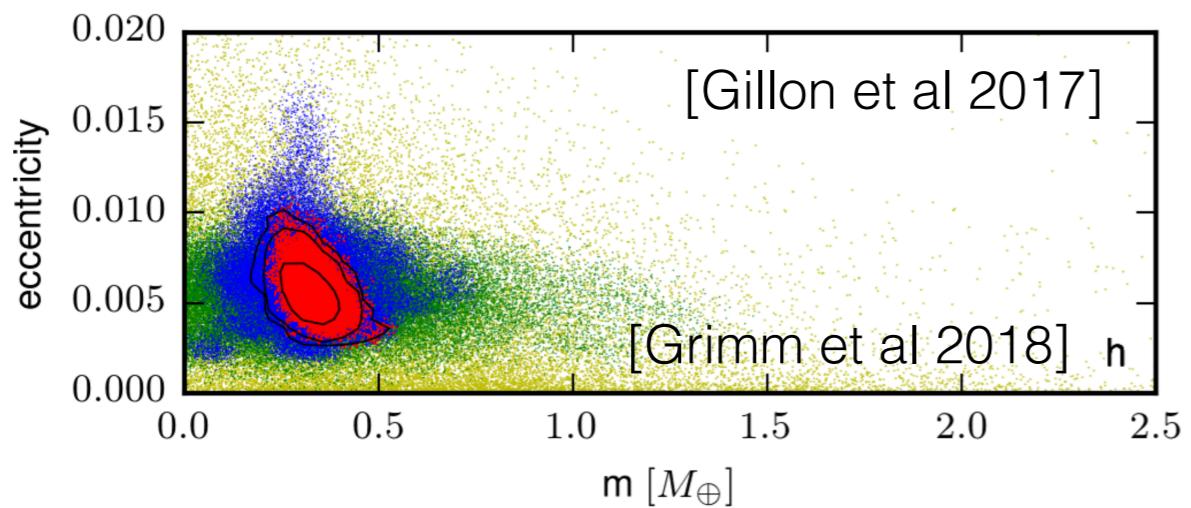


Variational Bayes and beyond: Foundations of scalable Bayesian inference

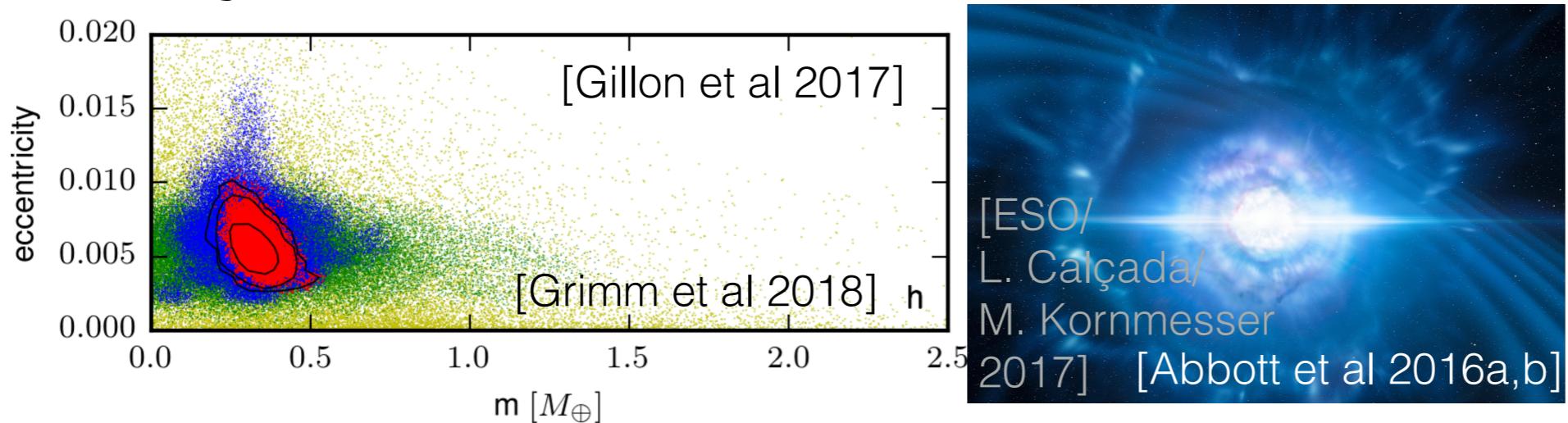
Tamara Broderick
Associate Professor
MIT

Bayesian inference

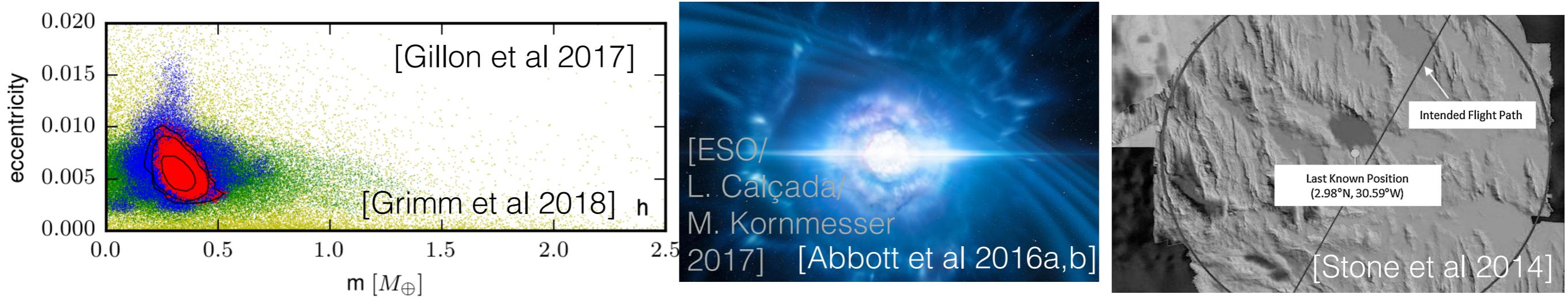
Bayesian inference



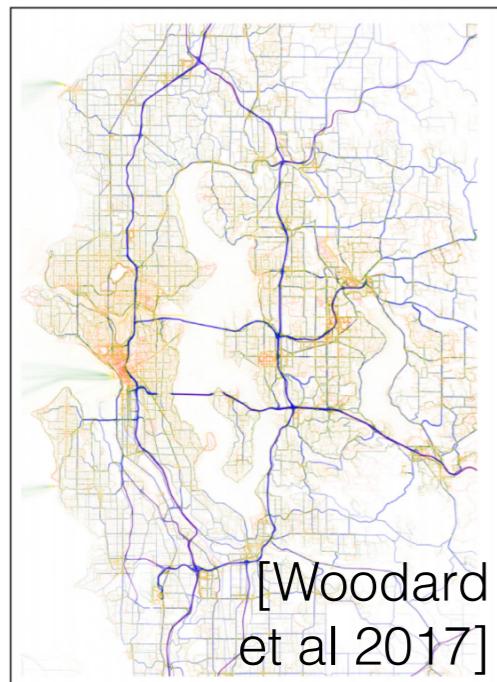
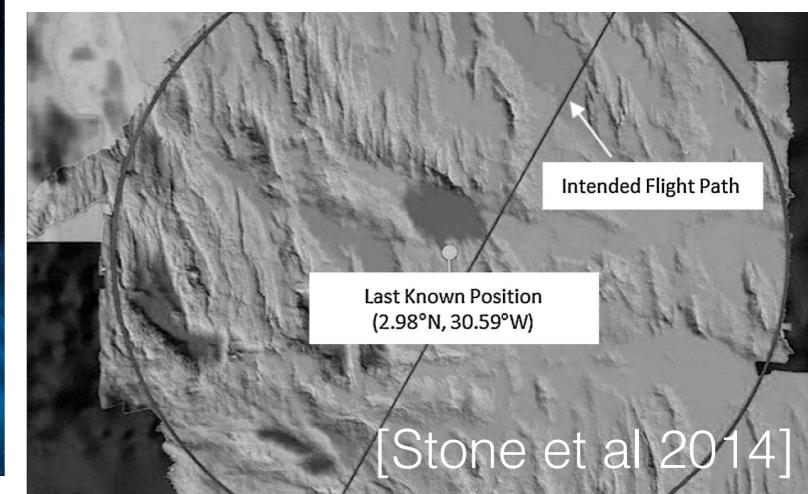
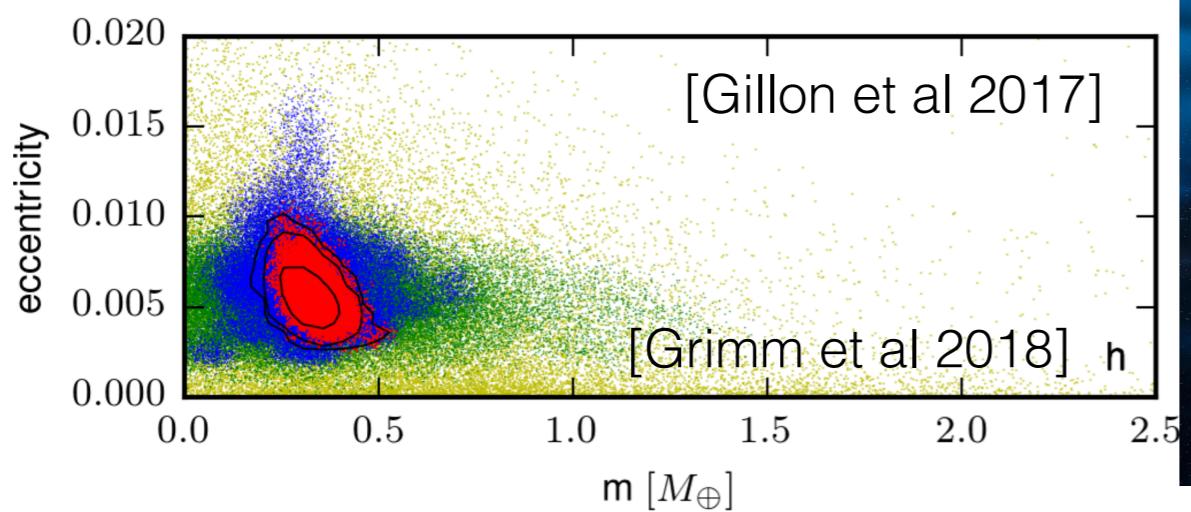
Bayesian inference



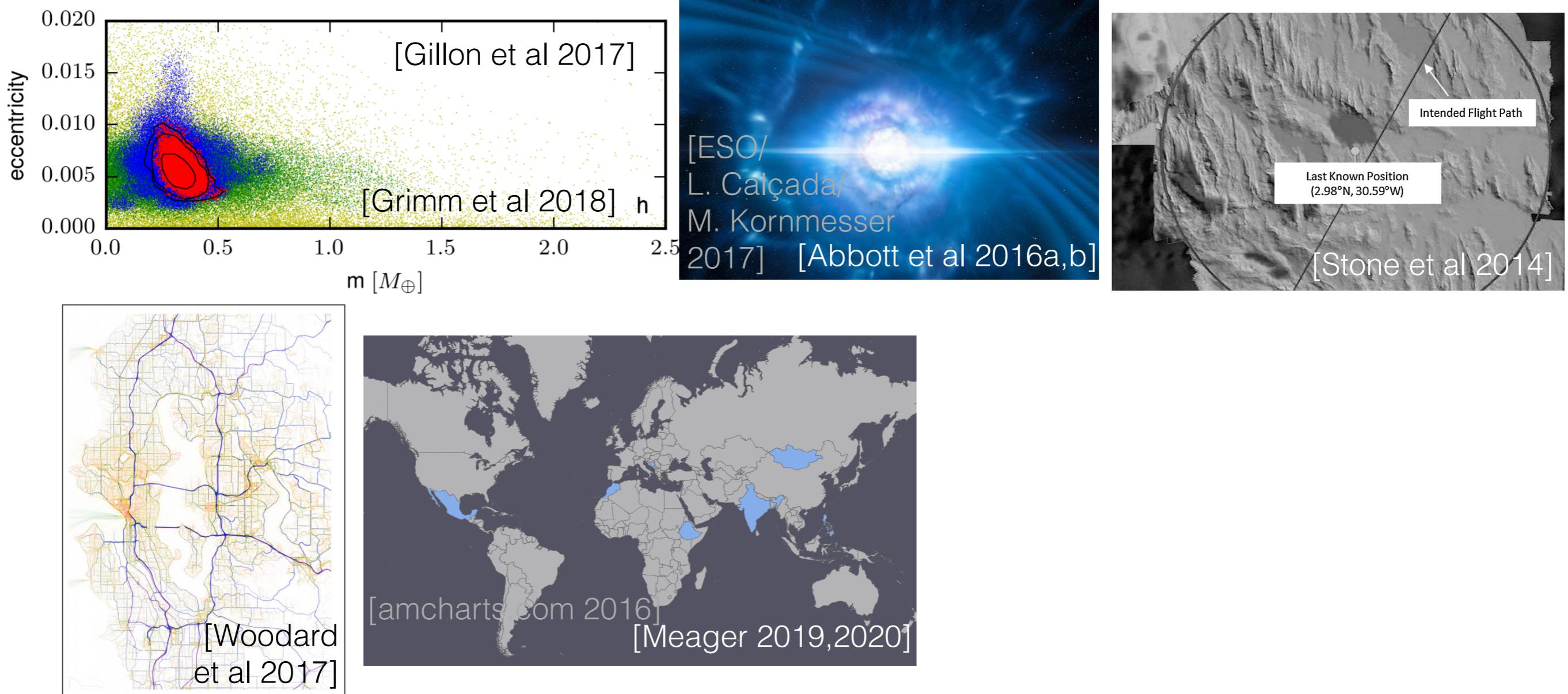
Bayesian inference



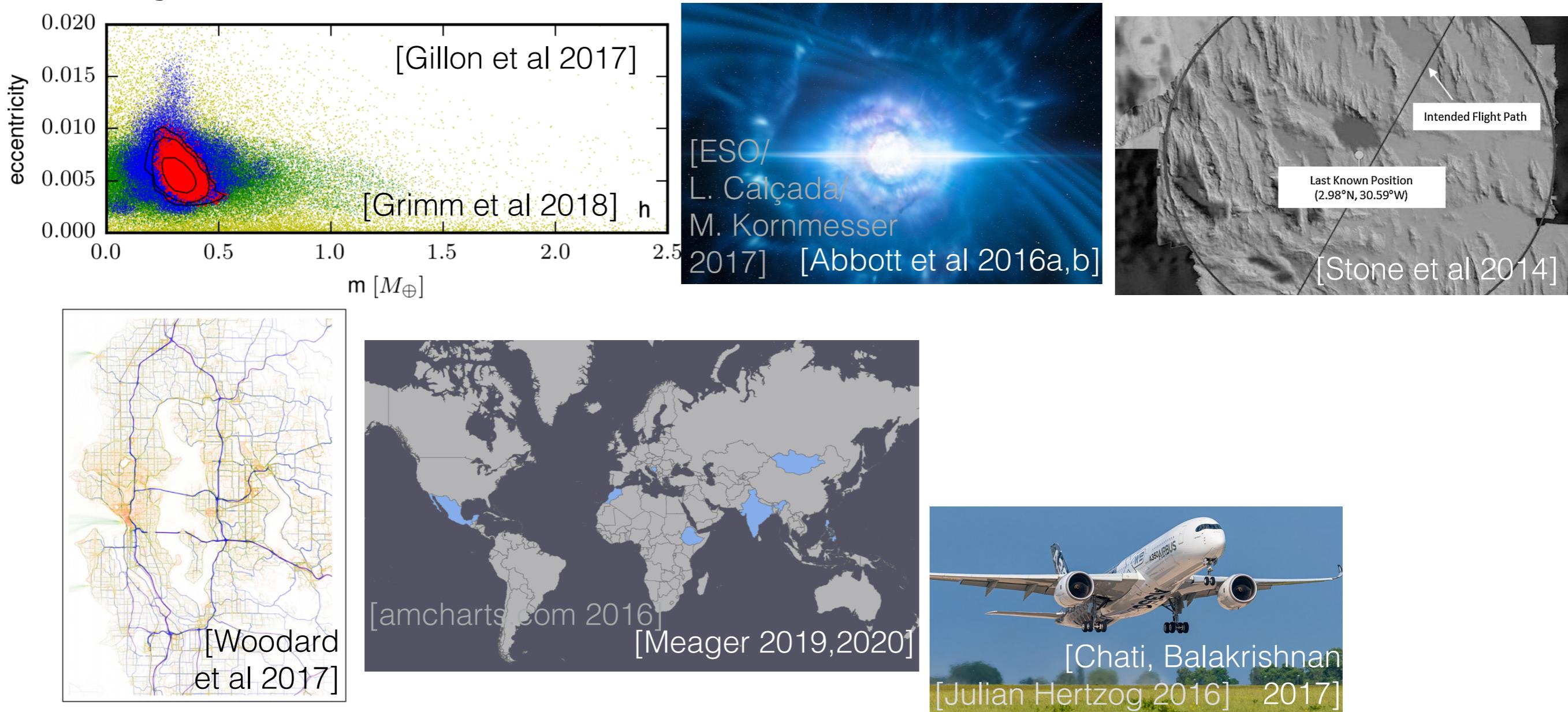
Bayesian inference



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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- 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
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 - Uncertainty doesn't have to disappear in large data sets

Variational Bayes

Variational Bayes

- Modern problems: often large data, large dimensions

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- Variational Bayes can be very fast

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NEW	MILLION	CHILDREN	SCHOOL	[Blei et al
FILM	TAX	WOMEN	STUDENTS	2003]
SHOW	PROGRAM	PEOPLE	SCHOOLS	
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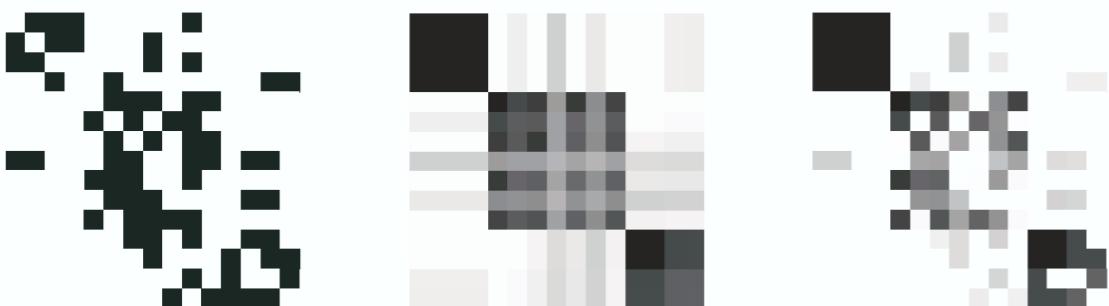
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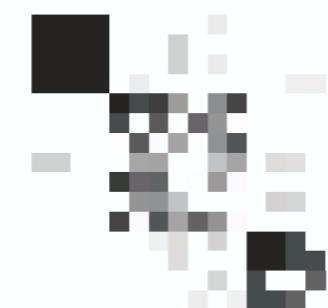
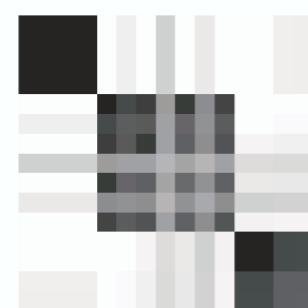
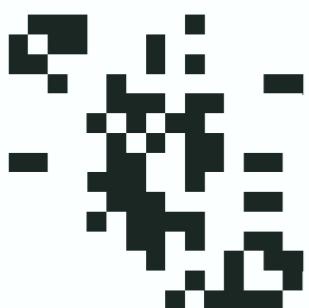


Variational Bayes

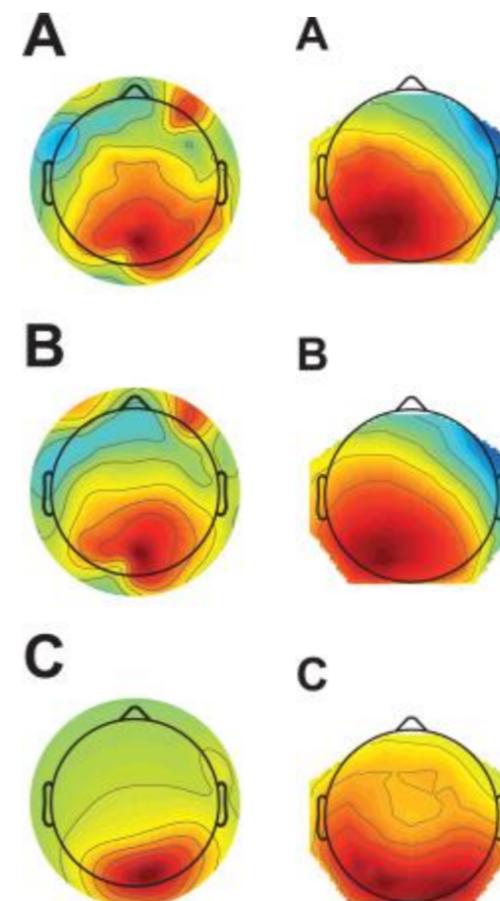
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[Airoldi et al 2008]



[Gershman et al 2014]

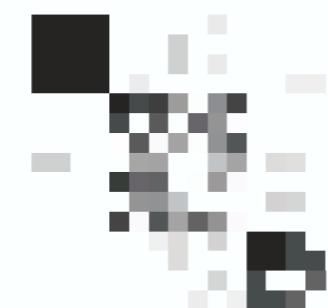
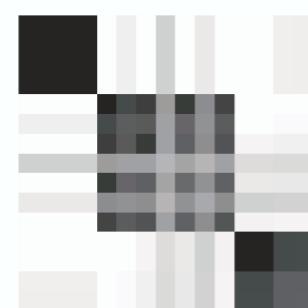
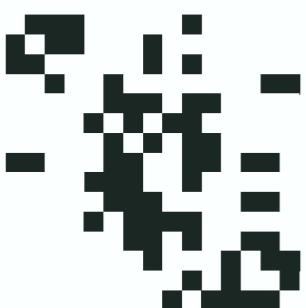
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Variational Bayes

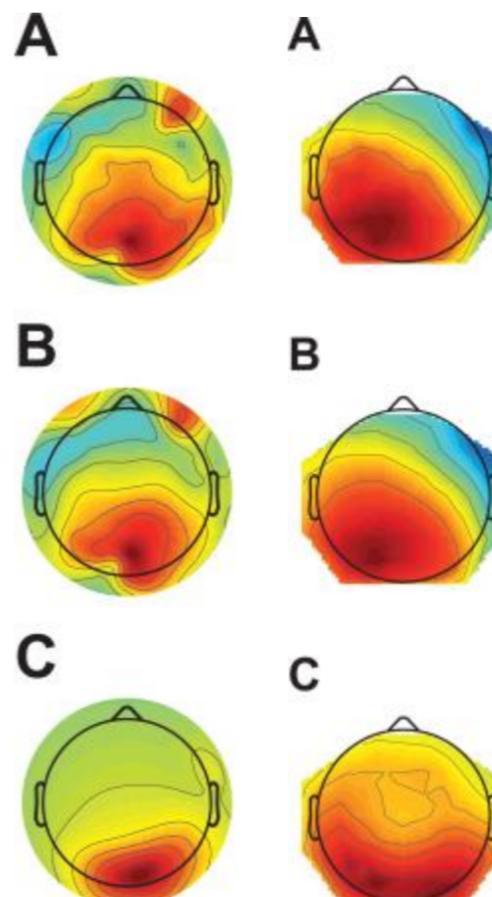
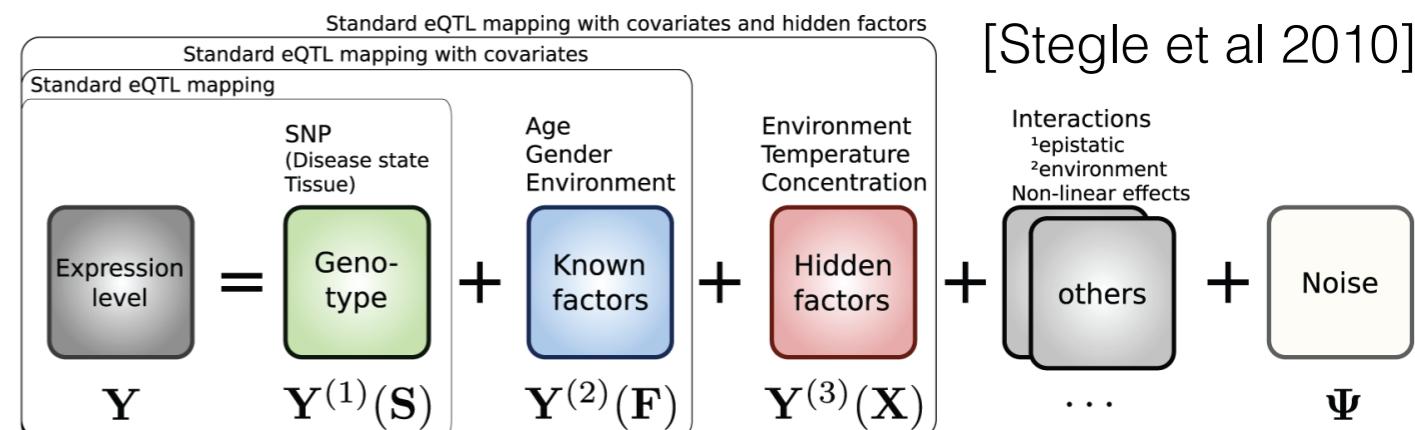
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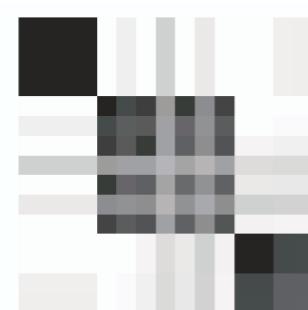
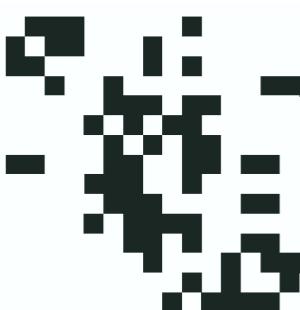
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Variational Bayes

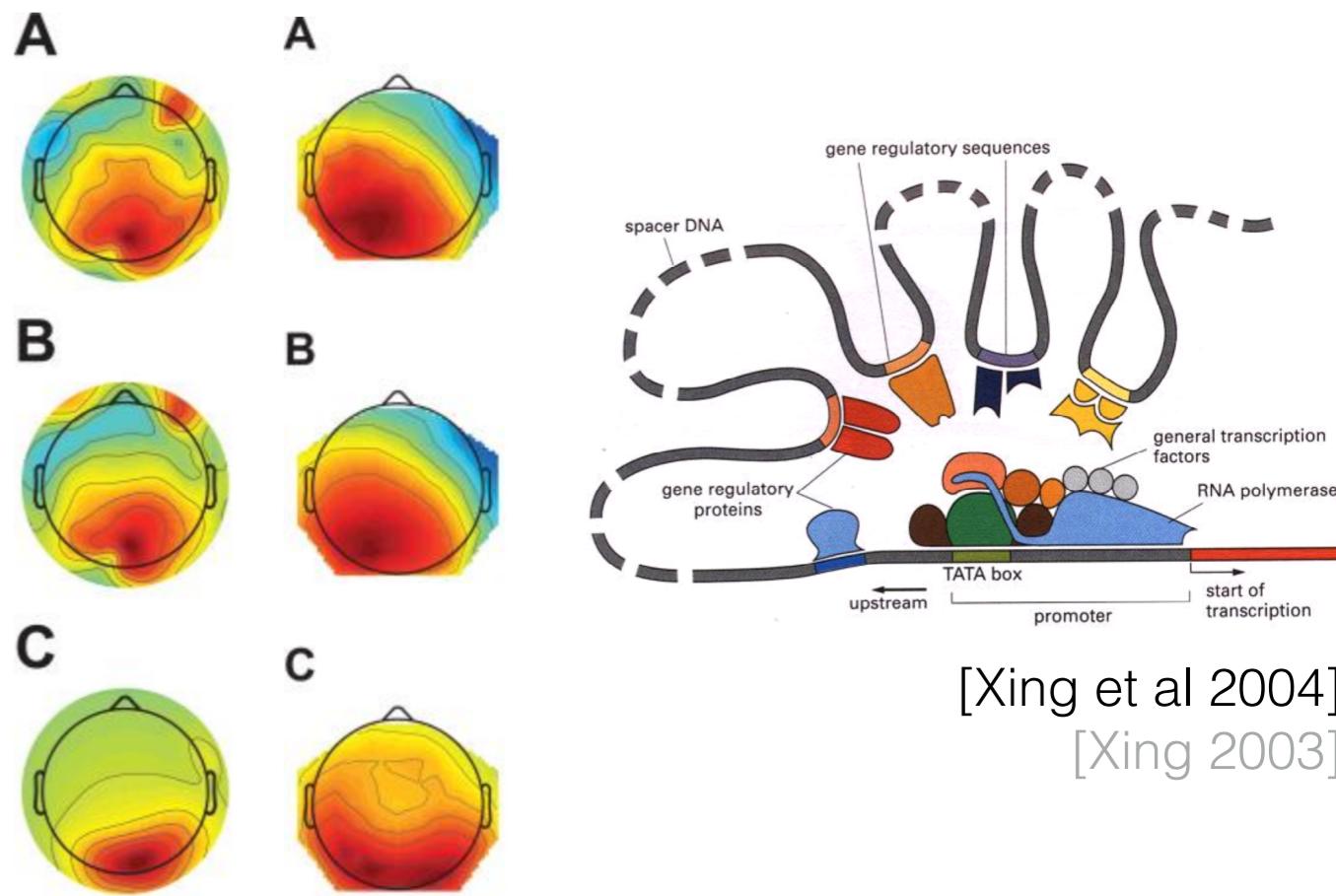
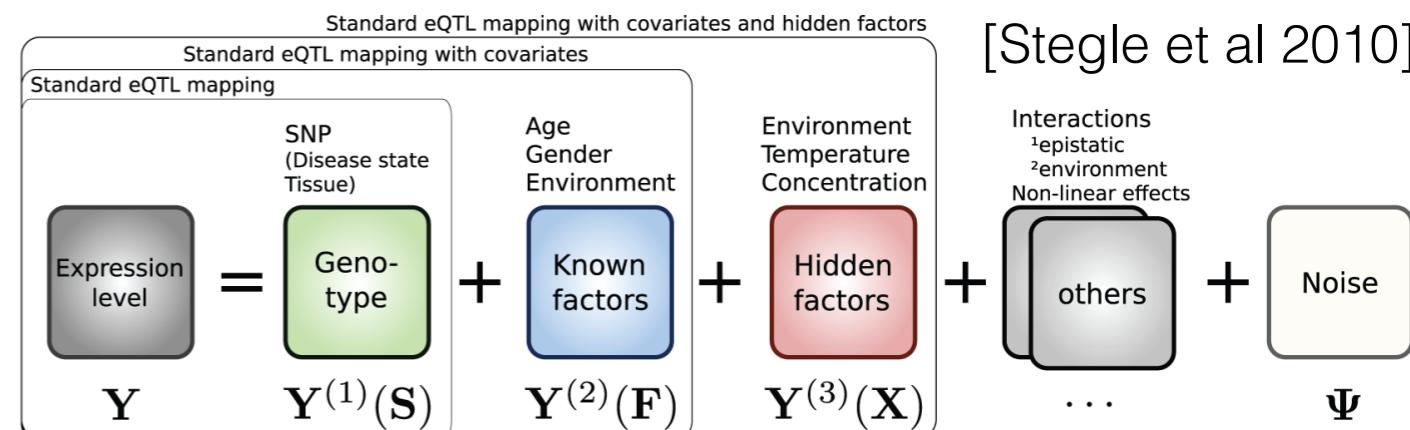
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Roadmap

- Bayes & Approximate Bayes review

Roadmap

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- What is:
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Roadmap

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Bayesian inference

Bayesian inference

parameters
 θ

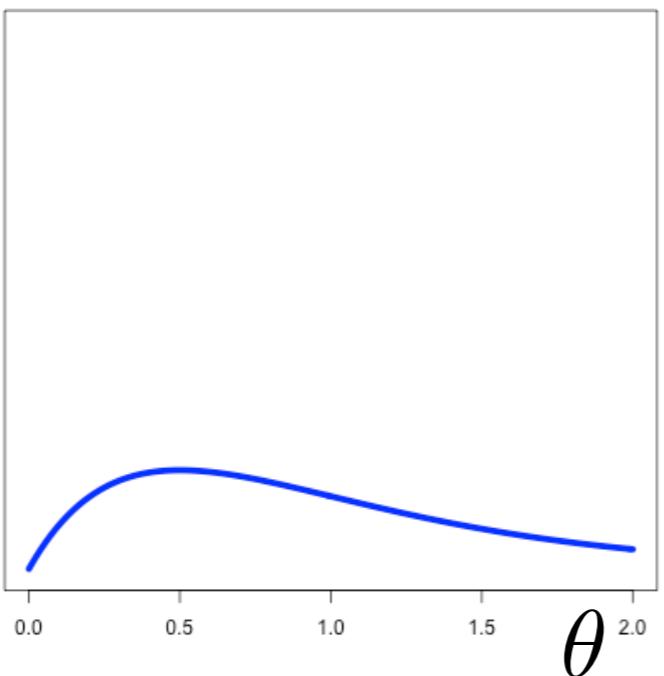
Bayesian inference

parameters
 $p(\theta)$
prior



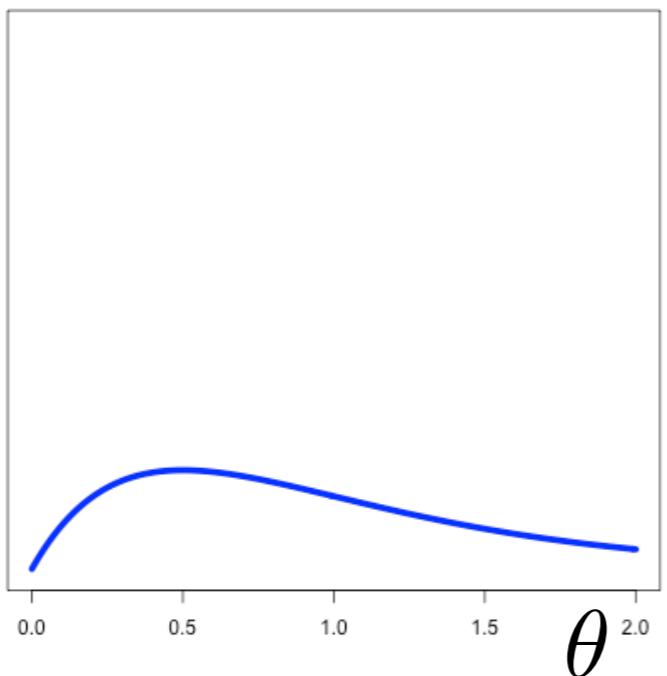
Bayesian inference

parameters
 $p(\theta)$
prior



Bayesian inference

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

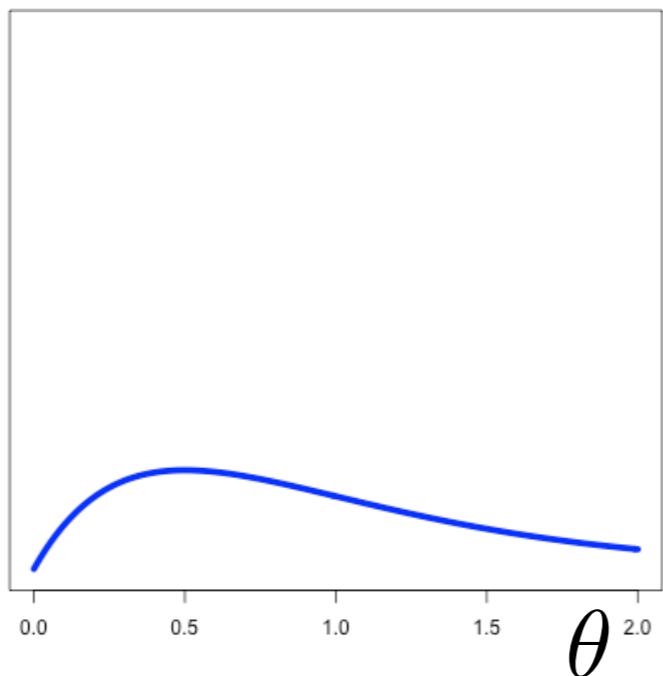


Bayesian inference

data parameters

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

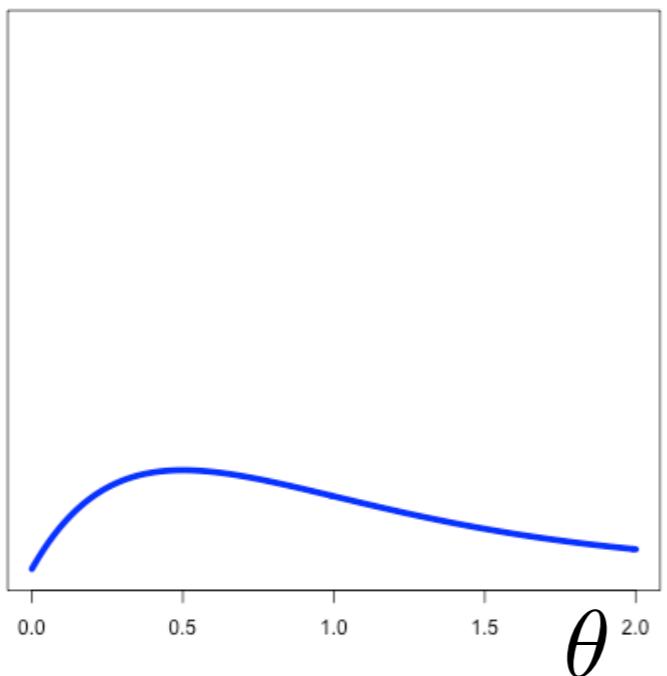
likelihood prior



Bayesian inference

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

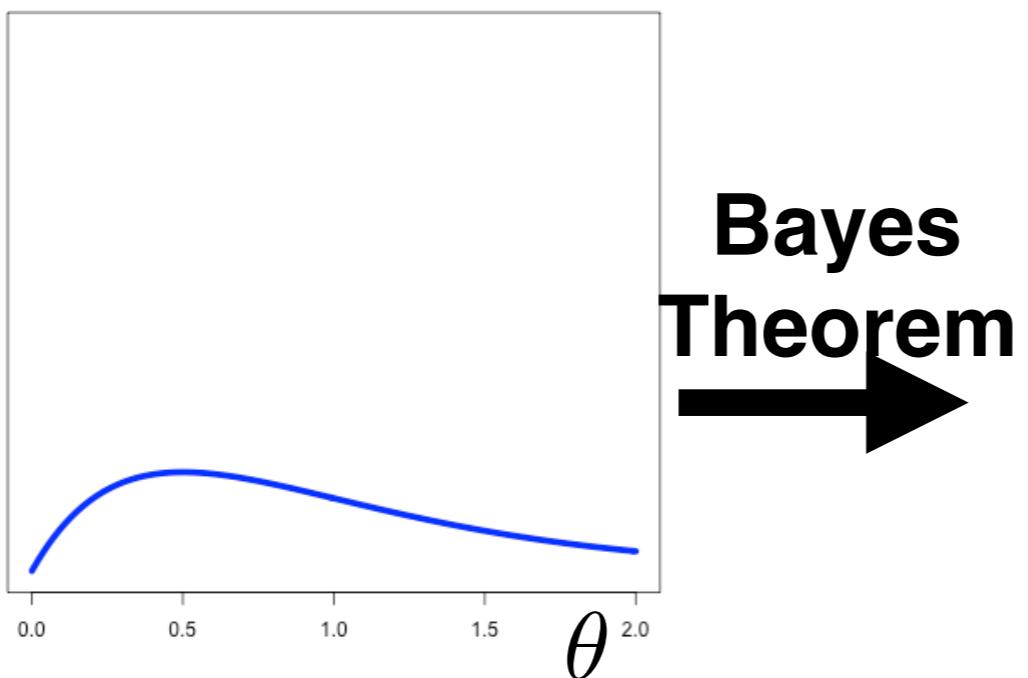
posterior likelihood prior



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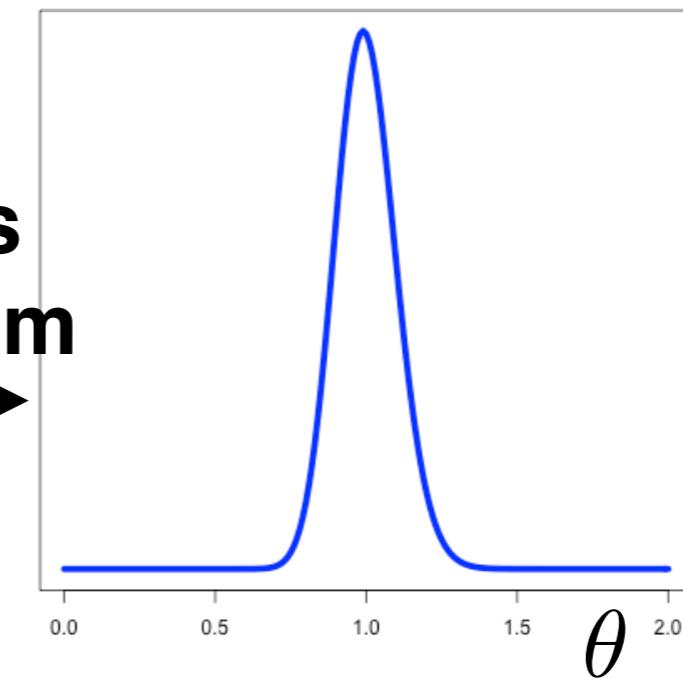
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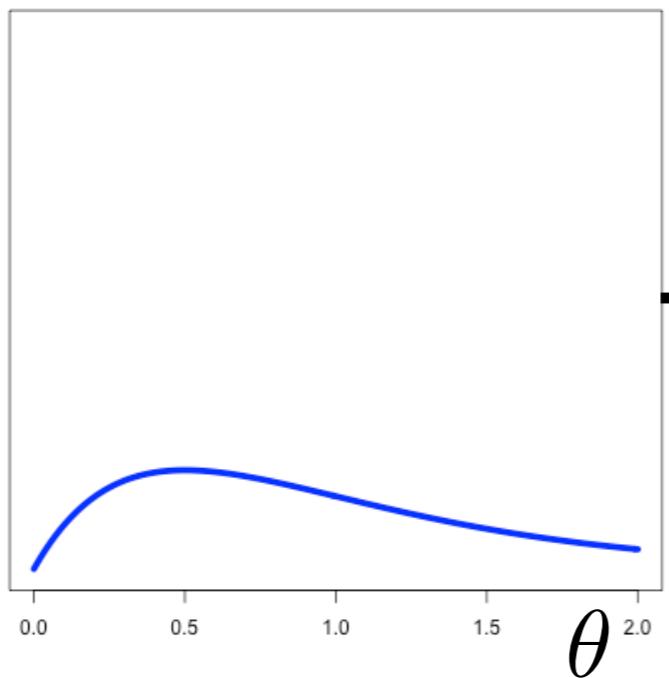
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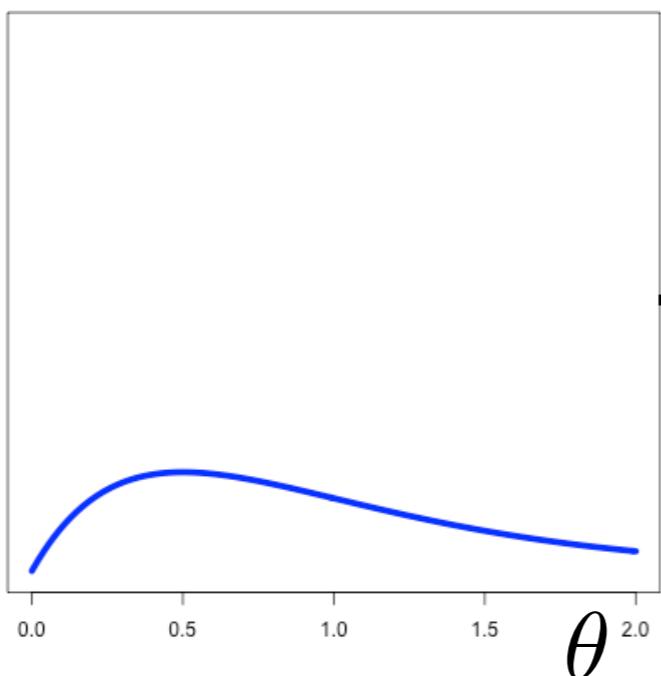
**Bayes
Theorem**
→



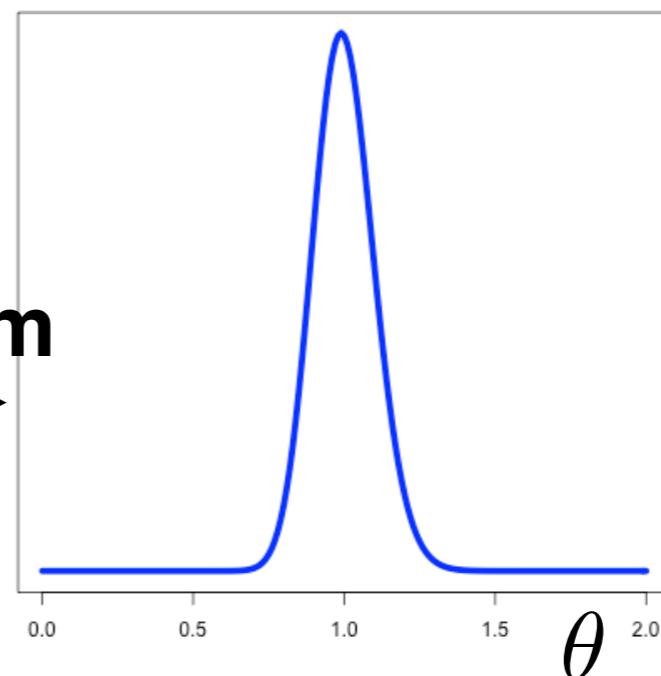
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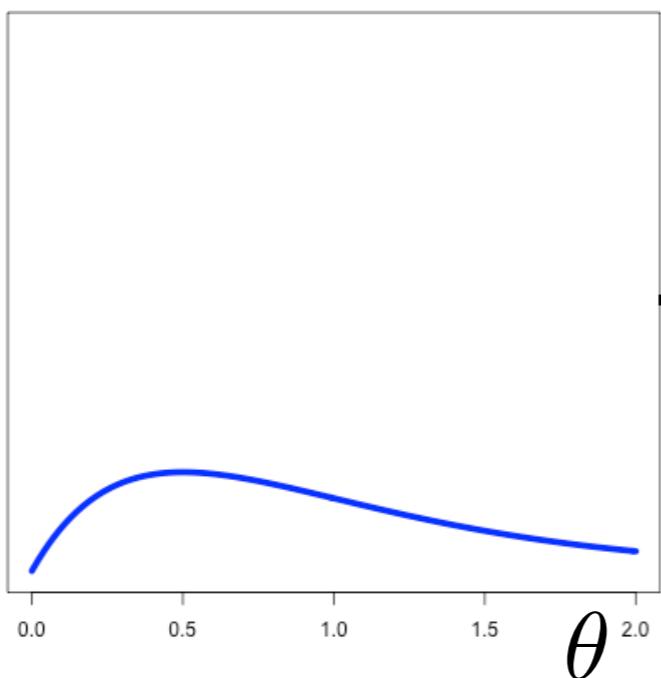


1. Build a model: choose prior & choose likelihood

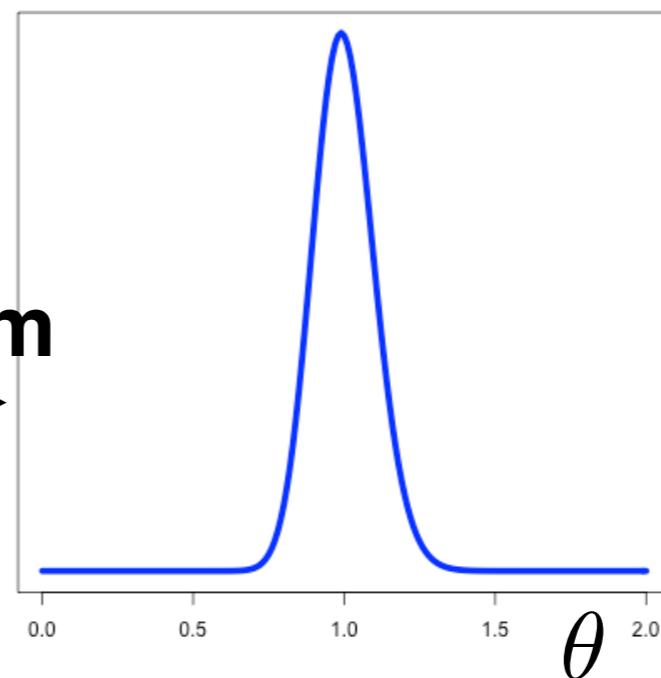
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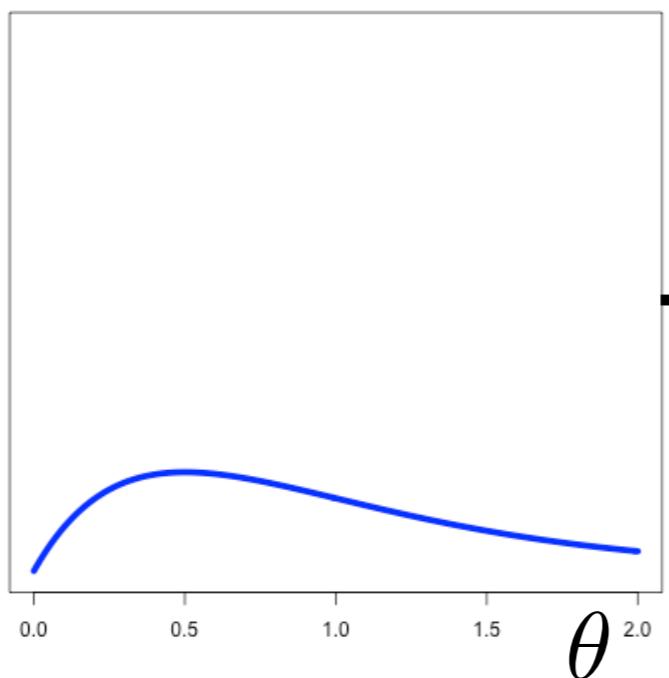


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2. Compute the posterior

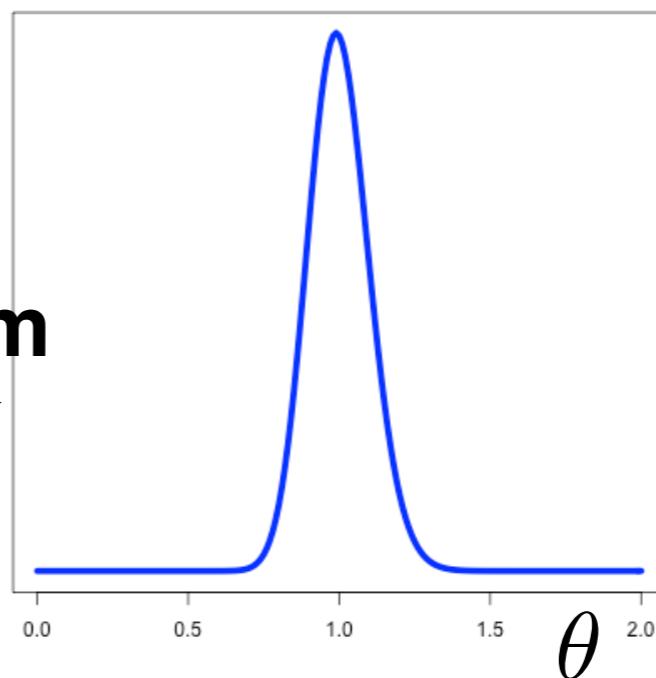
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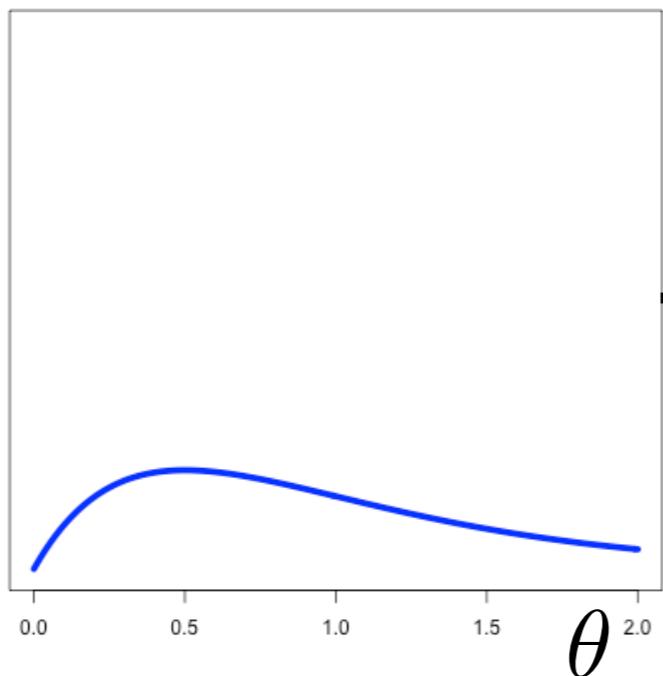


1. Build a model: choose prior & choose likelihood
2. Compute the posterior
3. Report a summary, e.g. posterior means and (co)variances

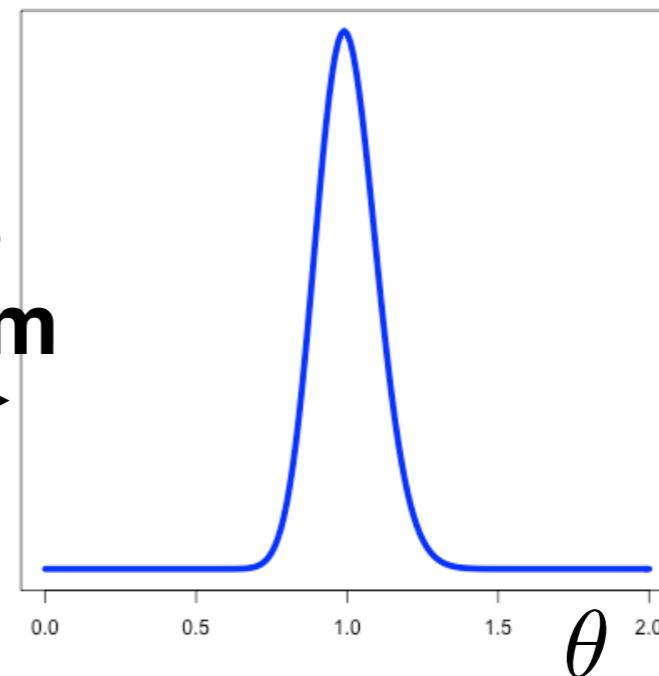
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**Bayes
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→

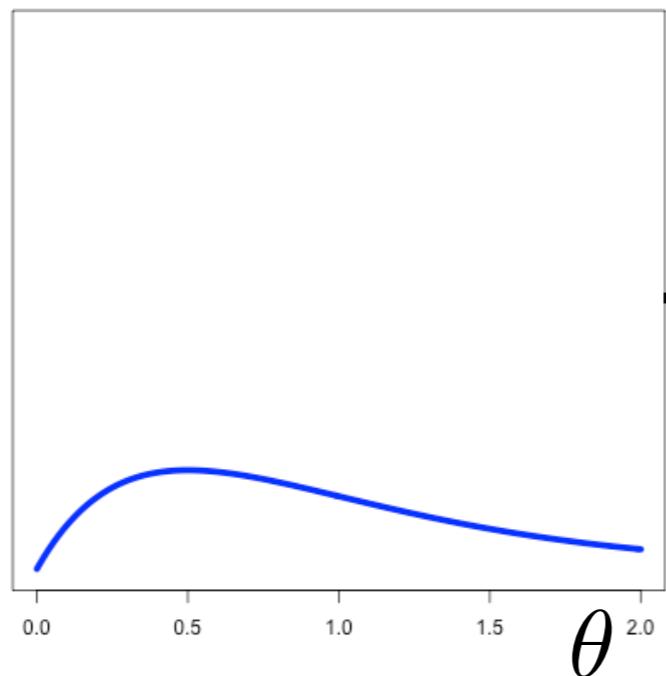


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- Why are steps 2 and 3 hard?

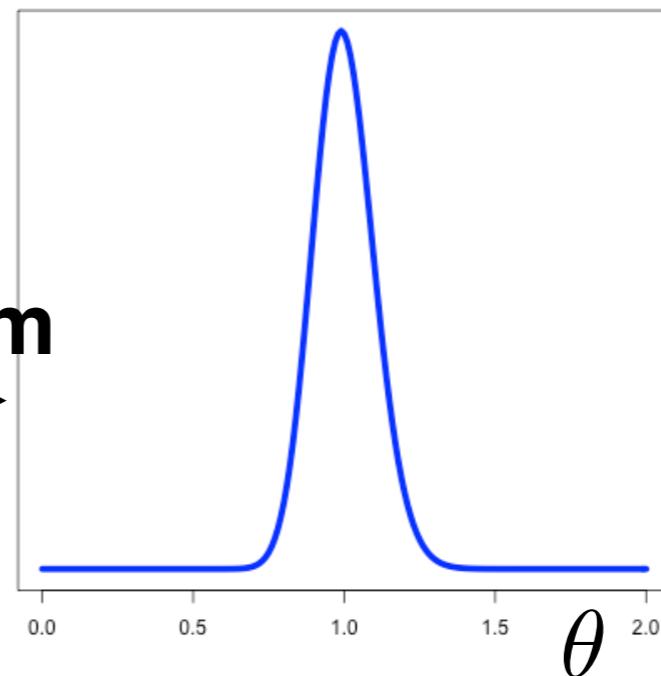
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**Bayes
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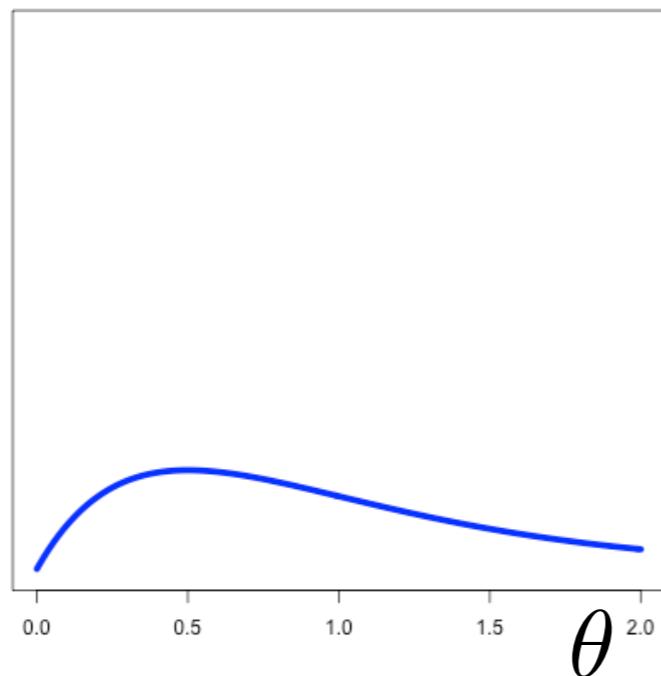


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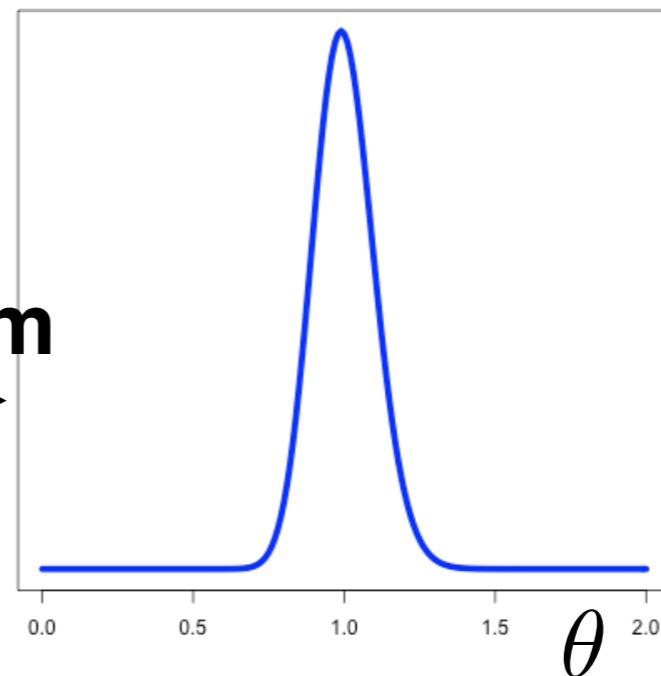
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**Bayes
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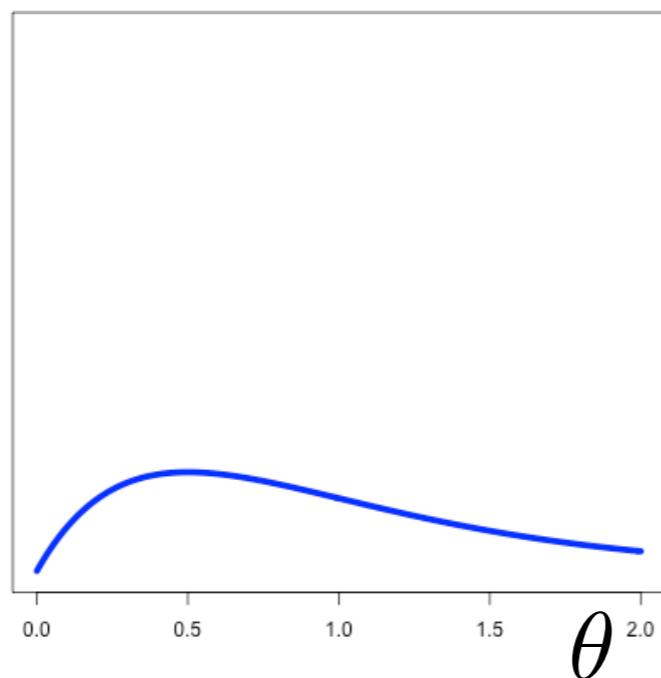


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- Why are steps 2 and 3 hard?
 - Typically no closed form, high-dimensional integration

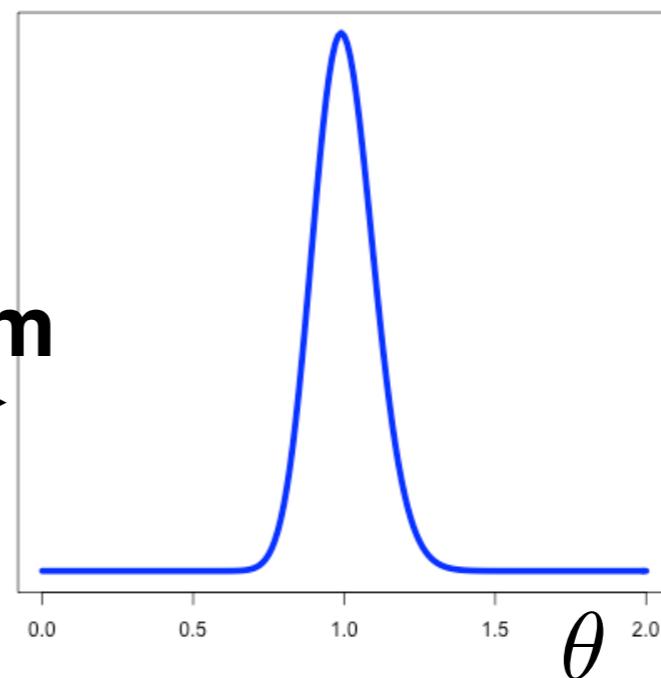
Bayesian inference

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

posterior likelihood prior



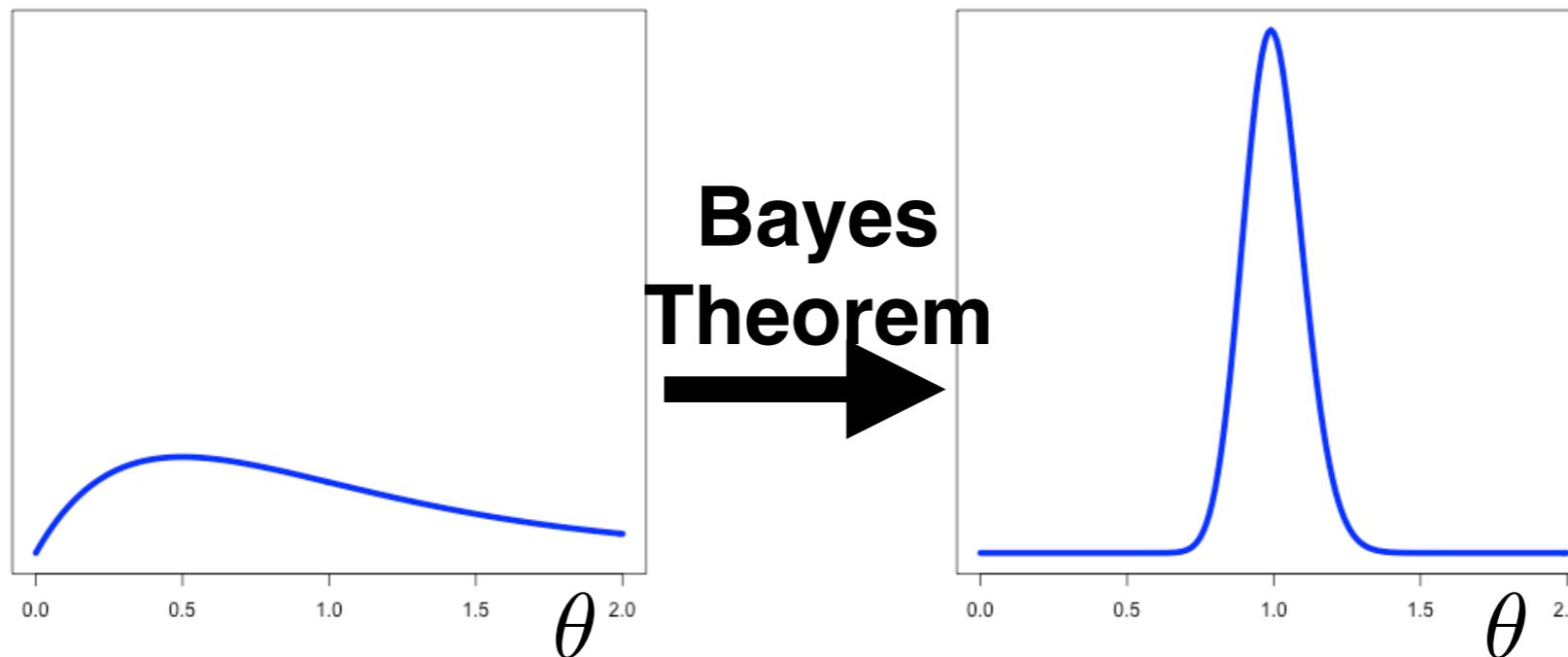
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Bayesian inference

data parameters
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posterior likelihood prior evidence



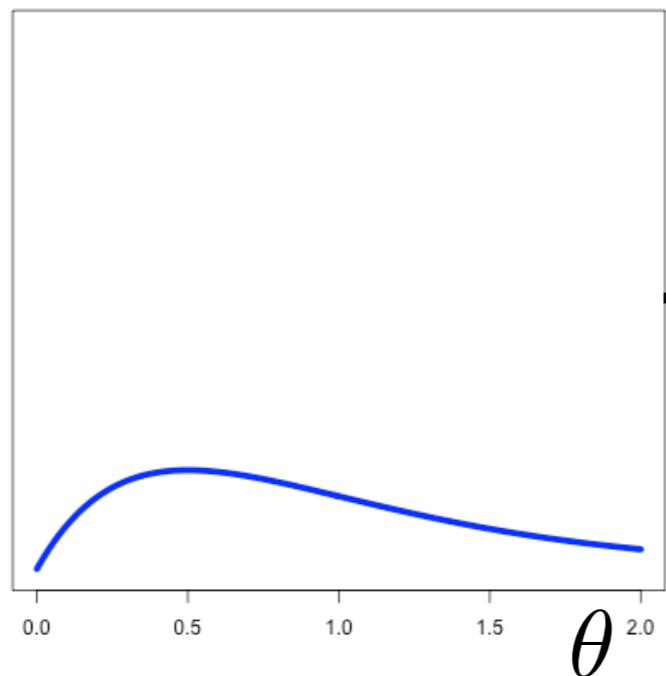
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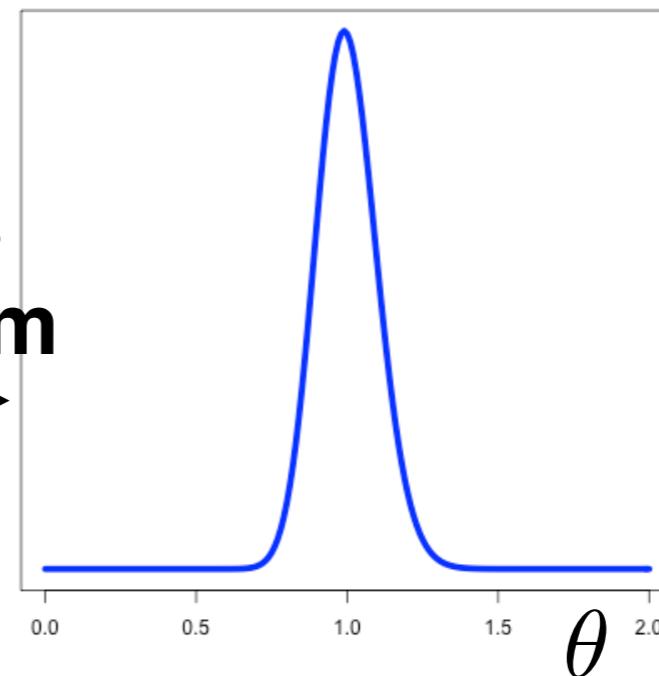
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posterior likelihood prior evidence



**Bayes
Theorem**

→



1. Build a model: choose prior & choose likelihood
 2. Compute the posterior
 3. Report a summary, e.g. posterior means and (co)variances
- Why are steps 2 and 3 hard?
 - Typically no closed form, high-dimensional integration

Approximate Bayesian Inference

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- Gold standard: Markov Chain Monte Carlo (MCMC)

[Bardenet,
Doucet,
Holmes
2017]

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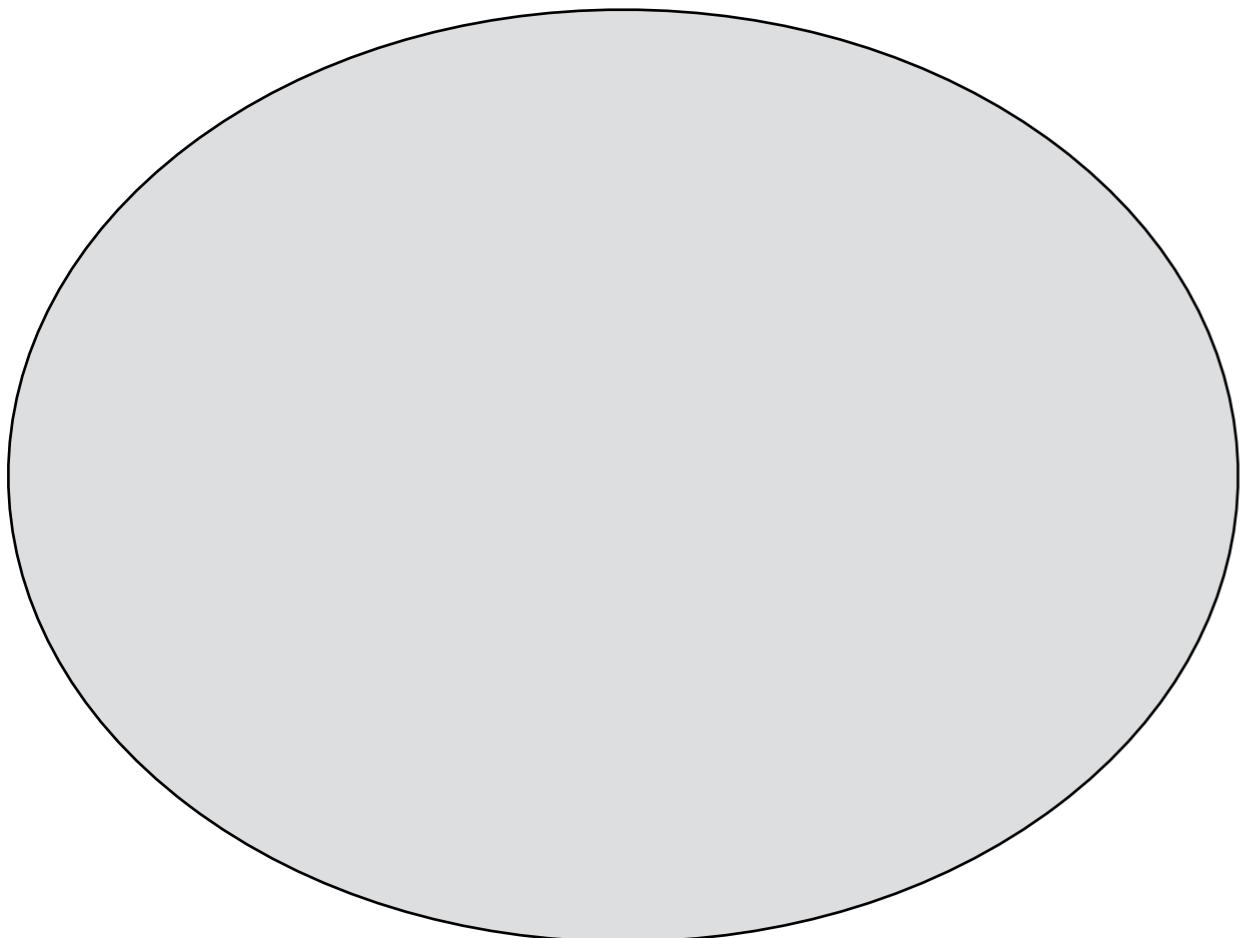
Instead: an optimization approach

