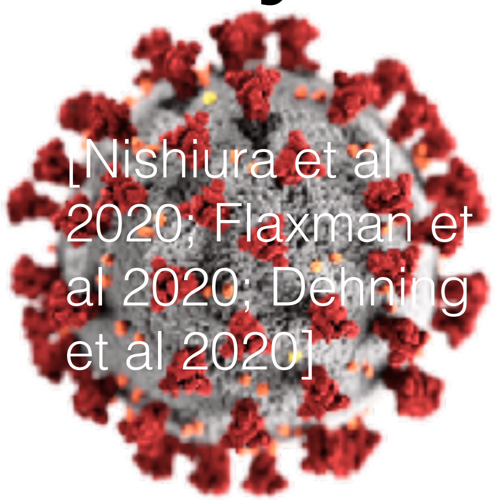
Variational Bayes and beyond: Foundations of scalable Bayesian inference (Part III)

Tamara Broderick
Associate Professor
MIT

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

Bayesian inference

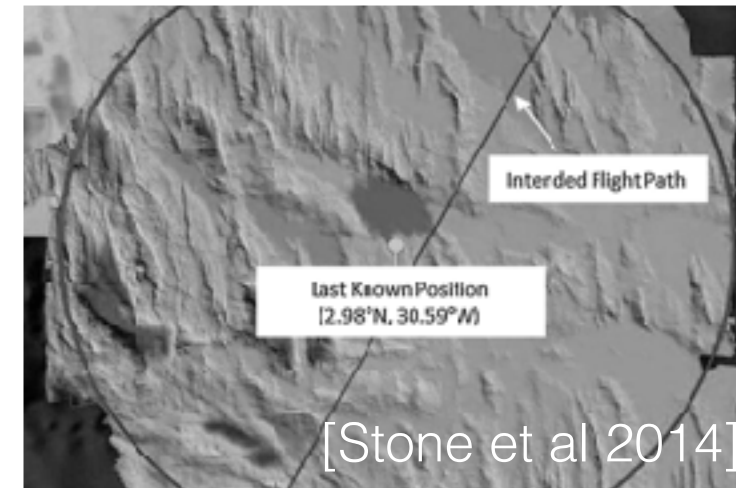


[Nishiura et al 2020; Flaxman et al 2020; Dehning et al 2020]

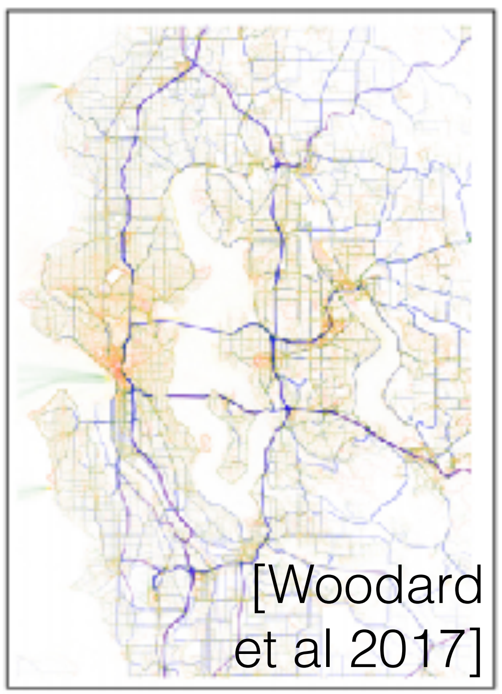
[Gillon et al 2017l Grimm et al 2018]

[Abbott et al 2016a,b]

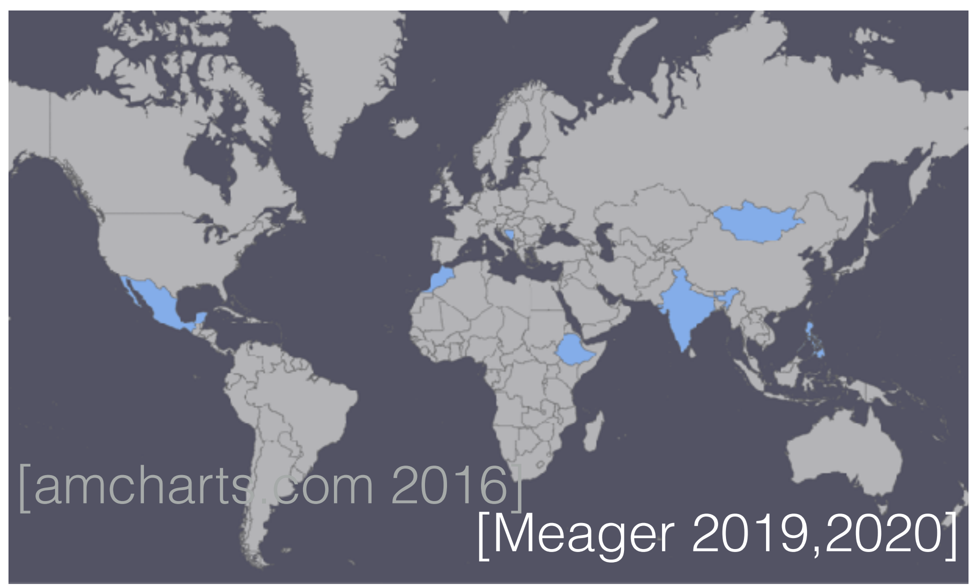
[ESO/ L. Calçada/ M. Kornmesser 2017]



