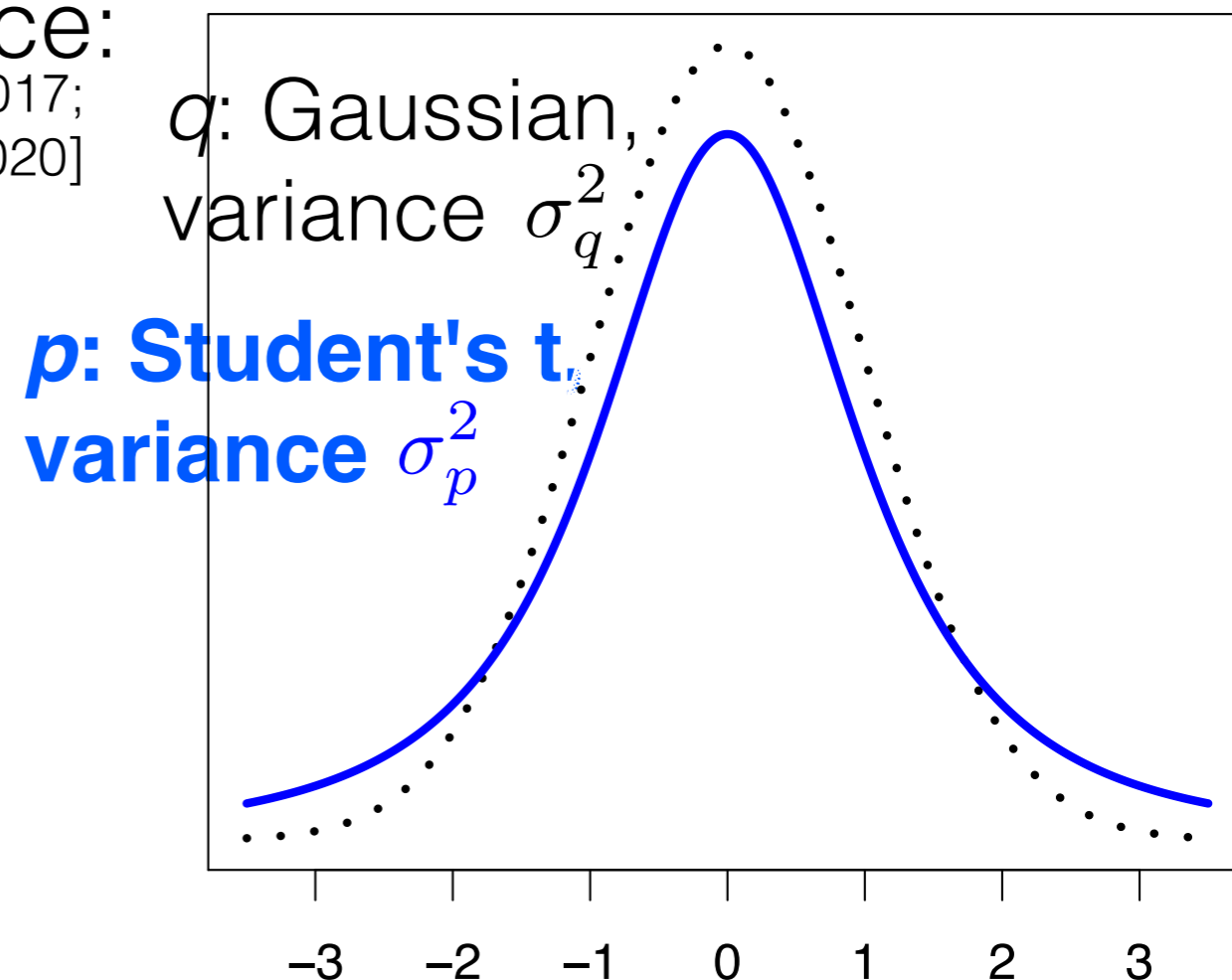


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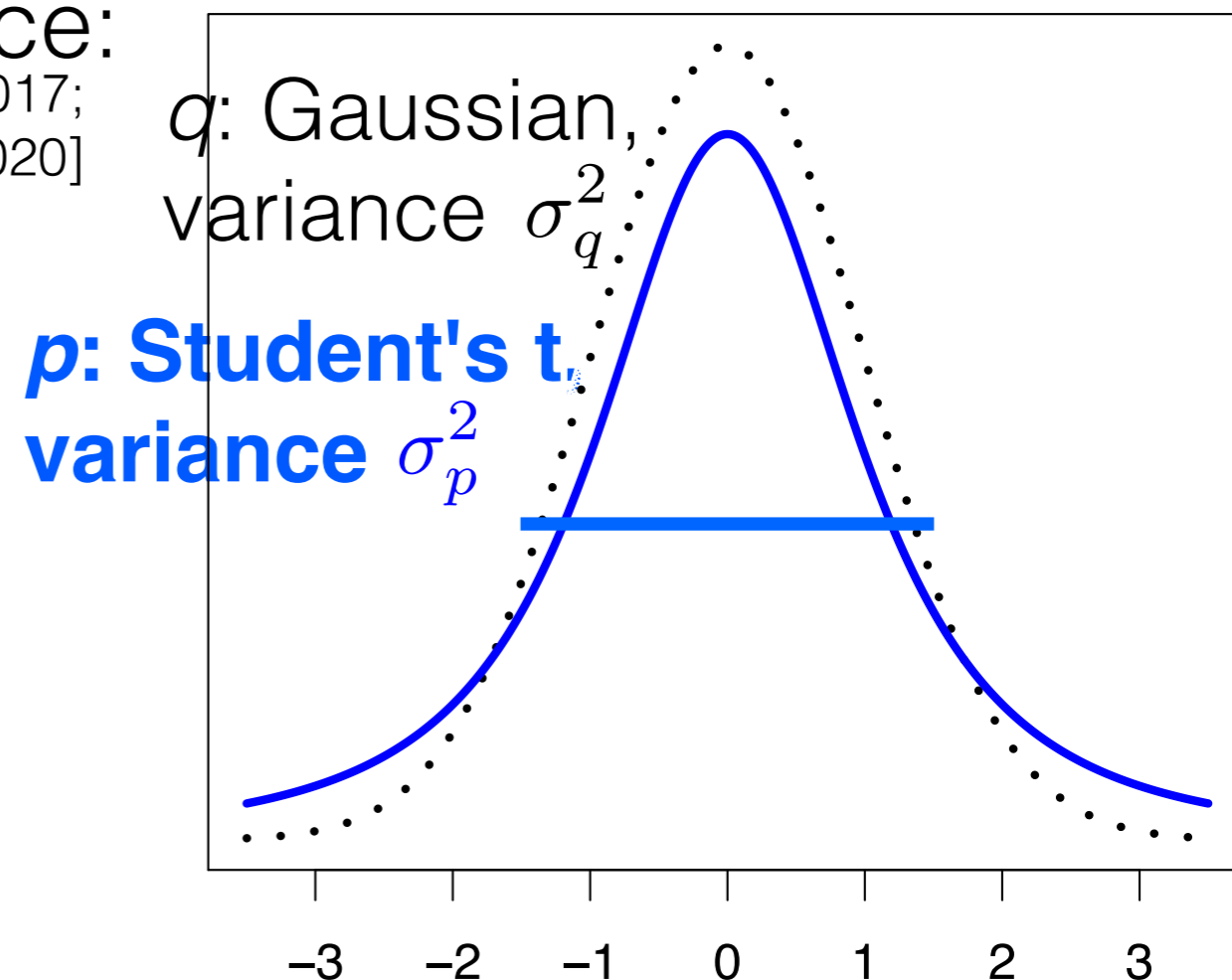


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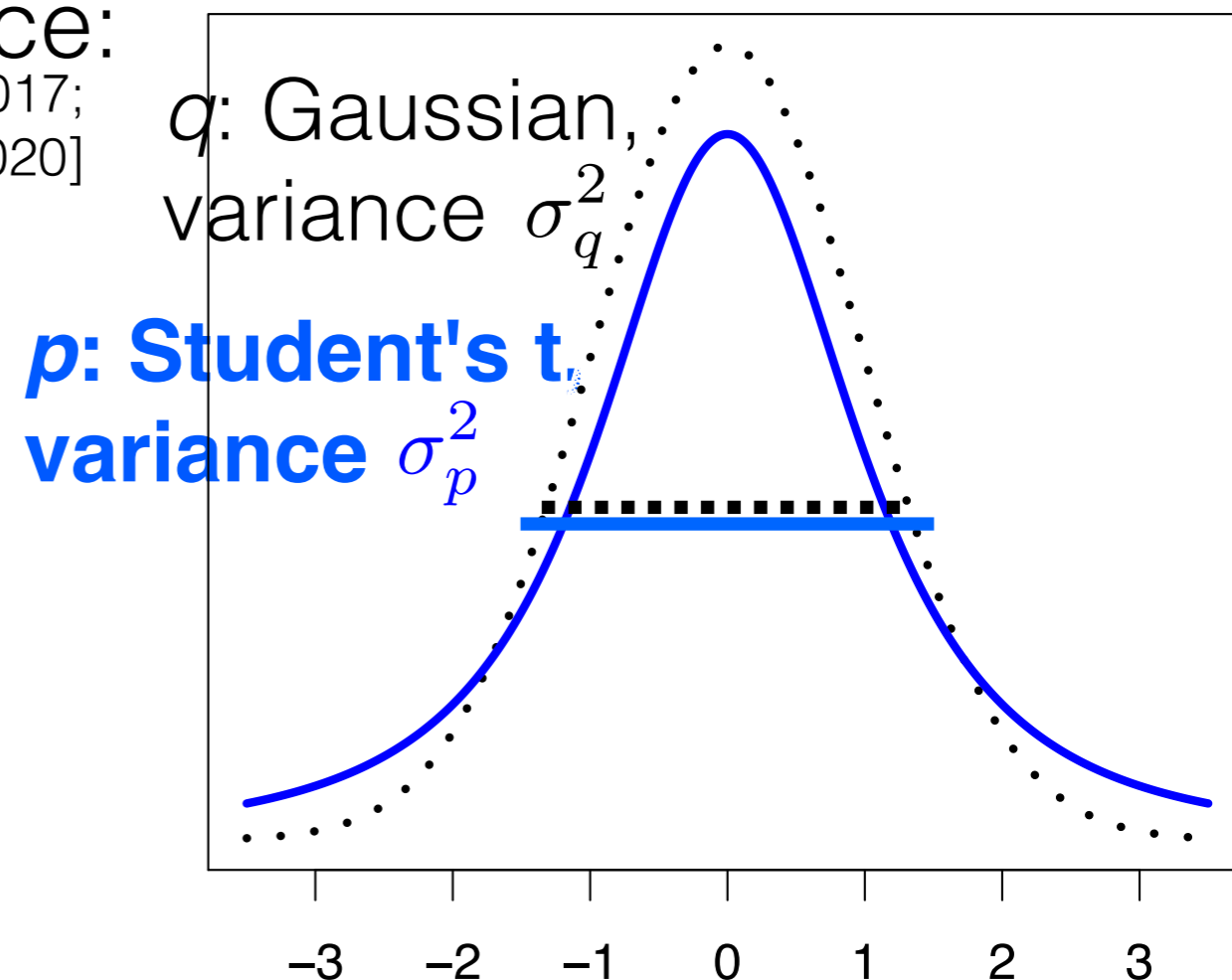


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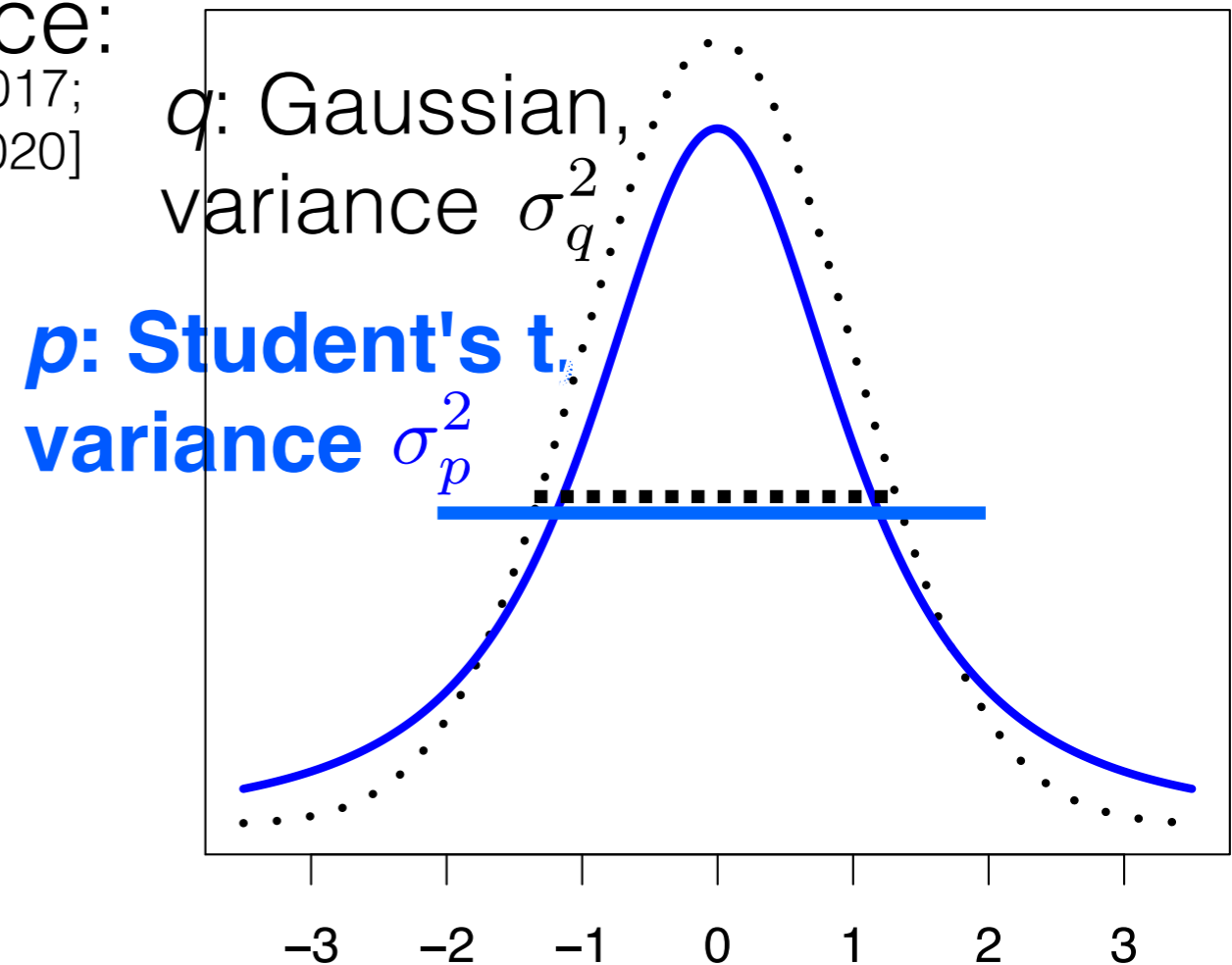


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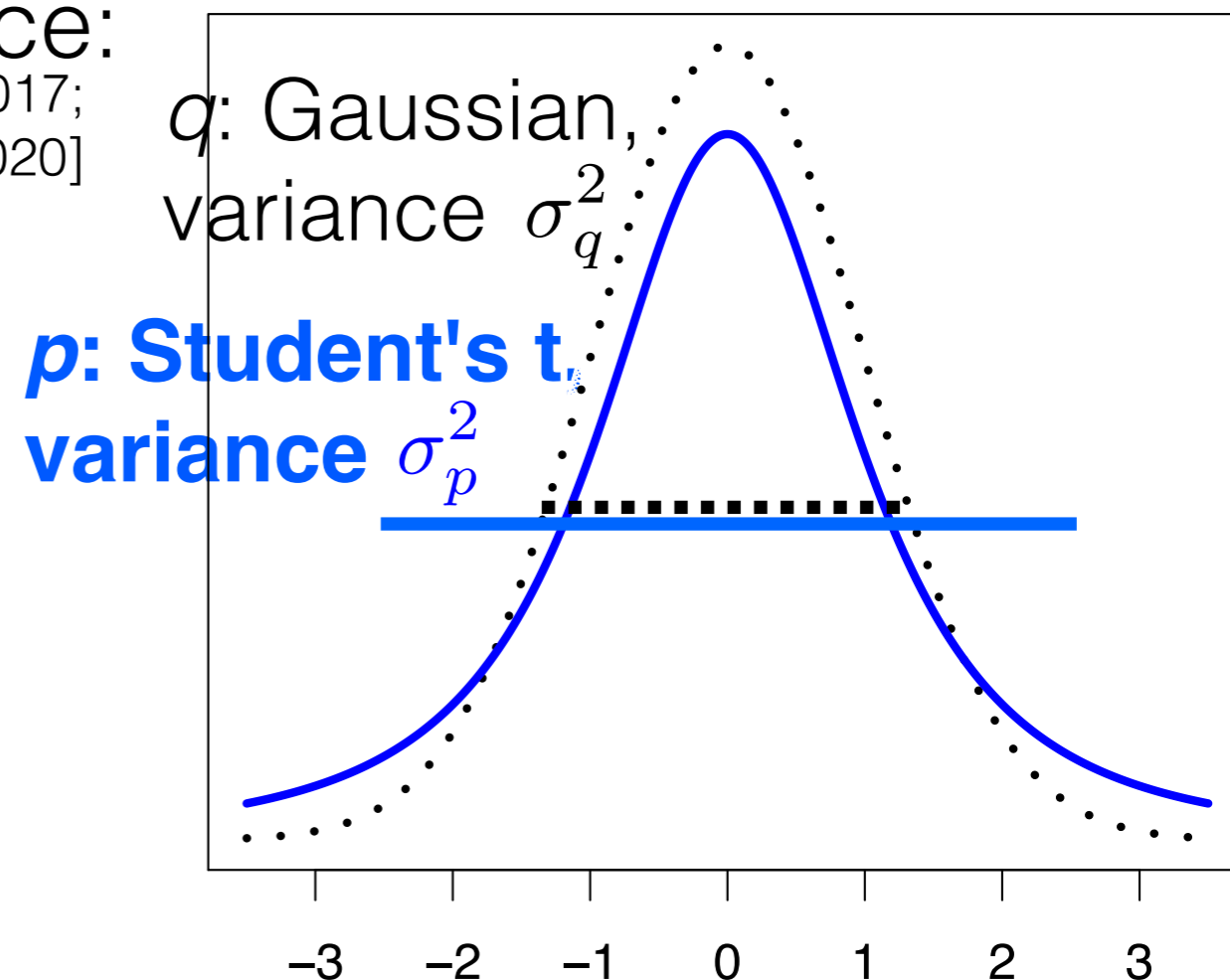


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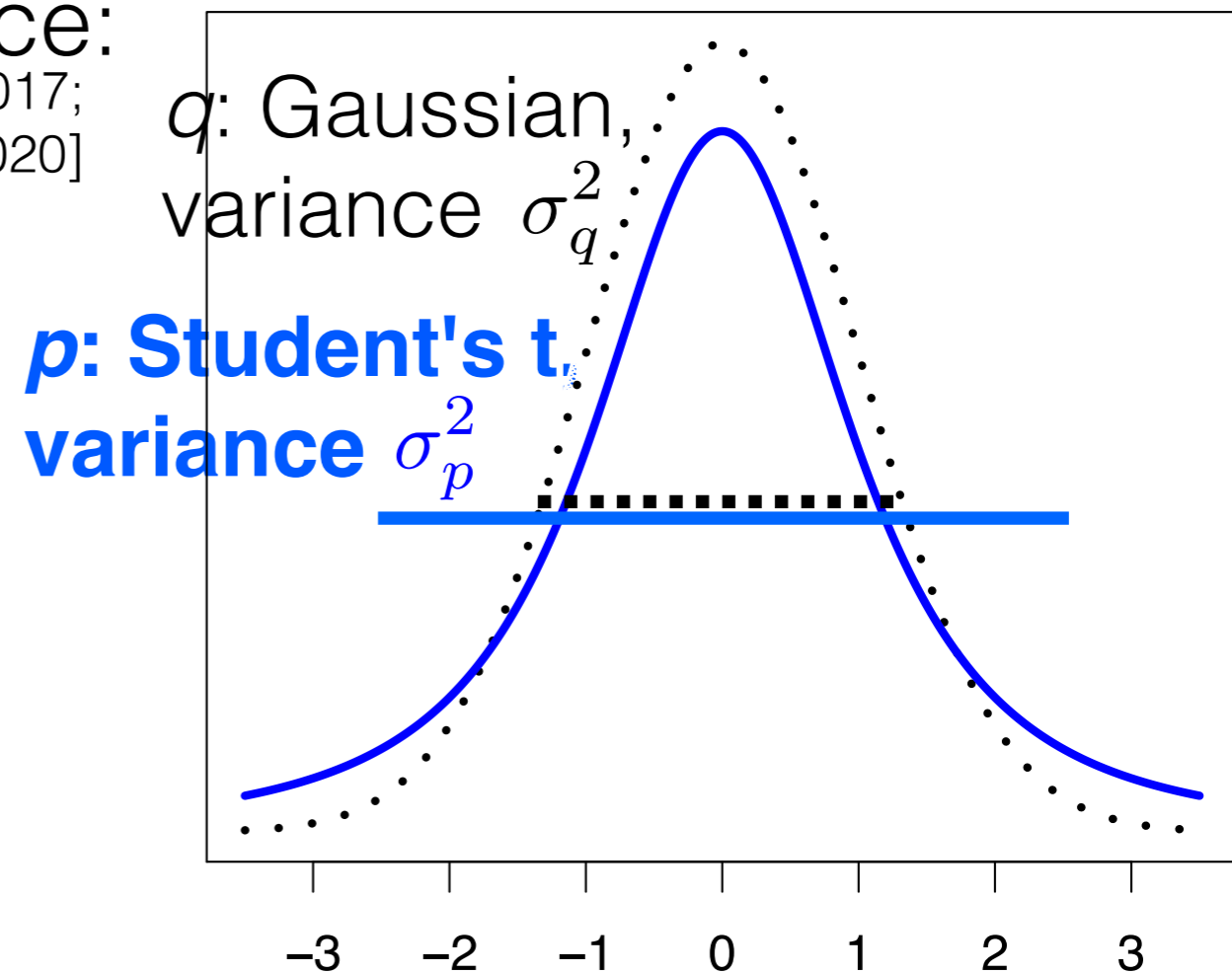