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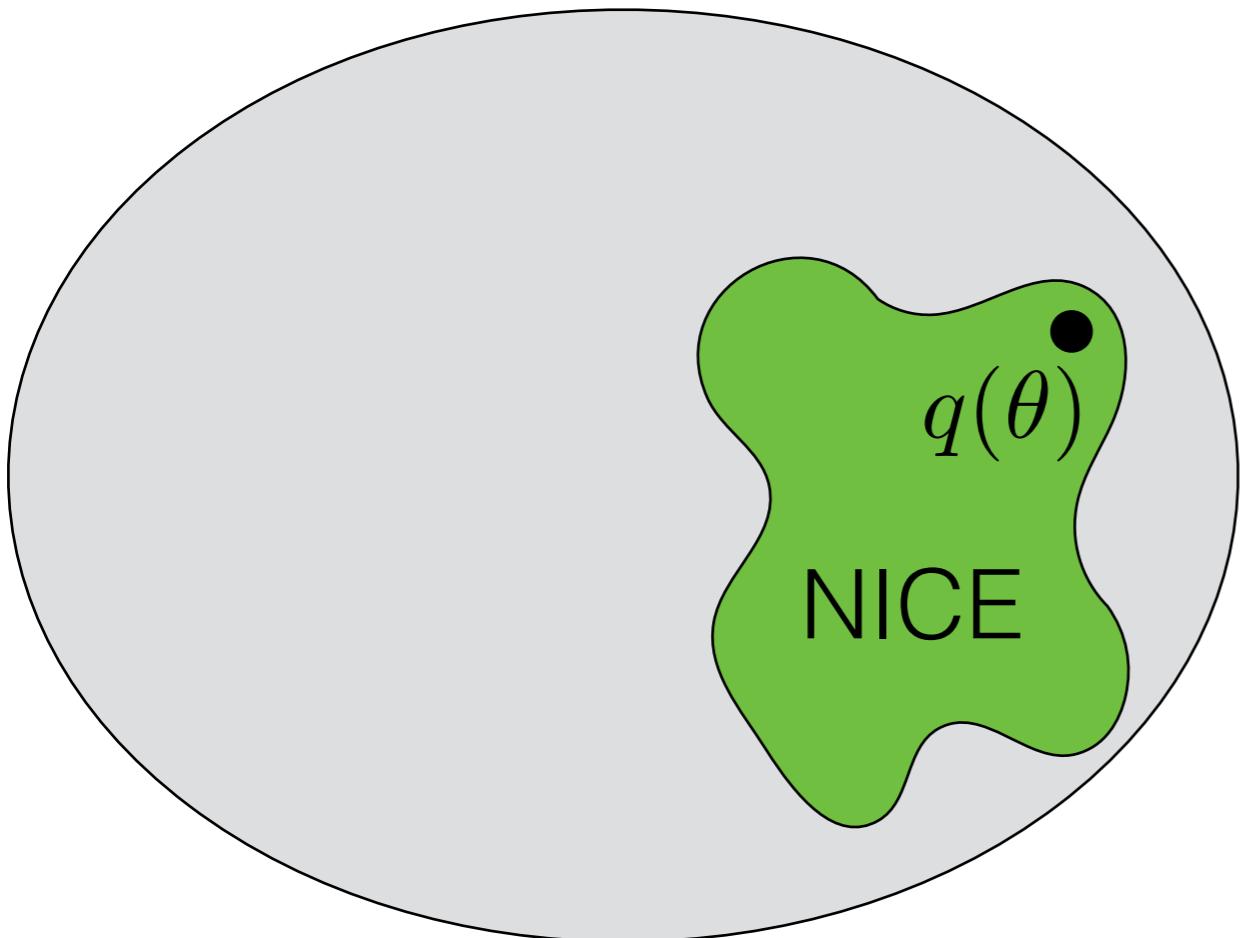
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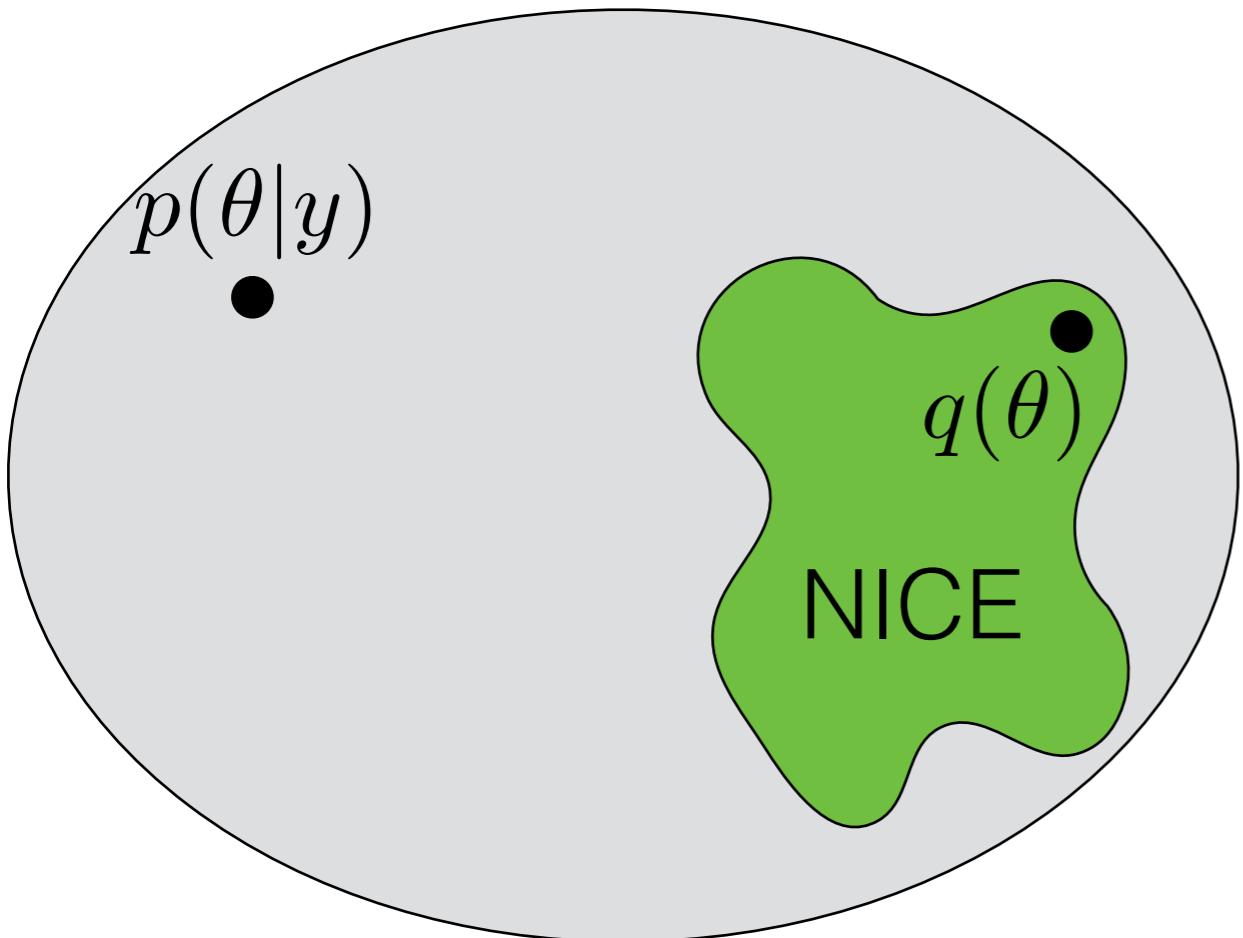
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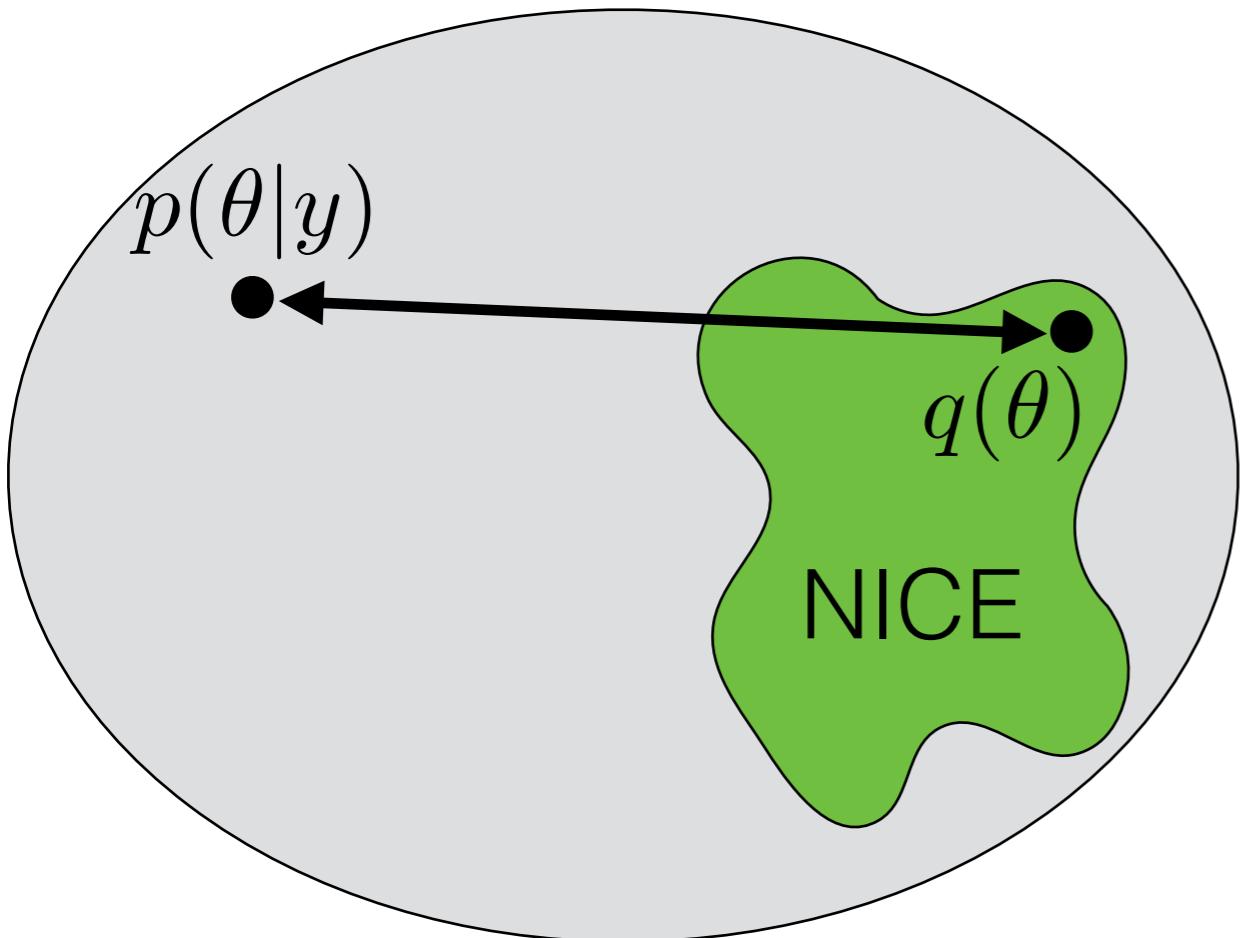
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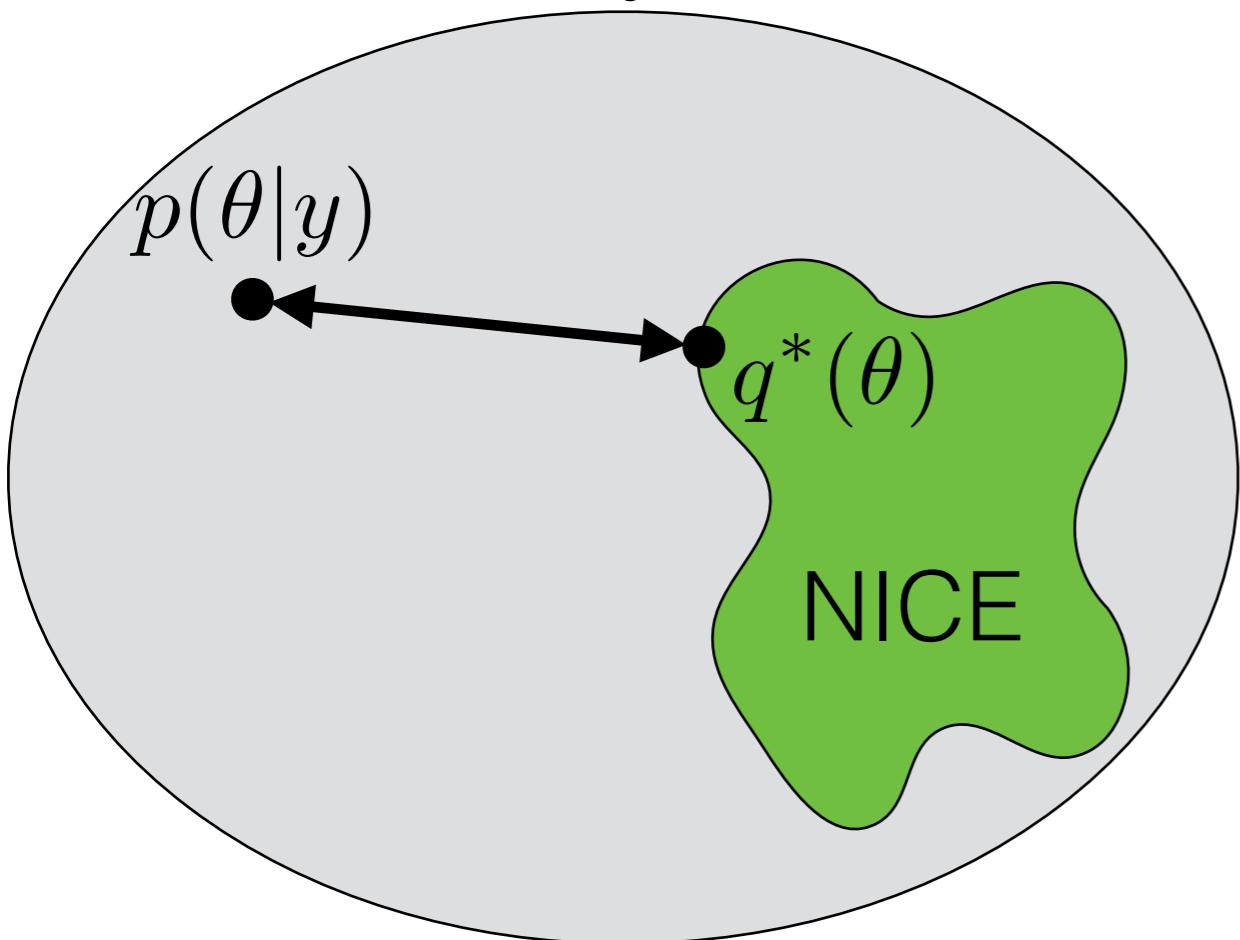
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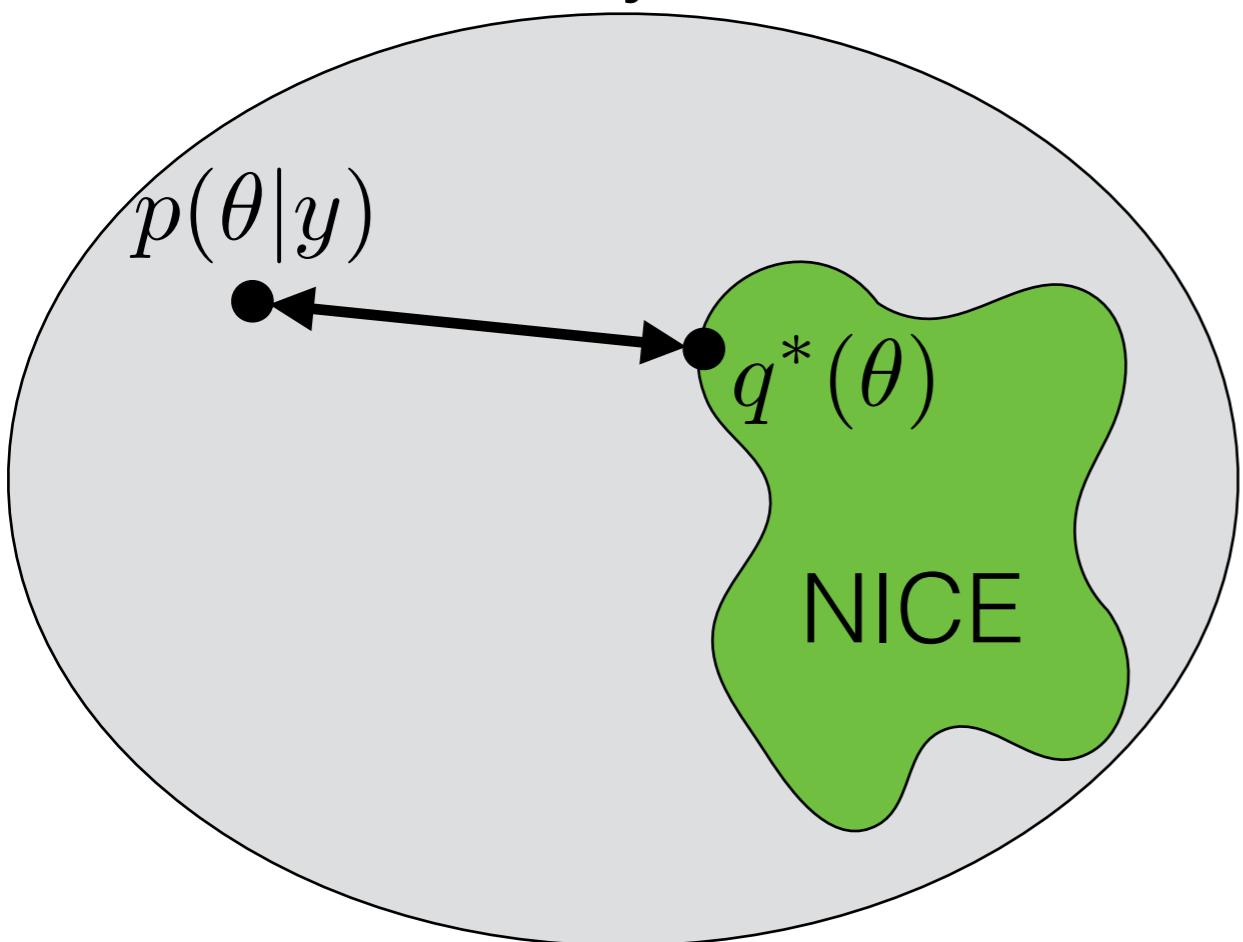
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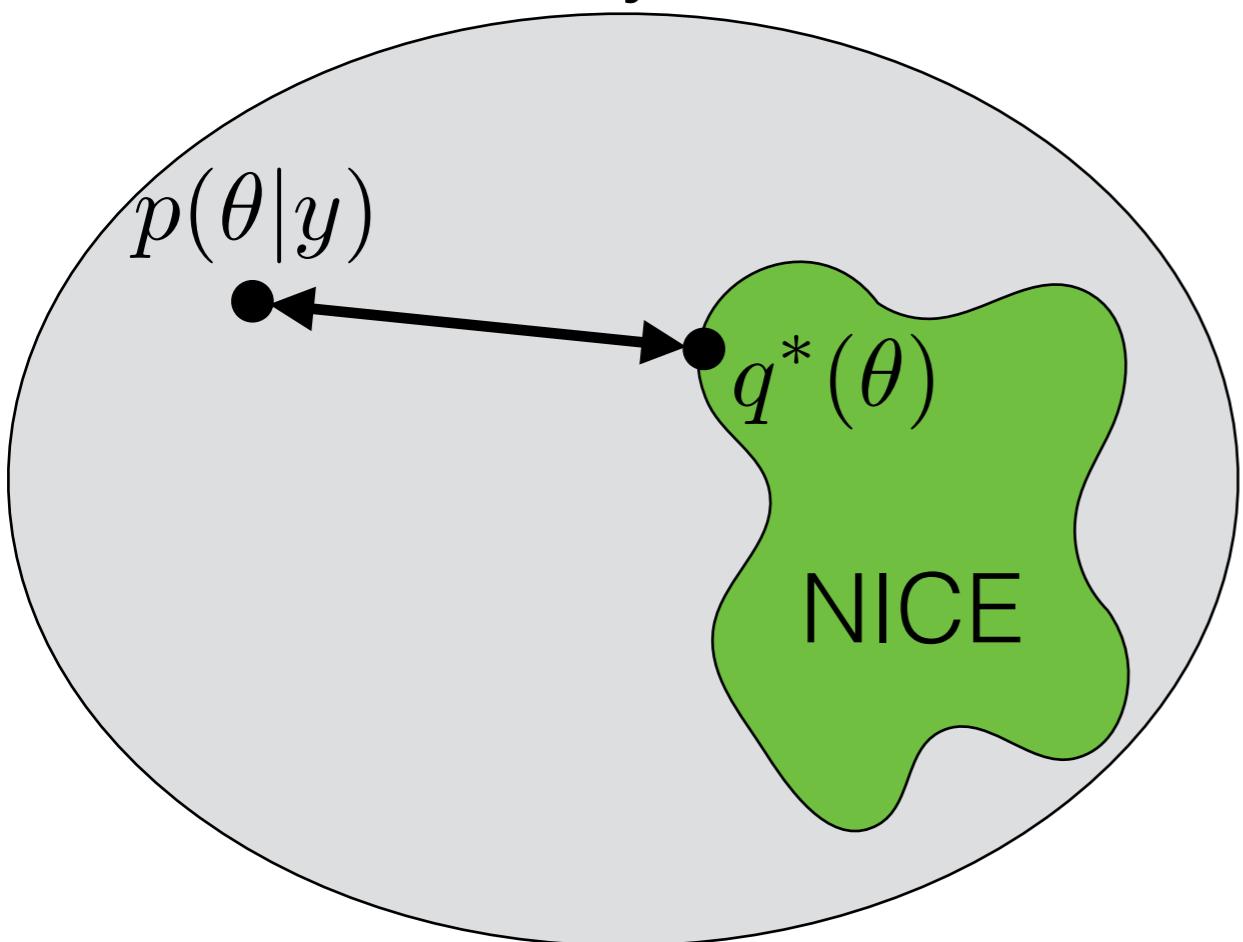
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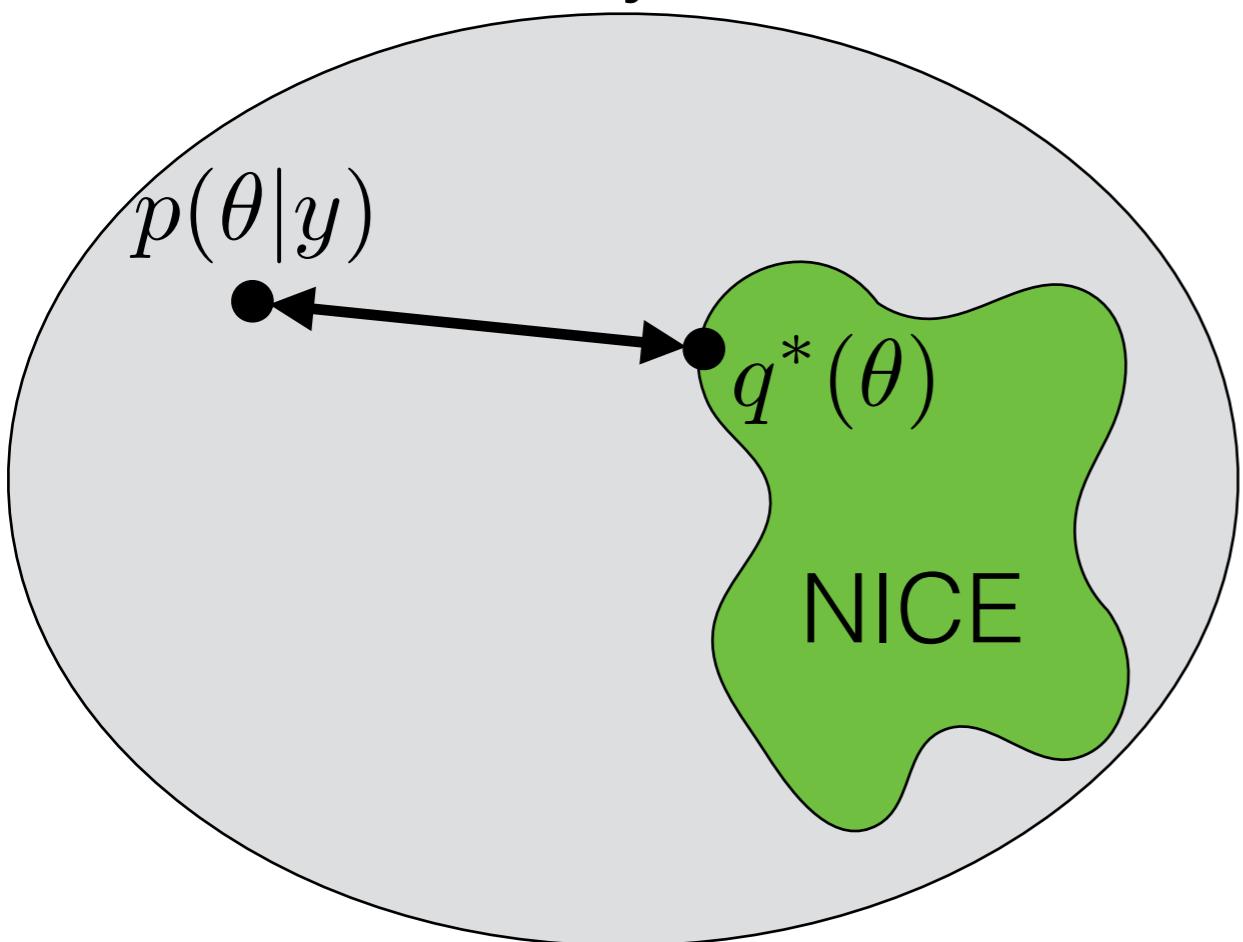
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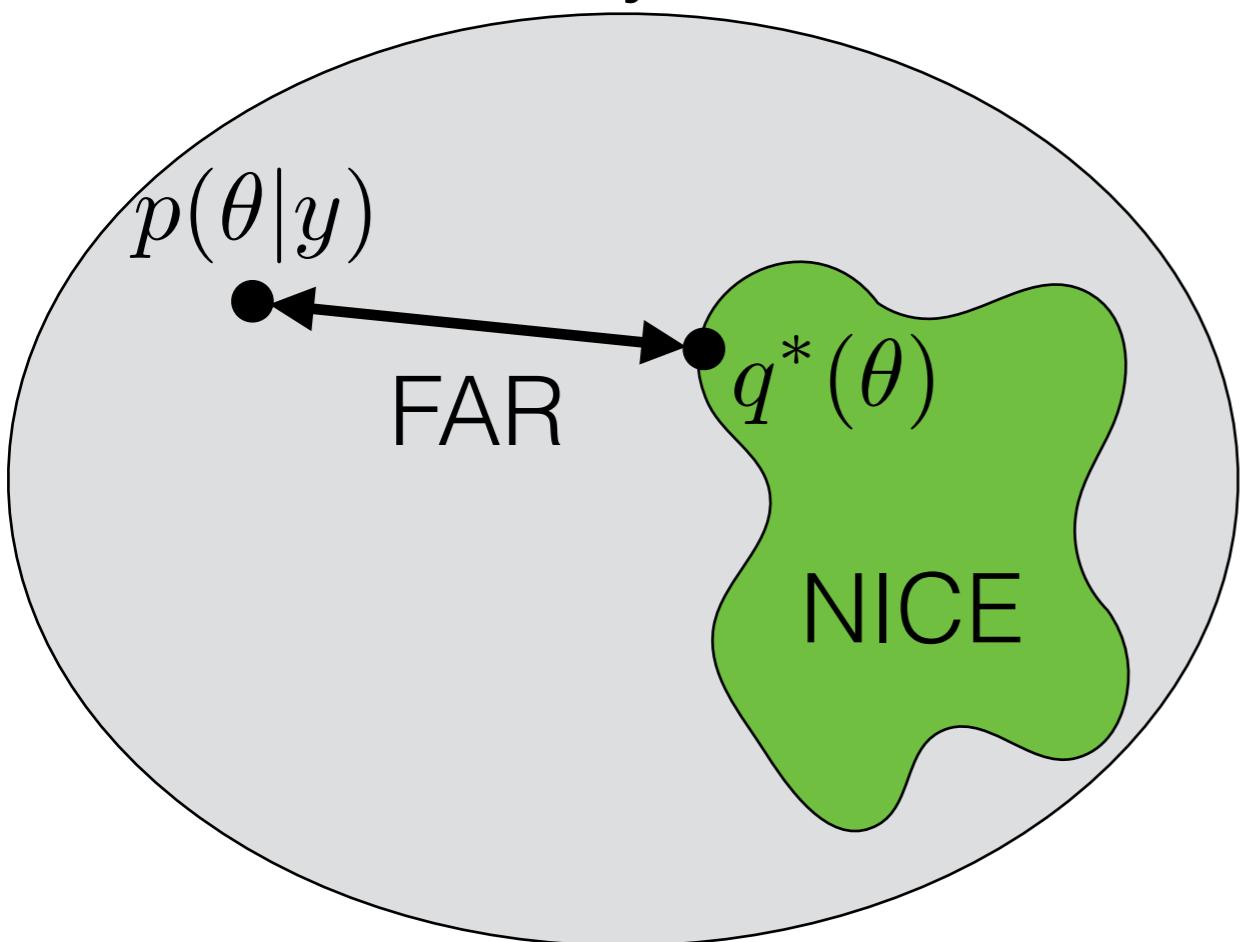
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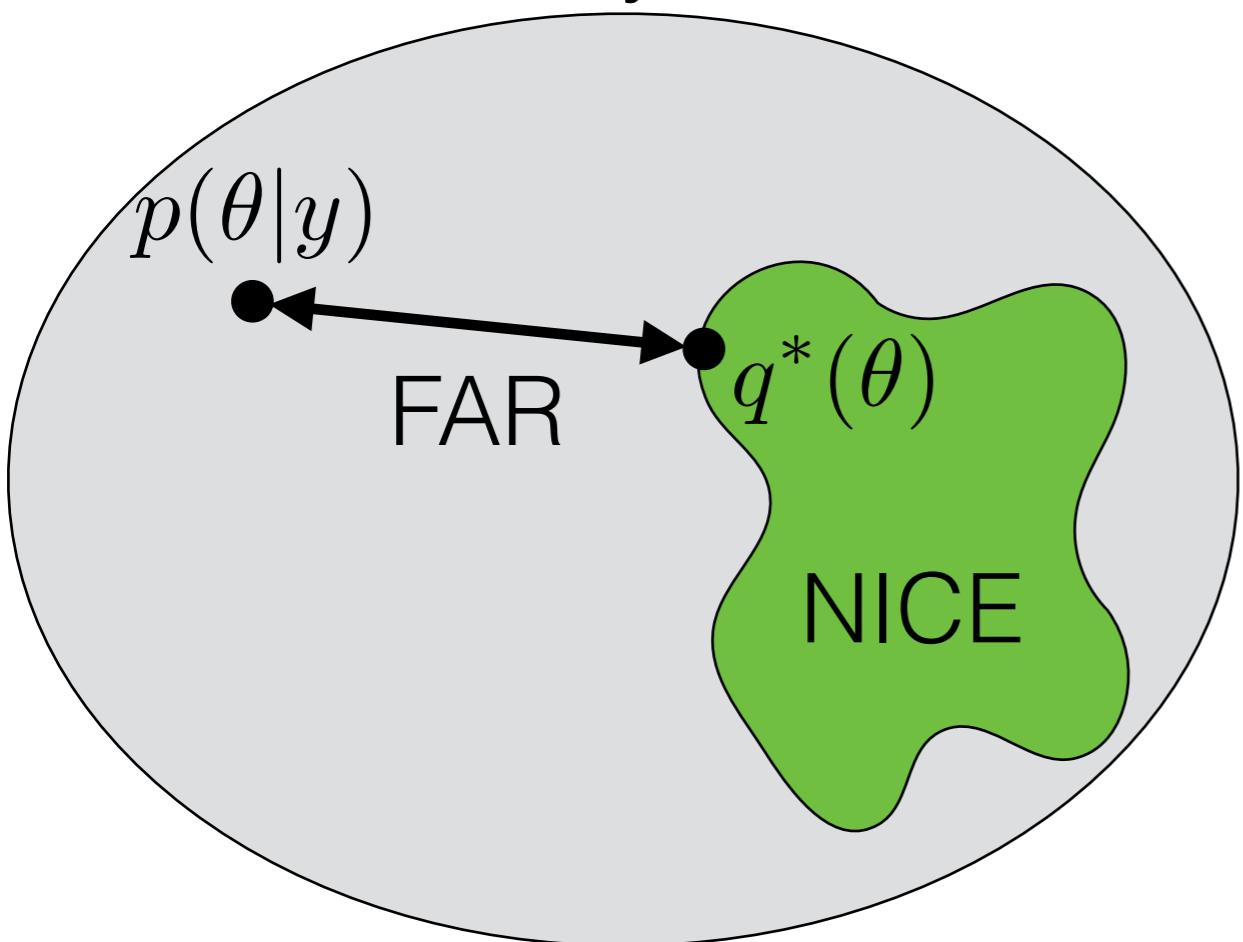
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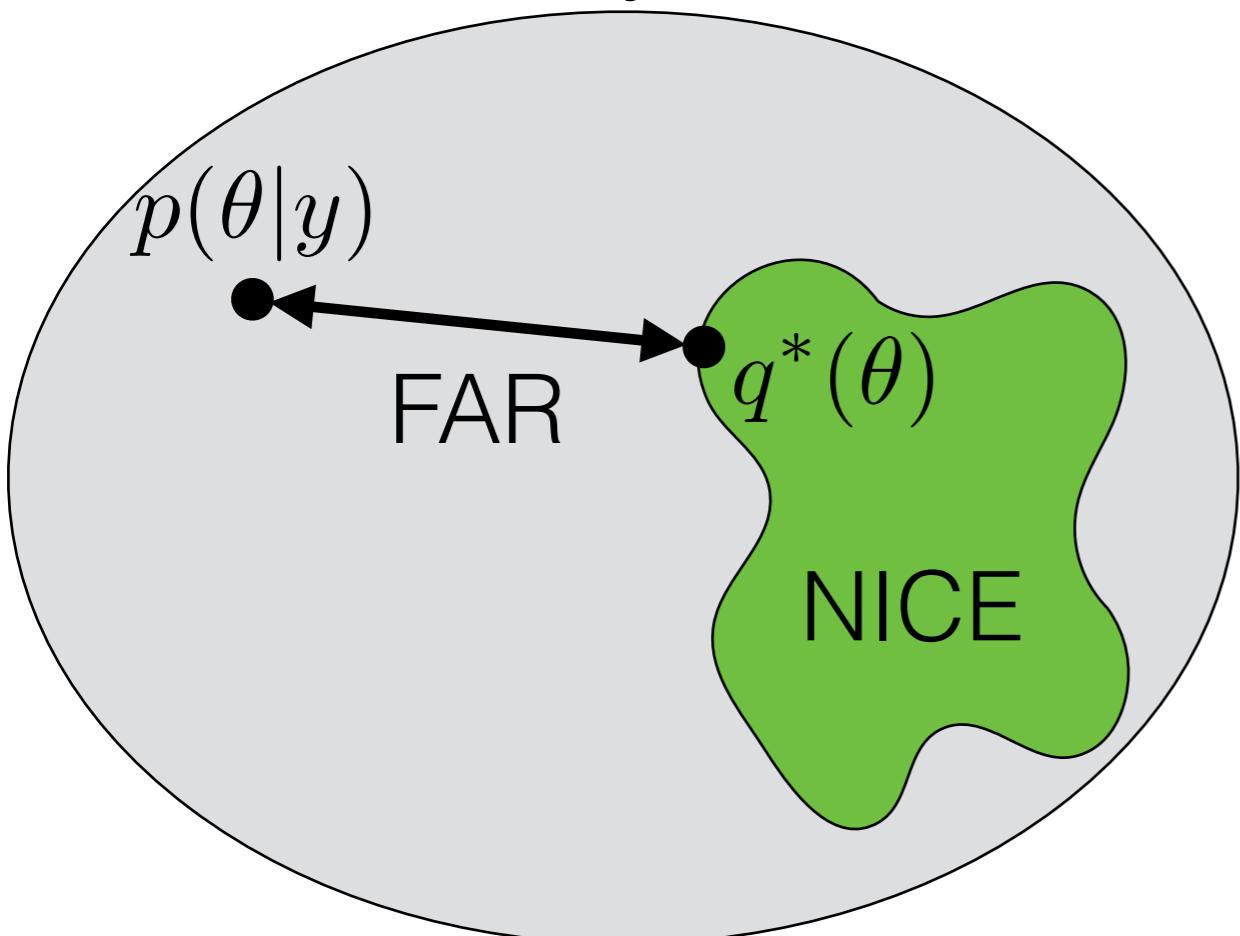
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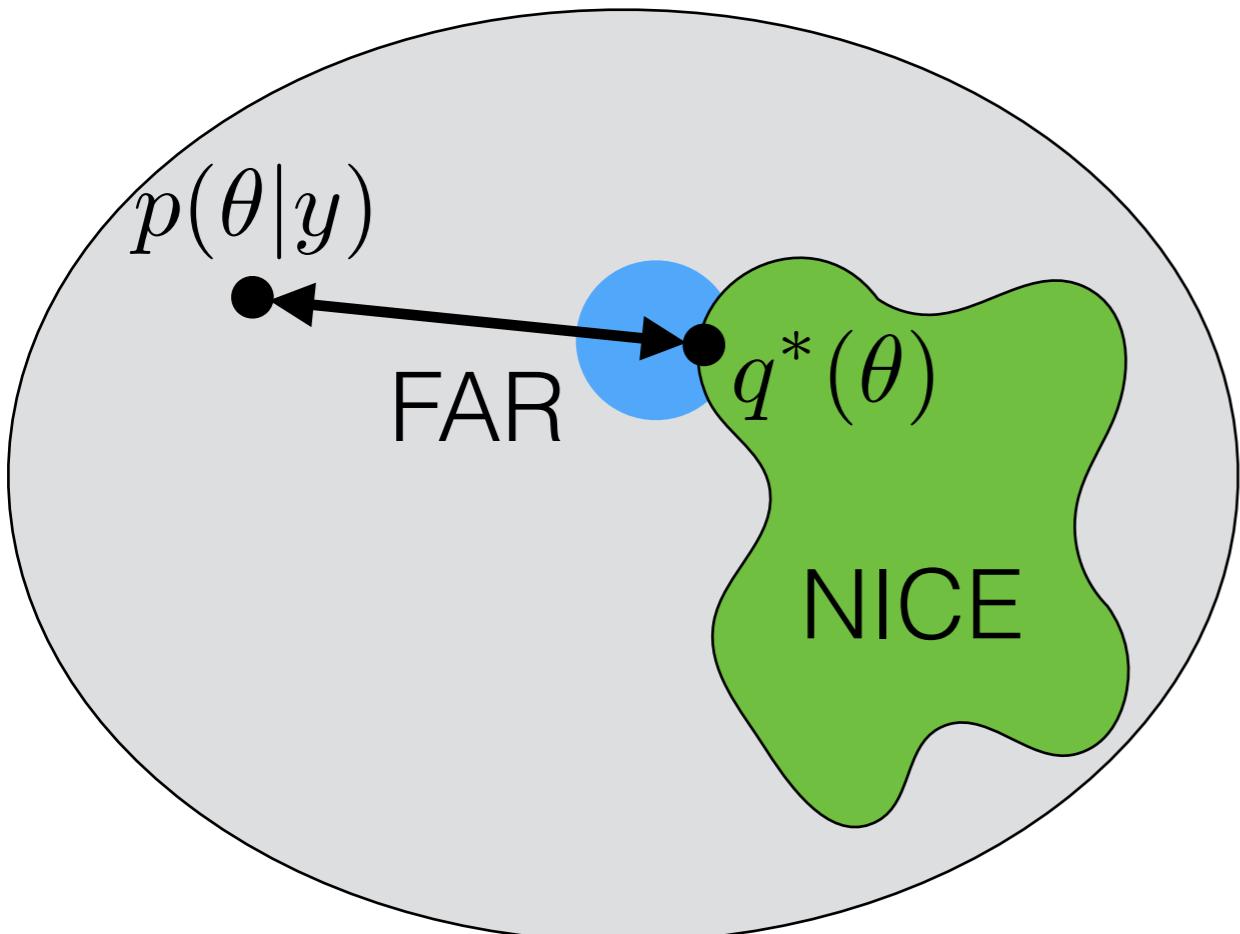
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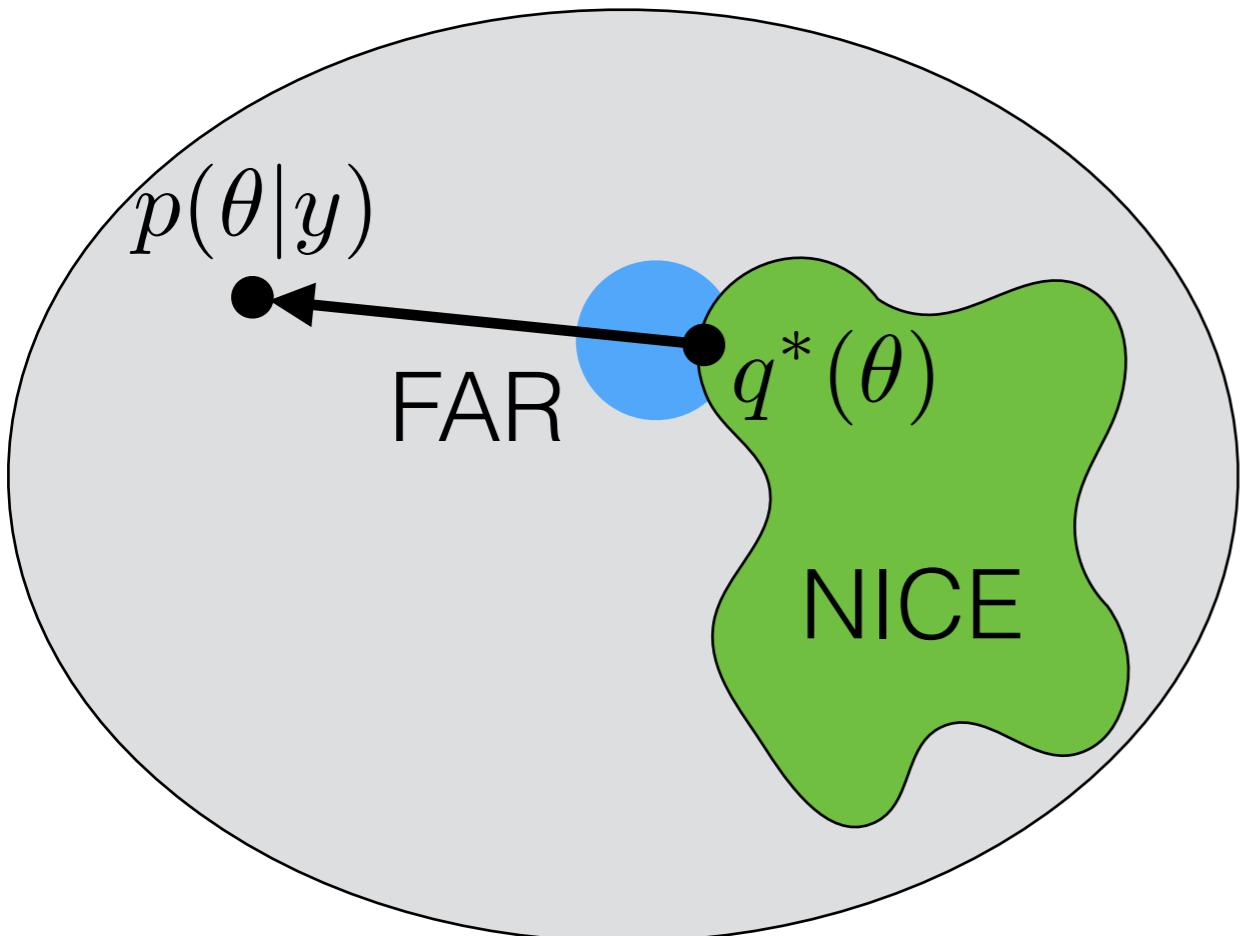
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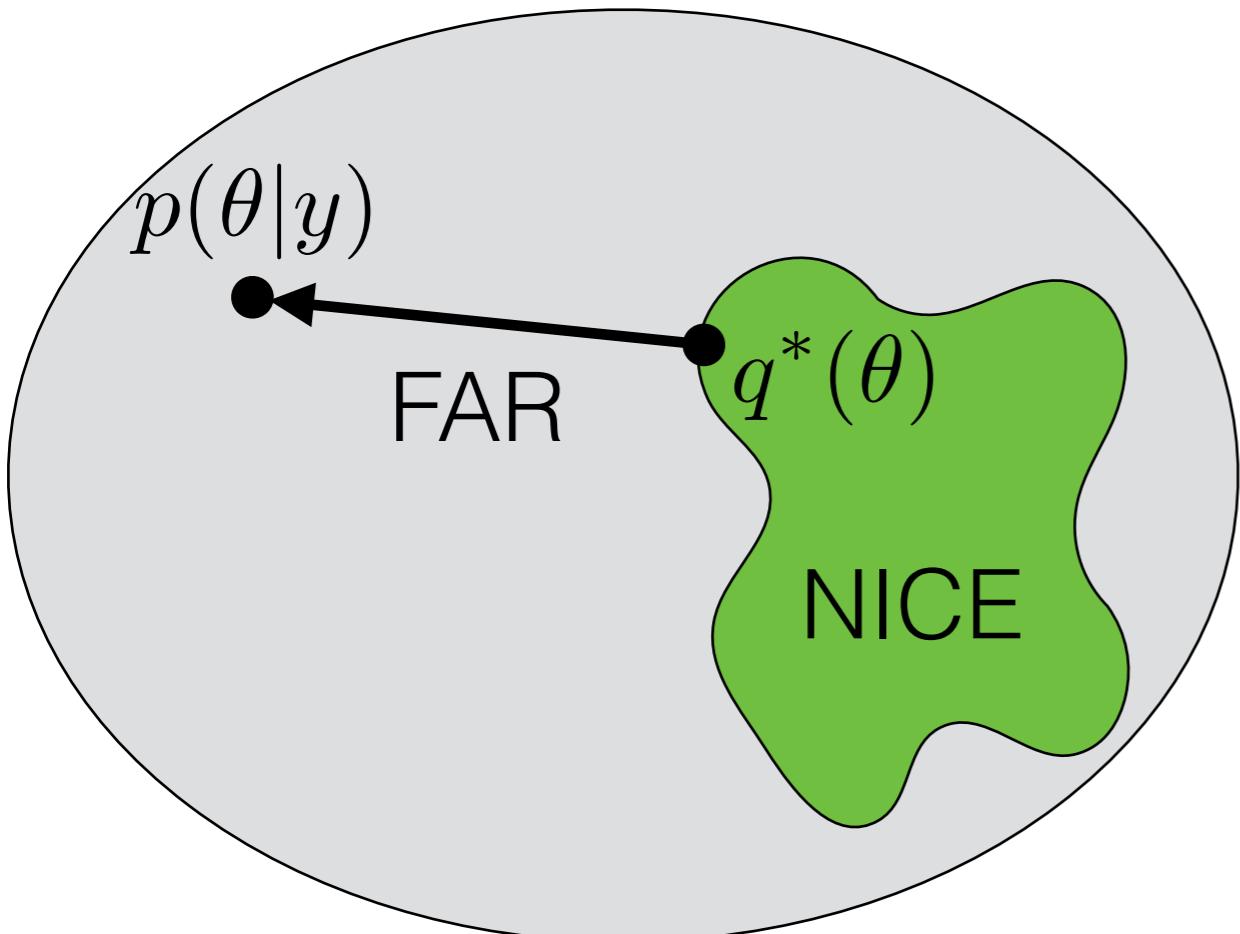
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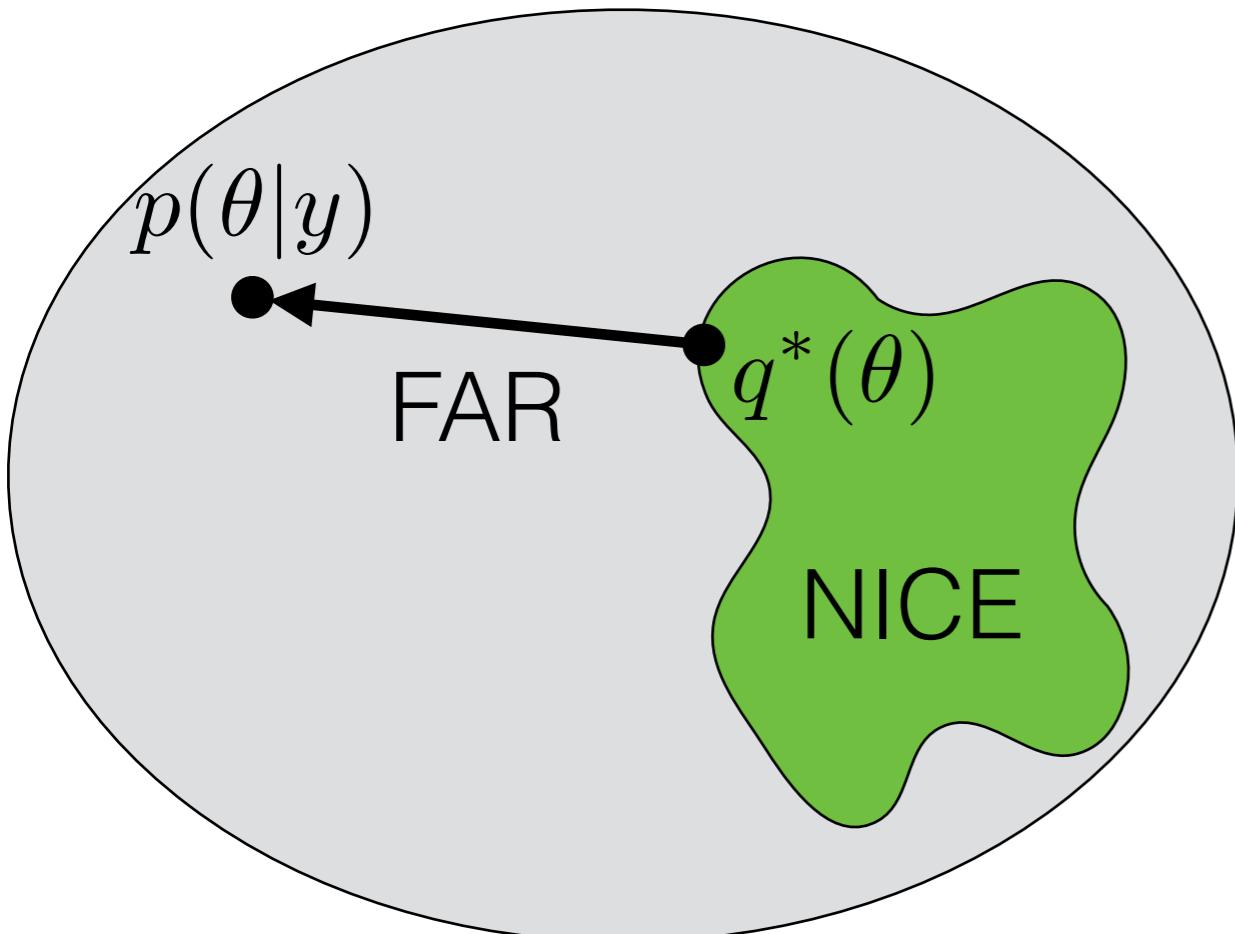
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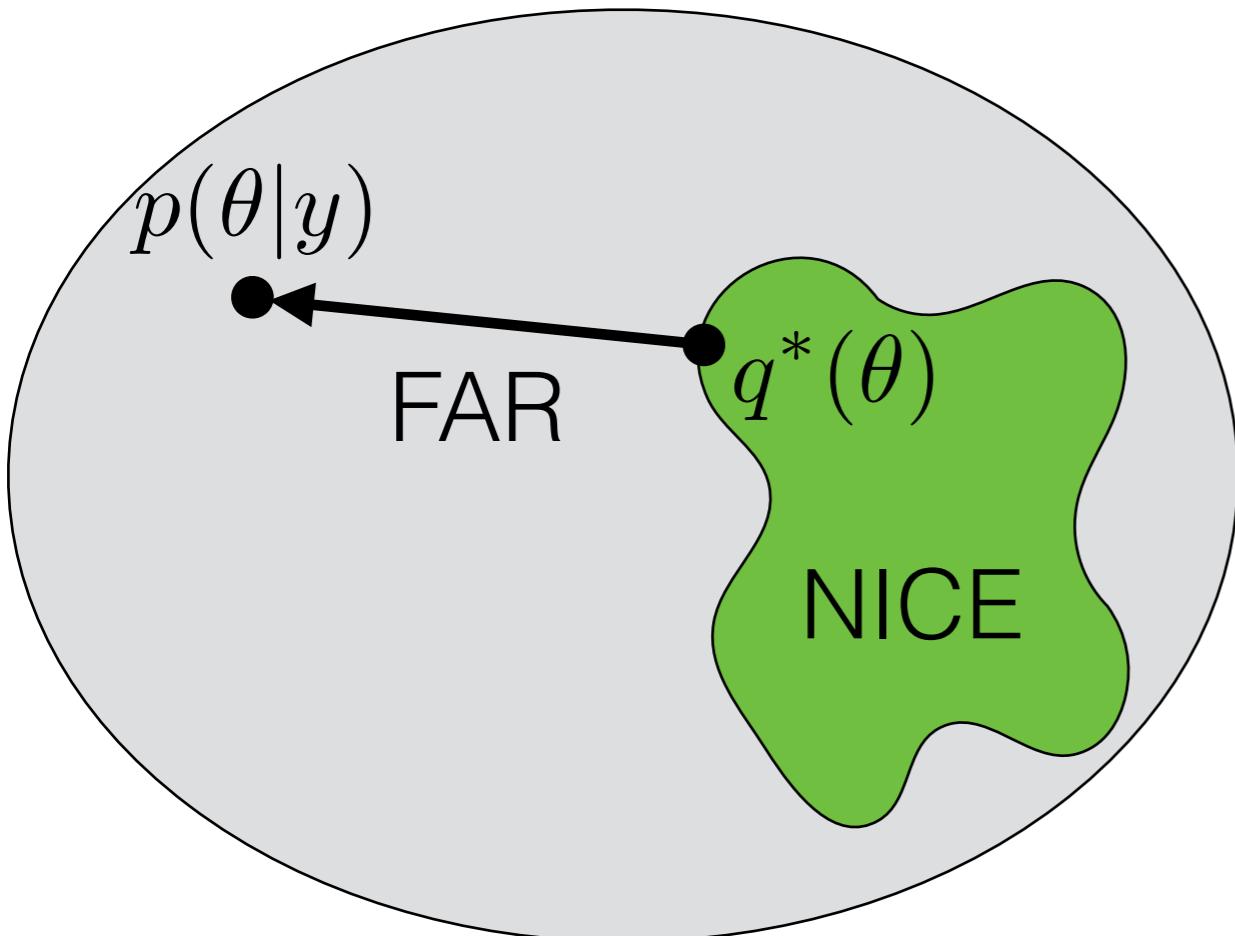
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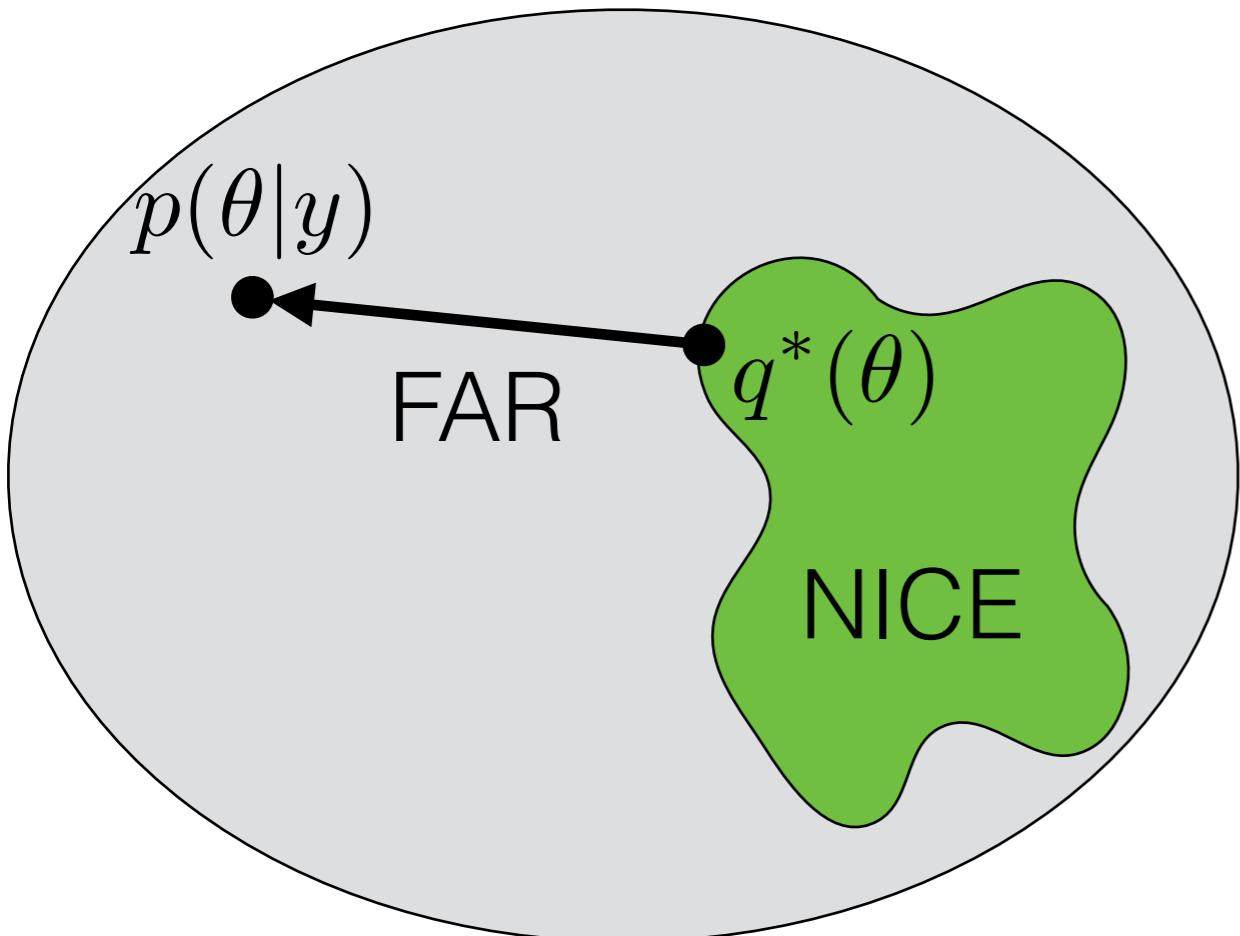
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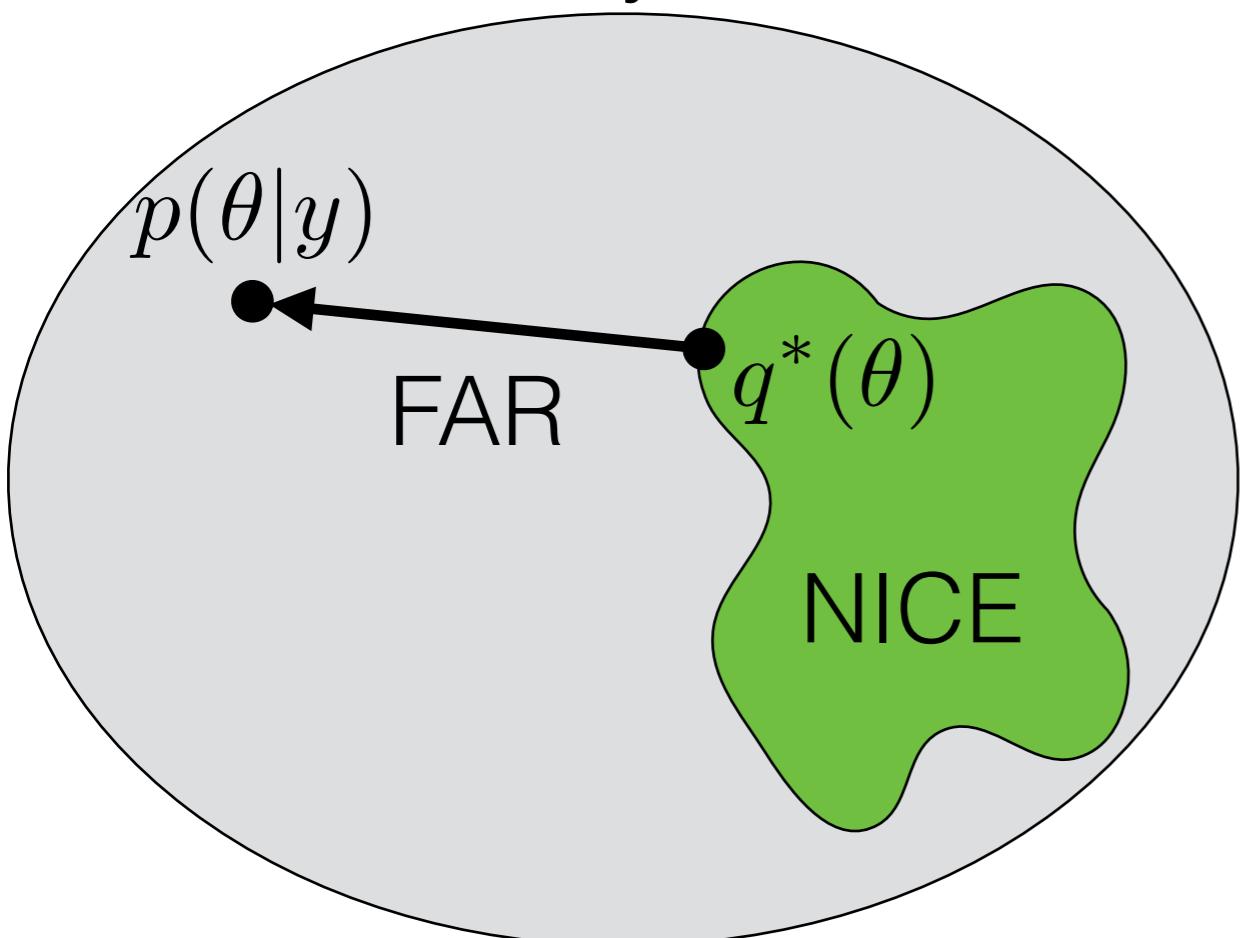
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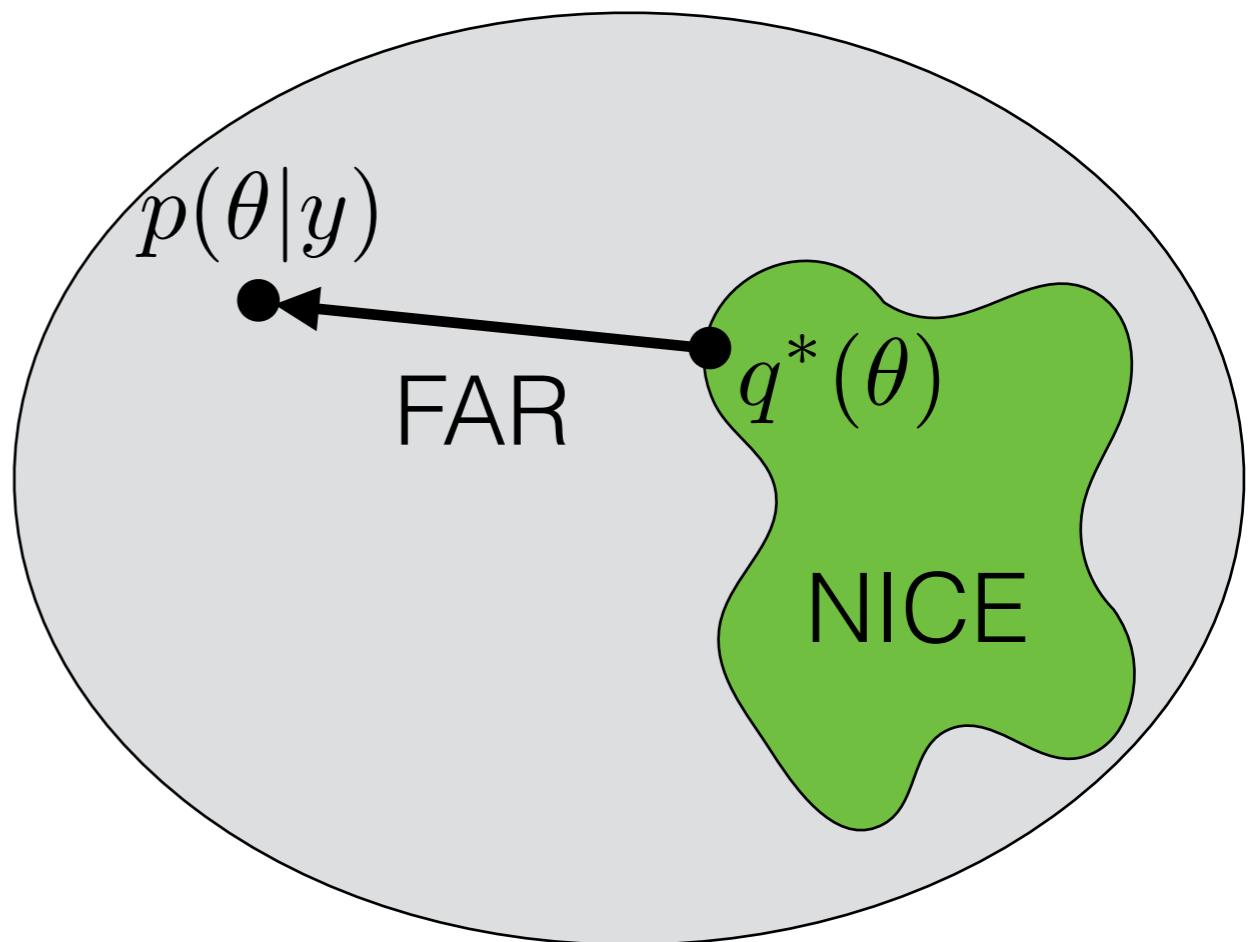
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- VB practical success: point estimates and prediction, fast, streaming, distributed (3.6M Wikipedia, 350K Nature)

Why KL?