[Stone et al 2014]



[Woodard et al 2017]



[amcharts.com 2016]

[Meager 2019,2020]

[Kuikka et al 2014]

[Baltic Salmon Fund]

[Chati, Balakrishnan 2017]

[Julian Hertzog 2016]

[mc-stan.org]

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

Criteo Online Ads Experiment

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

[Giordano, Broderick, Jordan 2018]

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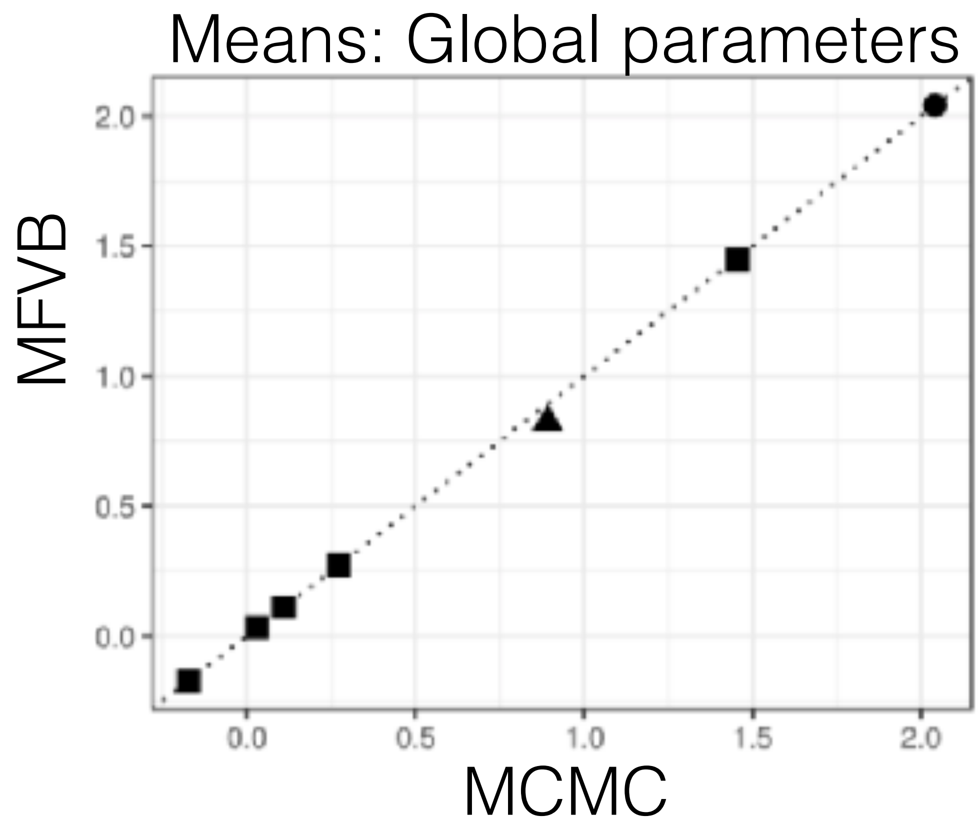