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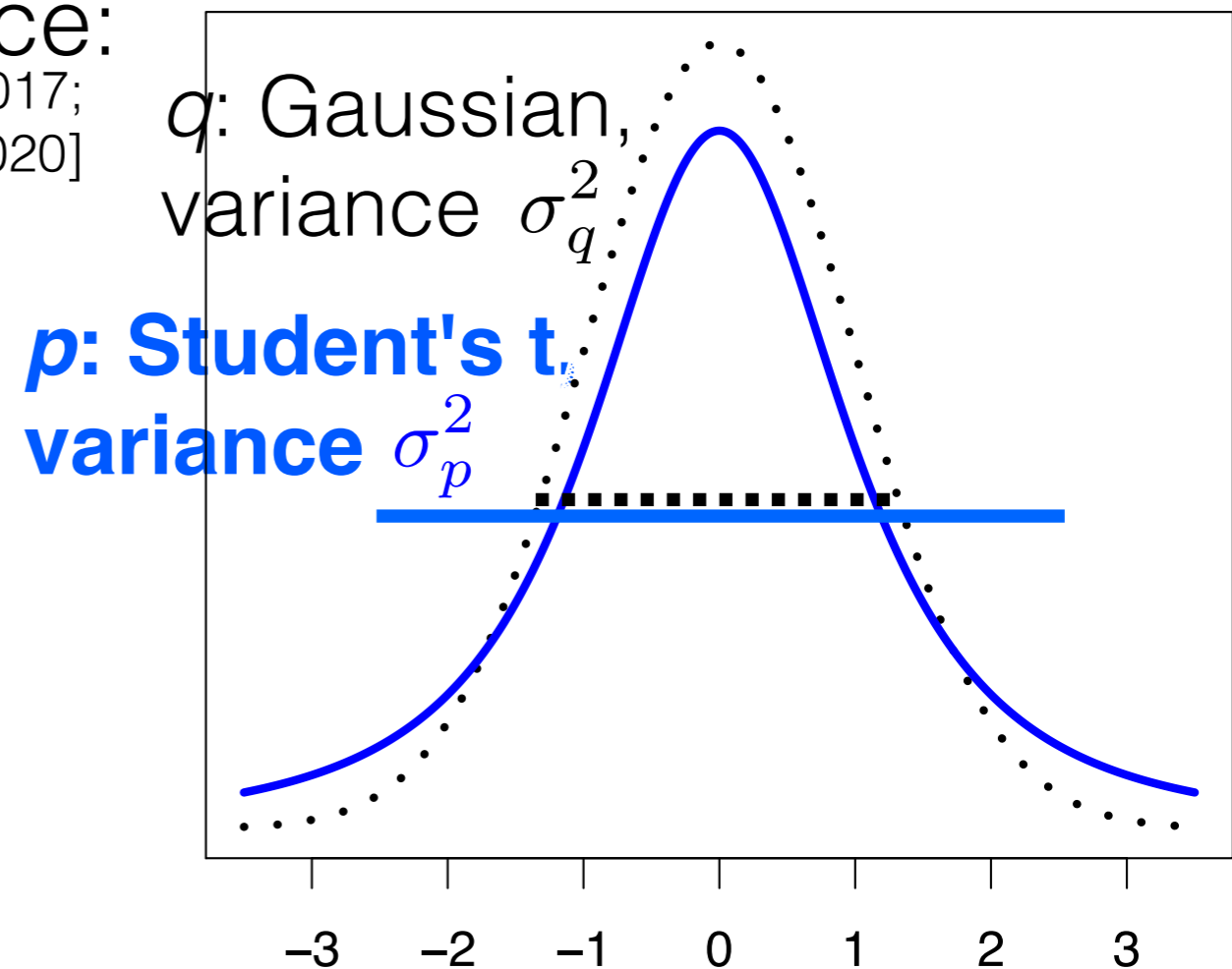
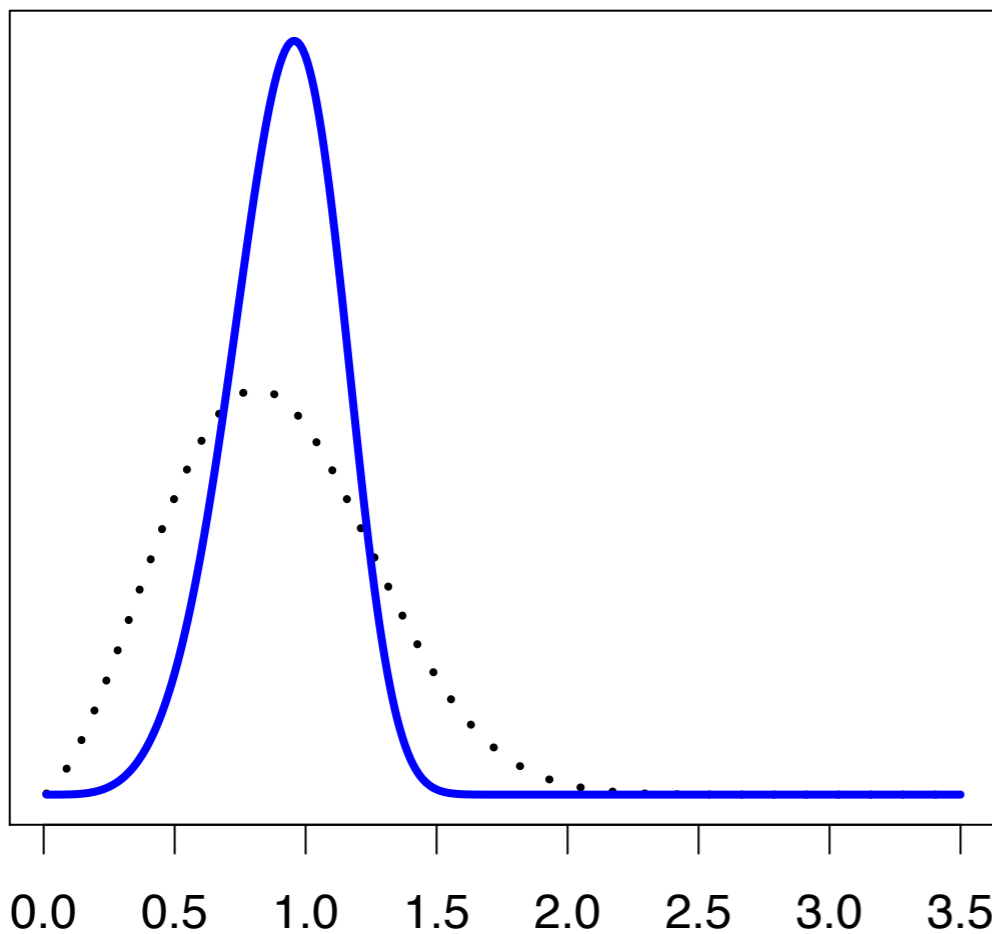
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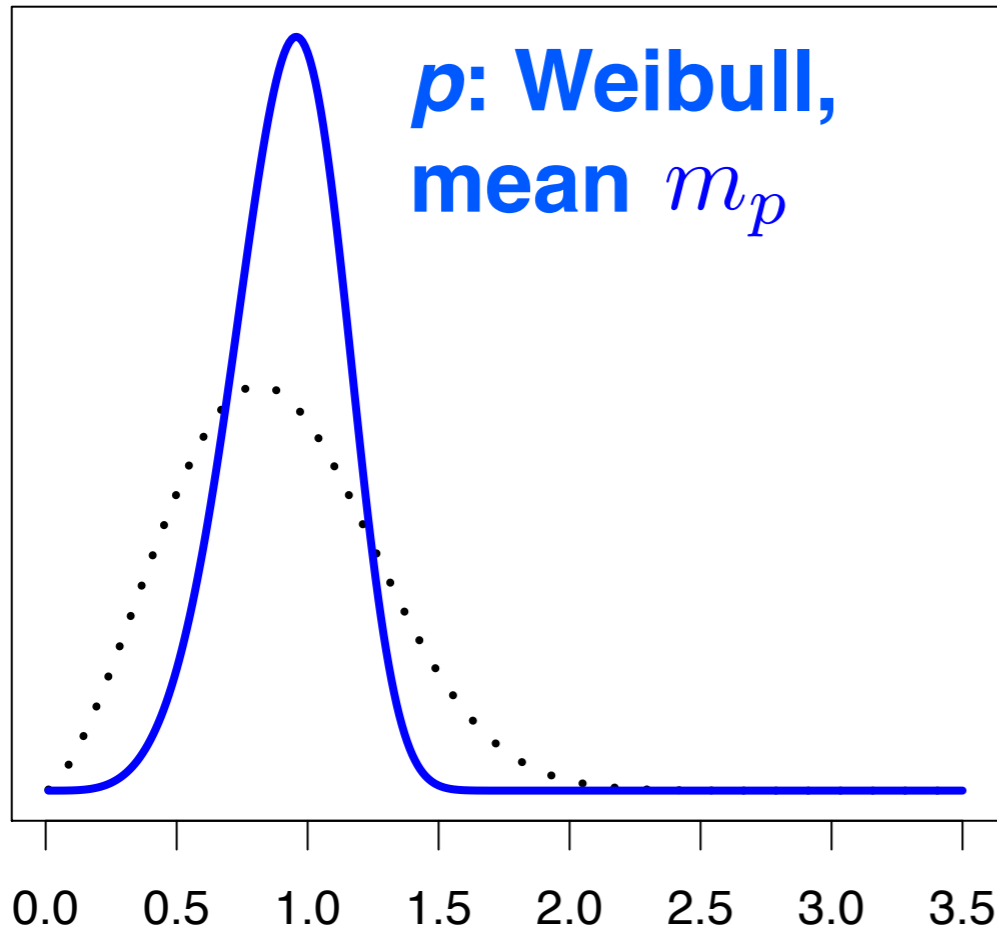
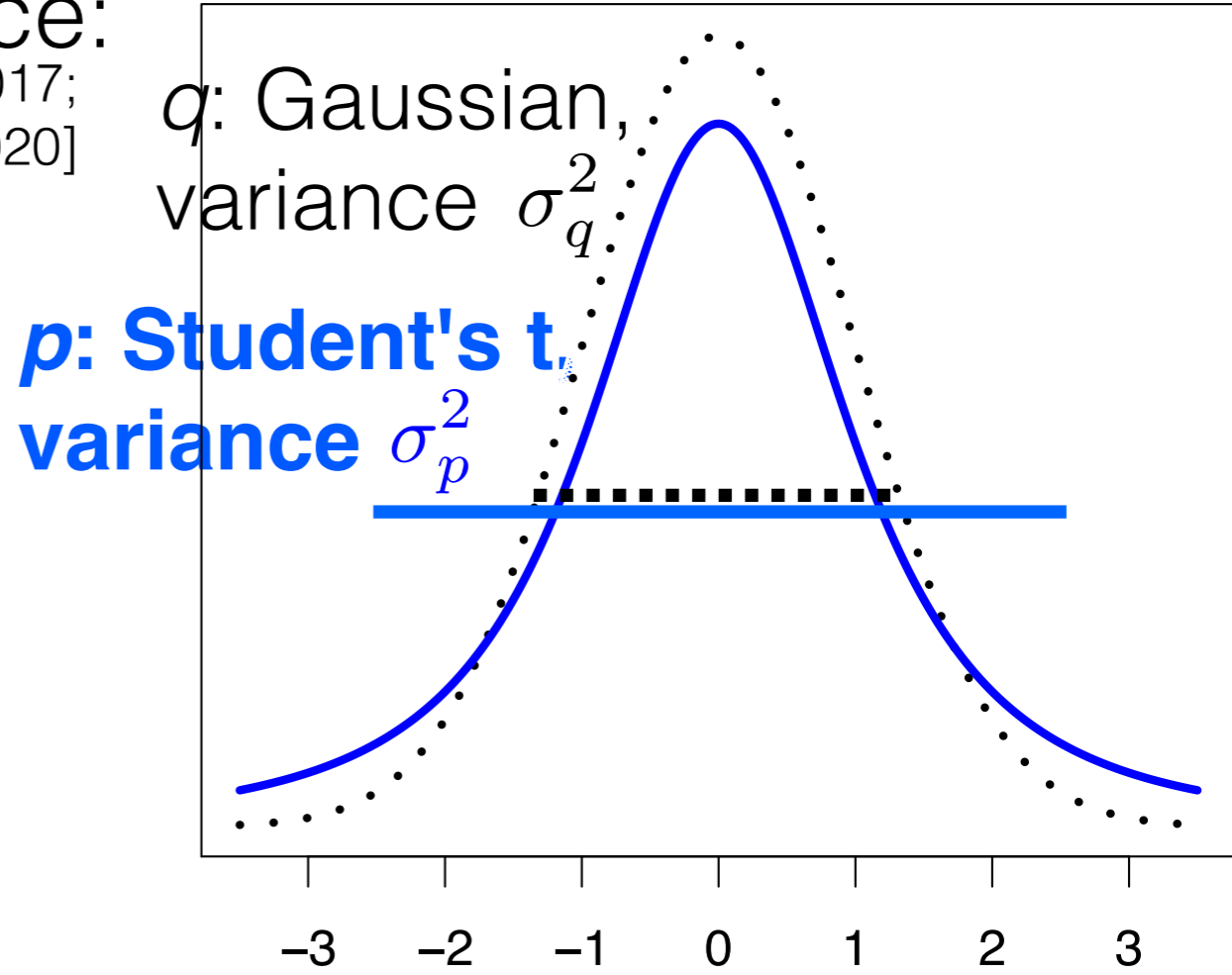
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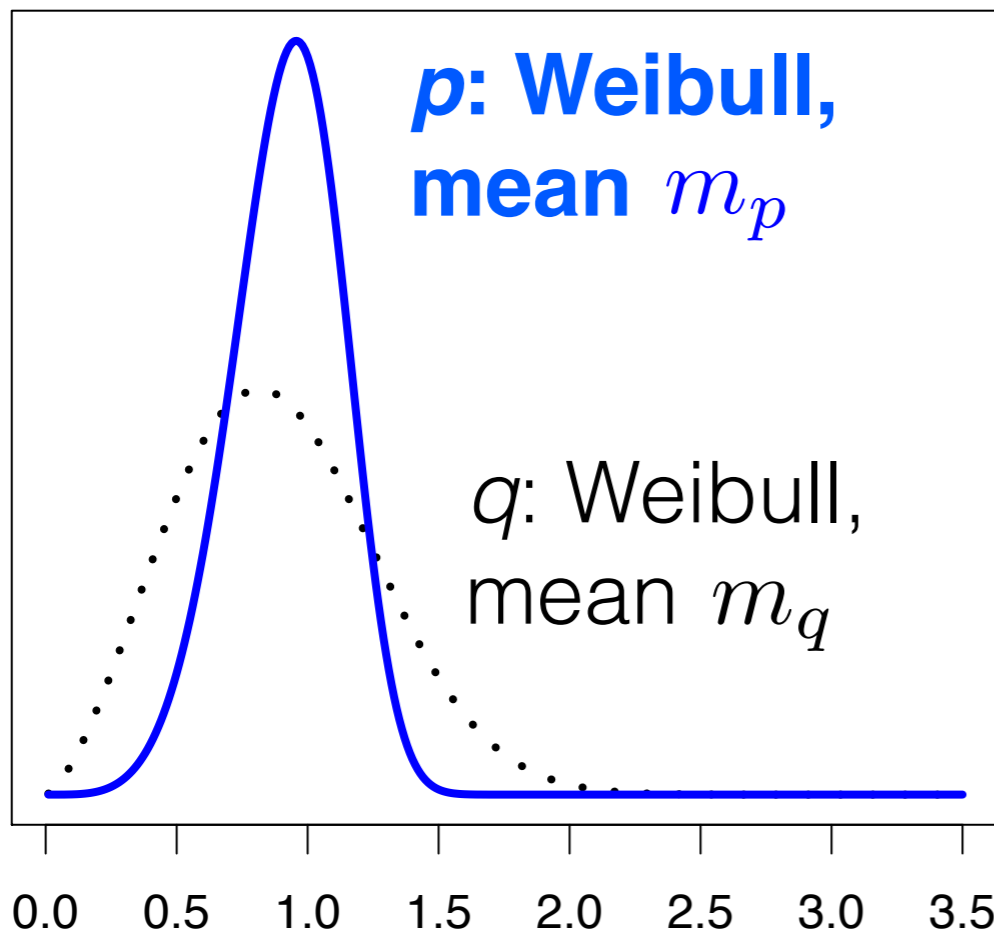
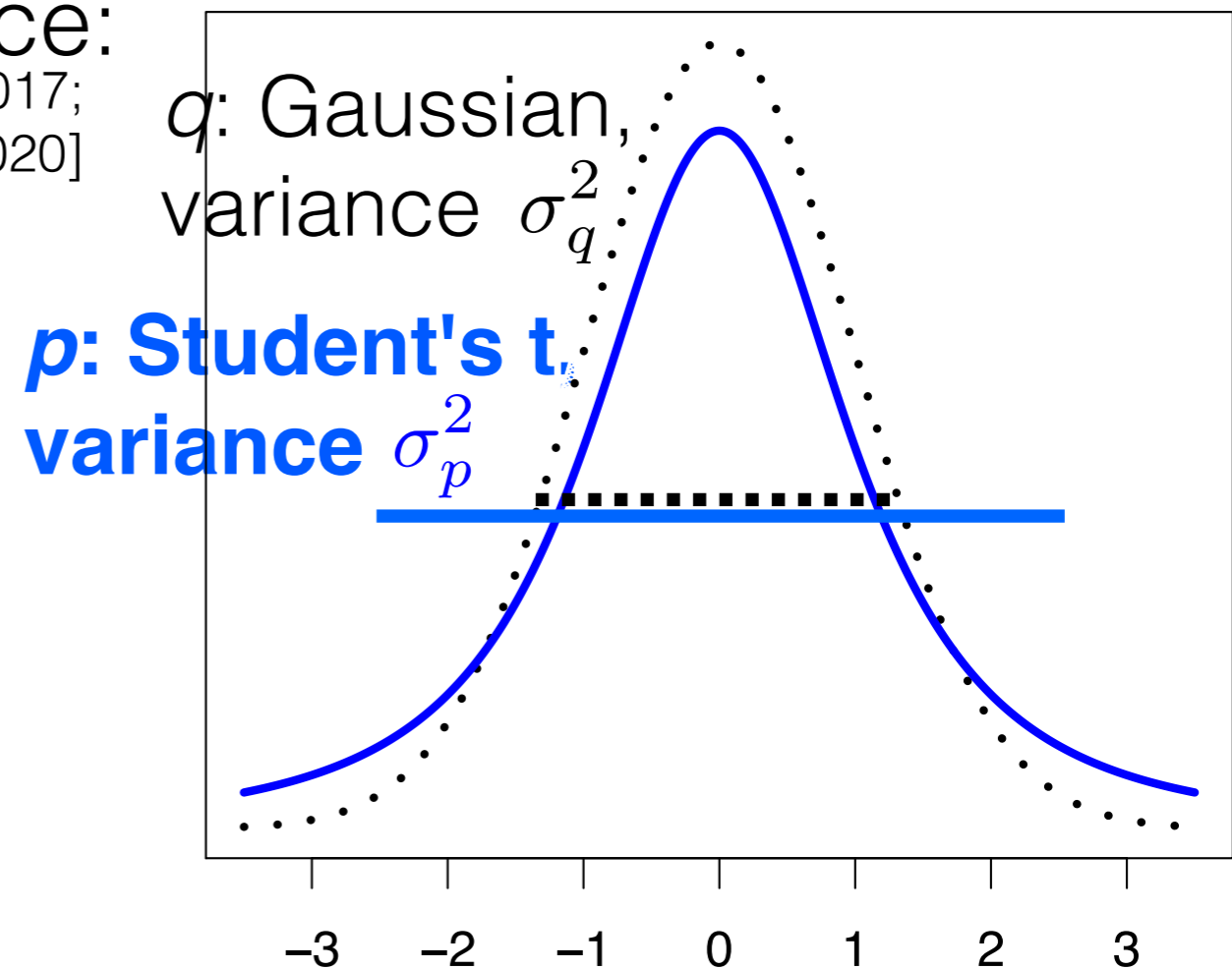
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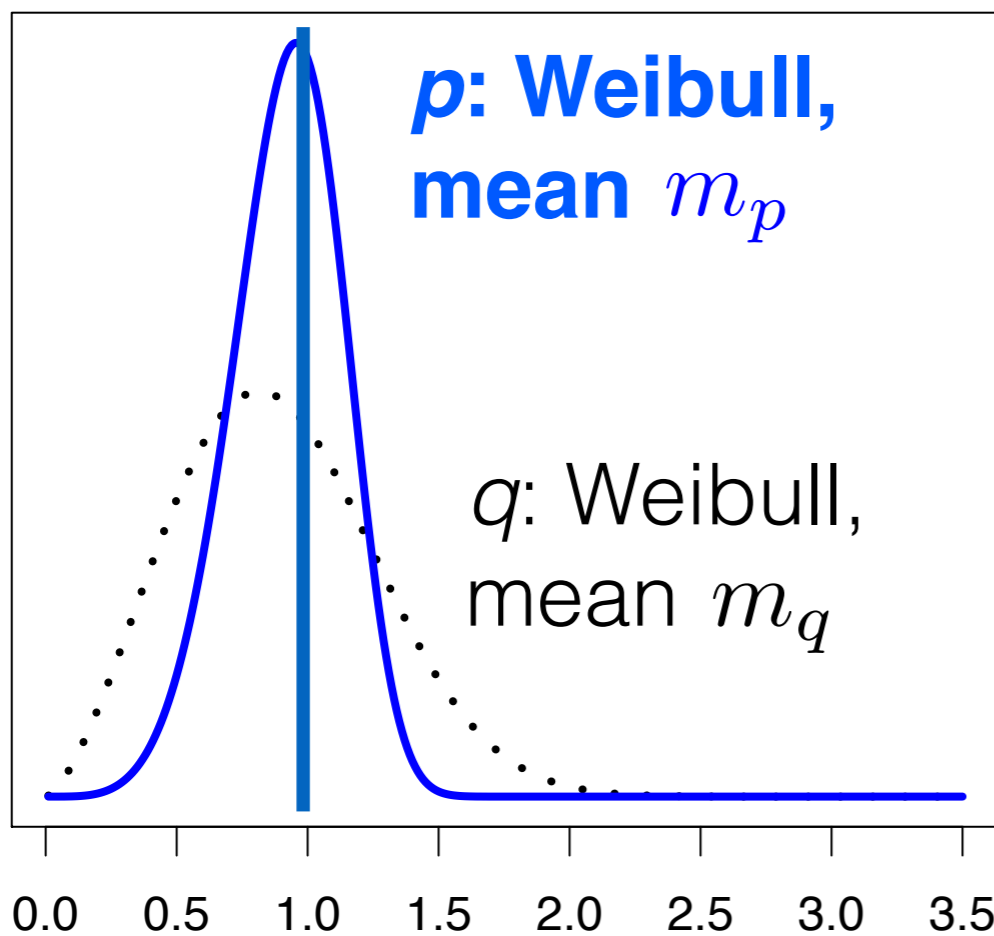
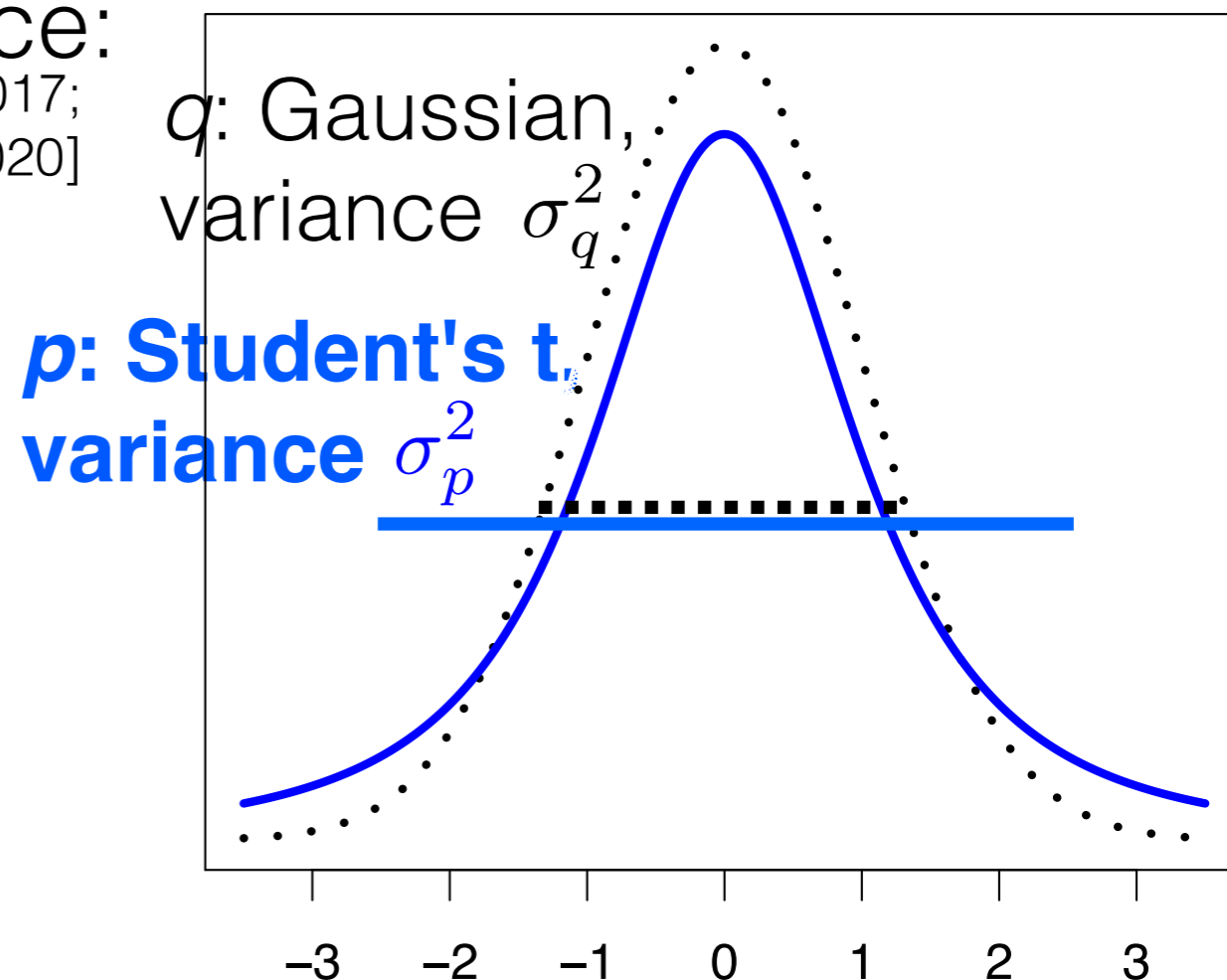
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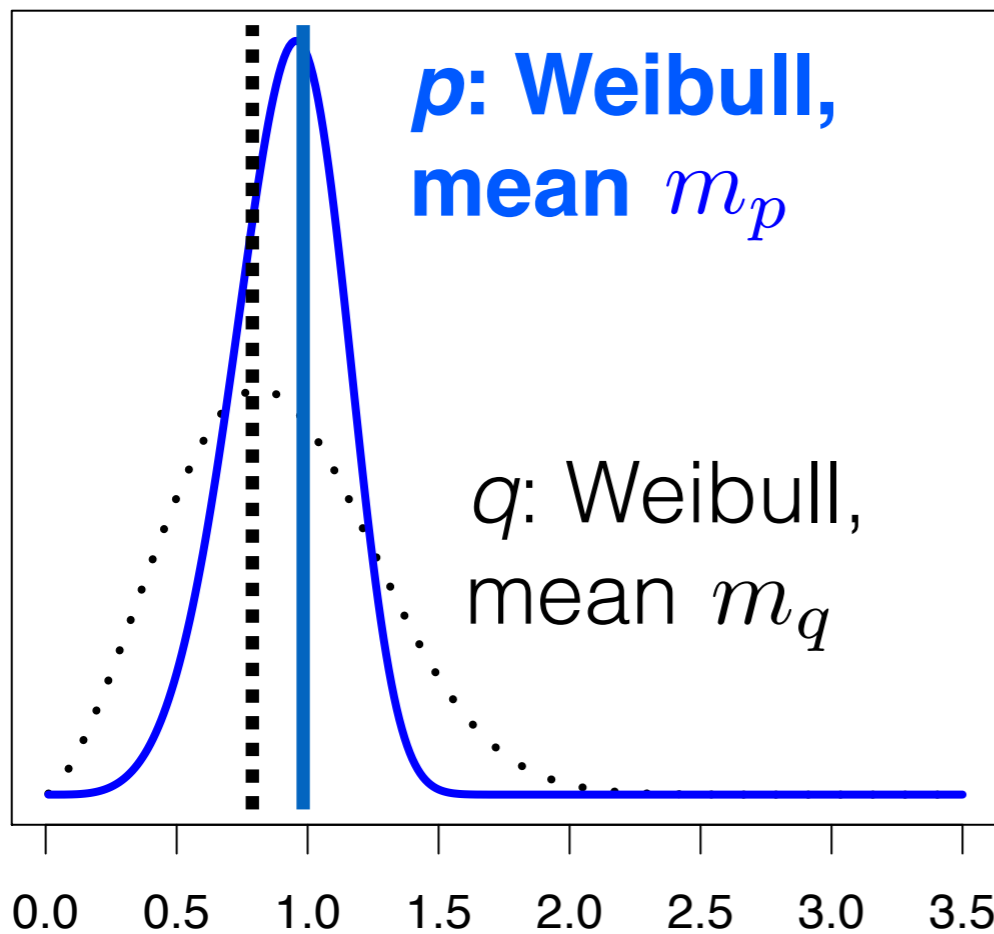
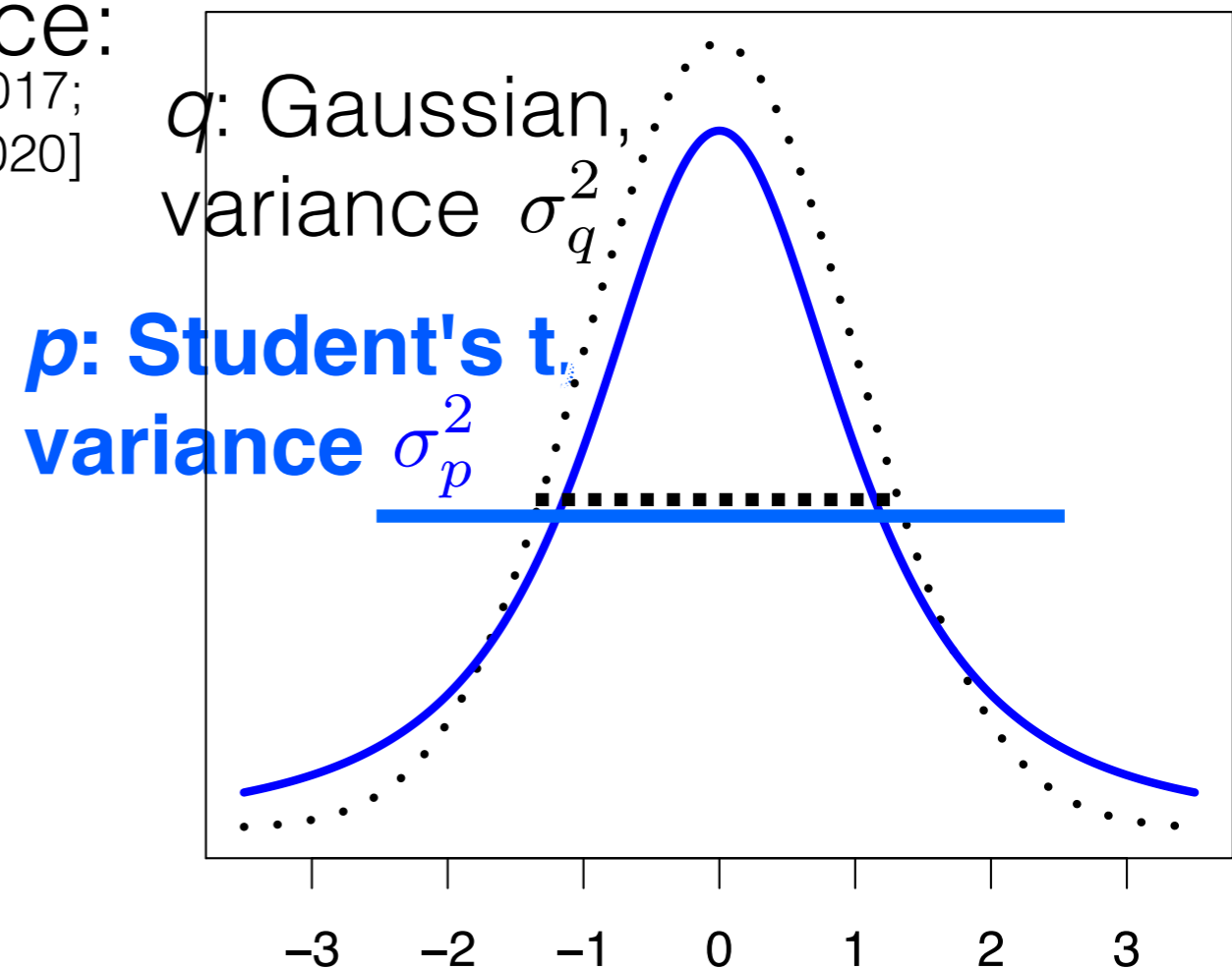
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Use q^* to approximate $p(\cdot|y)$