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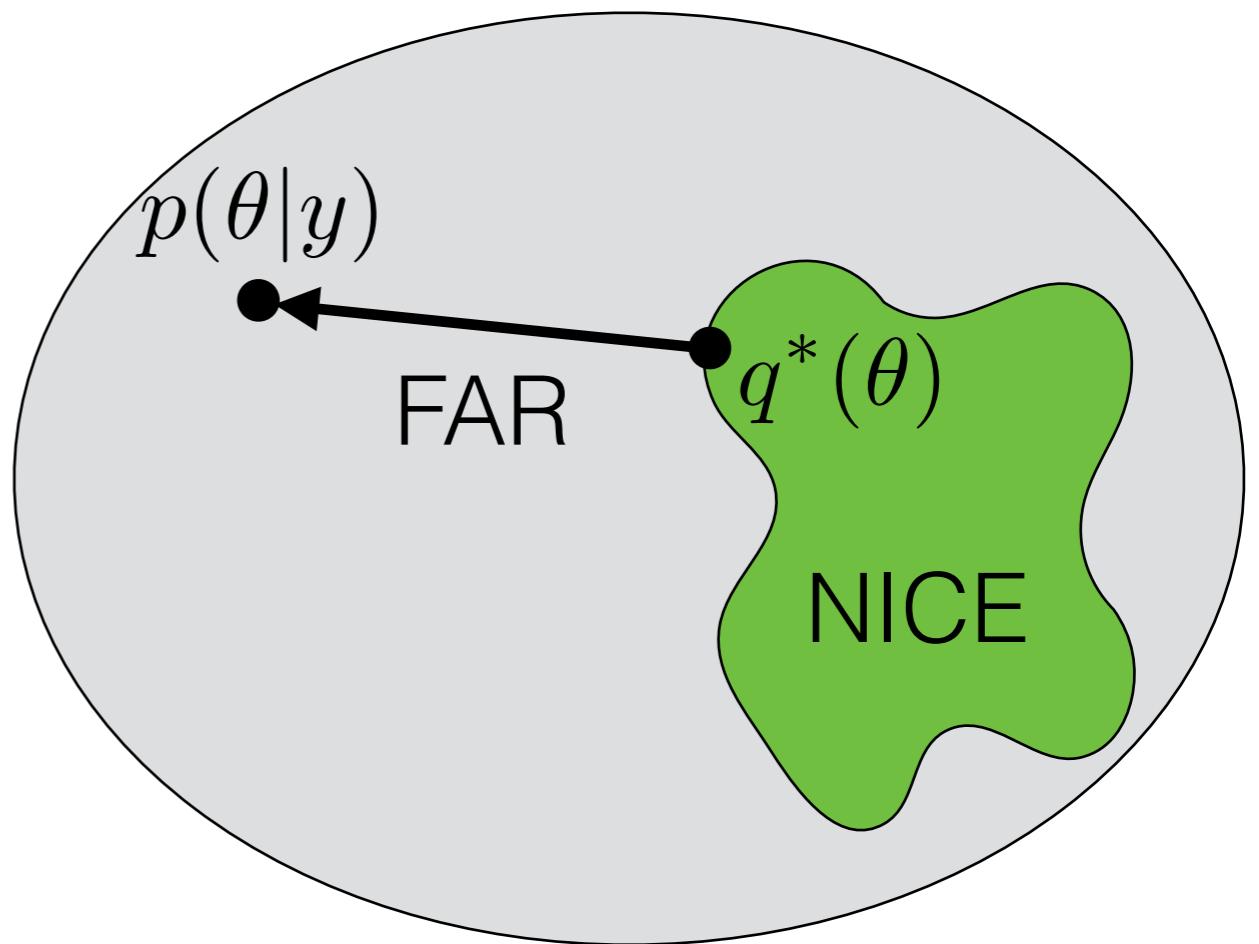
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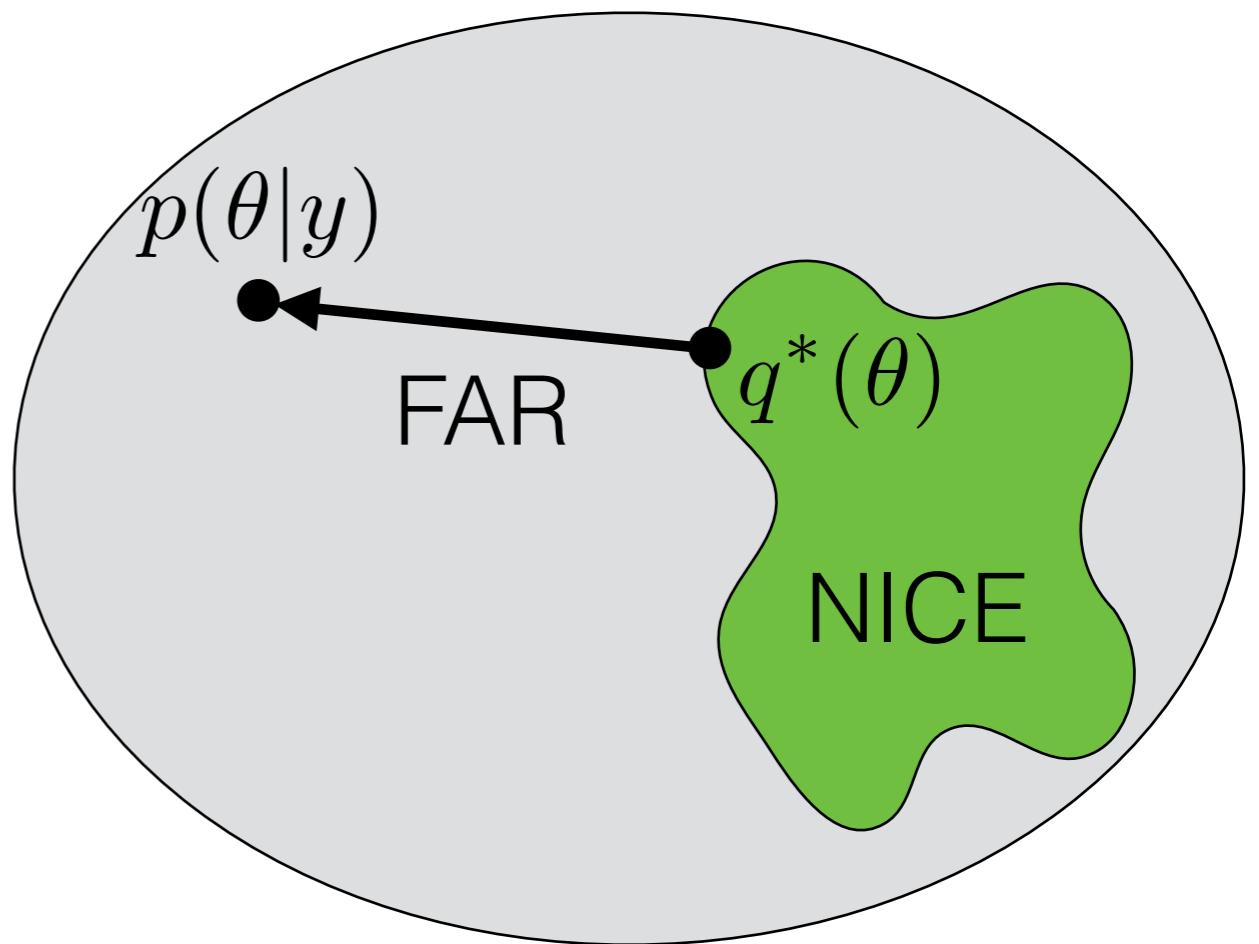
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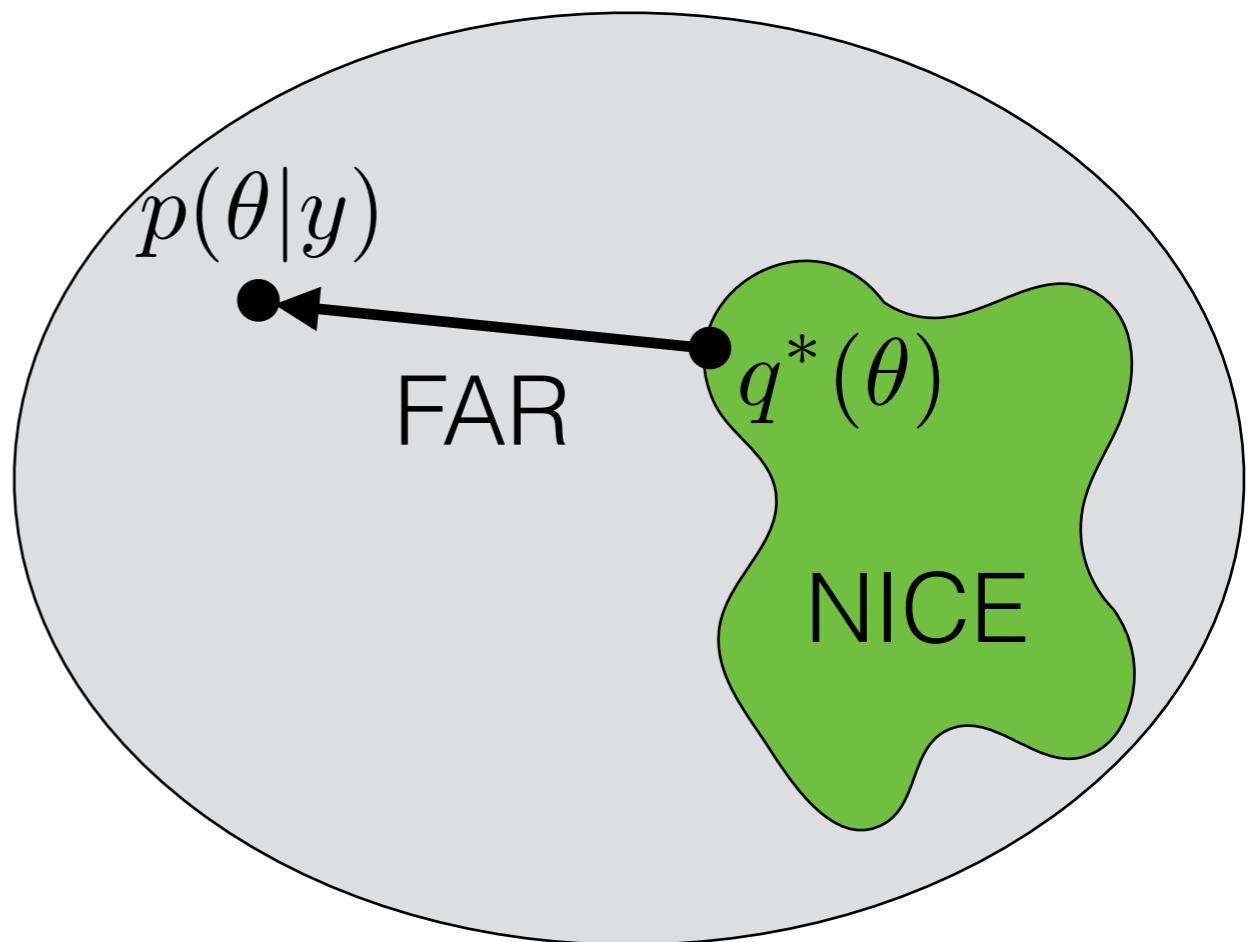
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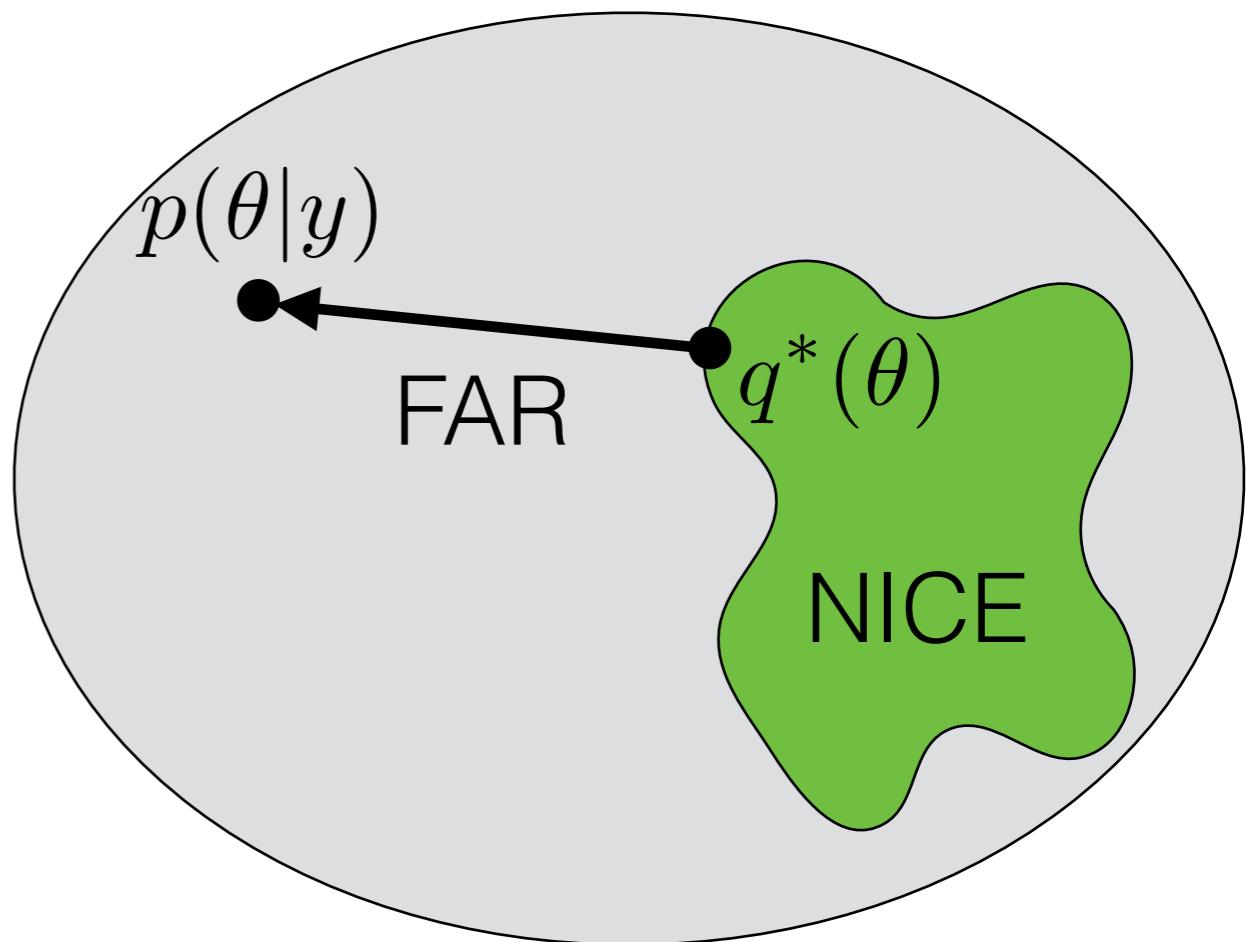
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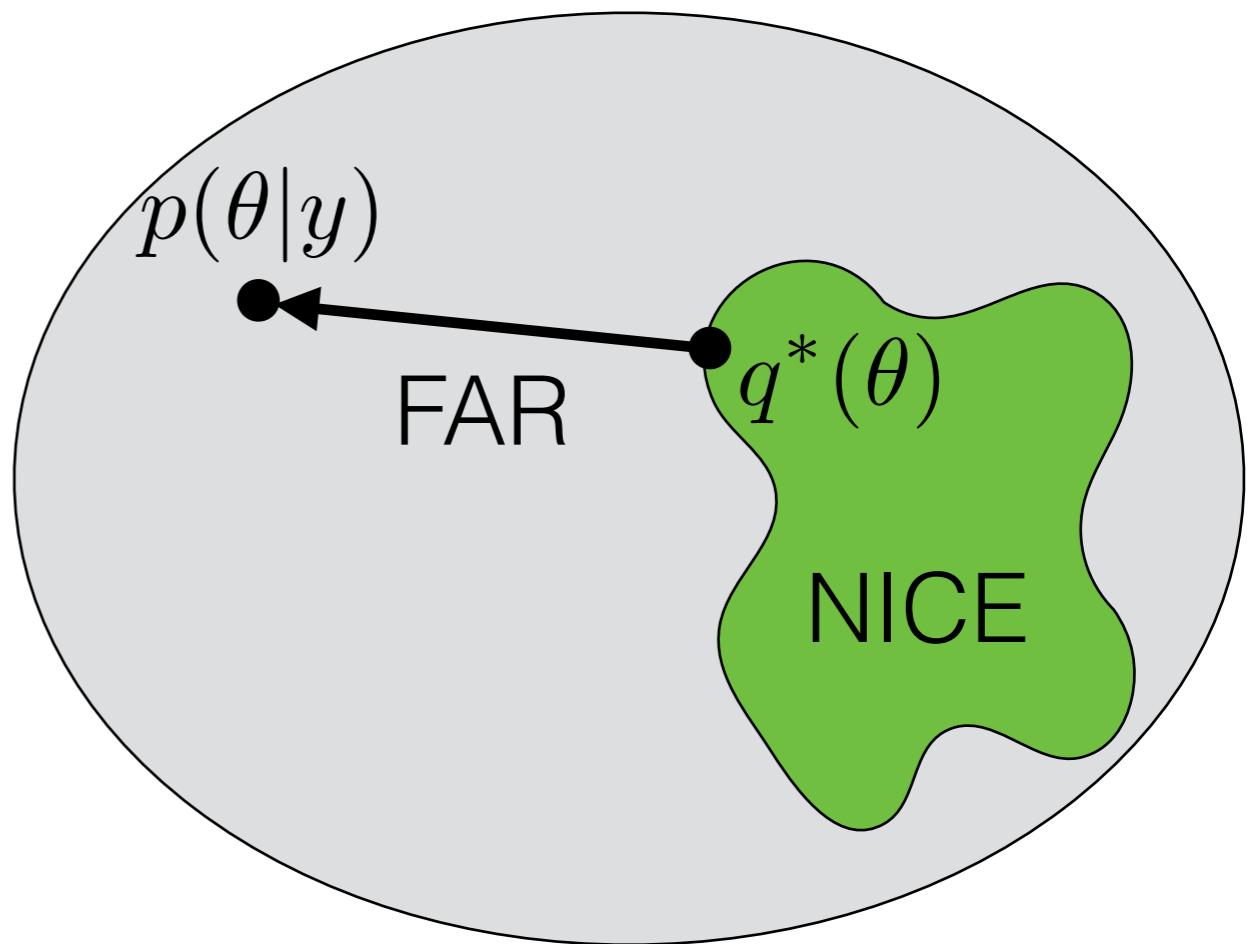
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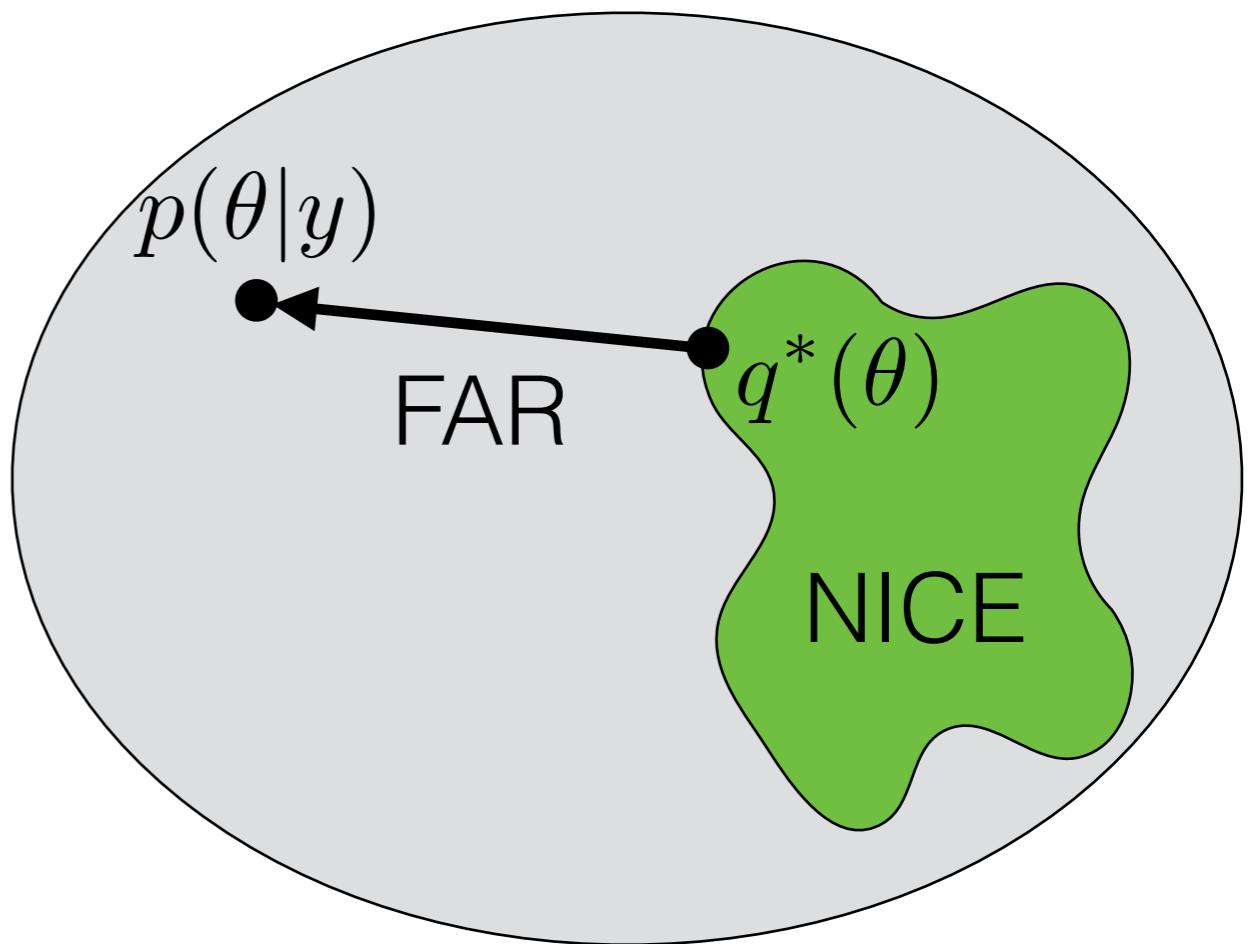
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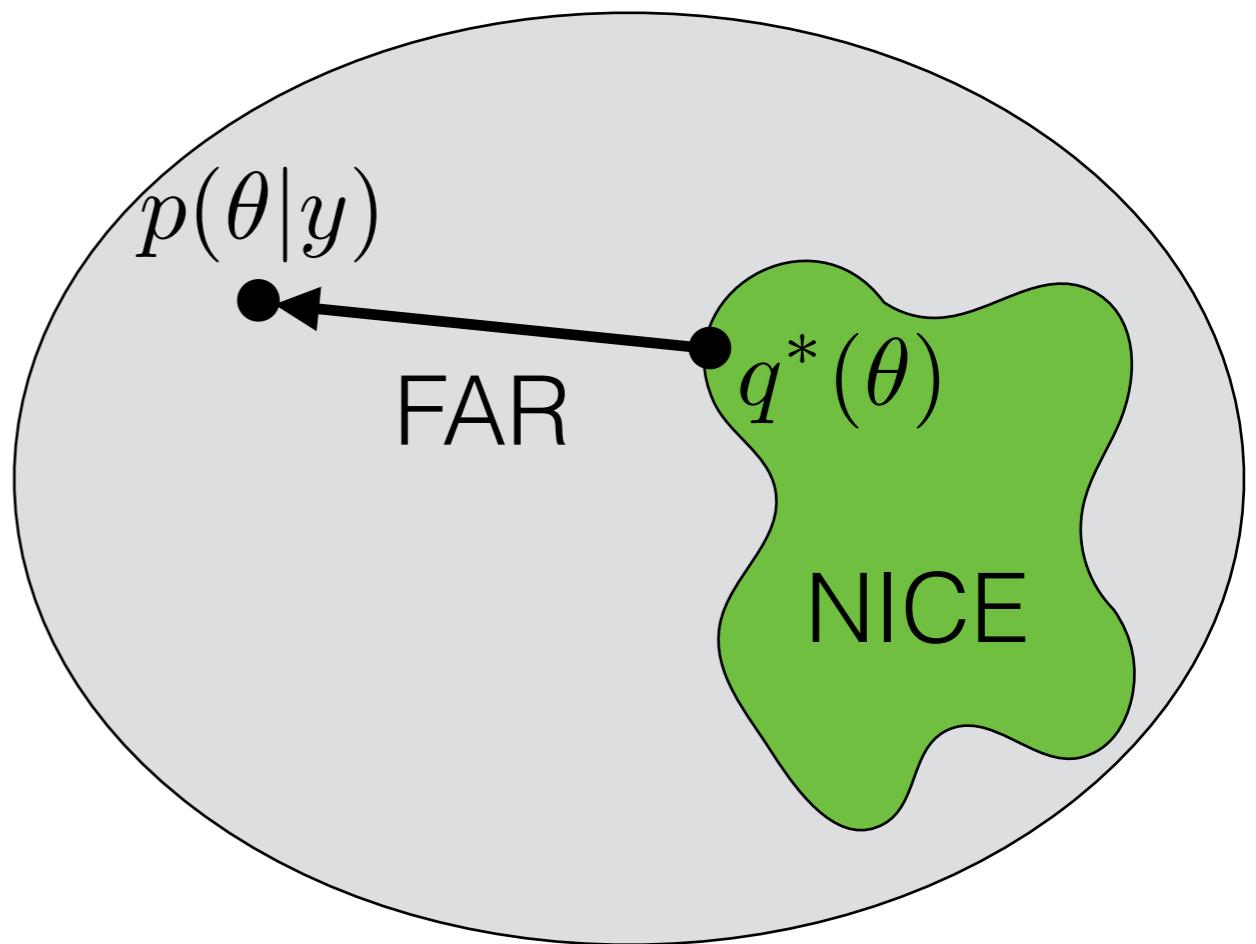
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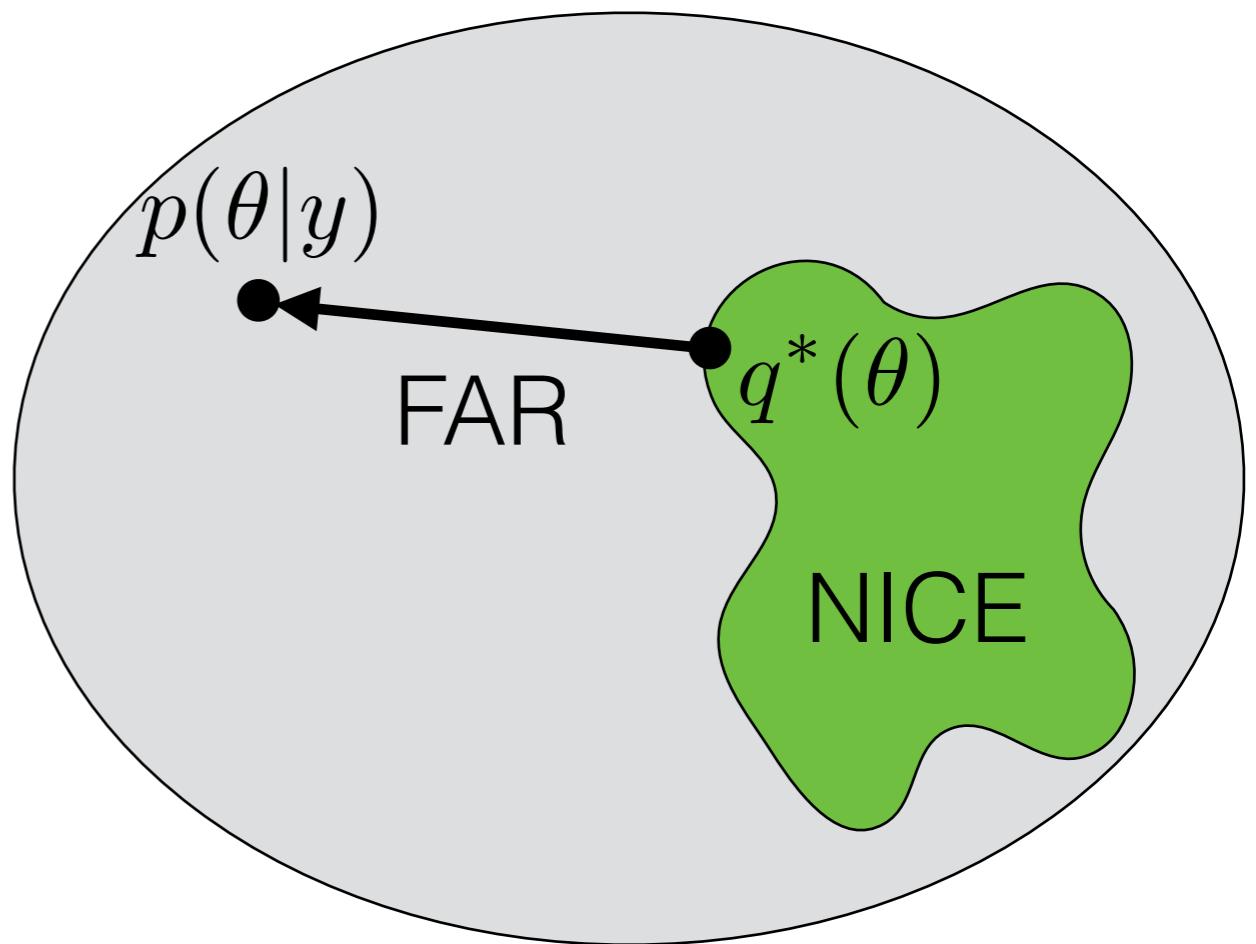
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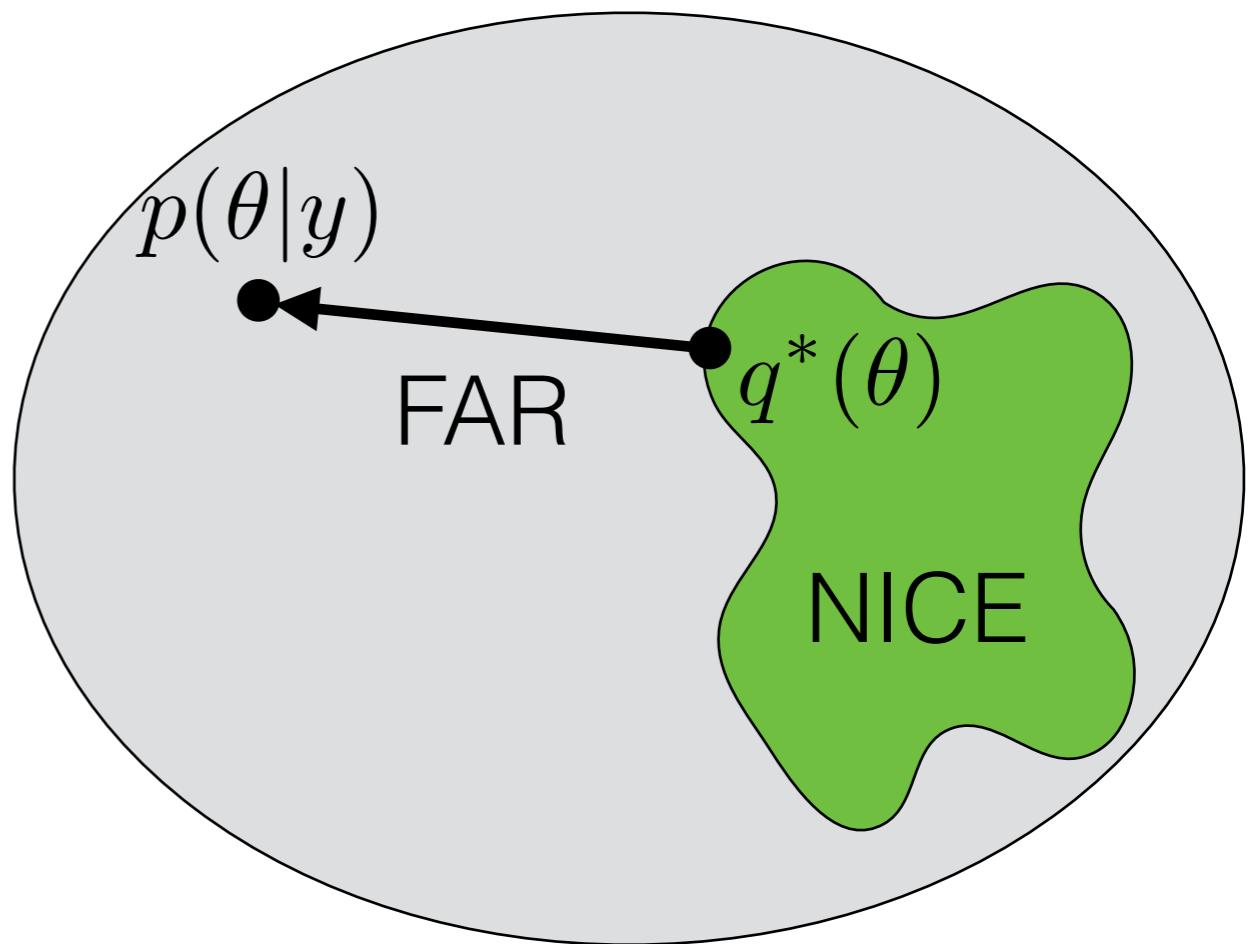
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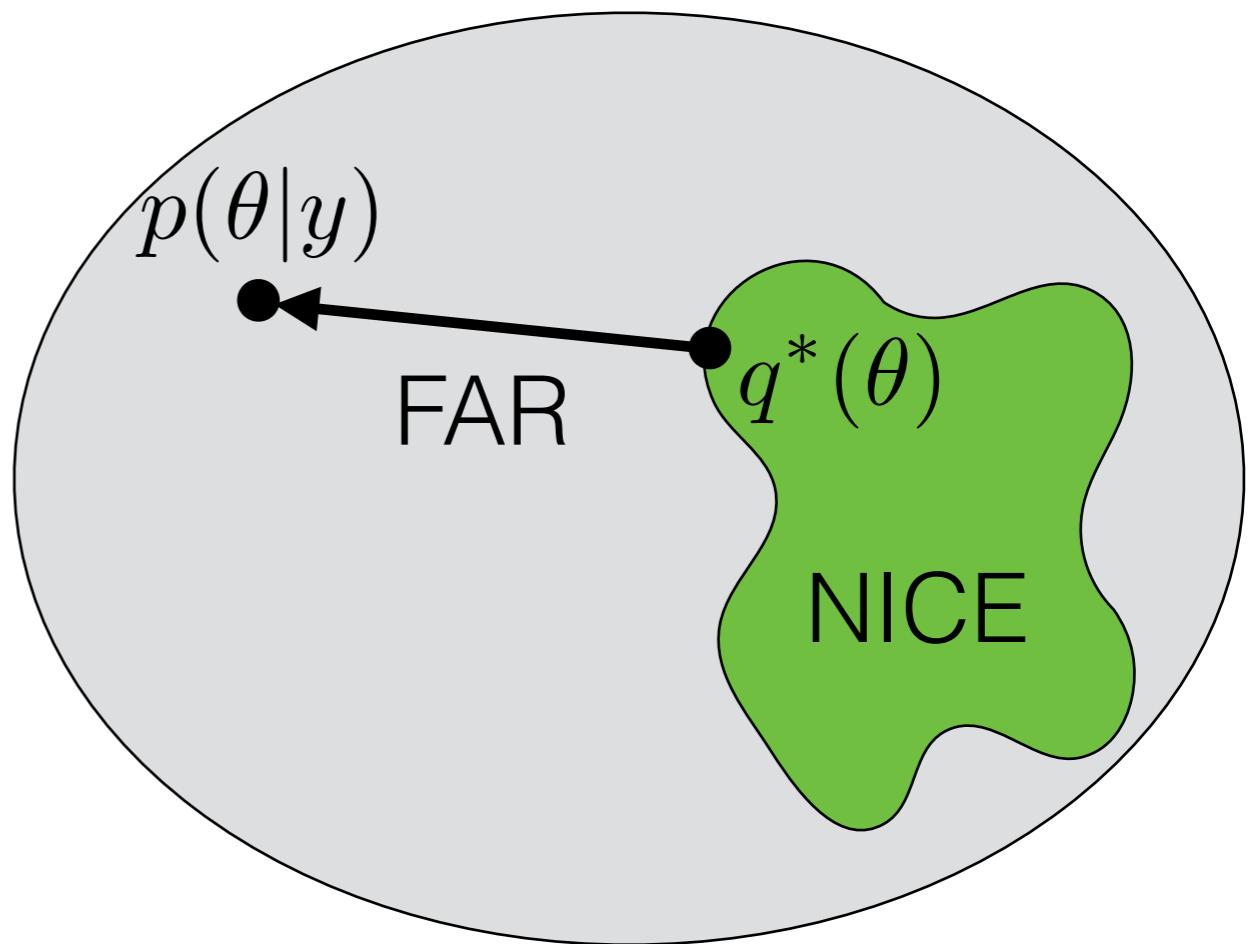
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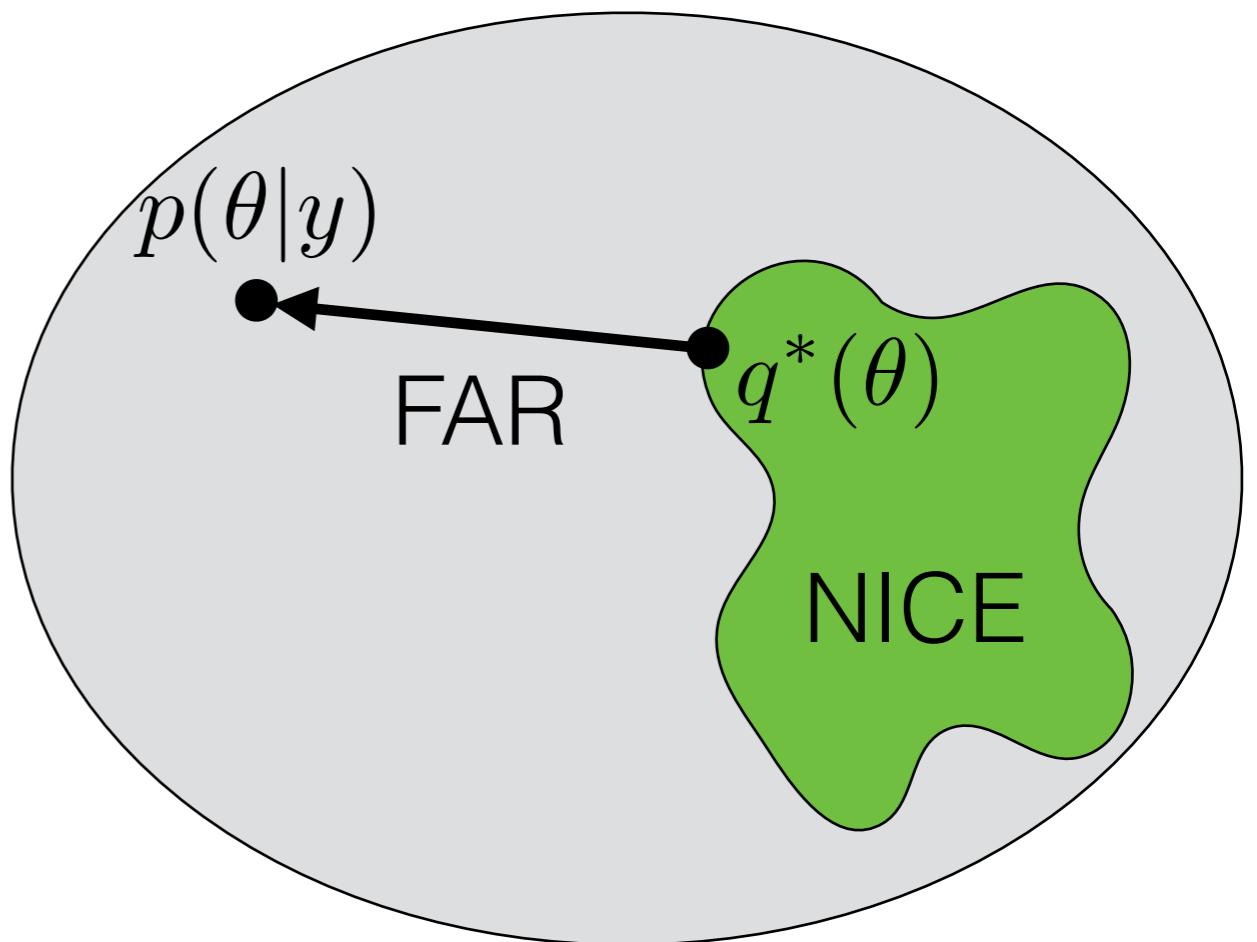
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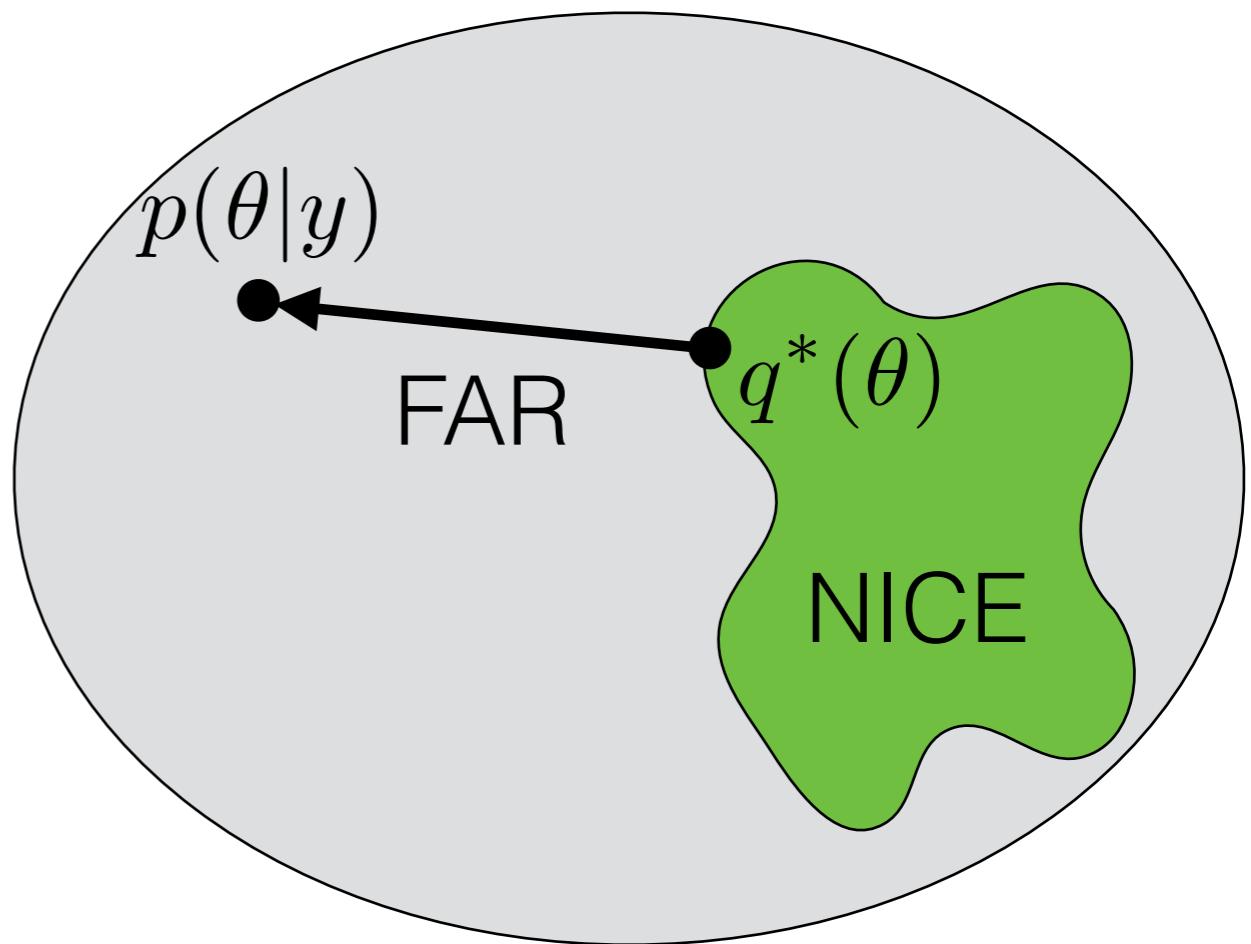
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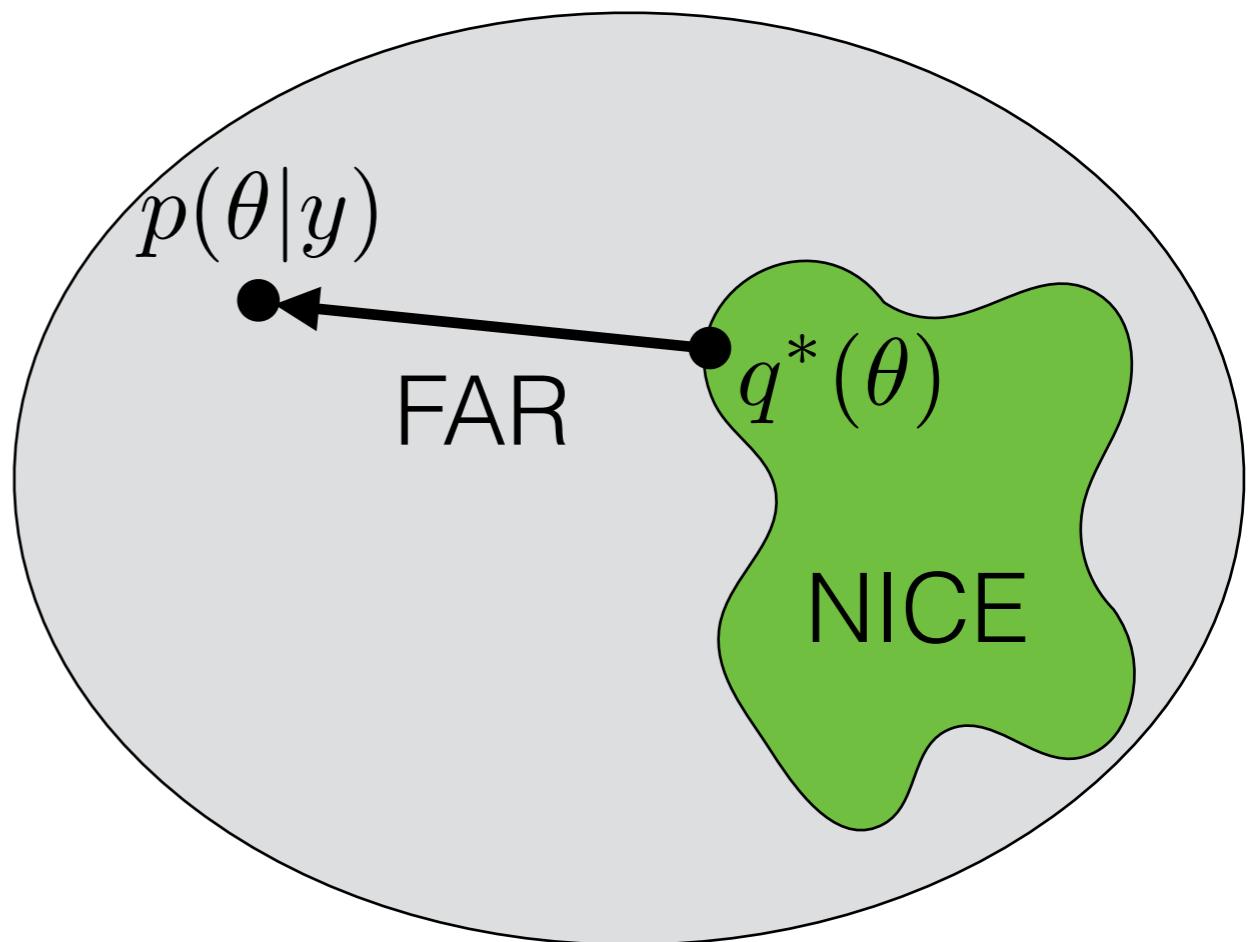
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“Evidence lower bound” (ELBO)

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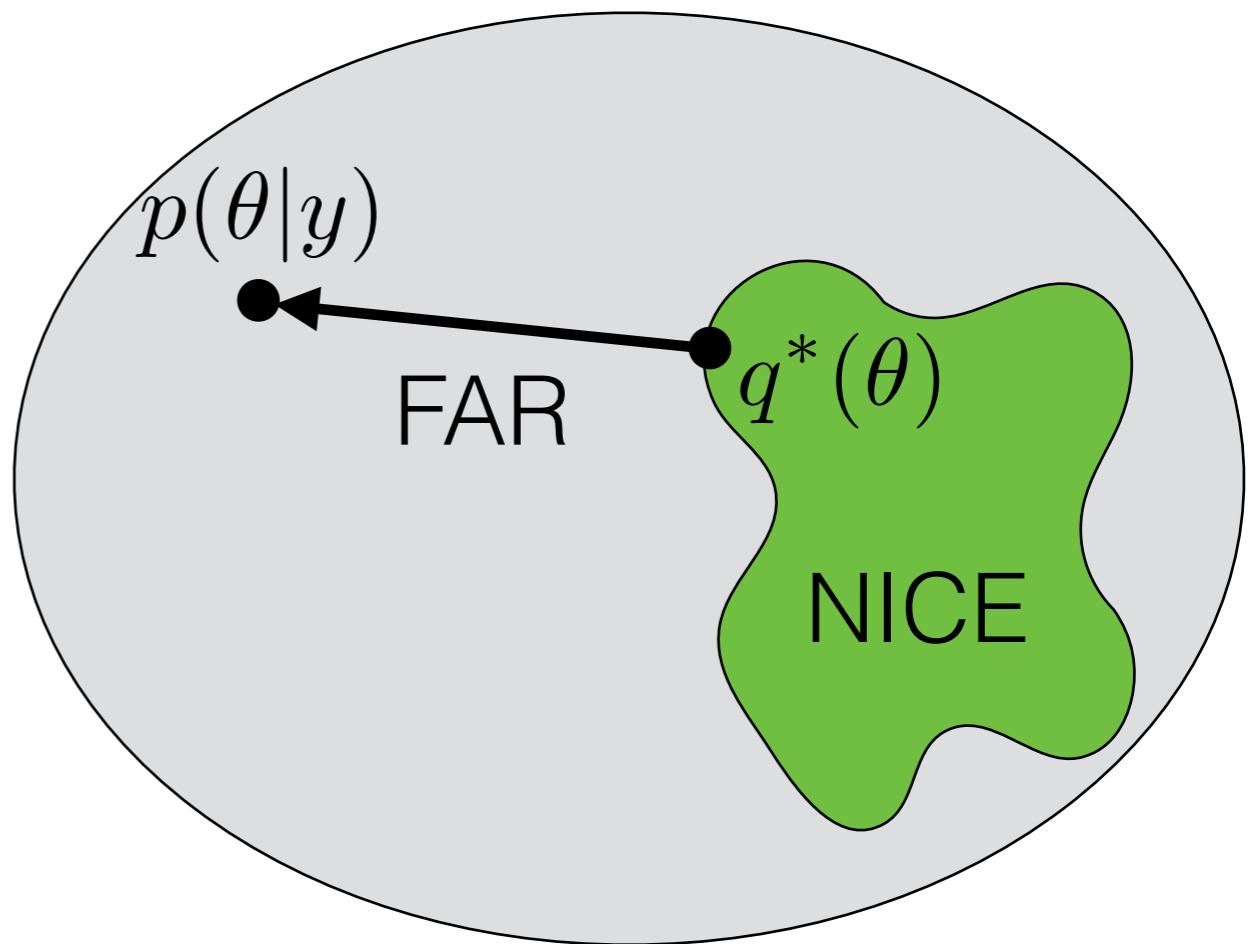
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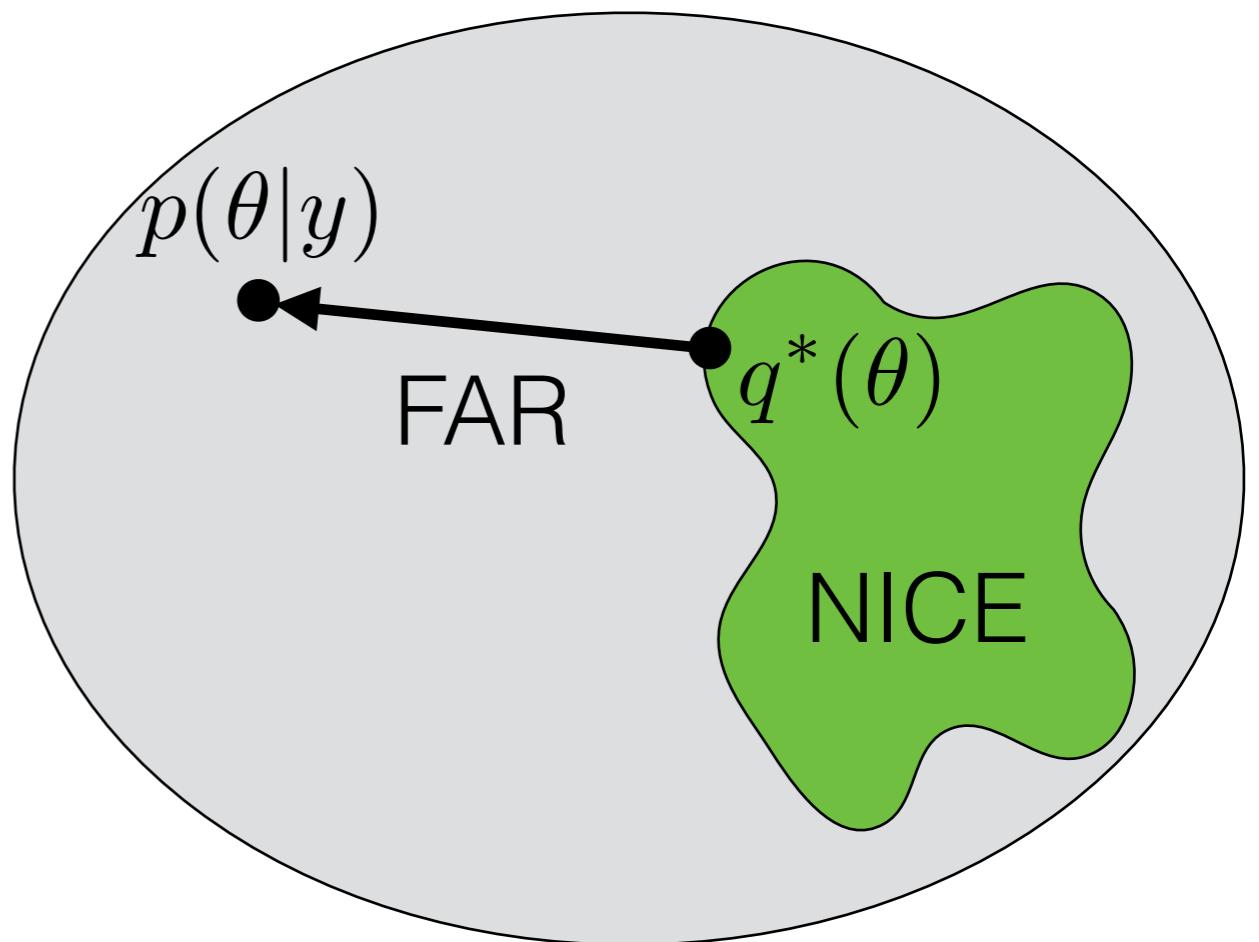
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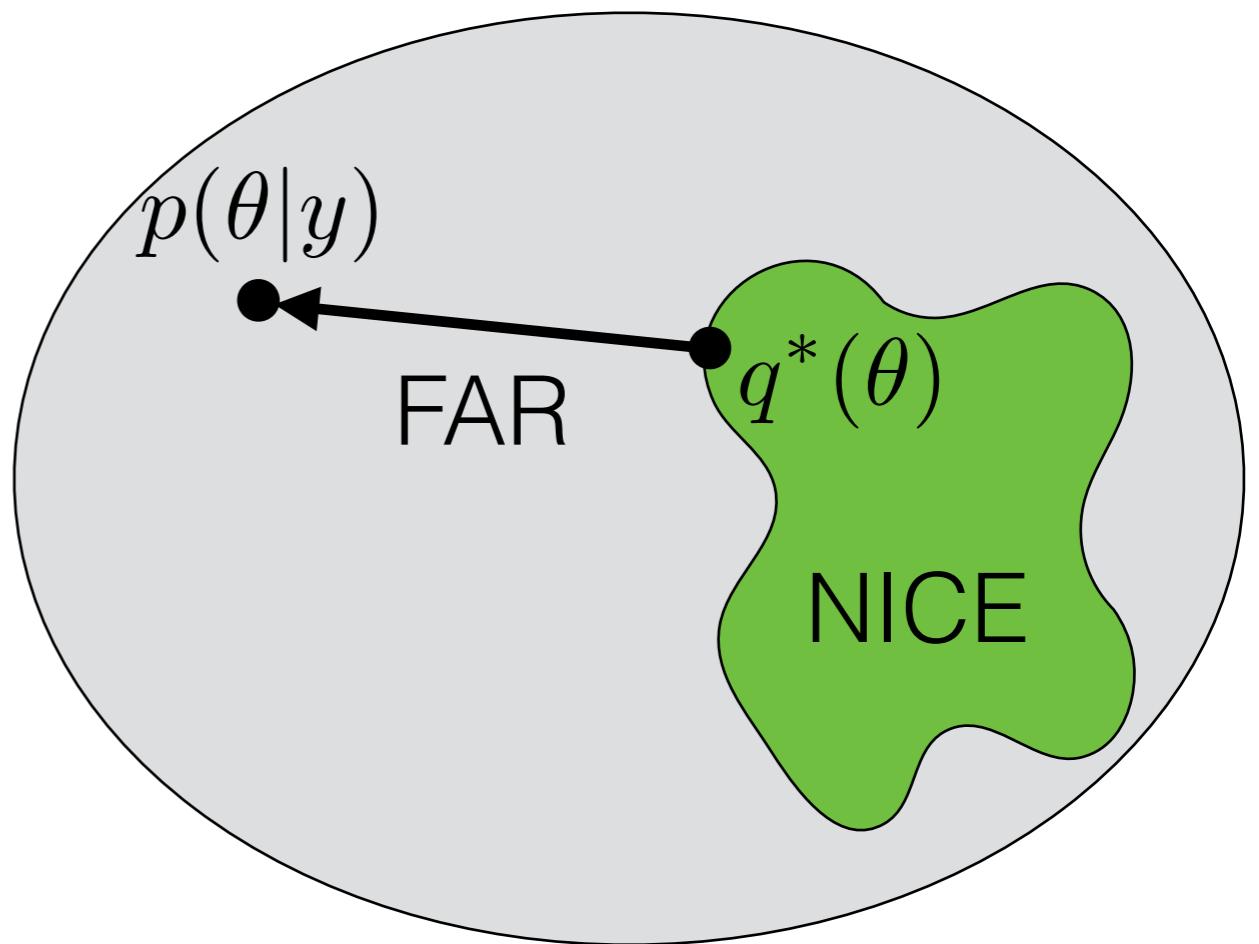
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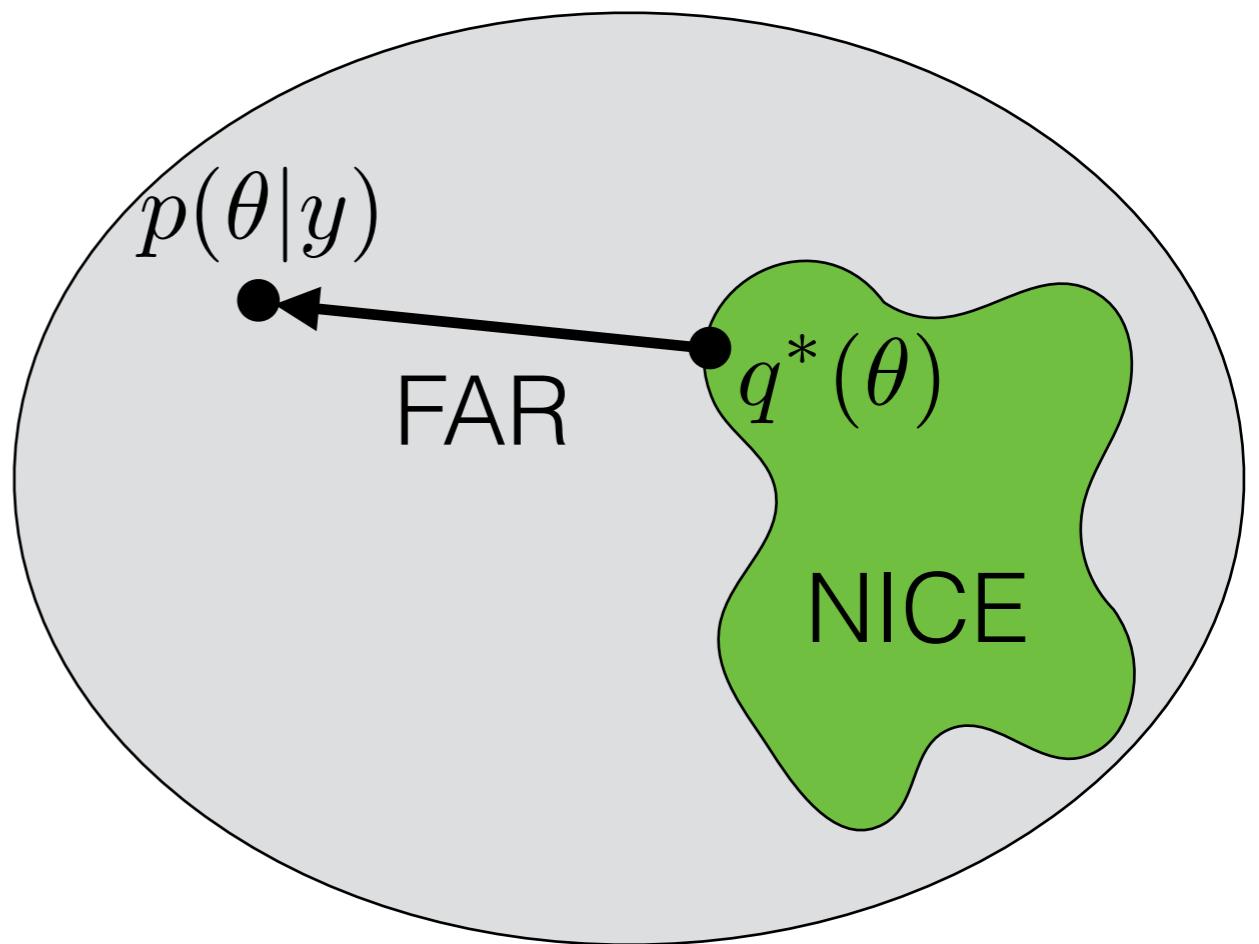
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- $q^* = \operatorname{argmax}_{q \in Q} \text{ELBO}(q)$

“Evidence lower bound” (ELBO)

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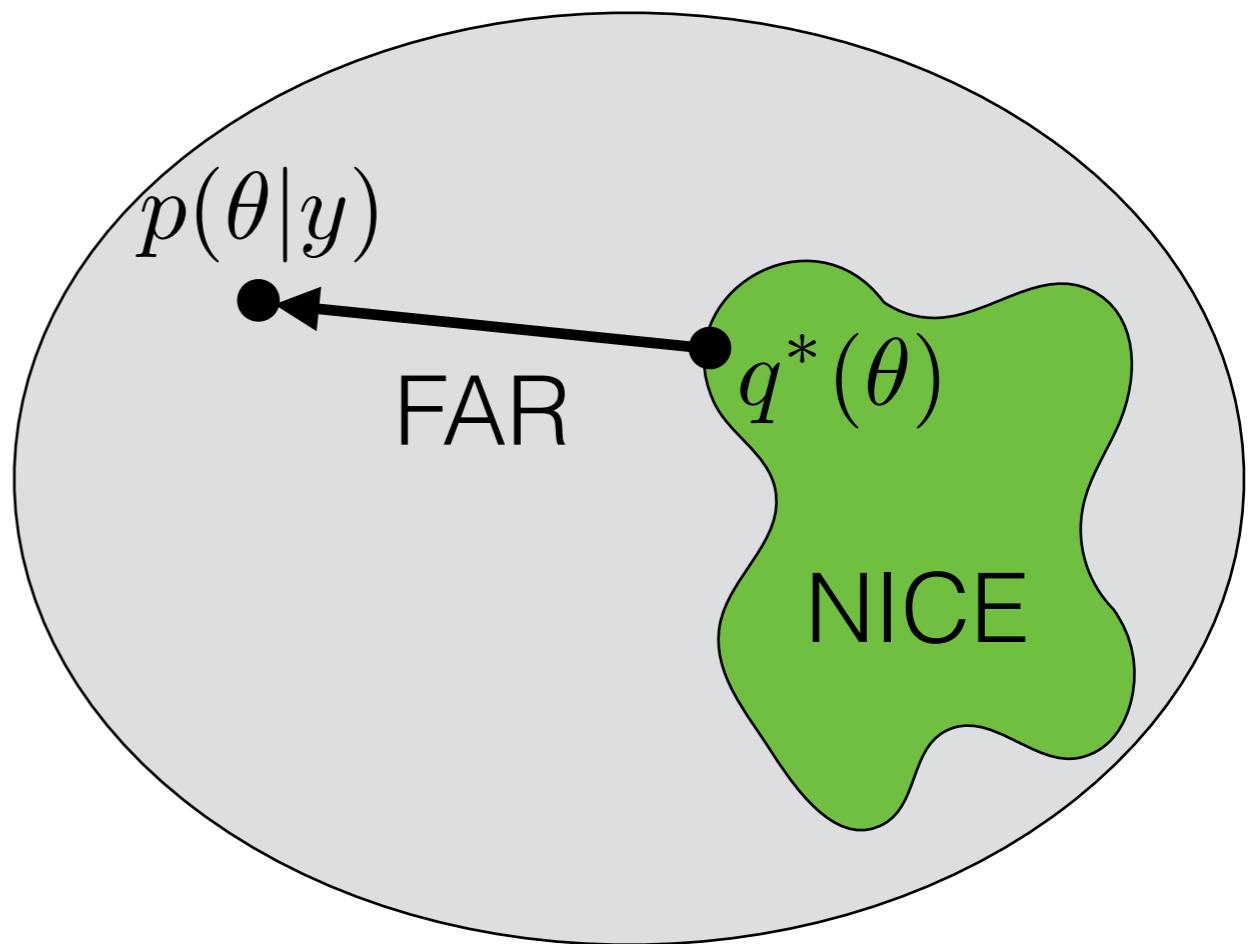
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$$:= \int q(\theta) \log \frac{q(\theta)}{p(\theta | y)} d\theta$$

$$= \int q(\theta) \log \frac{q(\theta)p(y)}{p(\theta, y)} d\theta = \log p(y) - \int q(\theta) \log \frac{p(\theta, y)}{q(\theta)} d\theta$$



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

“Evidence lower bound” (ELBO)

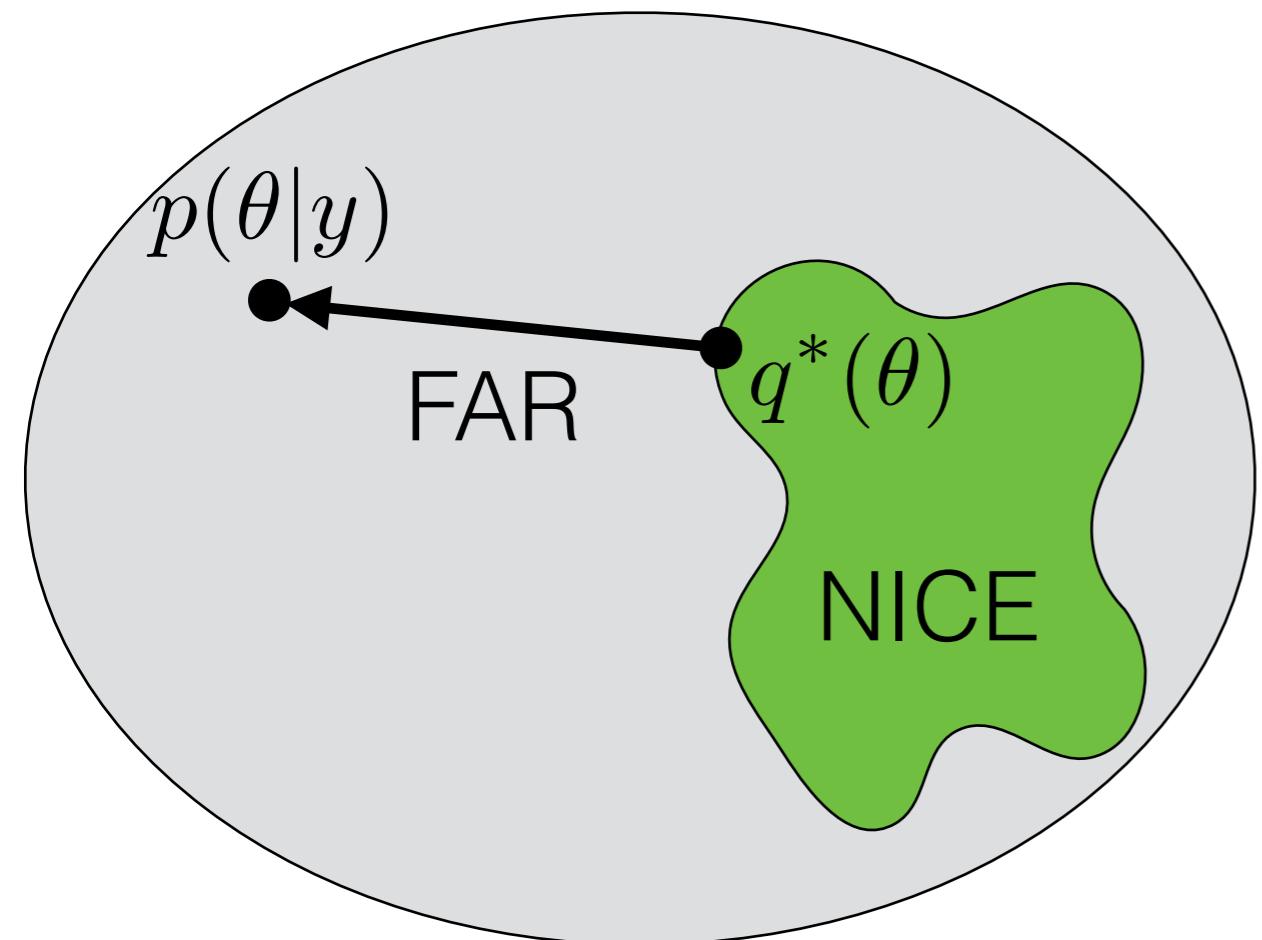
- $\text{KL} \geq 0 \Rightarrow \log p(y) \geq \text{ELBO}$

- $q^* = \operatorname{argmax}_{q \in Q} \text{ELBO}(q)$

- Why KL (in this direction)?

Variational Bayes

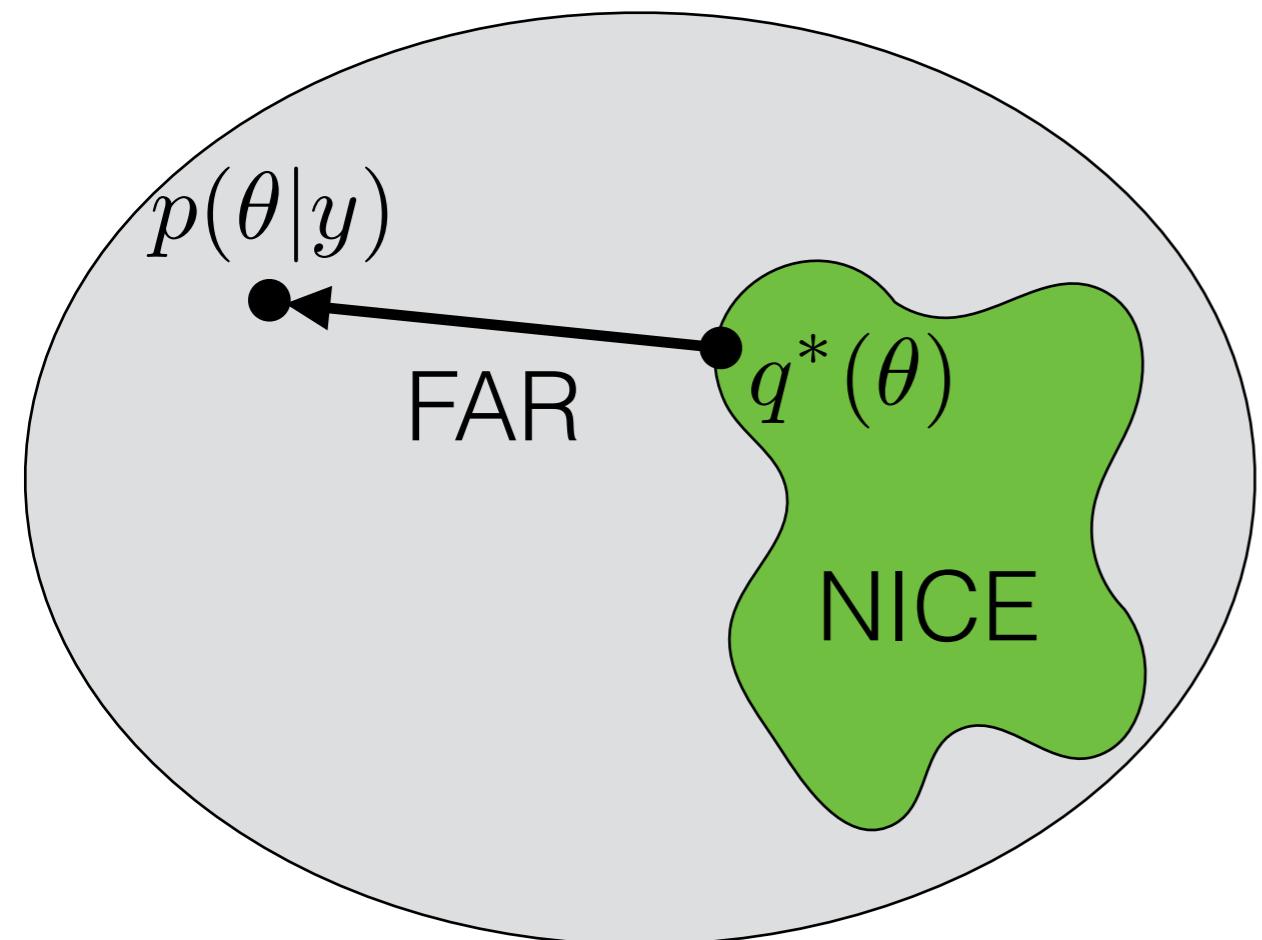
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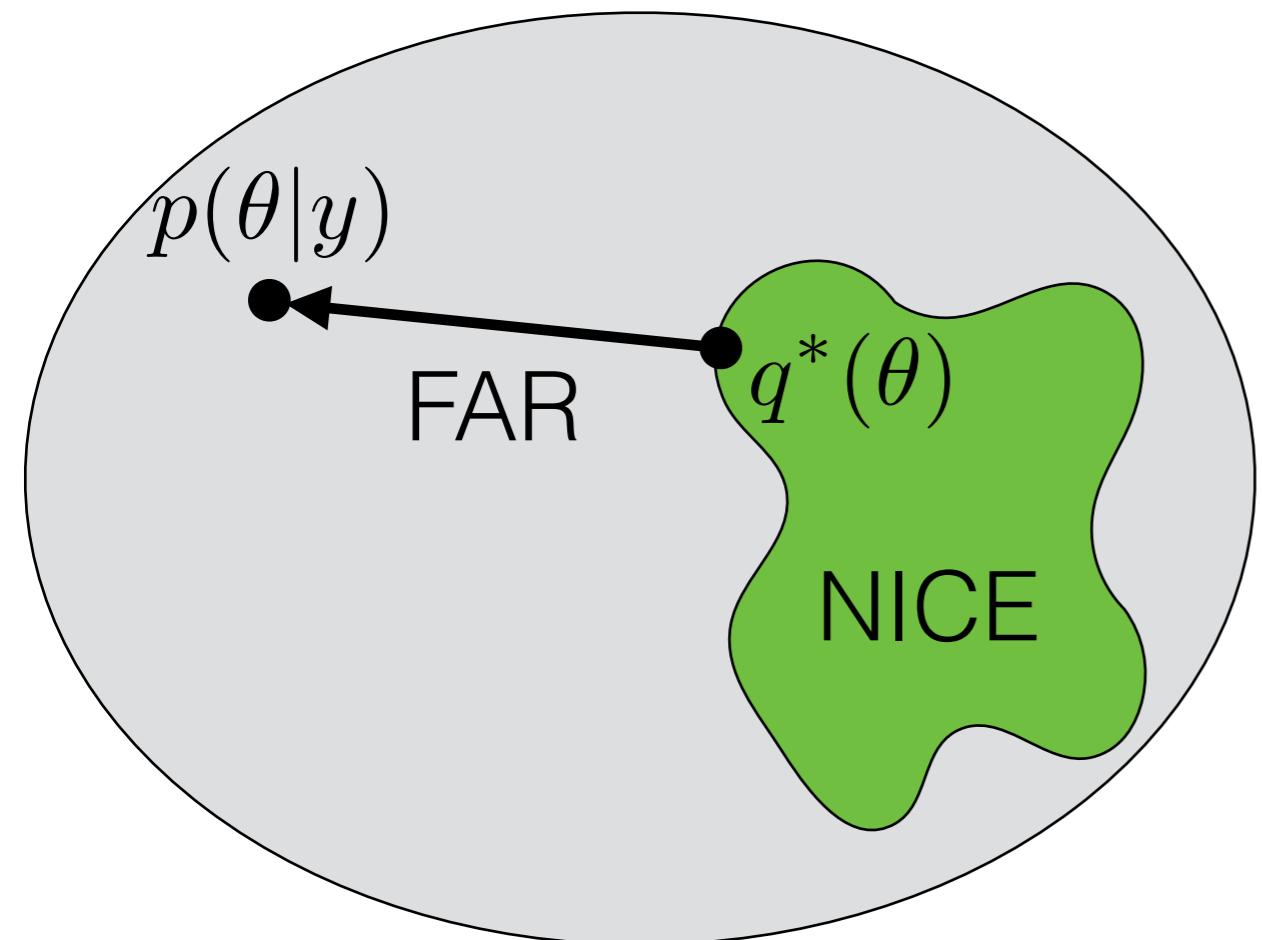
Choose “NICE” distributions



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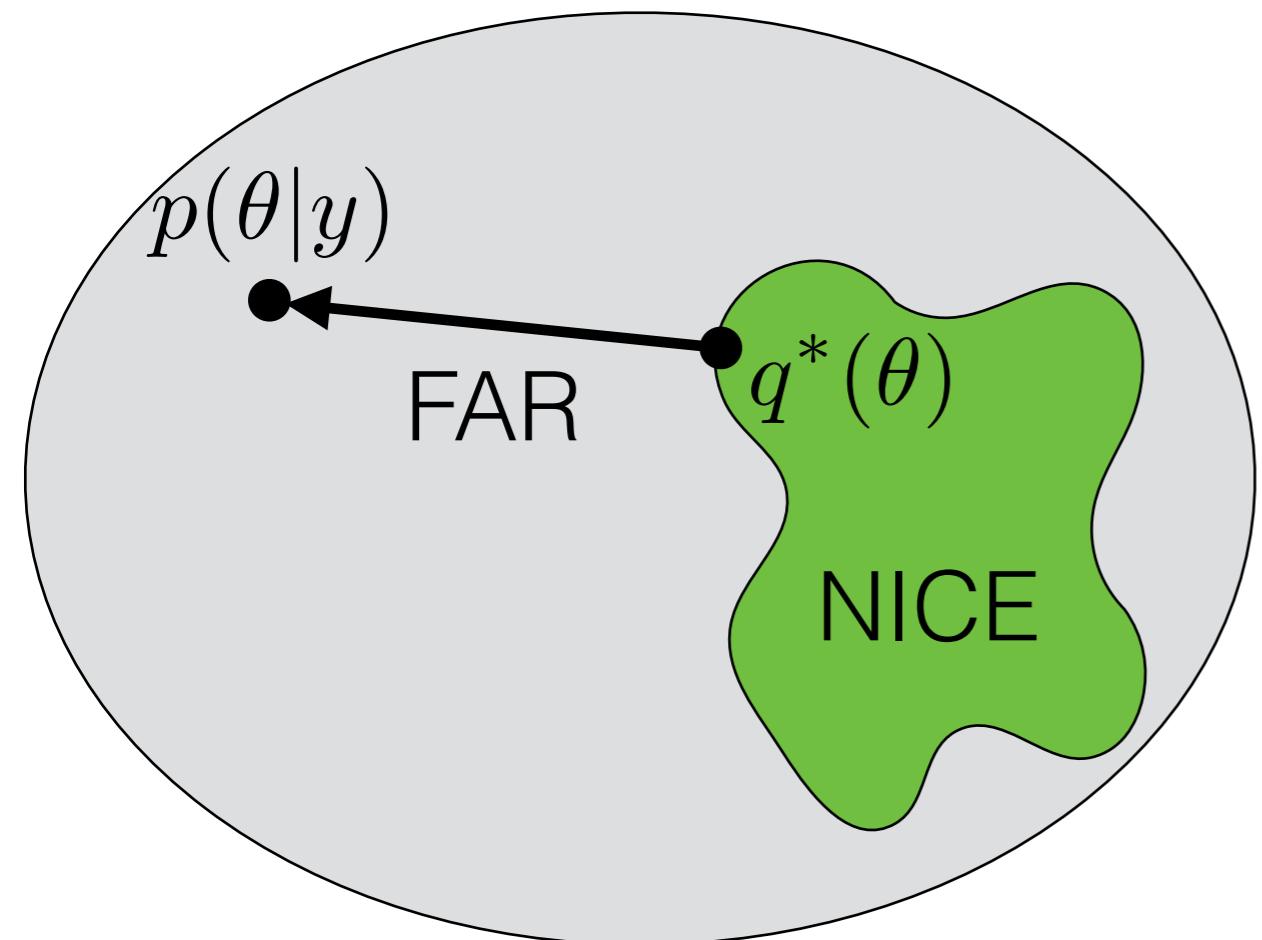
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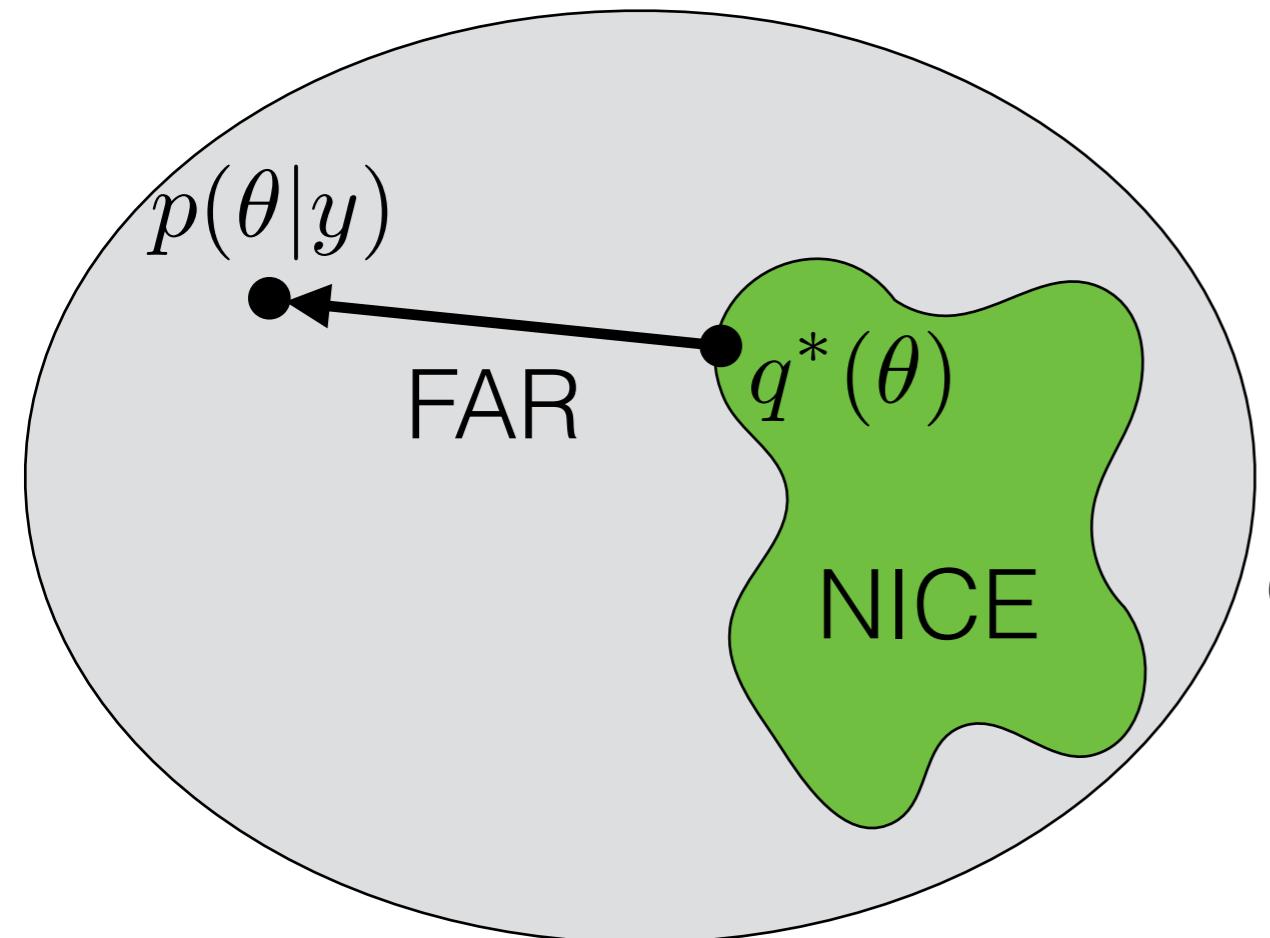
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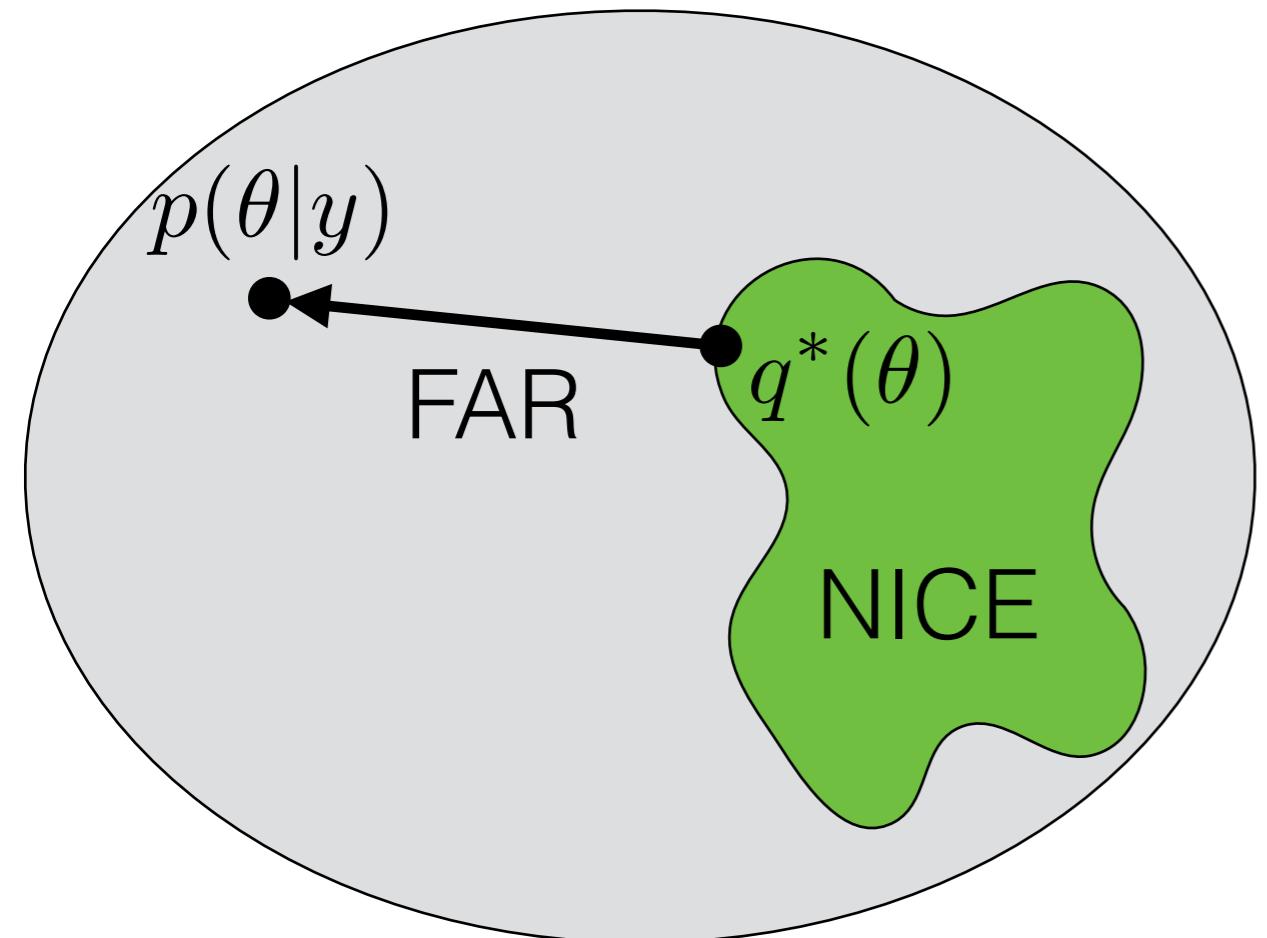
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$$Q_{MFVB} := \left\{ q : q(\theta) = \prod_{j=1}^J q_j(\theta_j) \right\}$$

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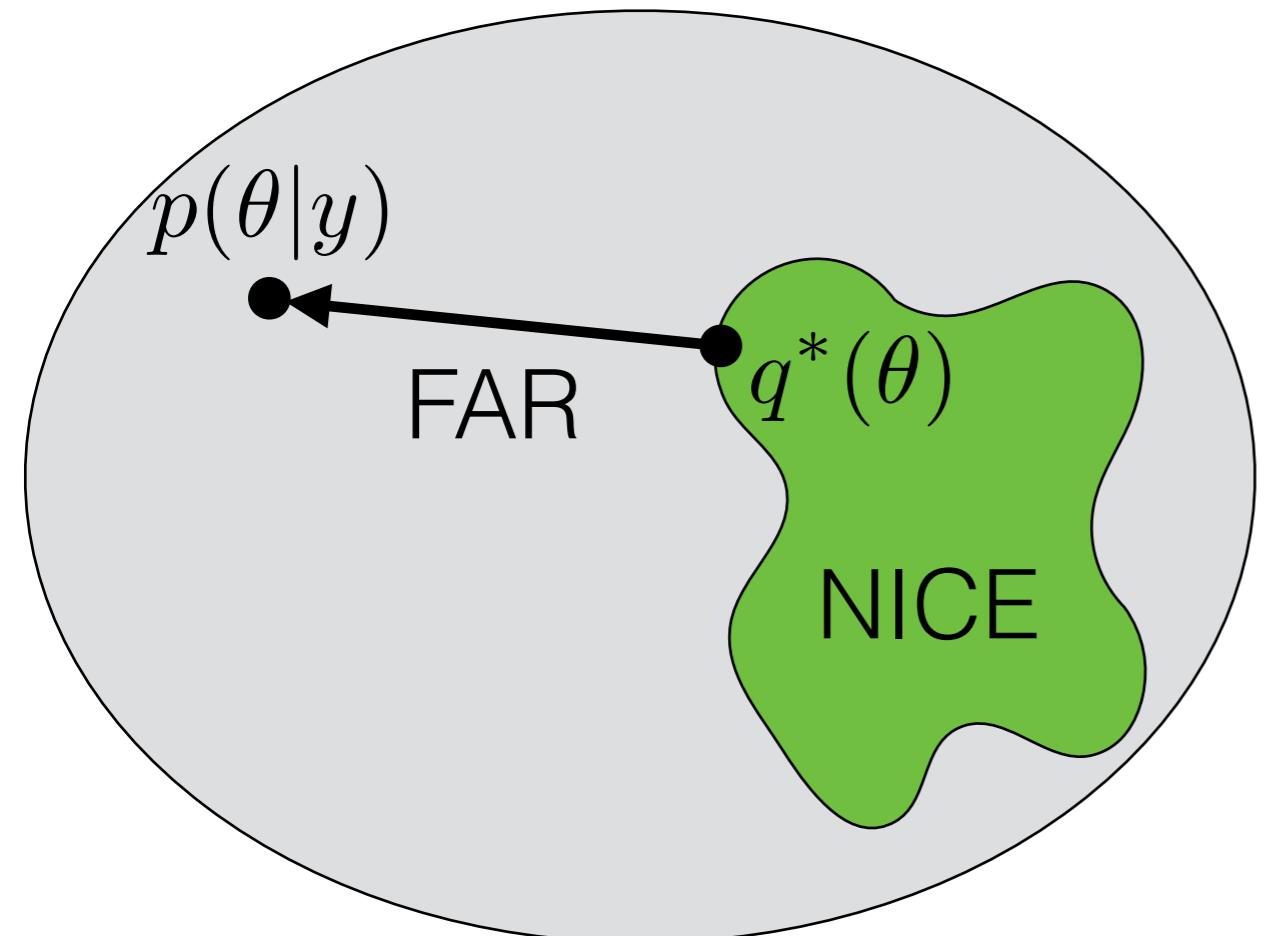
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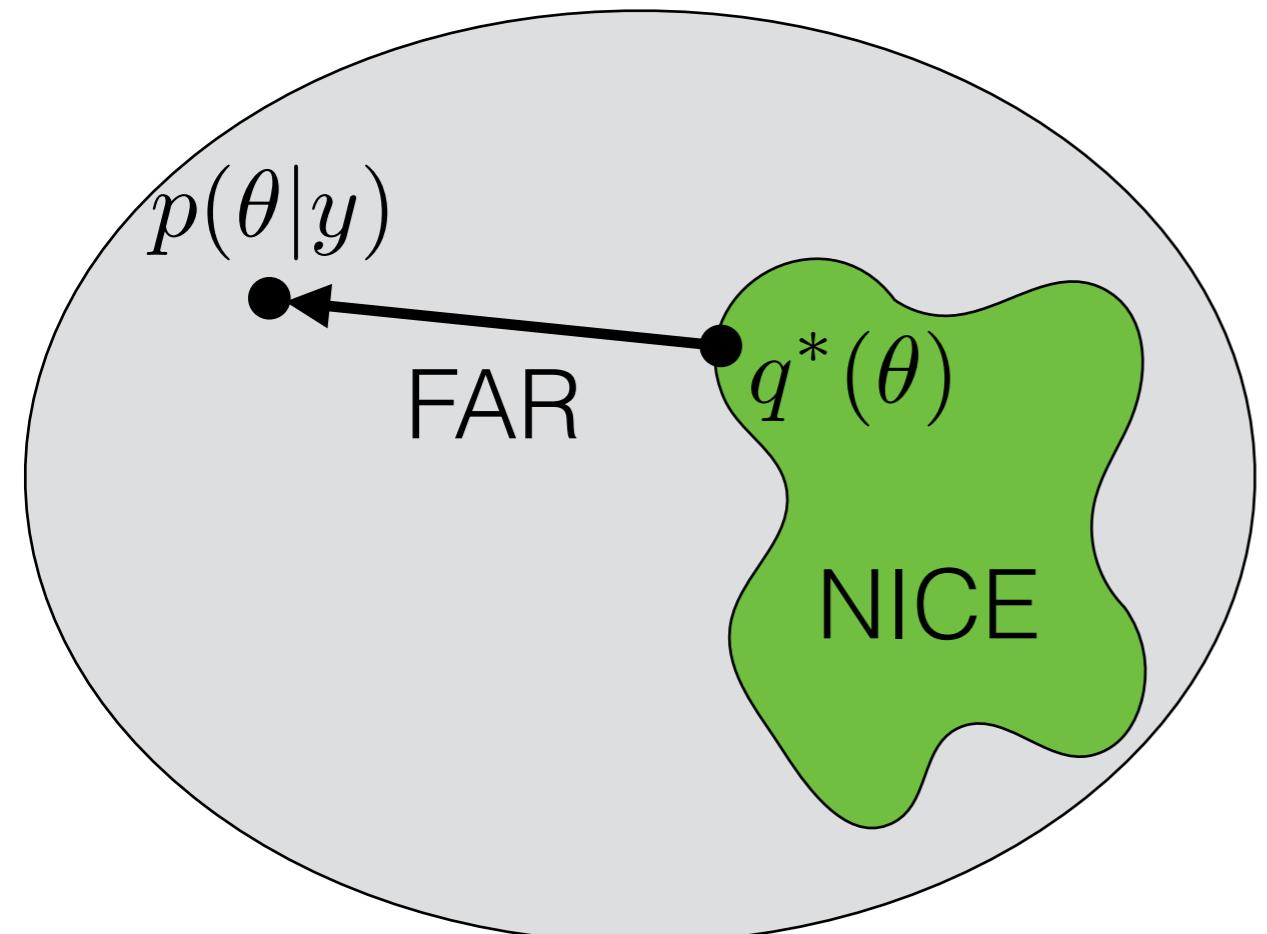
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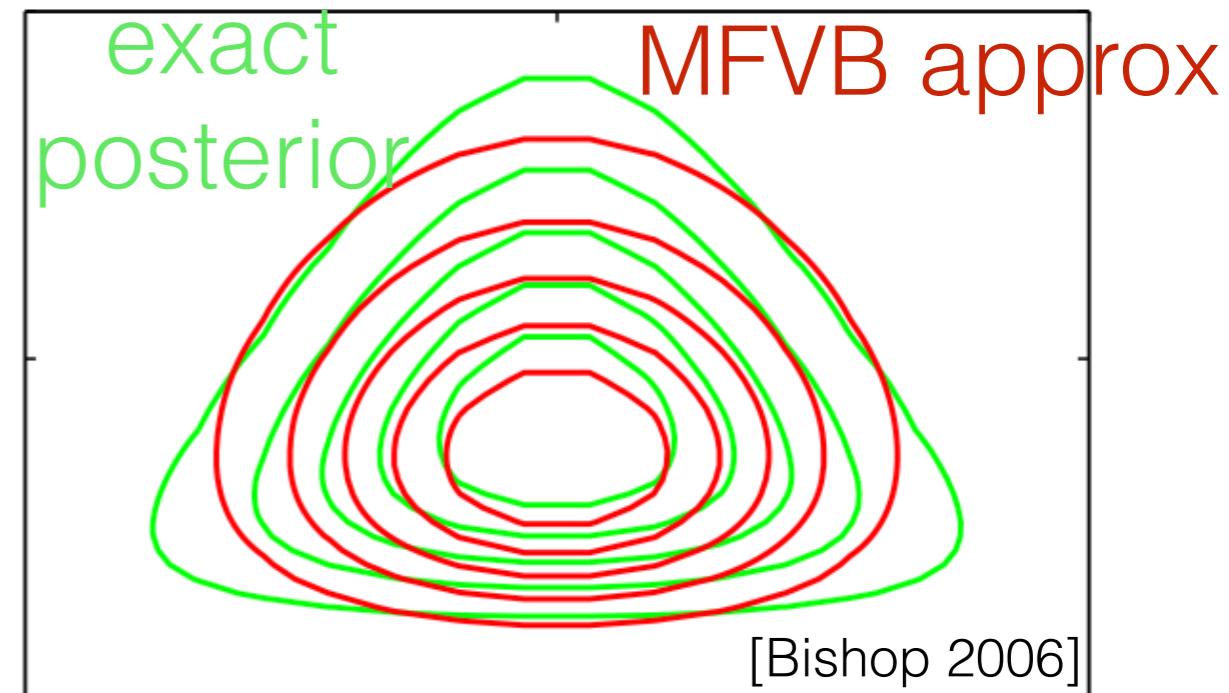