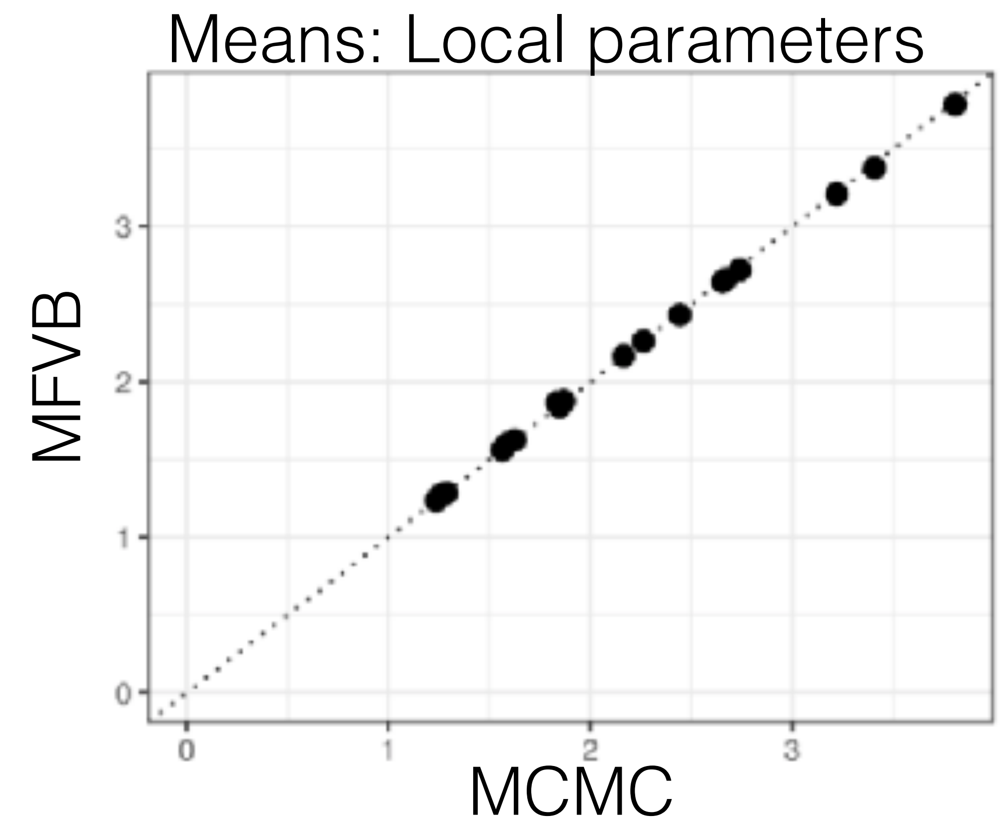

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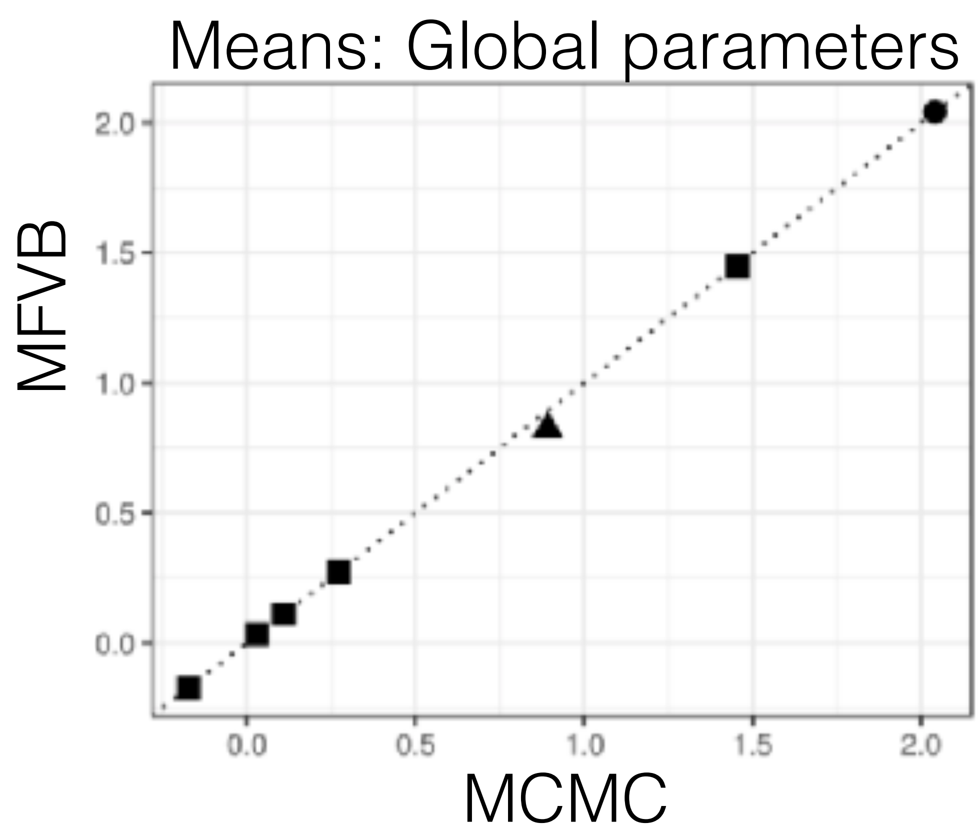