Optimization

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

Variational Bayes

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Implementation

Gaussian example
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**How
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- What is:
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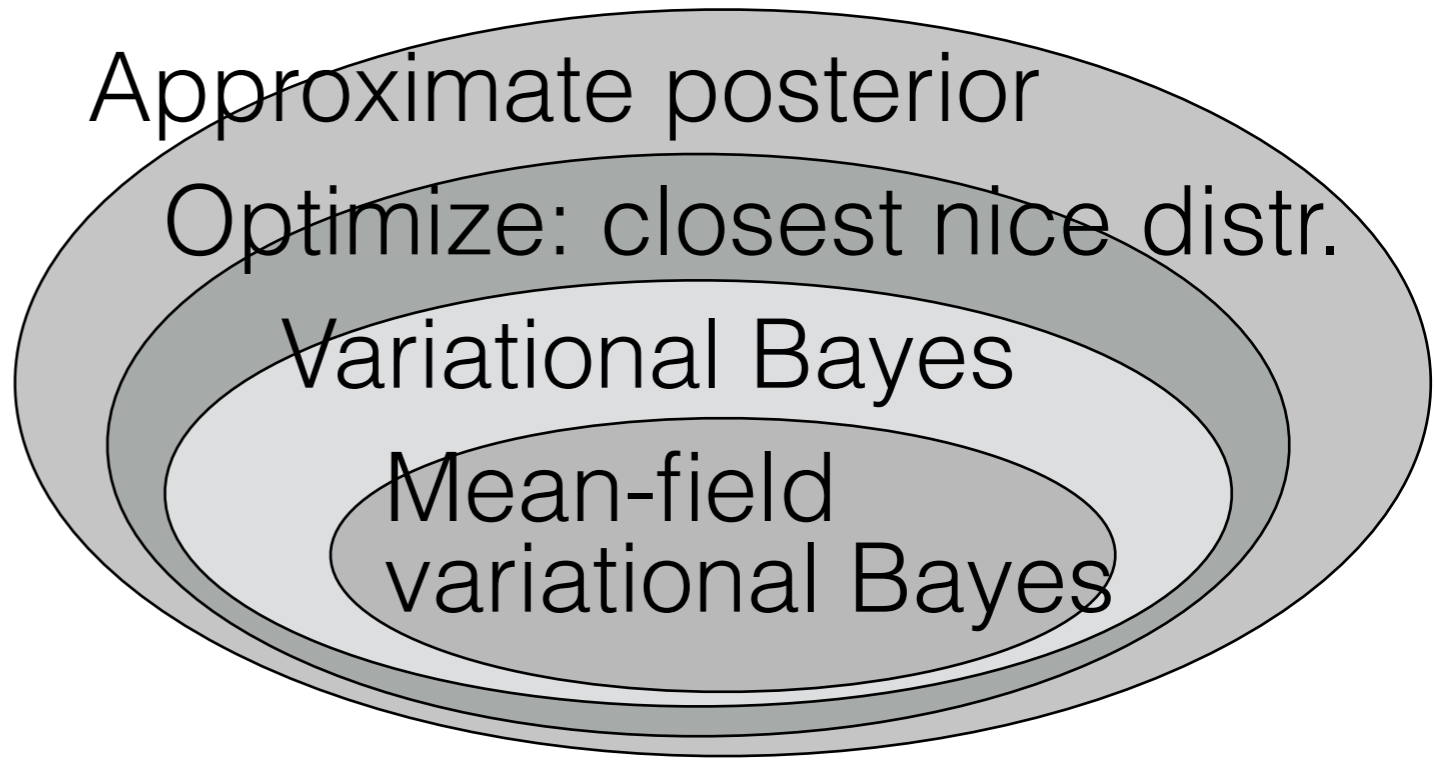
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Approximate posterior

Optimize: closest nice distr.

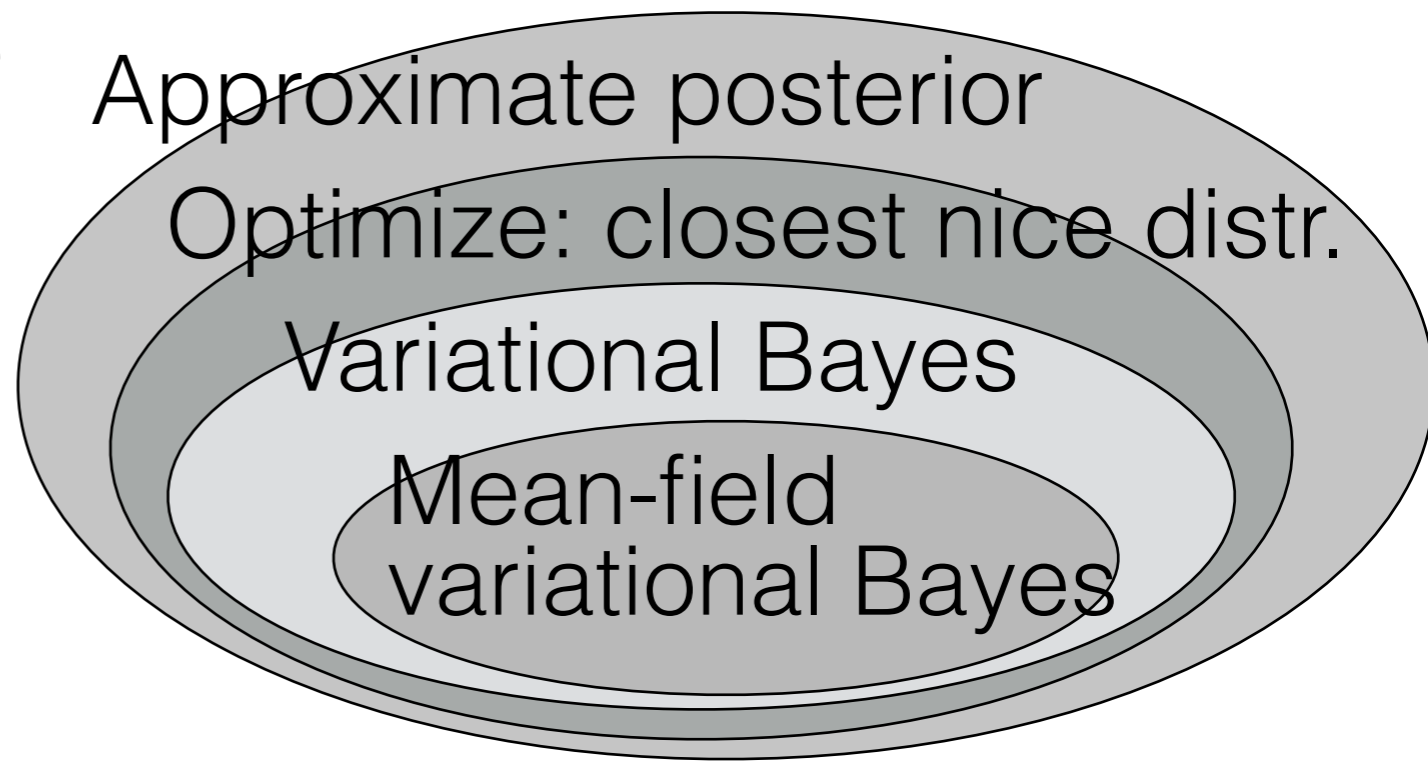
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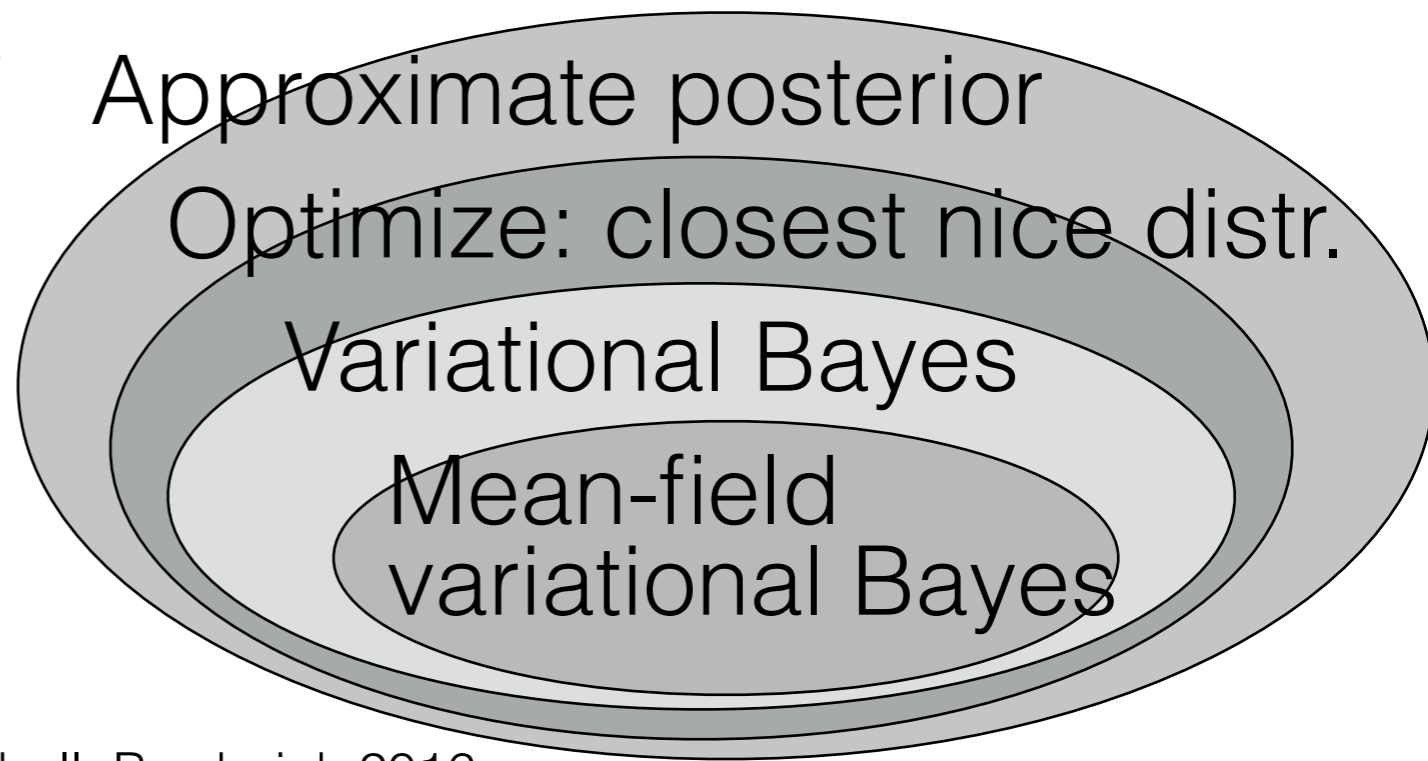
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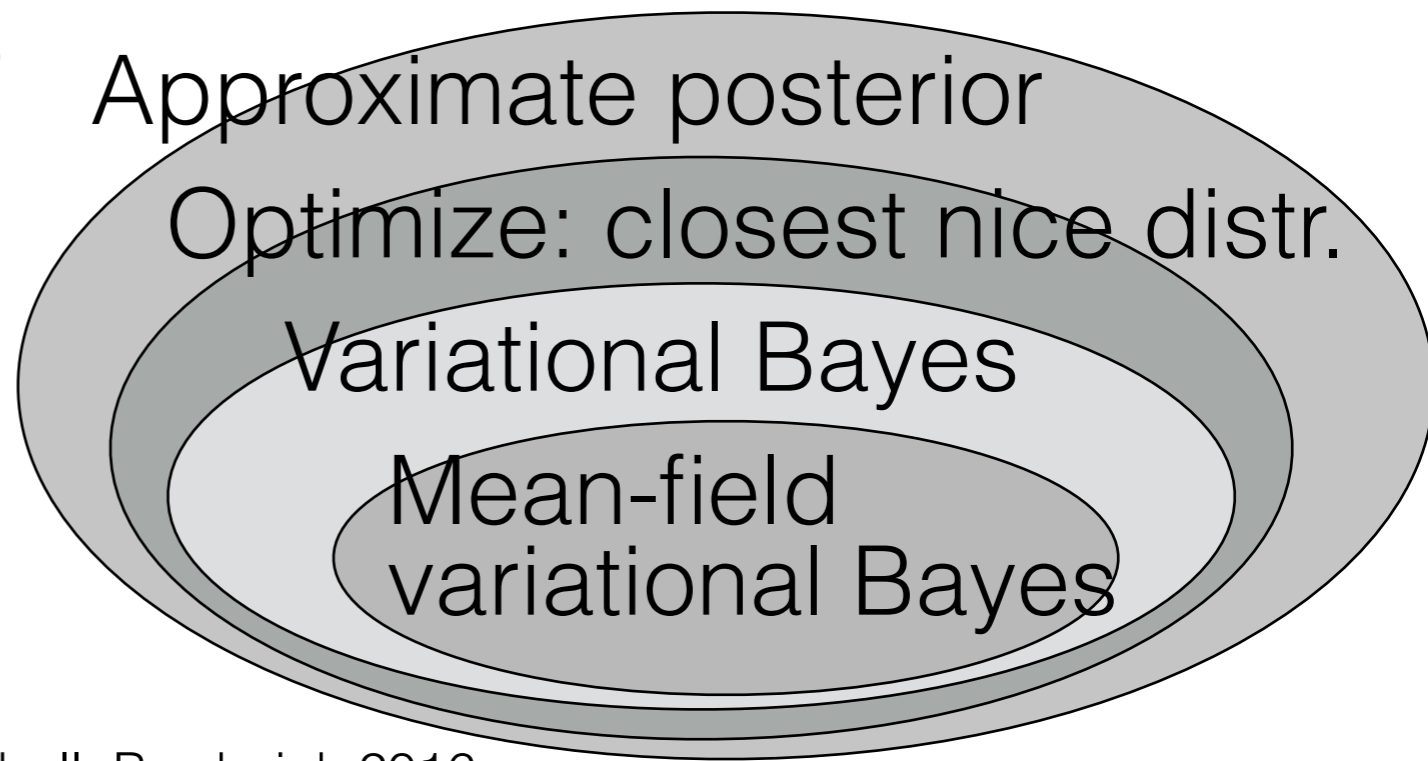


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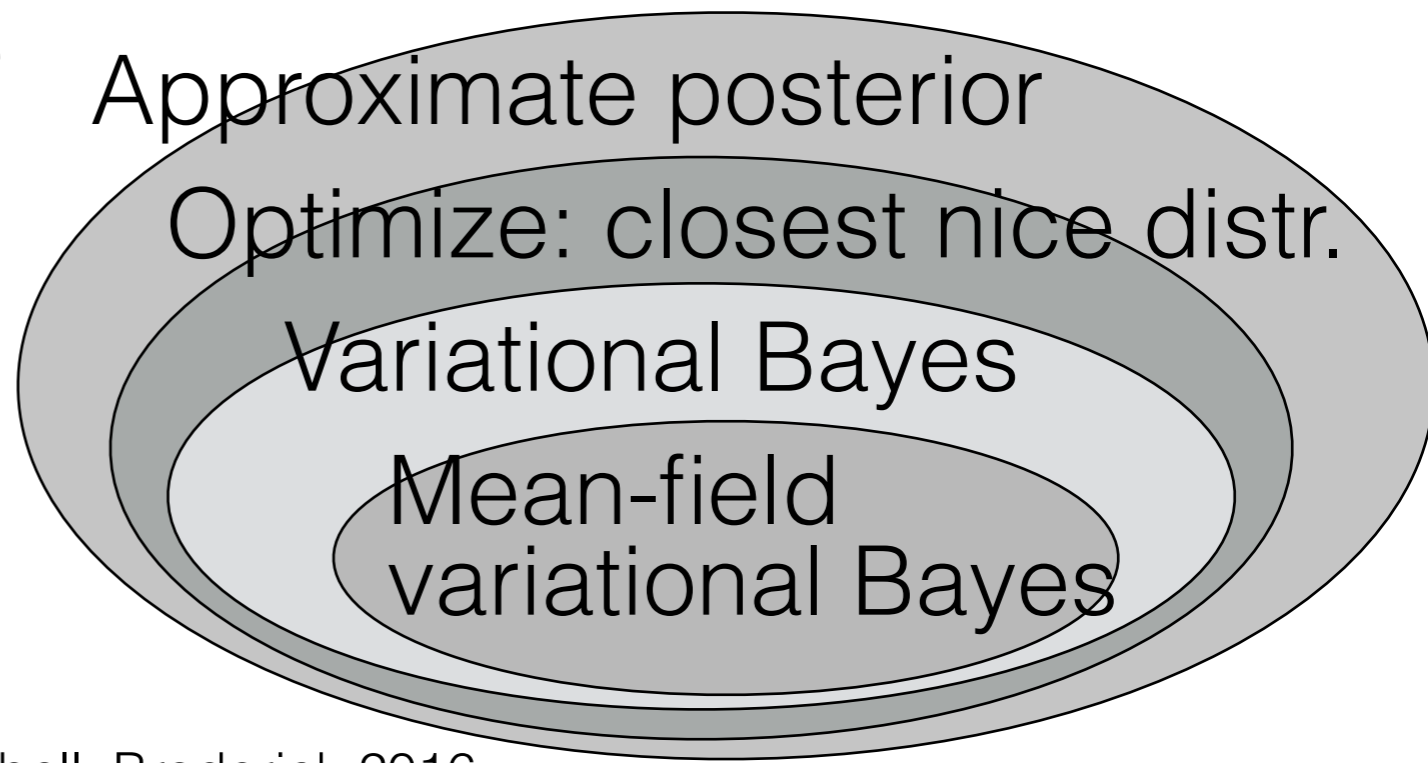


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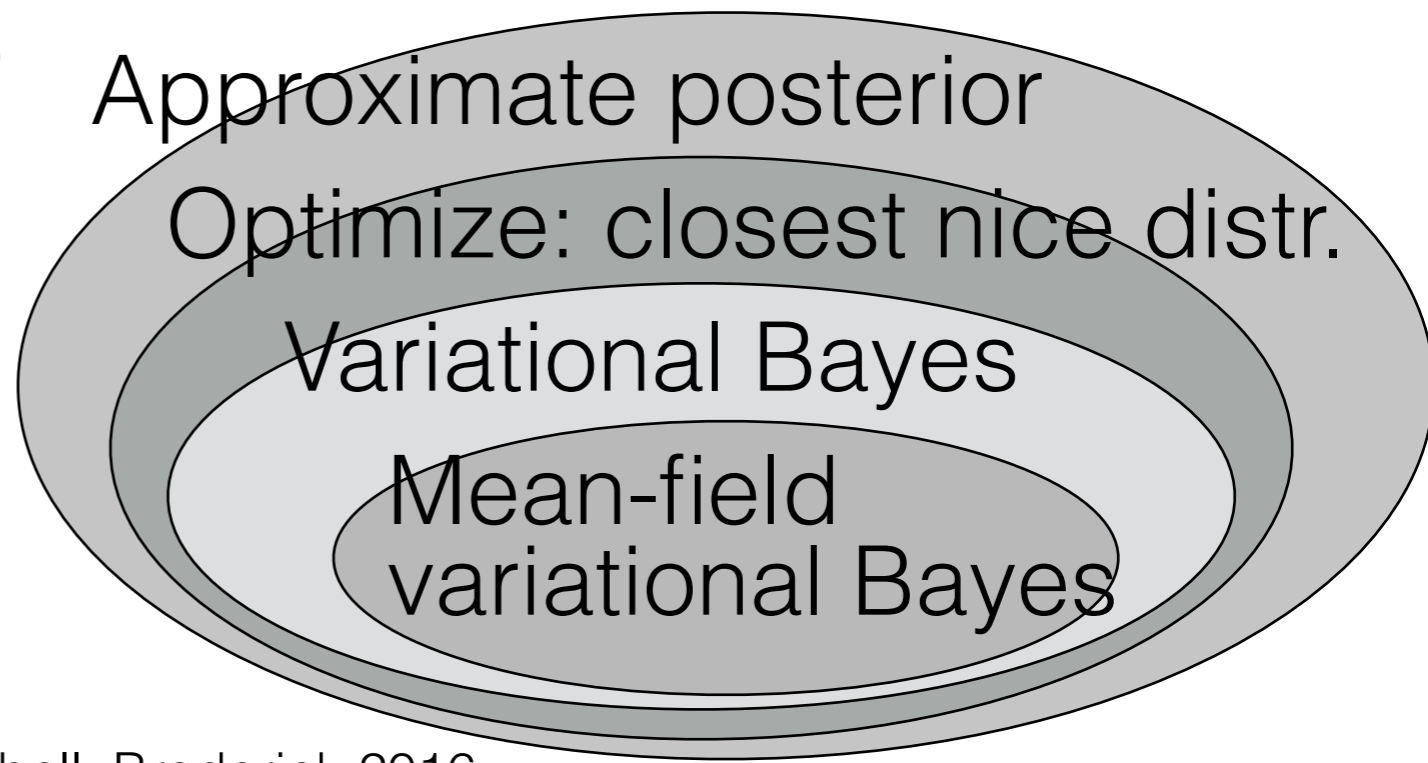