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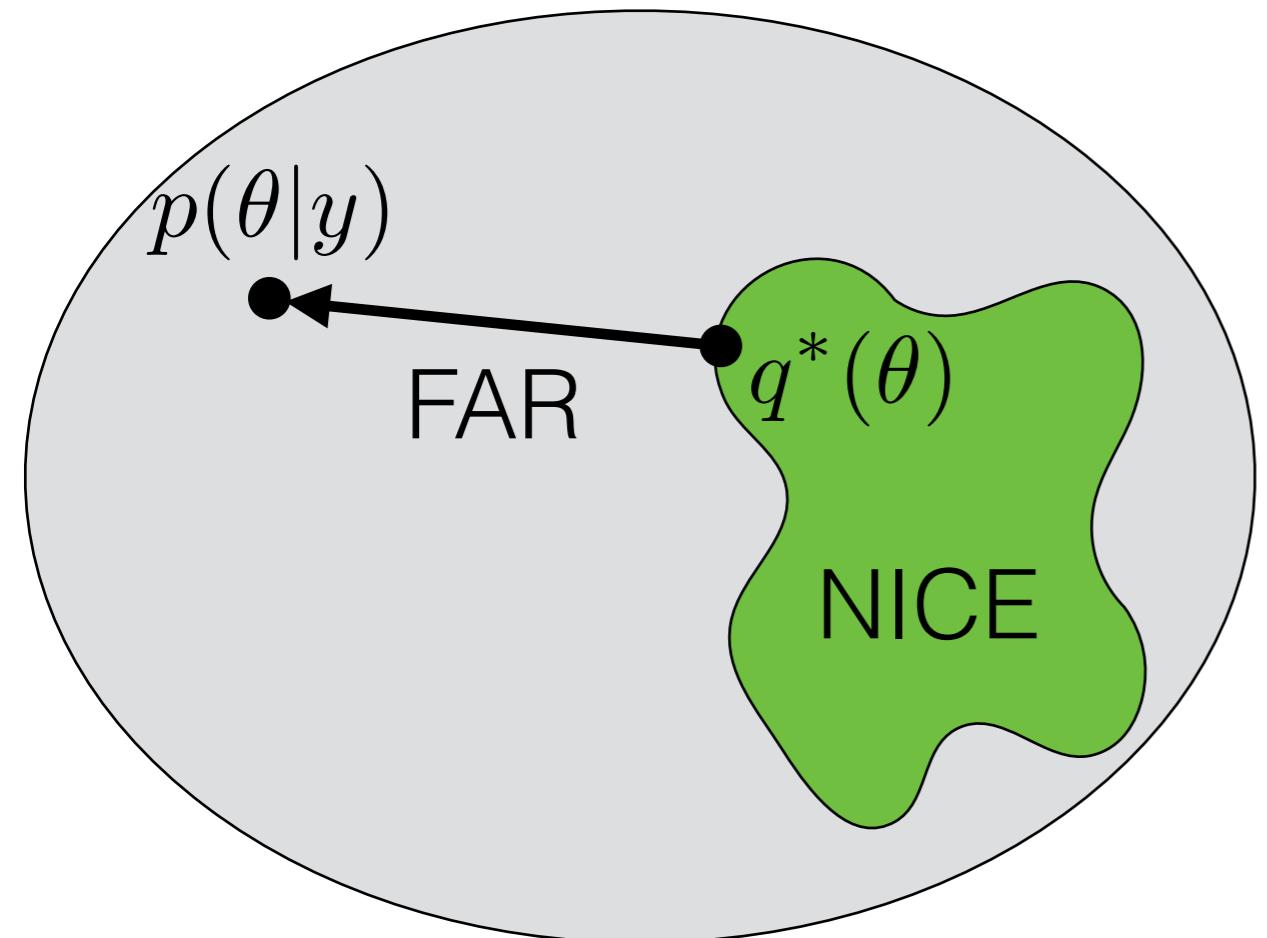
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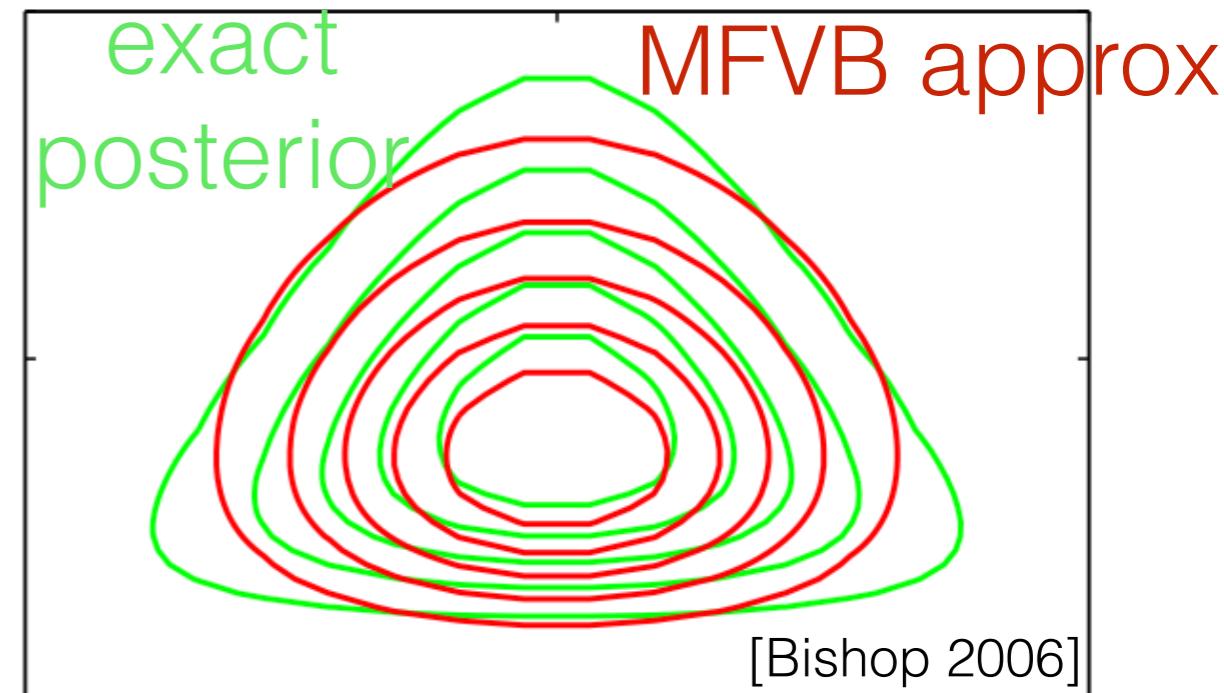
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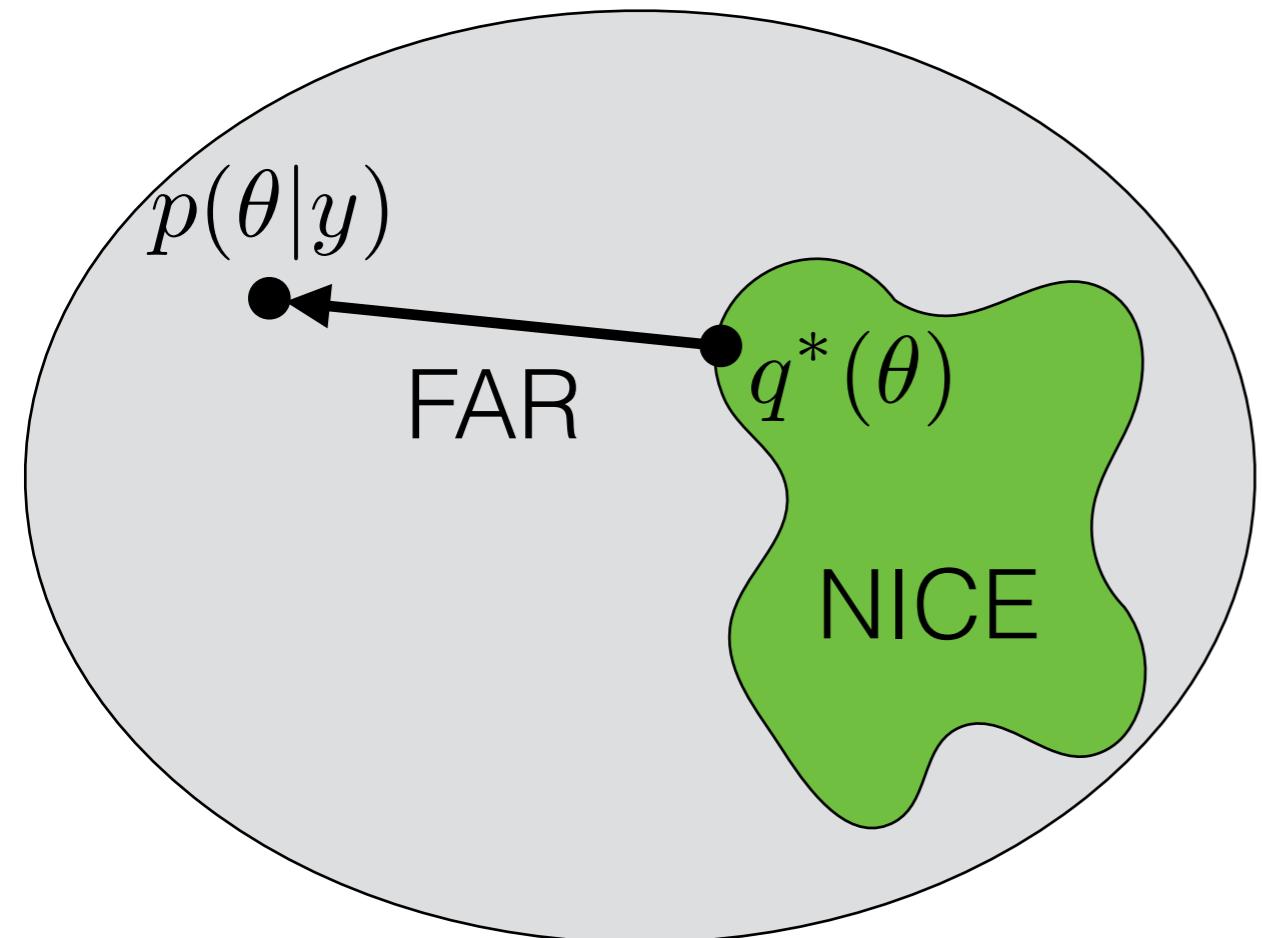
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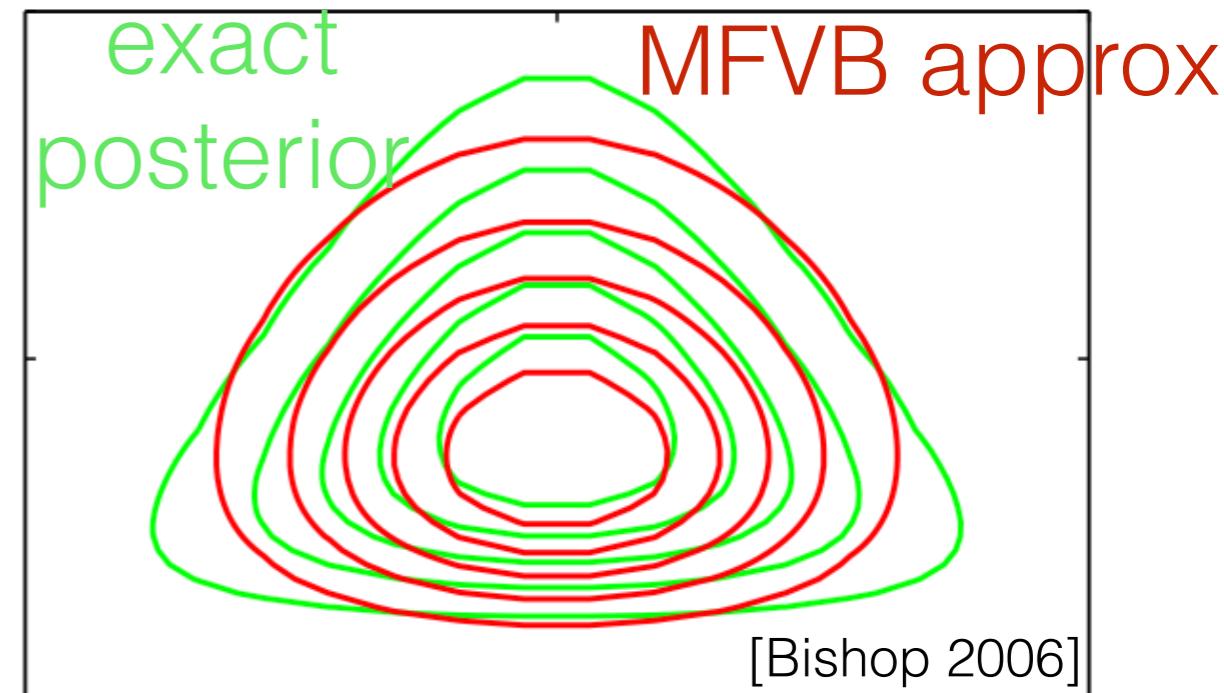
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- One option: Coordinate descent in q_1, \dots, q_J



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

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- What is:
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- Why use VB?
- When can we trust VB?
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Air pollution: Particulate matter



[Krongut 2020]

Air pollution: Particulate matter

- Sensor readings of log PM2.5 $y = (y_1, \dots, y_N)$

- Model:

$$p(y|\theta) : \quad y_n \stackrel{iid}{\sim} \mathcal{N}(\mu, \sigma^2)$$



[Krongut 2020]

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[MacKay 2003; Bishop 2006]

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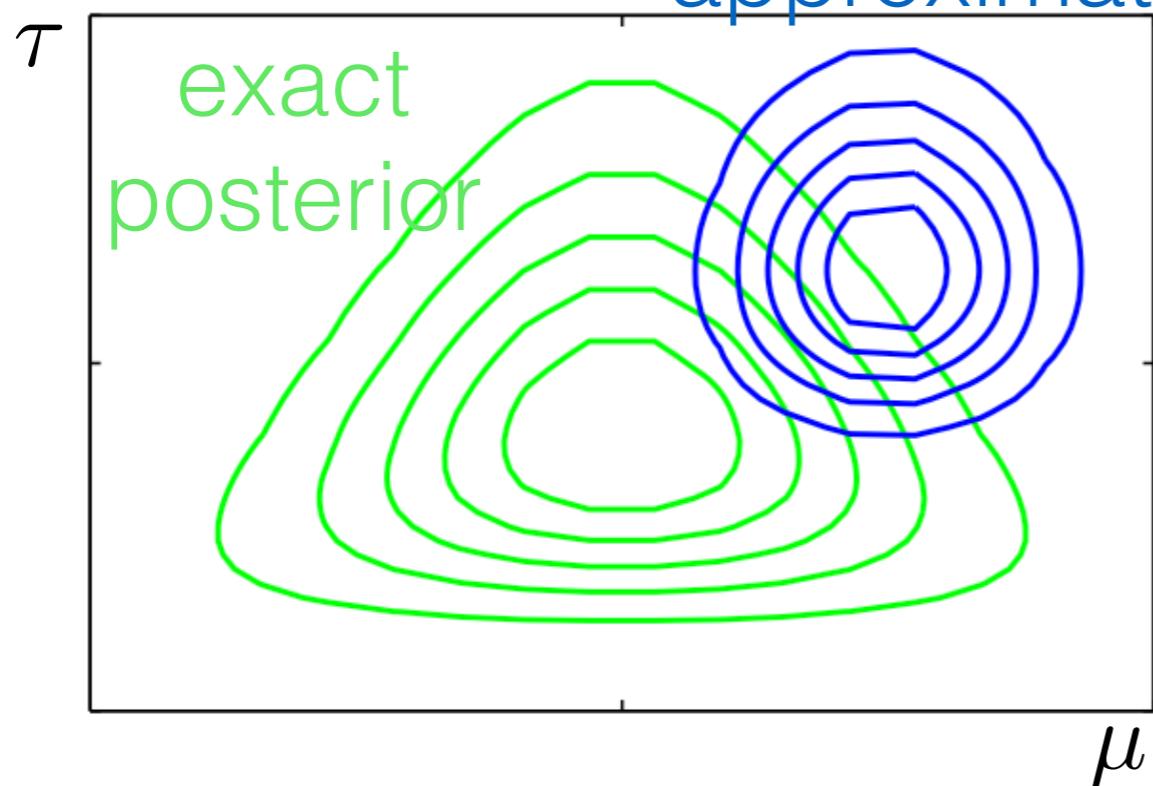
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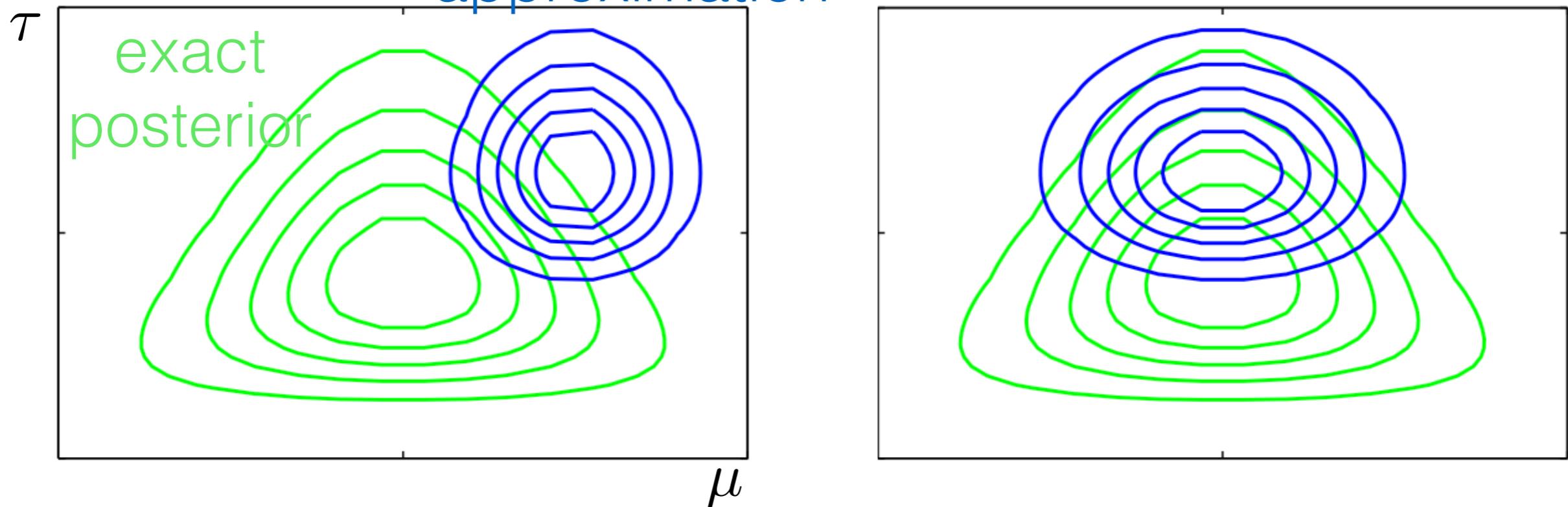
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Air pollution: Particulate matter approximation



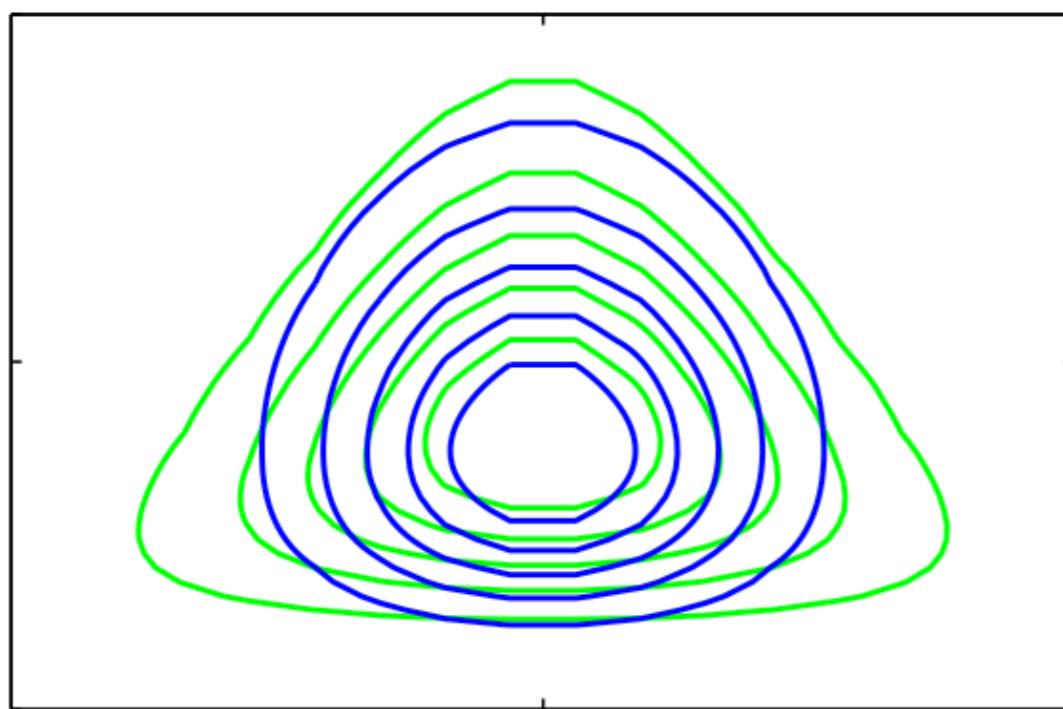
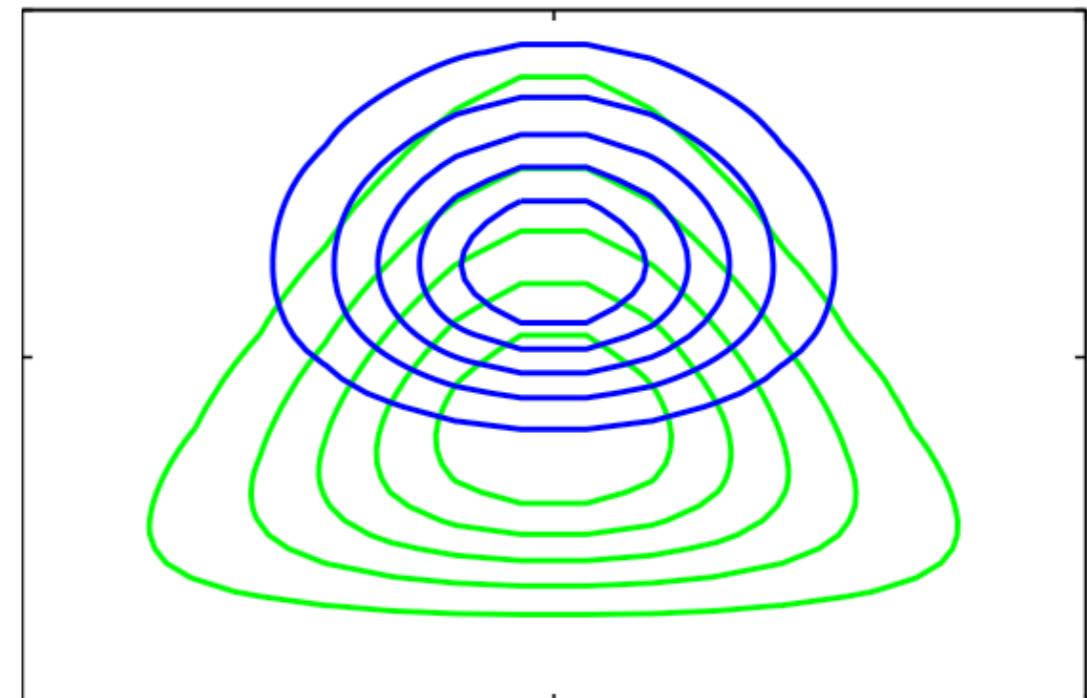
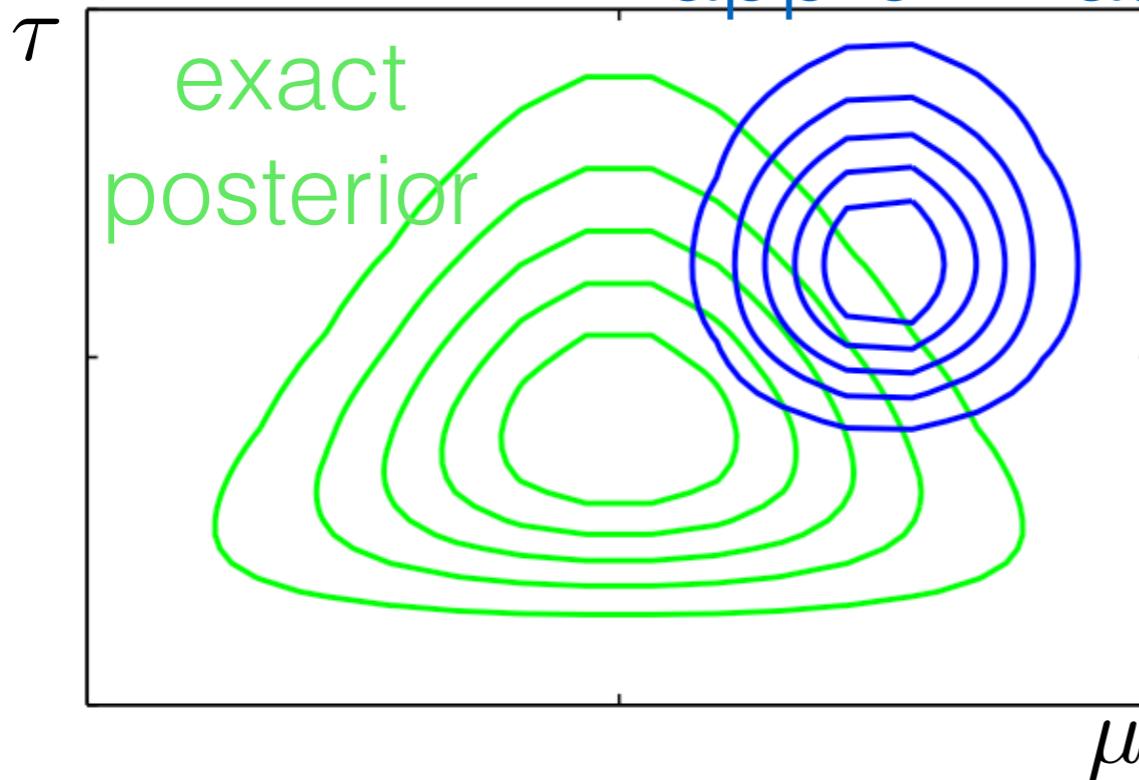
Air pollution: Particulate matter

approximation



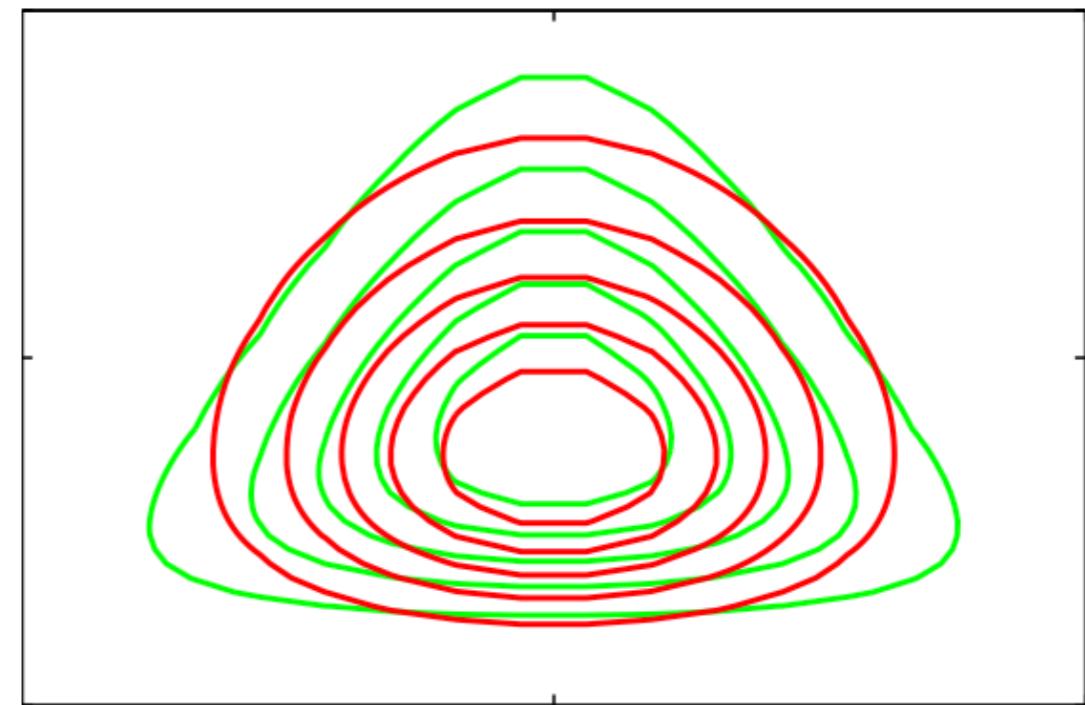
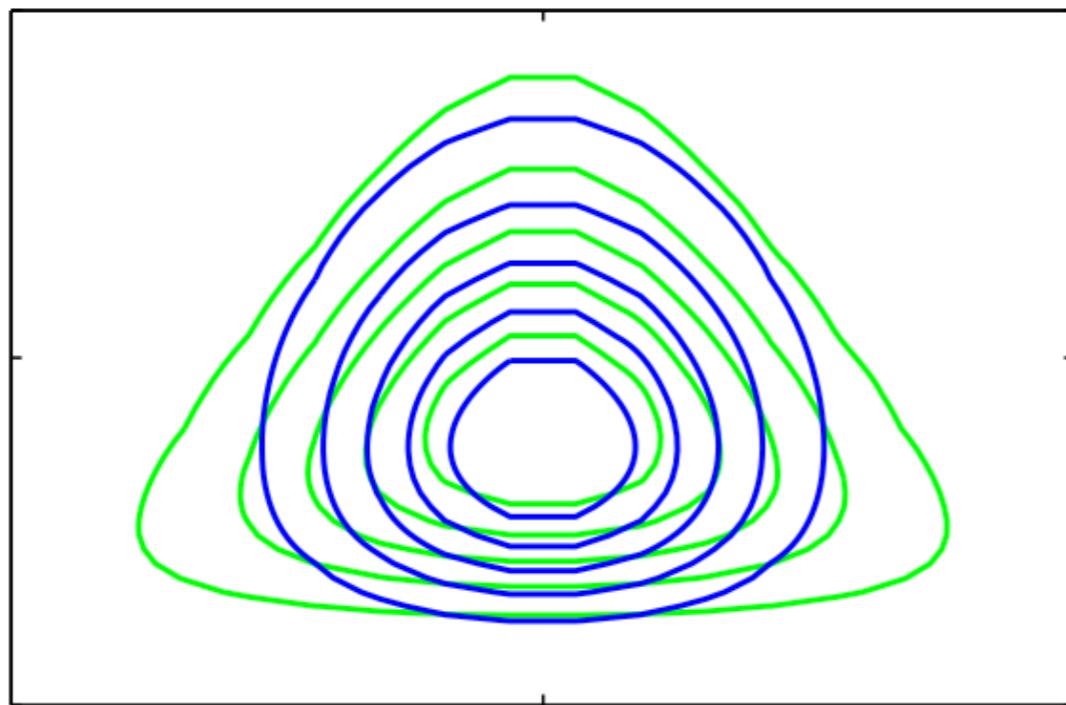
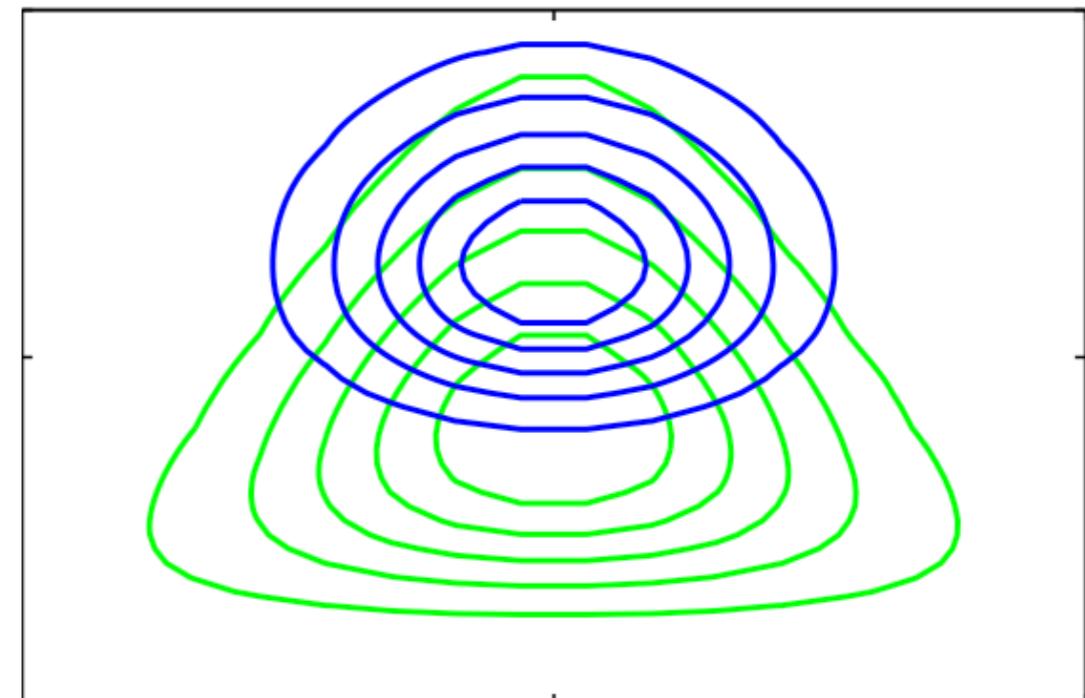
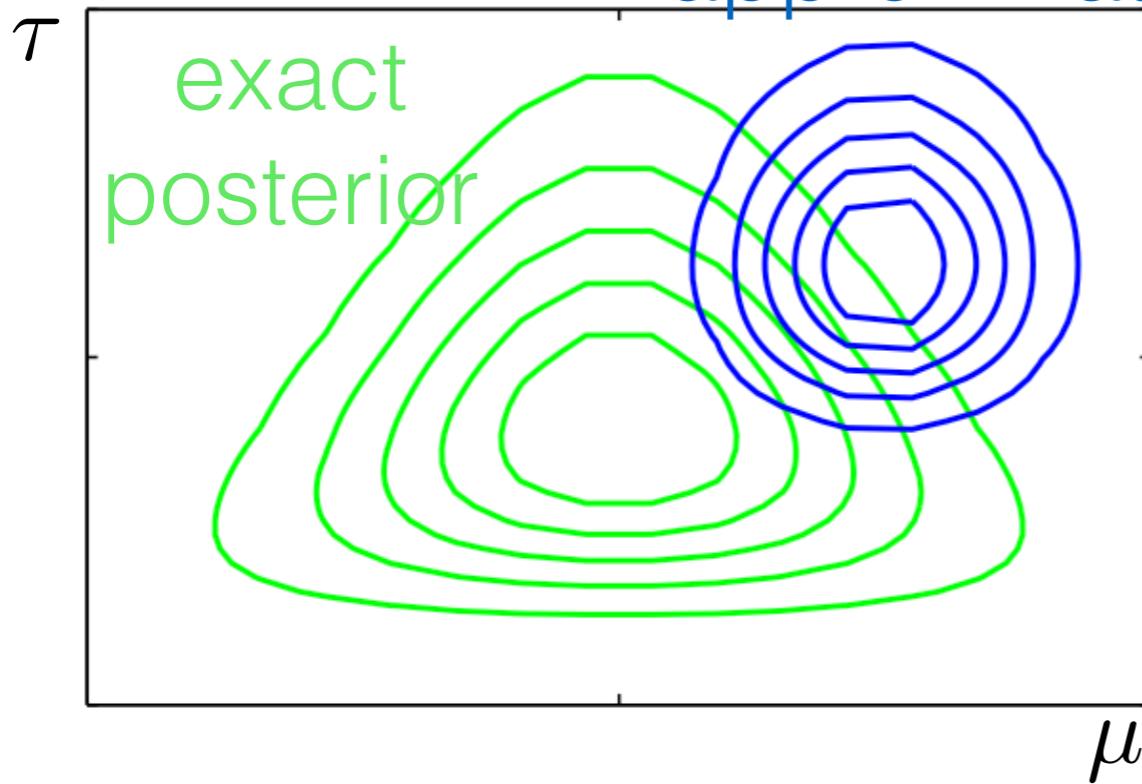
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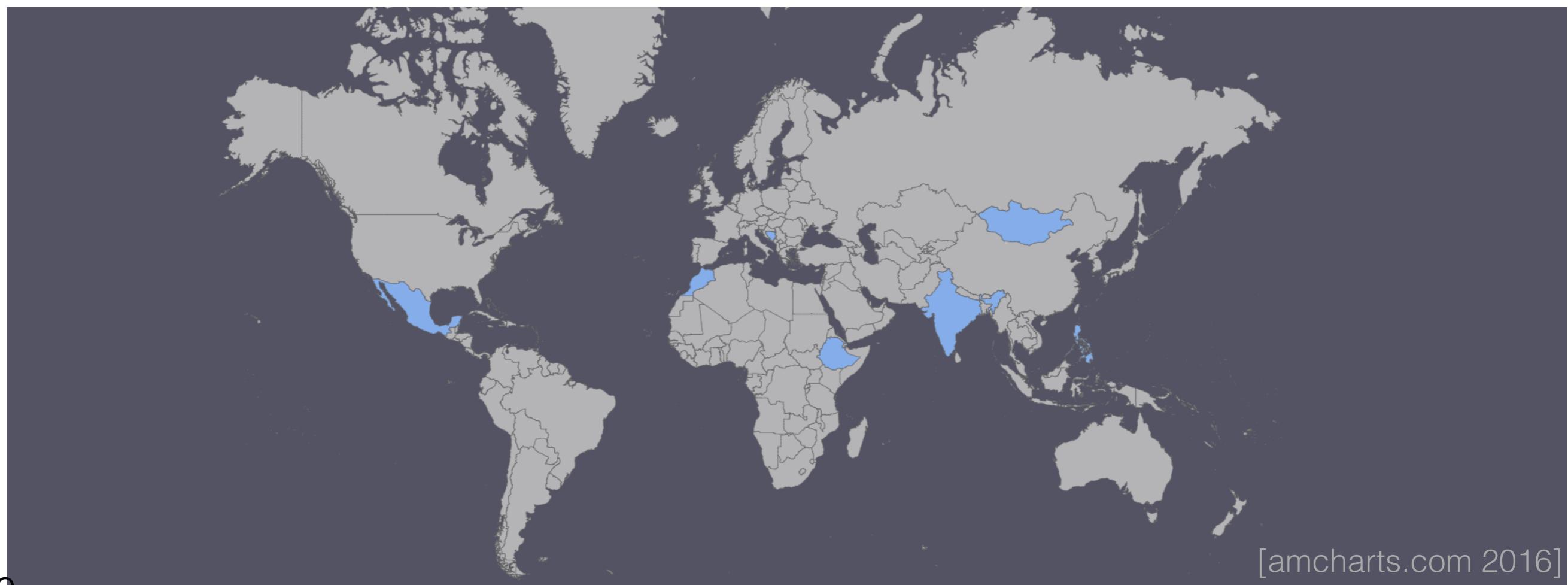


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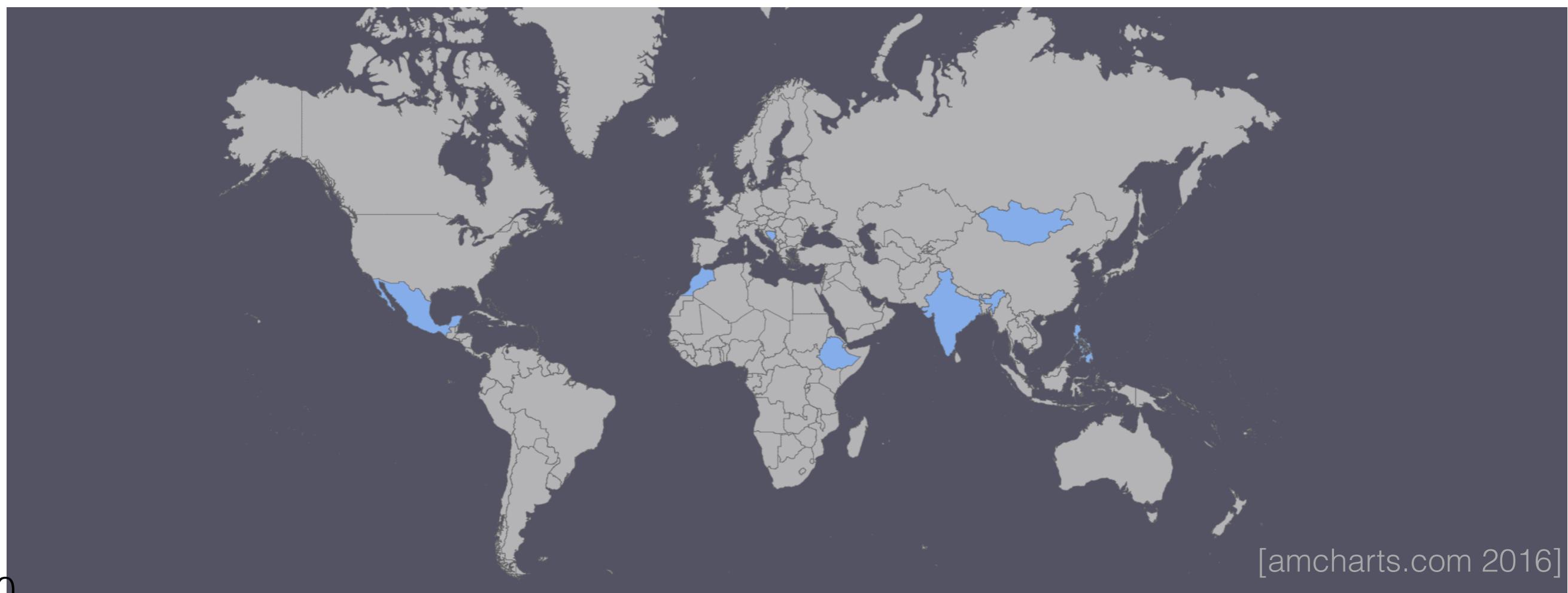
Microcredit Experiment



[amcharts.com 2016]

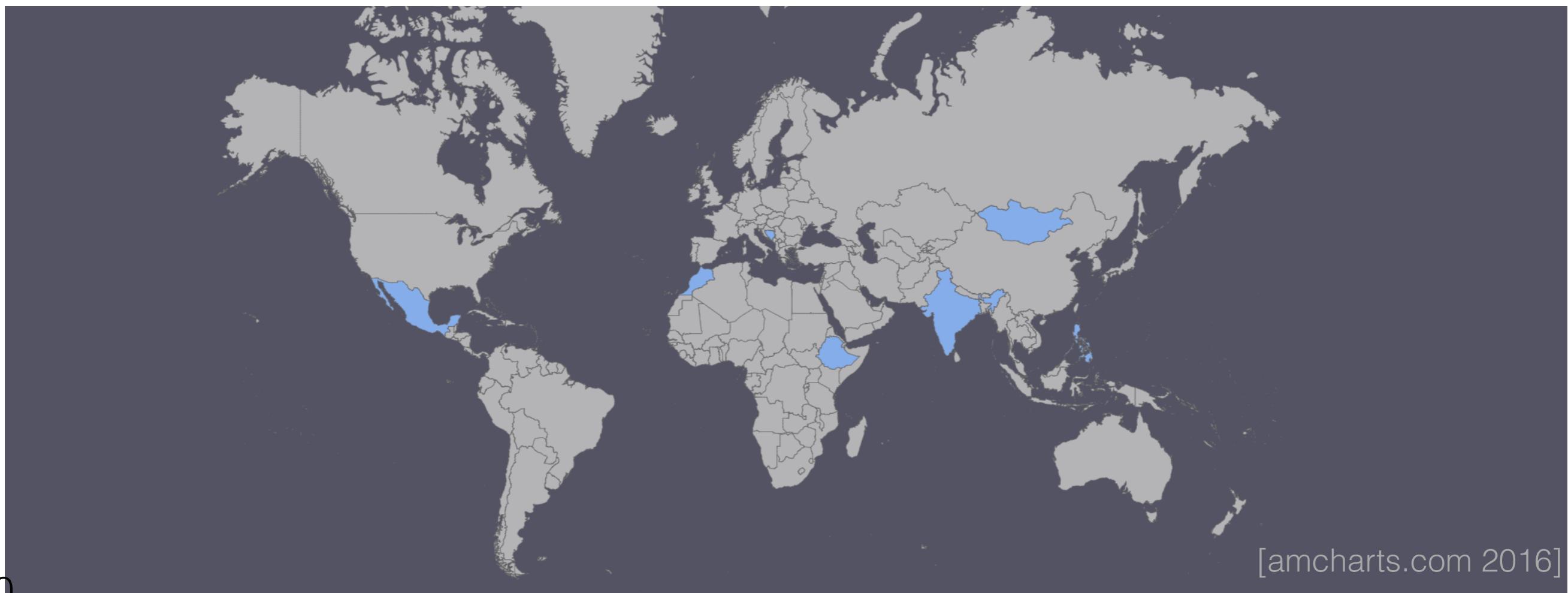
Microcredit Experiment

- Simplified from Meager (2019)



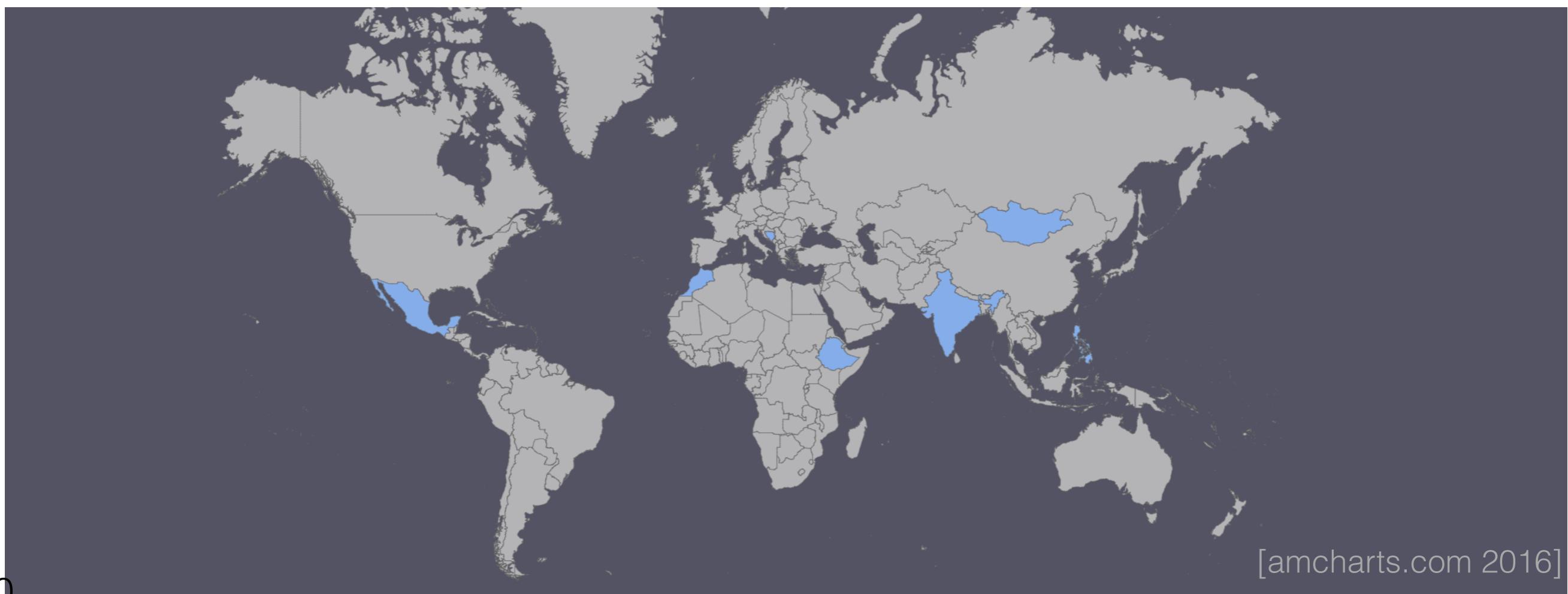
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- $K = 7$ microcredit trials (Mexico, Mongolia, Bosnia, India, Morocco, Philippines, Ethiopia)



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profit
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profit $\rightarrow y_{kn}$

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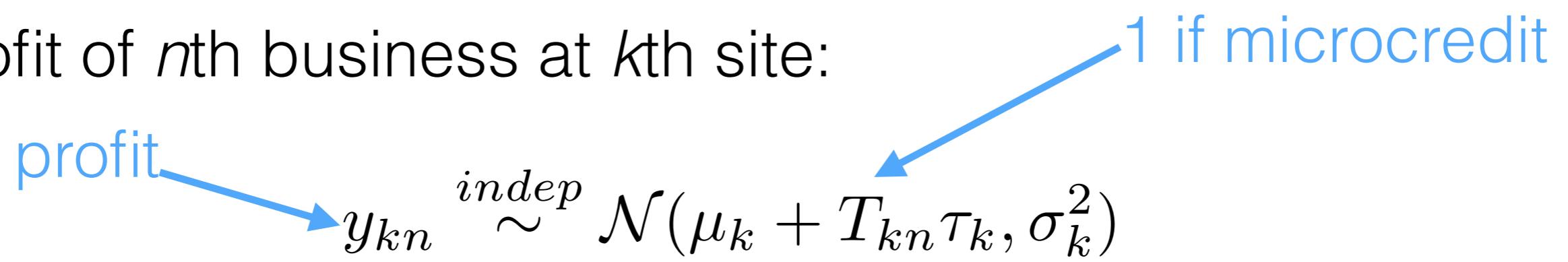
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- Priors and hyperpriors:

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profit → y_{kn} ← 1 if microcredit

- Priors and hyperpriors:

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

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

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

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

Microcredit

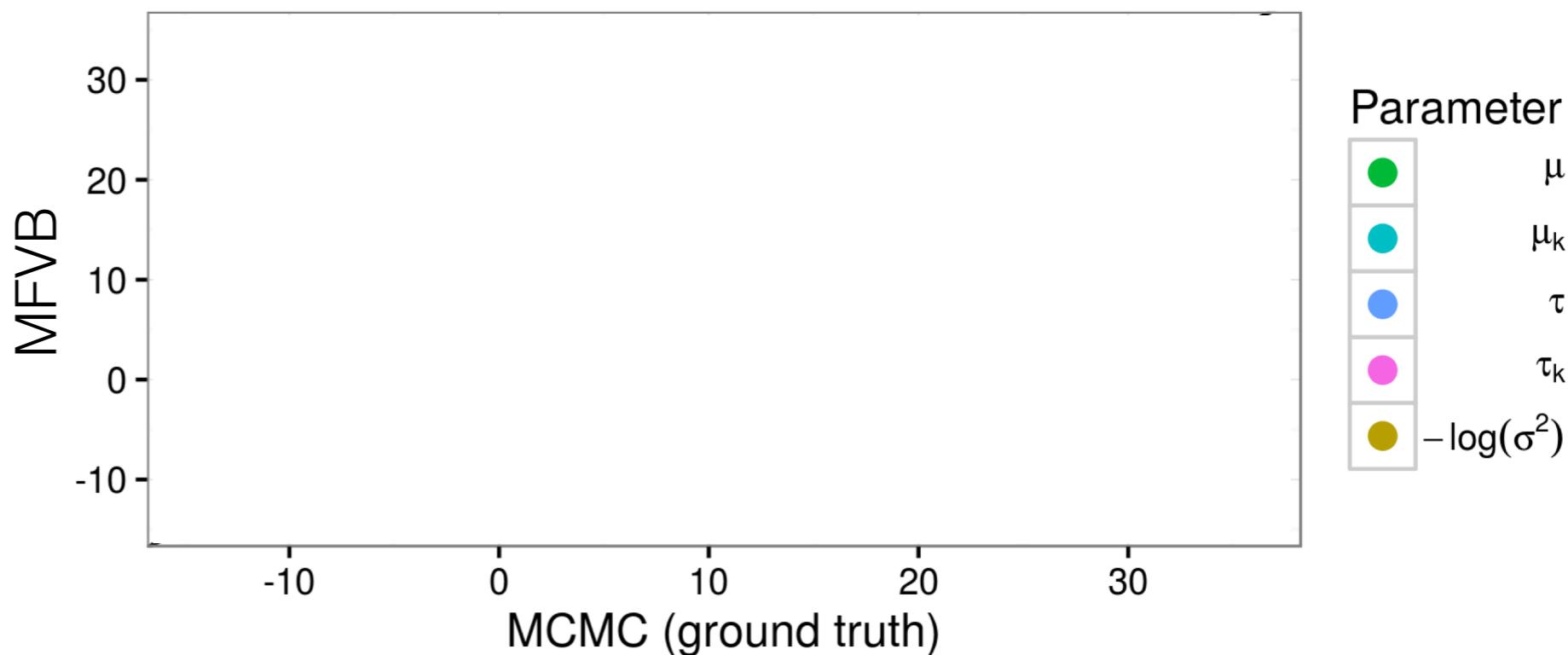
MFVB: Do we need to check the output?

Microcredit

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

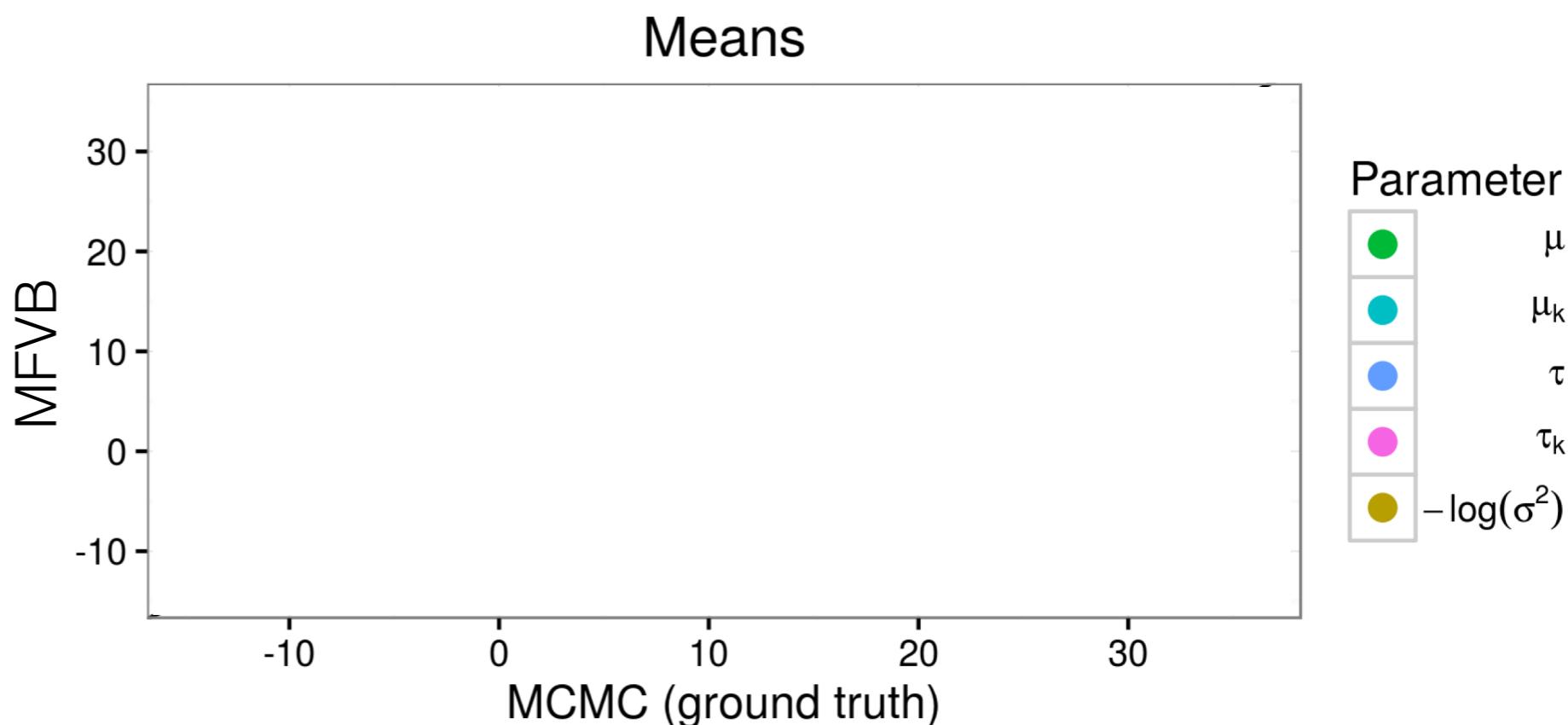
Microcredit

Means



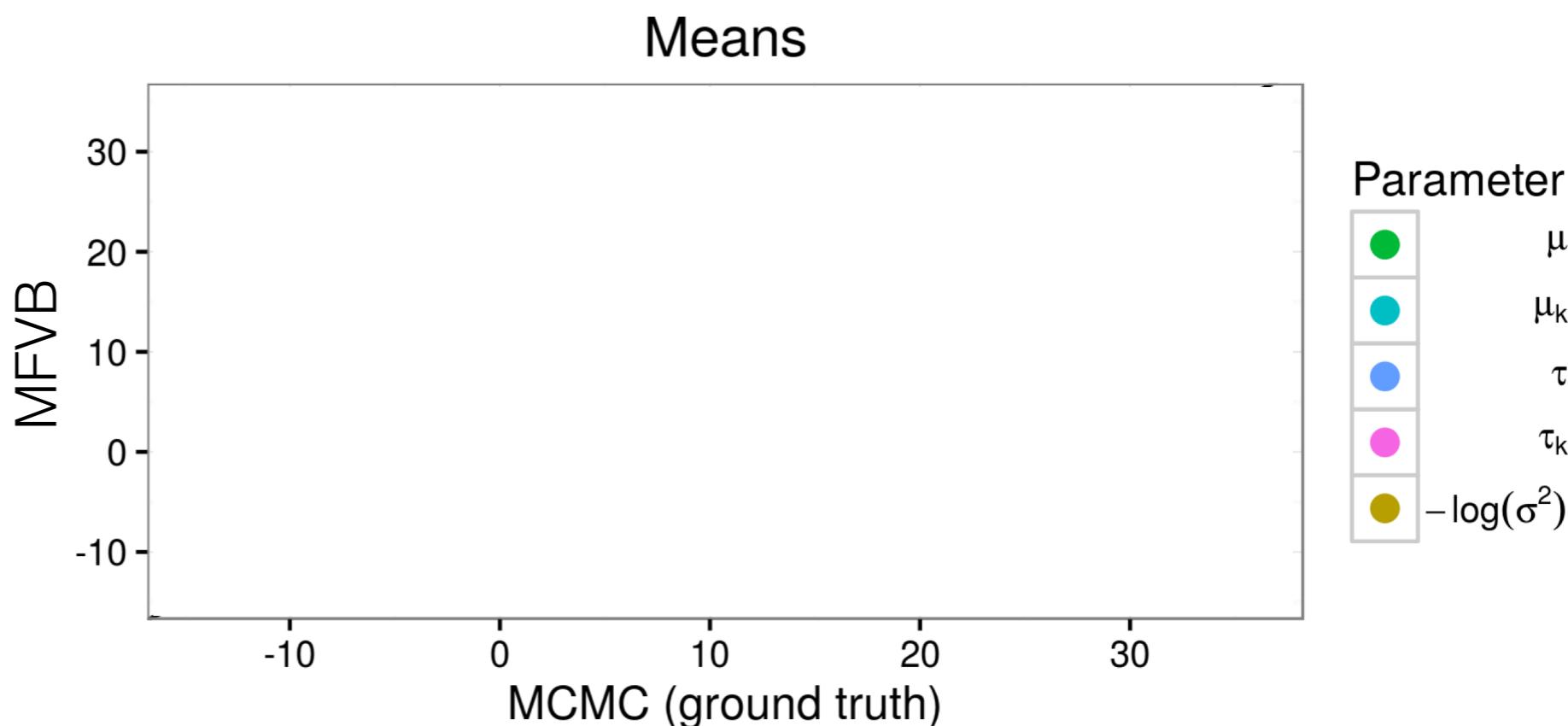
Microcredit

- One set of 2500 MCMC draws:
45 minutes



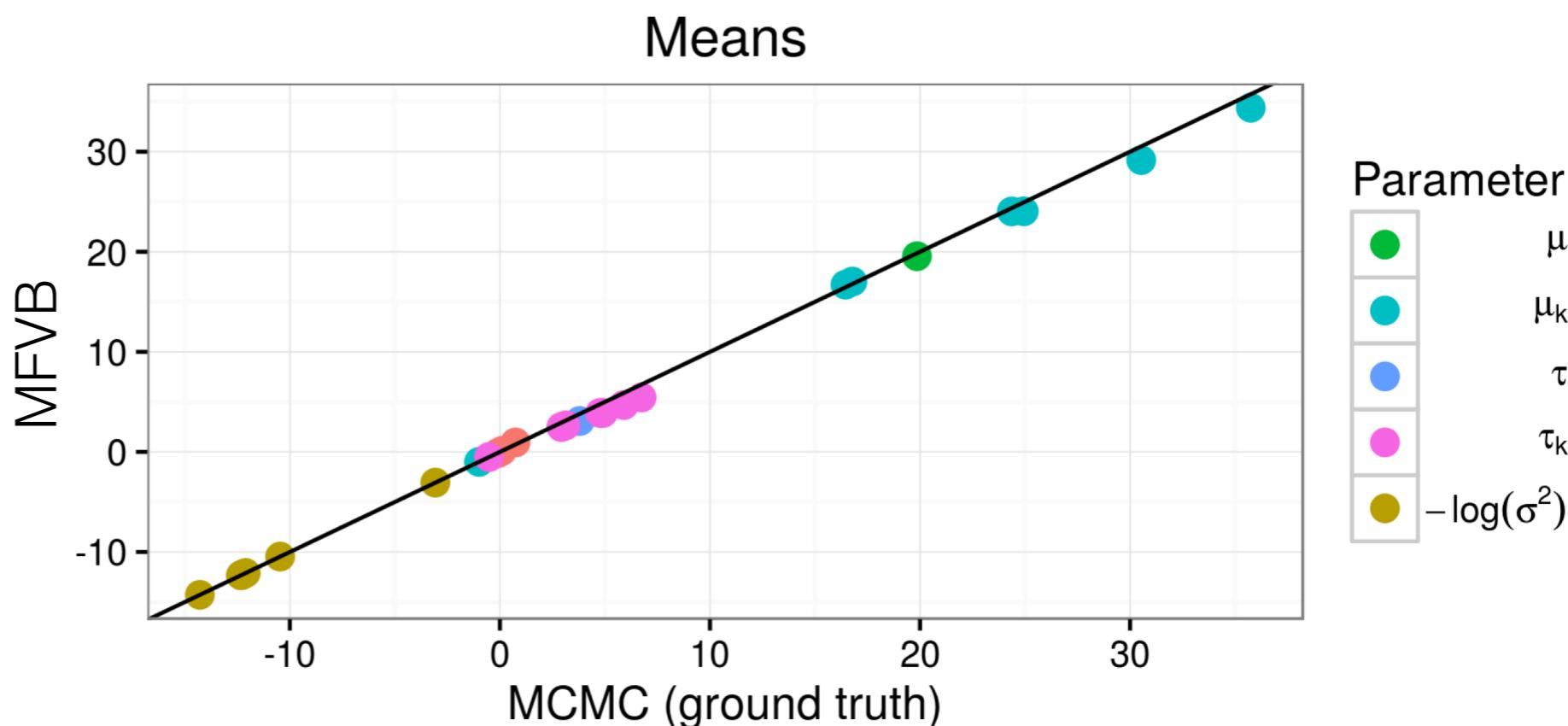
Microcredit

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



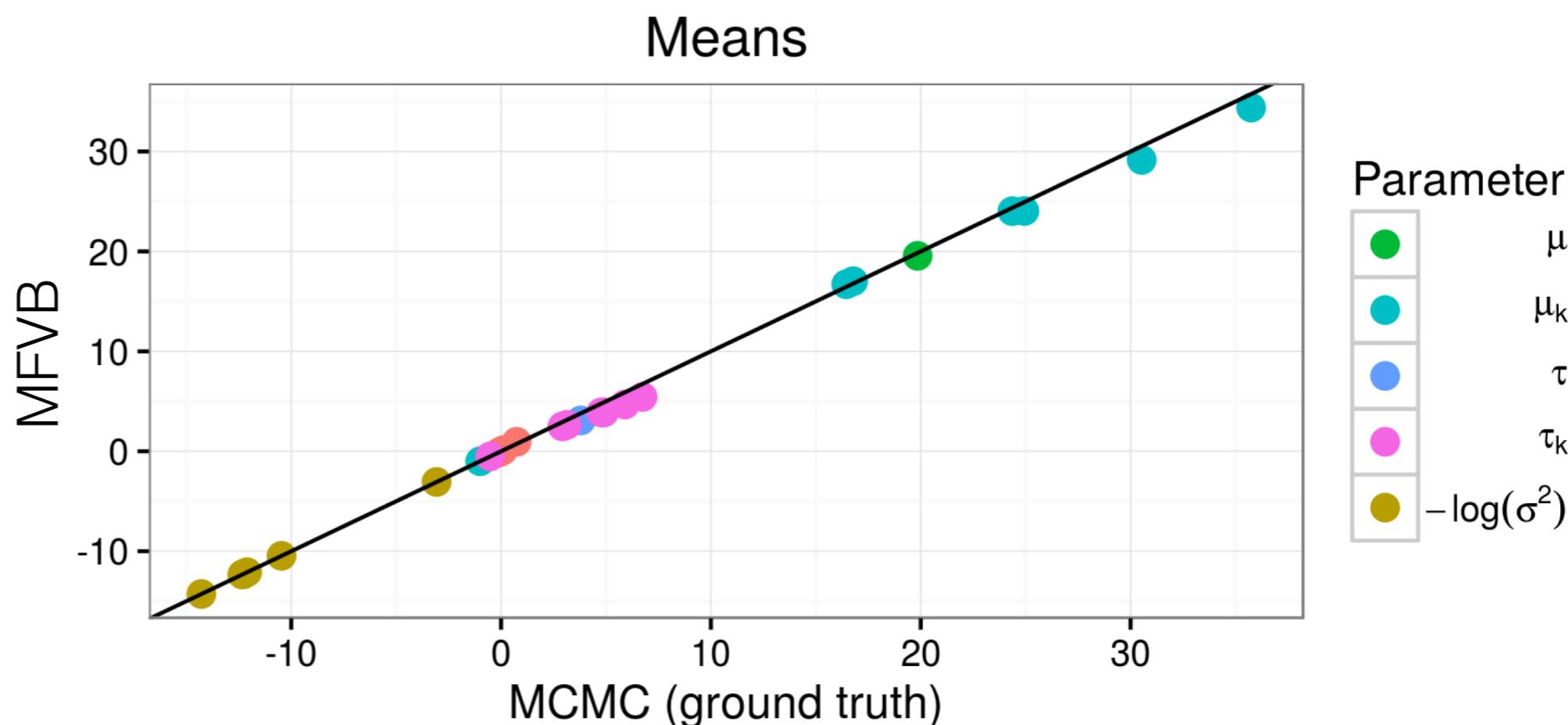
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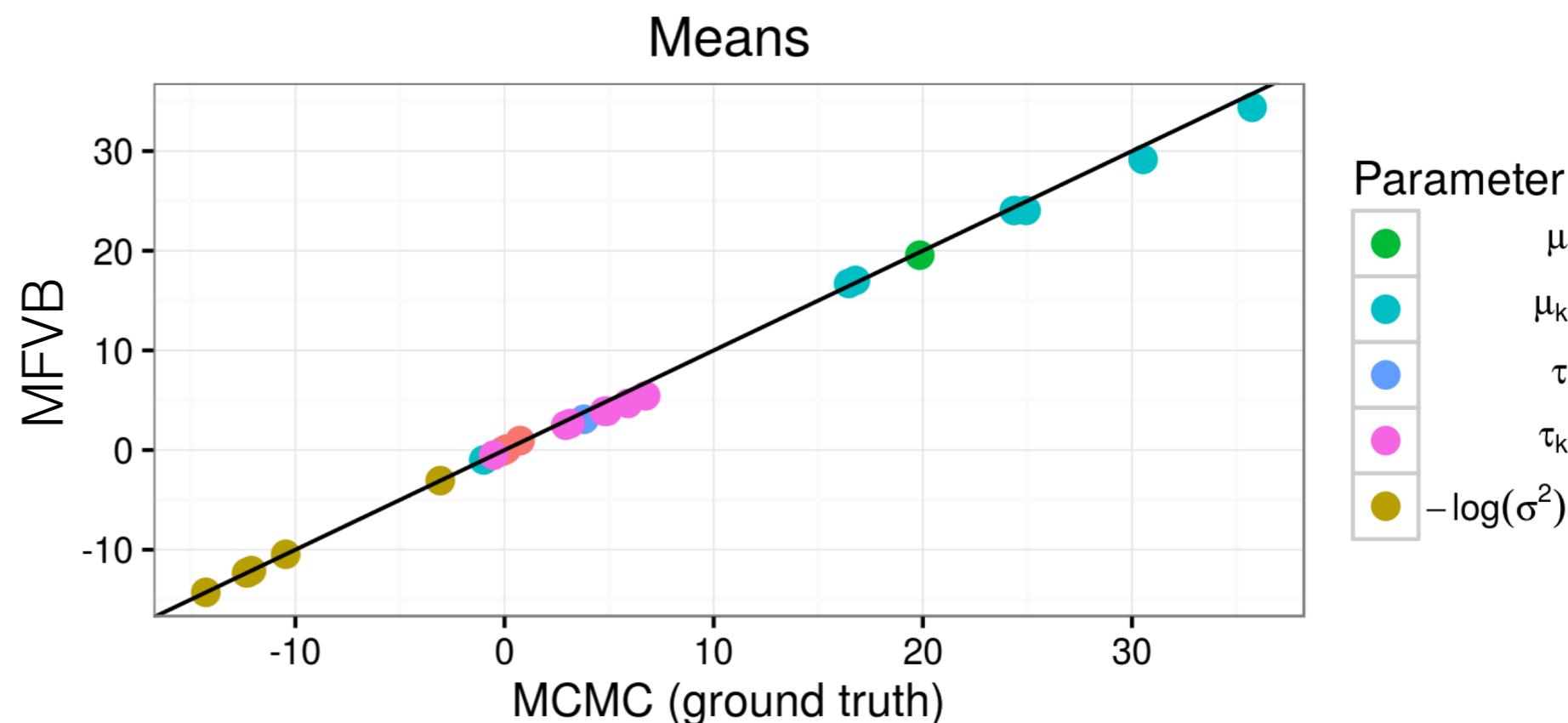


Criteo Online Ads Experiment

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

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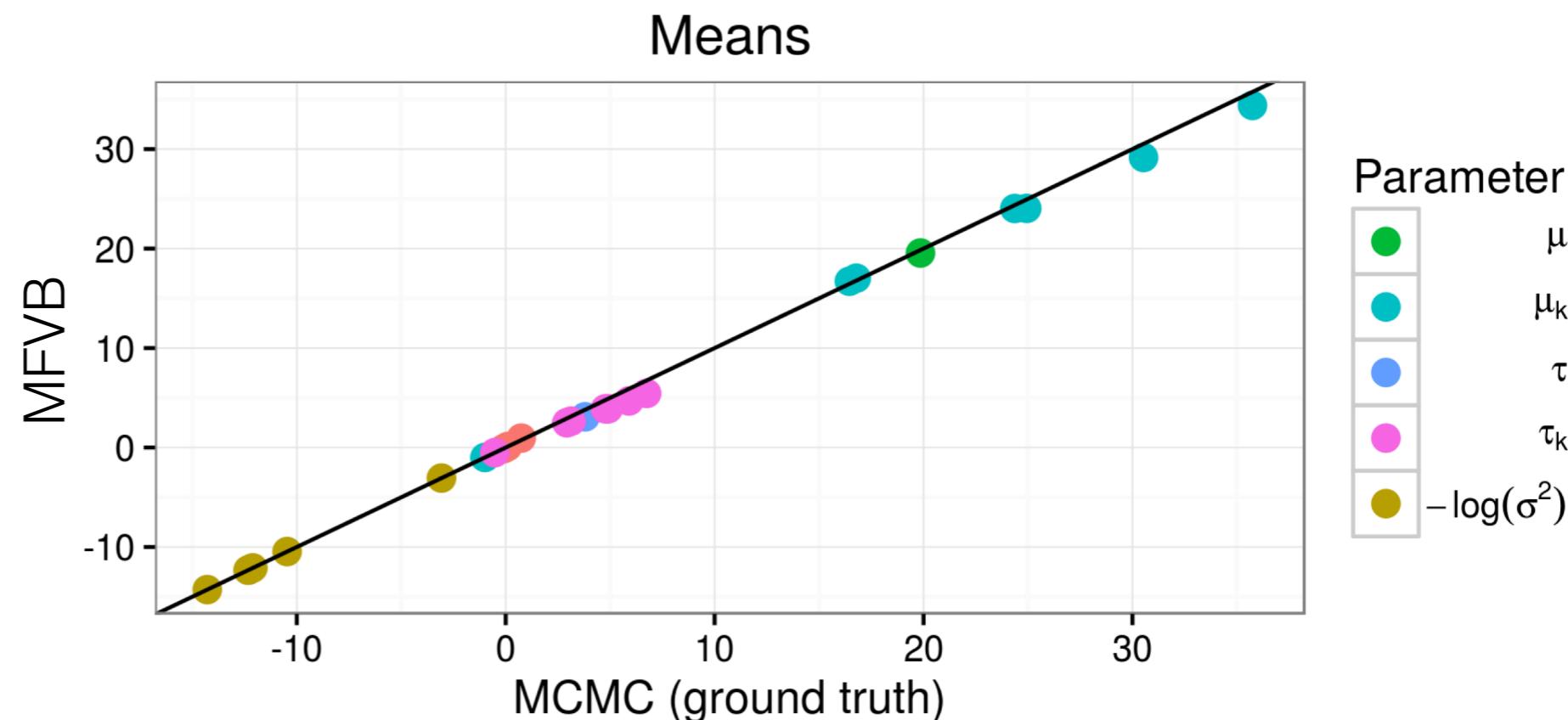


Criteo Online Ads Experiment

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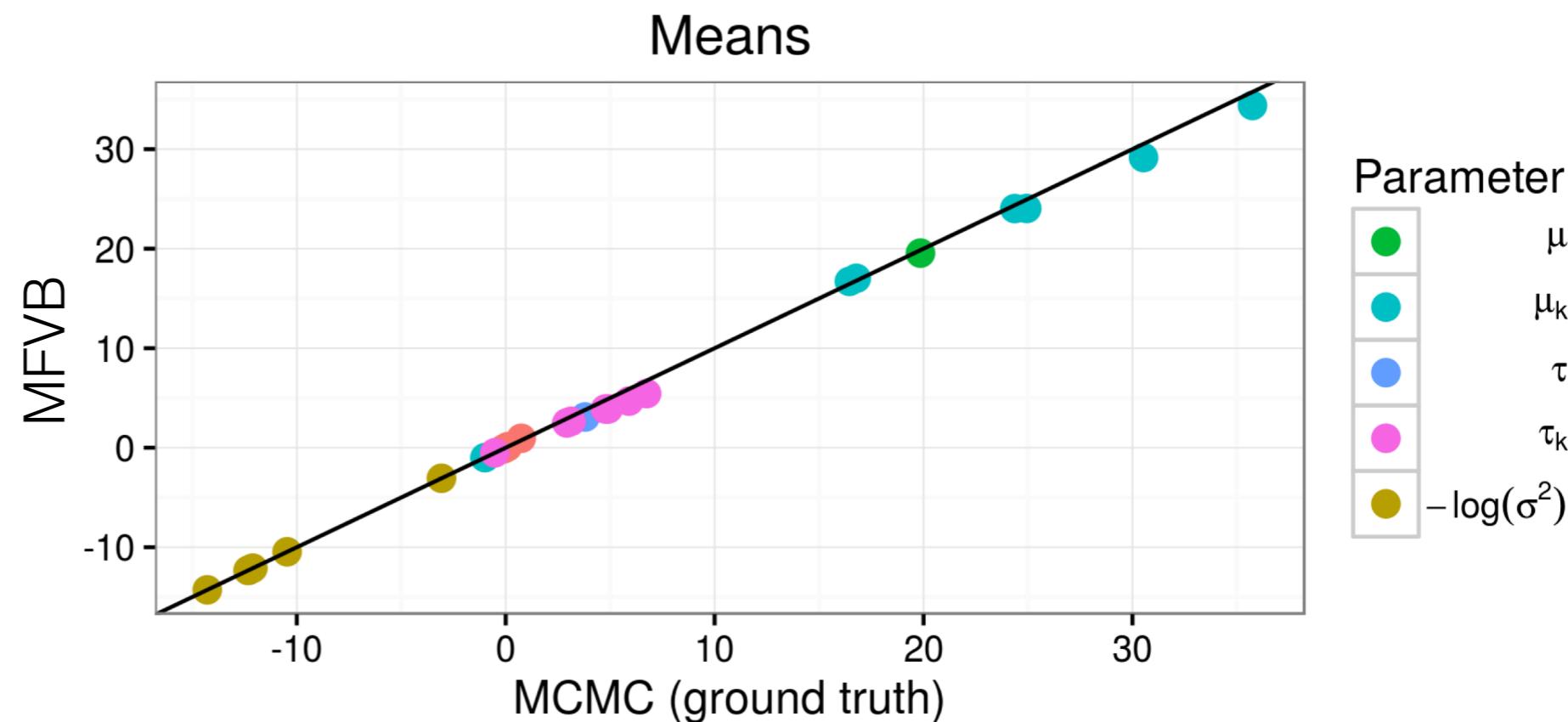


Criteo Online Ads Experiment

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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