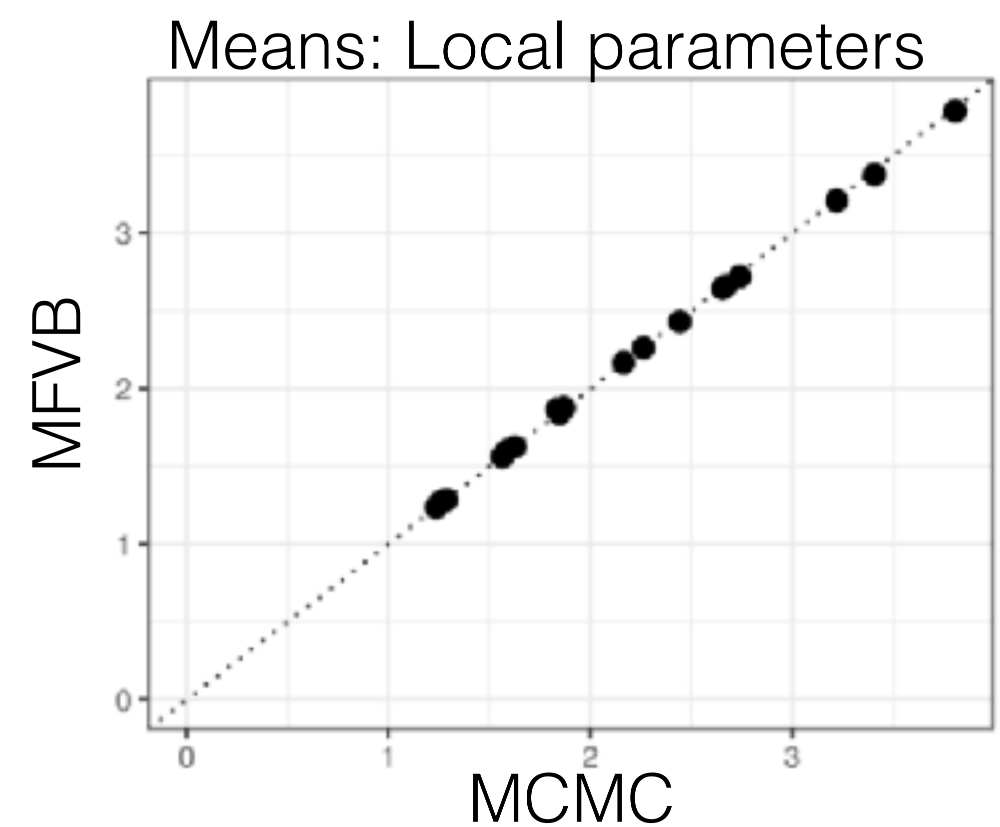

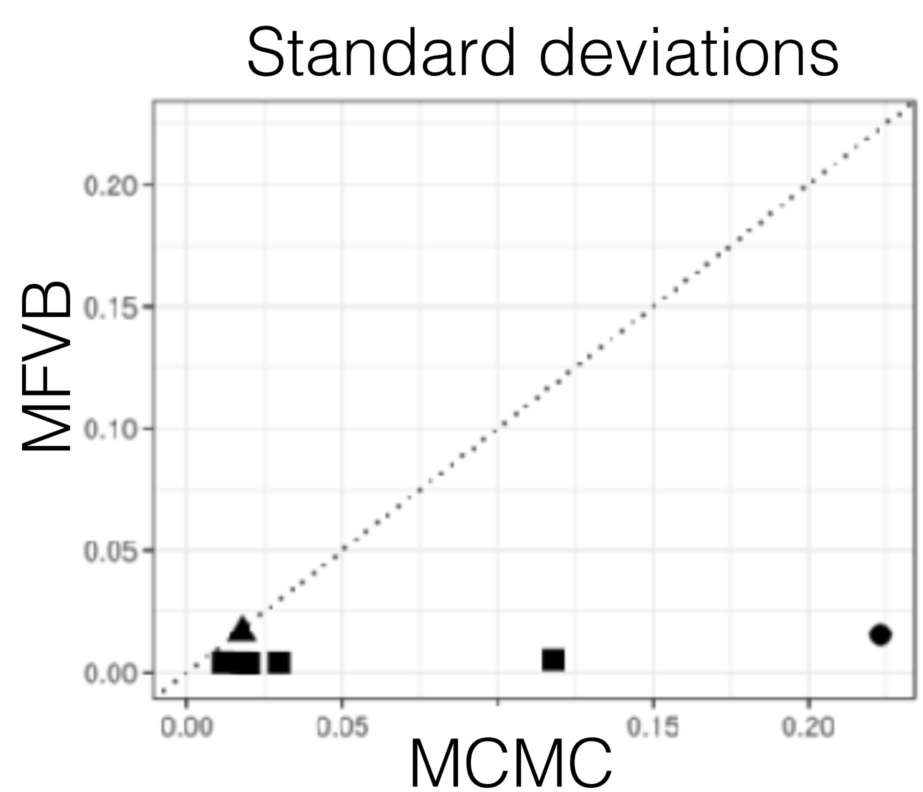

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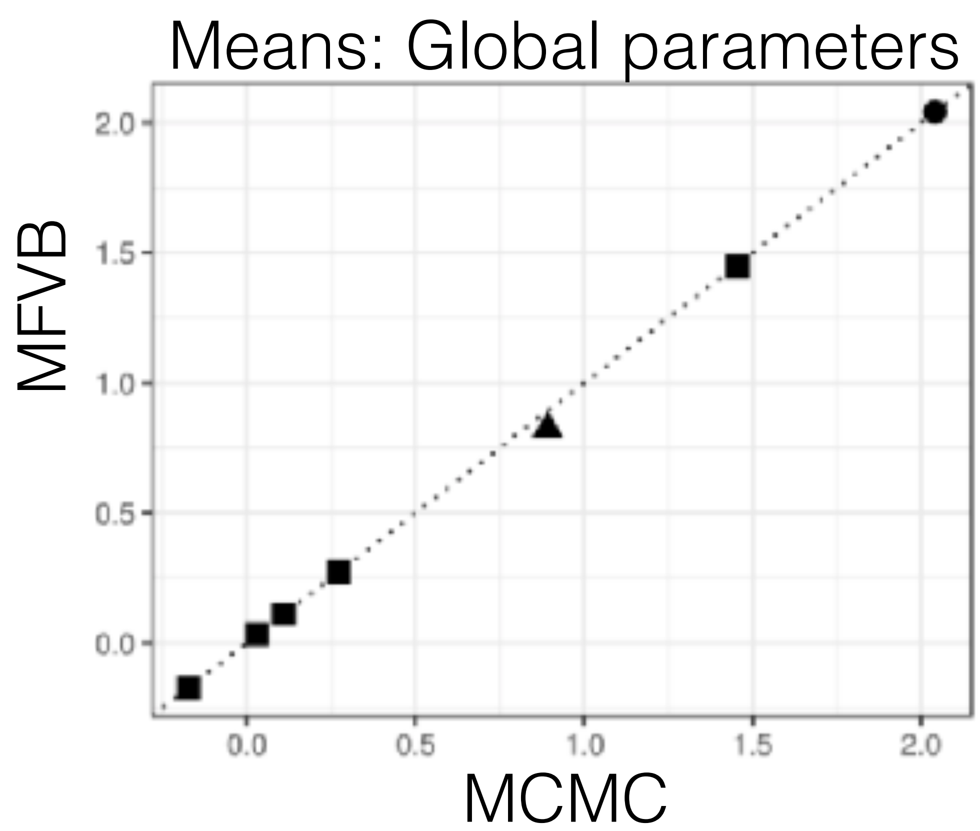