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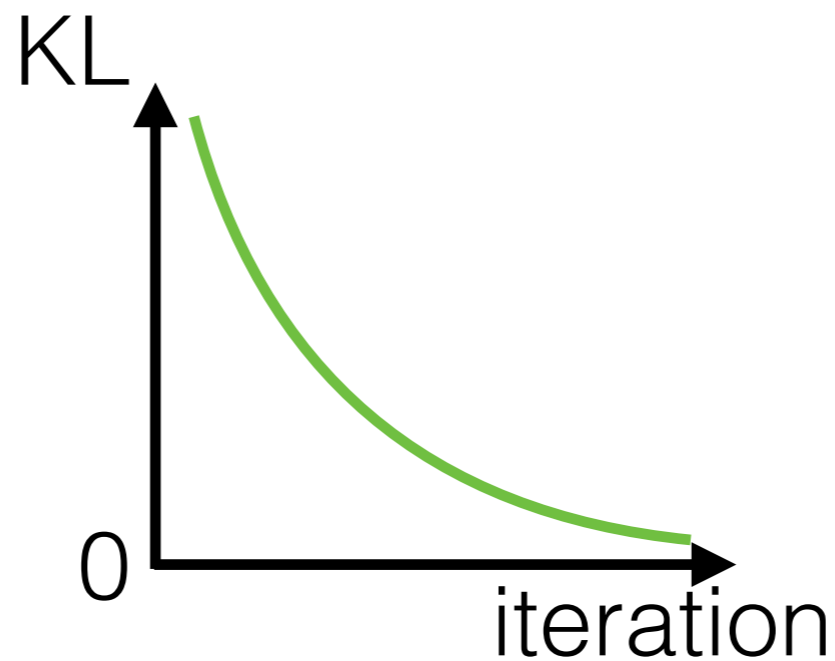
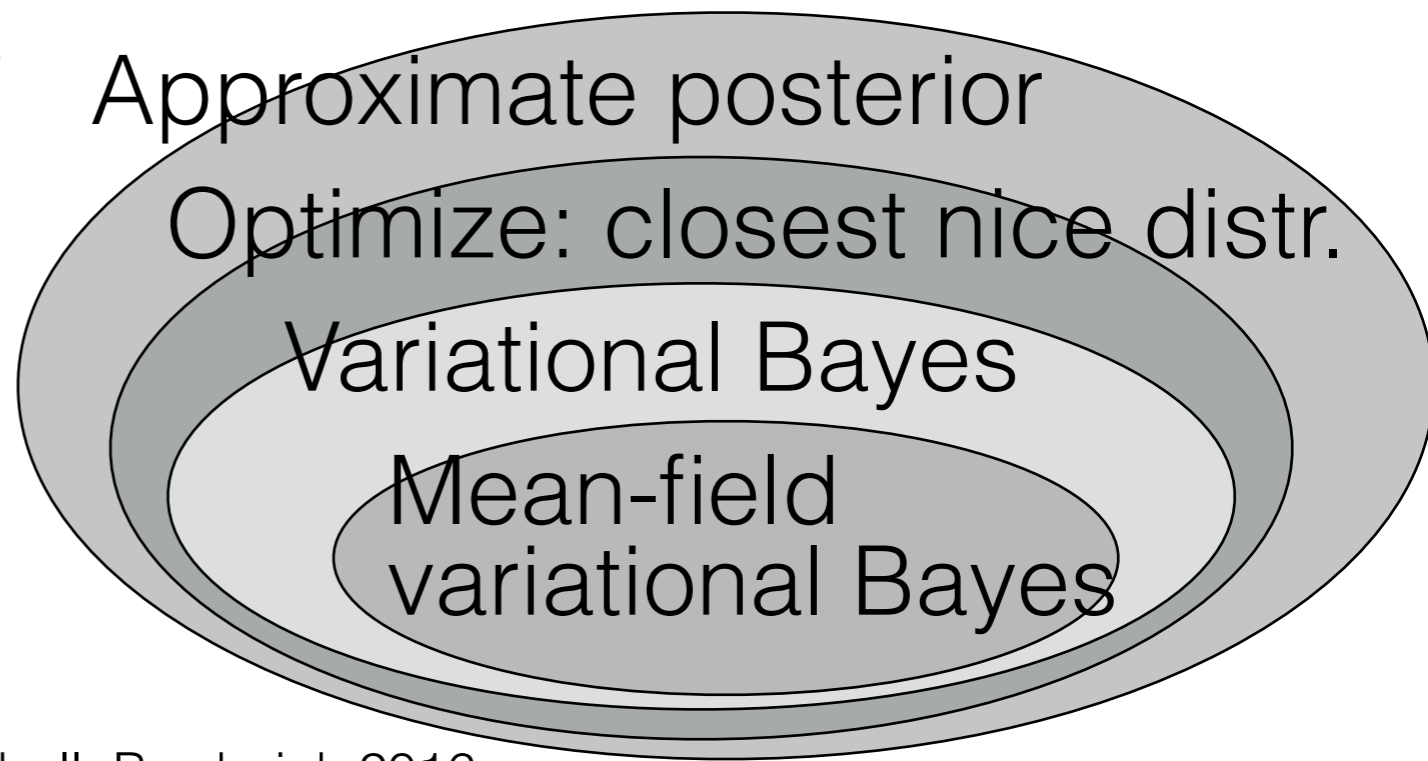


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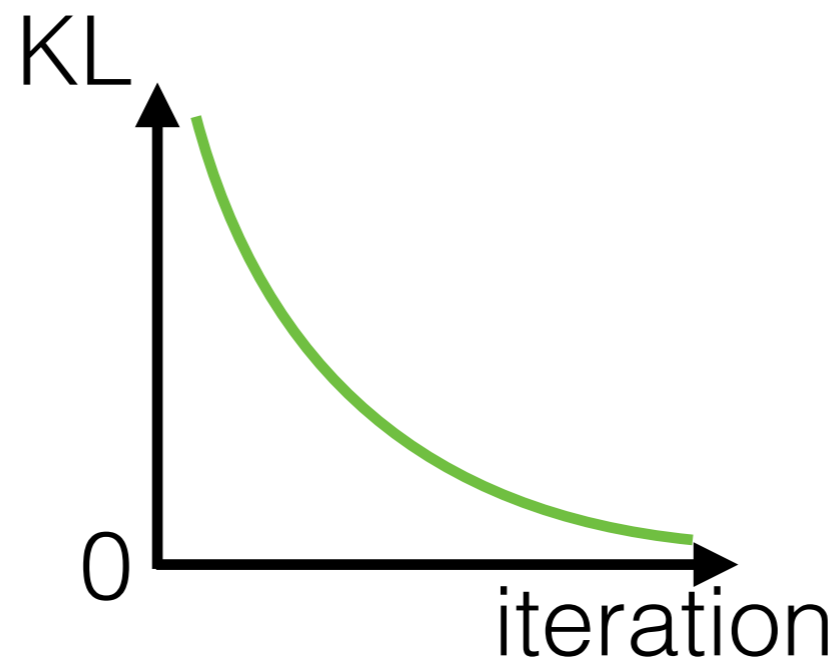
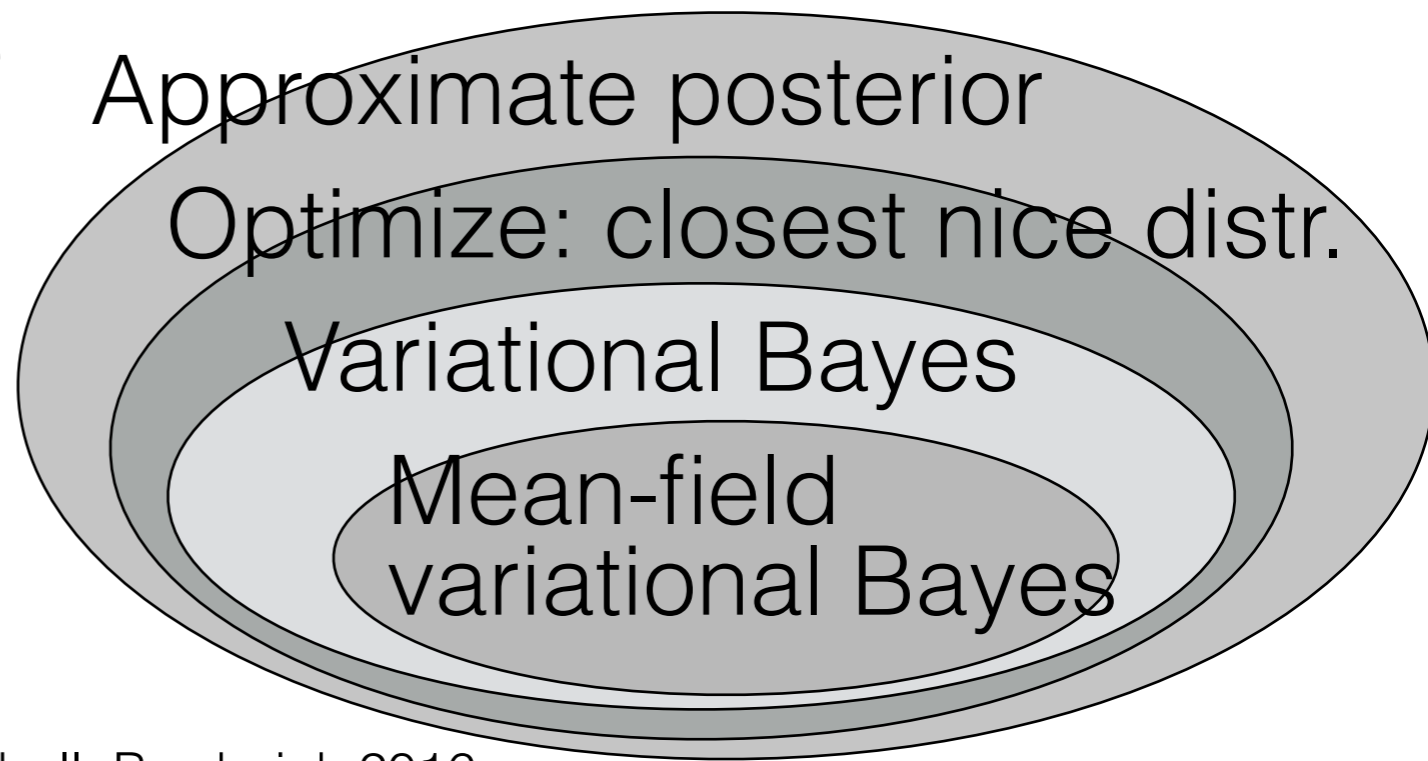


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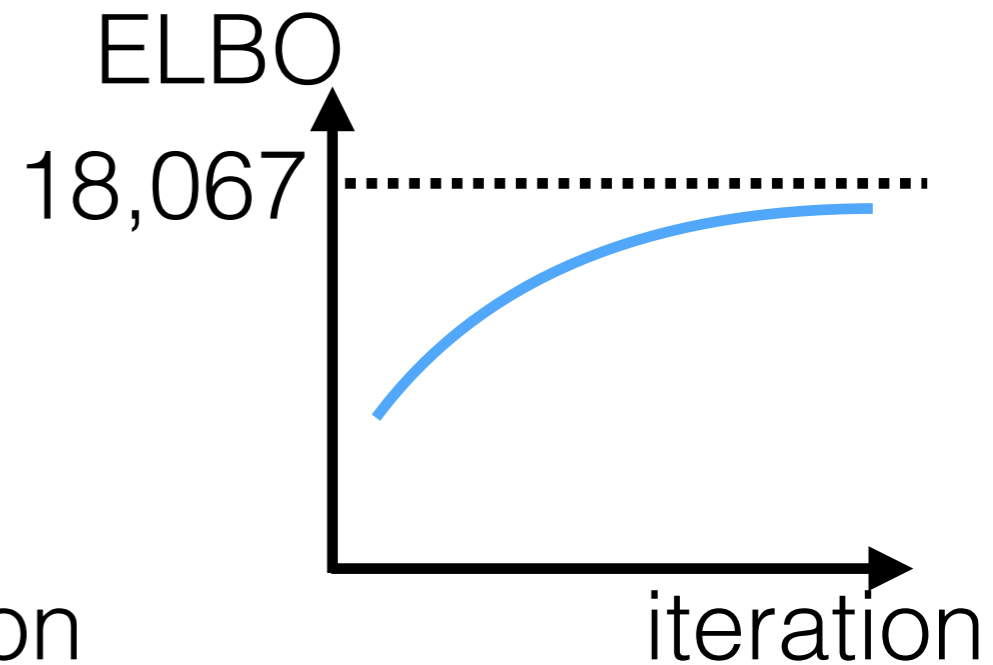
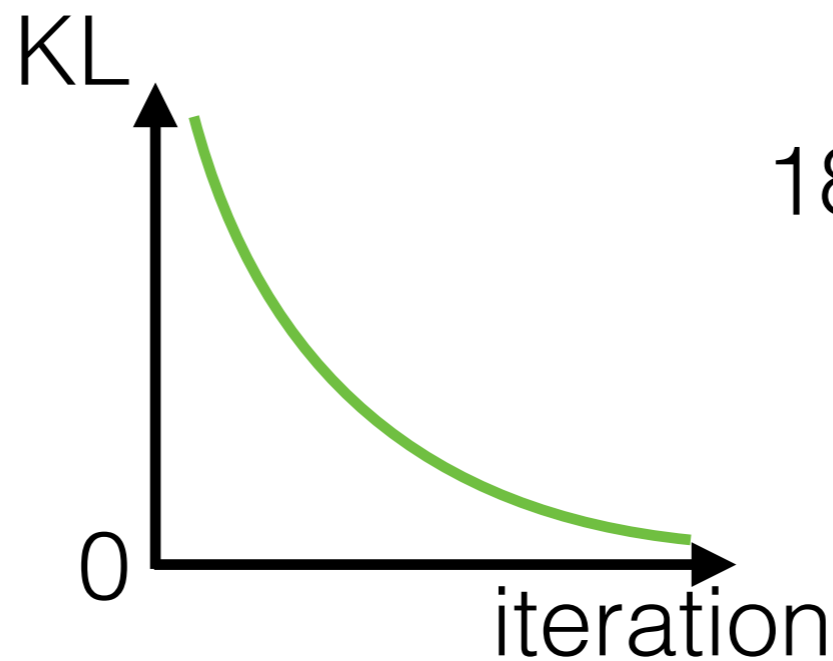
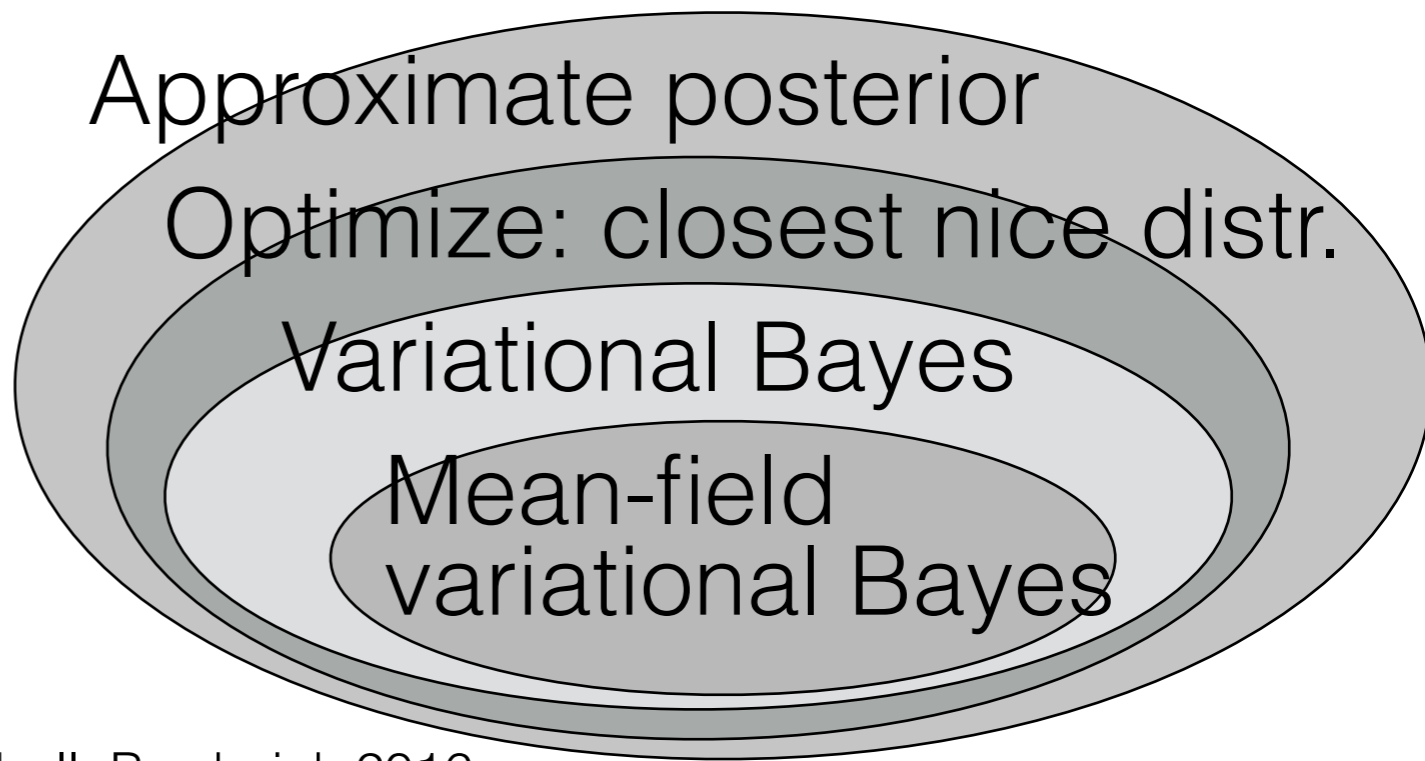


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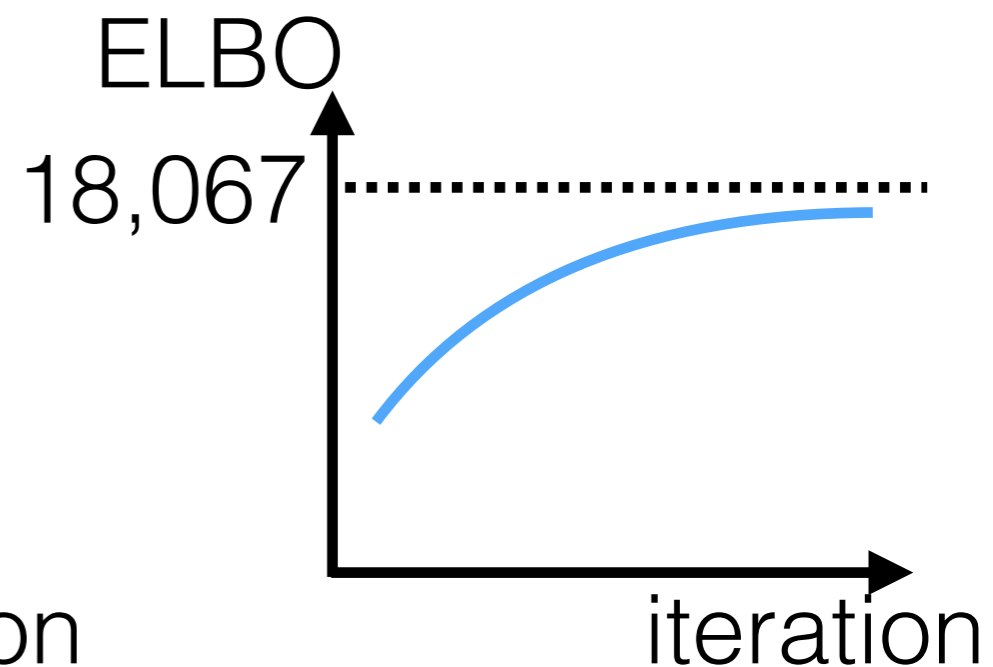
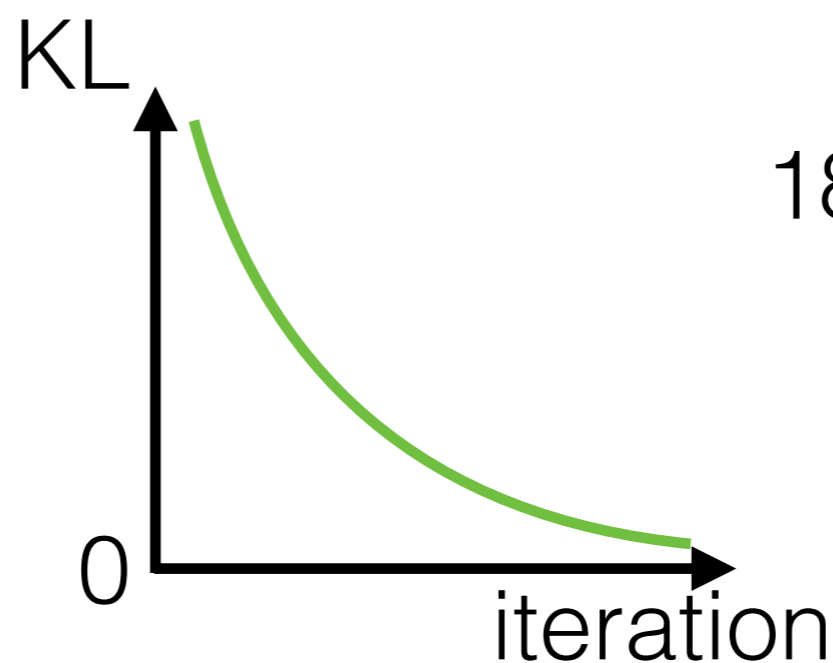
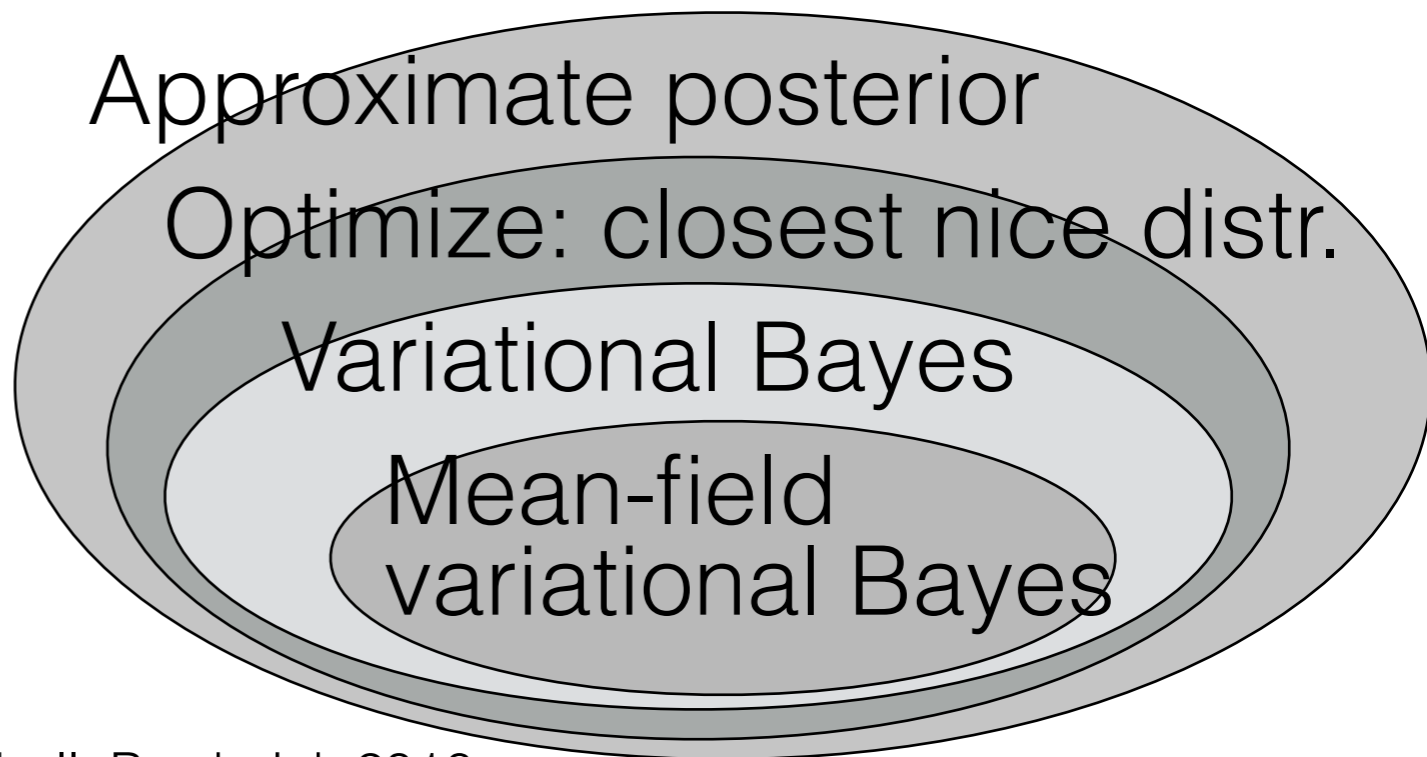
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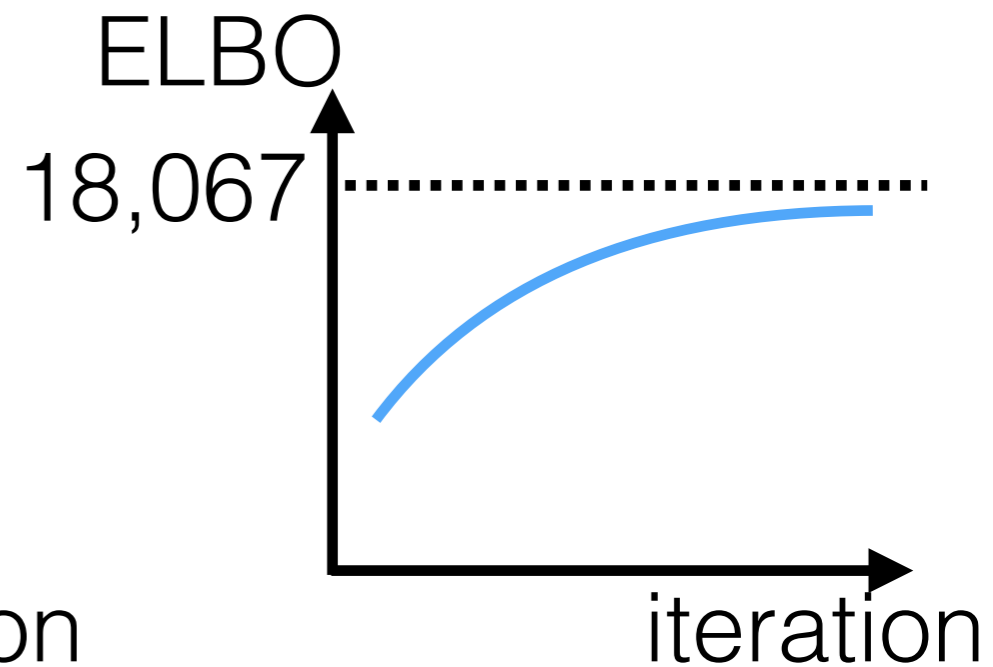
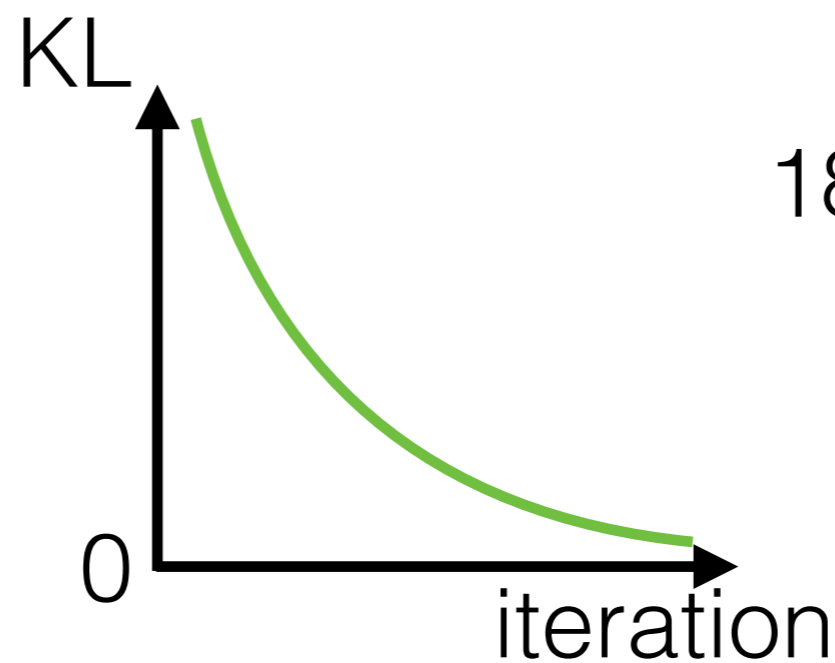
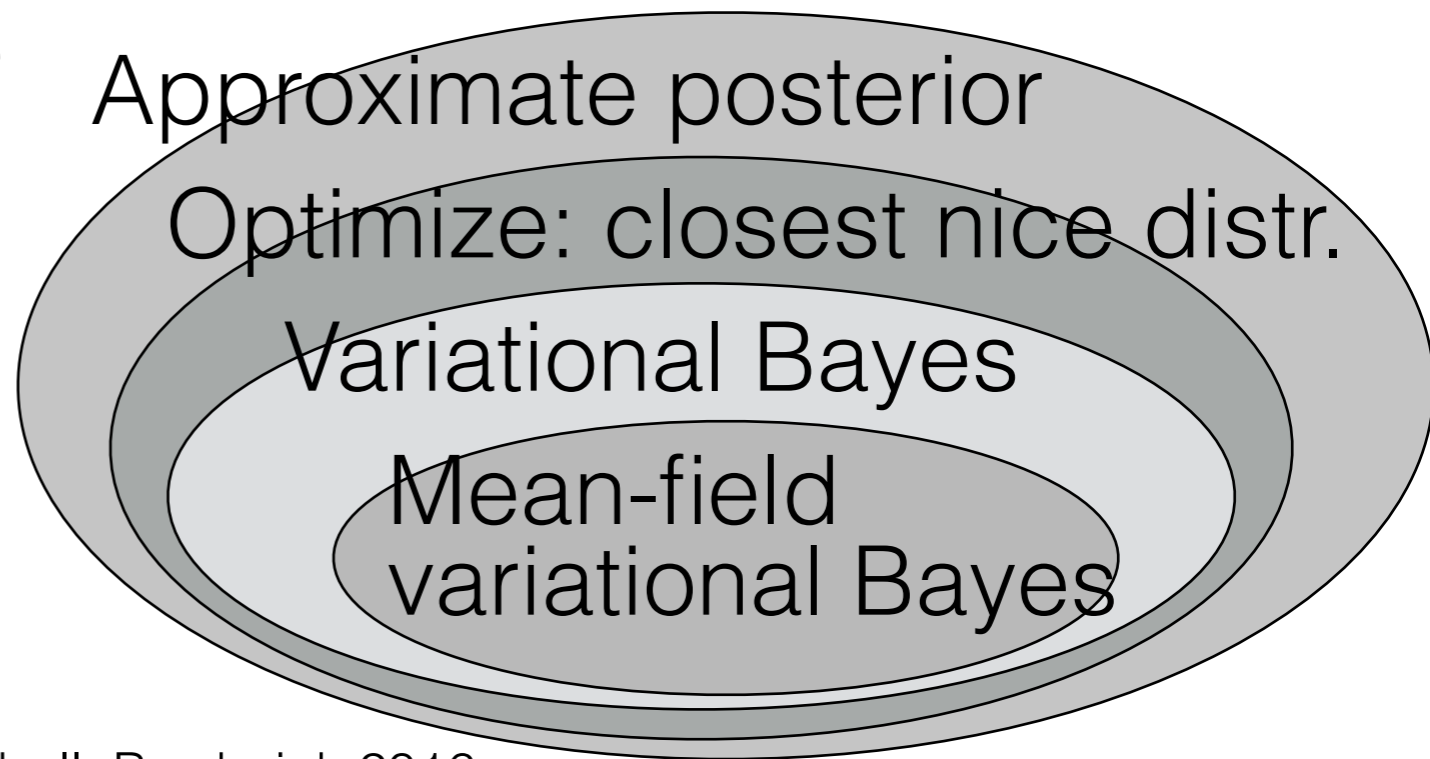
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- Diagnostics & workflow with theoretical guarantees
“Validated Variational Inference via Practical Posterior Error Bounds”