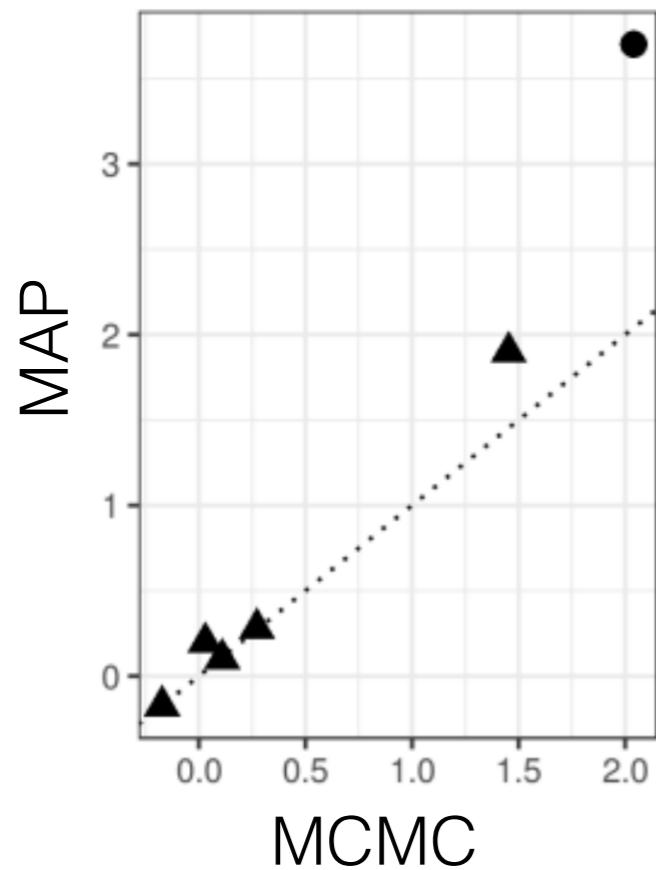
Criteo Online Ads Experiment

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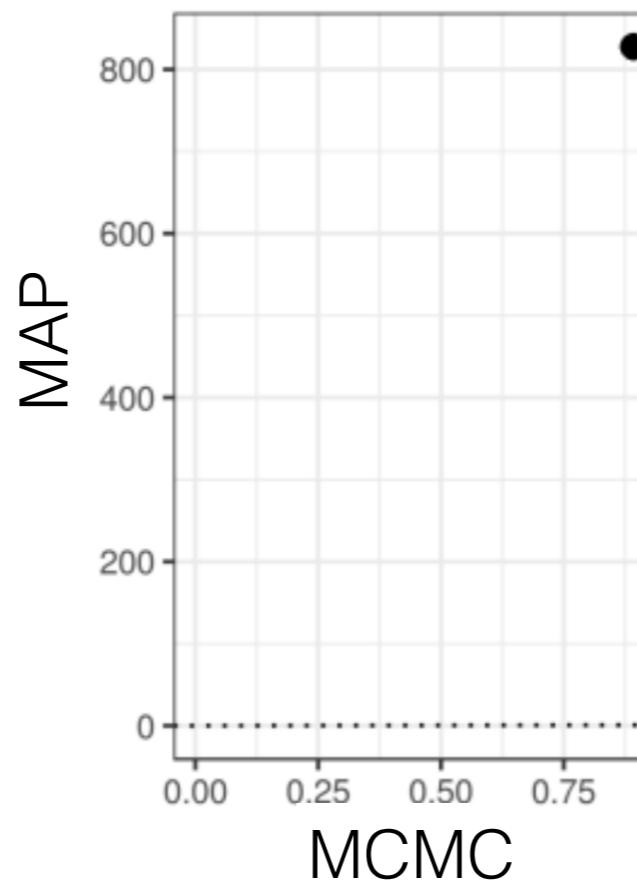
- MAP: **12 s**

Criteo Online Ads Experiment

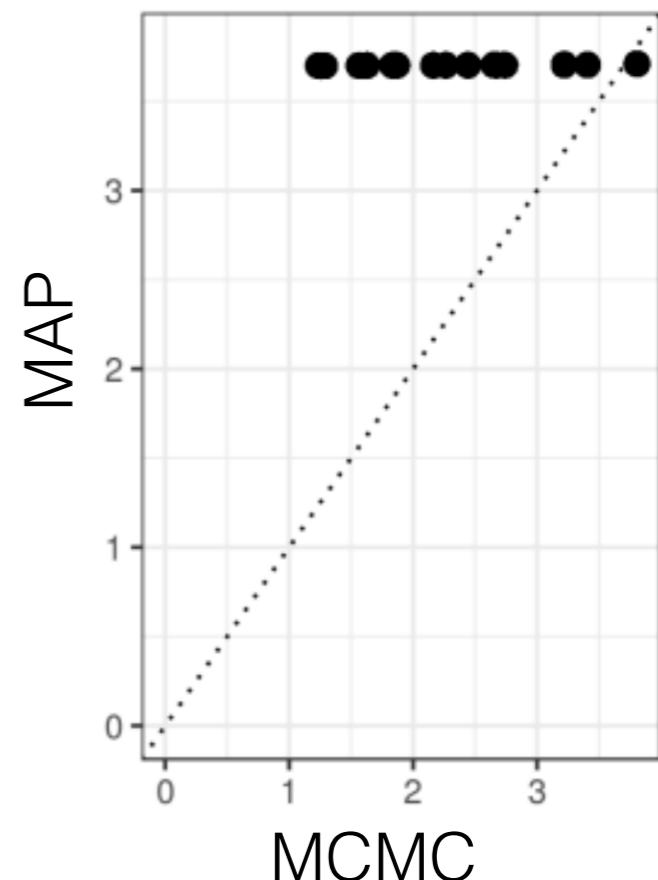
Global parameters ($-\tau$)



Global parameter τ



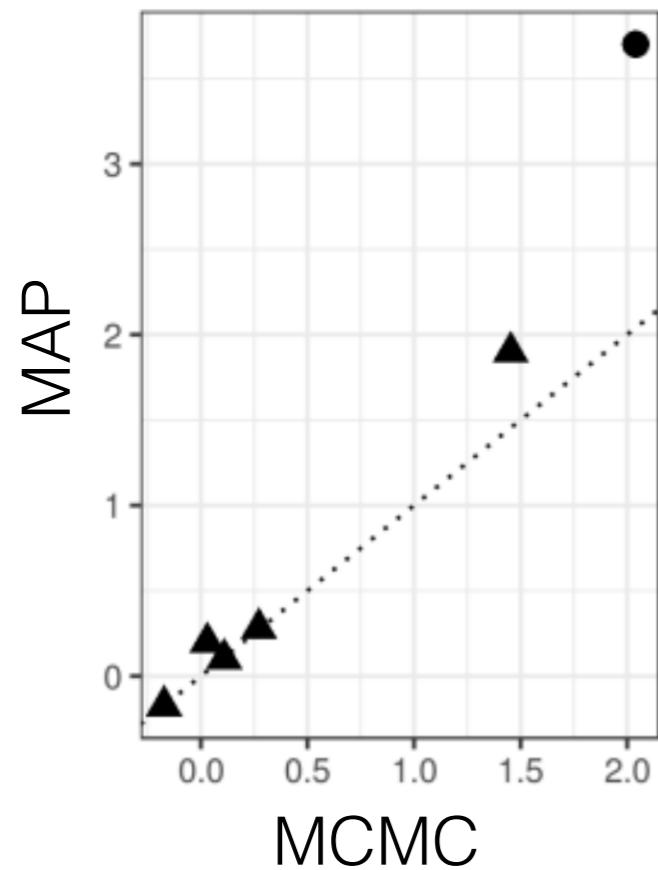
Local parameters



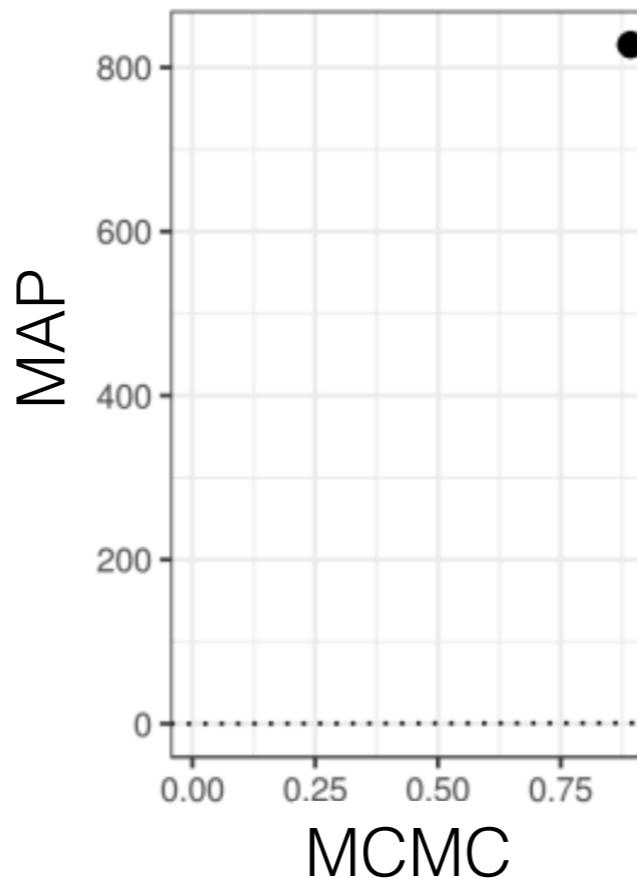
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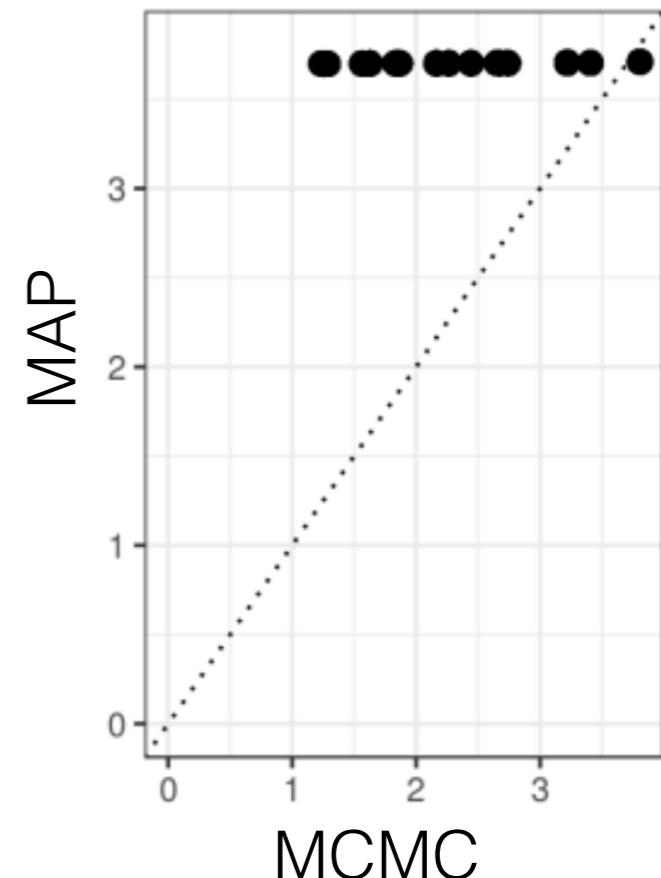
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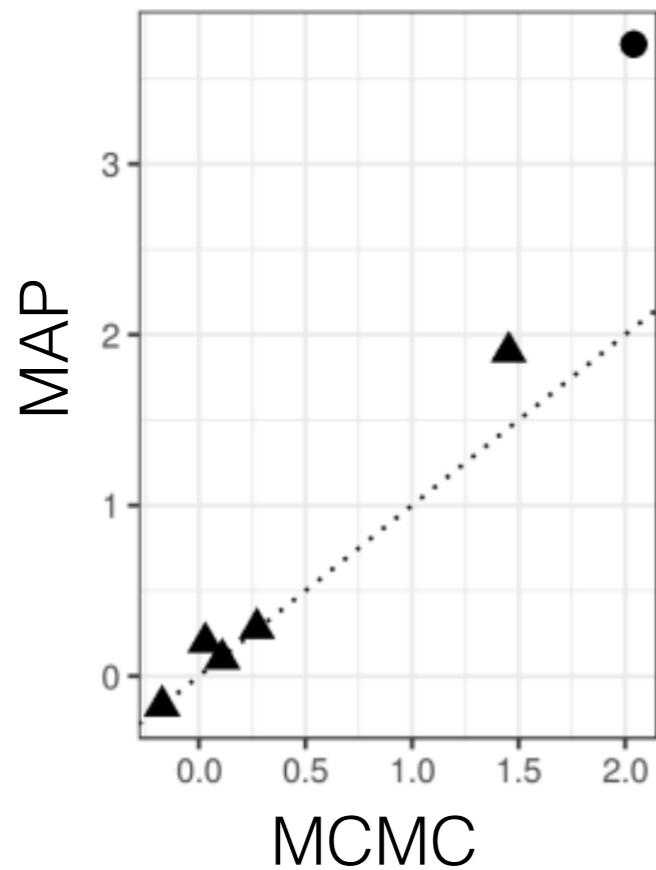
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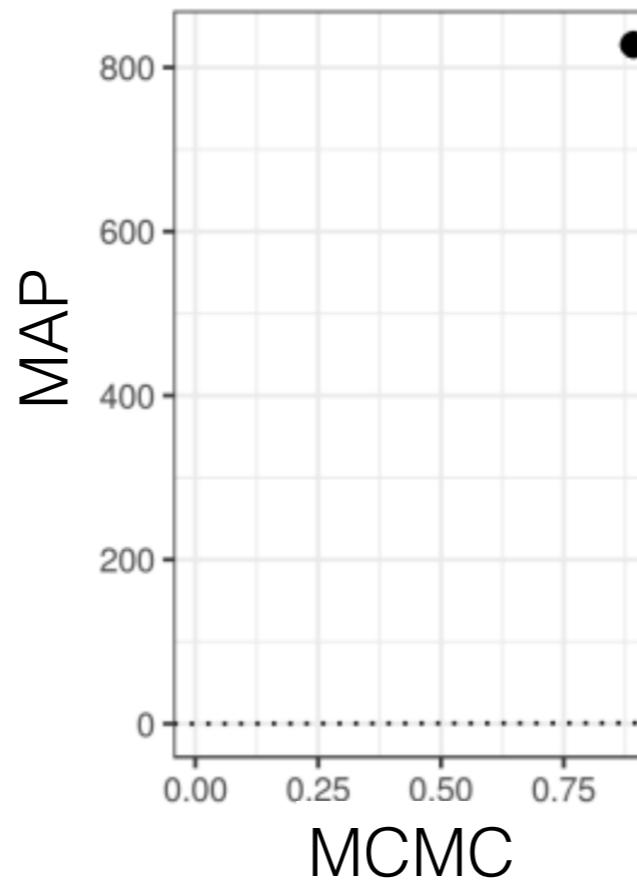
- MAP: **12 s**
- MFVB: **57 s**

Criteo Online Ads Experiment

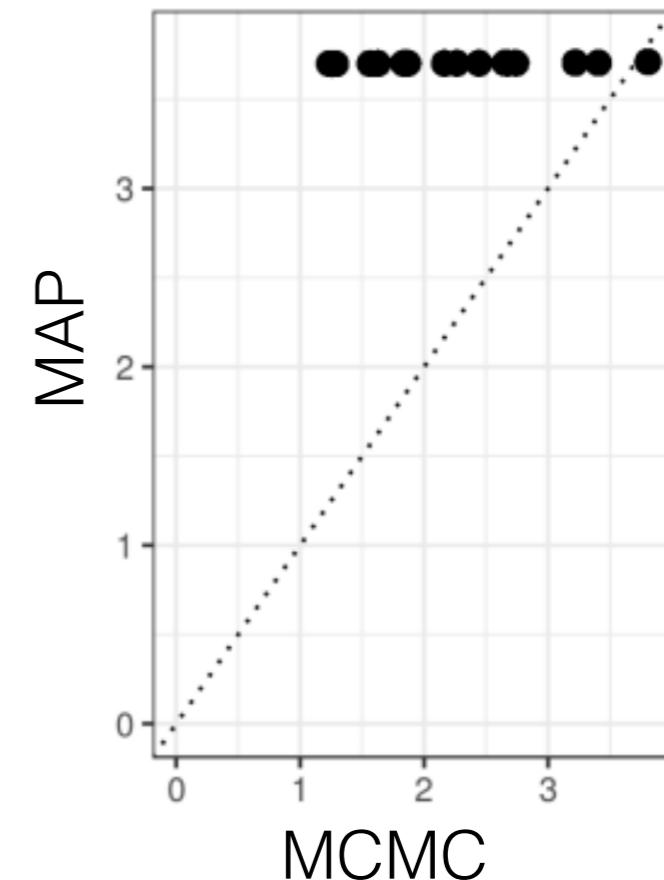
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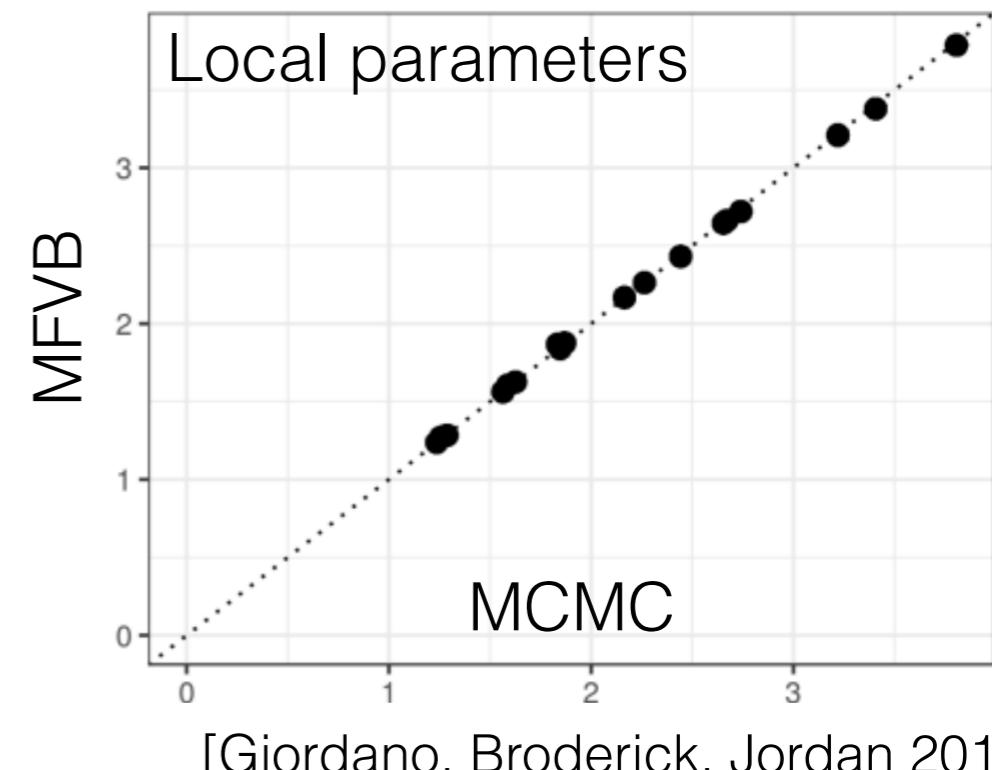
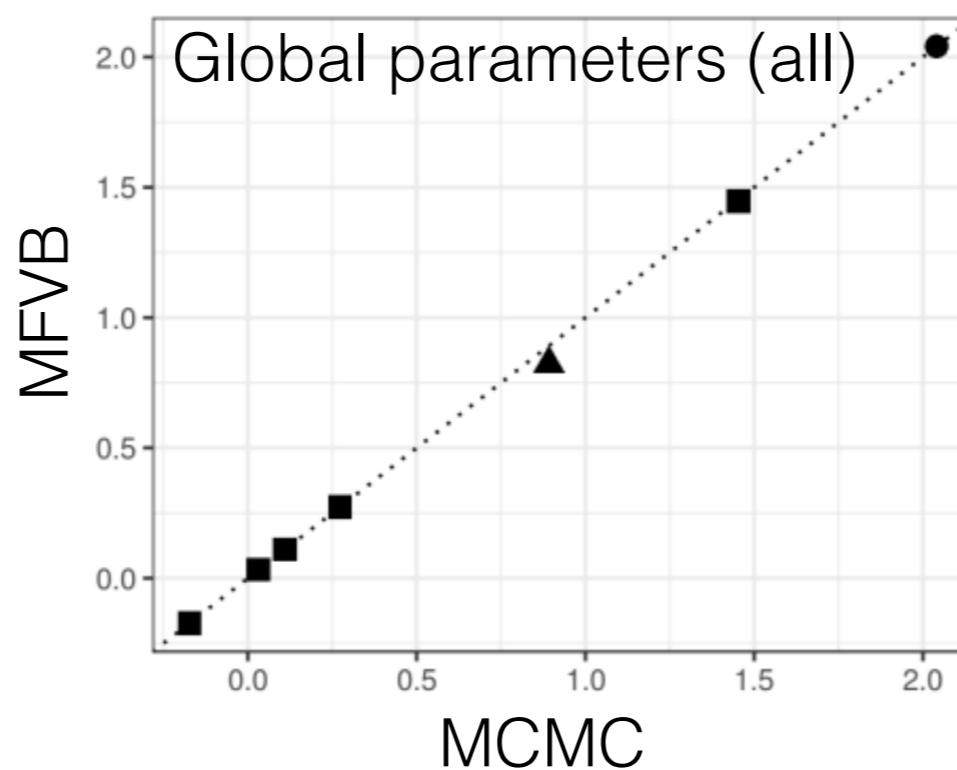
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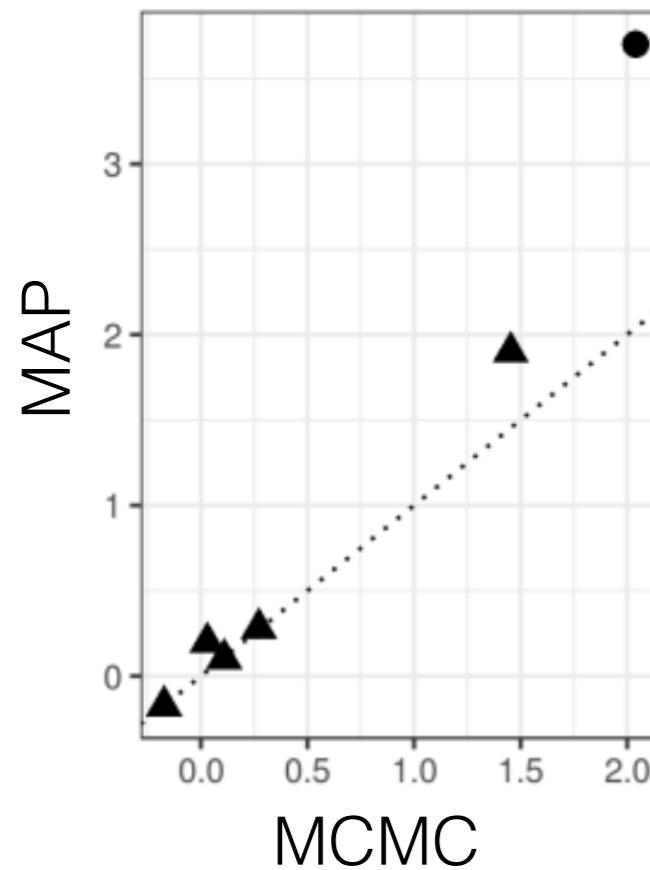


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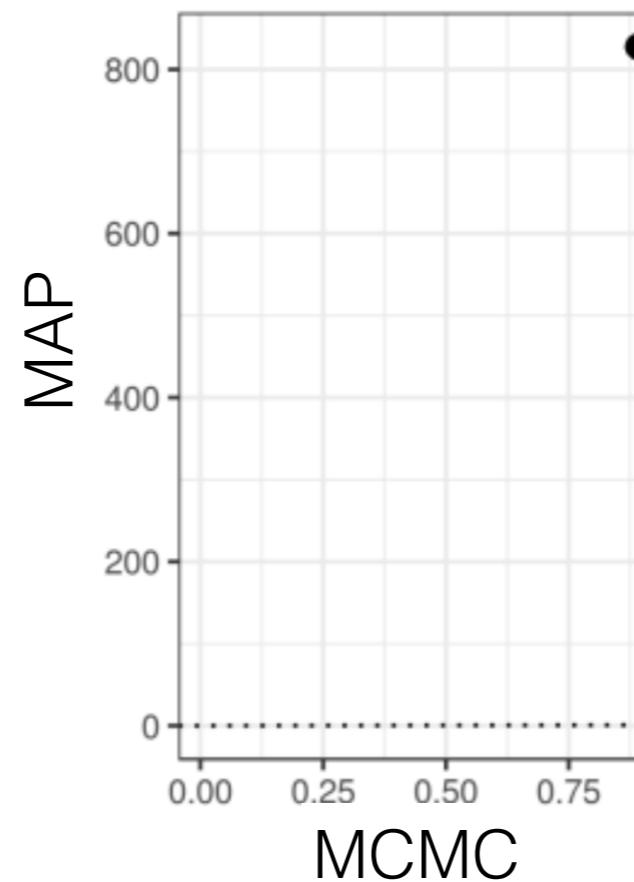


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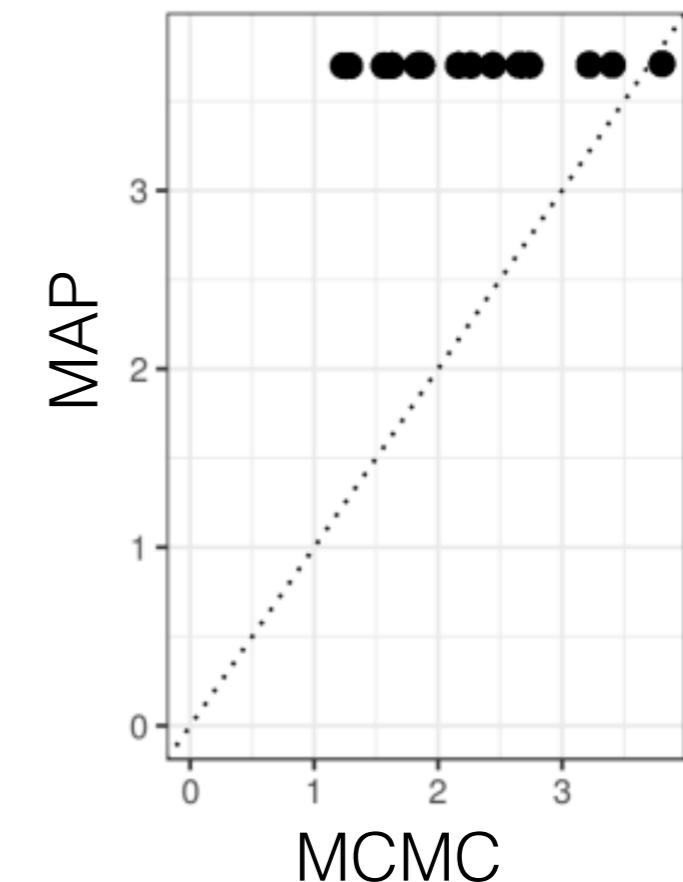
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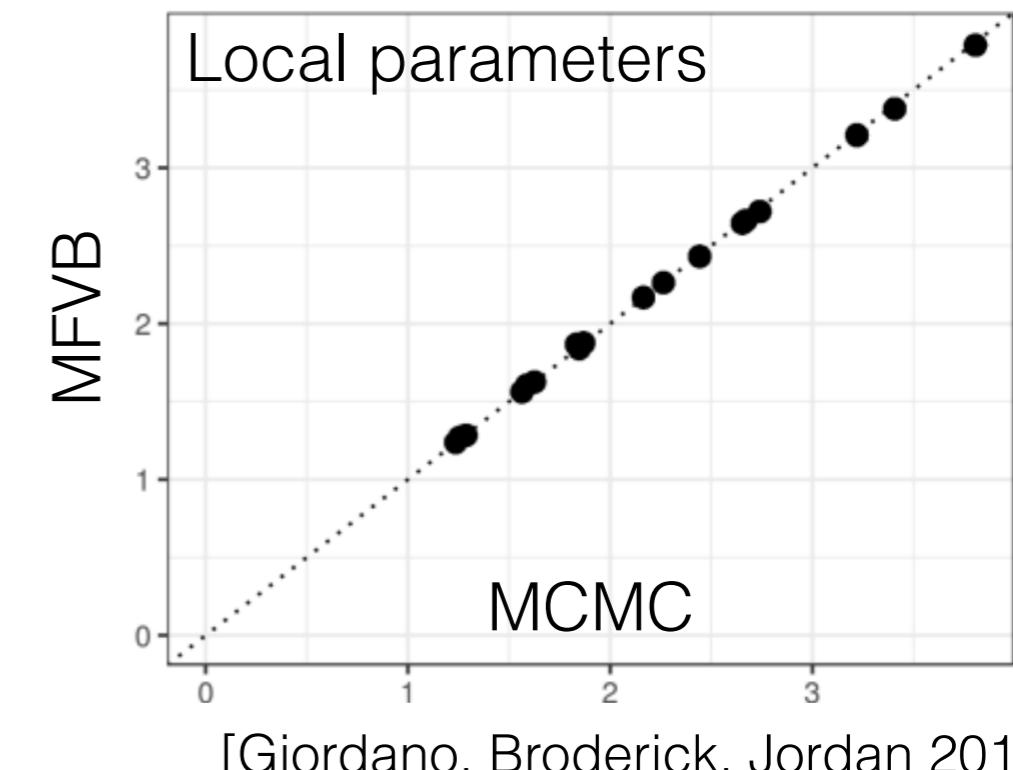
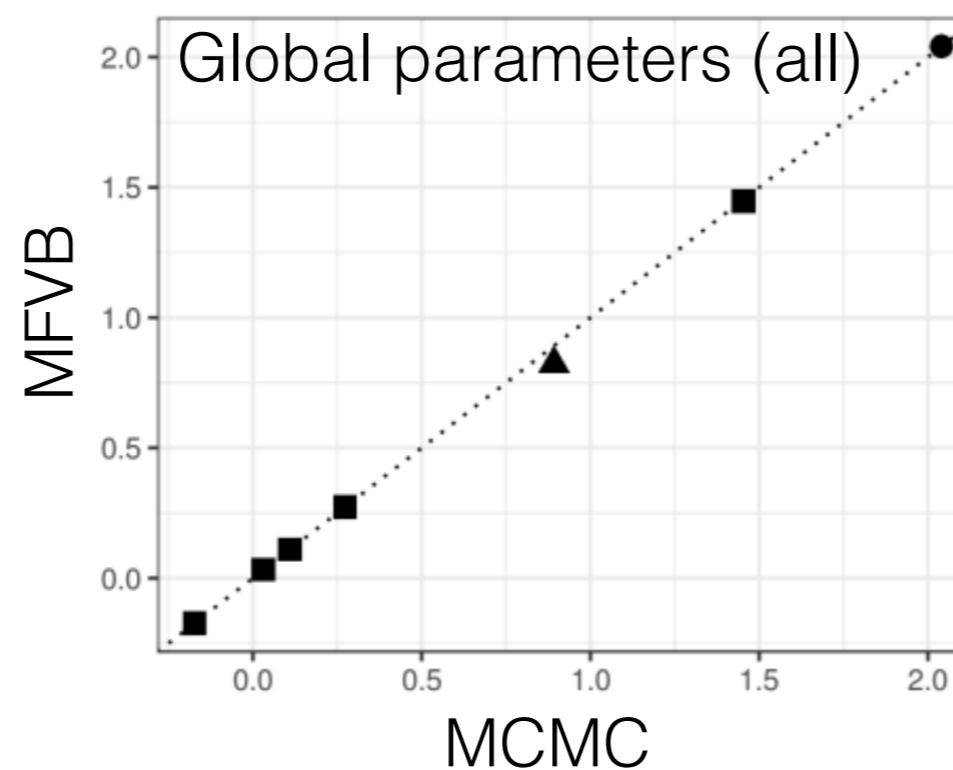
Global parameter τ



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.

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 - 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?

Roadmap

- Bayes & Approximate Bayes review
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What about uncertainty?

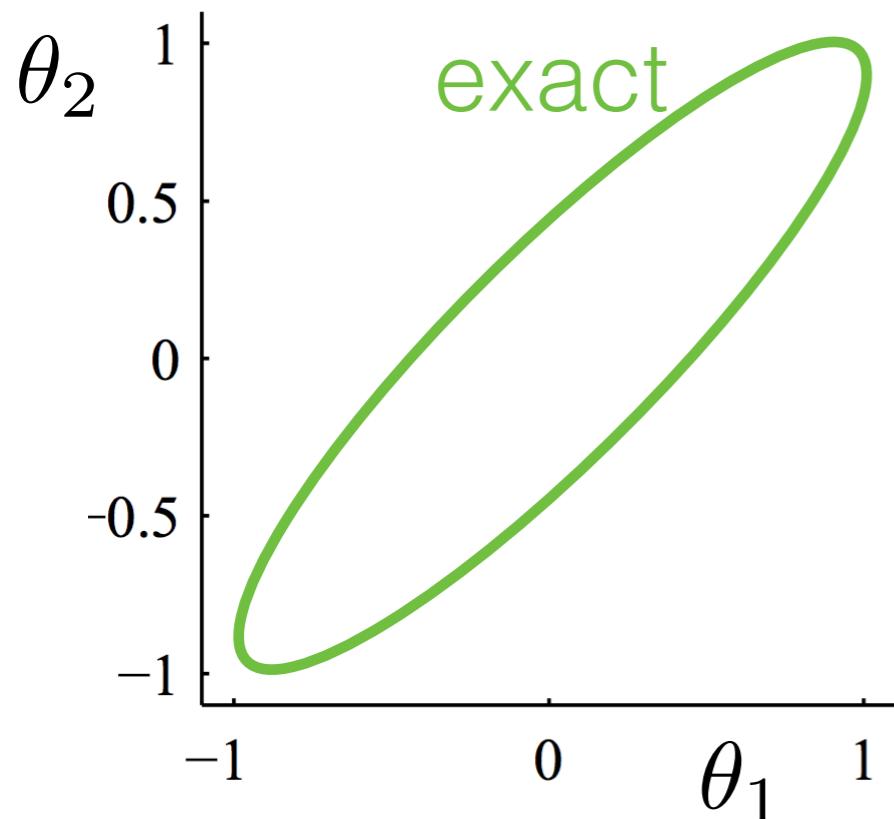
What about uncertainty?

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

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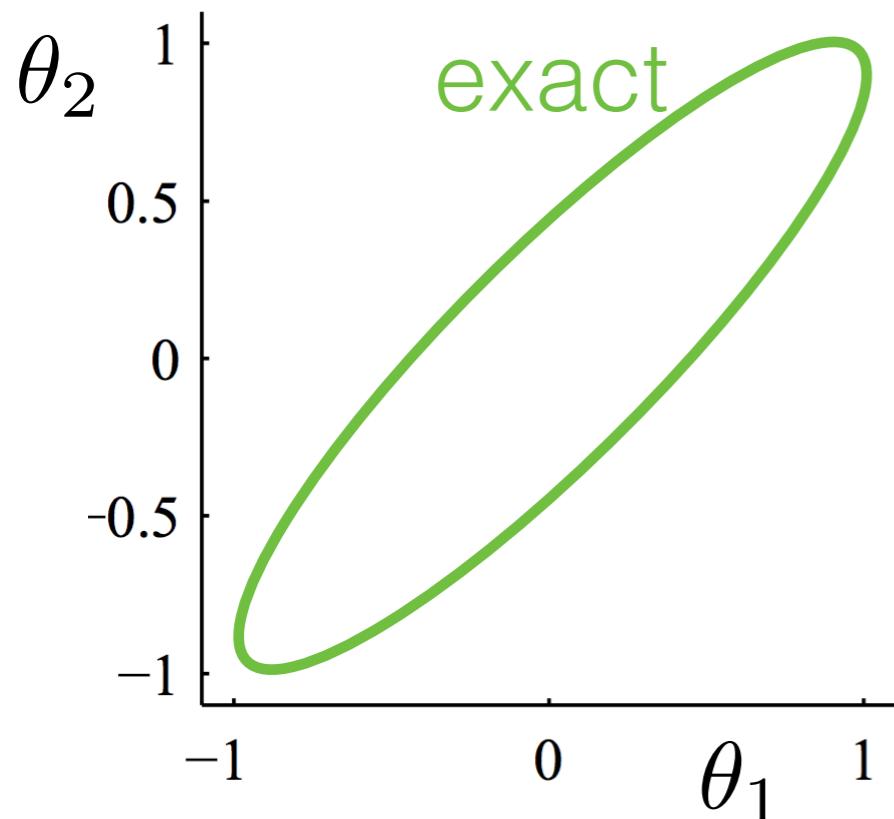


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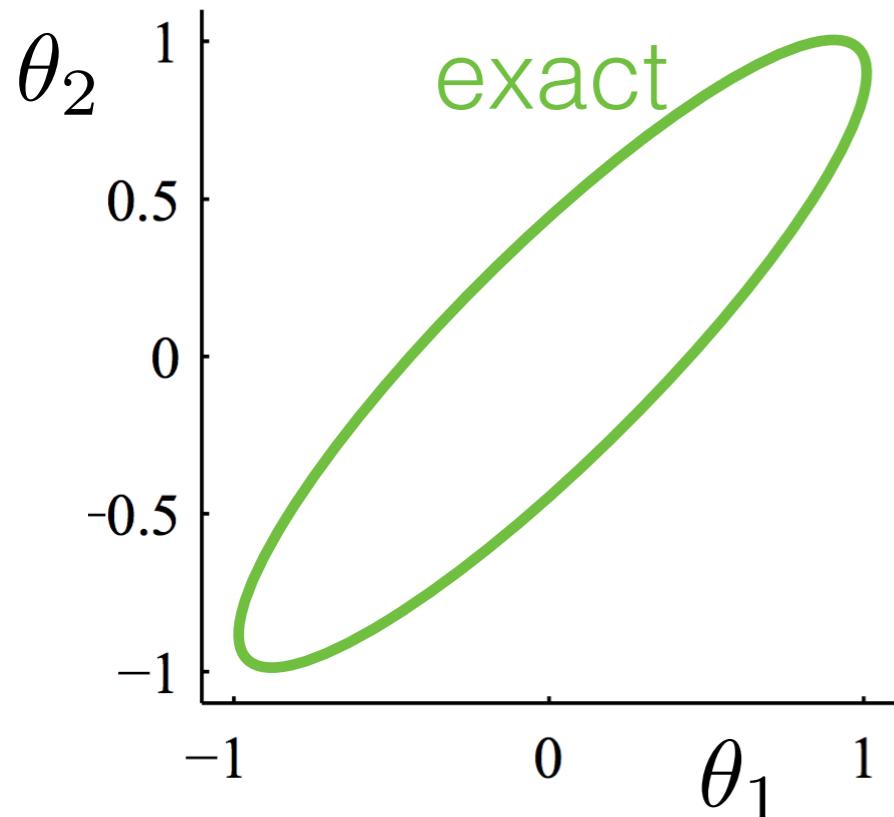
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- Conjugate linear regression

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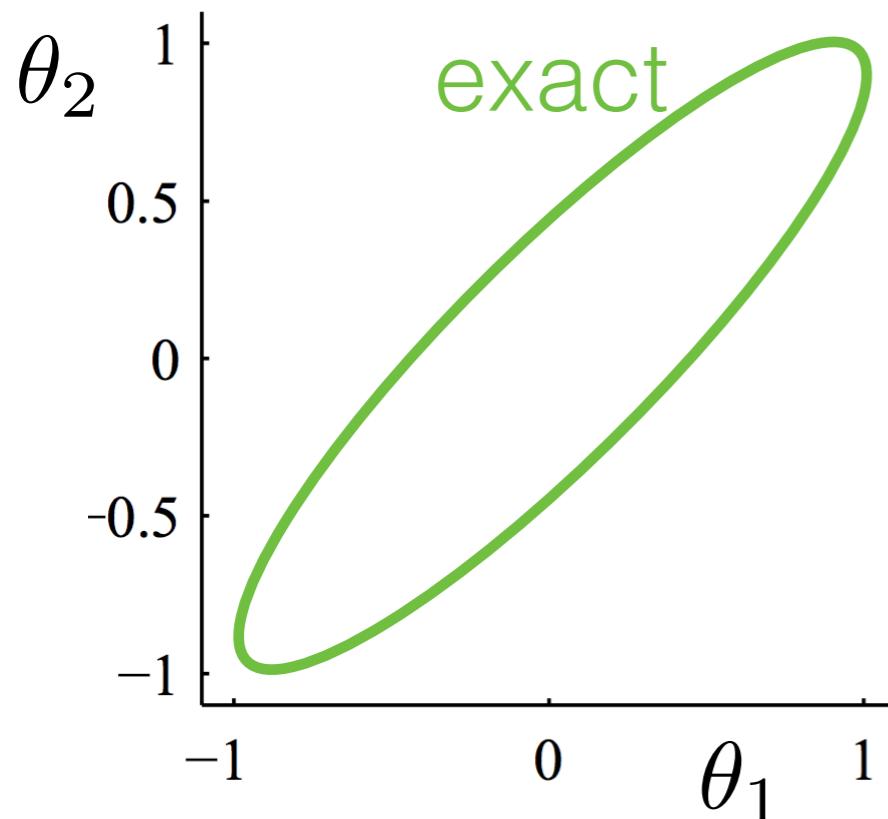
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- Conjugate linear regression
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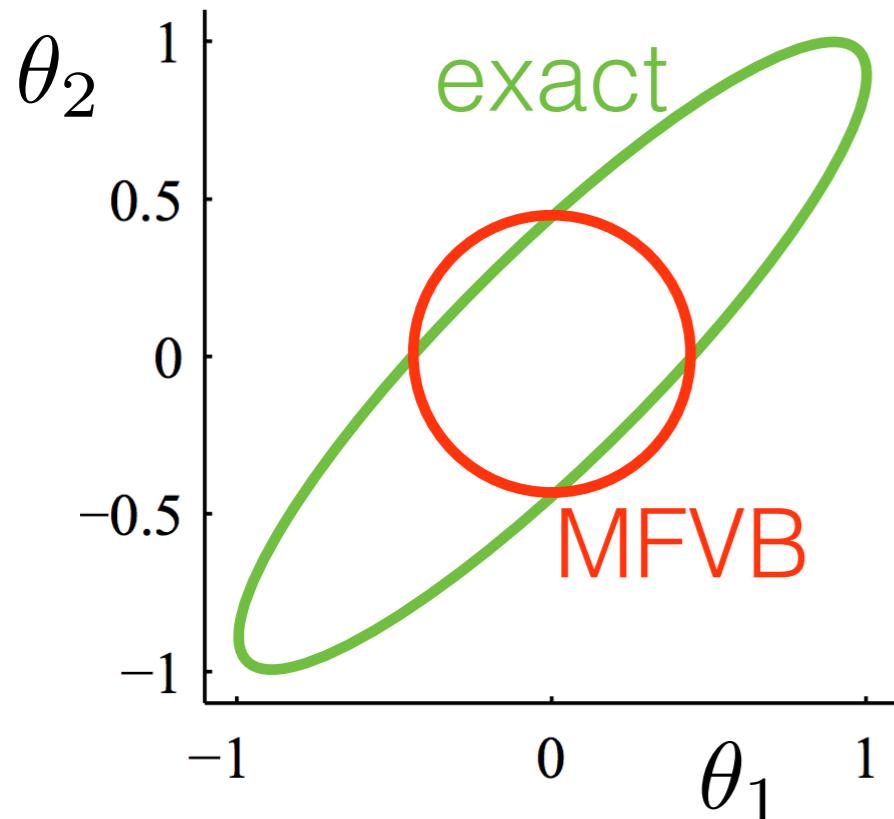
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[Exercise: derive the MFVB-CA steps. Hint: use precision matrix.]

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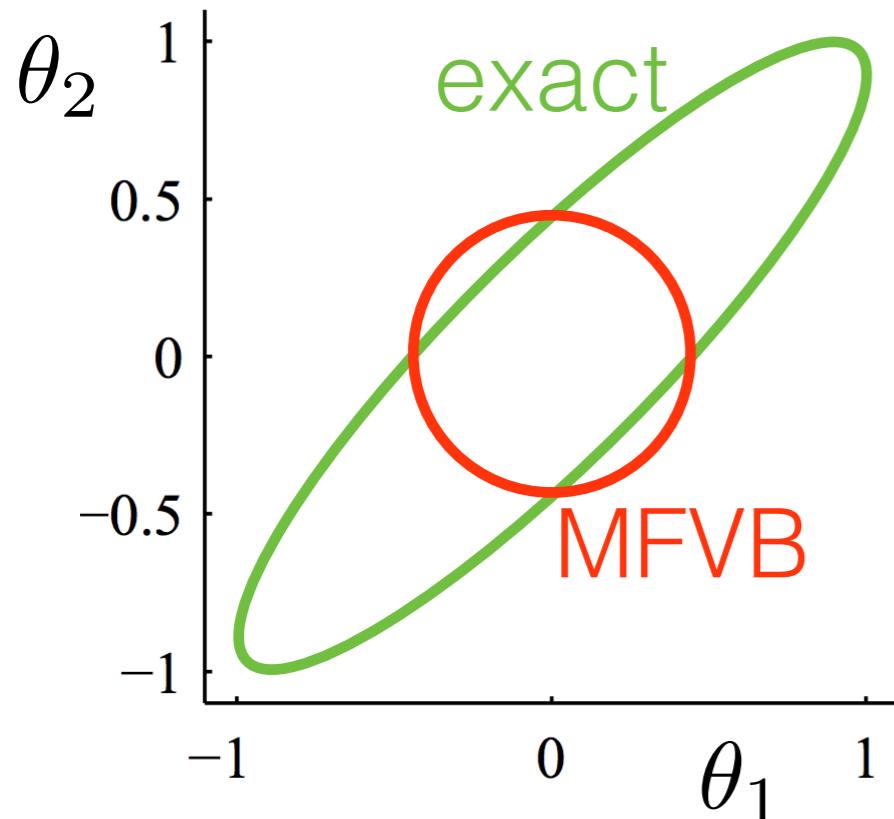
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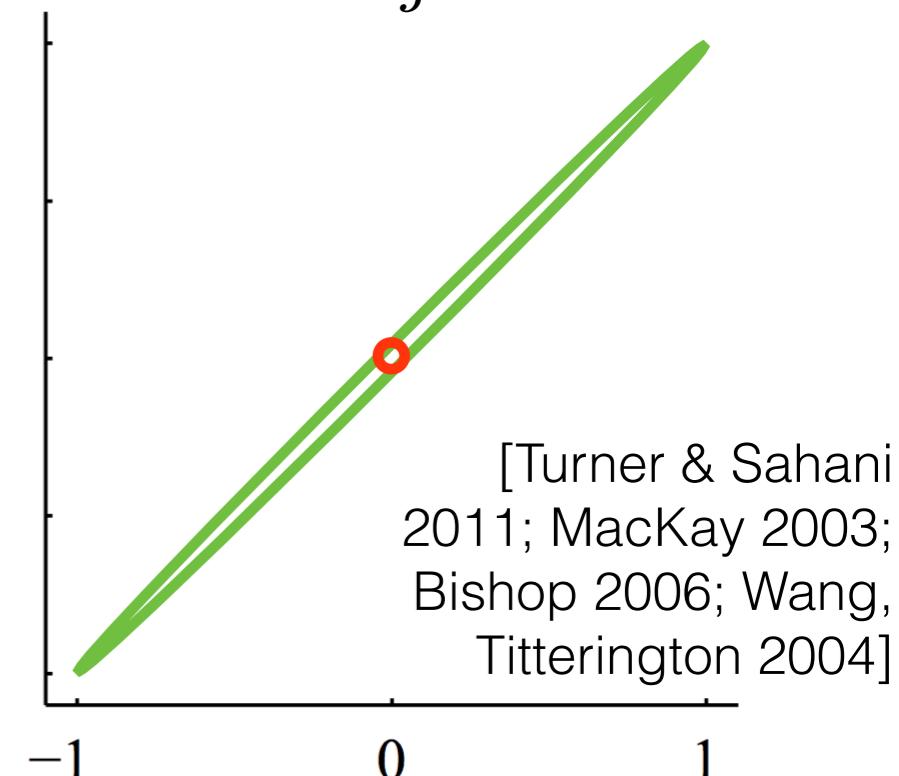
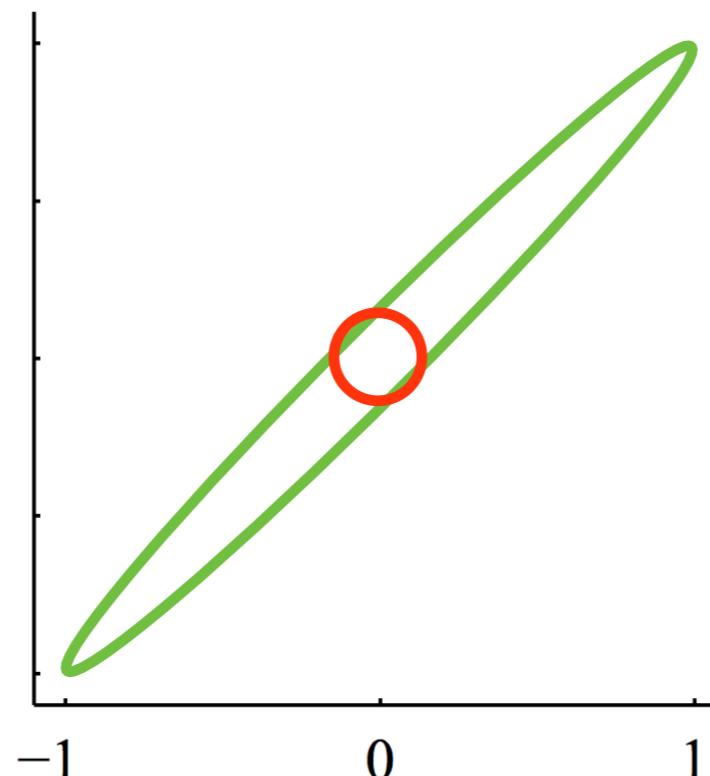
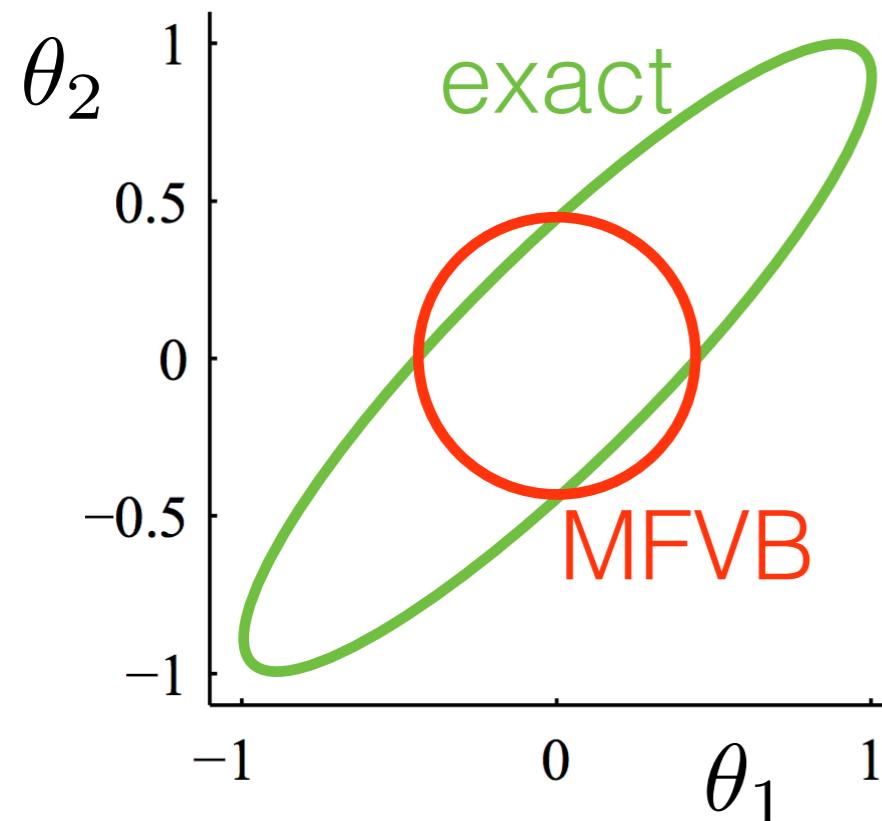
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- Underestimates variance (sometimes severely)

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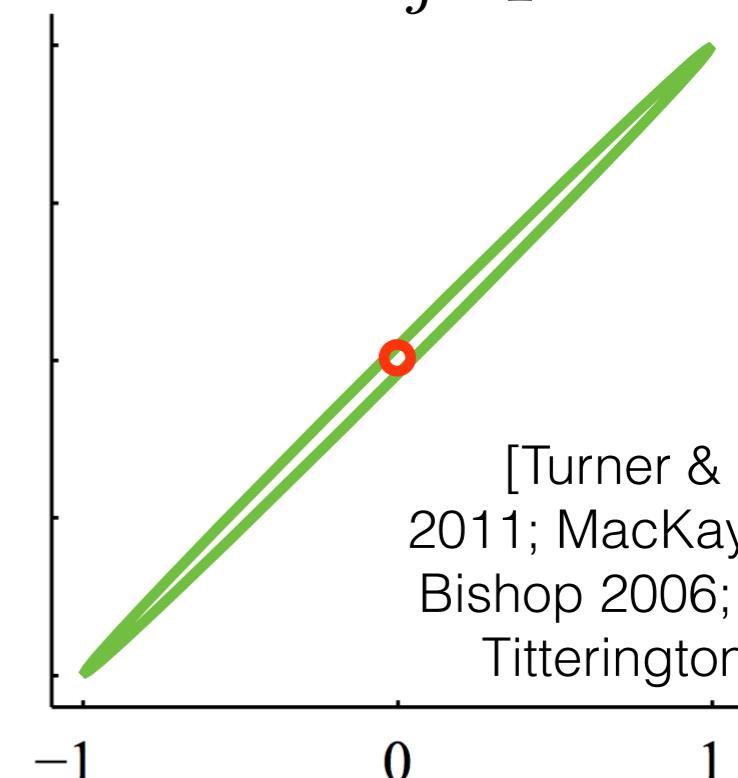
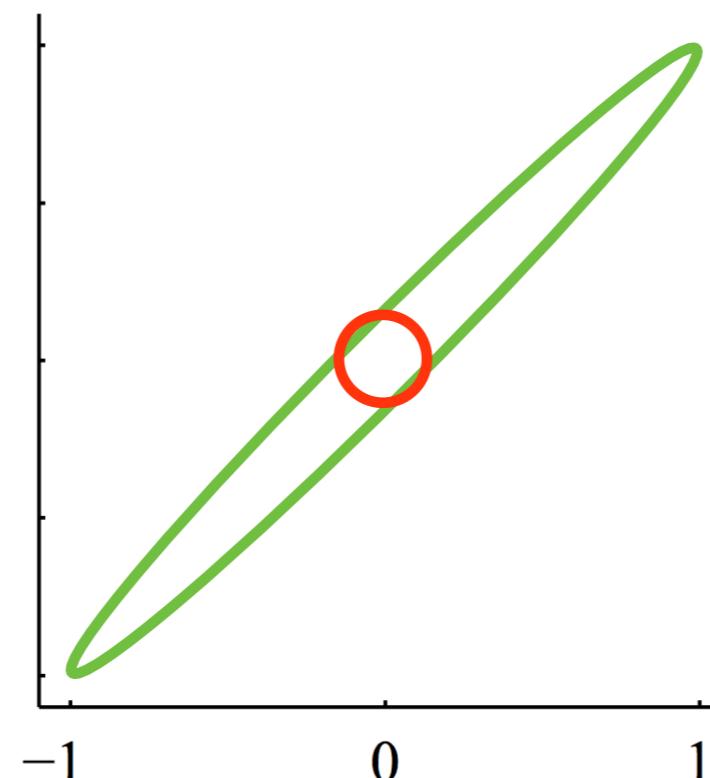
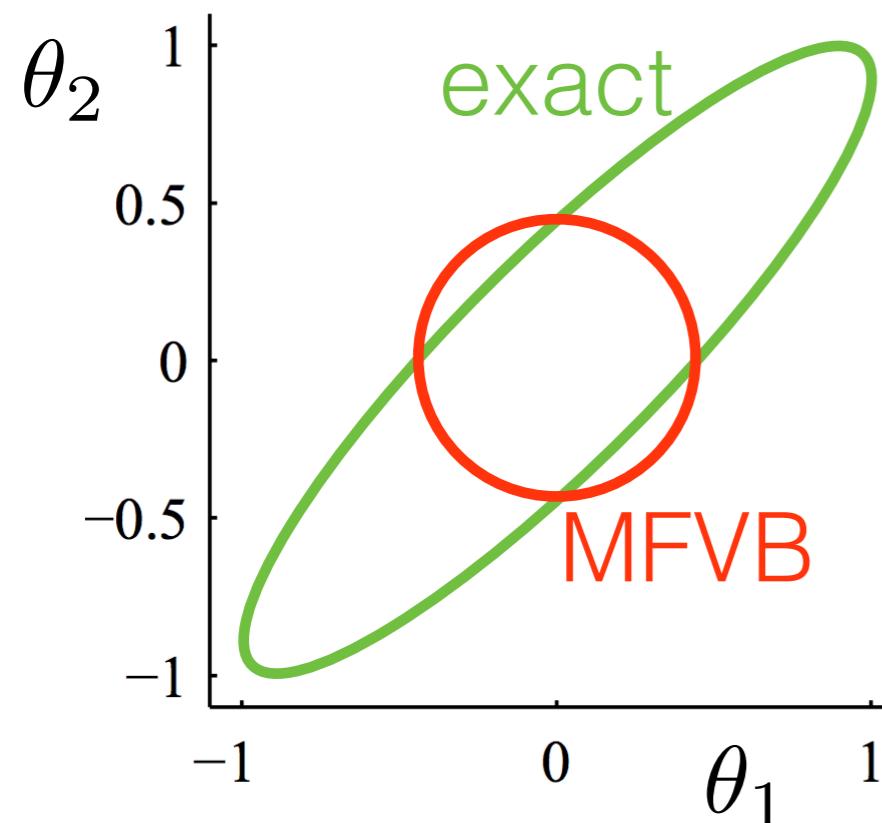
[Exercise: derive the MFVB-CA steps. Hint: use precision matrix.]

- Underestimates variance (sometimes severely)

What about uncertainty?

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

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



- Conjugate linear regression
- Bayesian central limit theorem

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

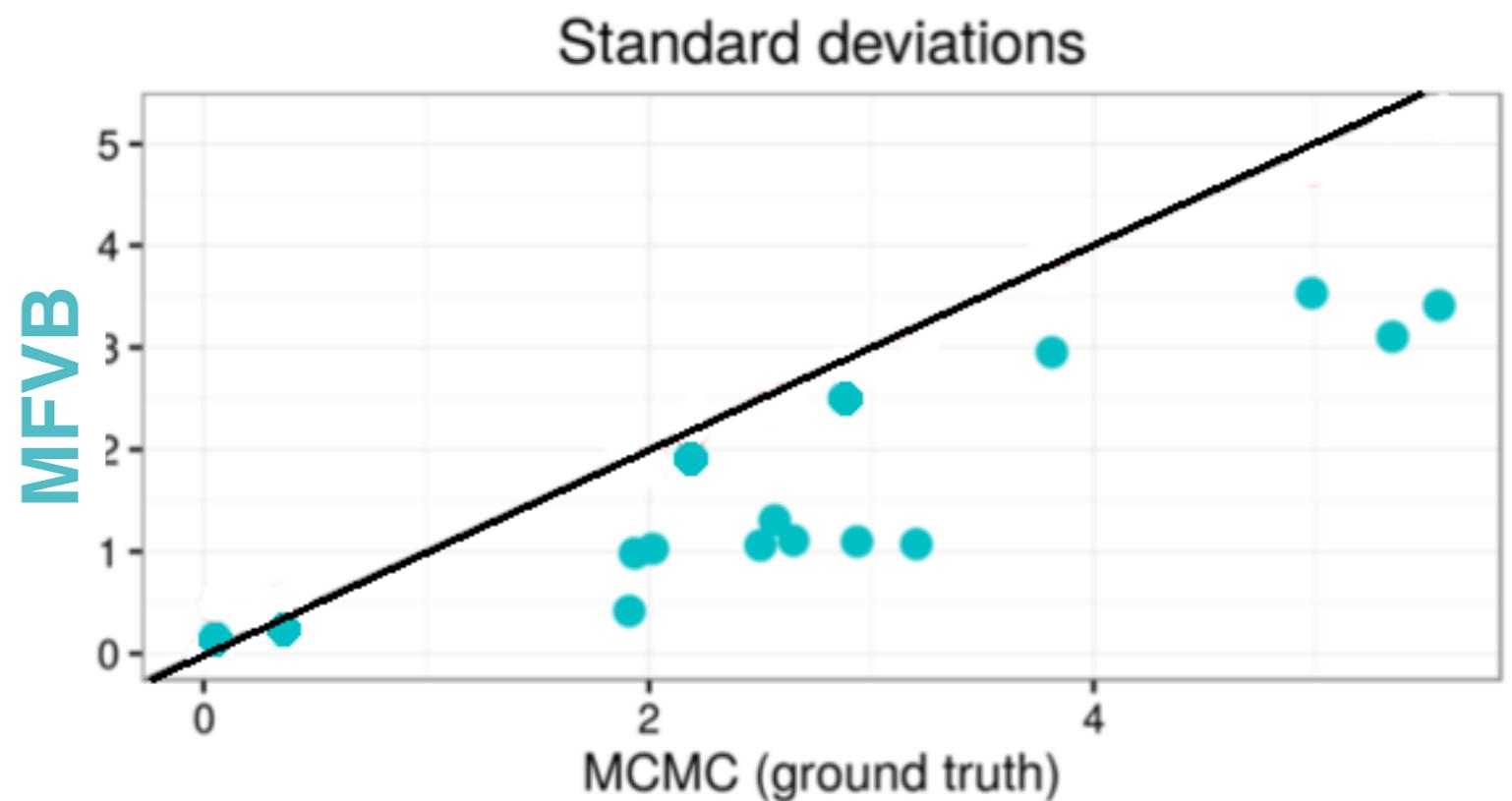
- Underestimates variance (sometimes severely)
- No covariance estimates

What about uncertainty?

- Microcredit

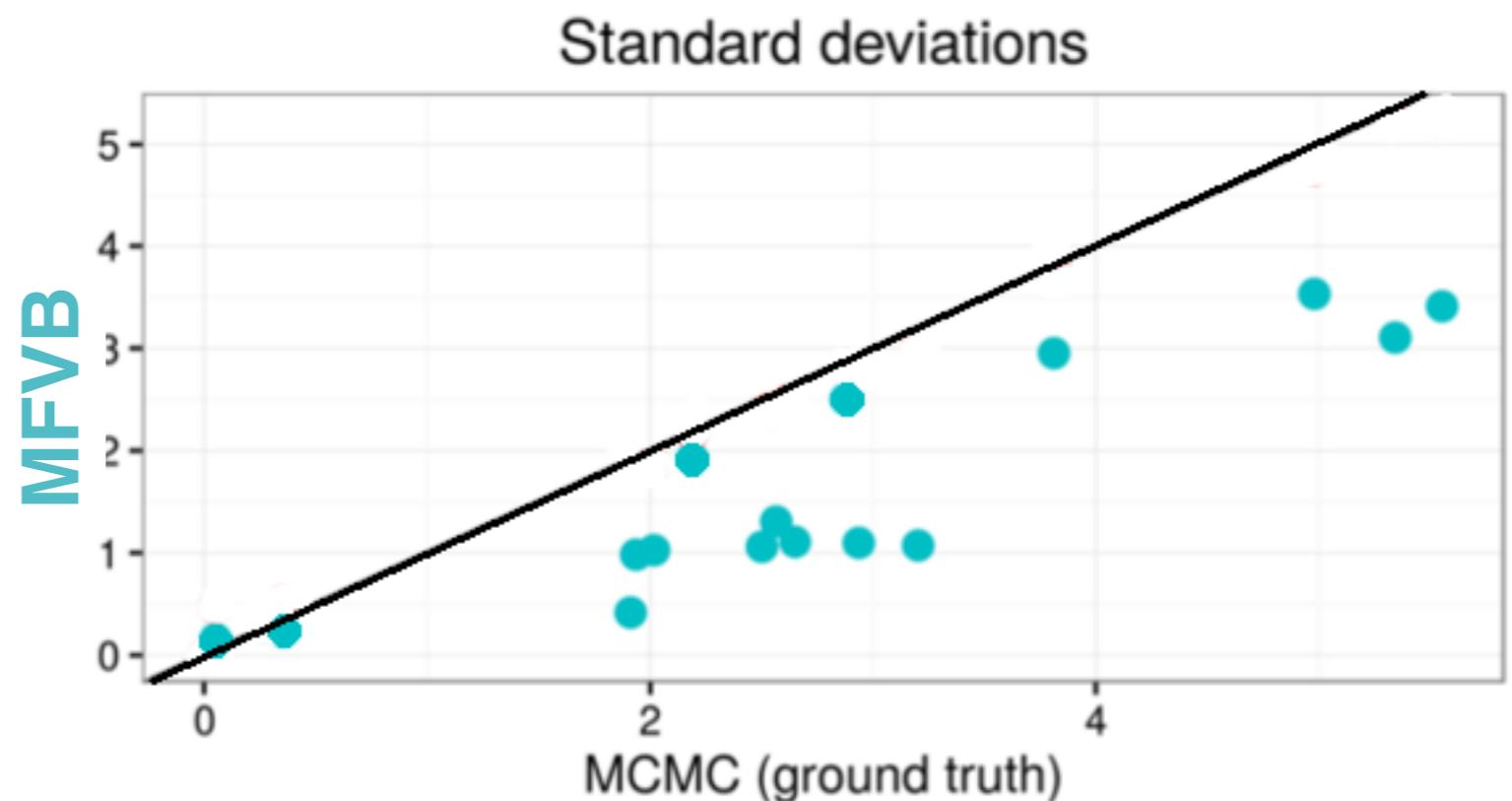
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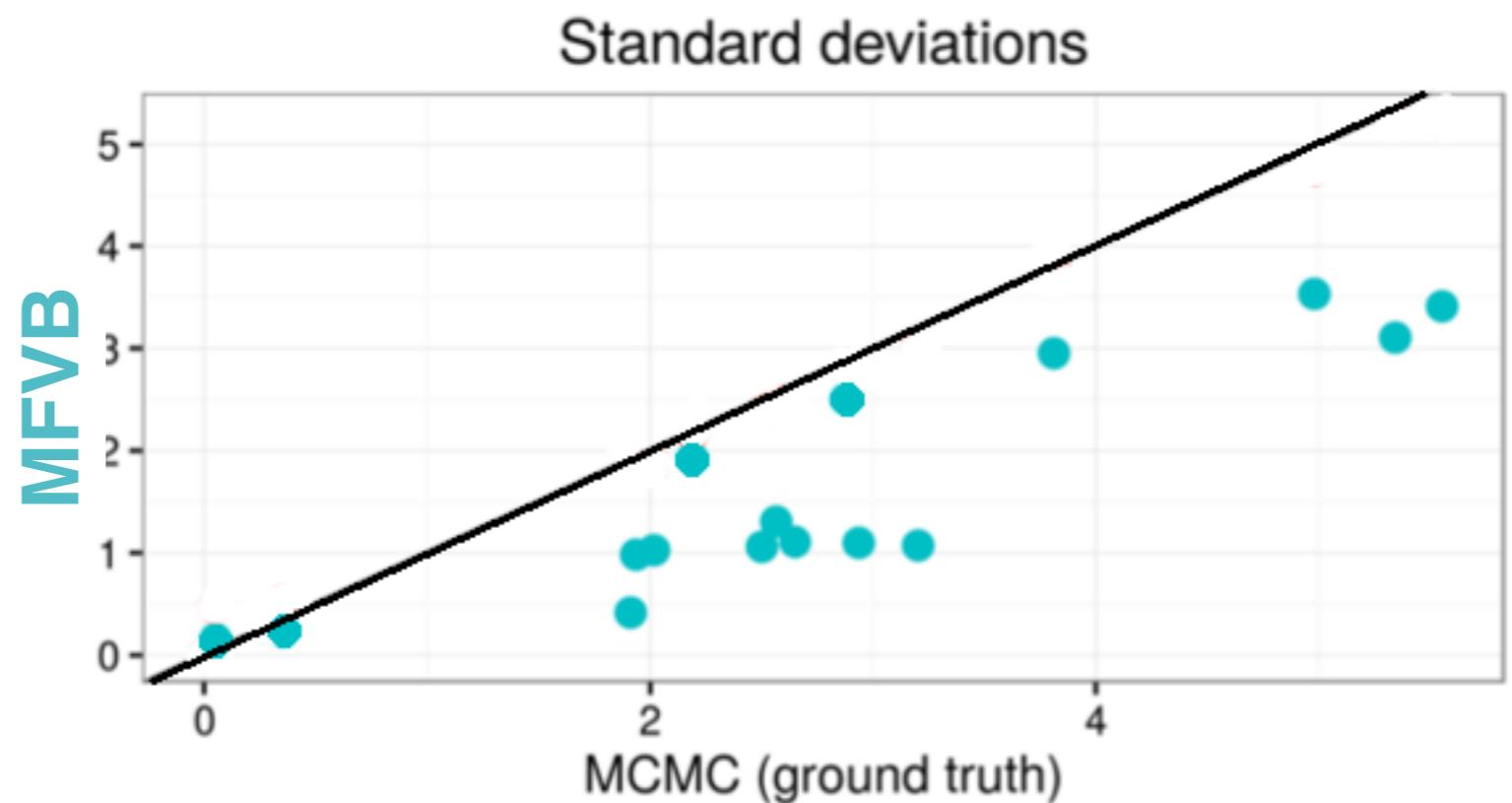
What about uncertainty?

- Microcredit effect
- τ mean:
3.08 USD PPP



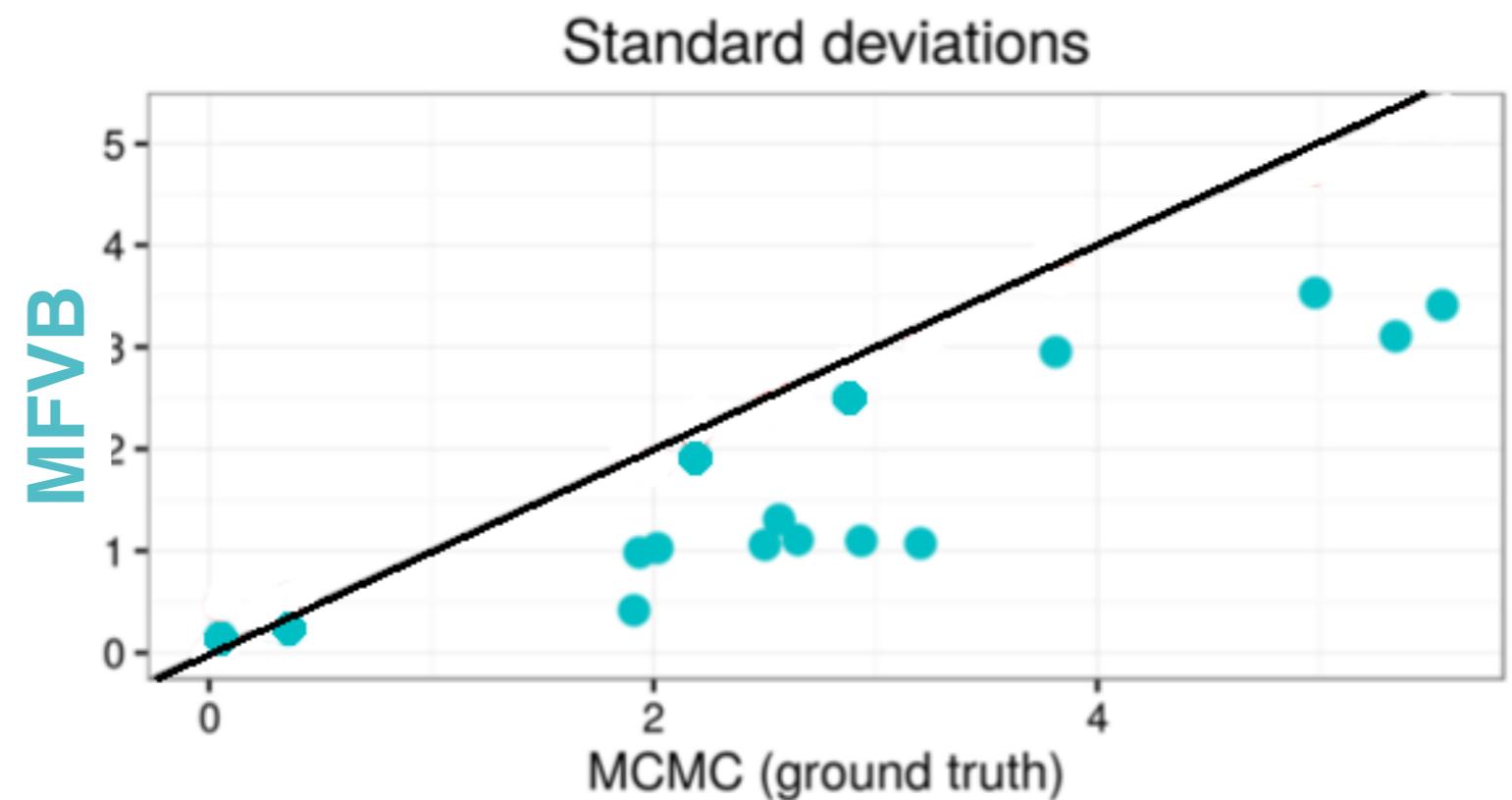
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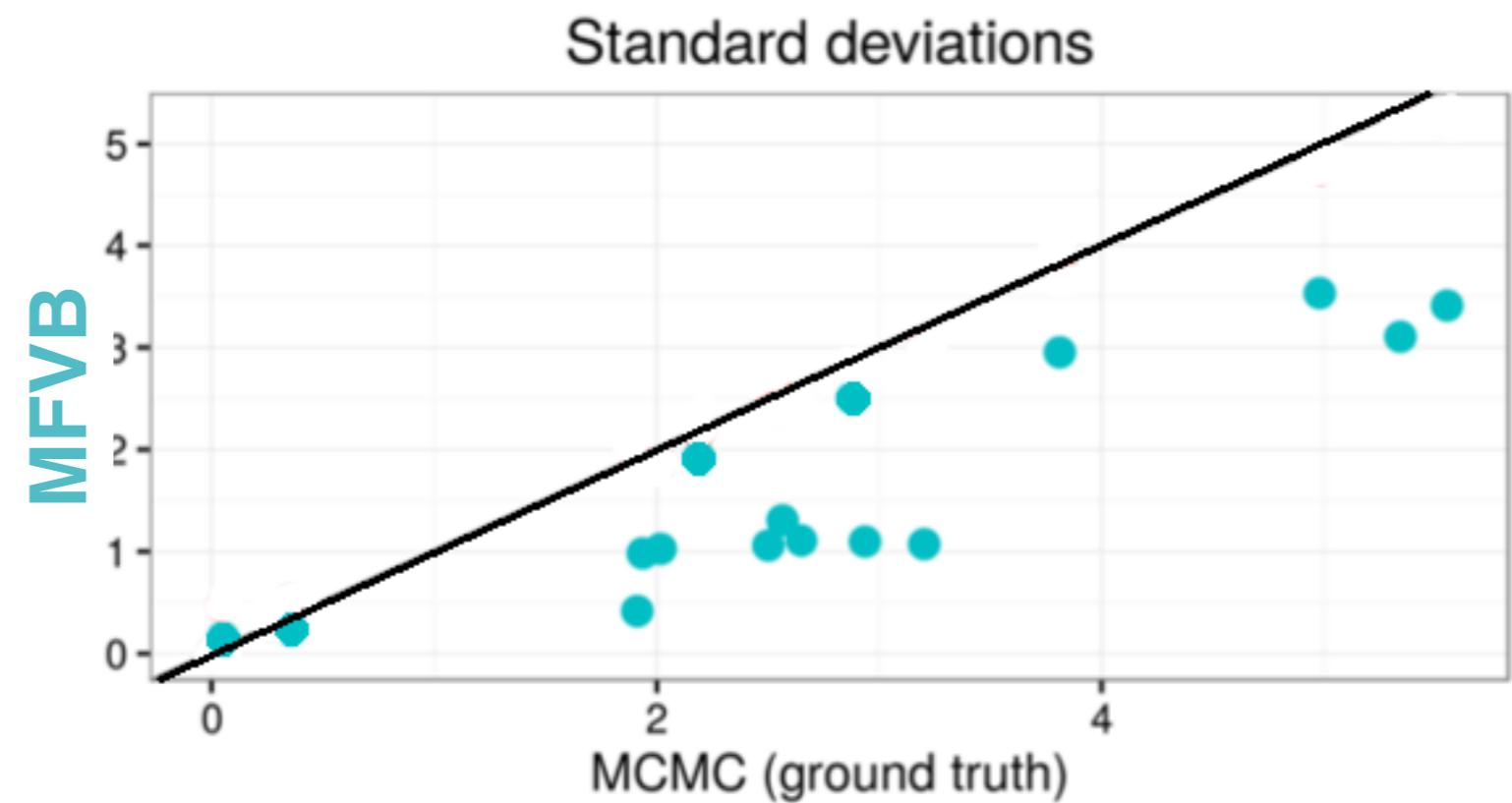
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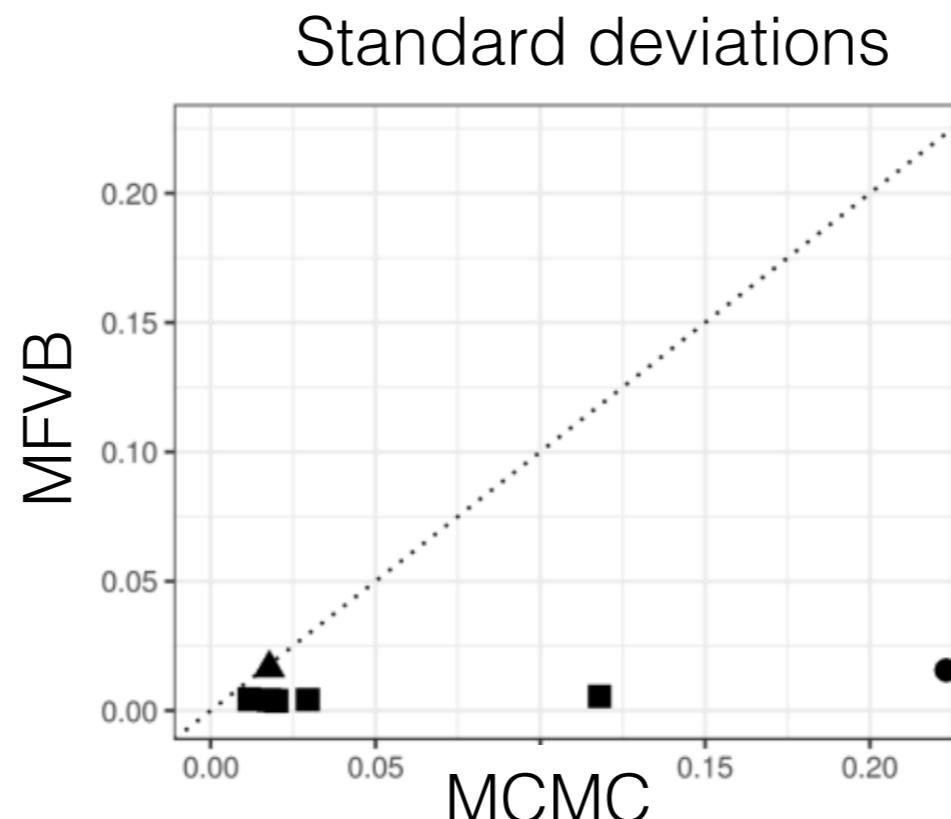


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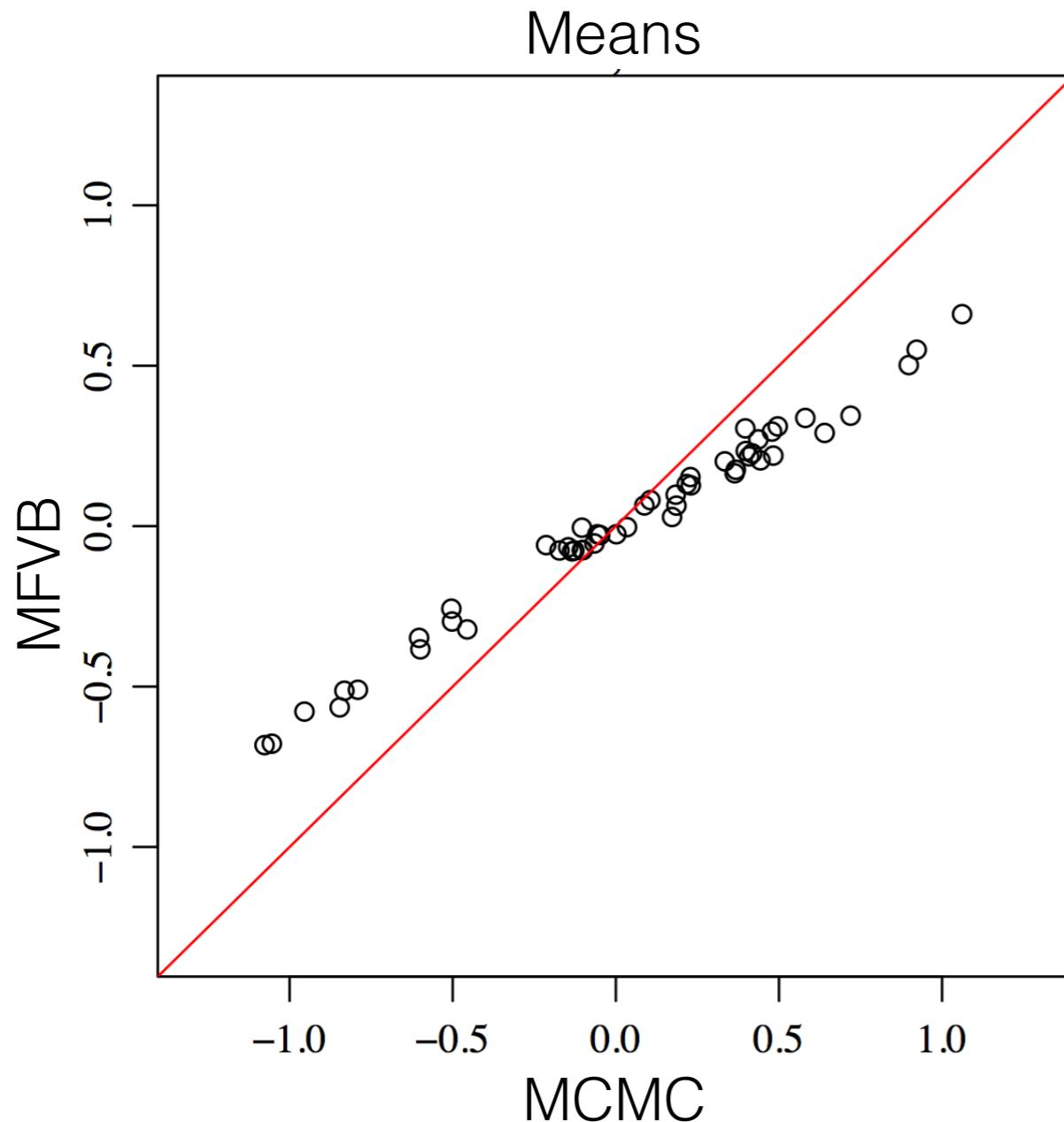


- Criteo
online ads
experiment



What about means?