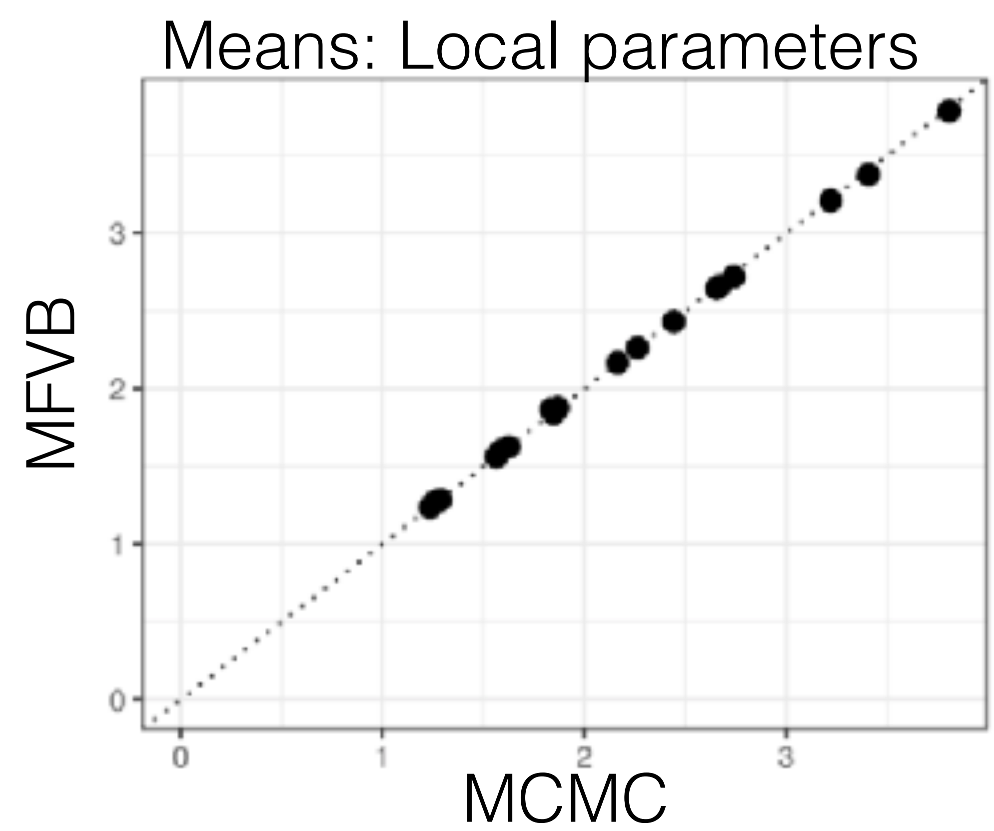

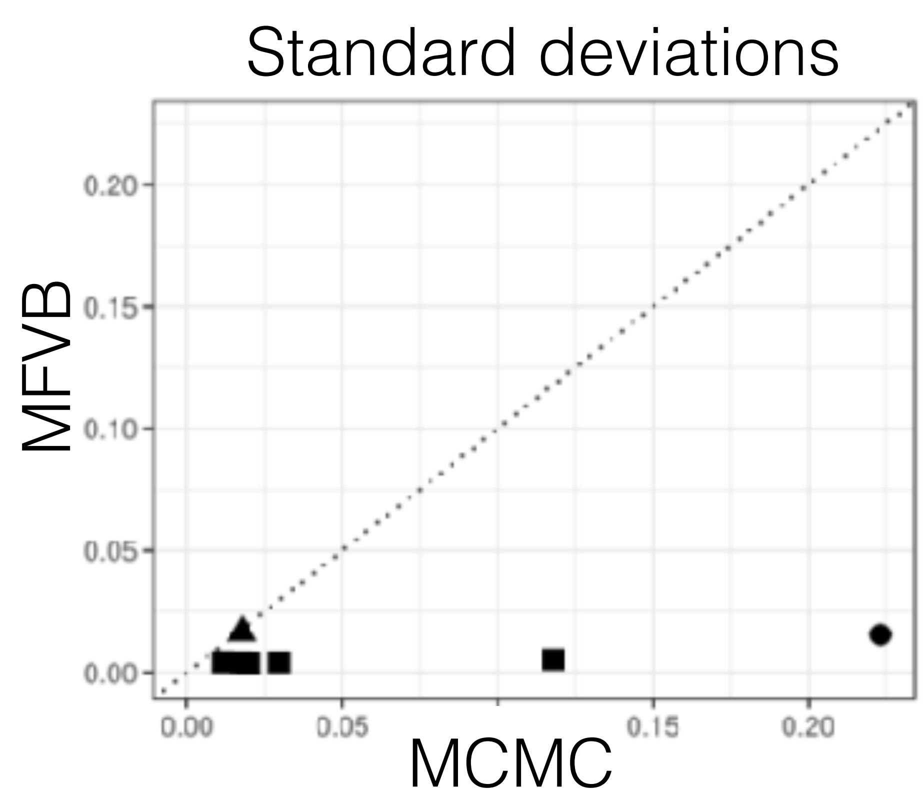

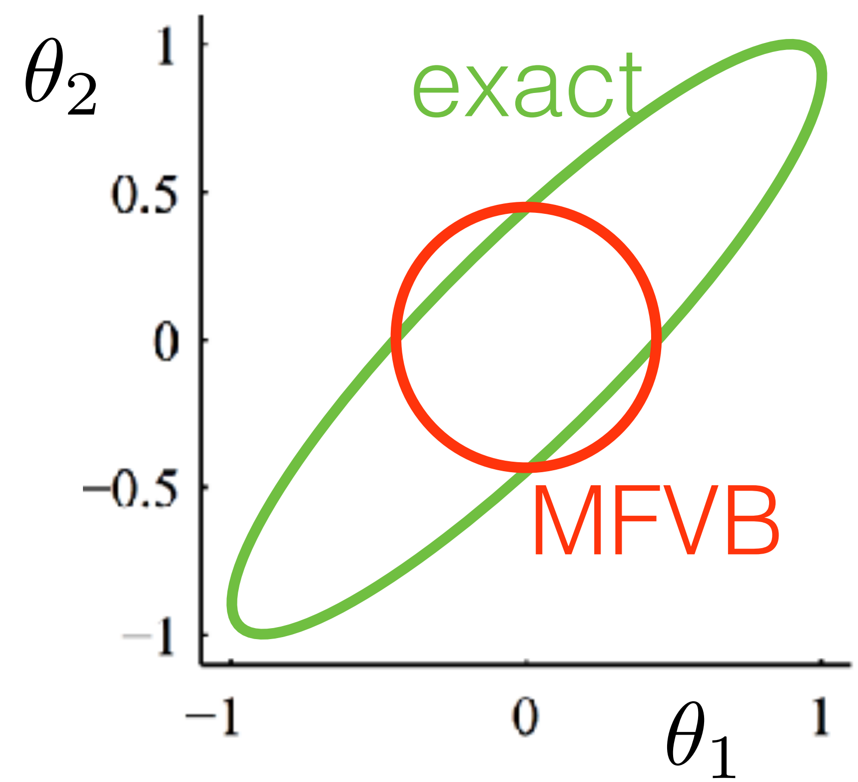