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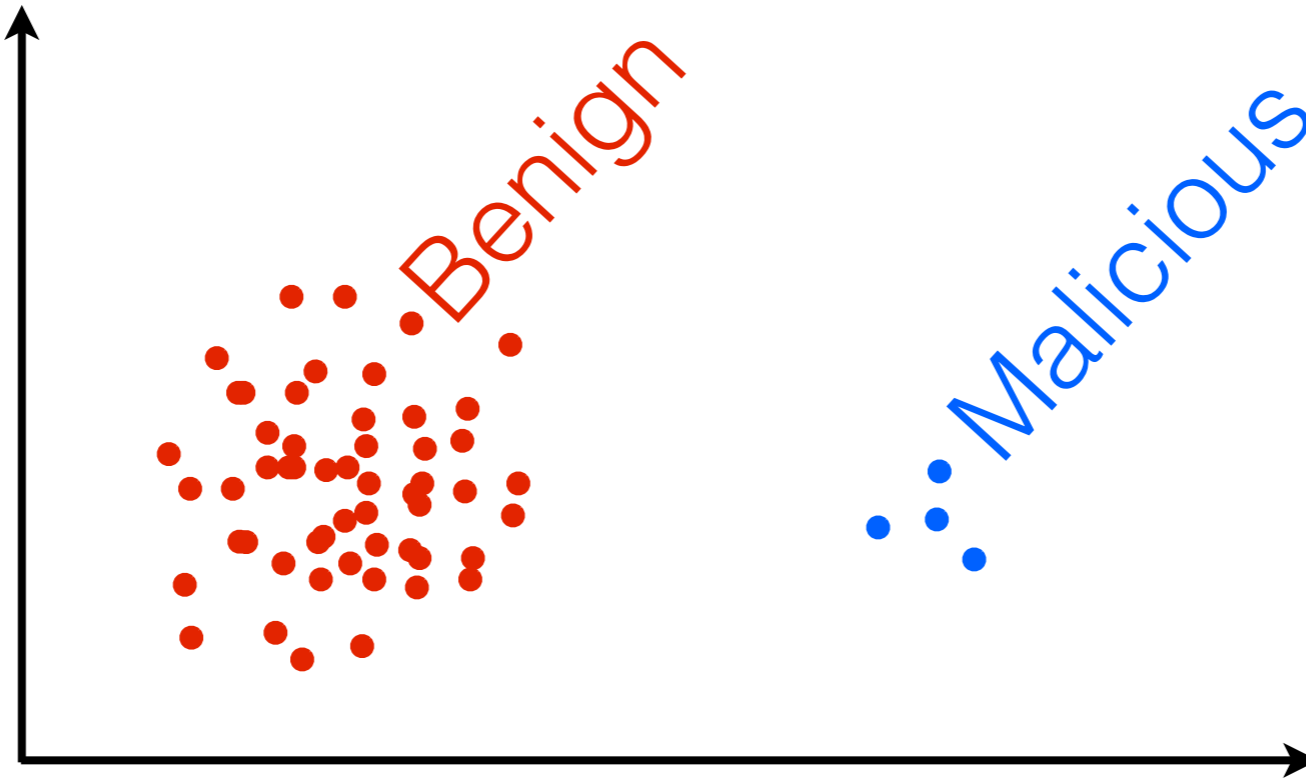
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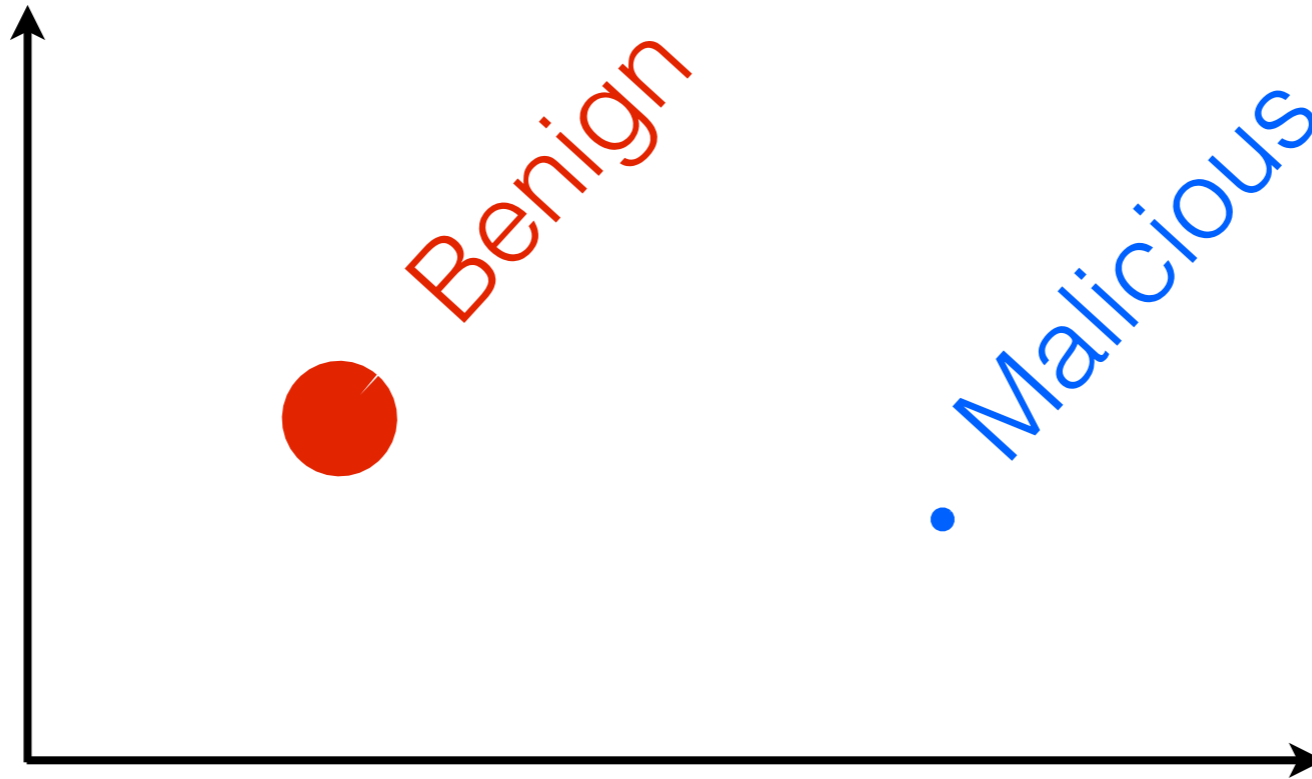
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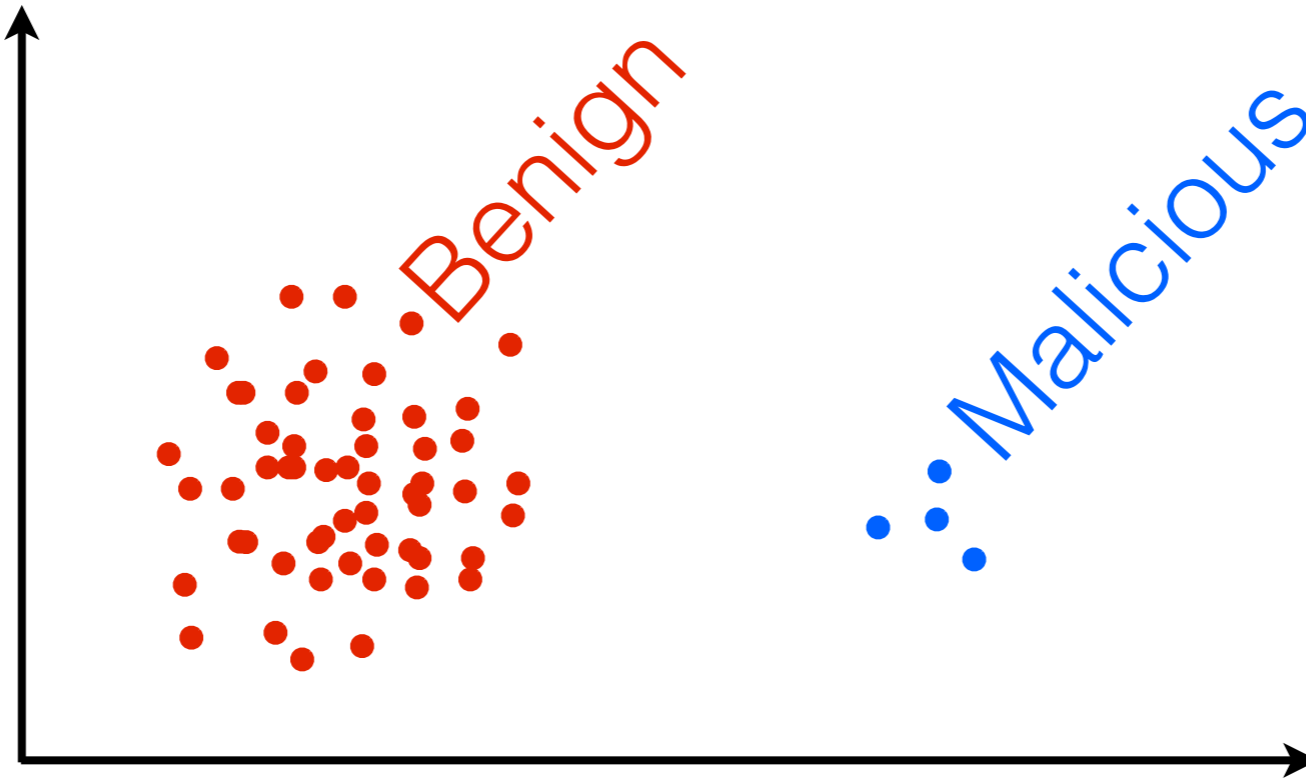
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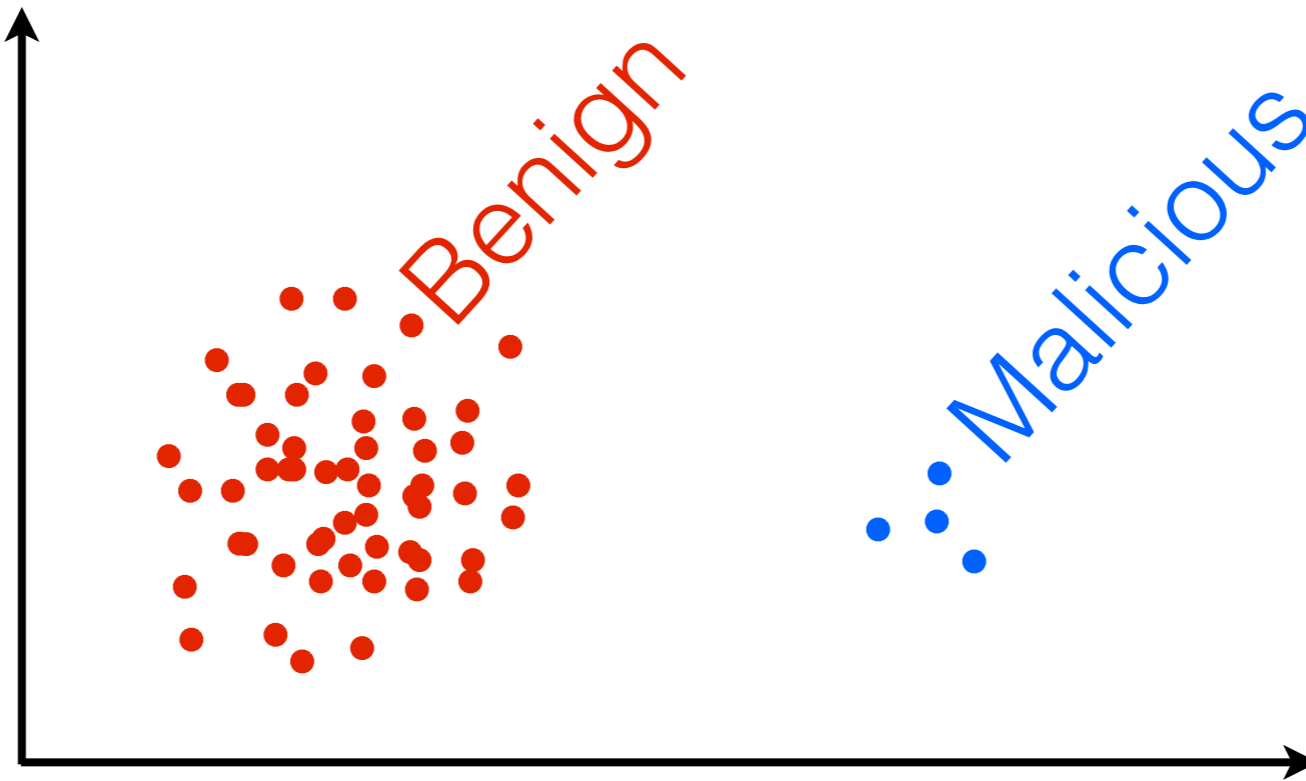
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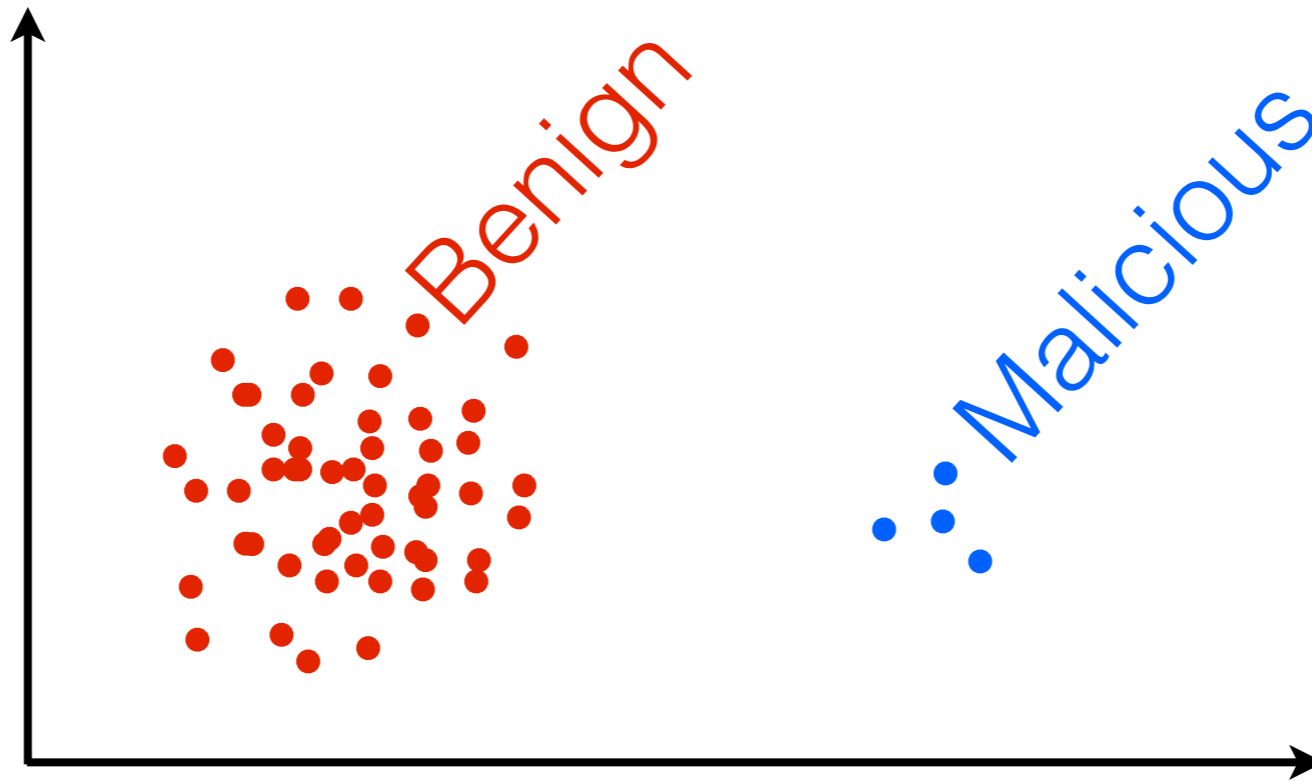
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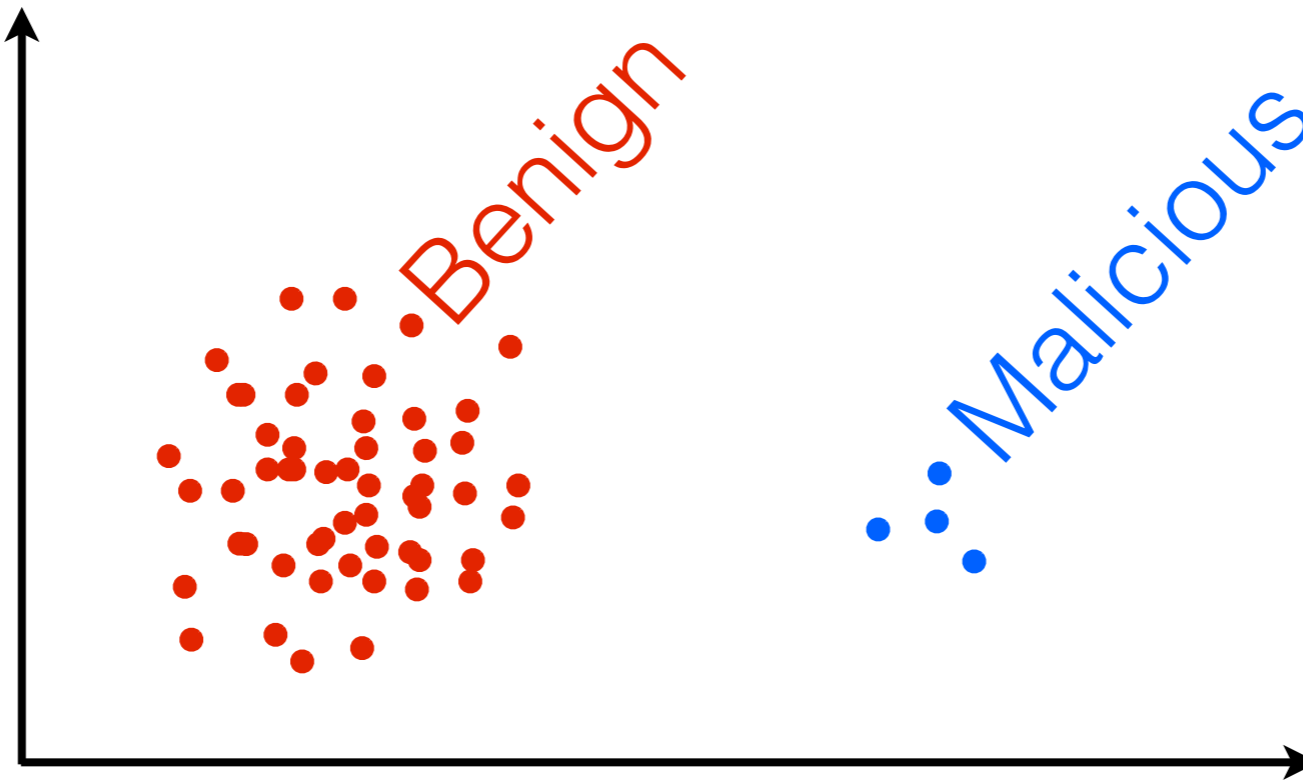
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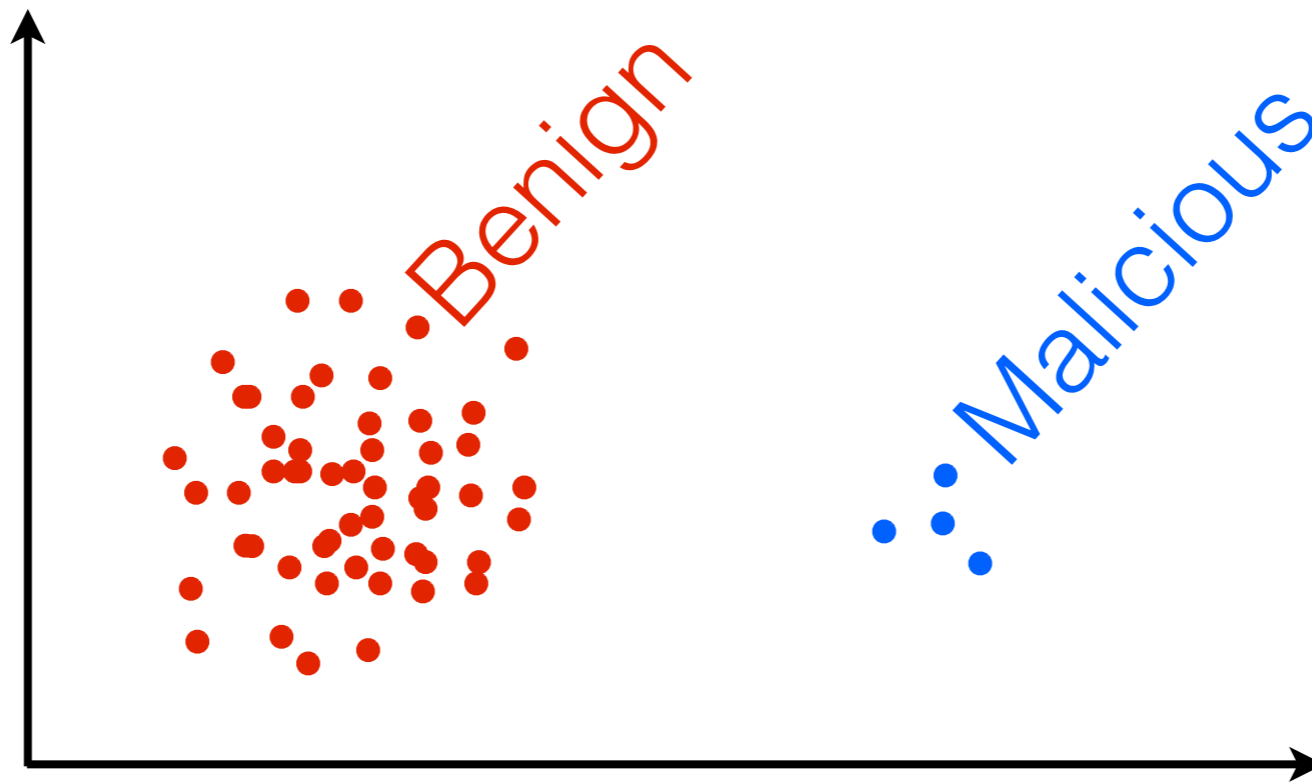
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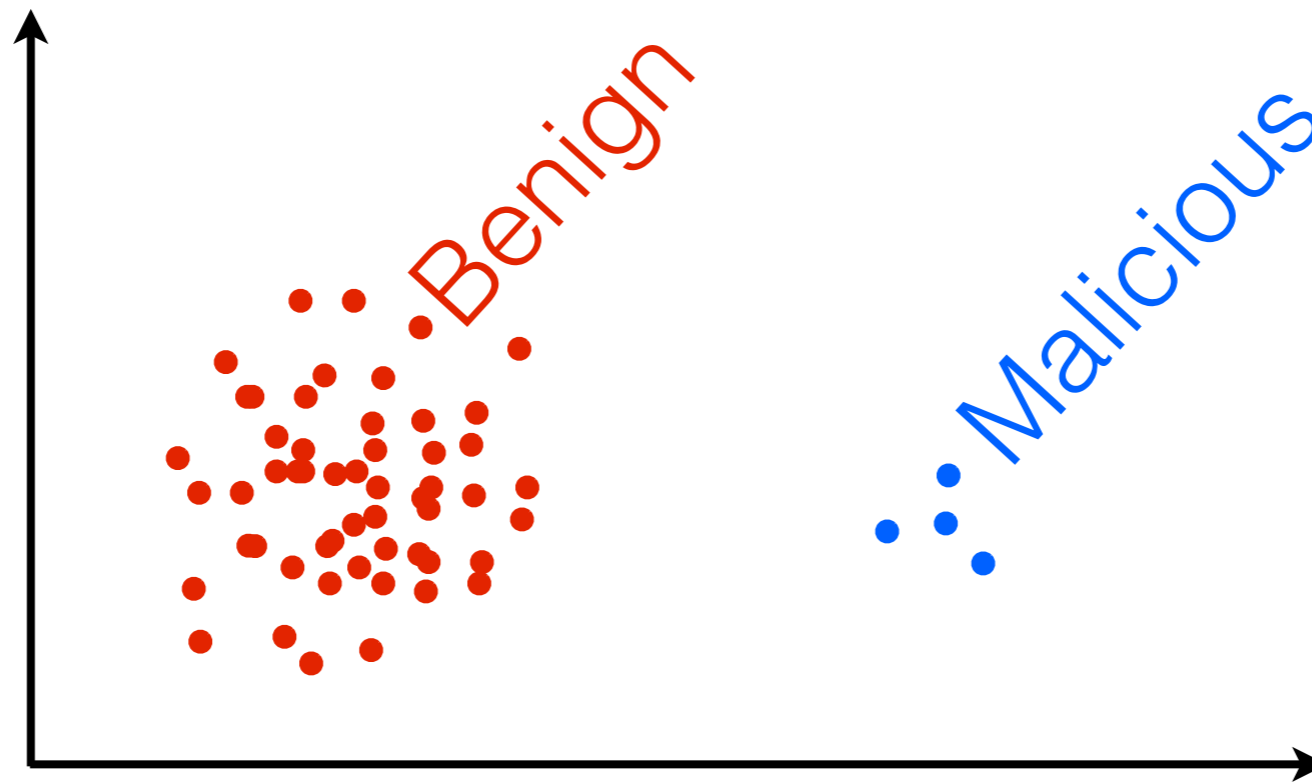
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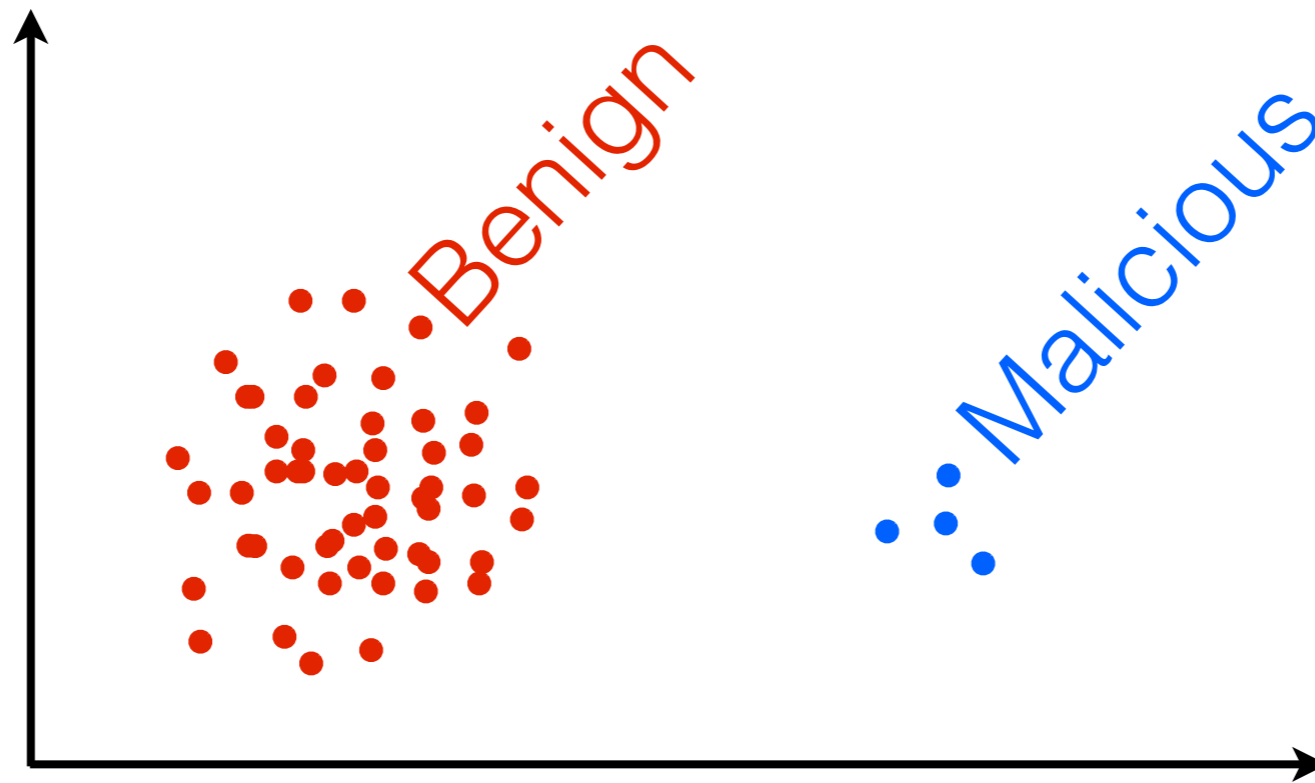
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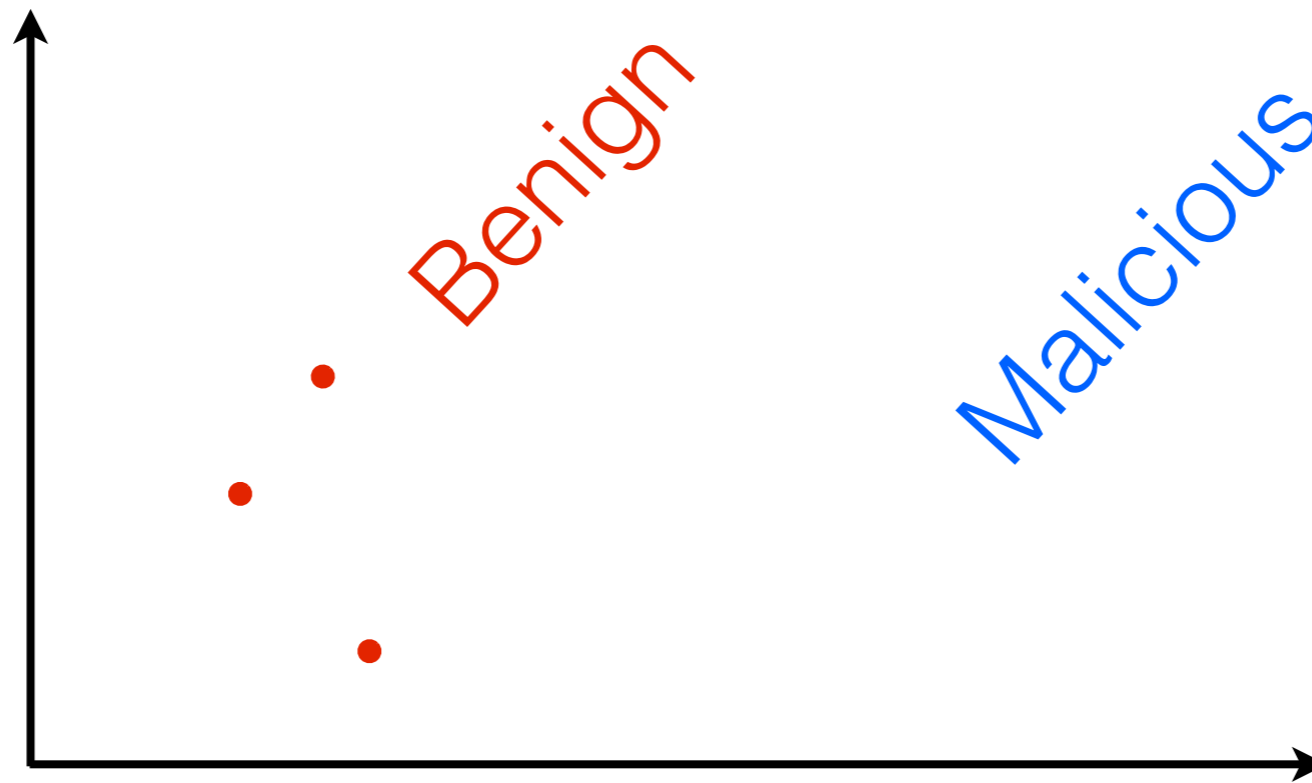