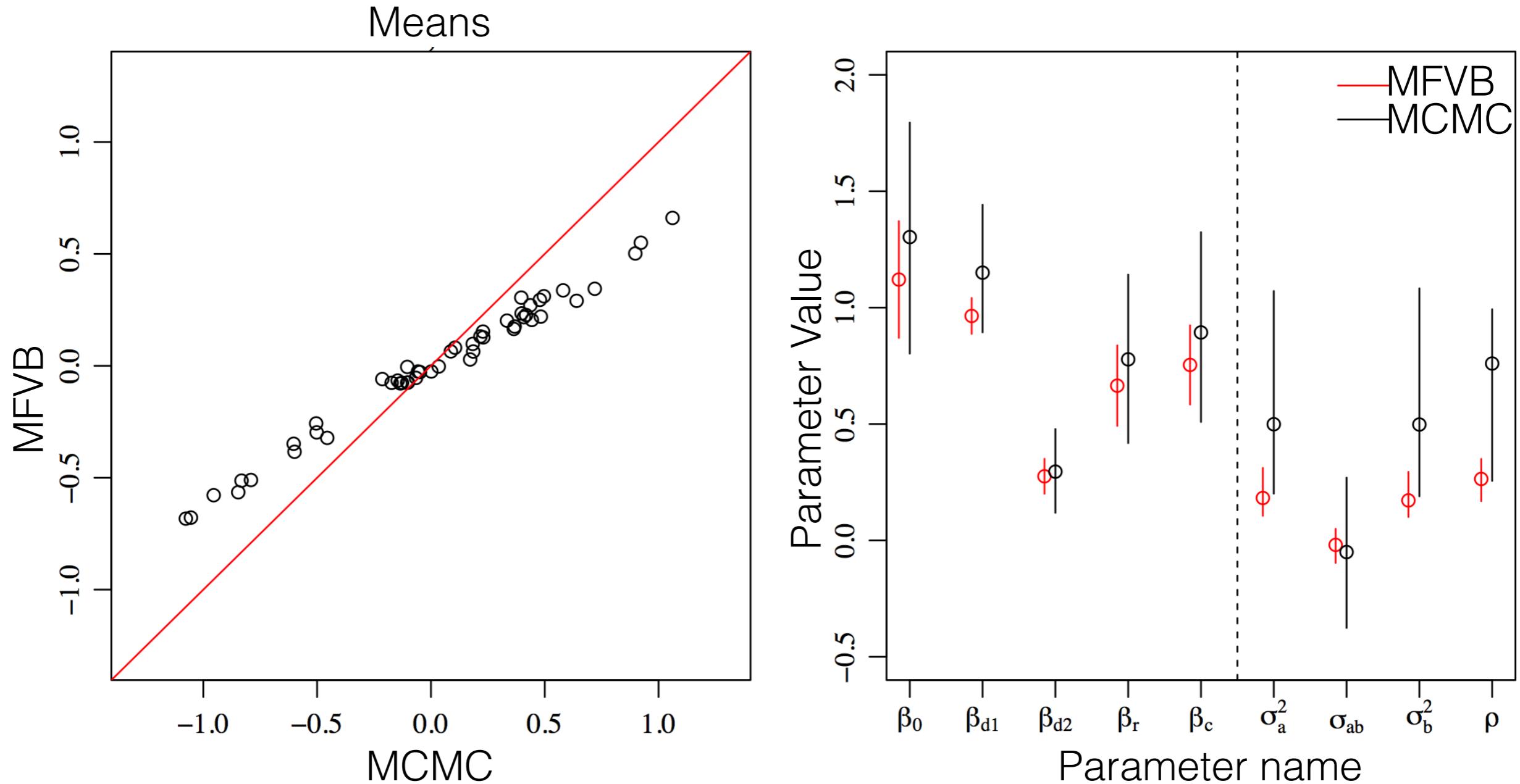
- Model for relational data with covariates
- When 1000+ nodes, MCMC > 1 day [Fosdick 2013, Ch 4]



[Fosdick 2013, Ch 4, Fig 4.3]

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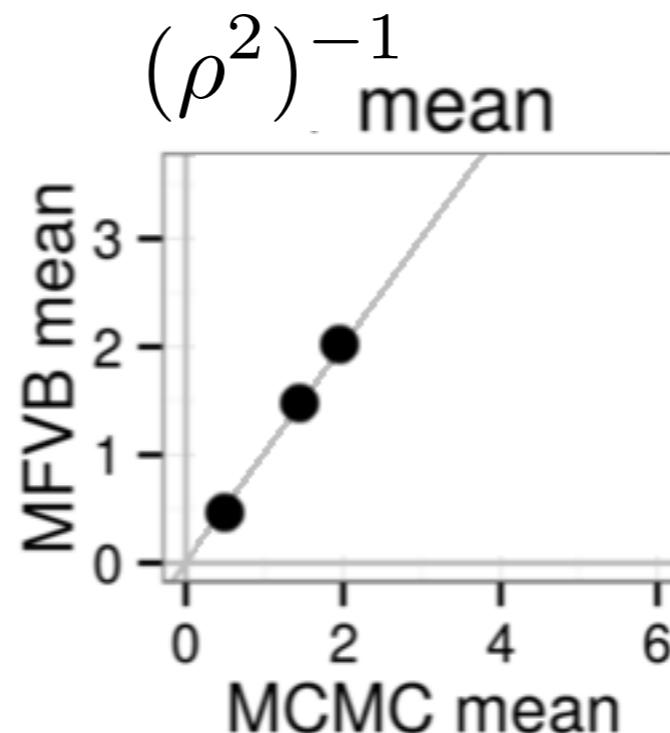
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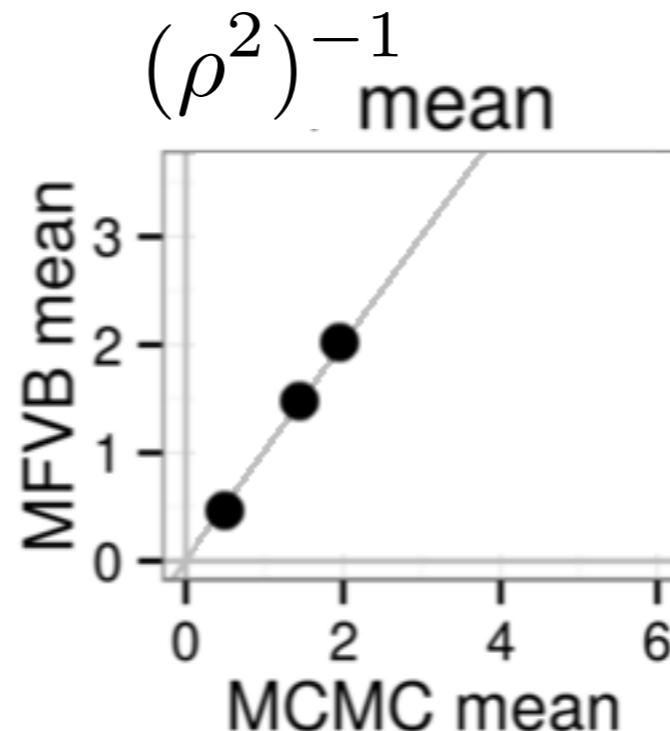
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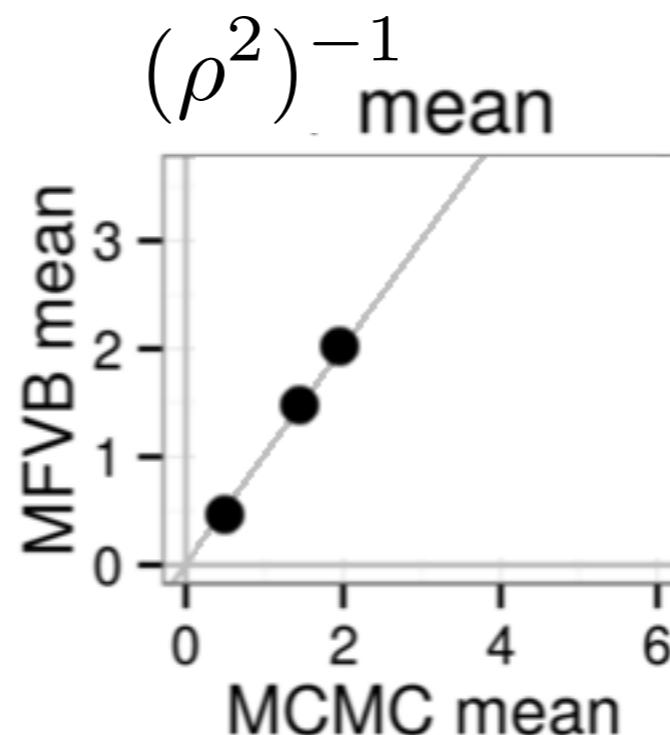
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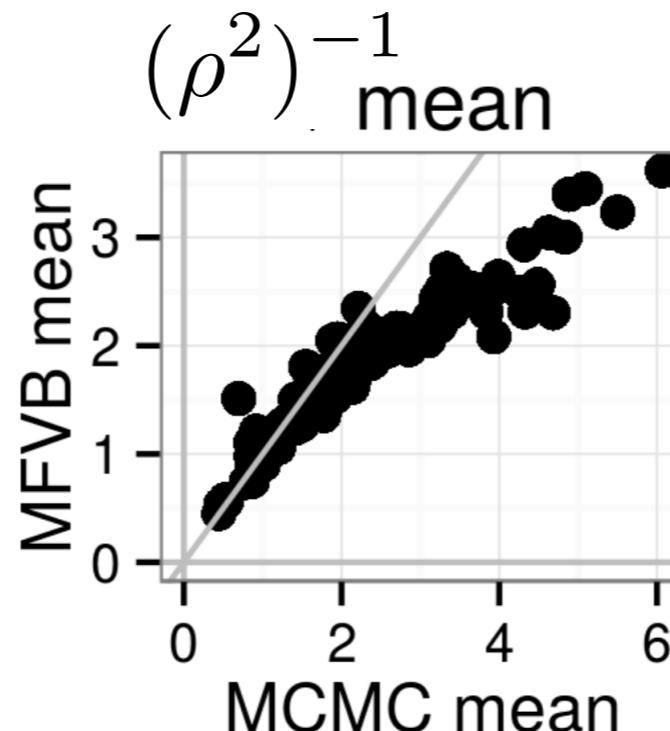
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Approximate Bayesian inference

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

Optimization

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

Variational Bayes

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

Mean-field variational Bayes

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**How
deep is
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issue?**

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

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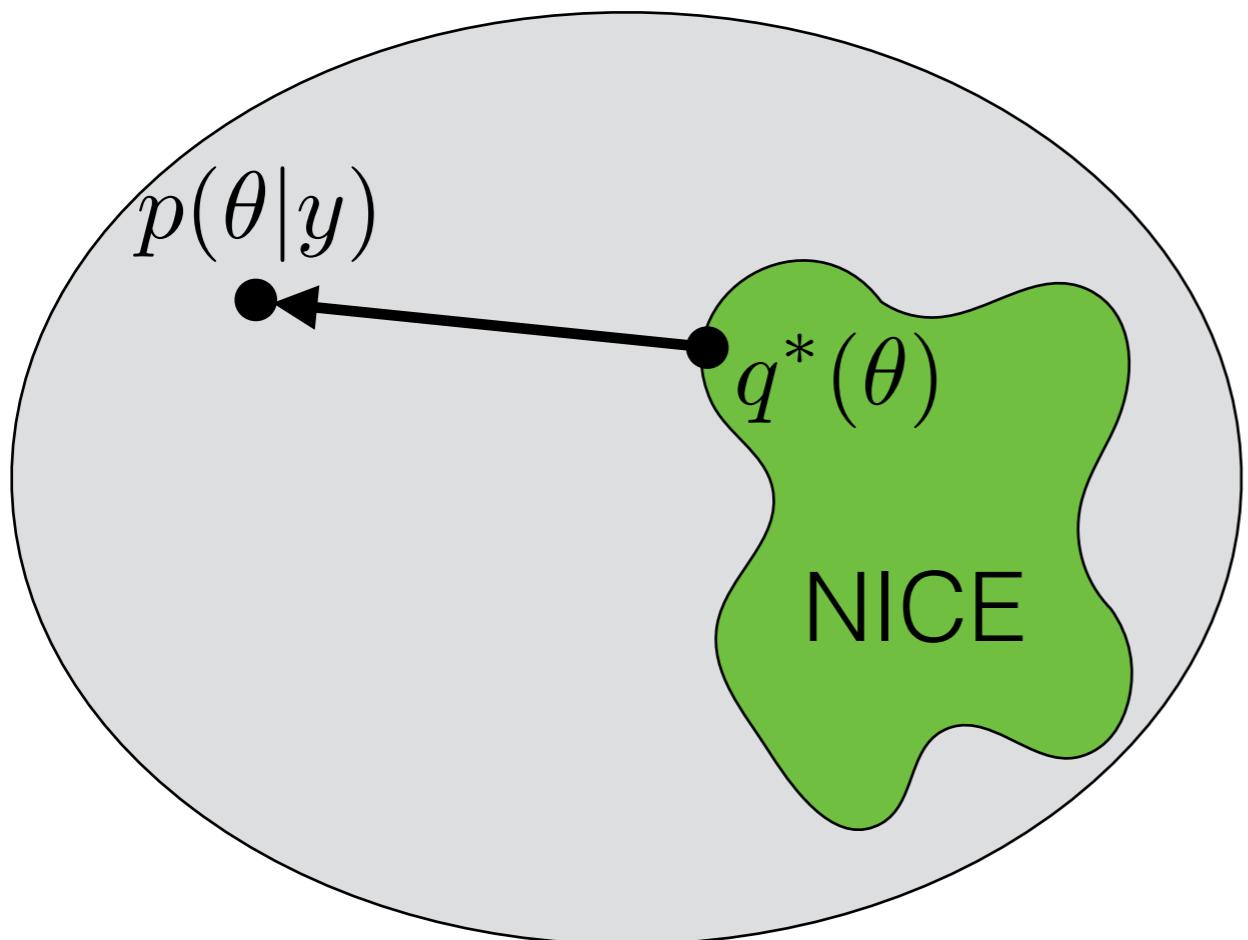
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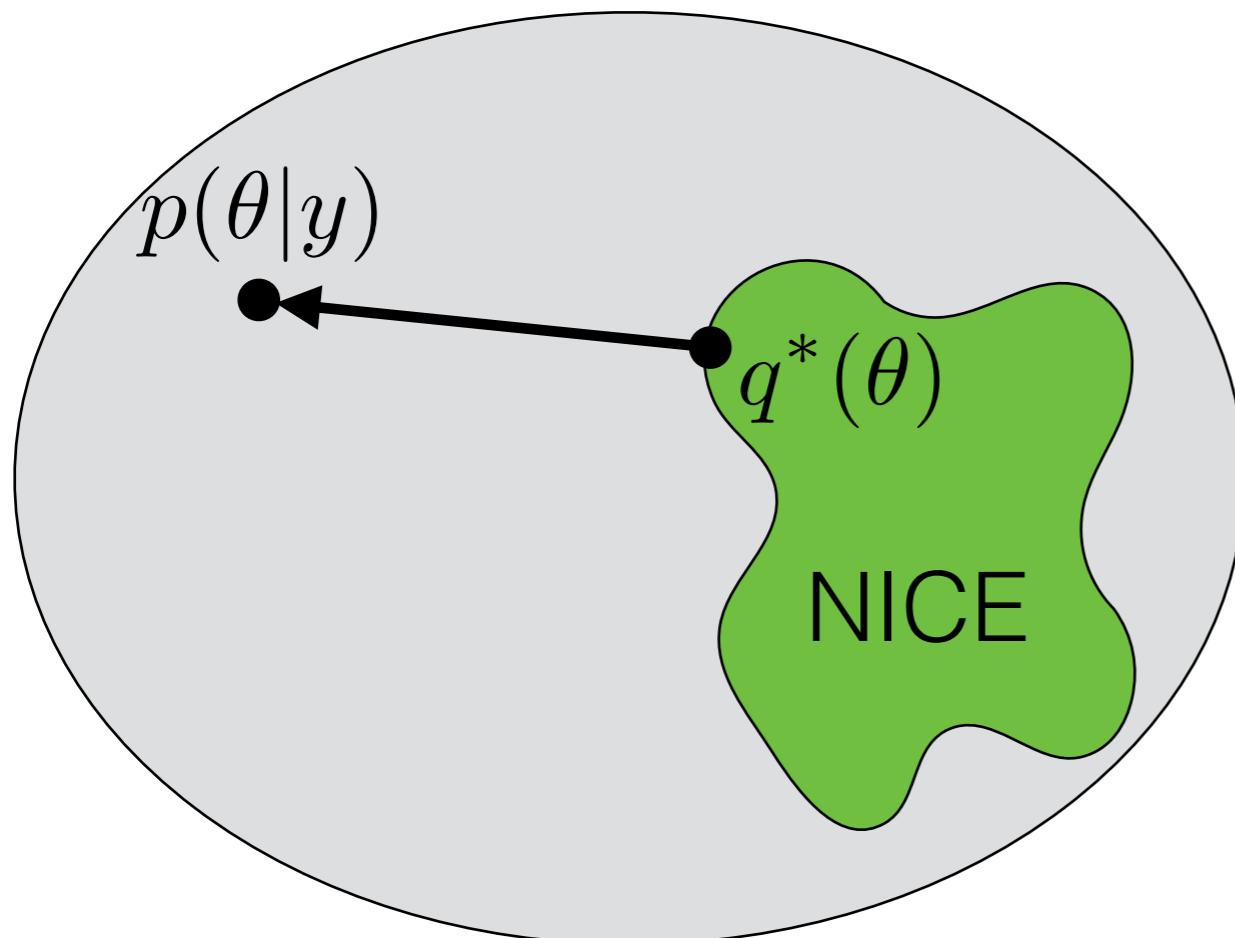
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Is it just MFVB?

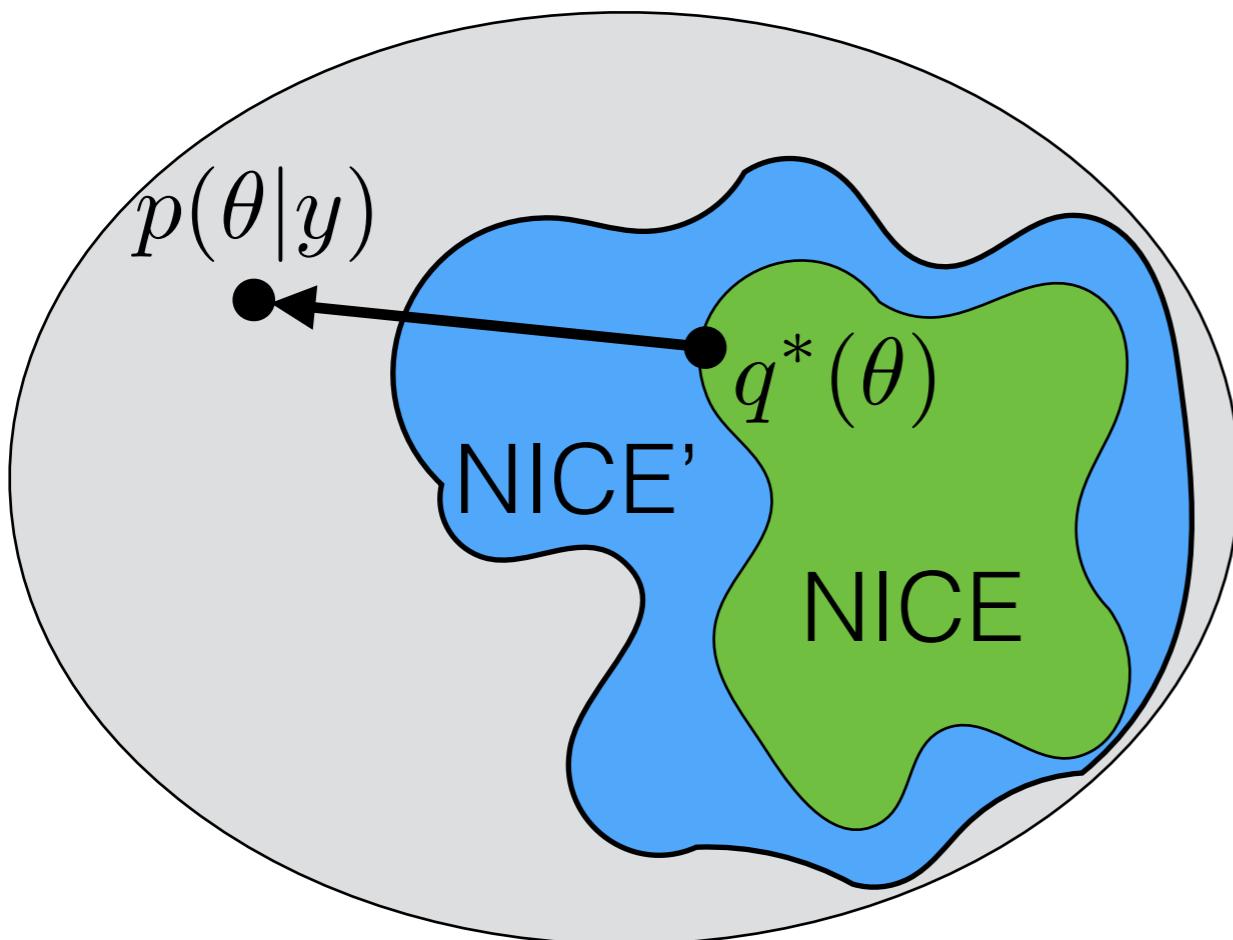


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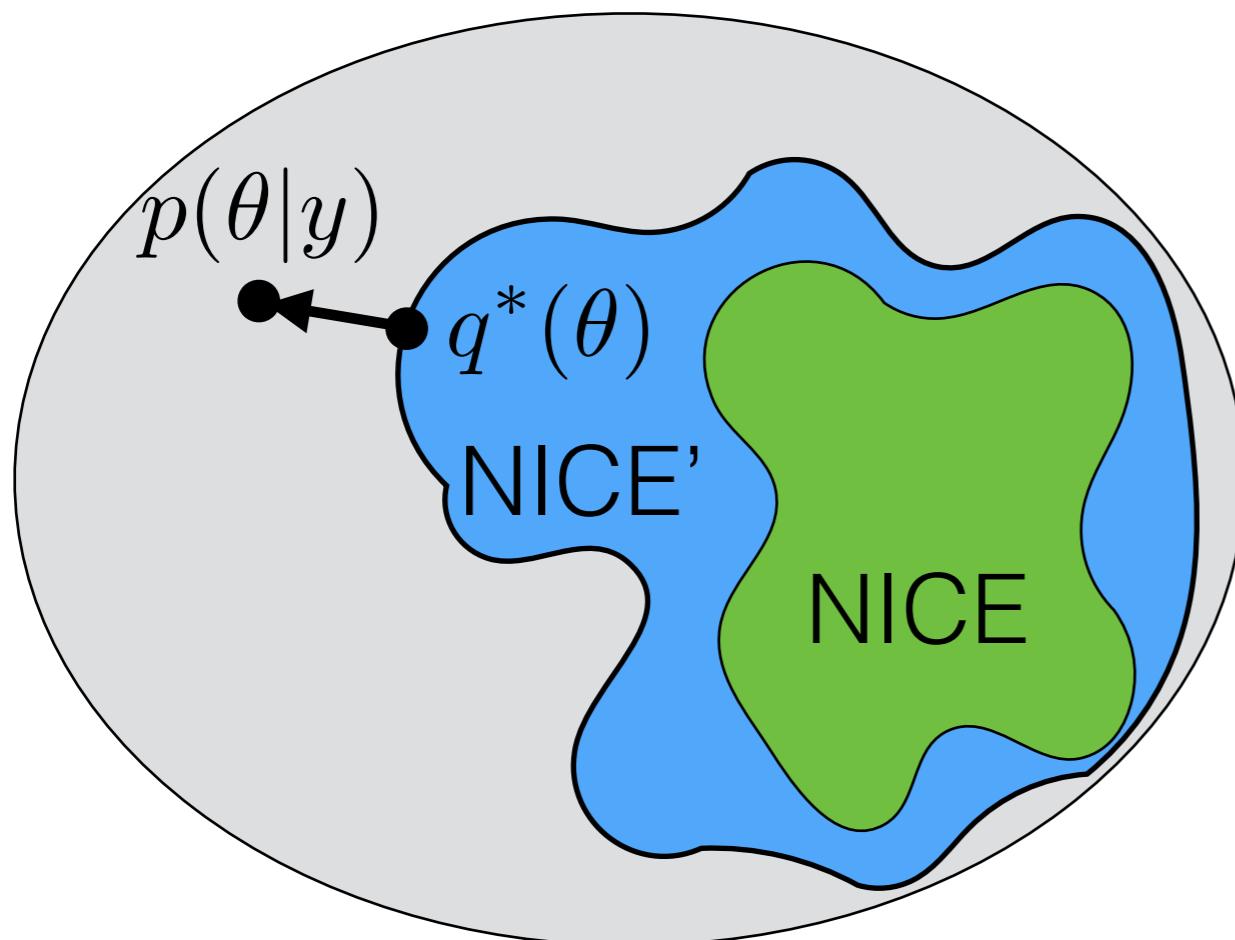
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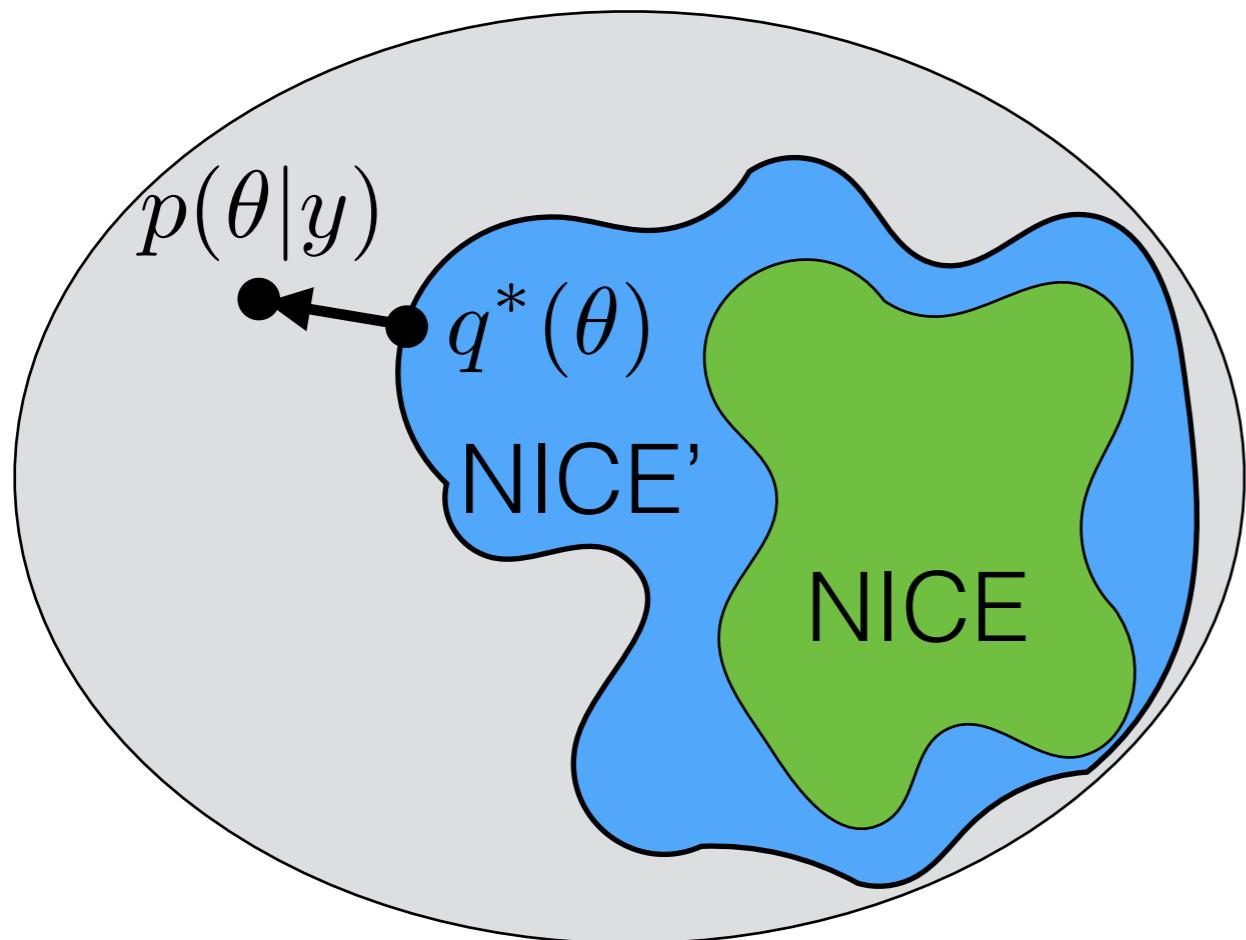
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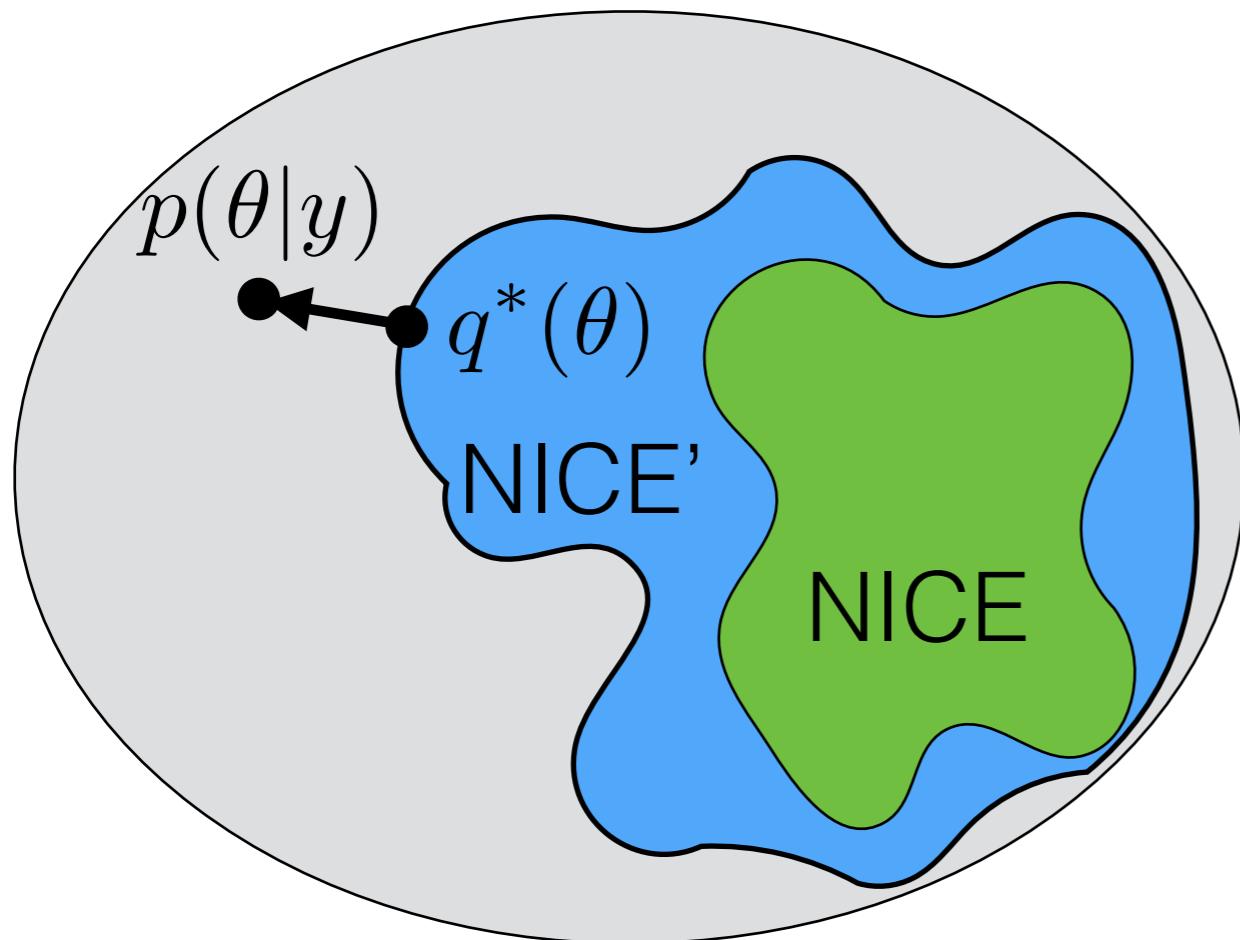
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- Exercise: Show, with a simple example, that a smaller KL does not imply better mean and variance estimates
- But how much worse can the estimates be? And could it have just been the implementation?

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- Some KL values seen in practice:
~1 to ~70, 0.5 to 3

[Baqué et al 2017;
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Proposition. Can have
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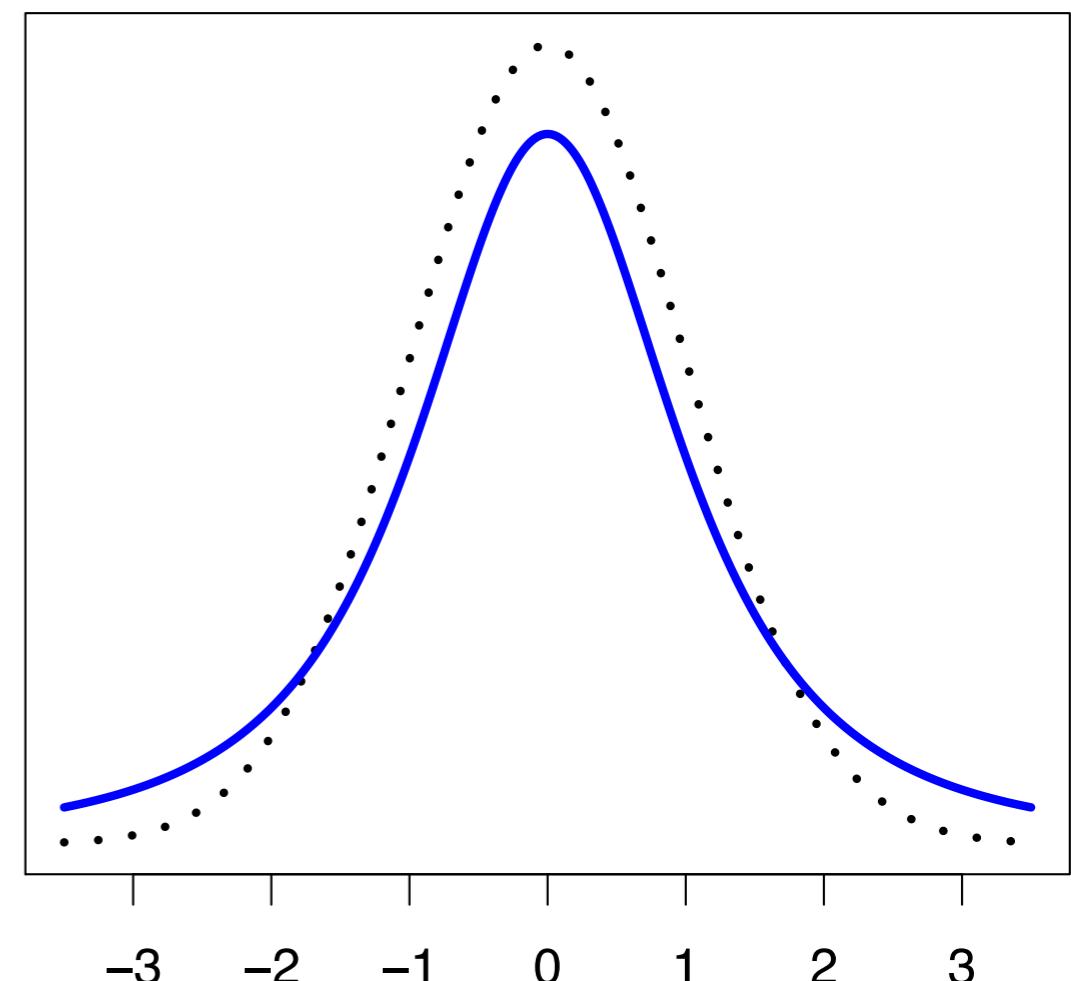
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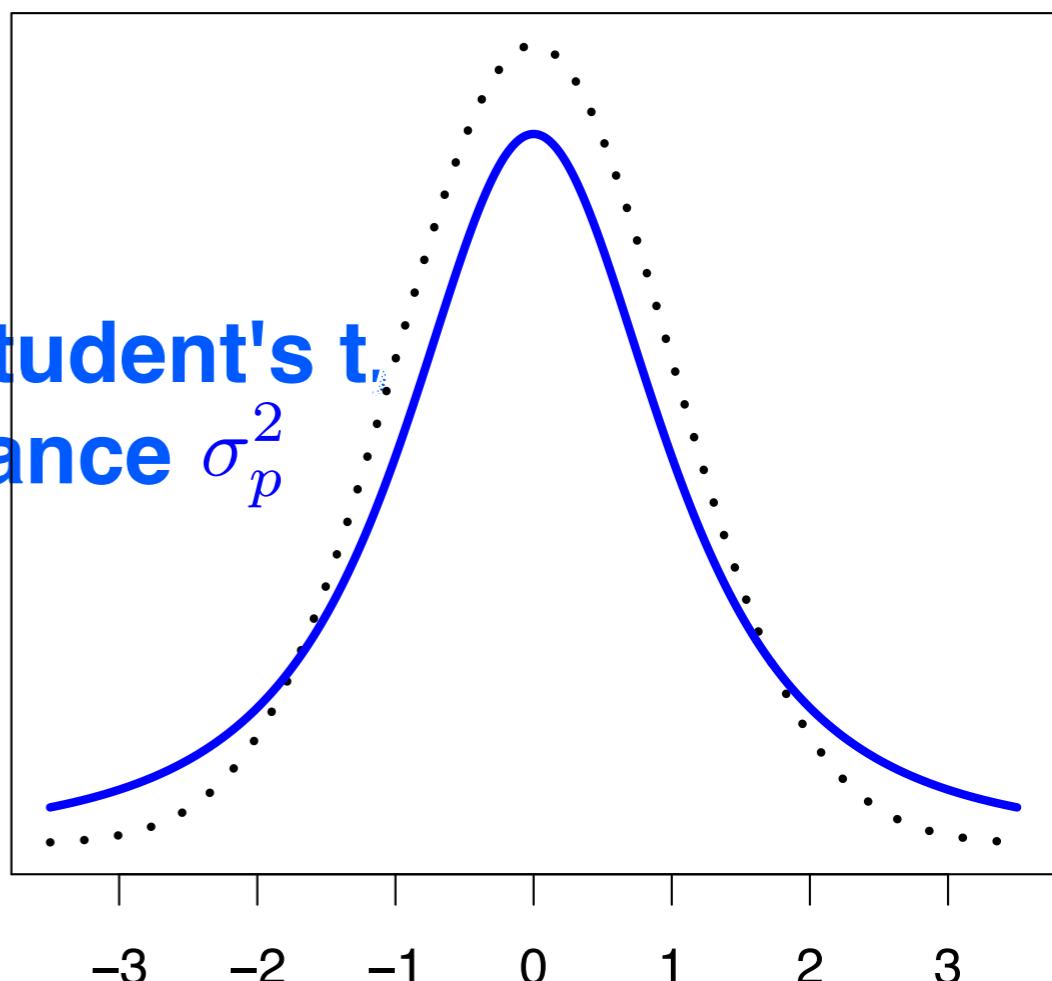
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**p : Student's t.
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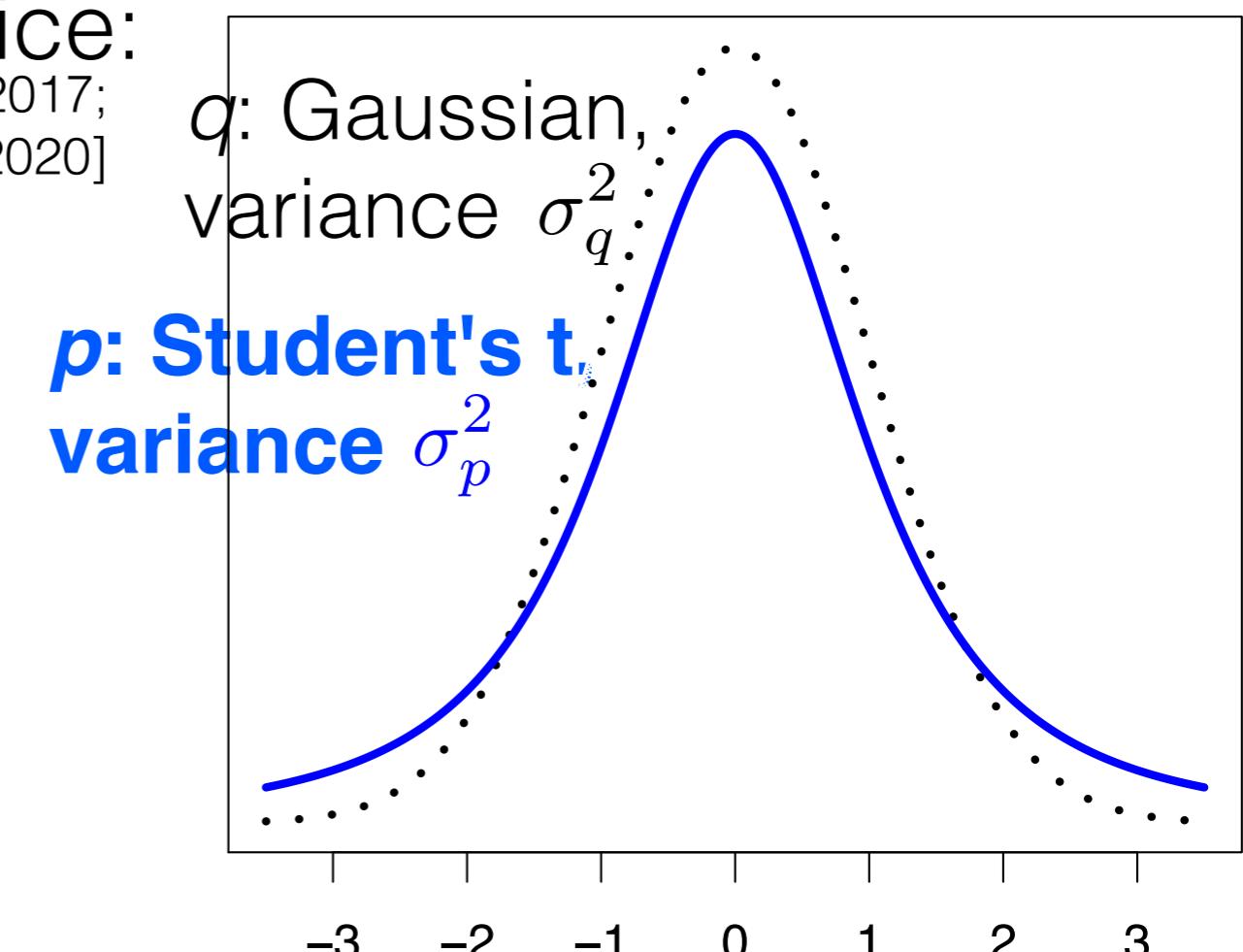


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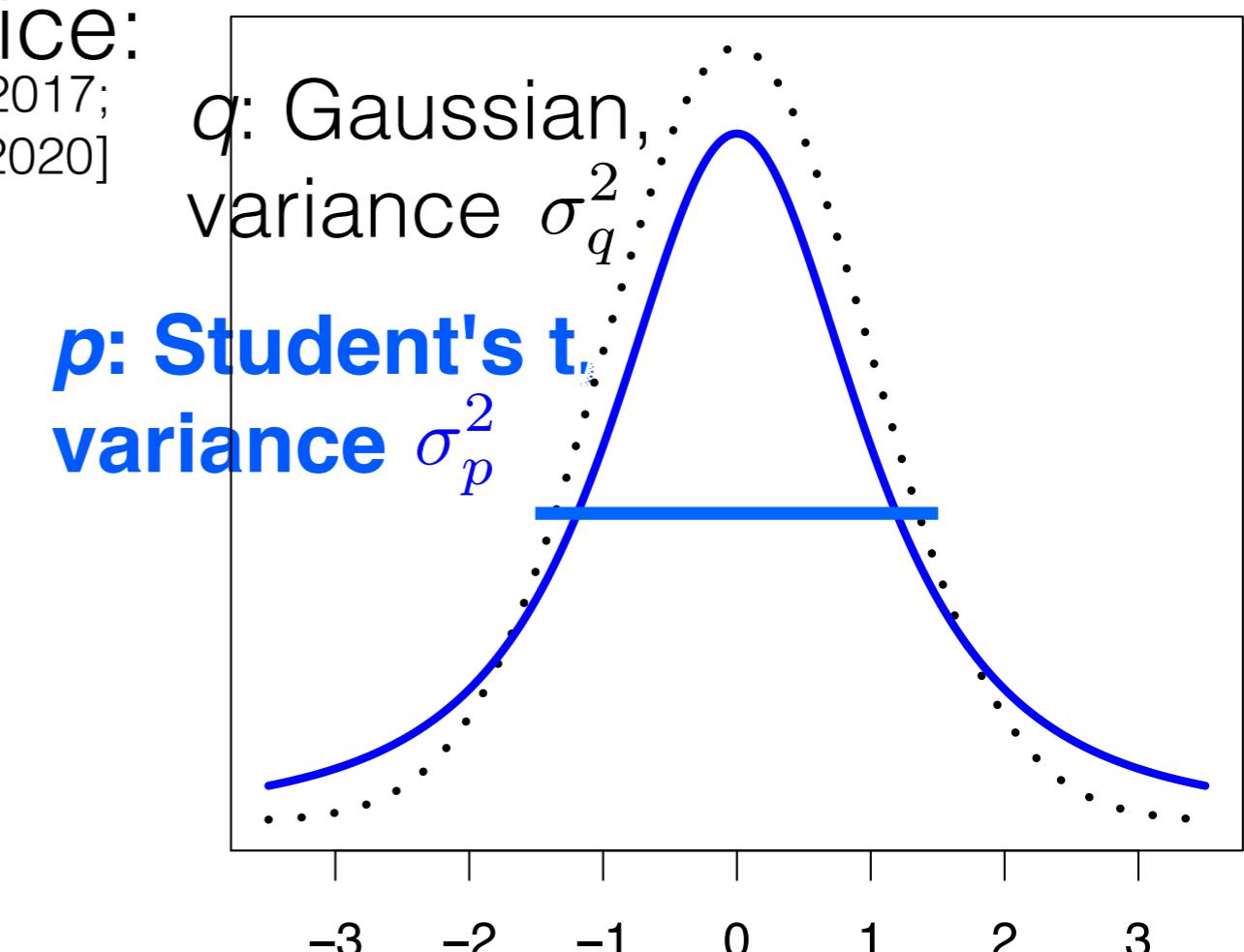


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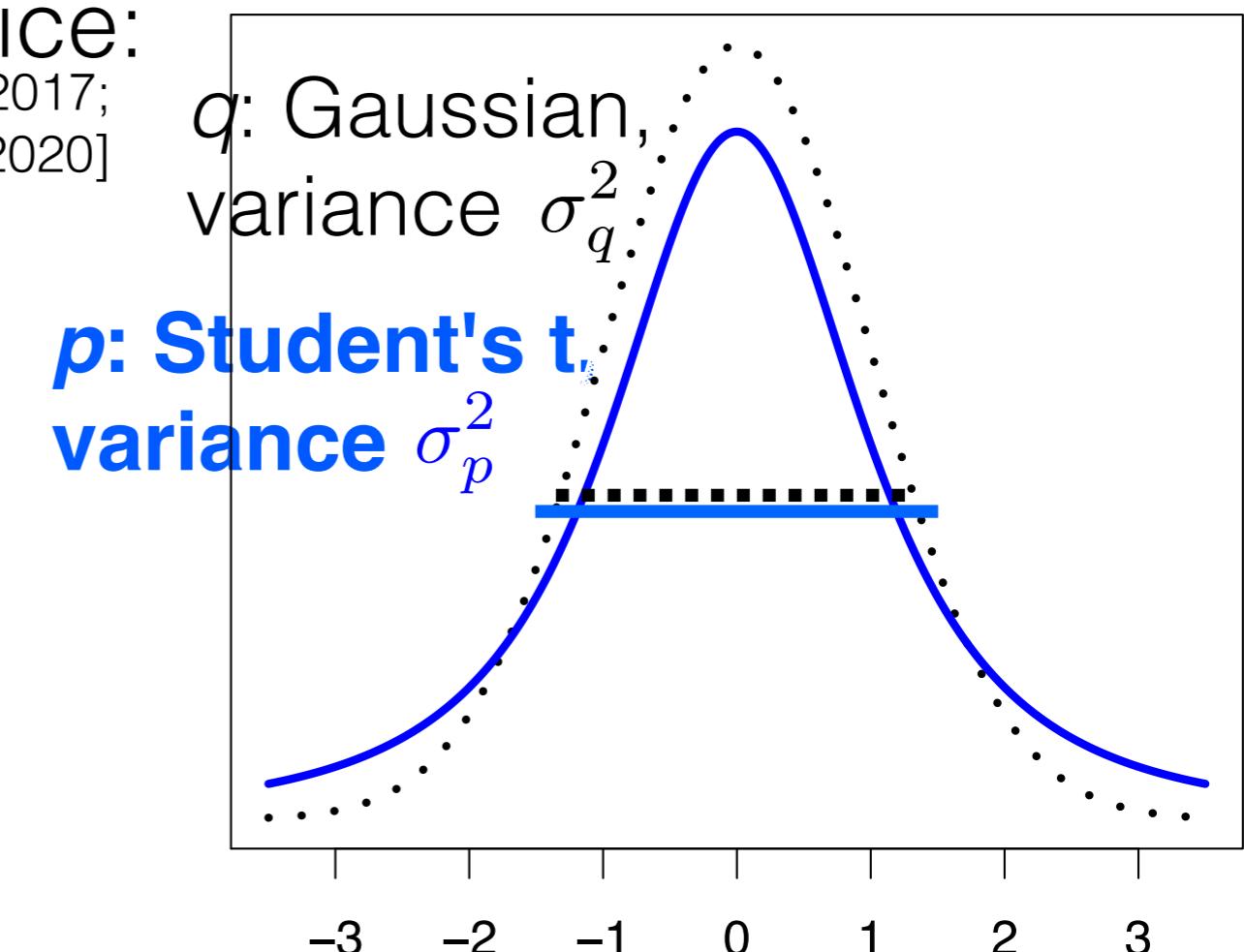


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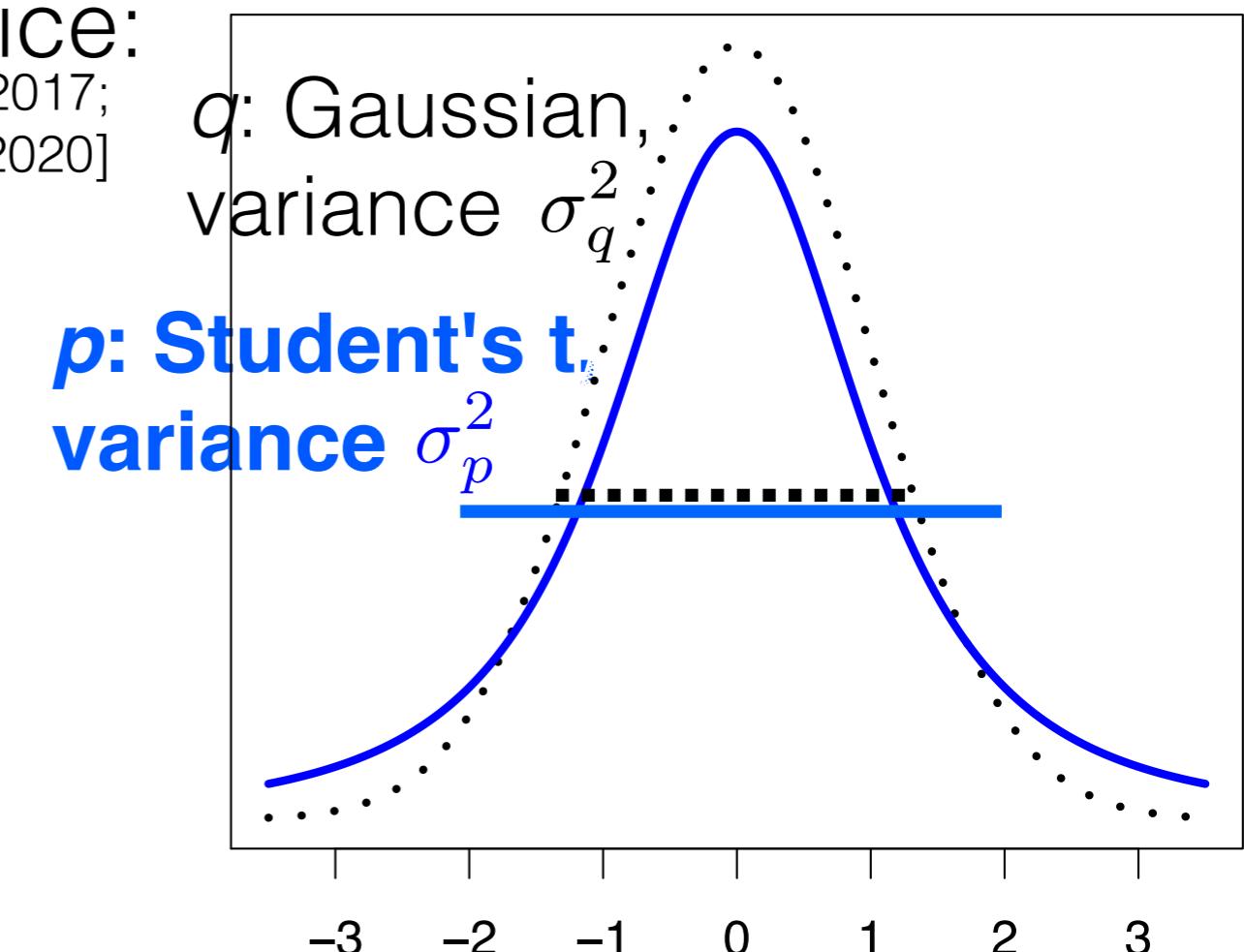


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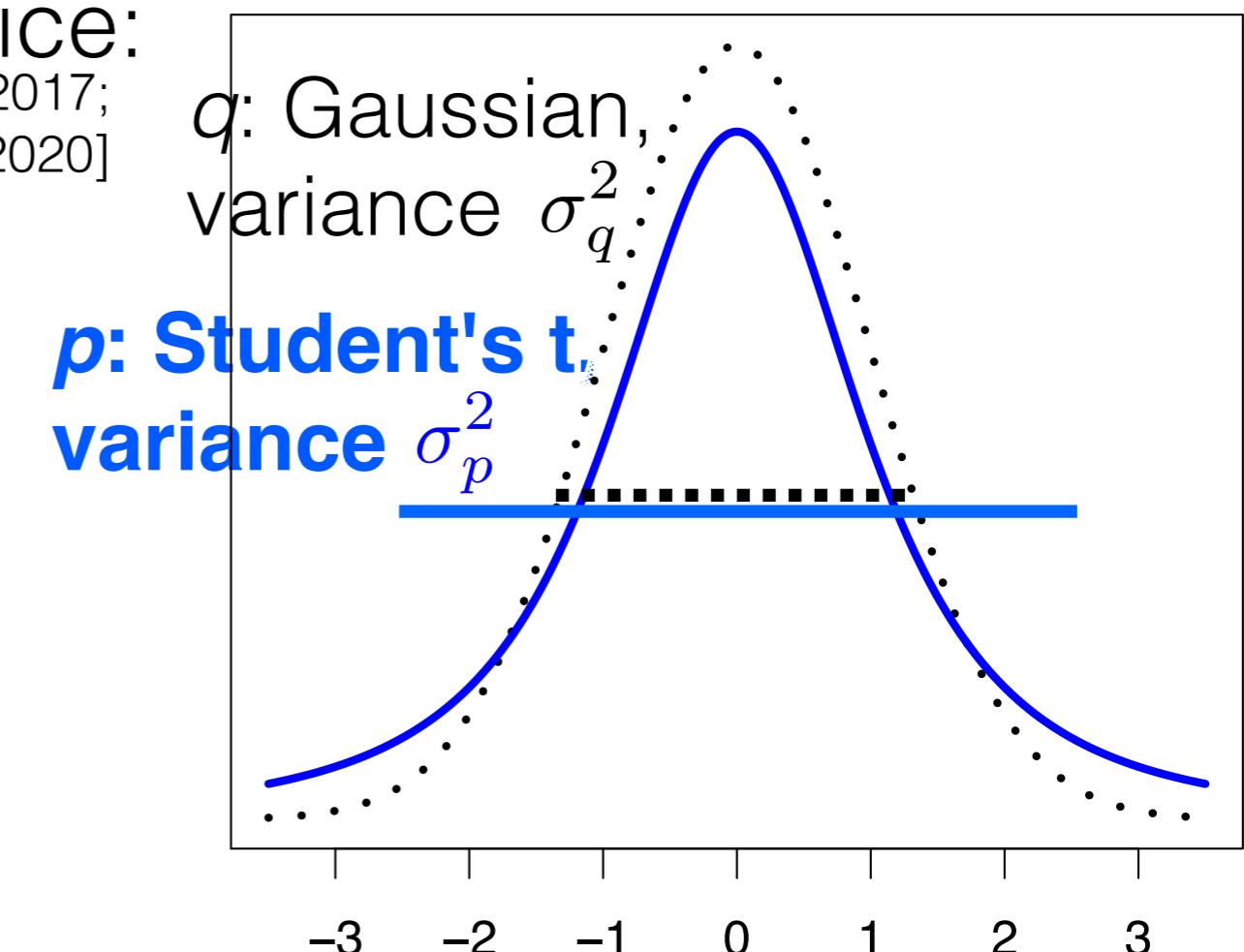


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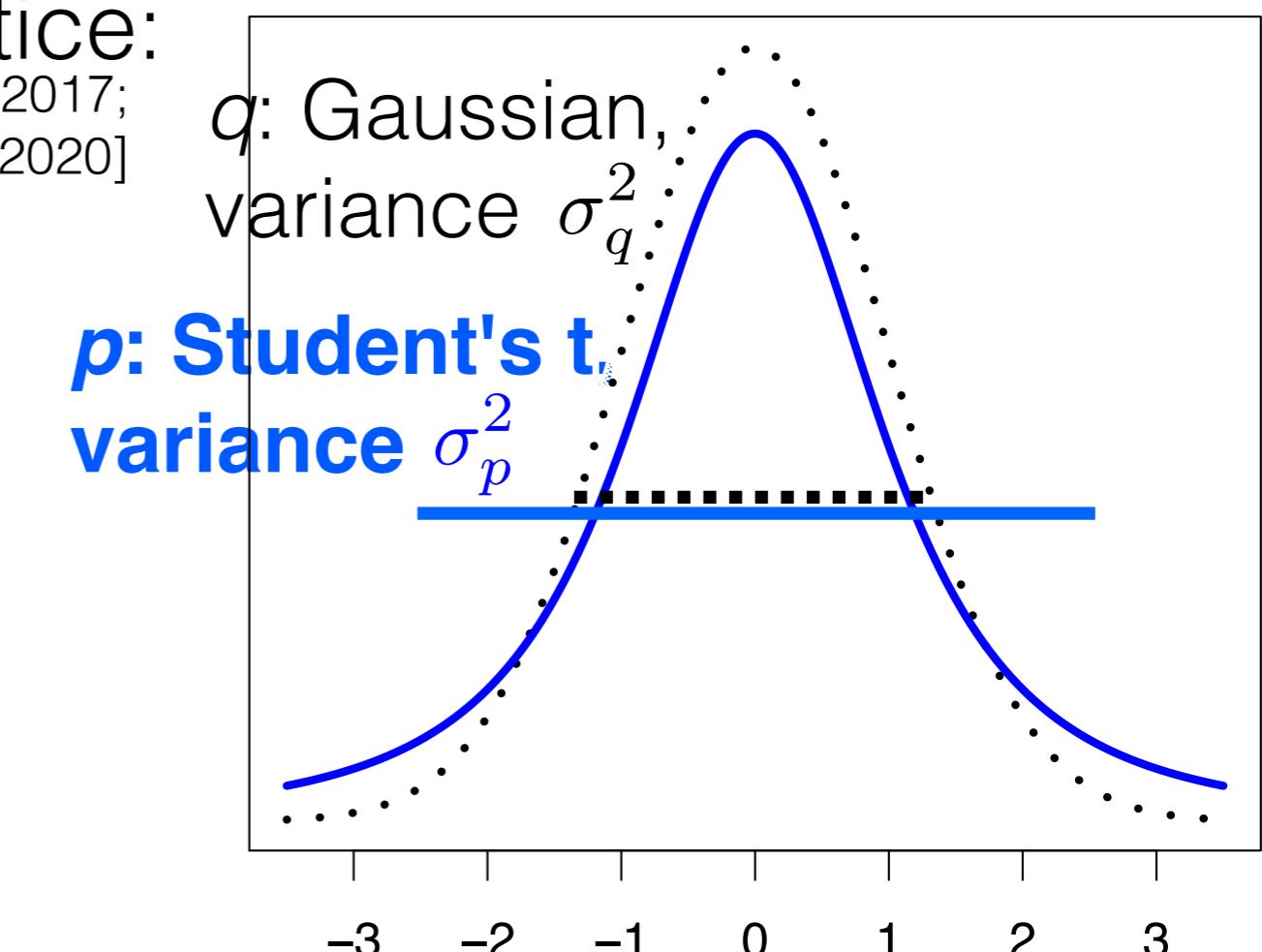