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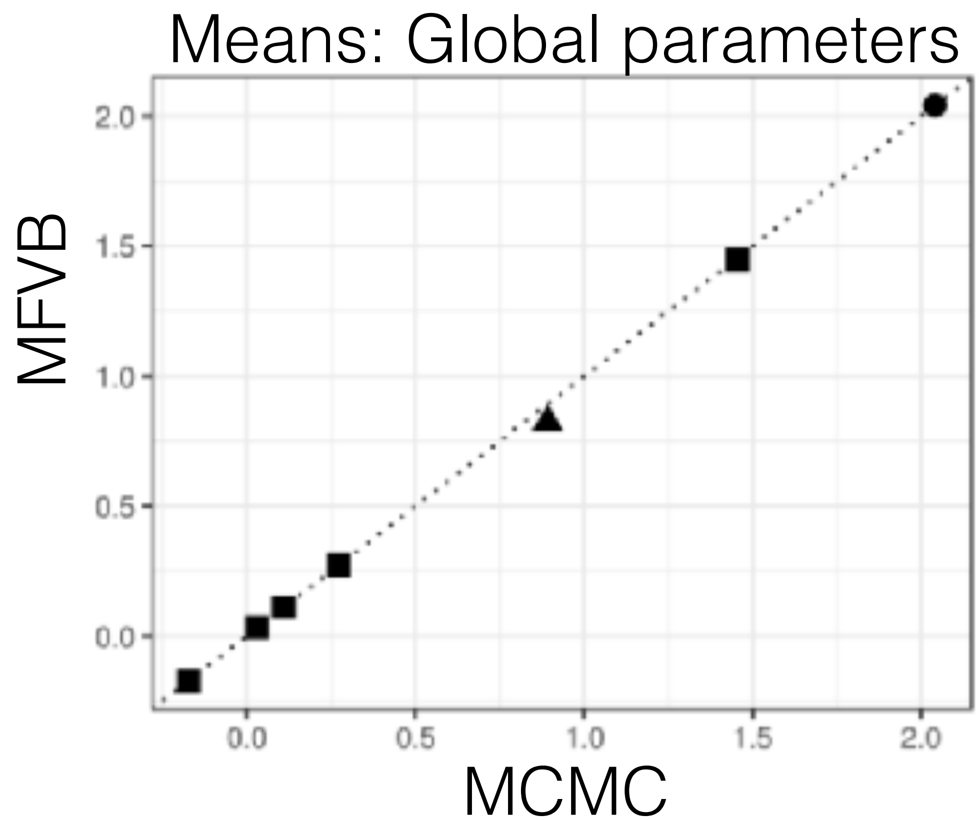