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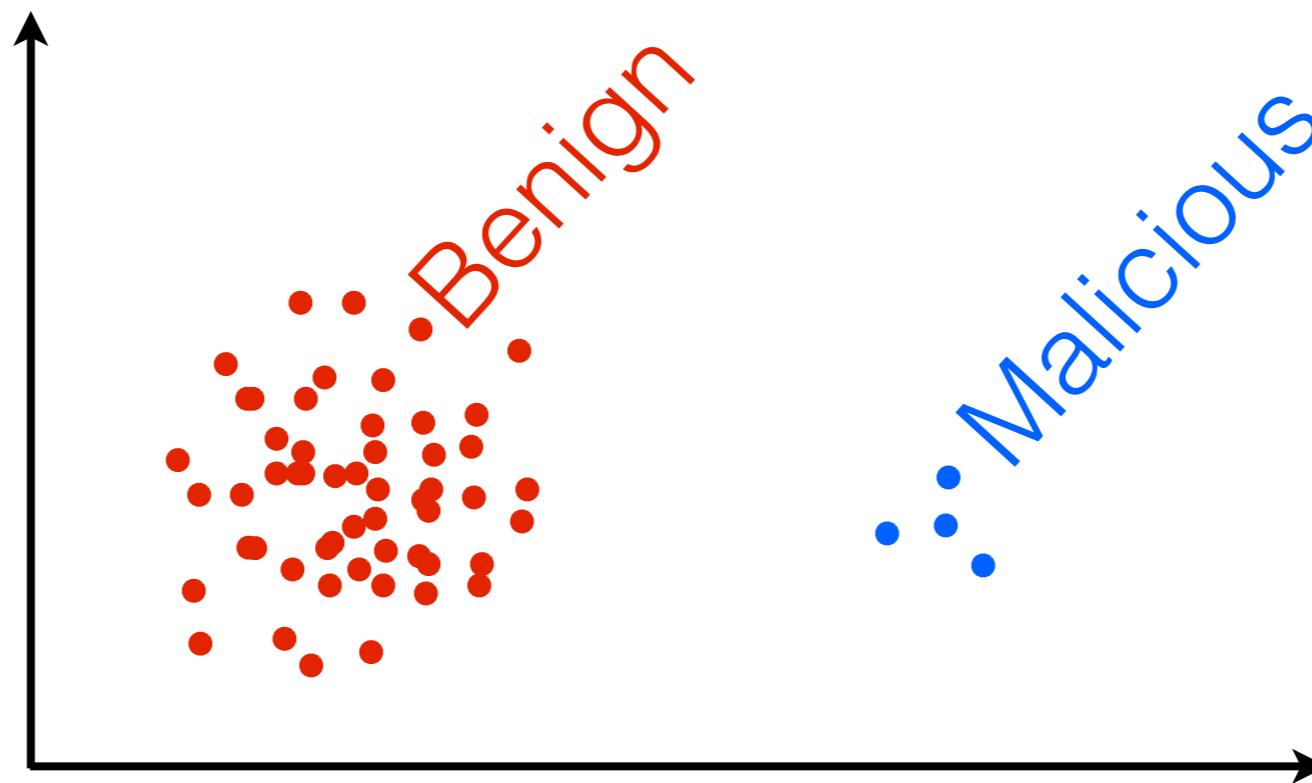


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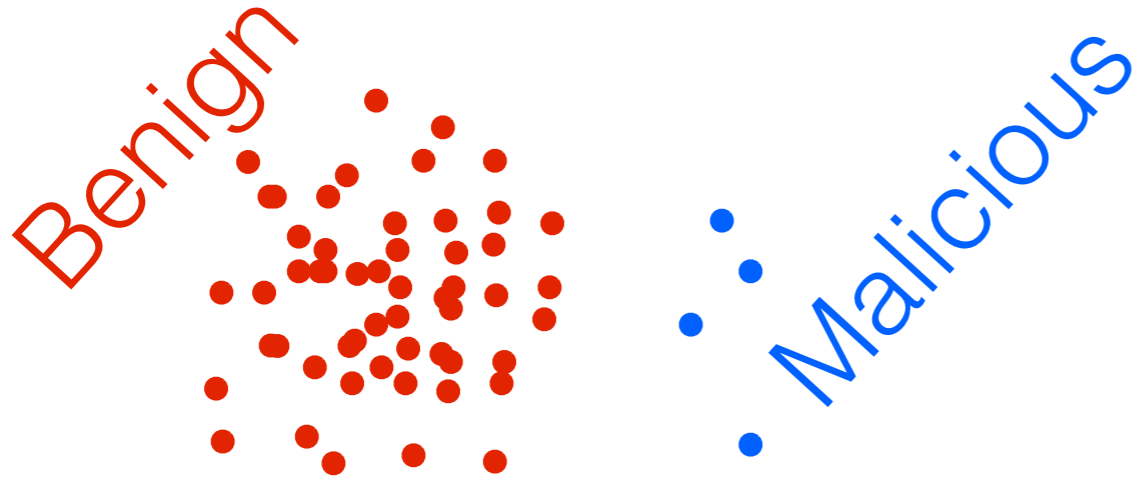
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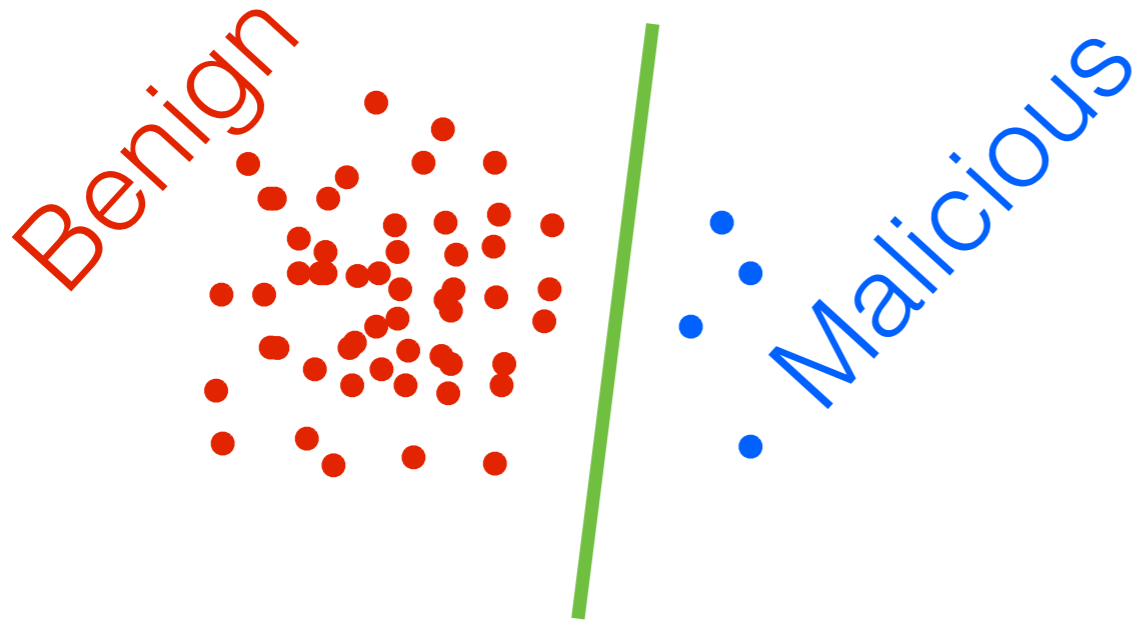
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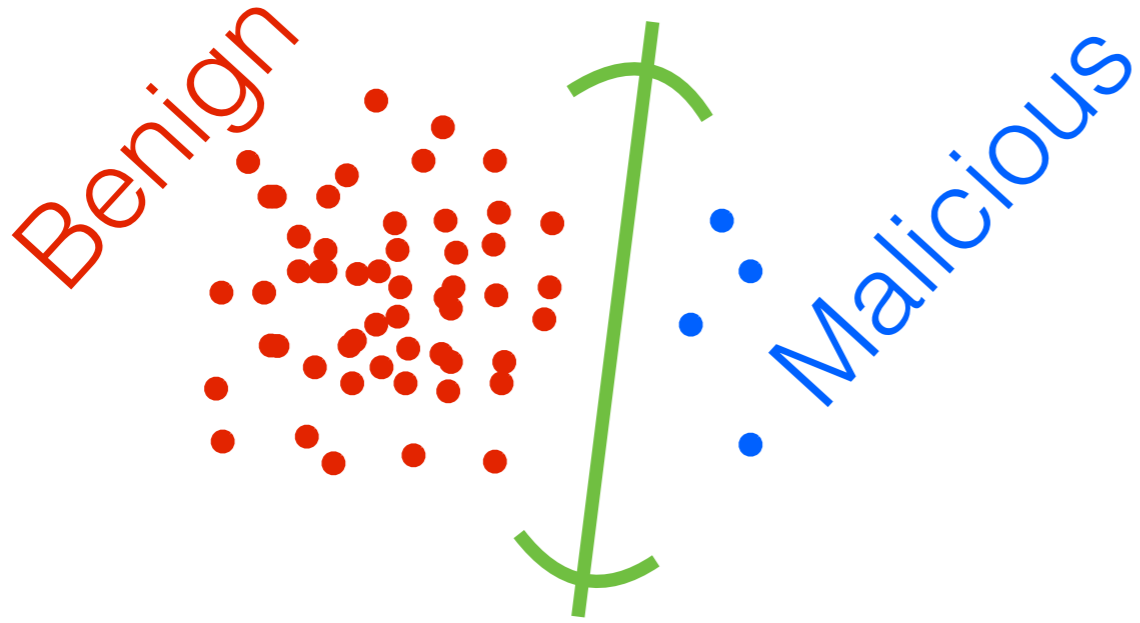
Uniform subsampling



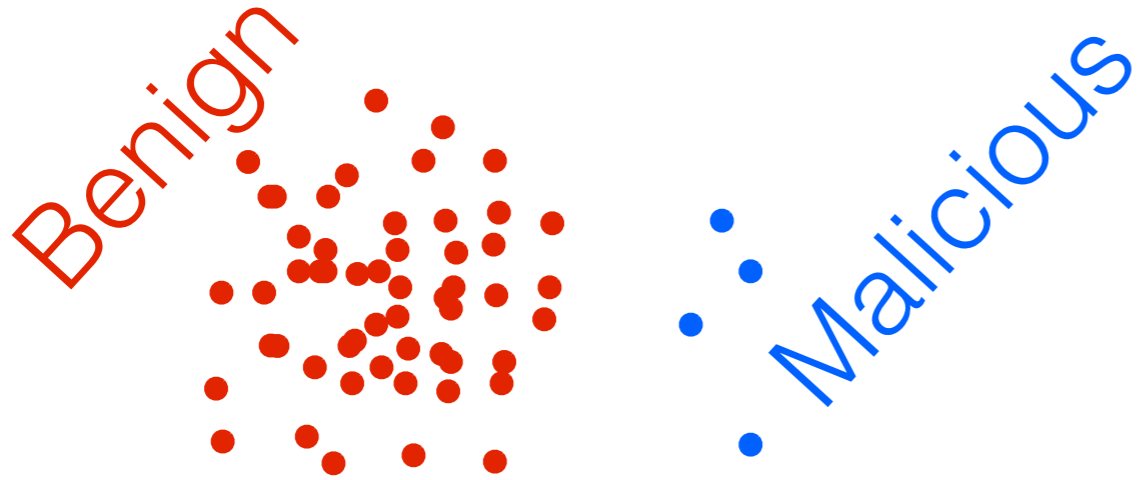
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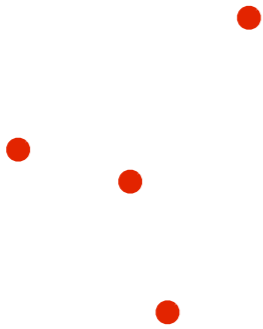