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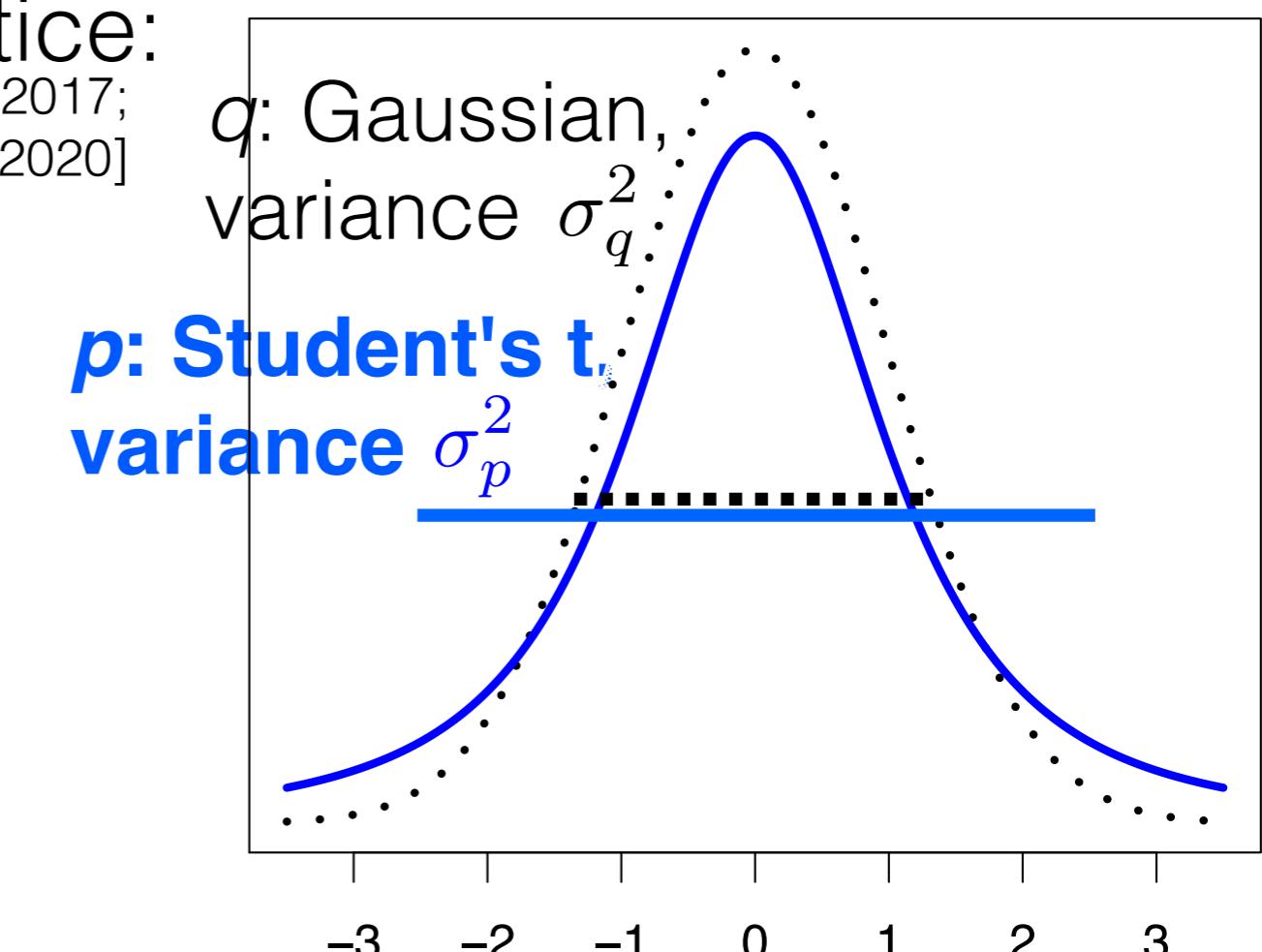
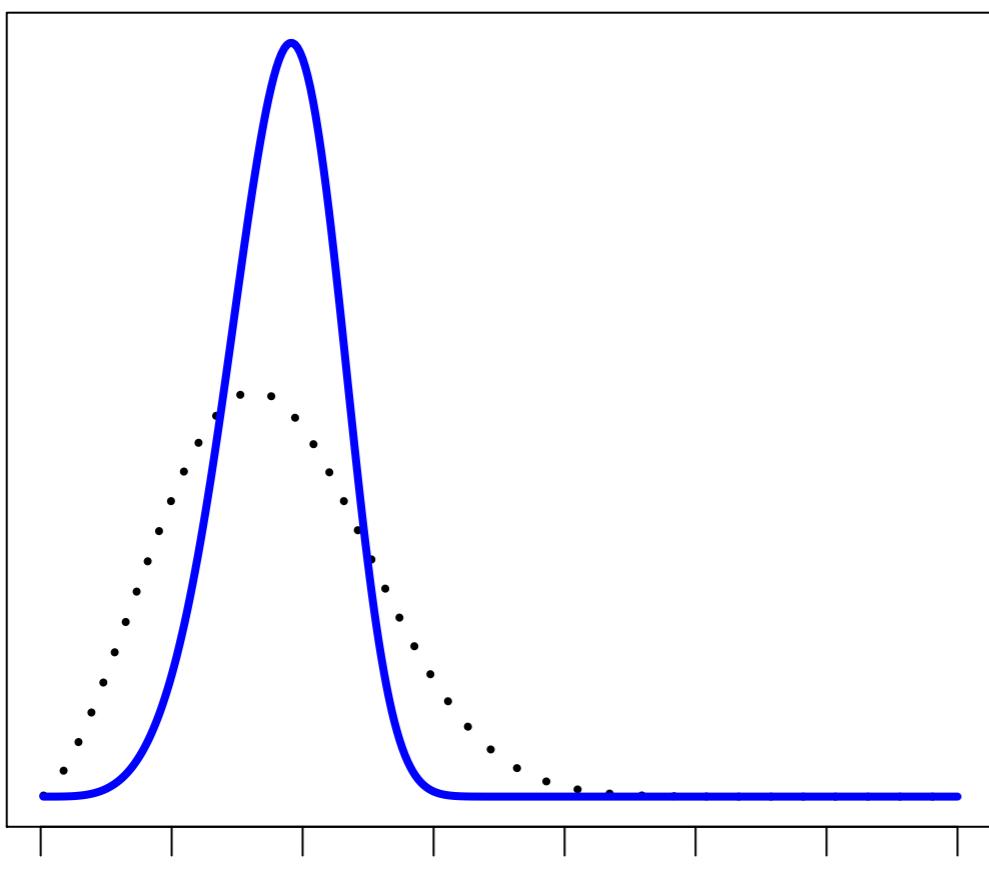
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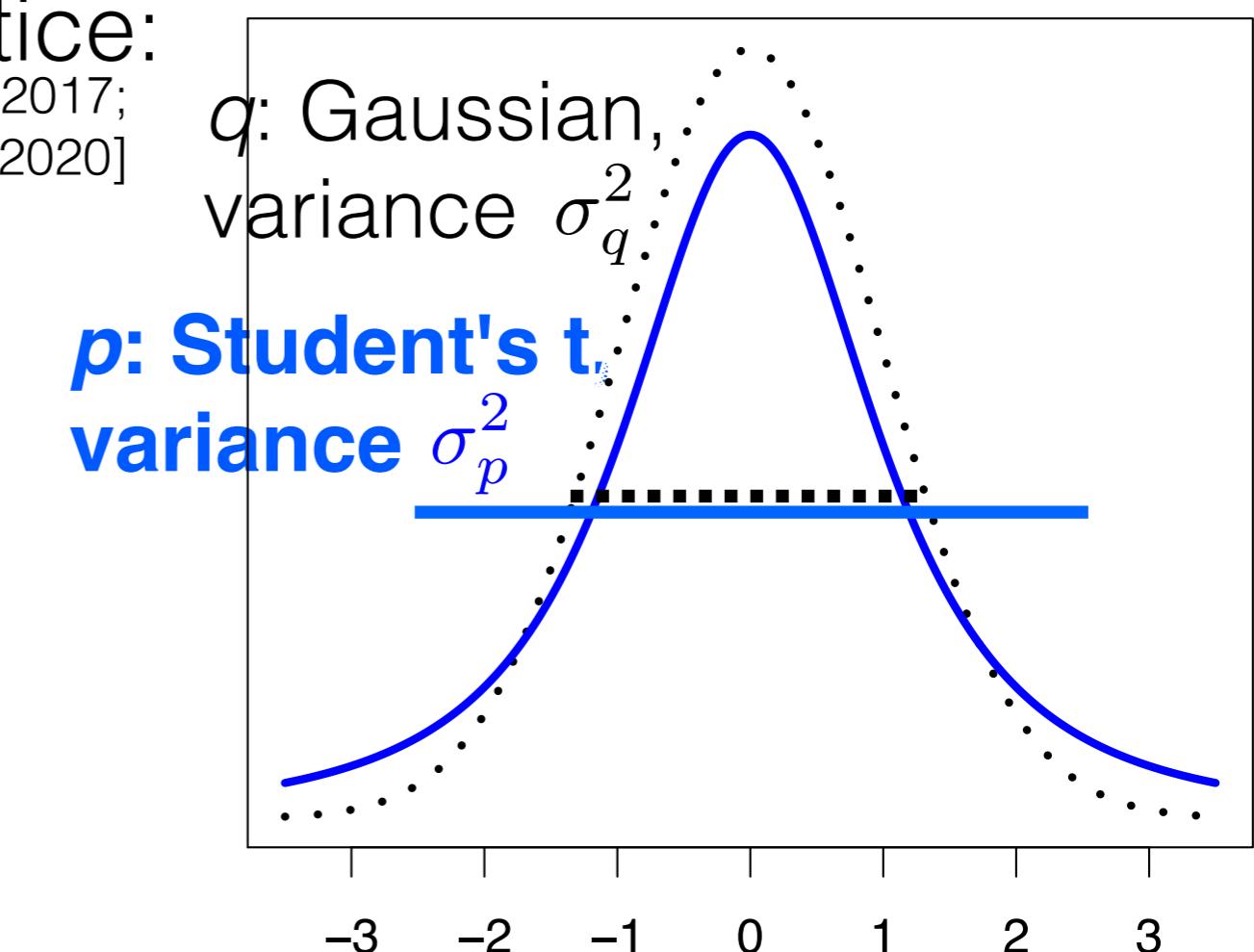
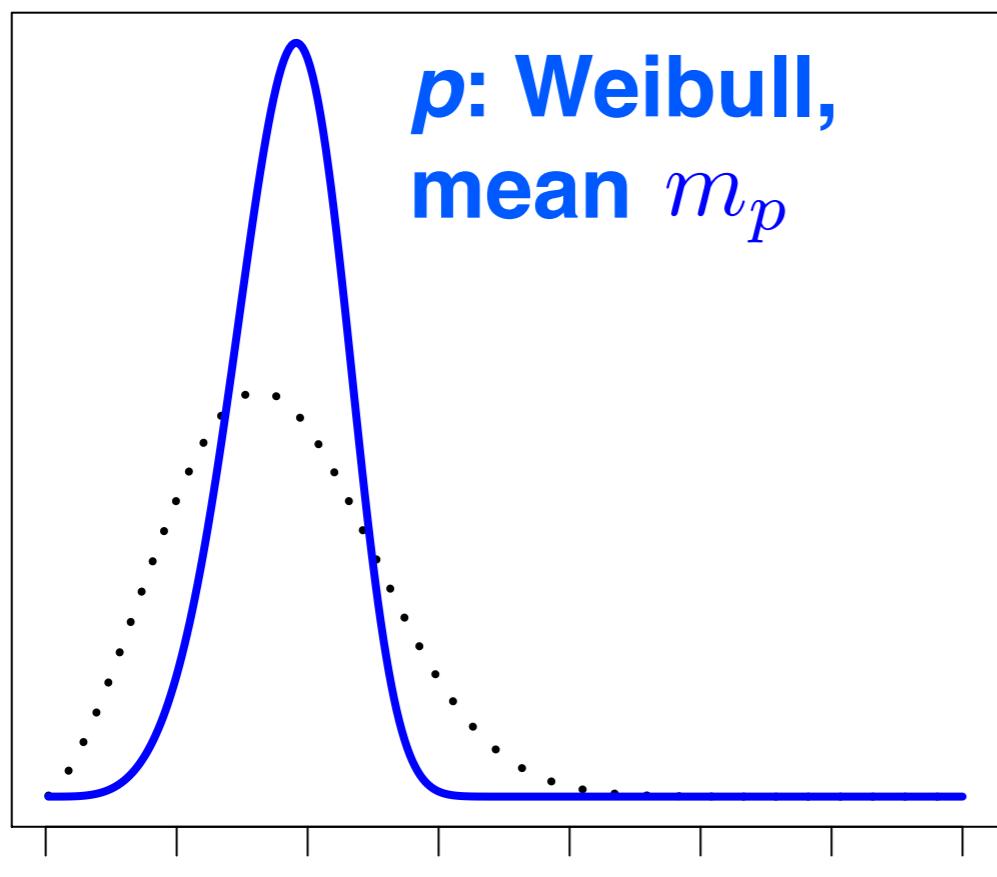
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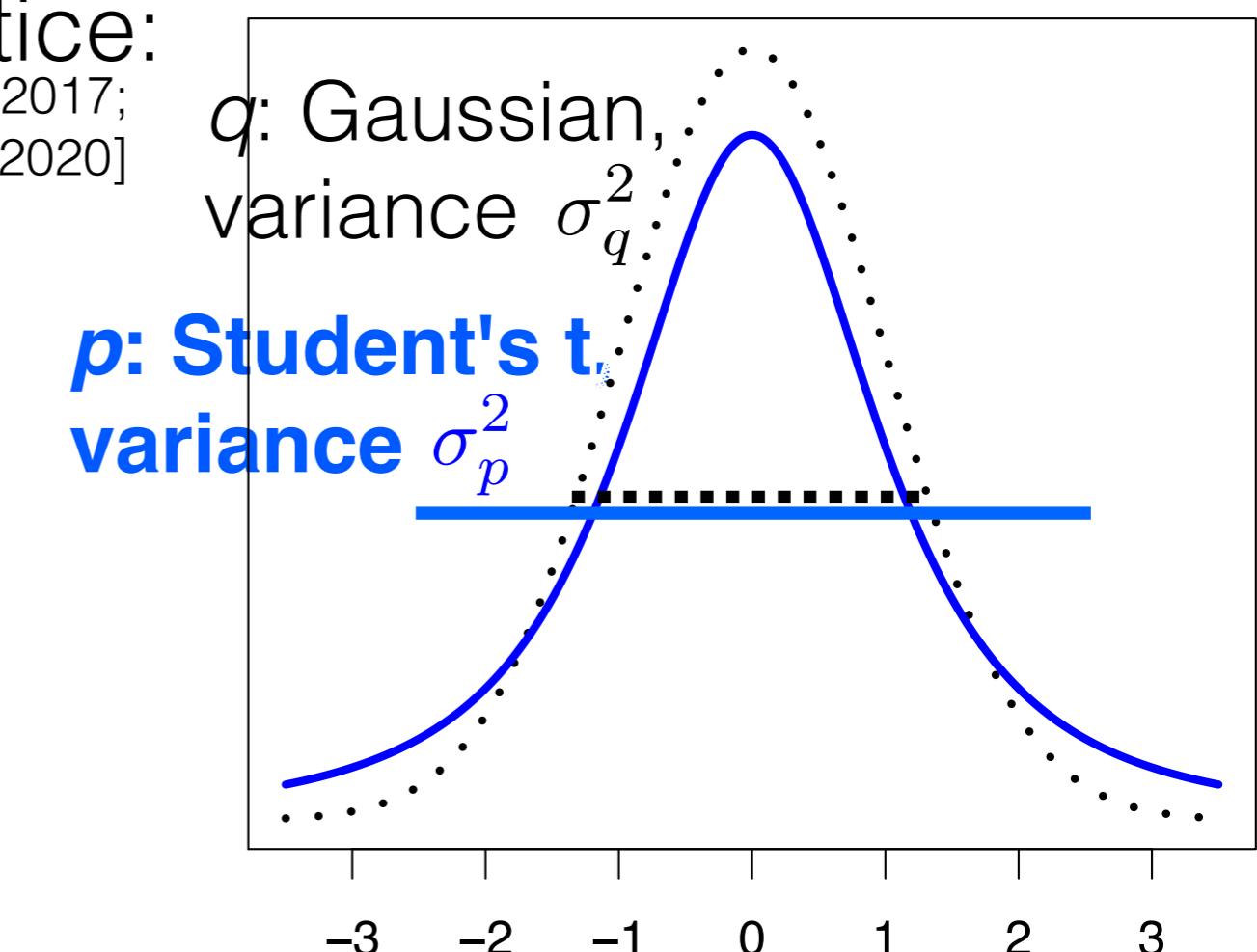
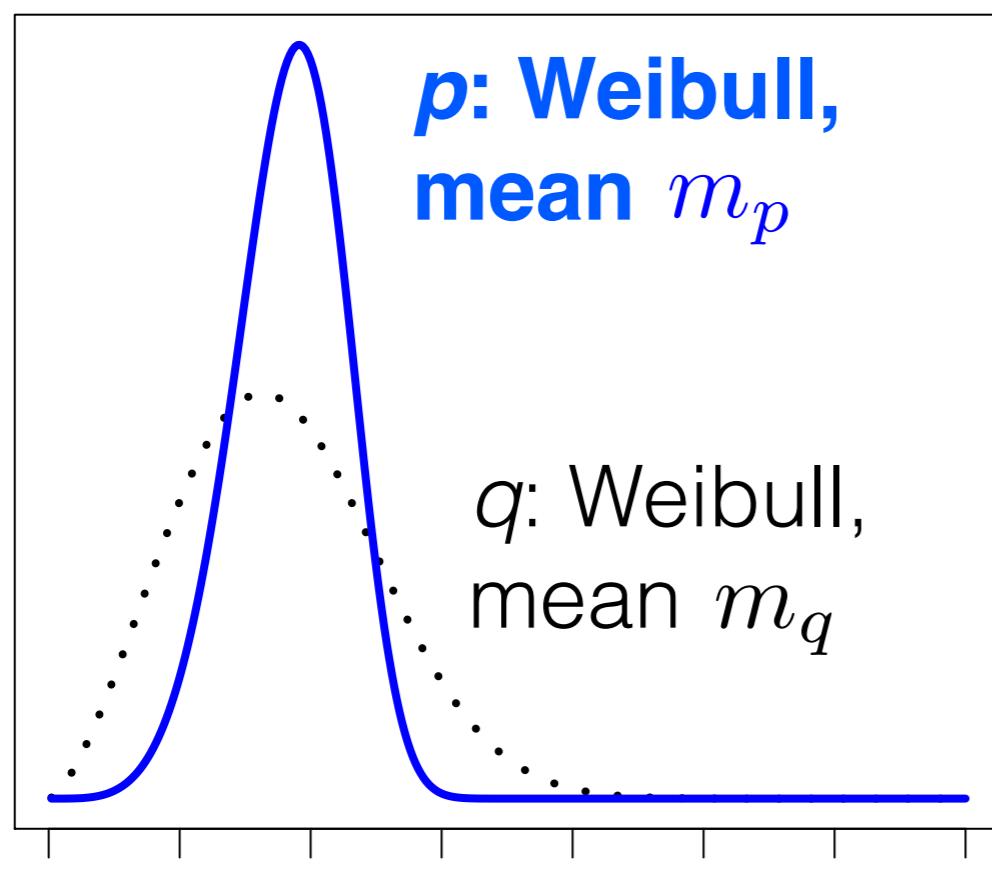
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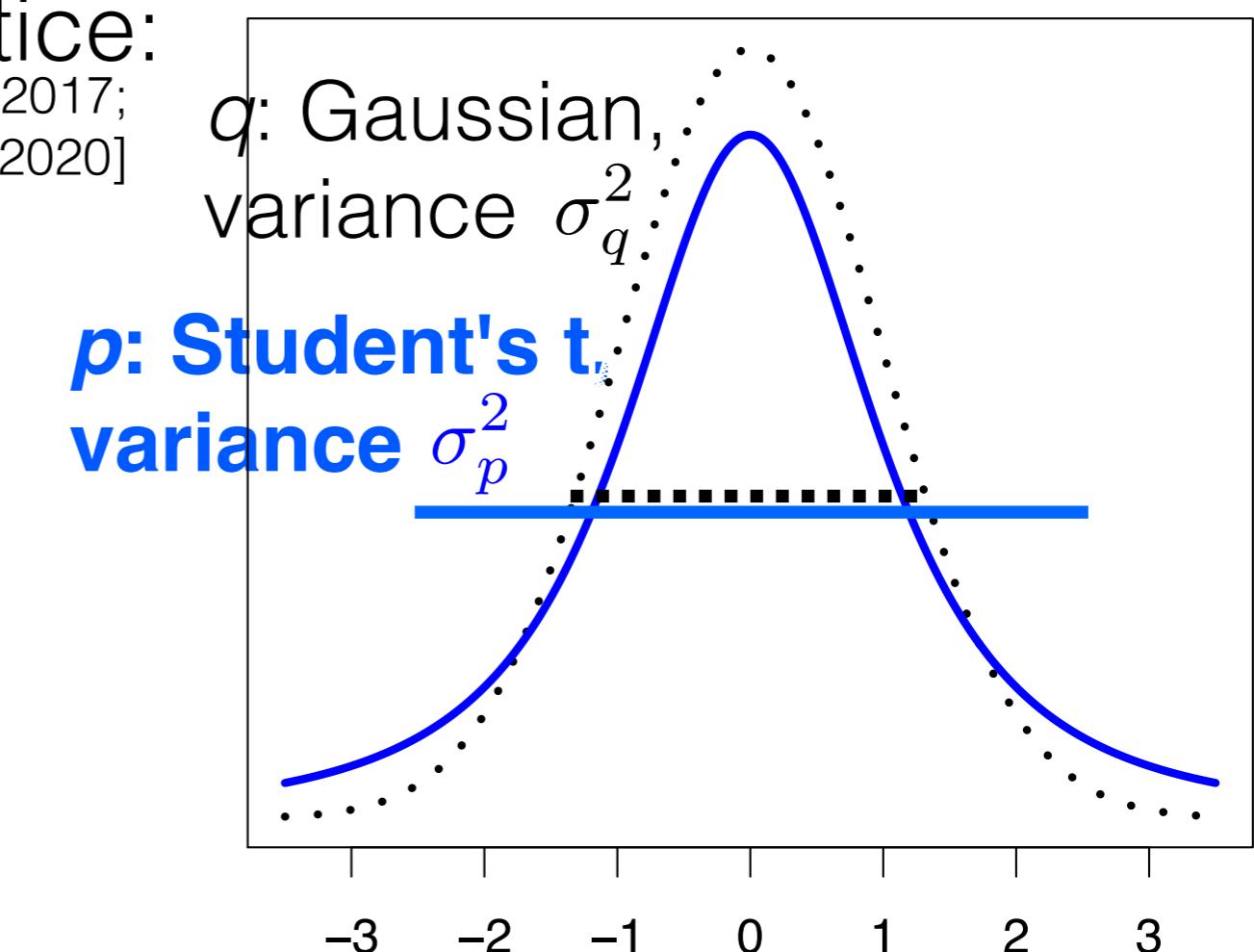
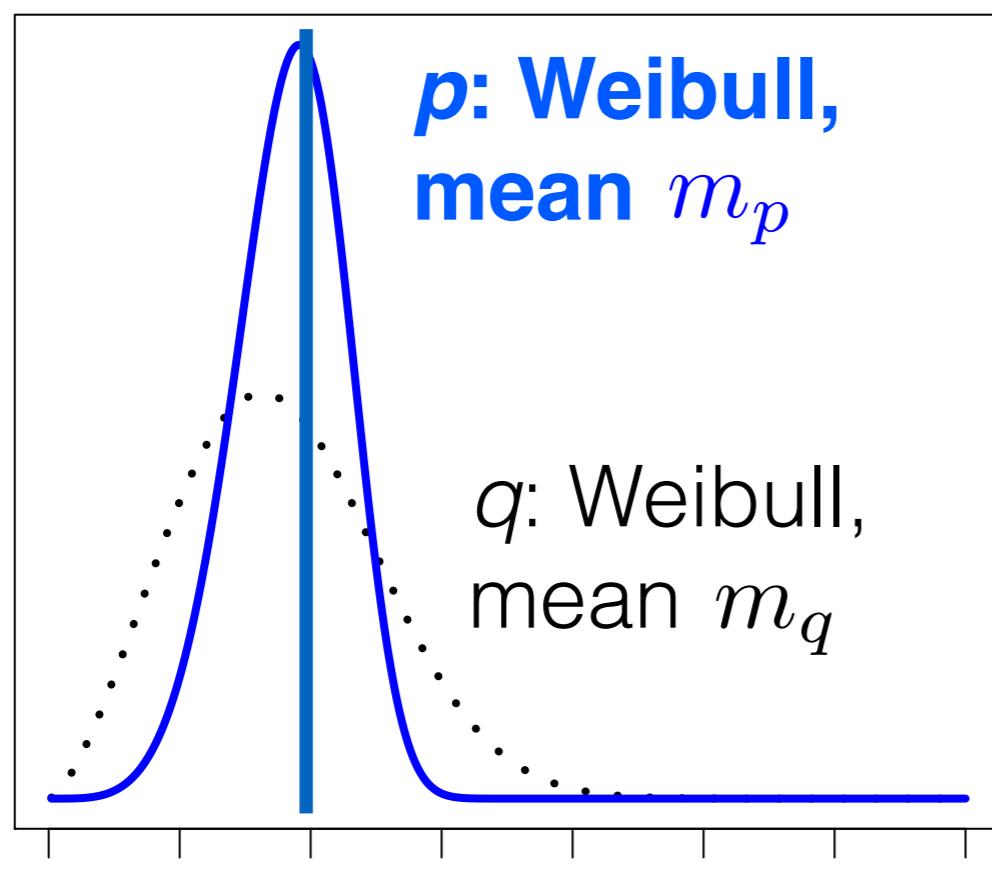
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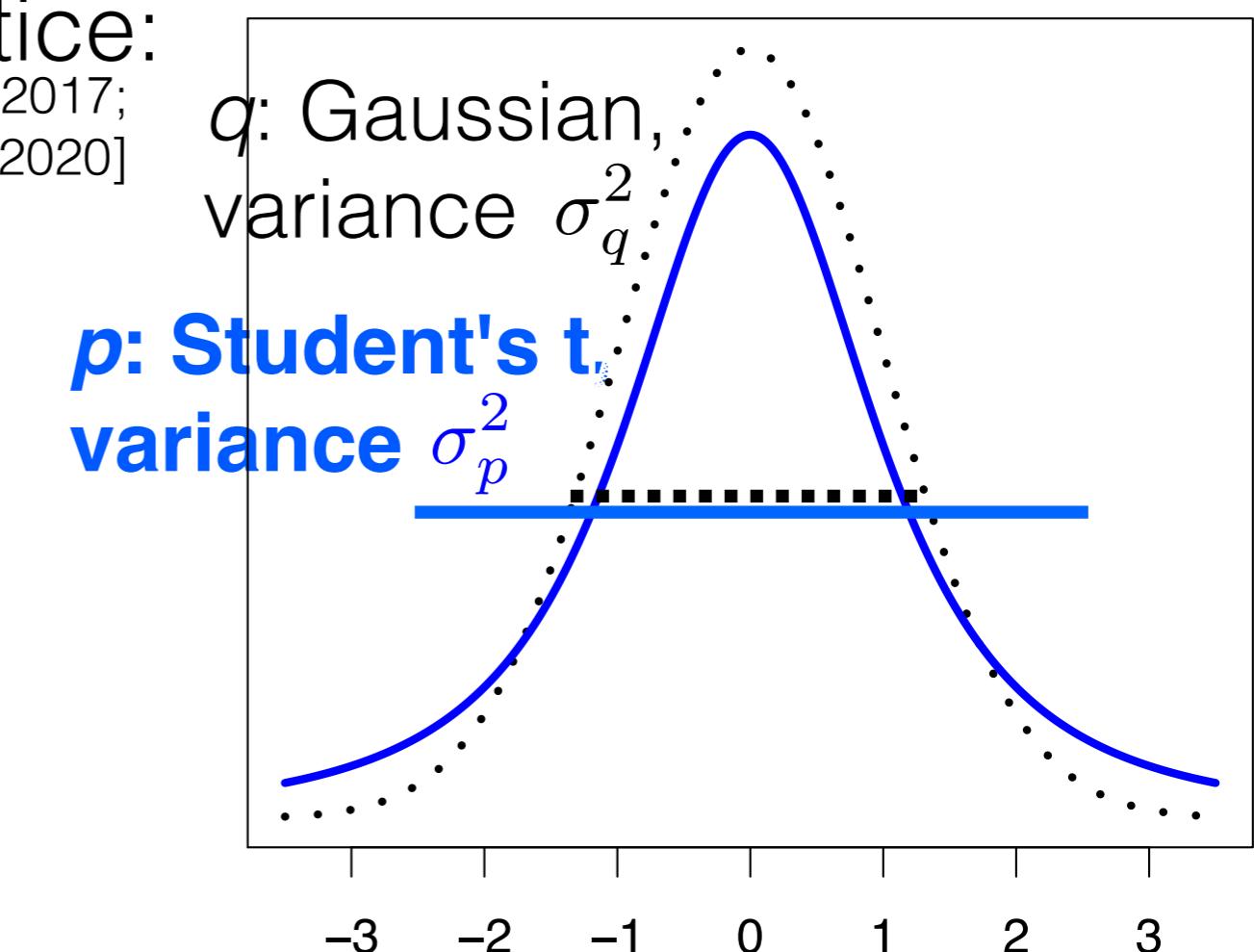
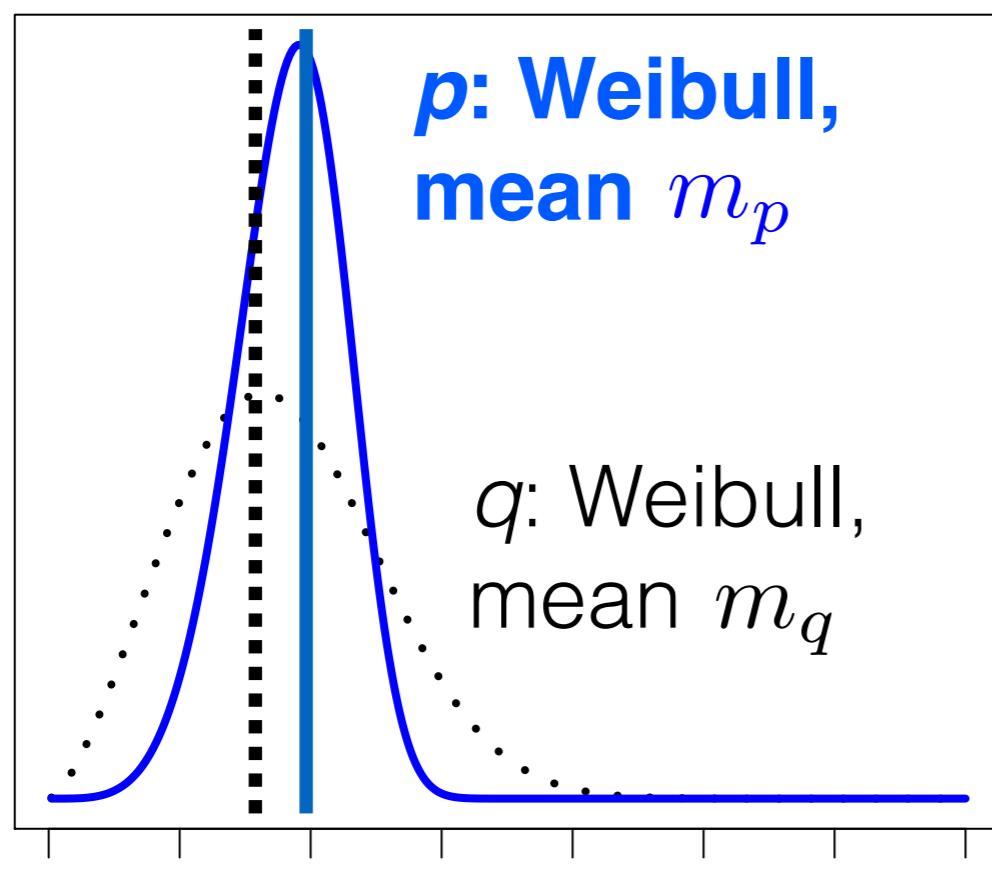
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$$\sigma_p^2 \geq c\sigma_q^2$$



Proposition. Can have small KL (<0.9) and arbitrarily bad mean estimate

$$(m_p - m_q)^2 \geq c\sigma_p^2$$

Approximate Bayesian inference

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

Optimization

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

Variational Bayes

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

How
deep is
the
issue?

Mean-field variational Bayes

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

Algorithm

Implementation

Gaussian example
was exact

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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?

Roadmap

- Bayes & Approximate Bayes review
- What is:
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What can we do?

What can we do?

Approximate posterior

Optimize: closest nice distr.

Variational Bayes

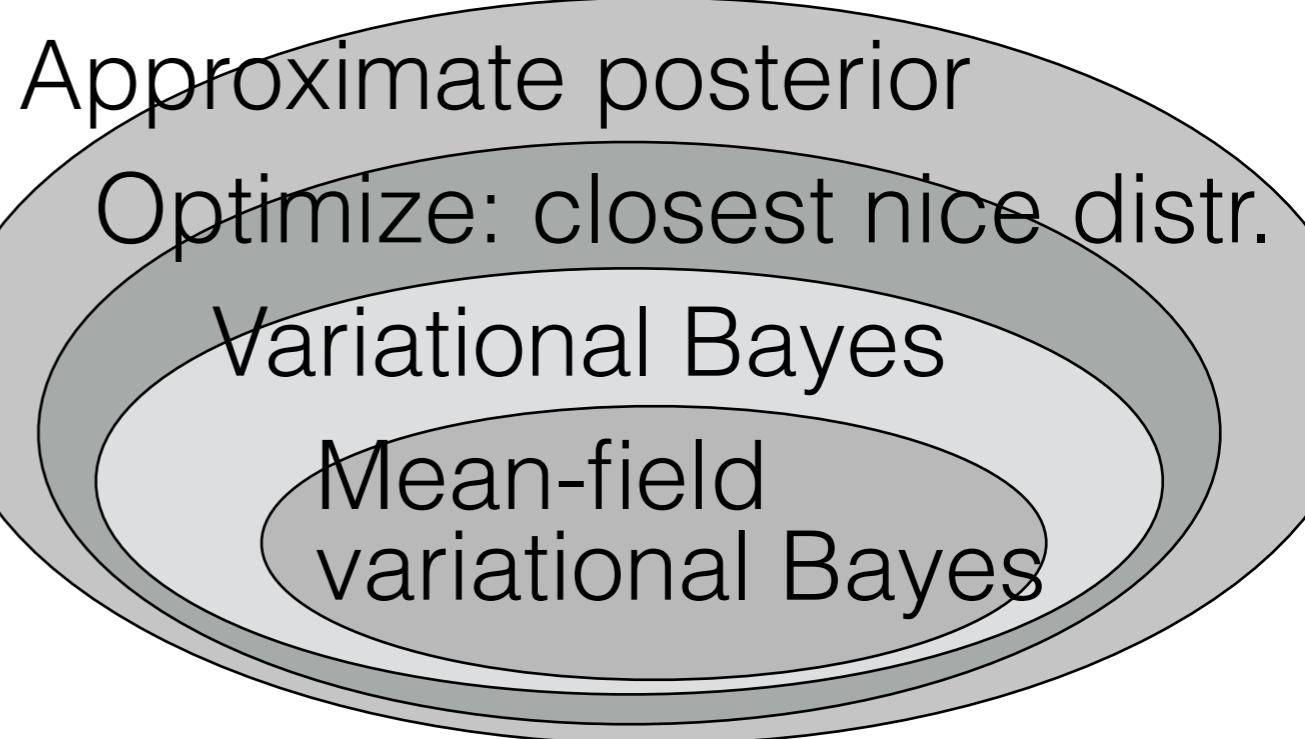
Mean-field
variational Bayes

What can we do?

- “Linear response” (LRVB) corrections fix the variance

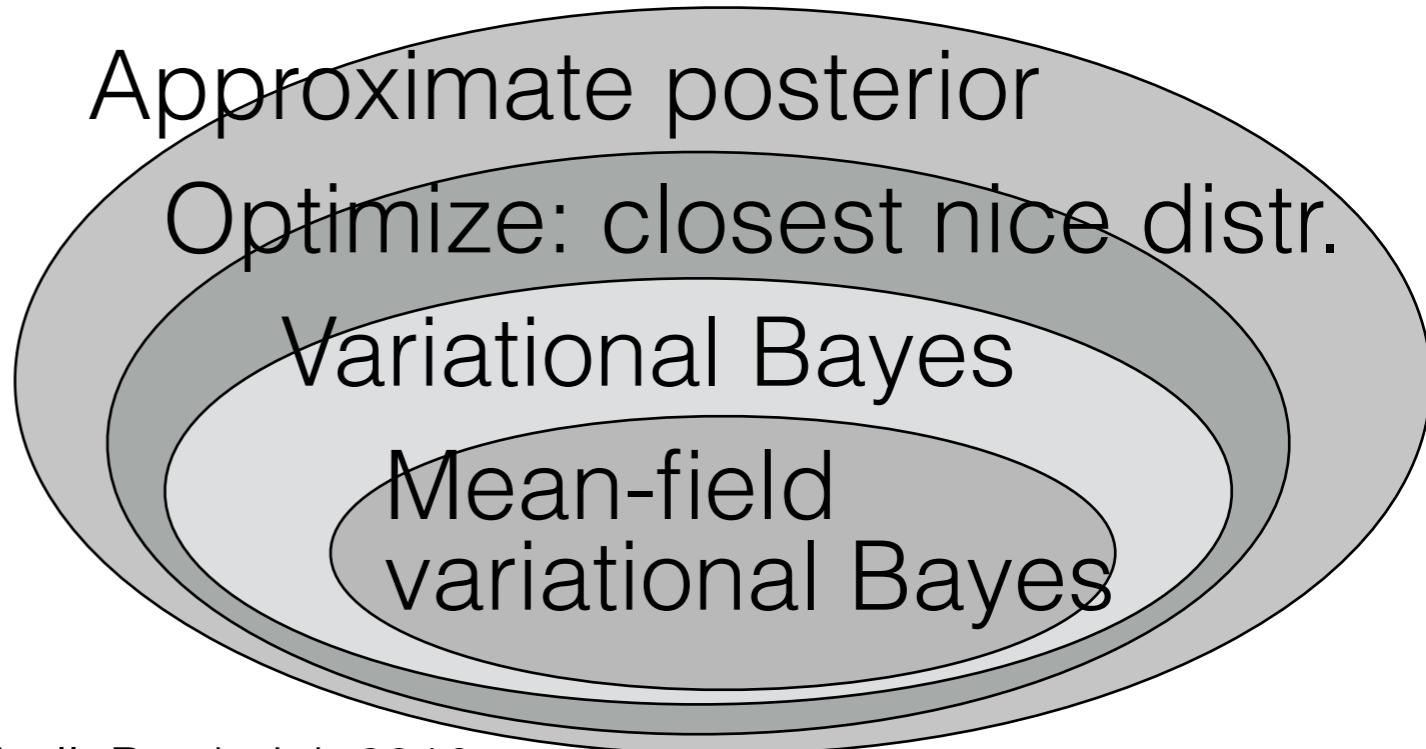
Broderick, Jordan 2015, 2018]

[Giordano,



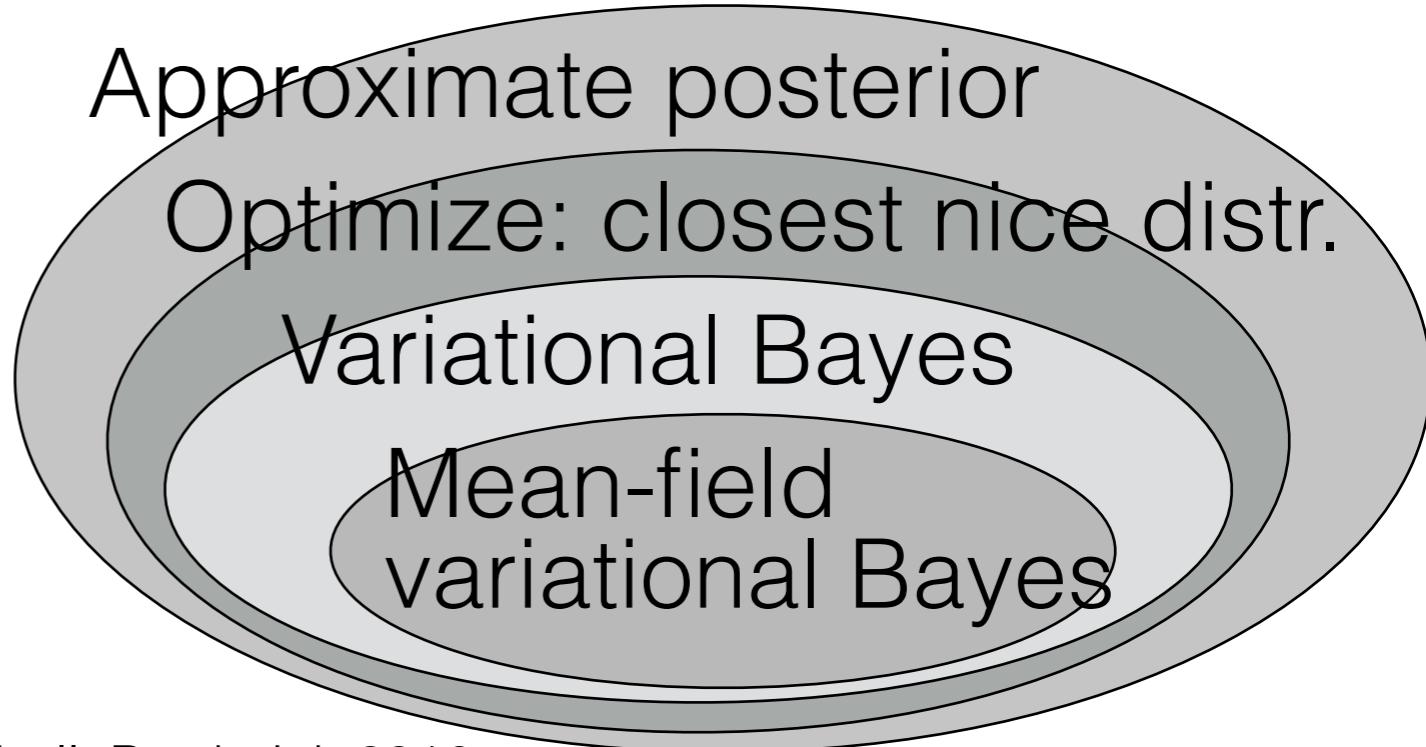
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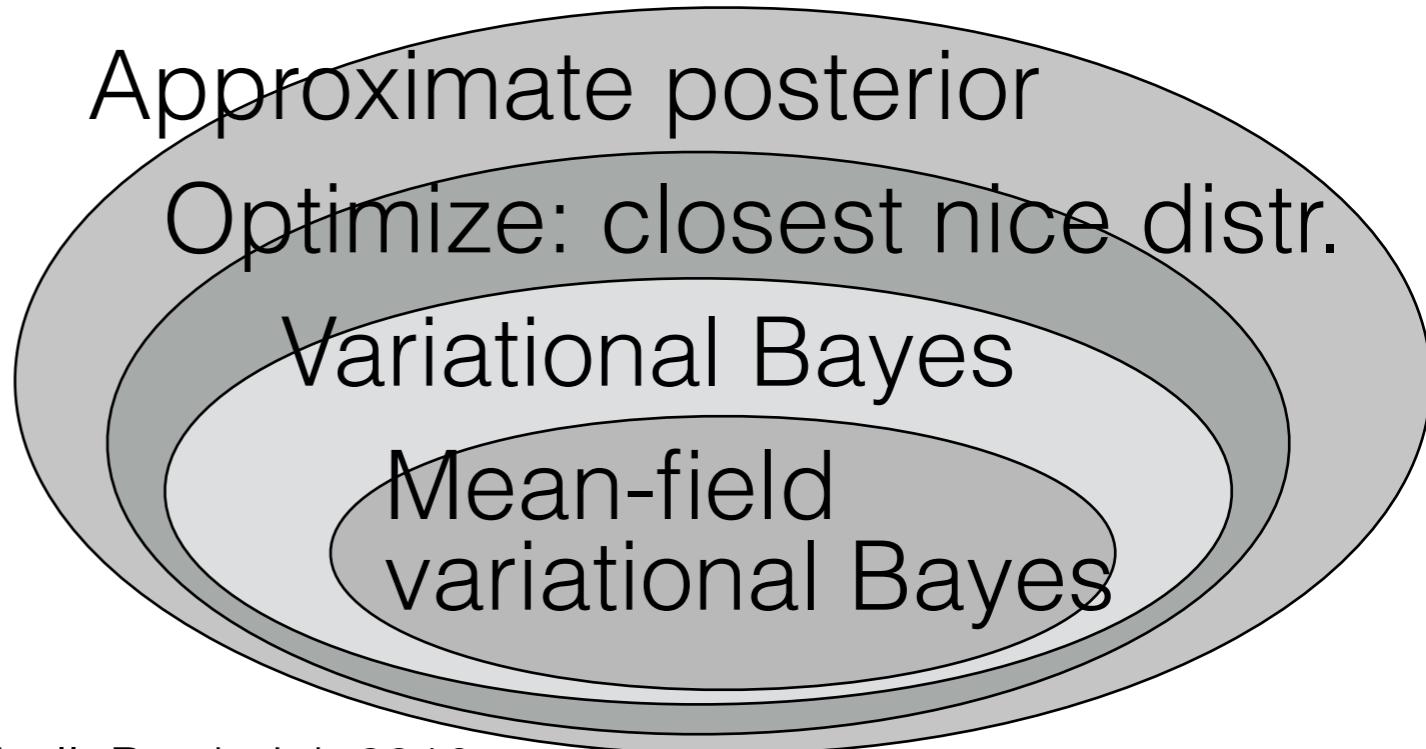
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- Reliable diagnostics



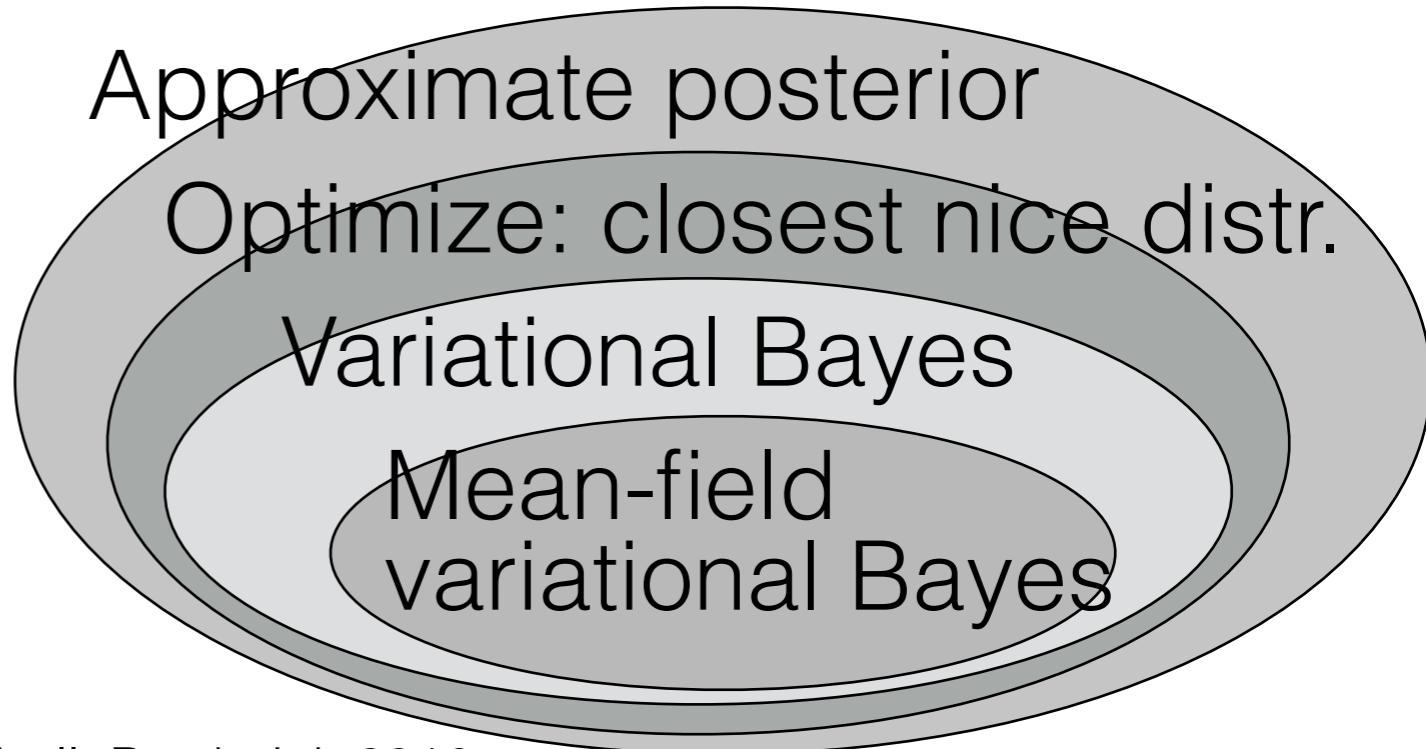
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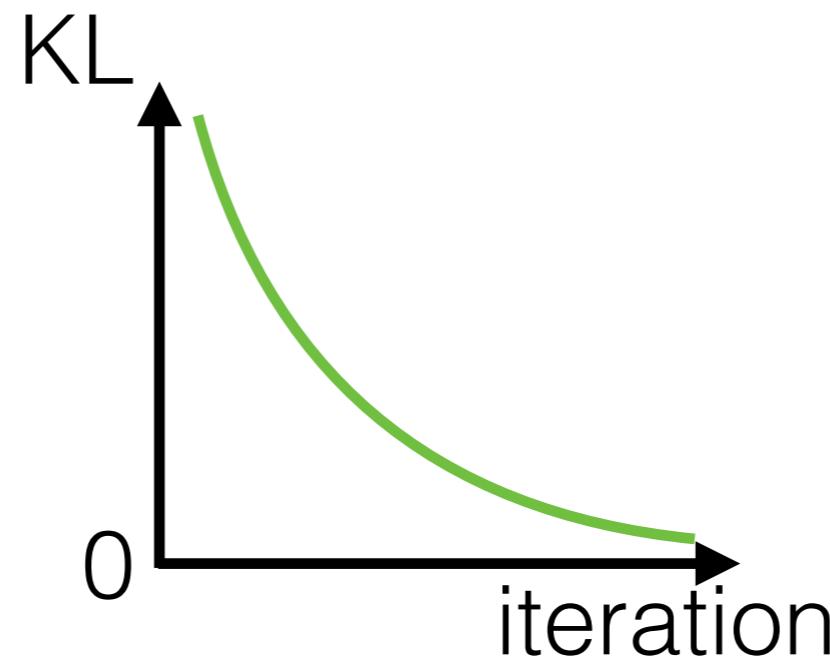
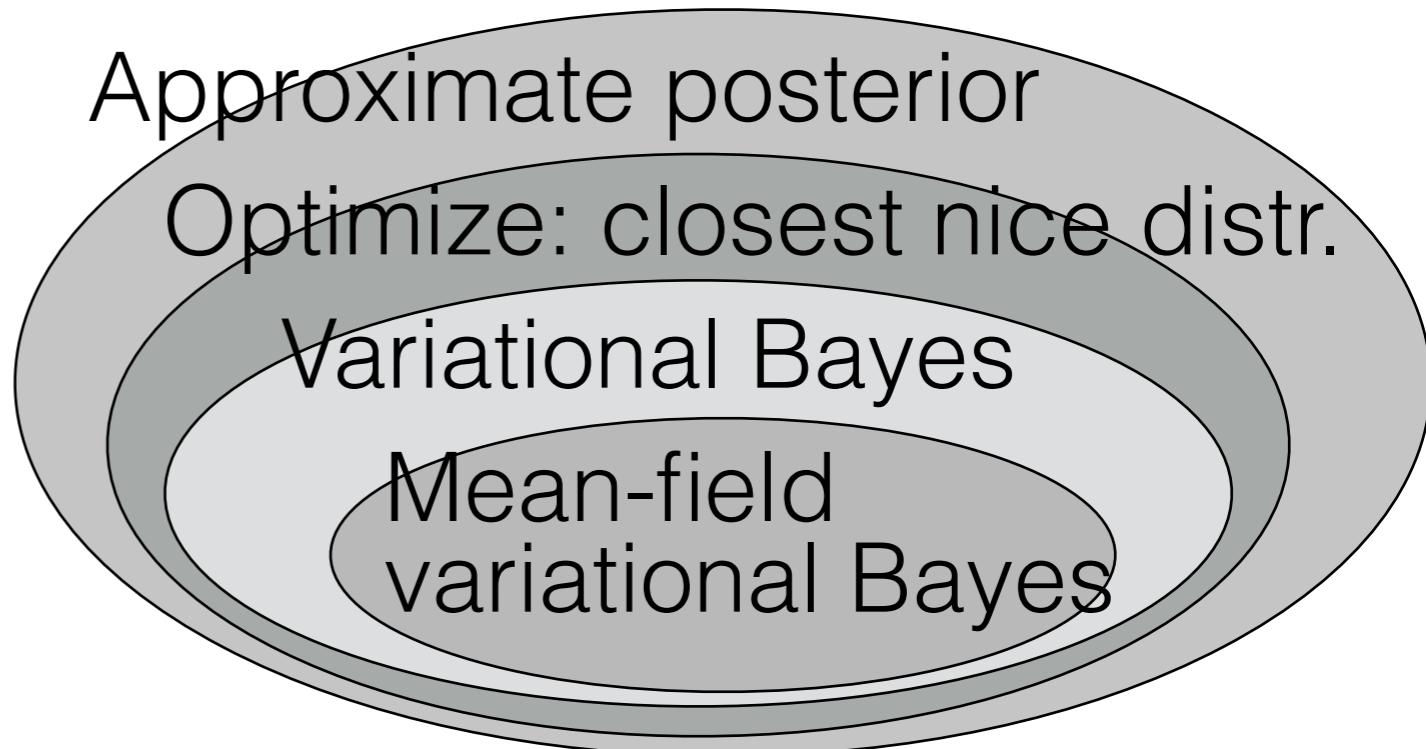
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 - cf. KL



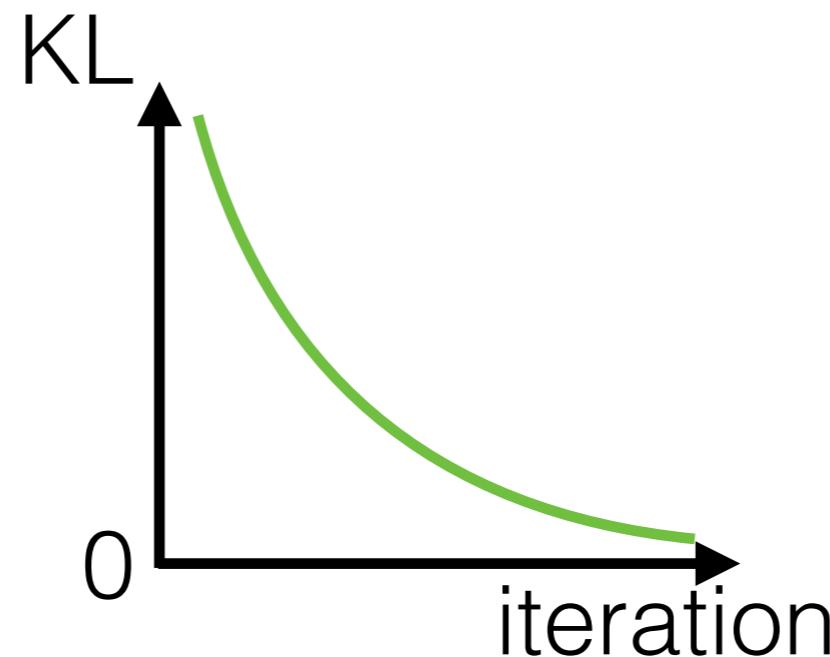
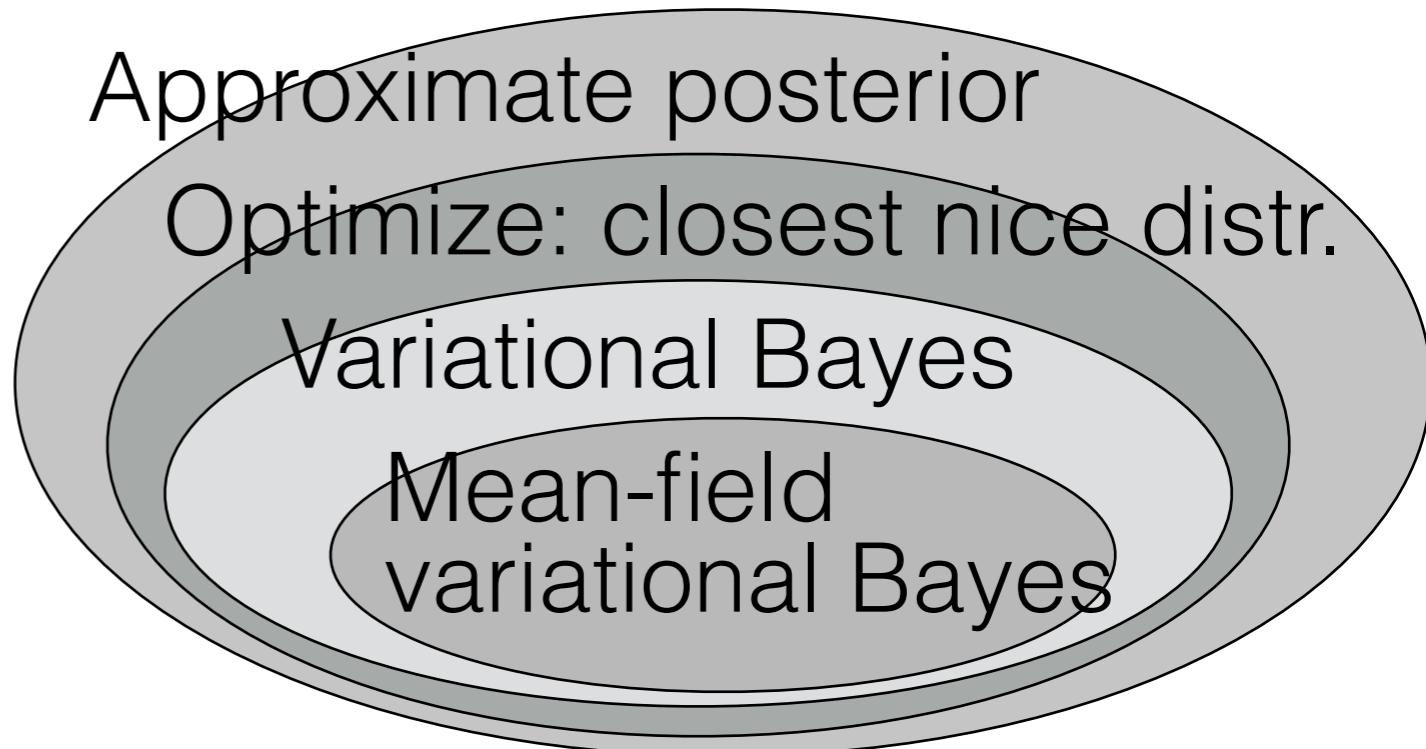
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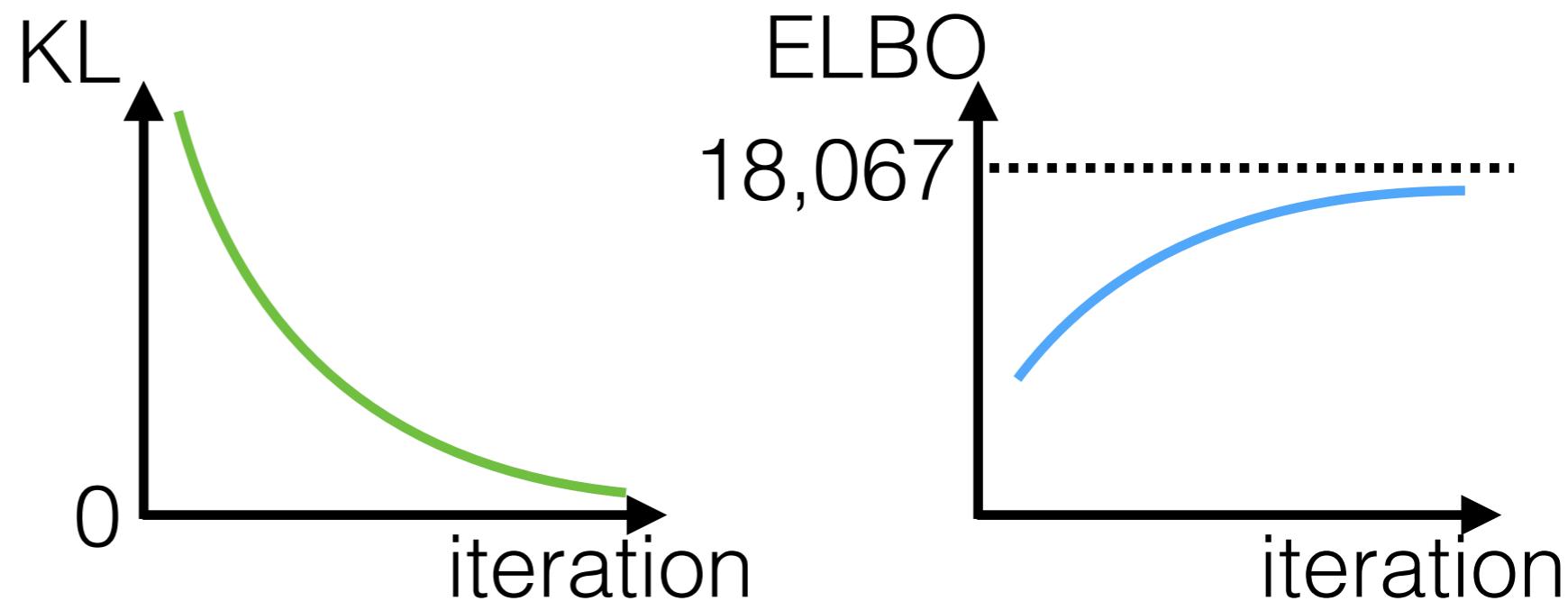
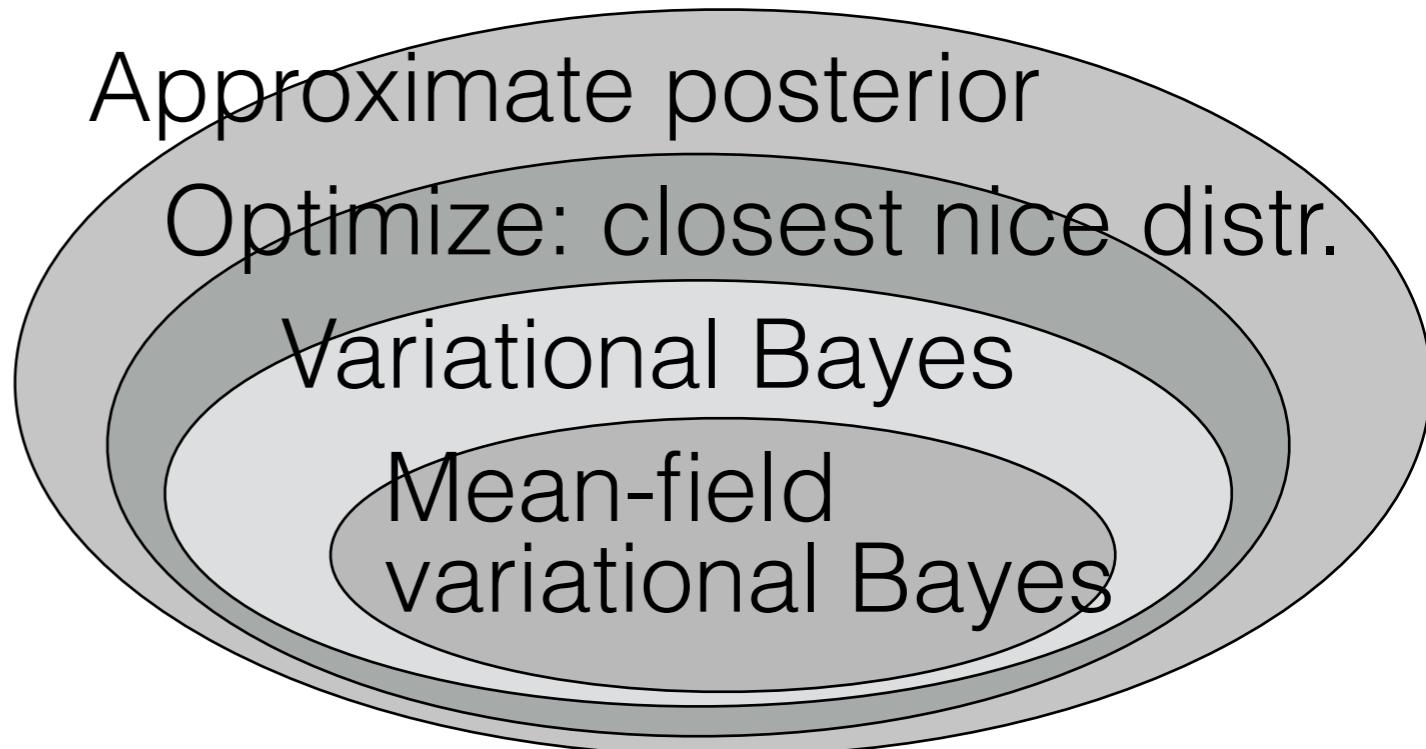
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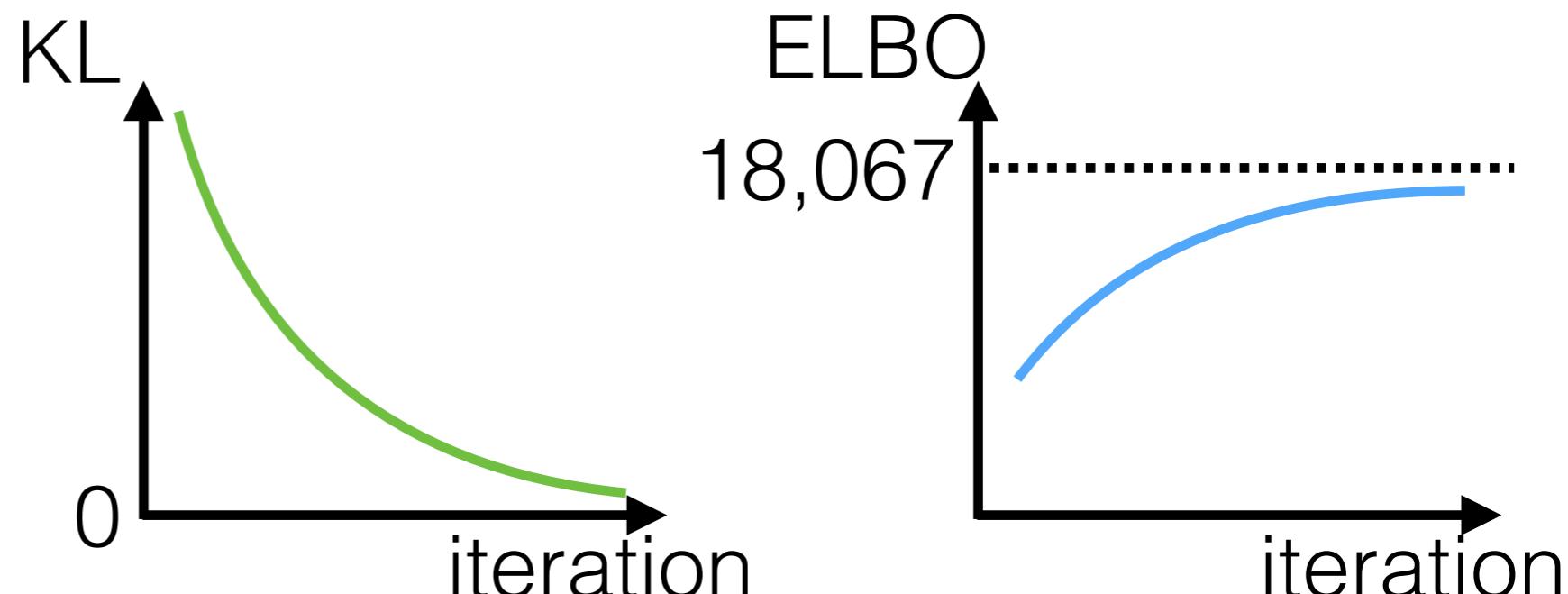
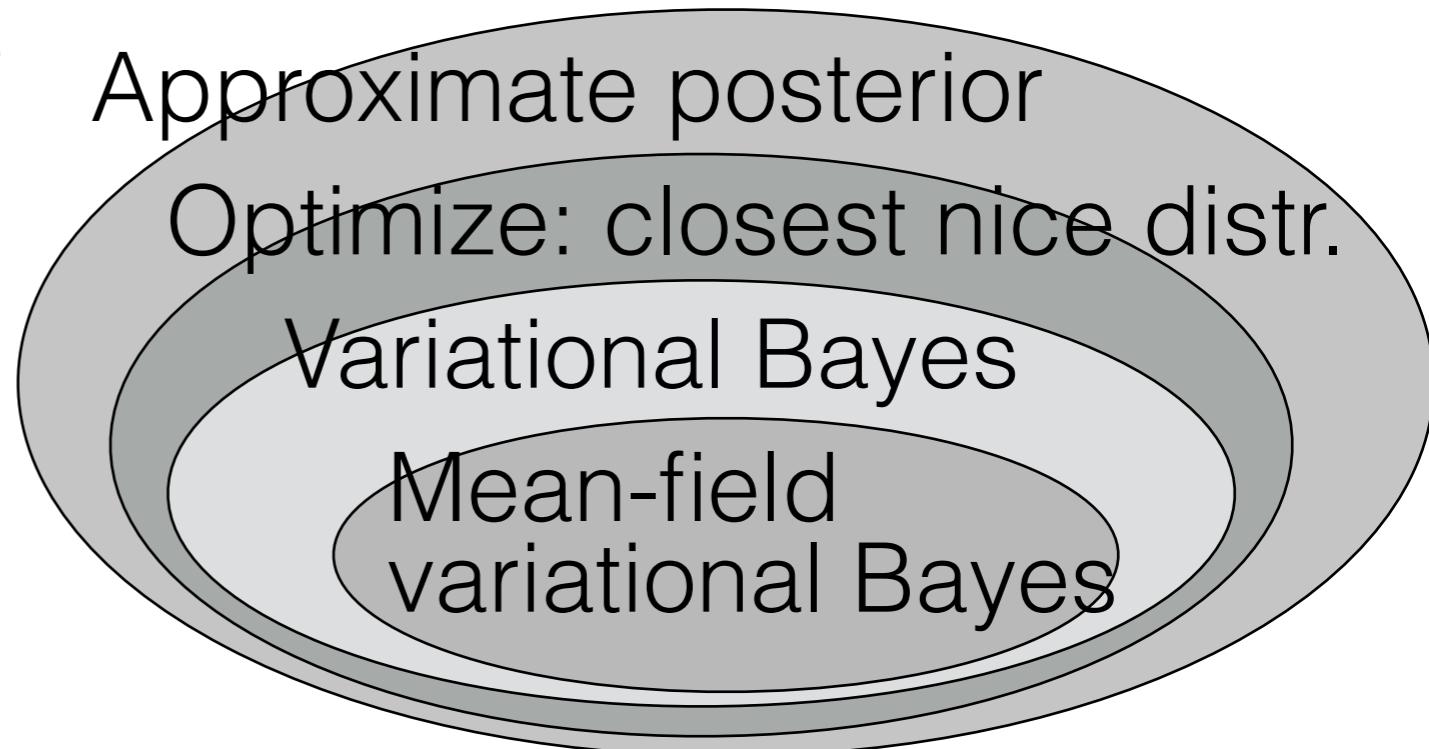
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[Gorham, Mackey 2015, 2017; Chwialkowski, Strathmann, Gretton 2016; Jitkrittum et al 2017; Talts et al 2018; Yao et al 2018, etc.]

→ “Yes, but did it work?”

Evaluating variational inference” ICML 2018



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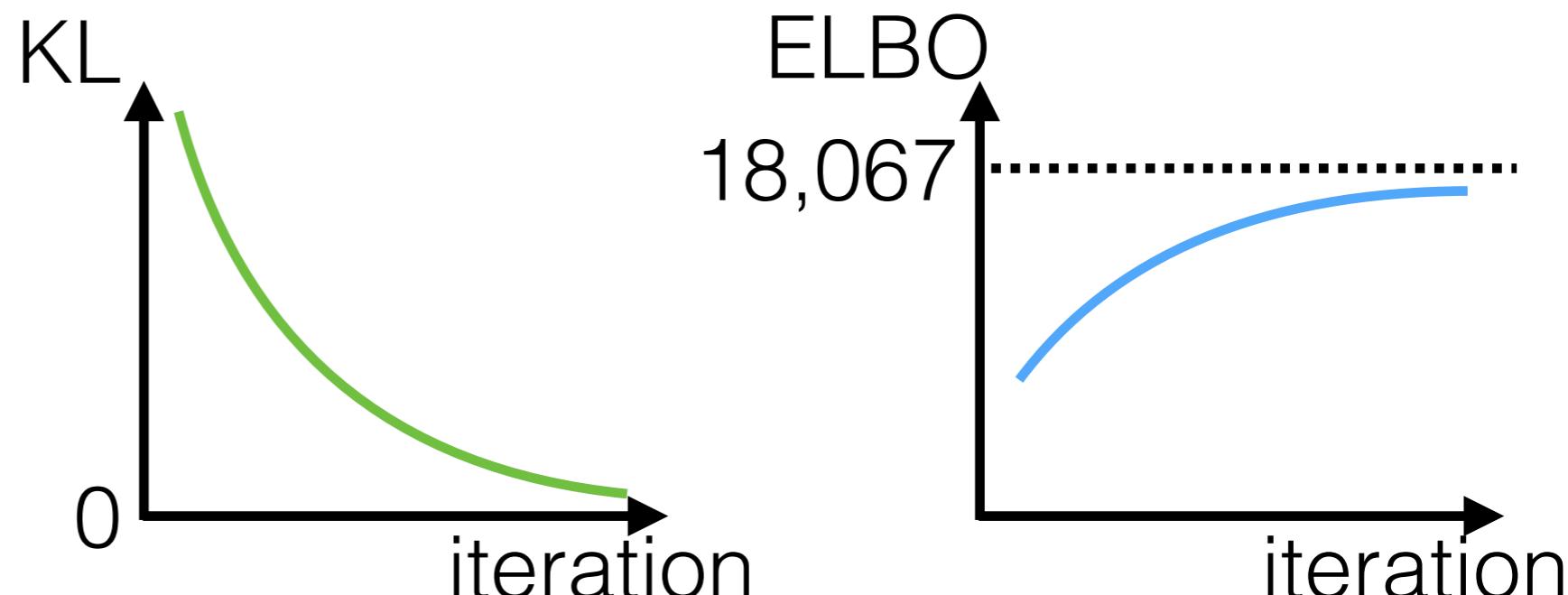
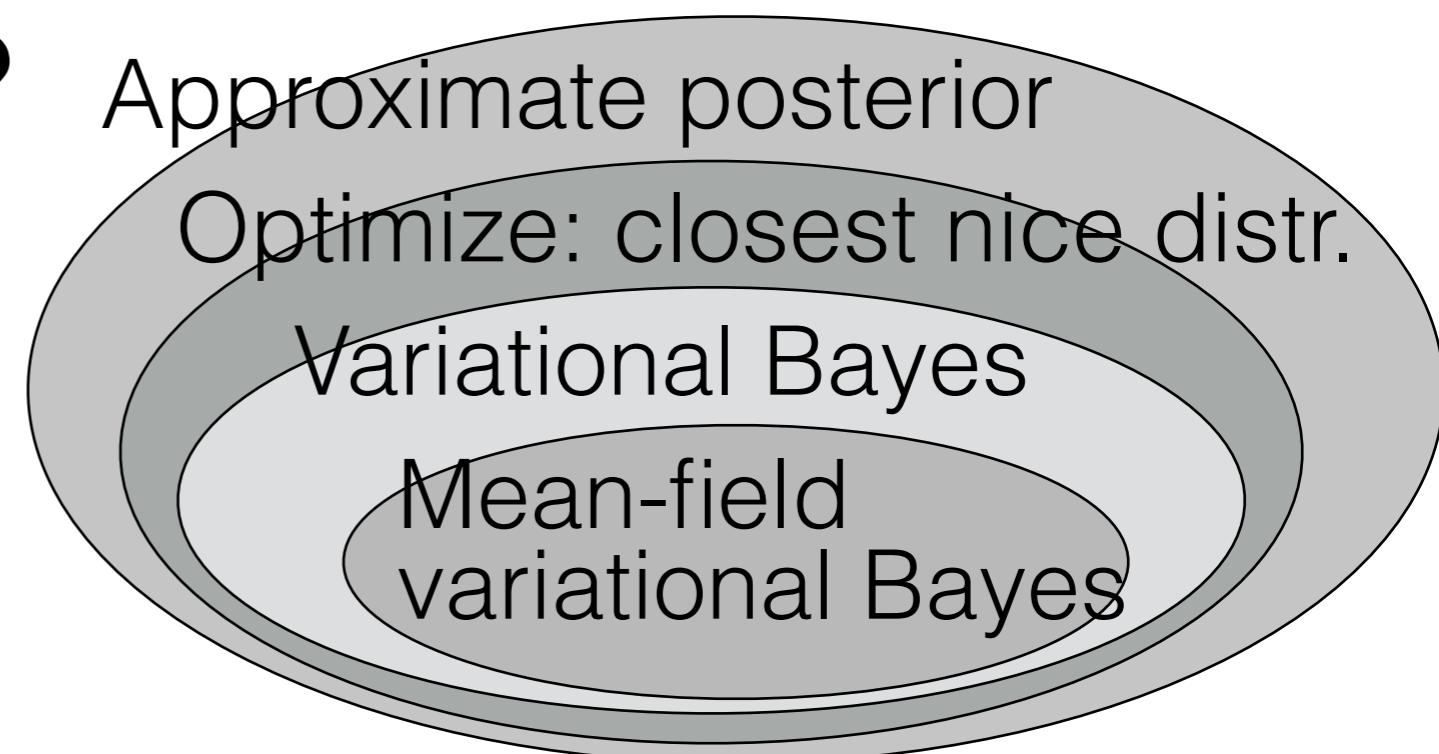
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- Diagnostics & workflow with theoretical guarantees
“Validated Variational Inference via Practical Posterior Error Bounds”

[Huggins, Kasprzak, Campbell, Broderick, 2020]



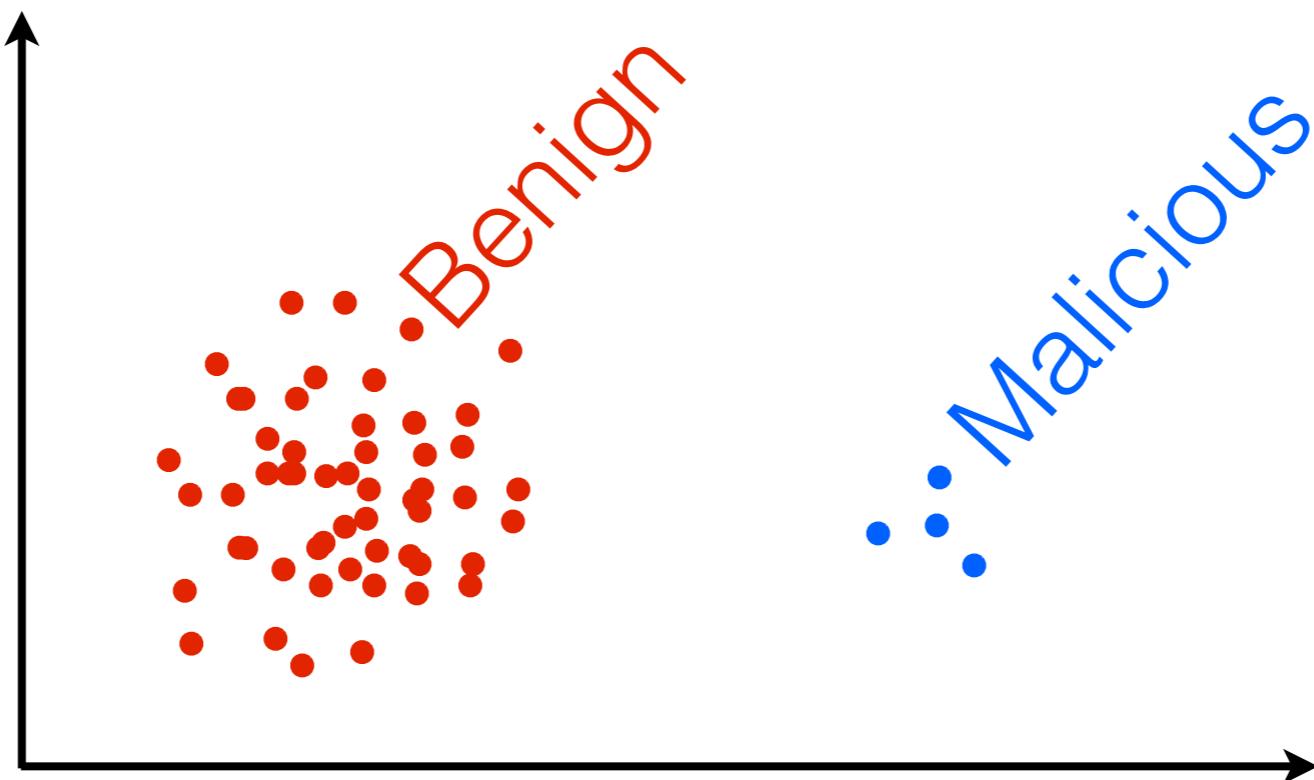
“Core” of the data set

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- Observe: redundancies can exist even if data isn't “tall”