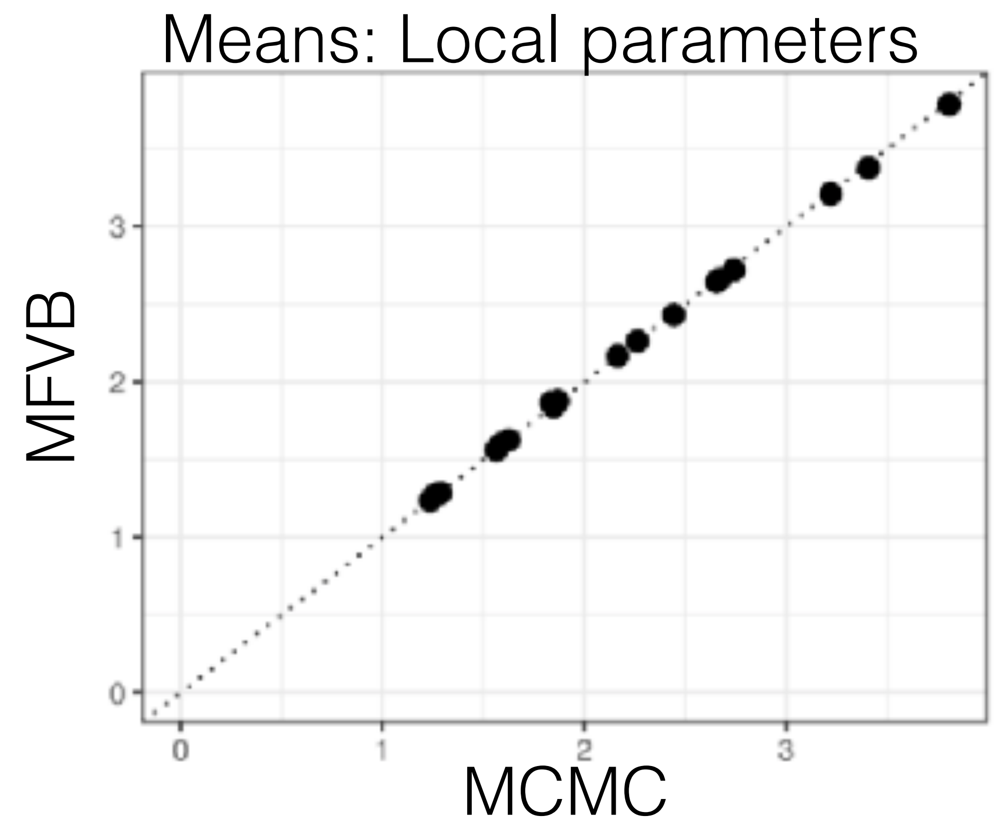

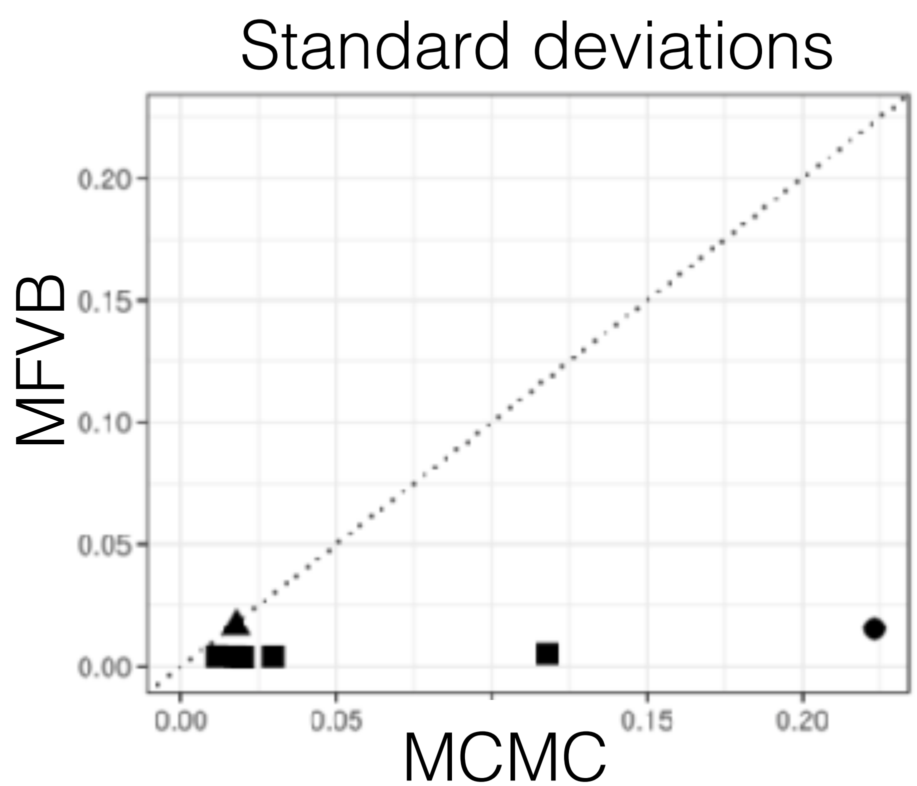

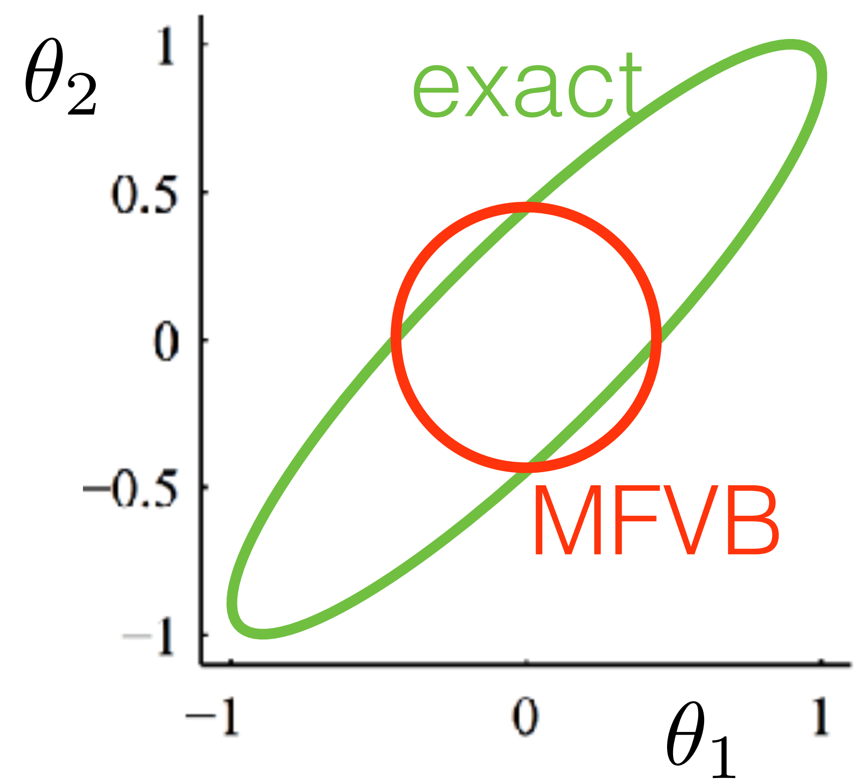