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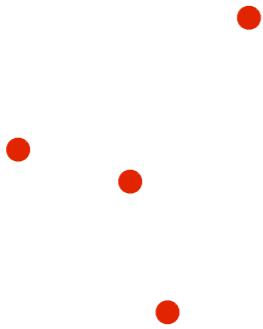
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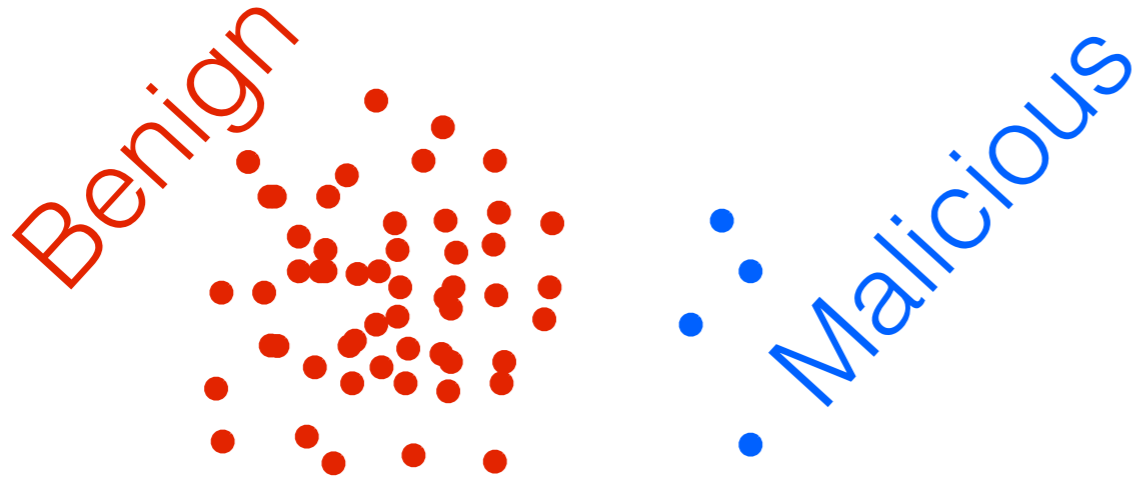
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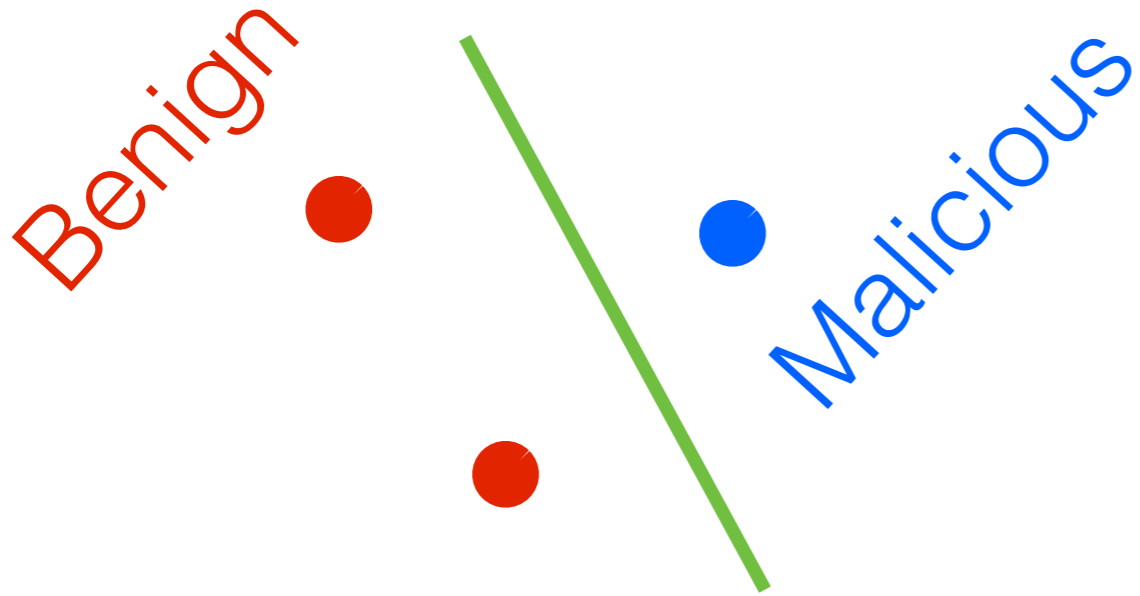
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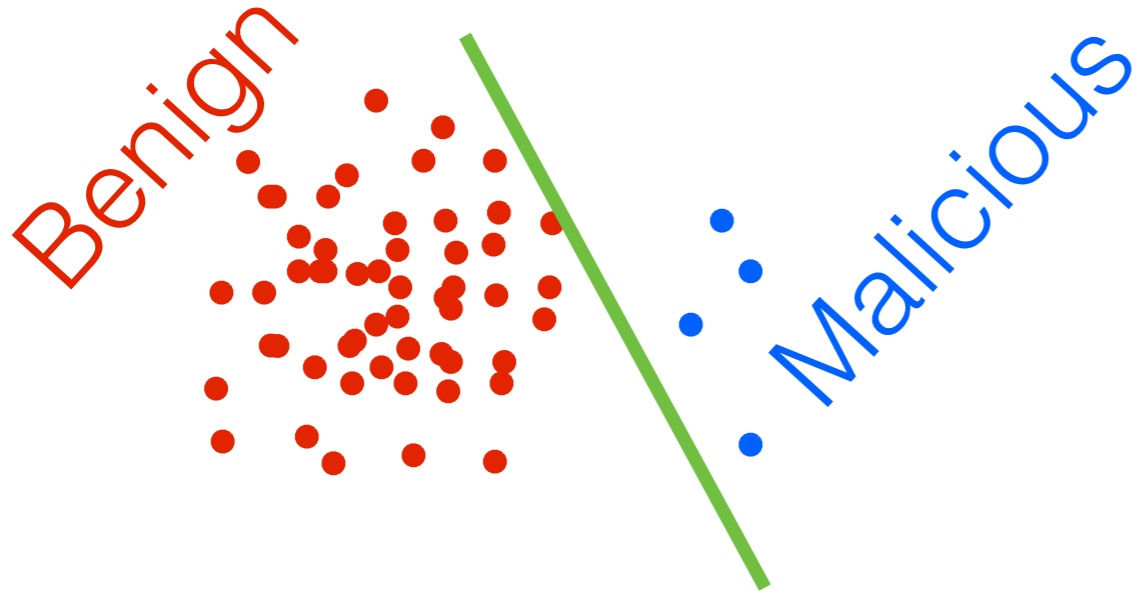
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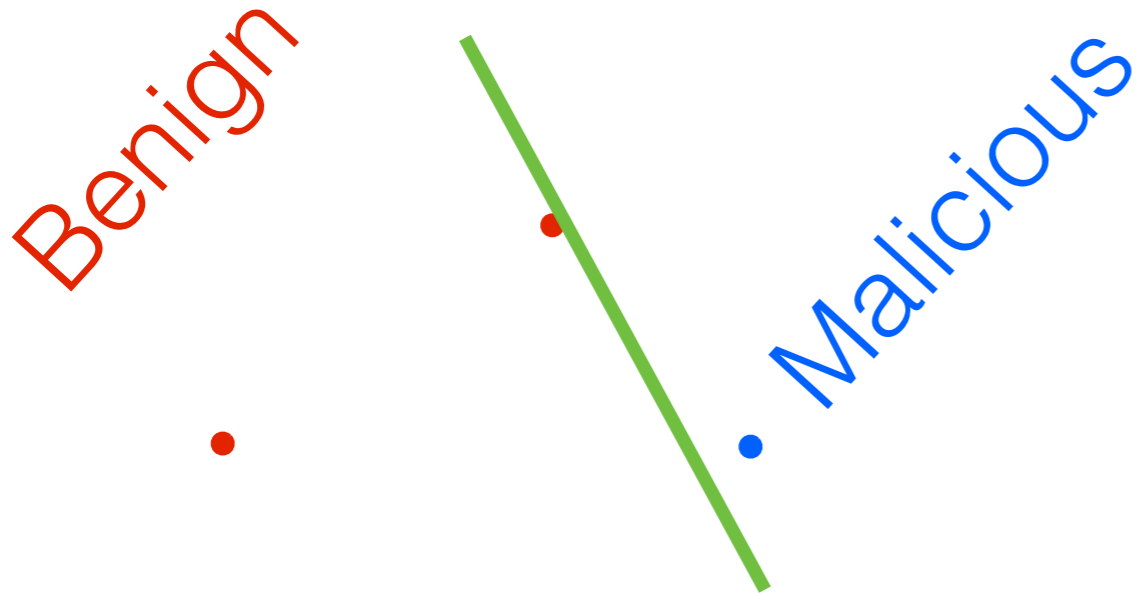
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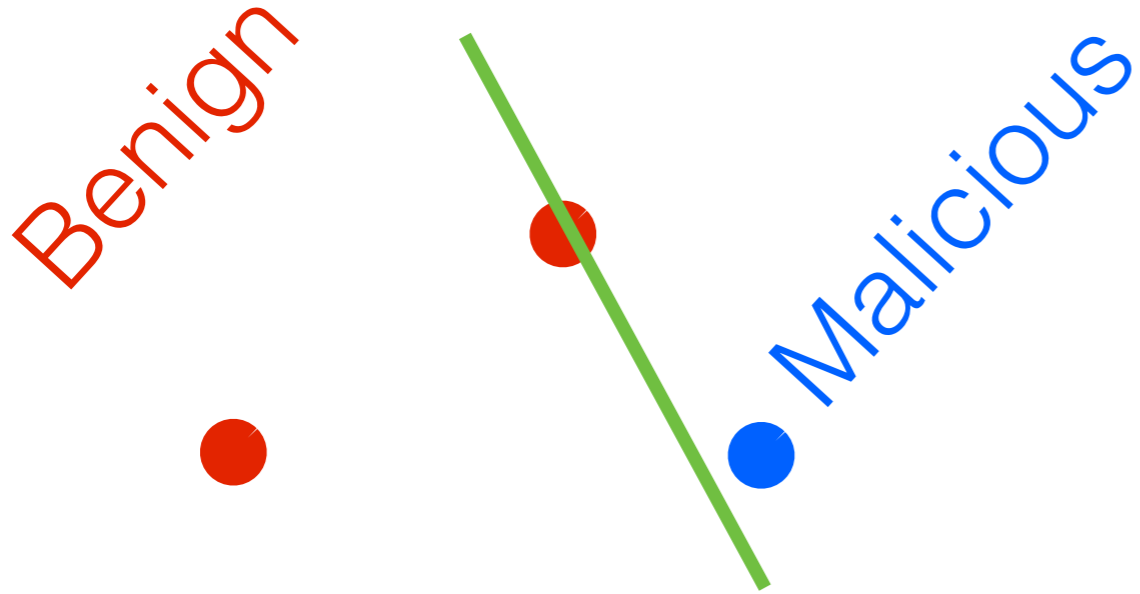
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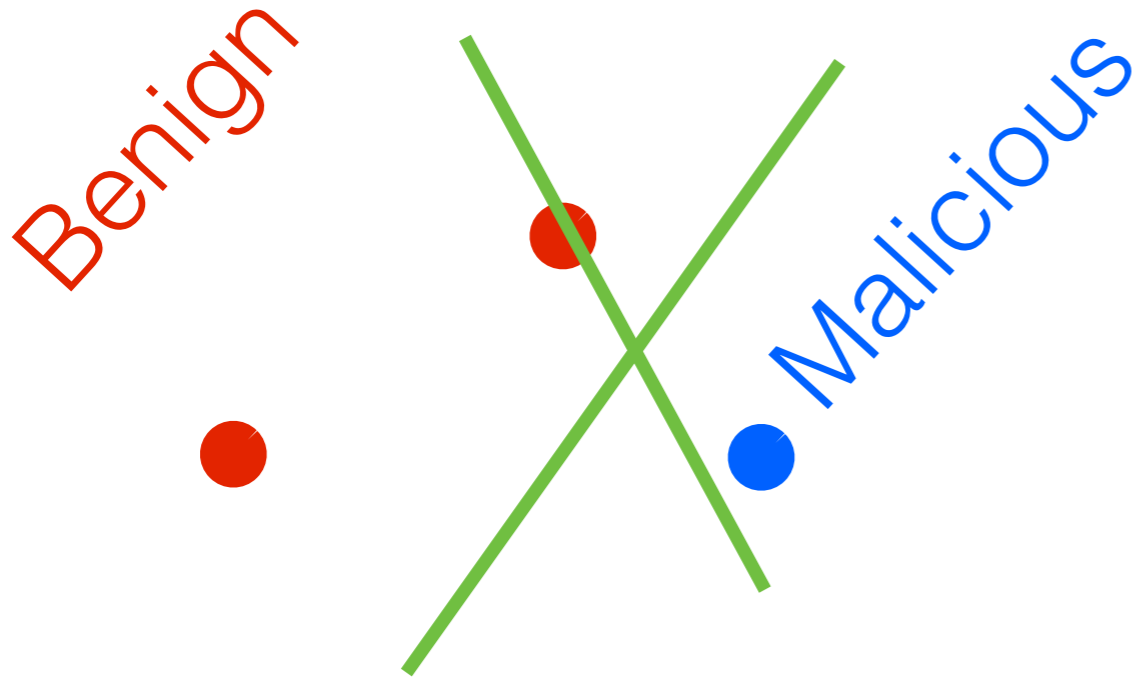
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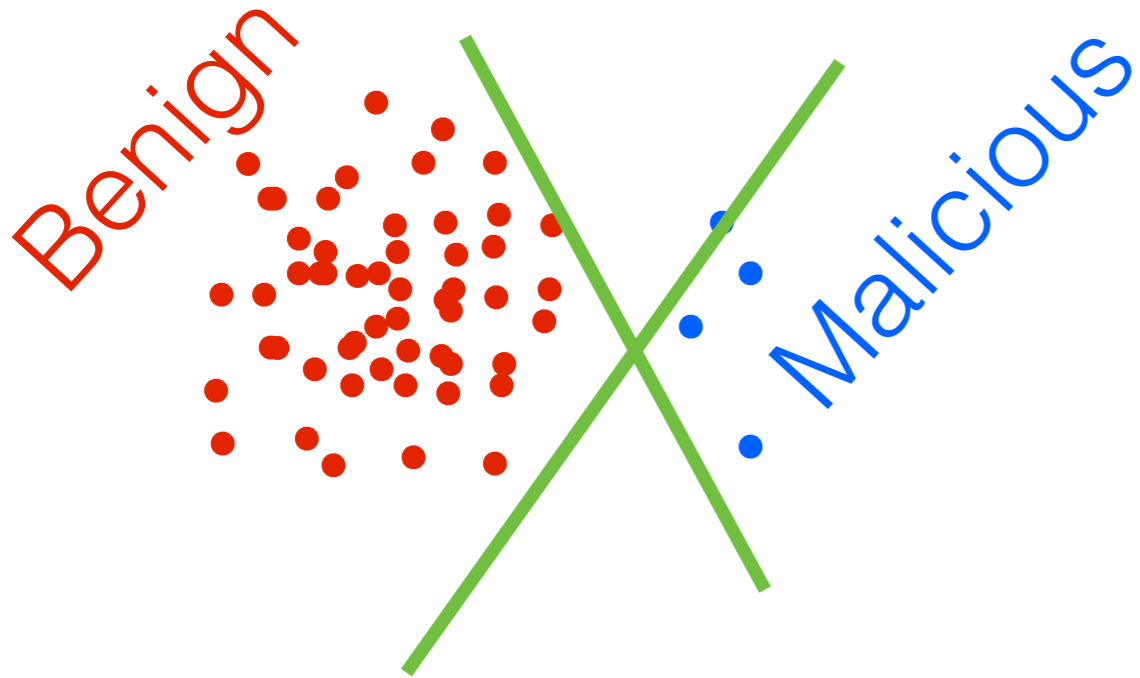
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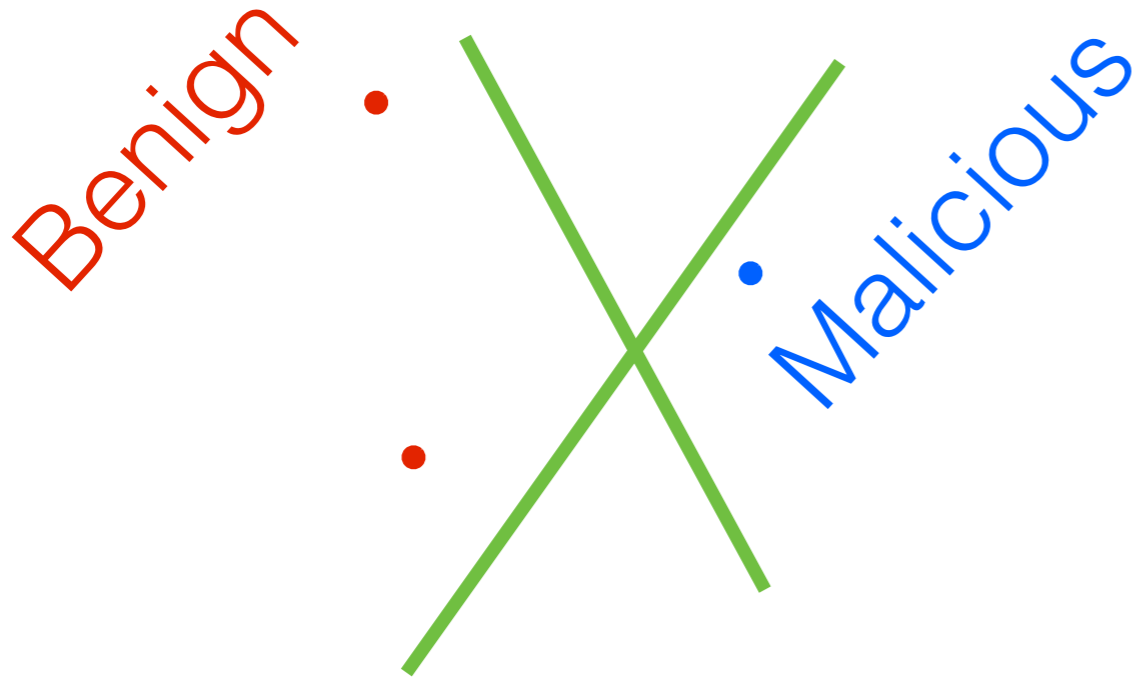
- Might miss important data