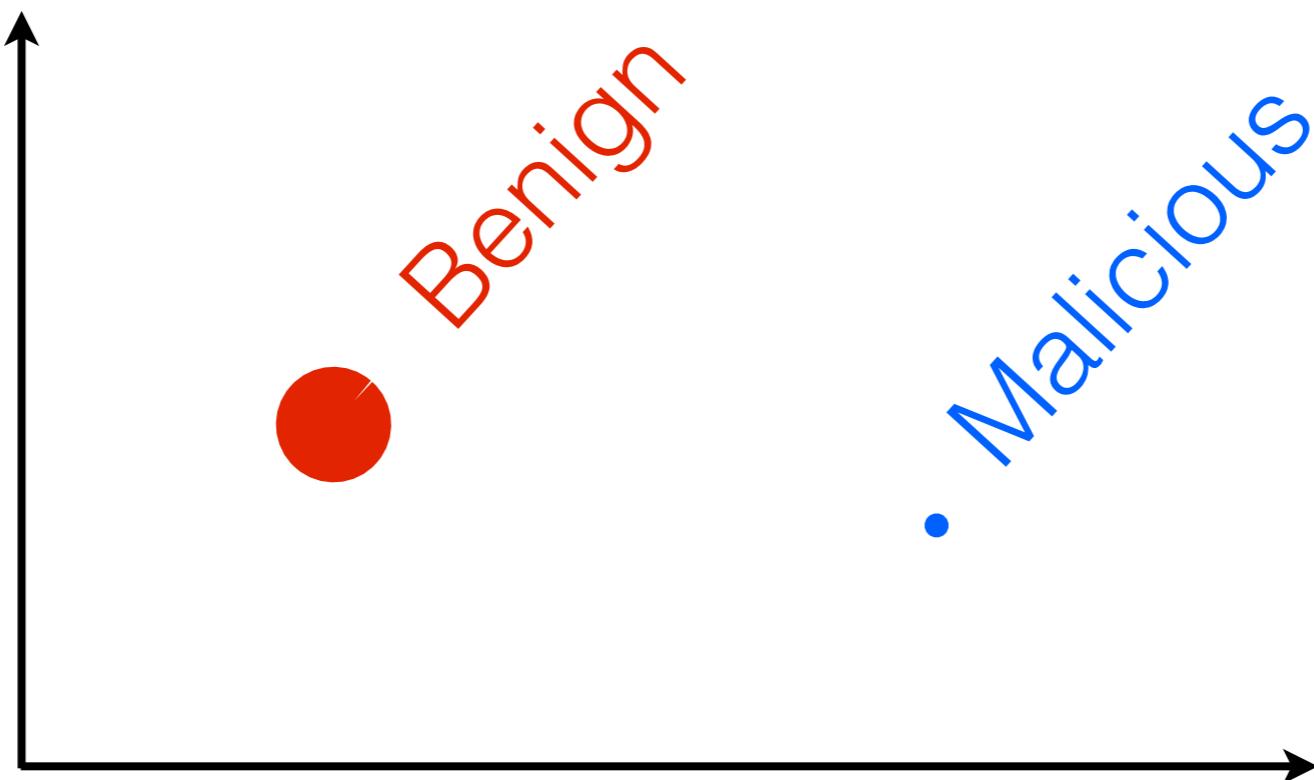
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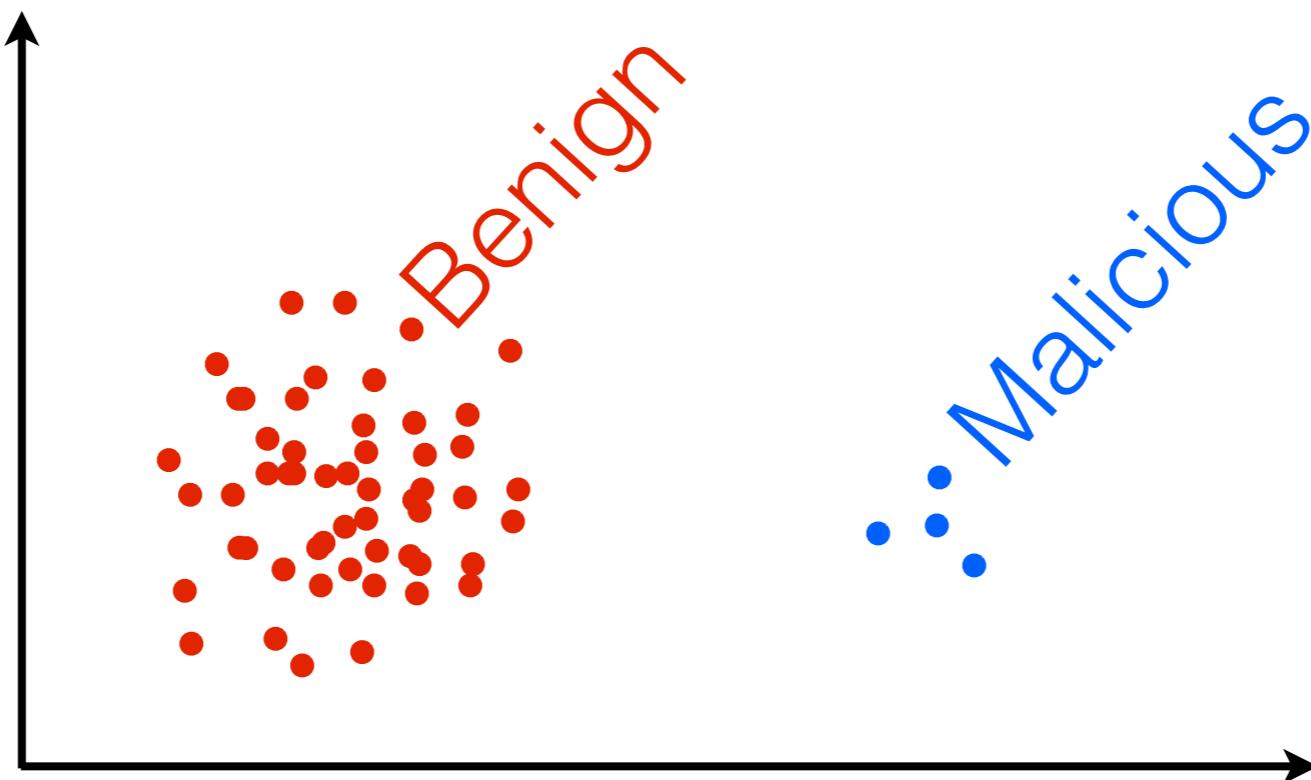
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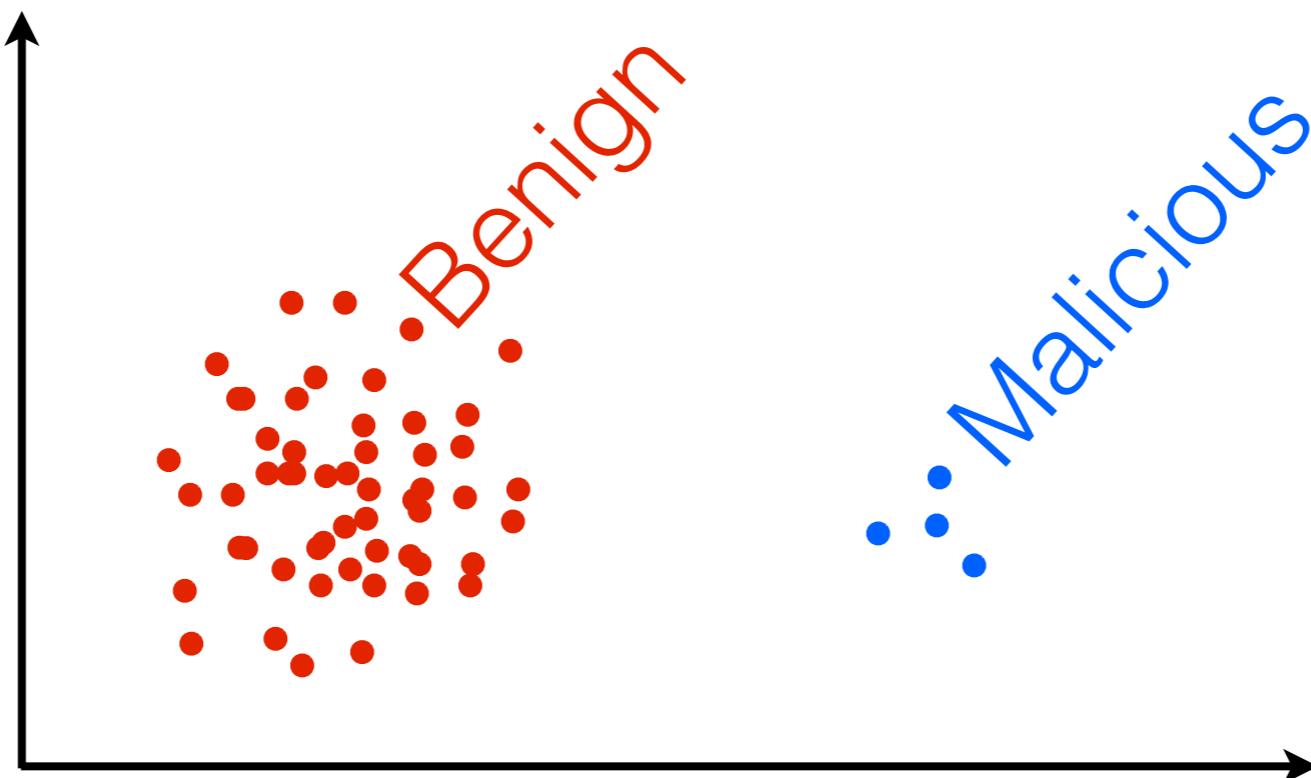
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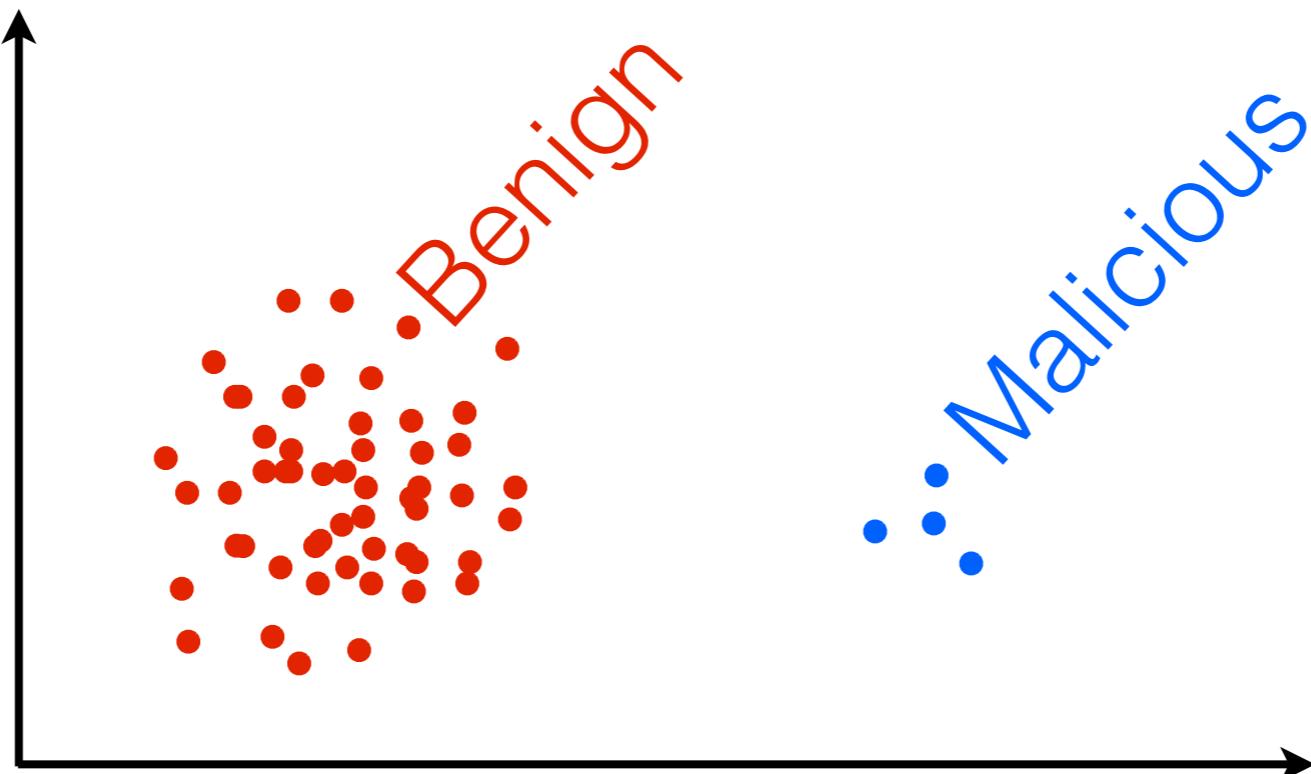
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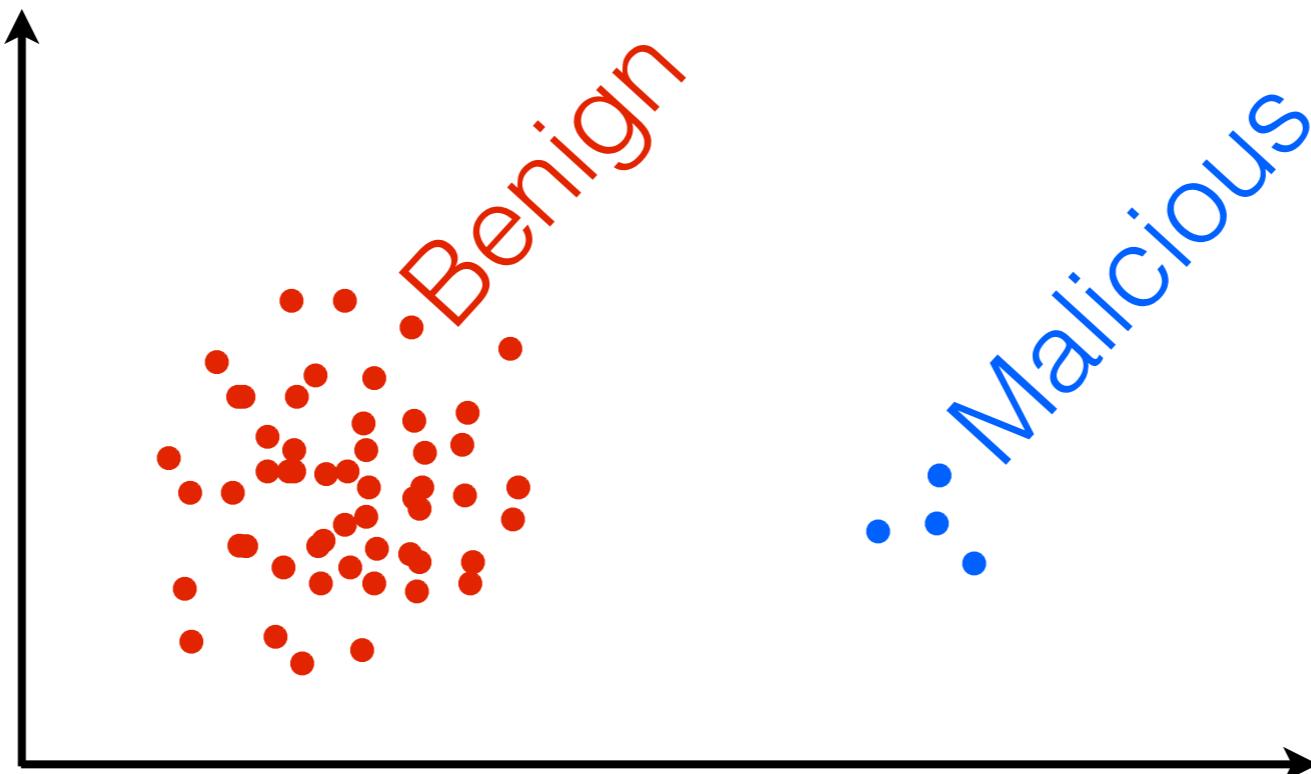
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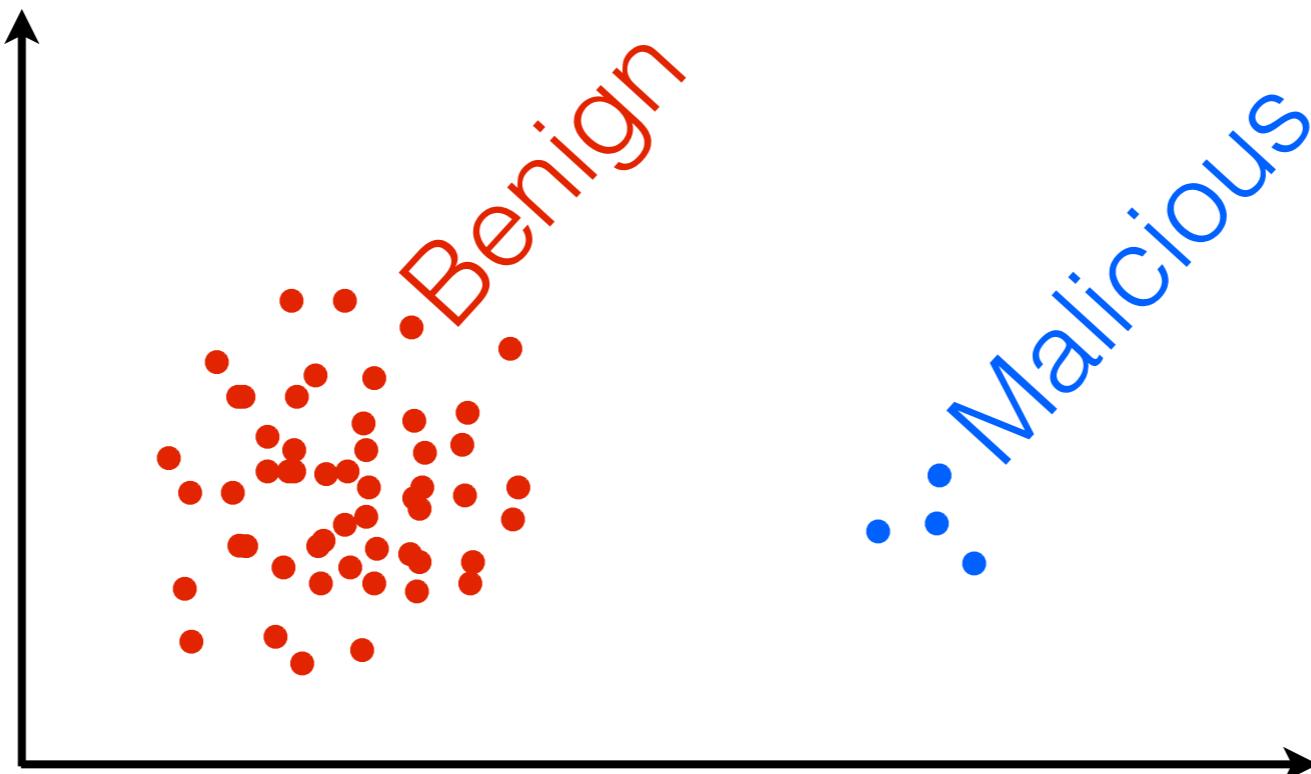
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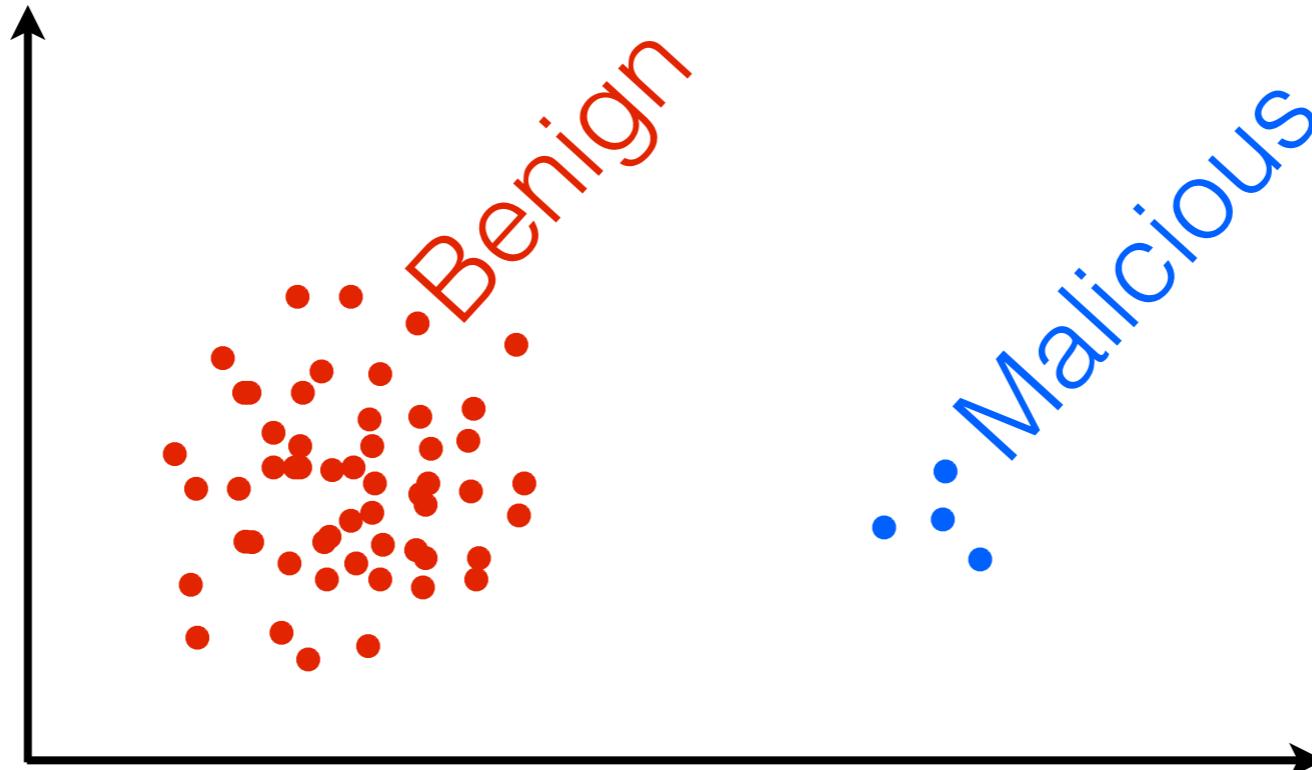
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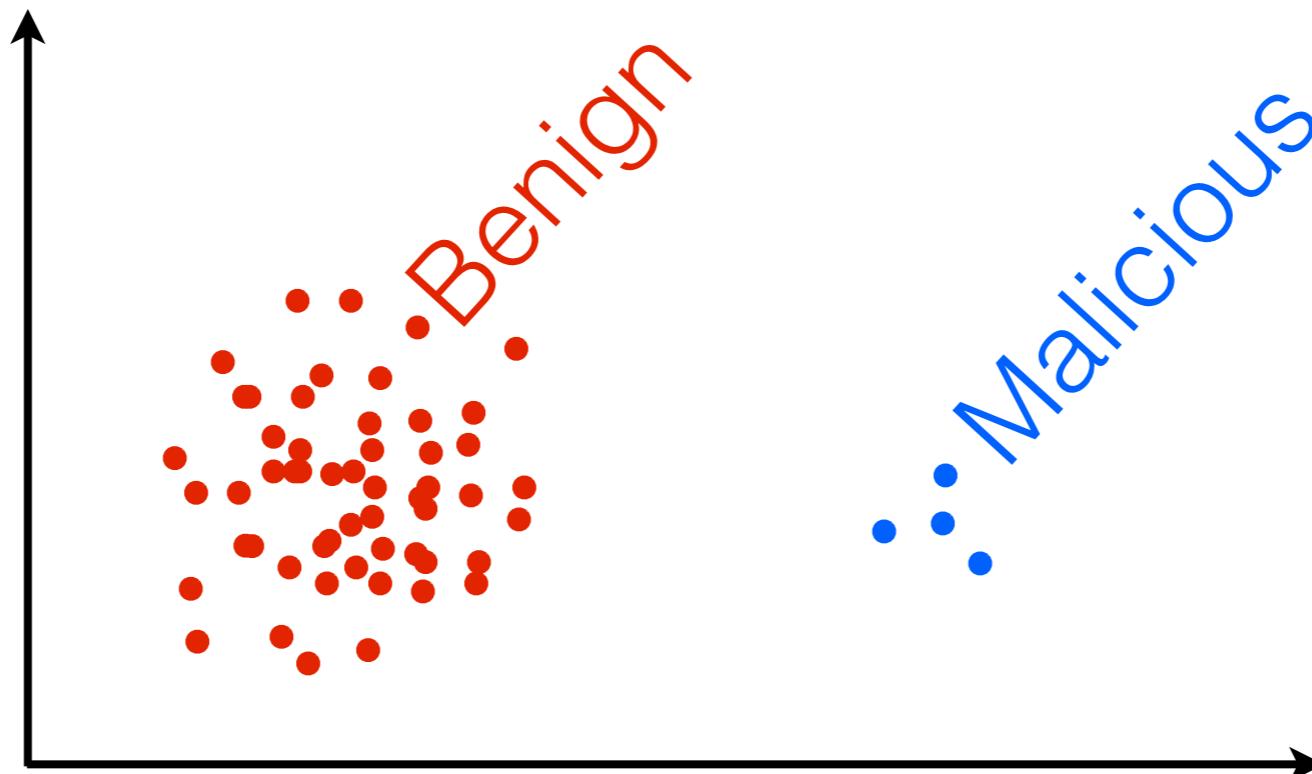
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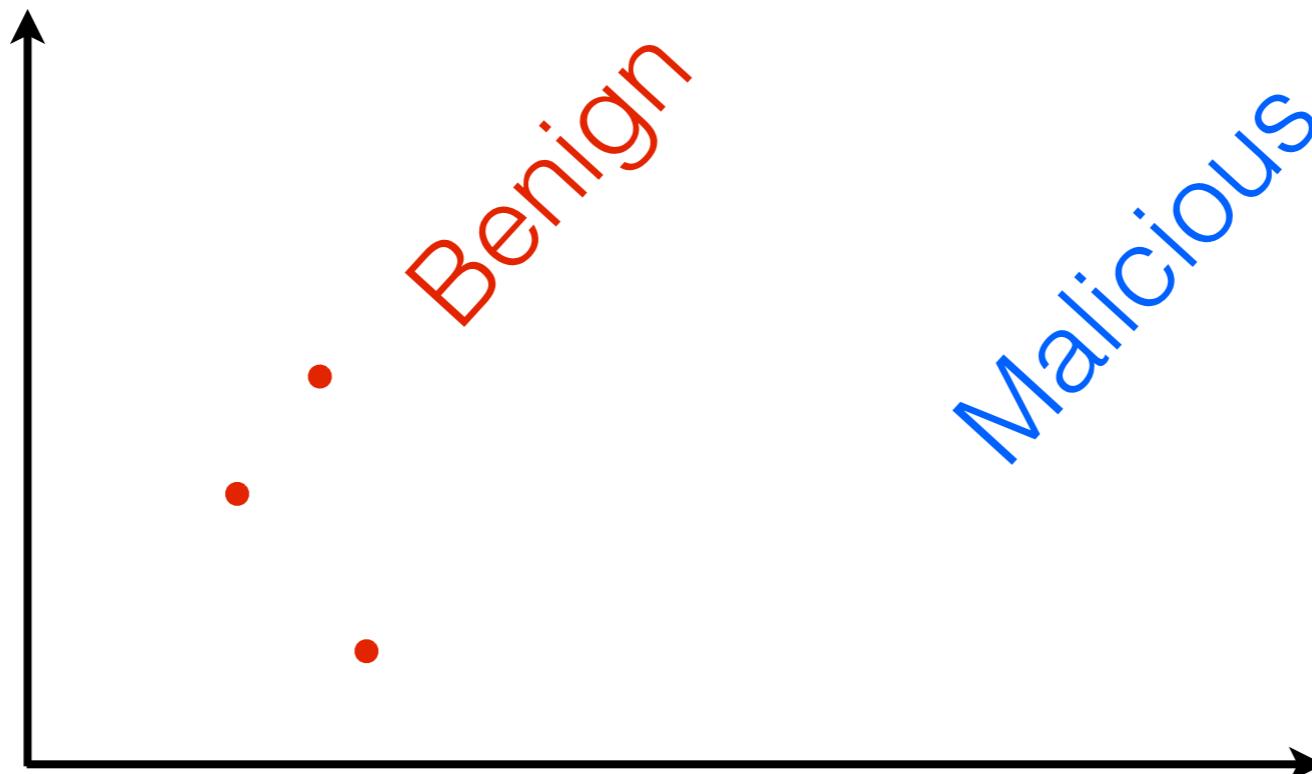
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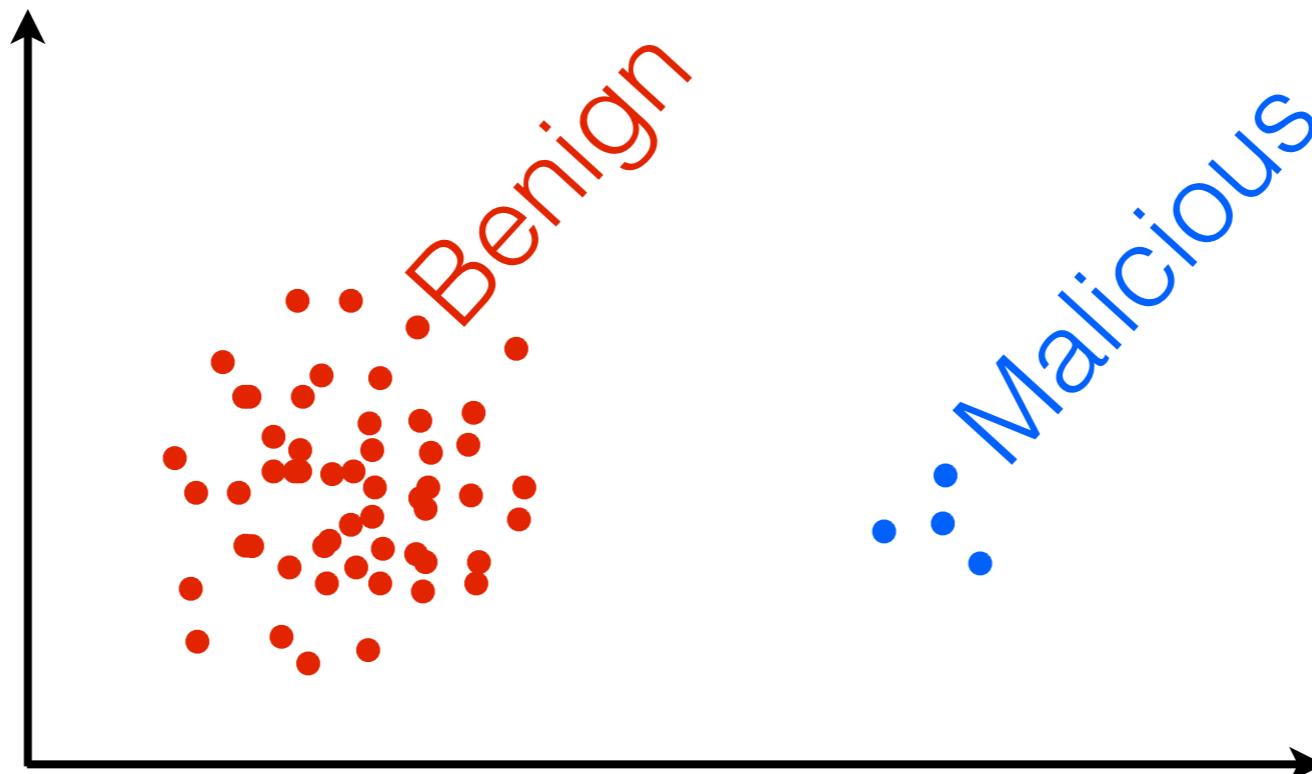
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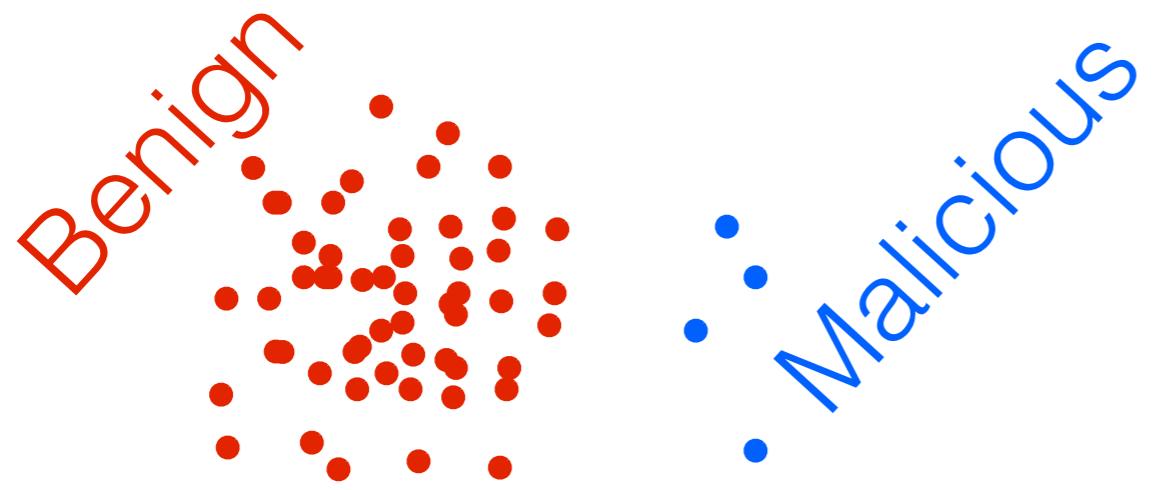
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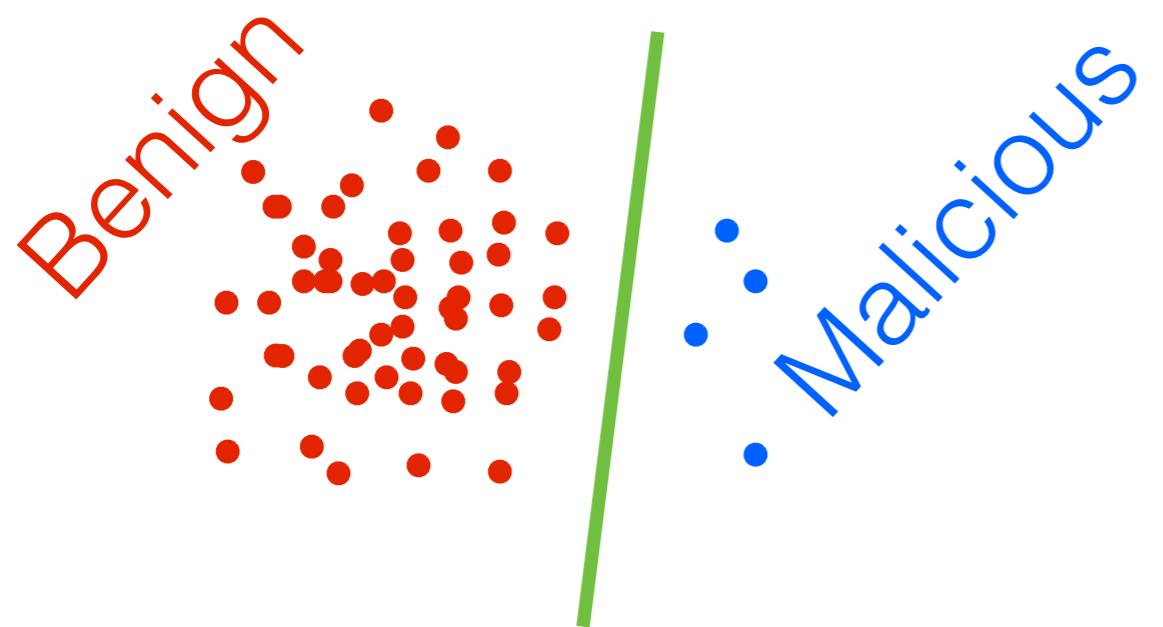
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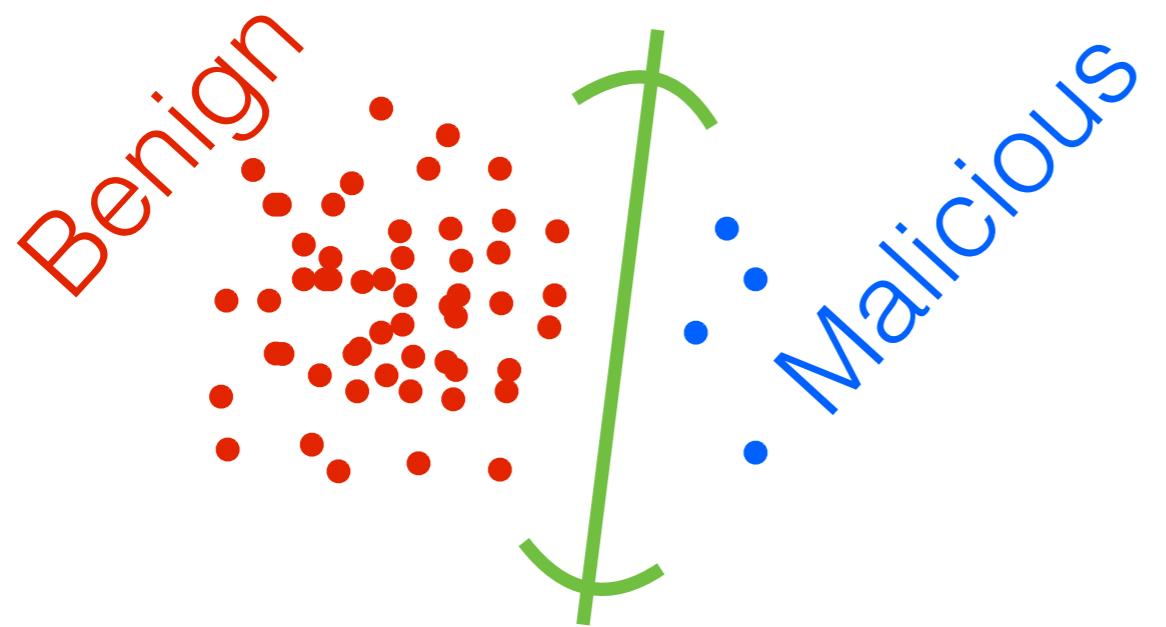
Uniform subsampling



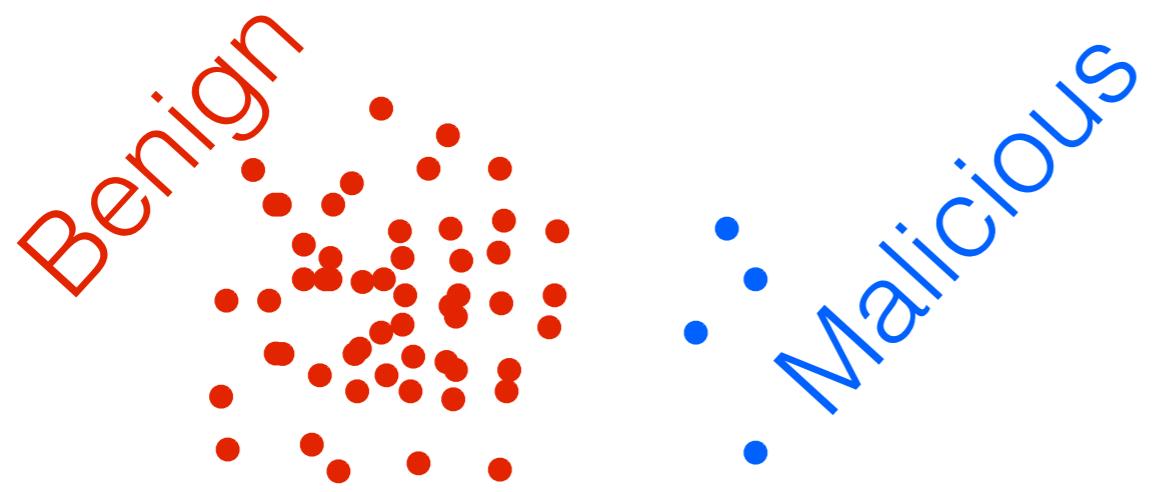
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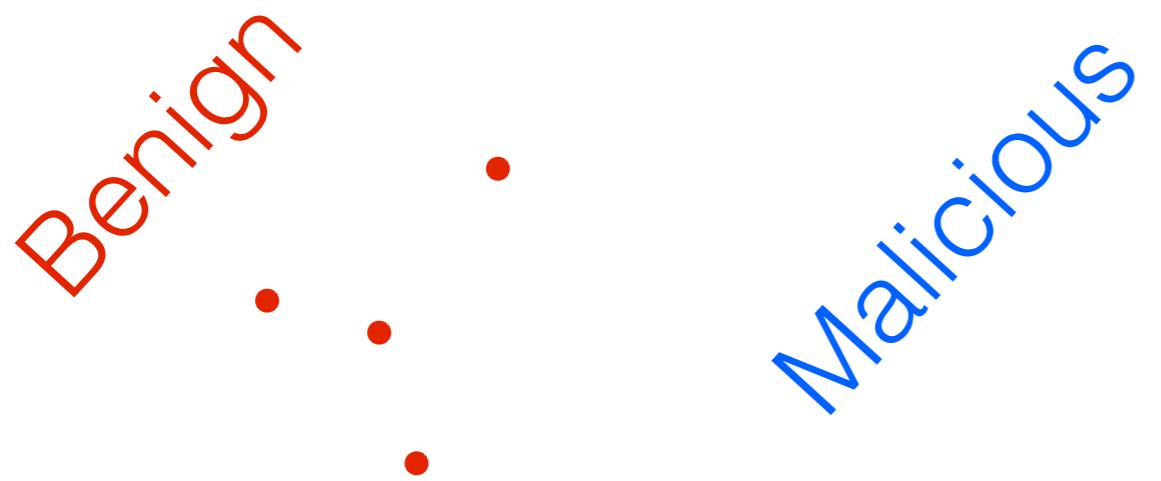
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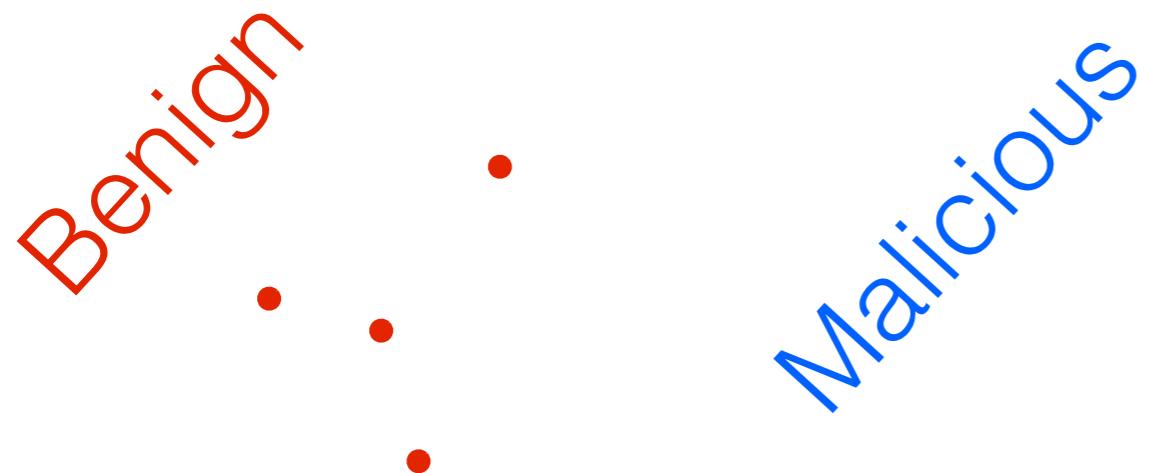
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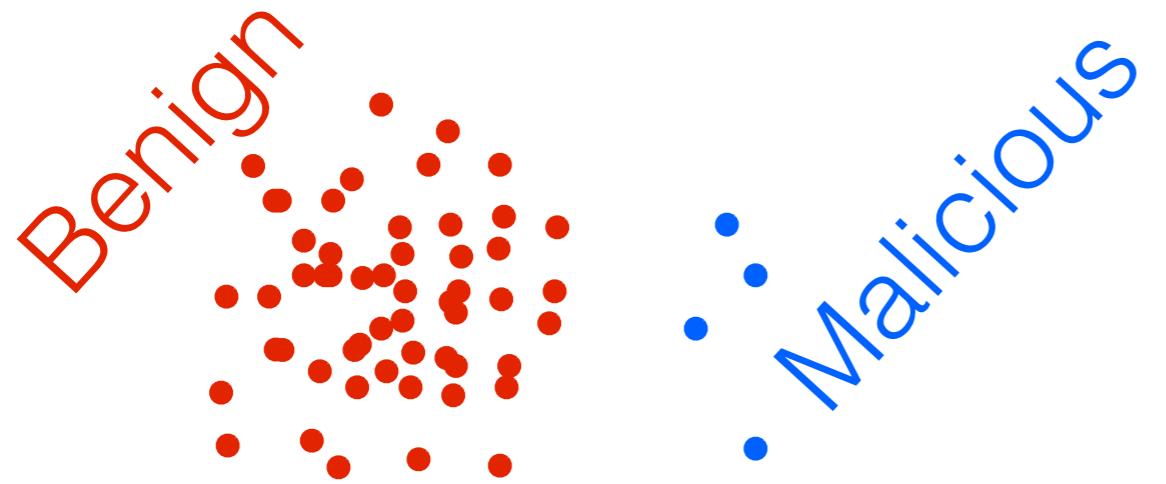


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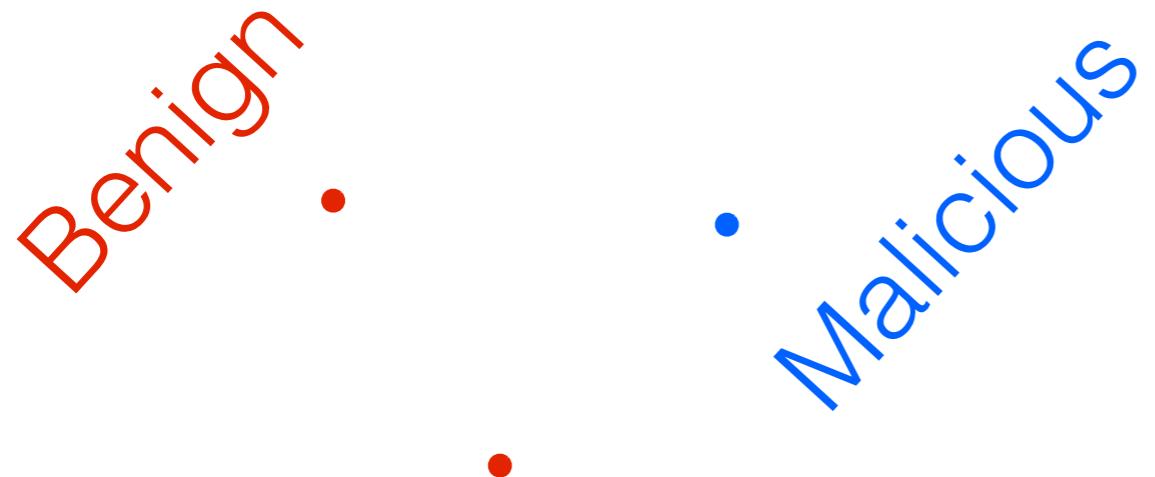
- Might miss important data

Uniform subsampling



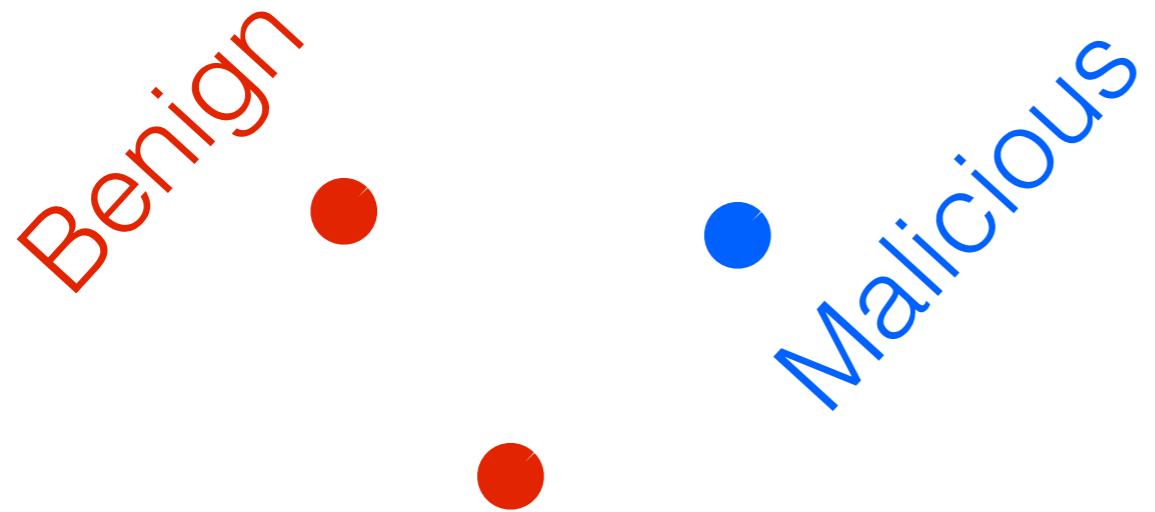
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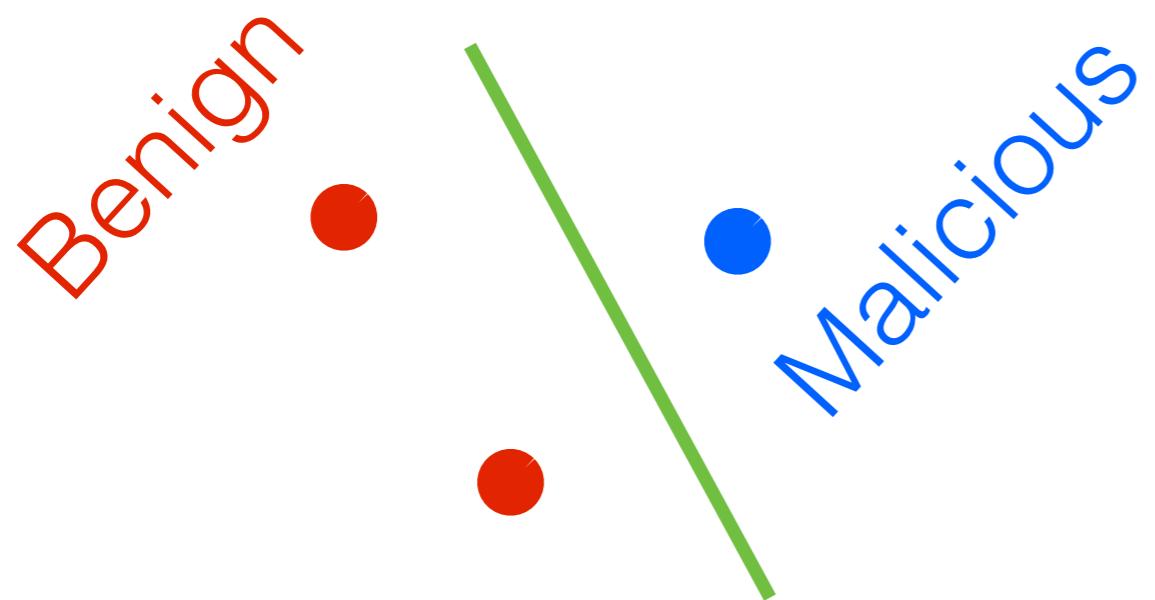
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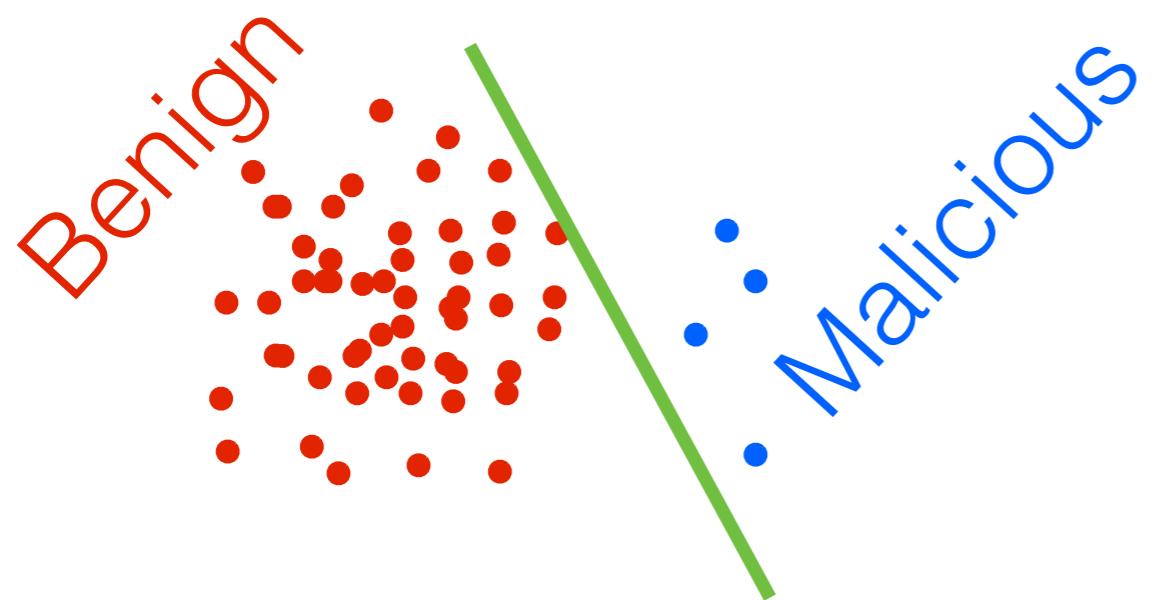
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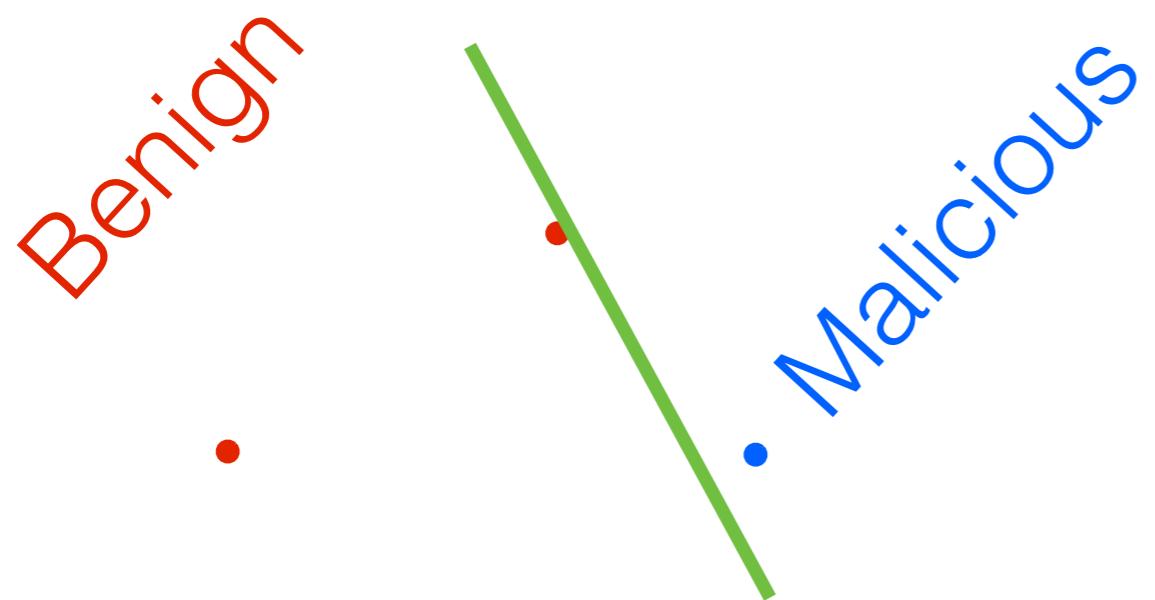
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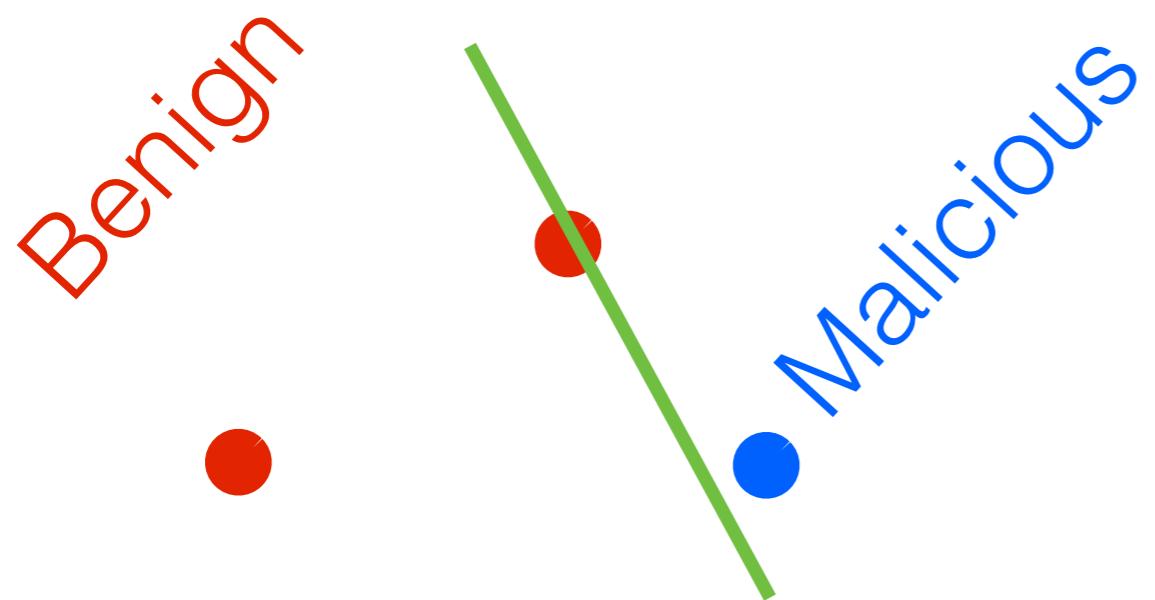
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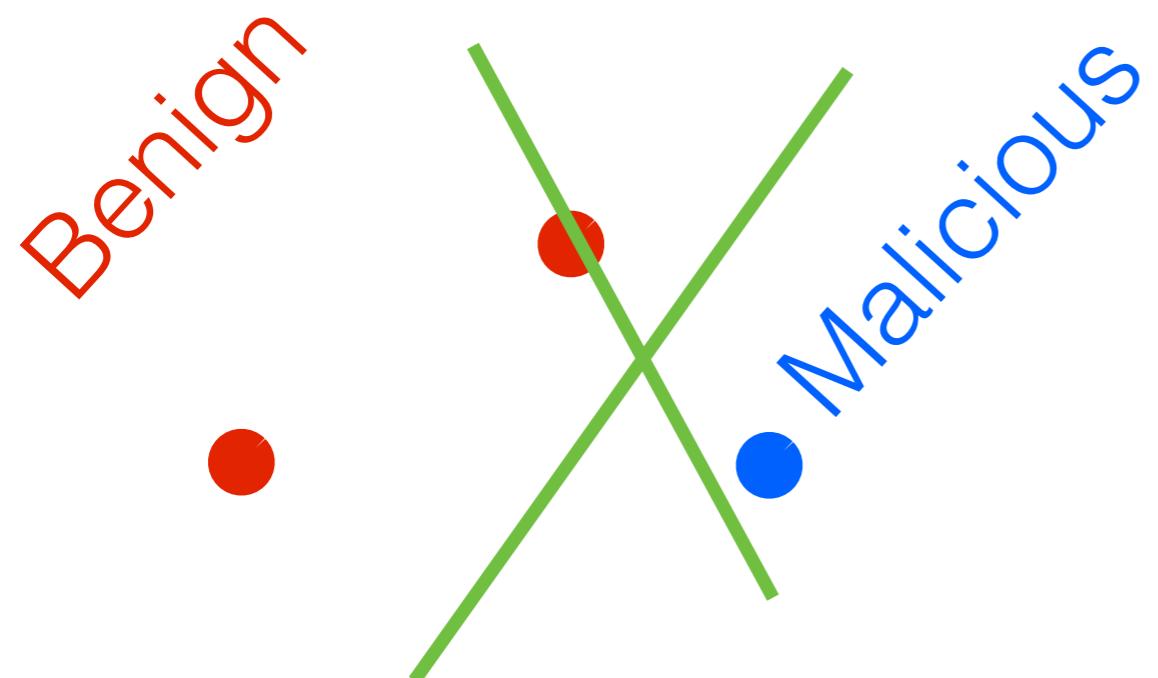
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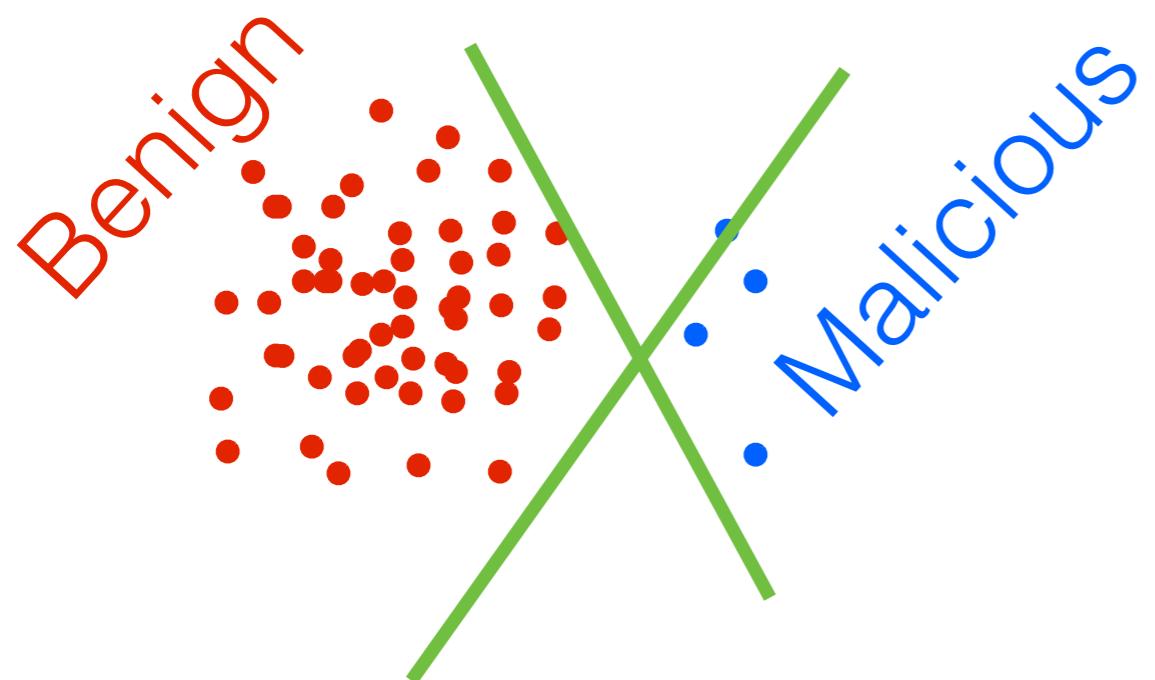
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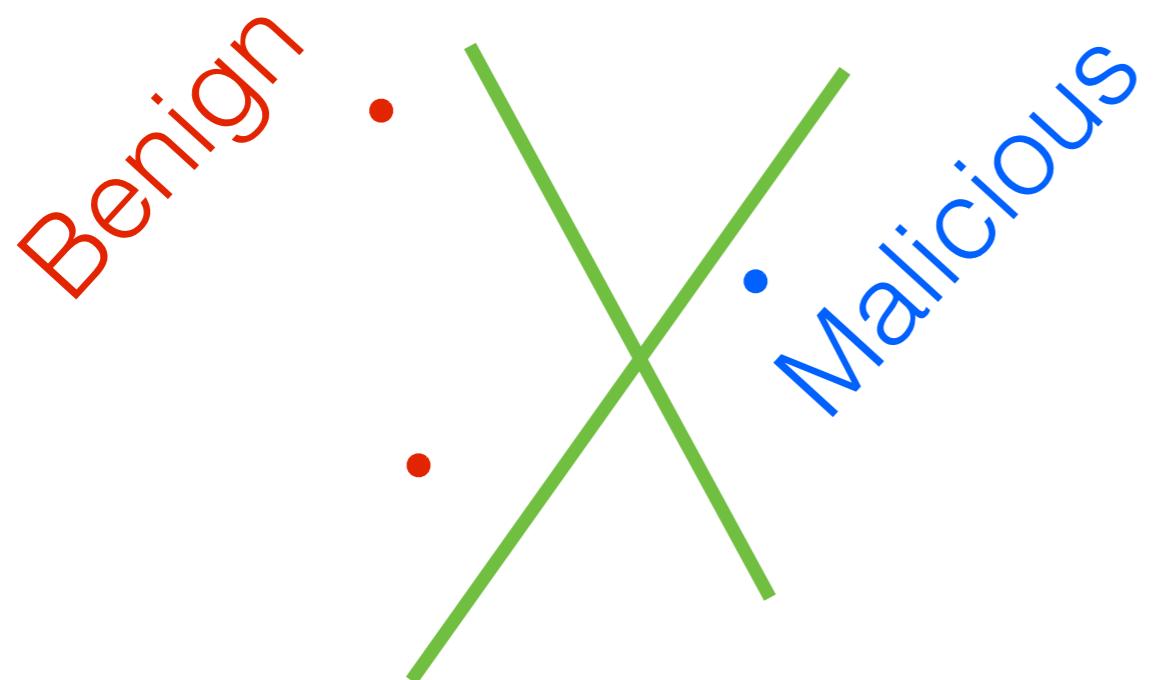
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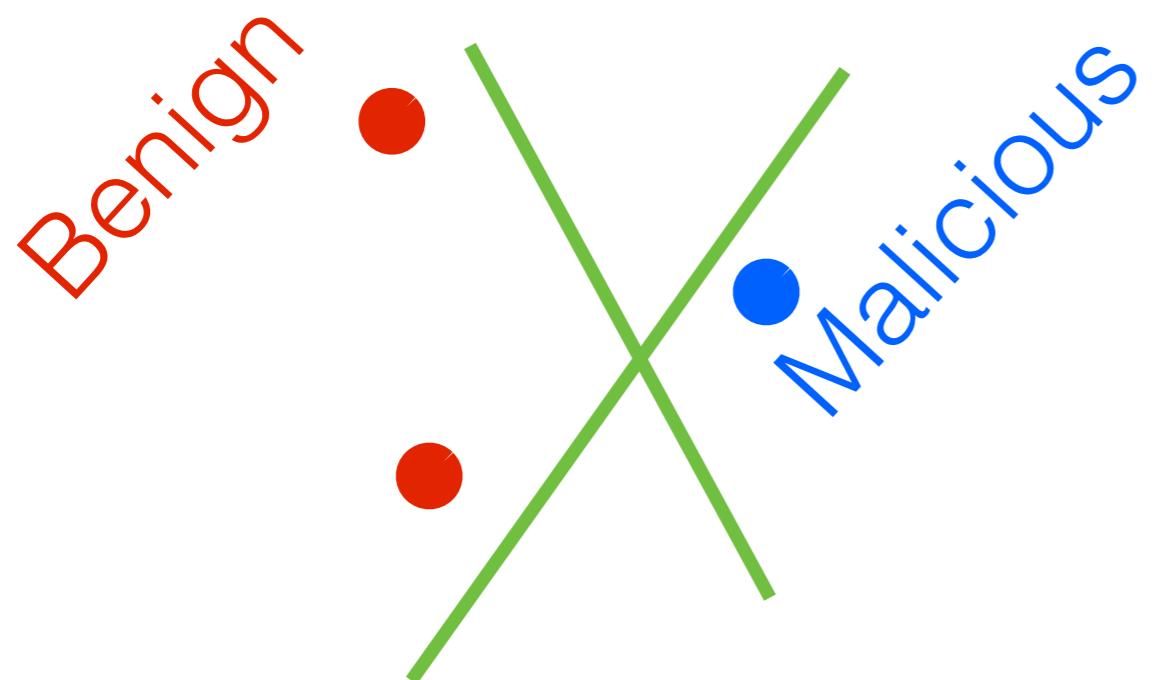
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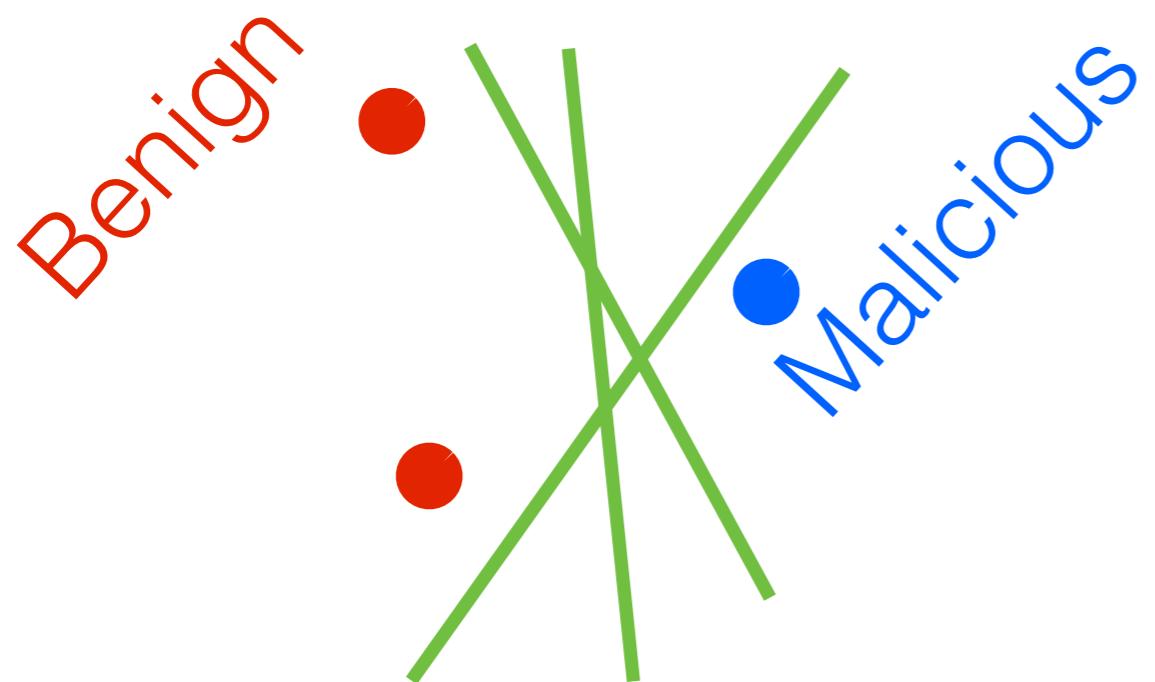
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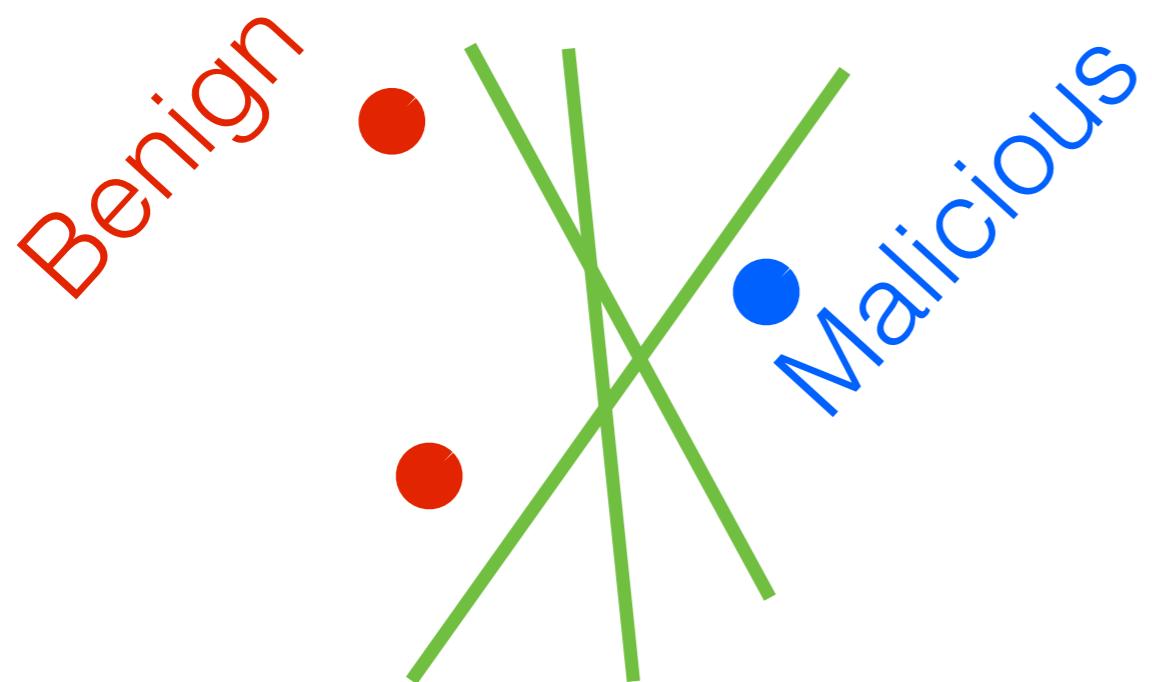
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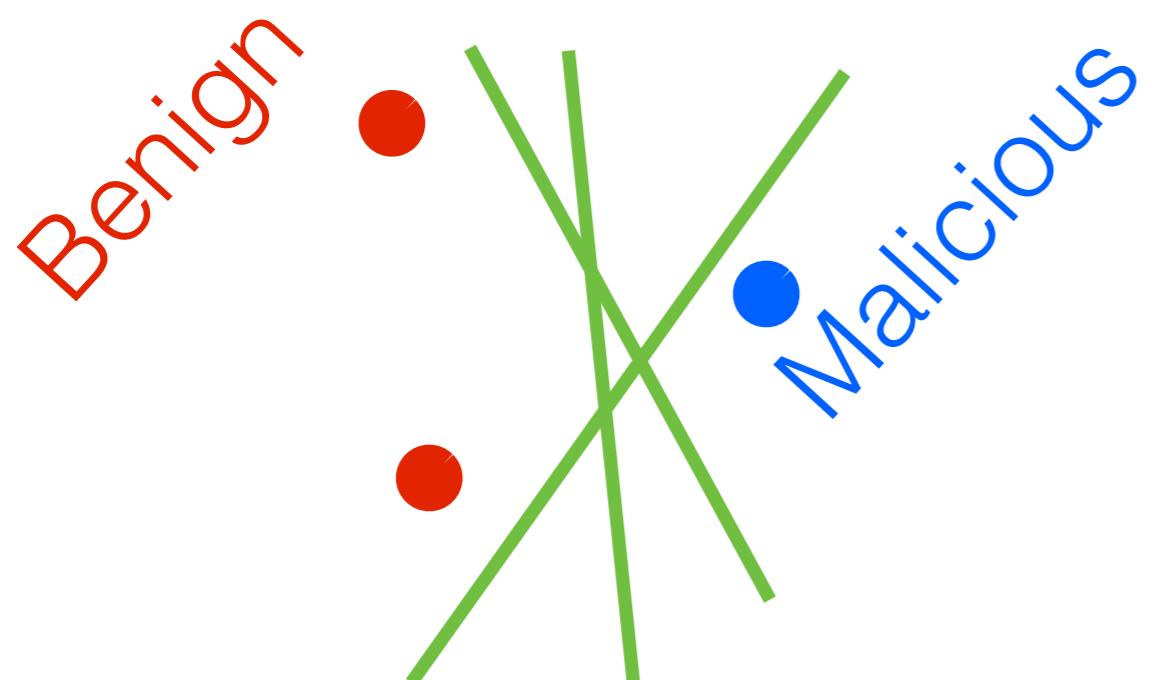
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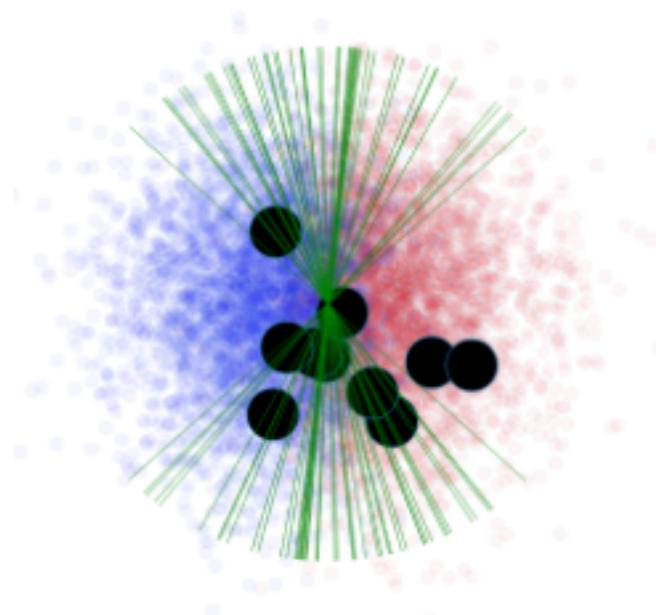


- Might miss important data
- Noisy estimates

Uniform subsampling

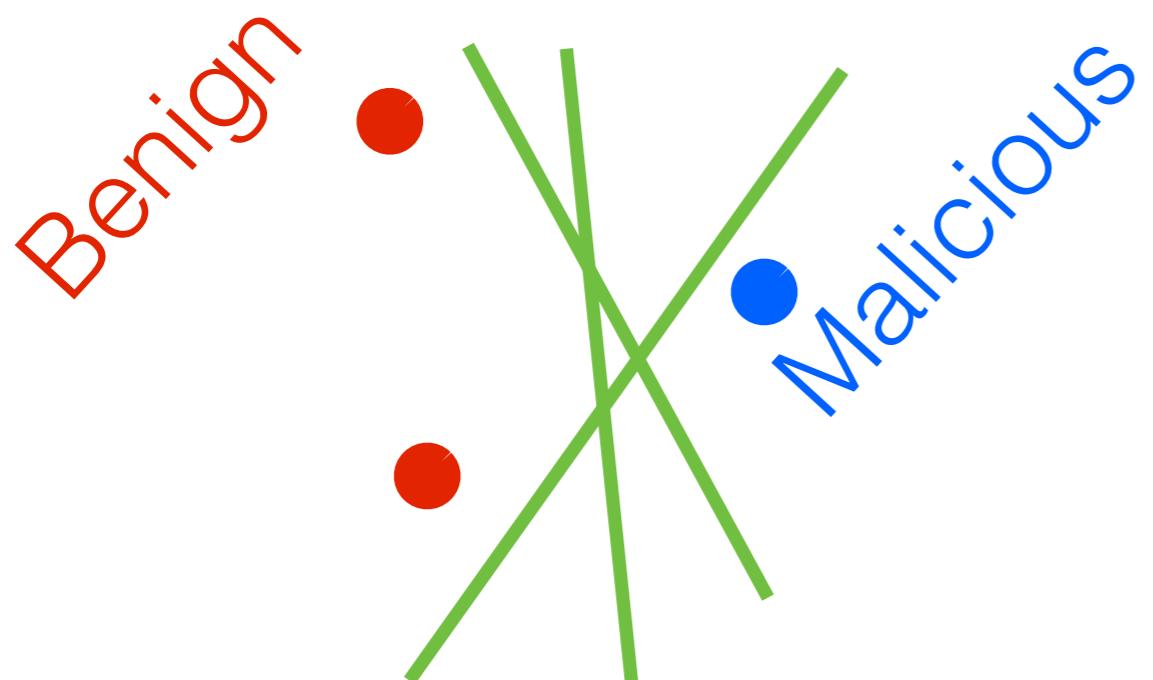


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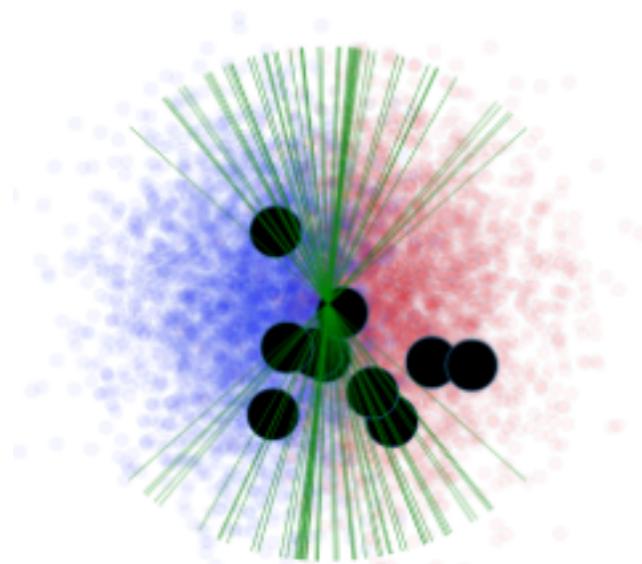


$M = 10$

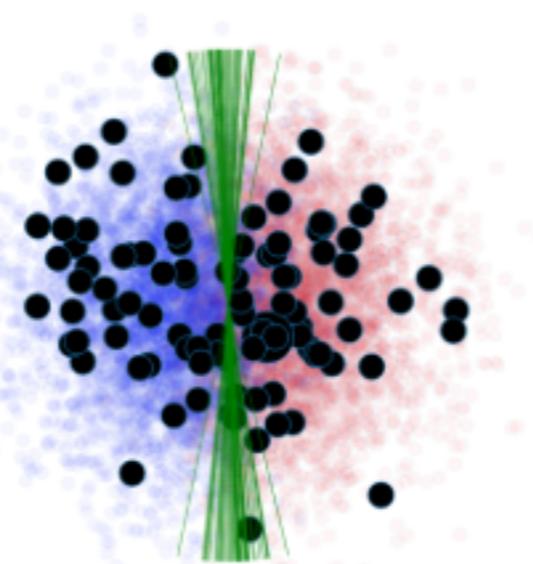
Uniform subsampling



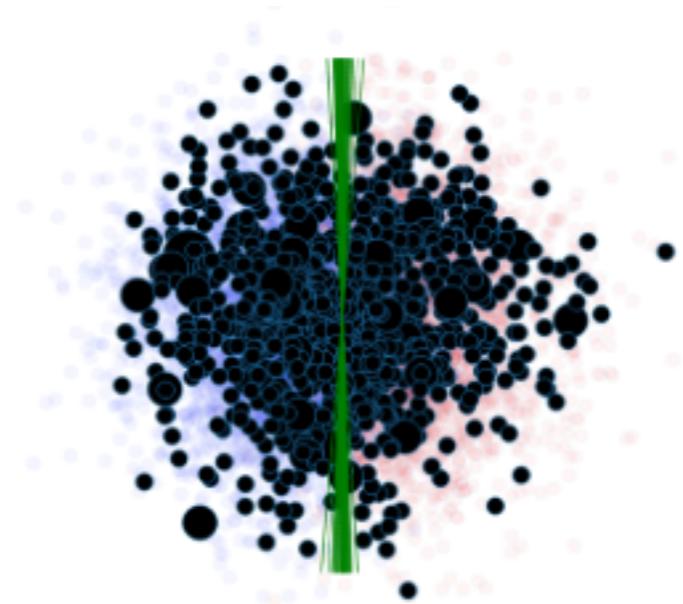
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$M = 10$



$M = 100$

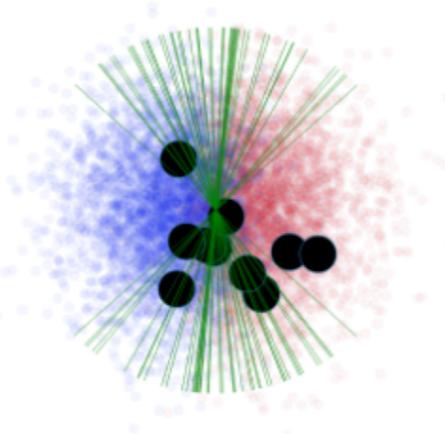


$M = 1000$

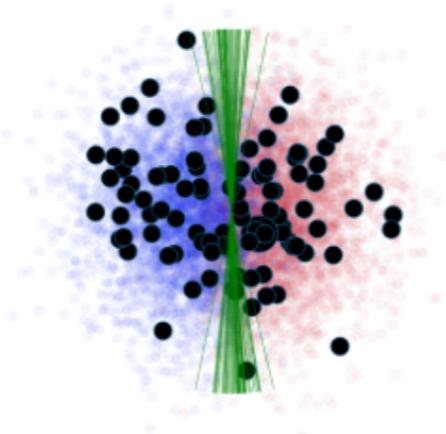
[Campbell, Broderick 2018, 2019]

Data summarization alternatives

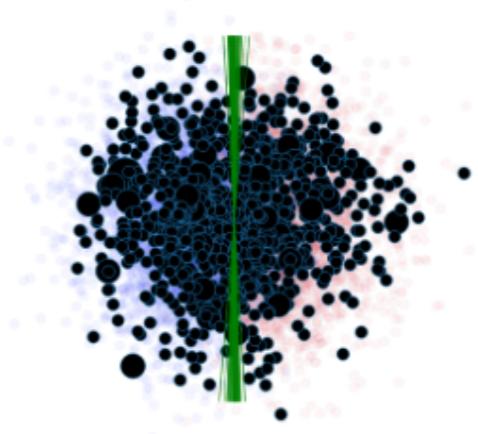
Uniform
subsampling



$$M = 10$$



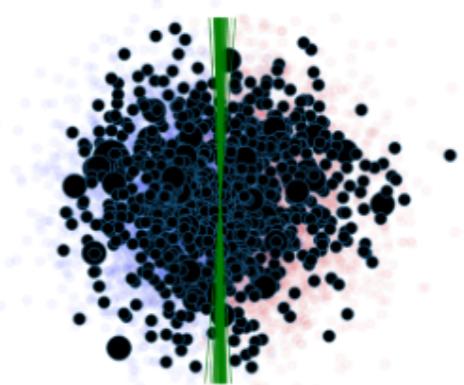
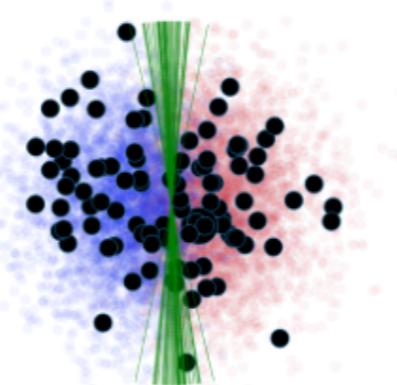
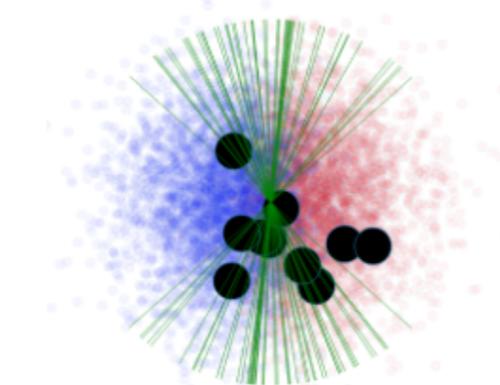
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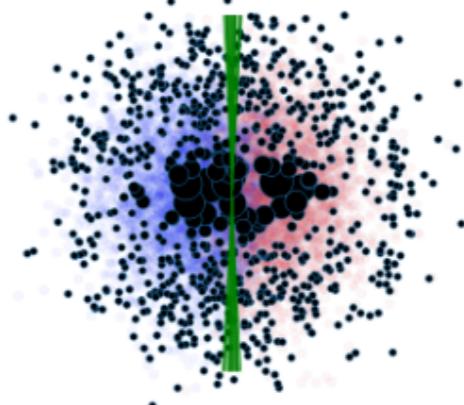
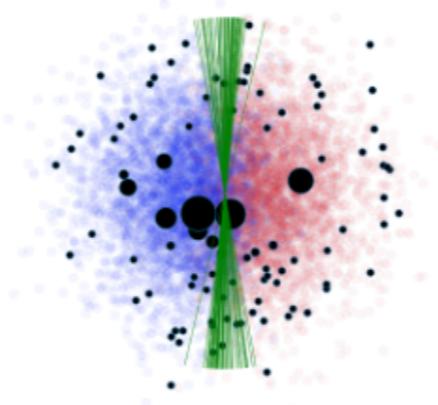
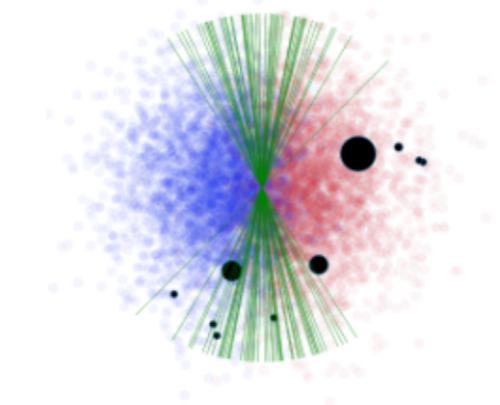
$$M = 1000$$

Data summarization alternatives

Uniform
subsampling



Importance
sampling



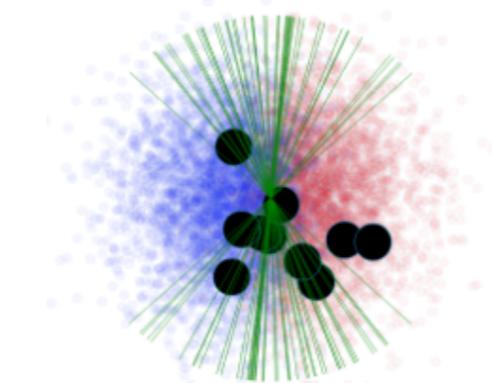
$M = 10$

$M = 100$

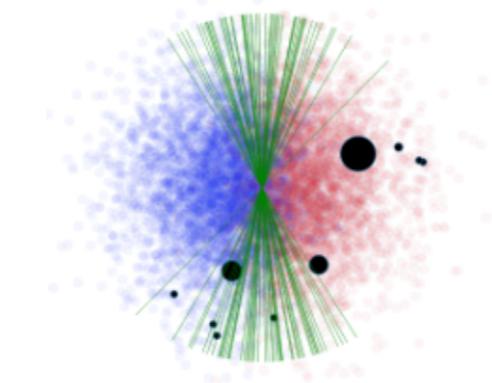
$M = 1000$

Data summarization alternatives

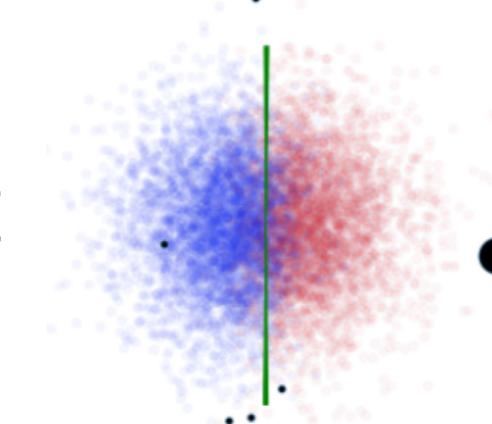
Uniform
subsampling



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.
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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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