Uniform subsampling



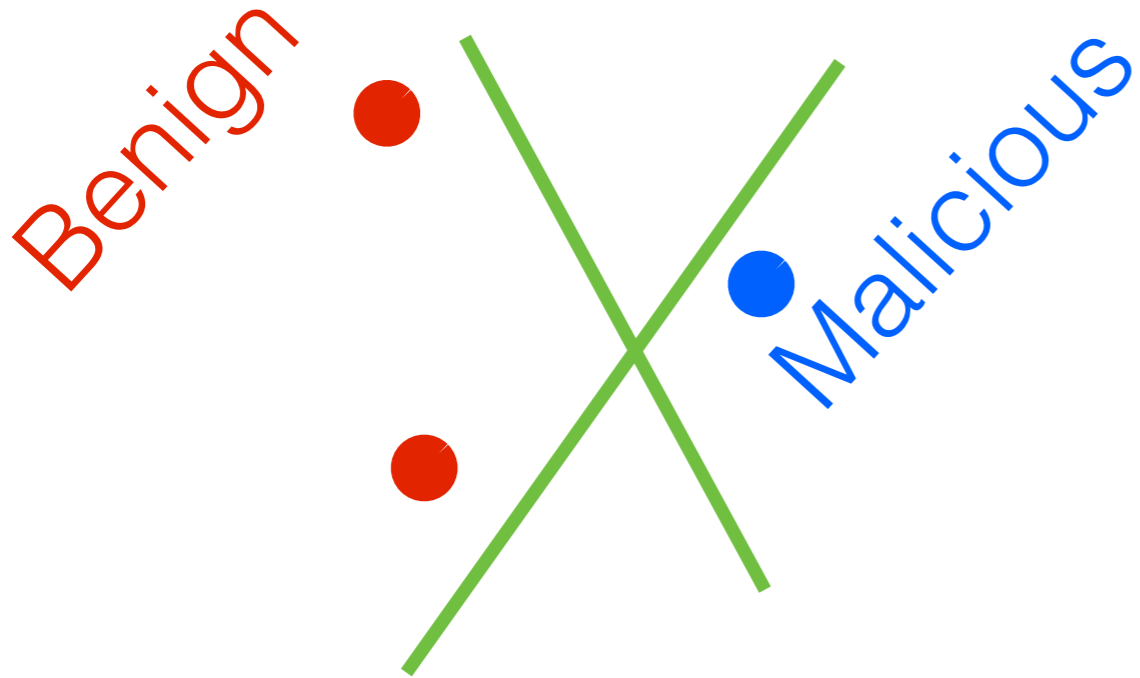
- Might miss important data

Uniform subsampling



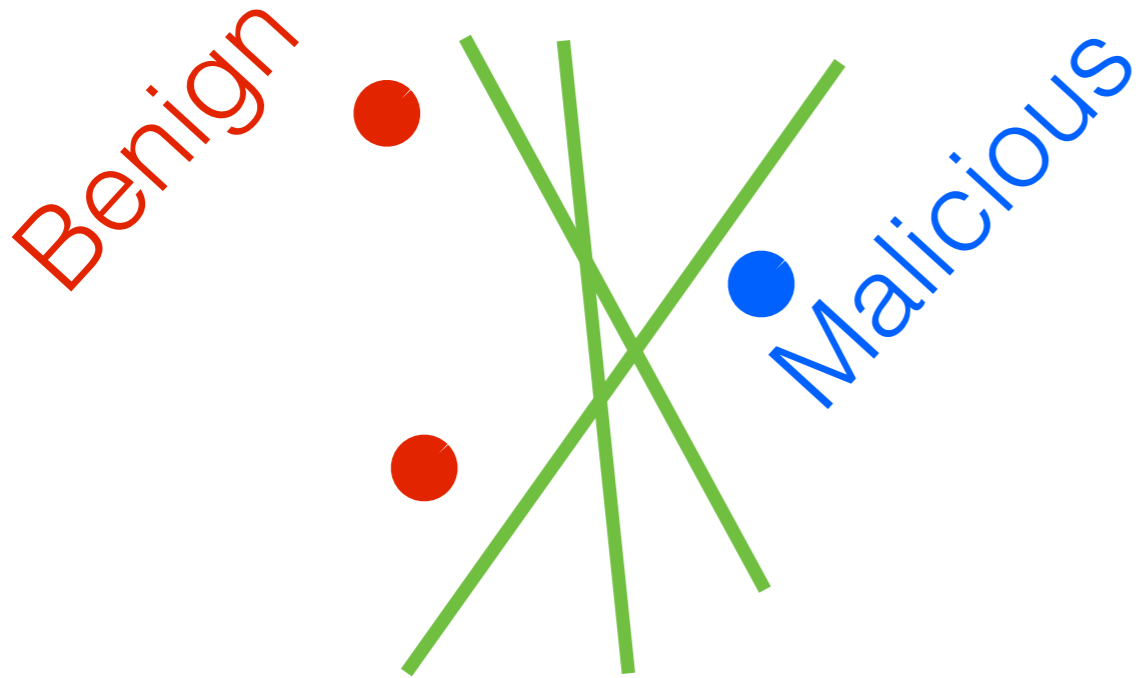
- Might miss important data

Uniform subsampling



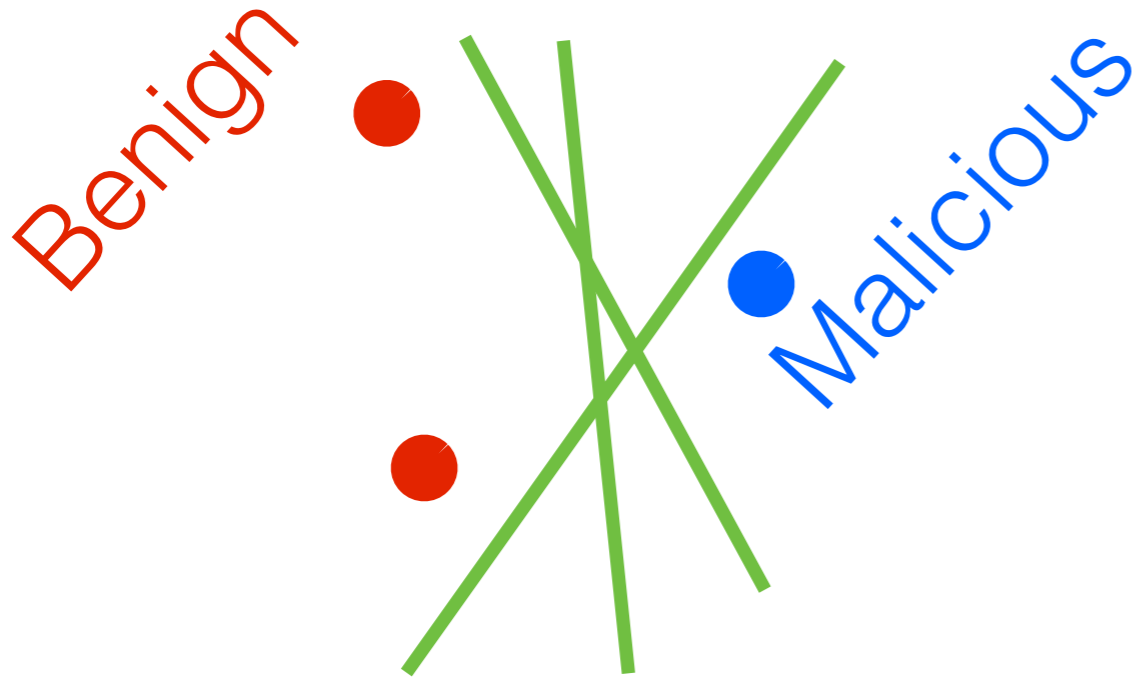
- Might miss important data

Uniform subsampling



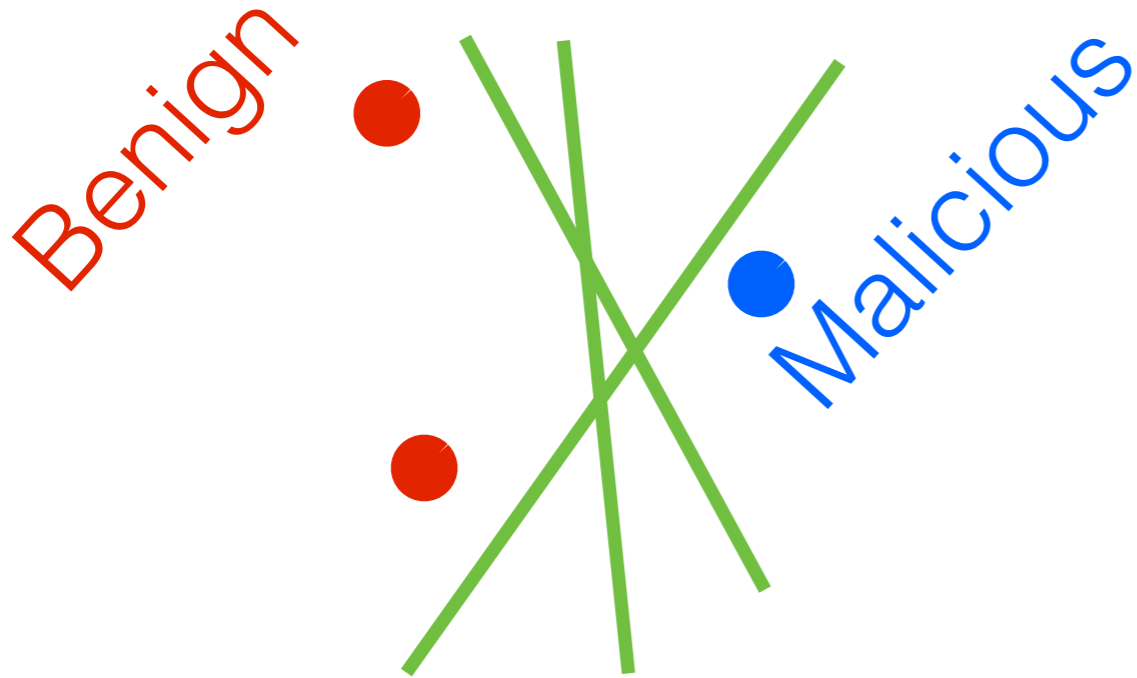
- Might miss important data

Uniform subsampling

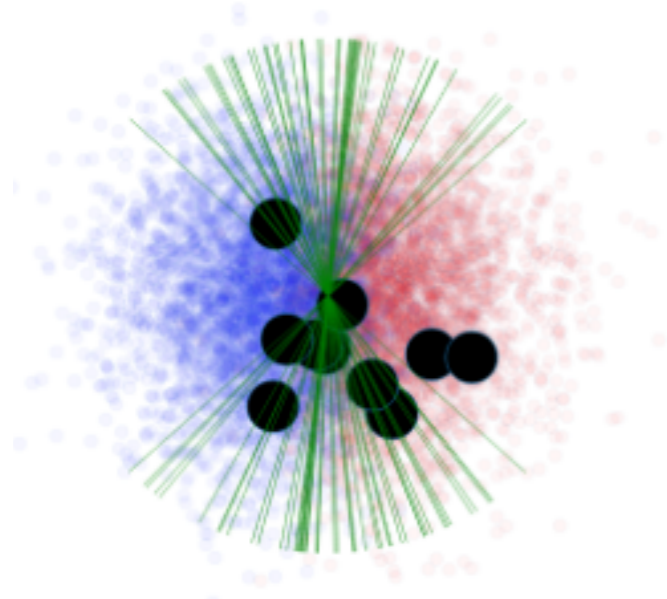


- Might miss important data
- Noisy estimates

Uniform subsampling

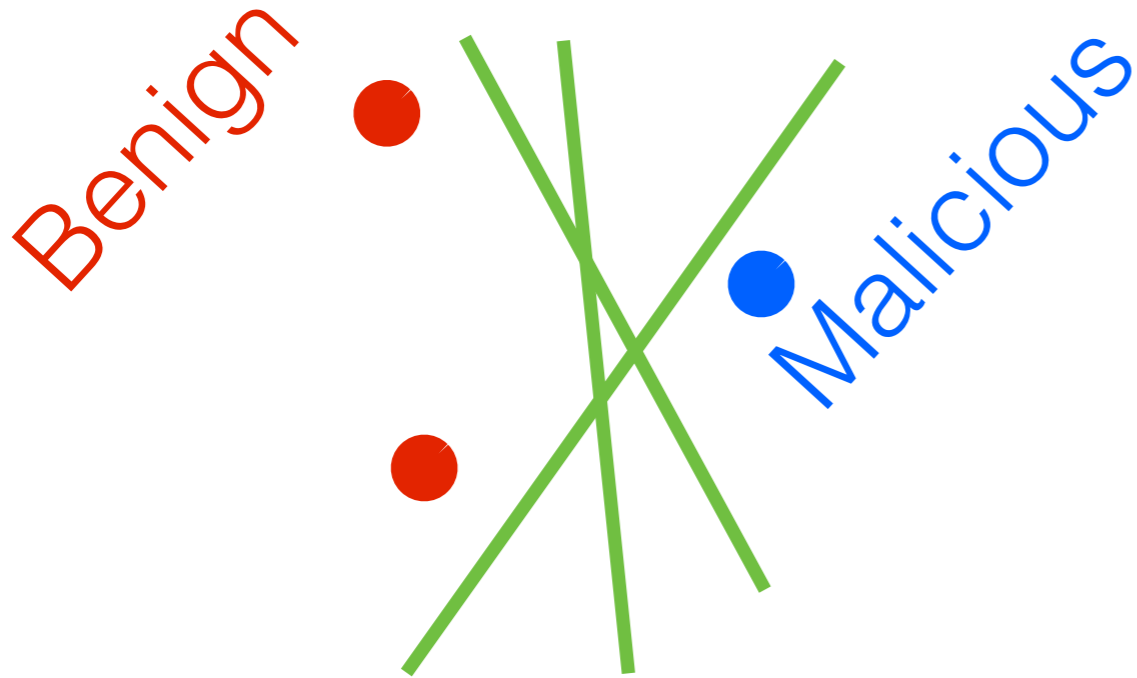


- Might miss important data
- Noisy estimates

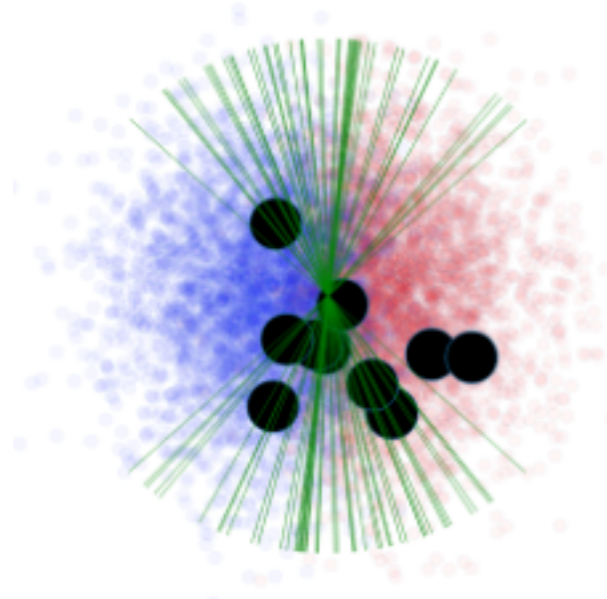


$M = 10$

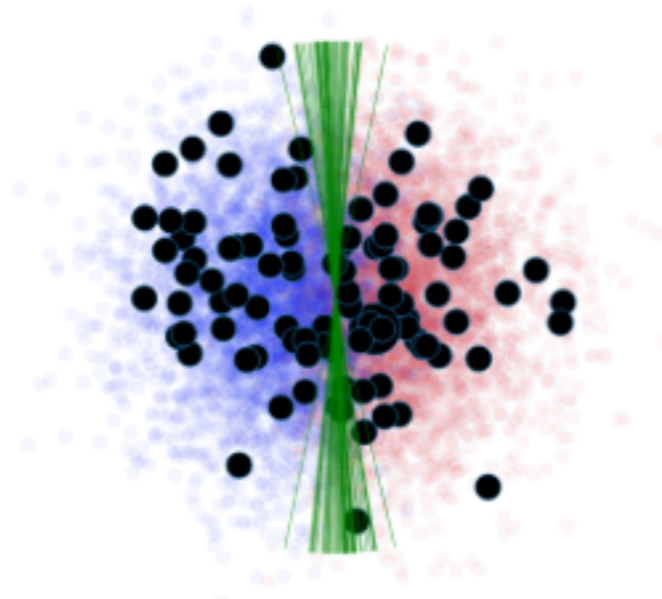
Uniform subsampling



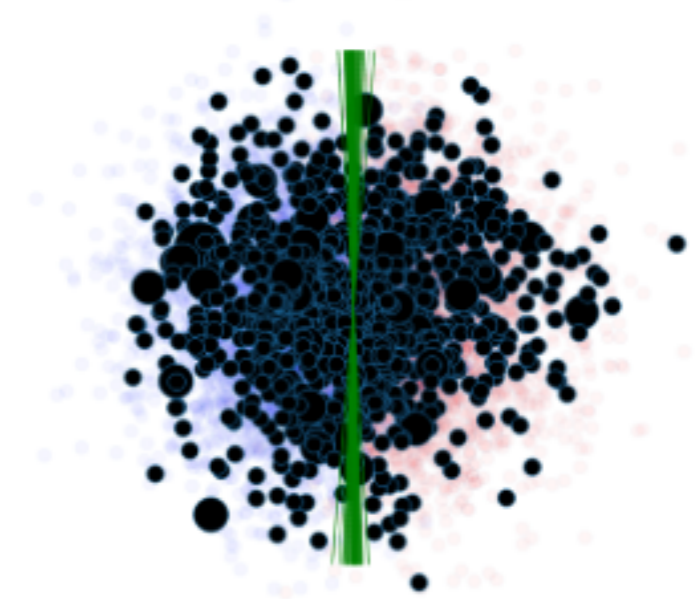
- Might miss important data
- Noisy estimates



$M = 10$



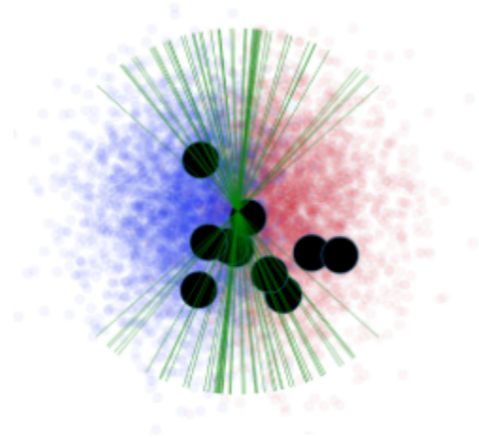
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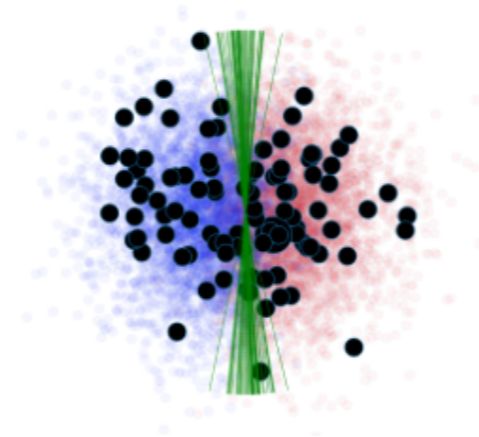
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Data summarization alternatives

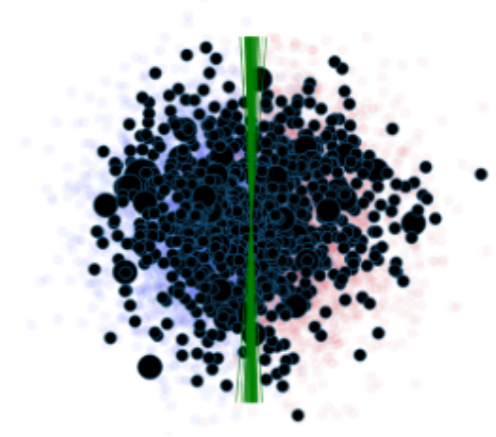
Uniform
subsampling



$M = 10$



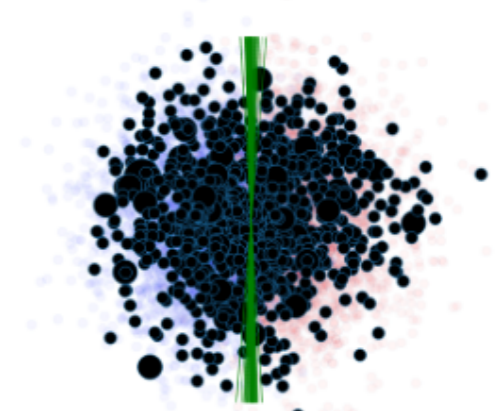
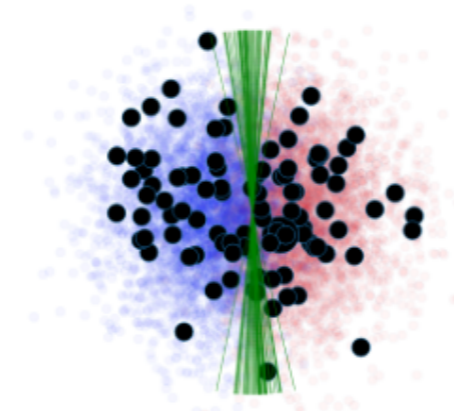
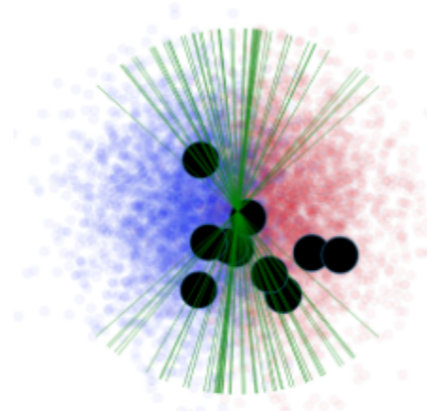
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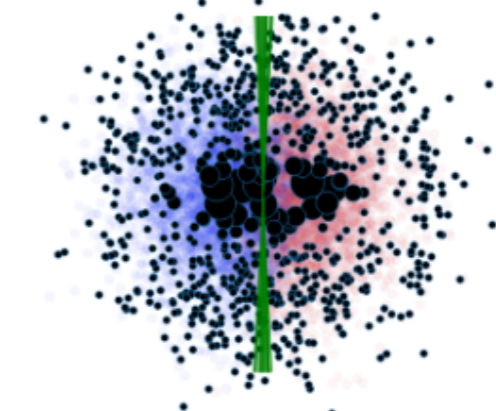
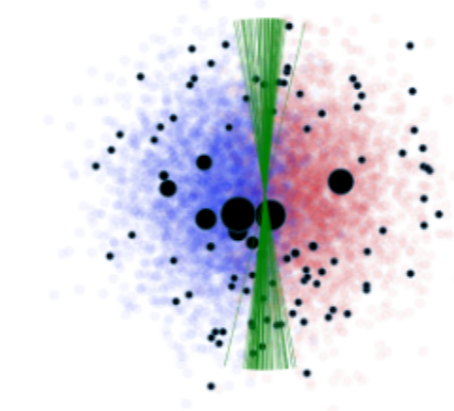
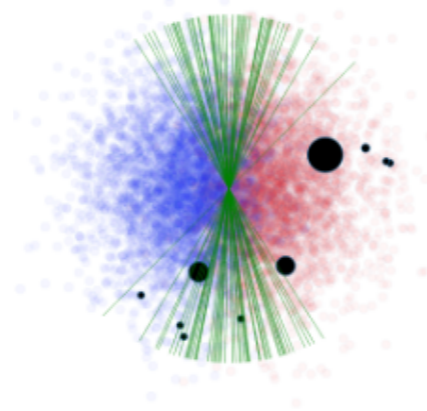
$M = 1000$

Data summarization alternatives

Uniform
subsampling



Importance
sampling



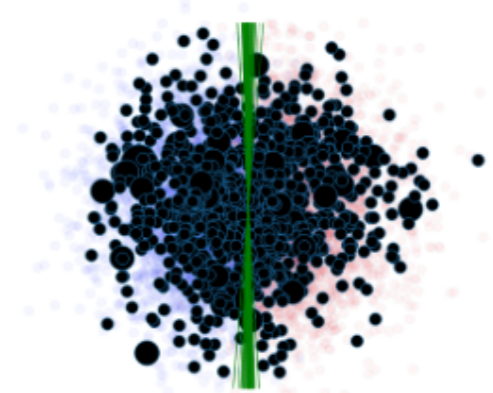
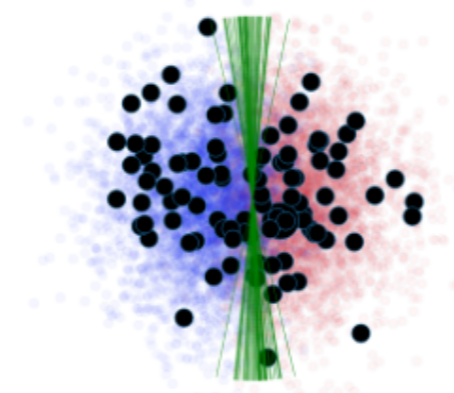
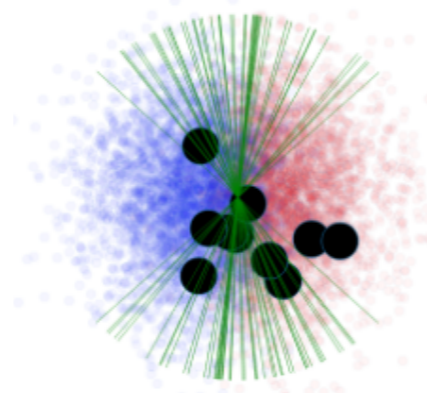
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$M = 100$

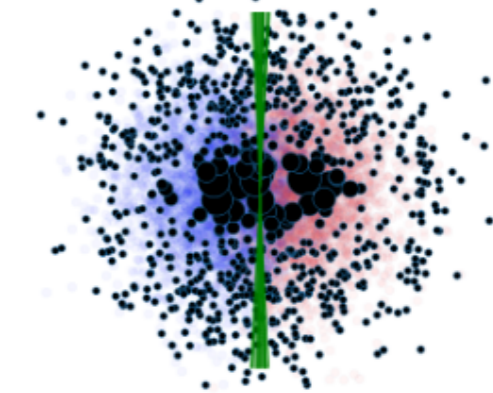
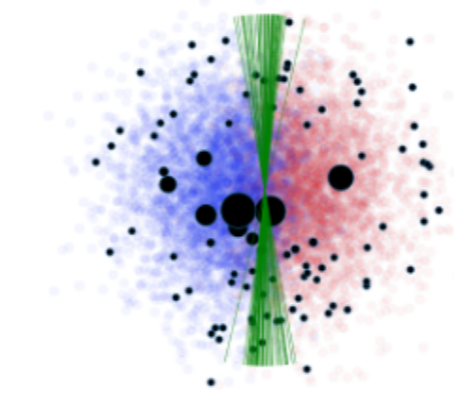
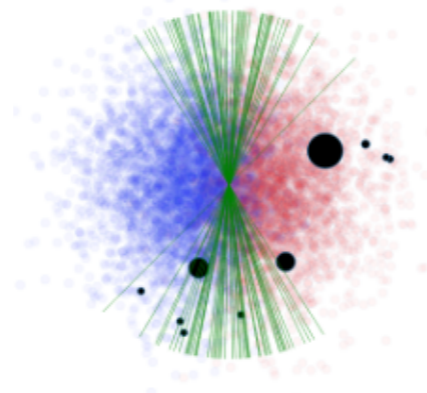
$M = 1000$

Data summarization alternatives

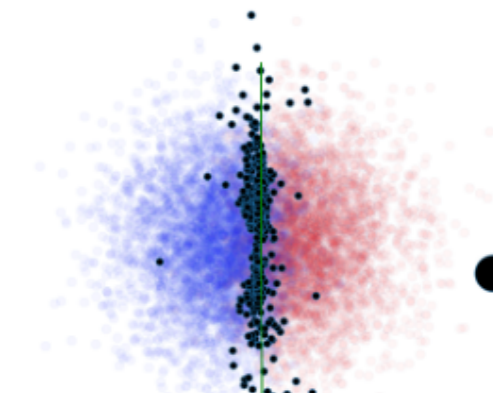
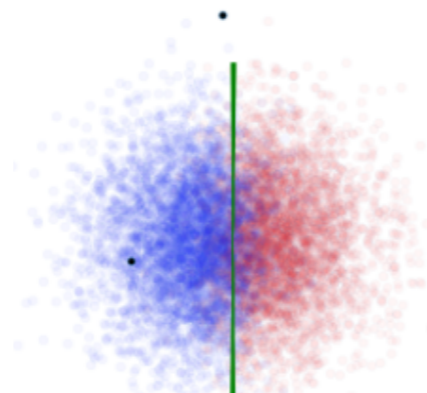
Uniform
subsampling



Importance
sampling



Bayesian/Hilbert
coresets



$M = 10$

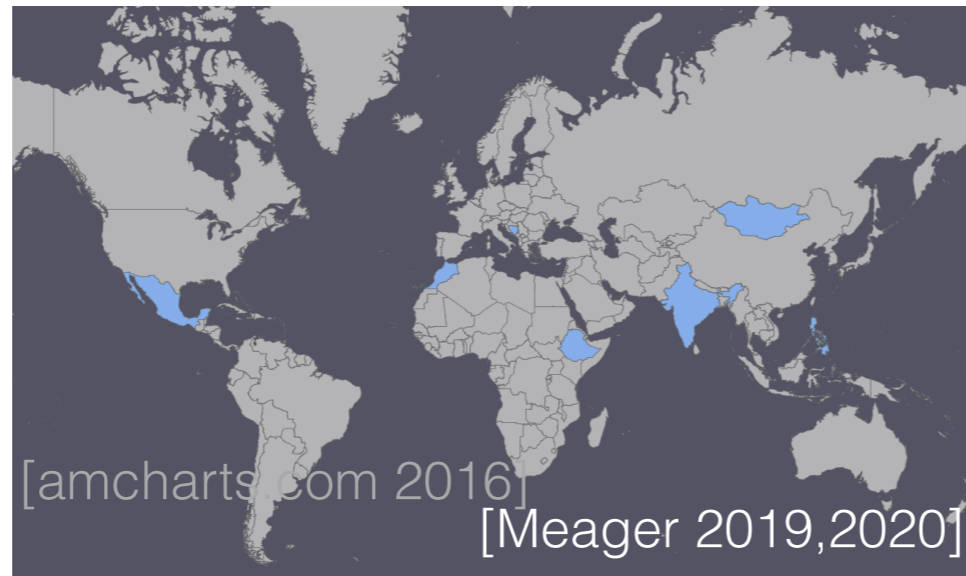
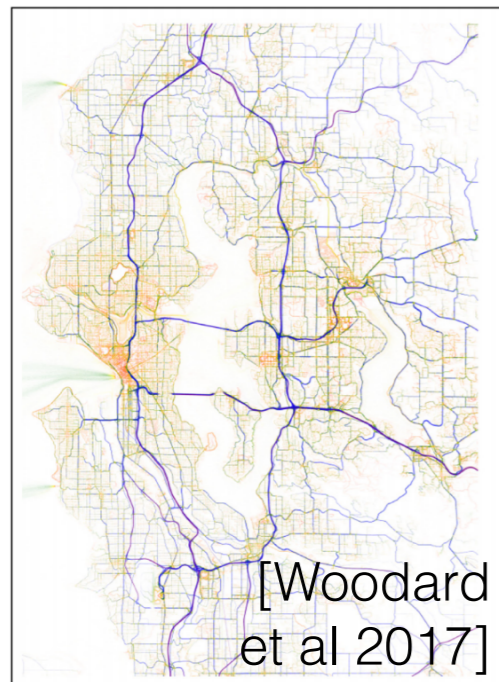
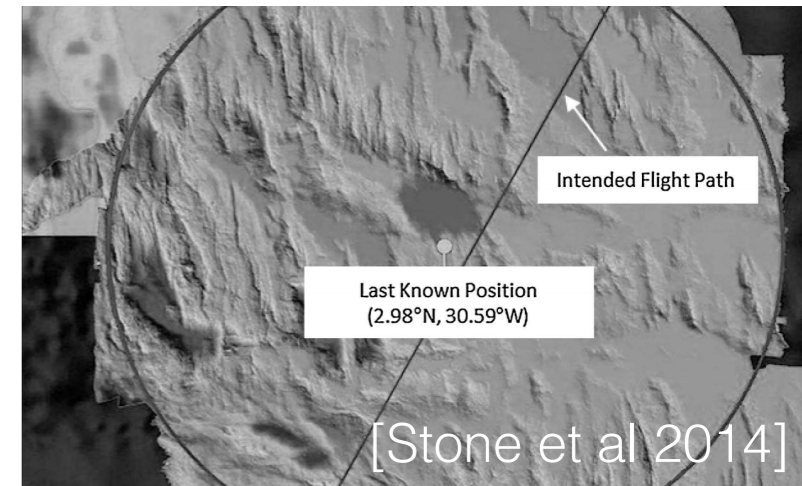
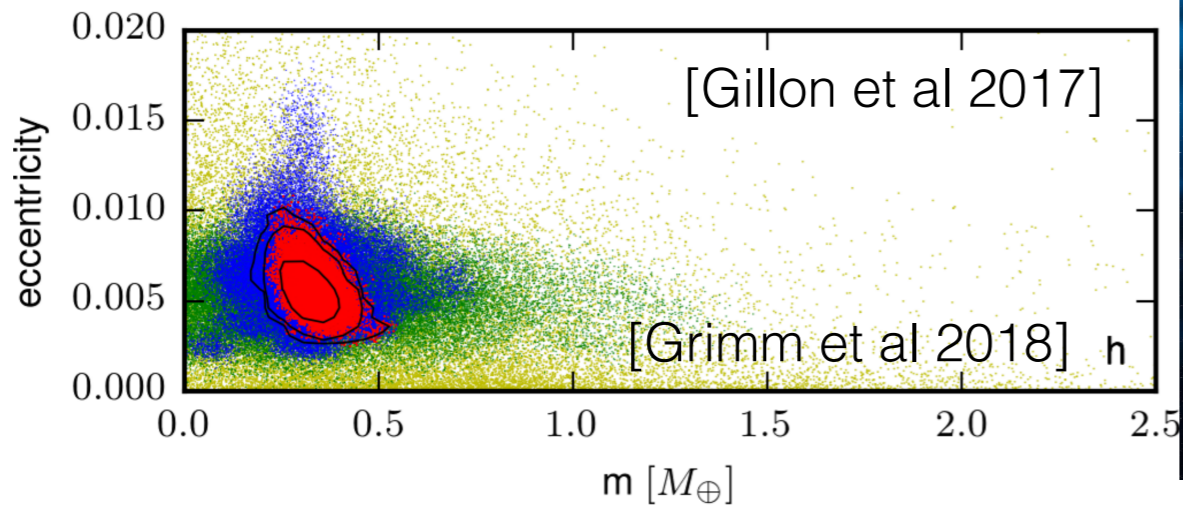
$M = 100$

$M = 1000$

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



- 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.
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- T Campbell and T Broderick. Automated scalable Bayesian inference via Hilbert coresets. *JMLR* 2019.
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- RJ Giordano, T Broderick, and MI Jordan. Covariances, robustness, and variational Bayes. *Journal of Machine Learning Research*, 2018.

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- J Gorham, and L Mackey. "Measuring sample quality with kernels." ArXiv:1703.01717 (2017).
- PD Hoff. *A first course in Bayesian statistical methods*. Springer Science & Business Media, 2009.
- MD Hoffman, DM Blei, C Wang, and J Paisley. "Stochastic variational inference." *The Journal of Machine Learning Research* 14.1 (2013): 1303-1347.
- JH Huggins, T Campbell, and T Broderick. Coresets for scalable Bayesian logistic regression. *NeurIPS* 2016.
- JH Huggins, RP Adams, and T Broderick. PASS-GLM: Polynomial approximate sufficient statistics for scalable Bayesian GLM inference. *NeurIPS* 2017.
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