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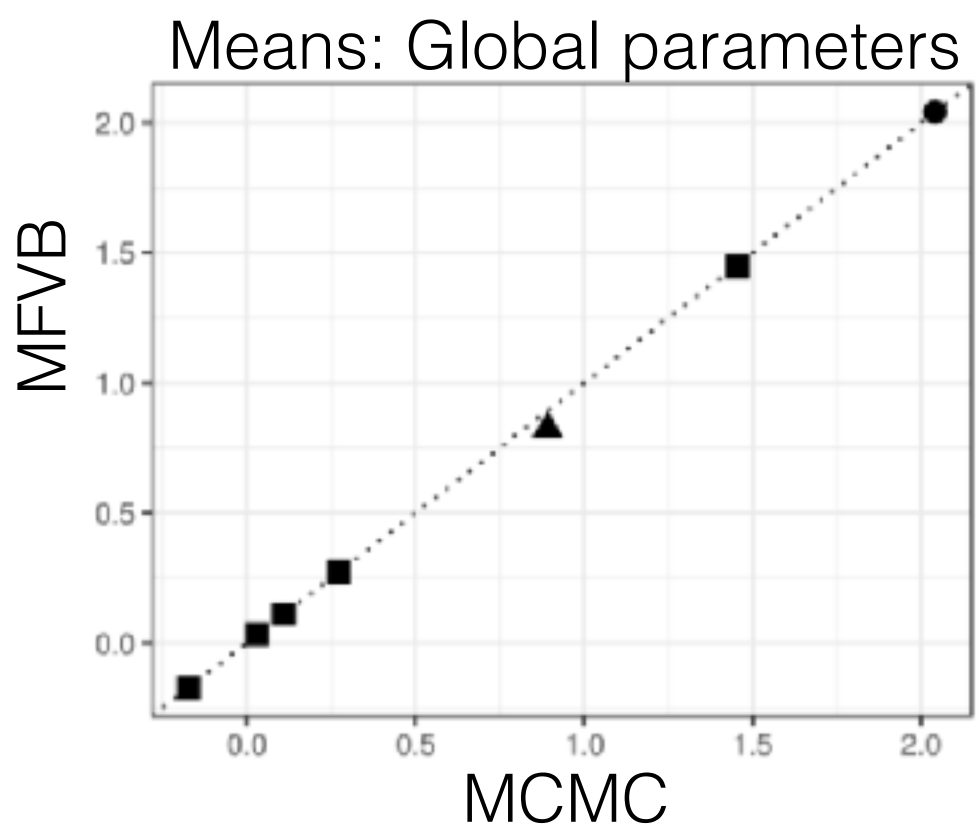

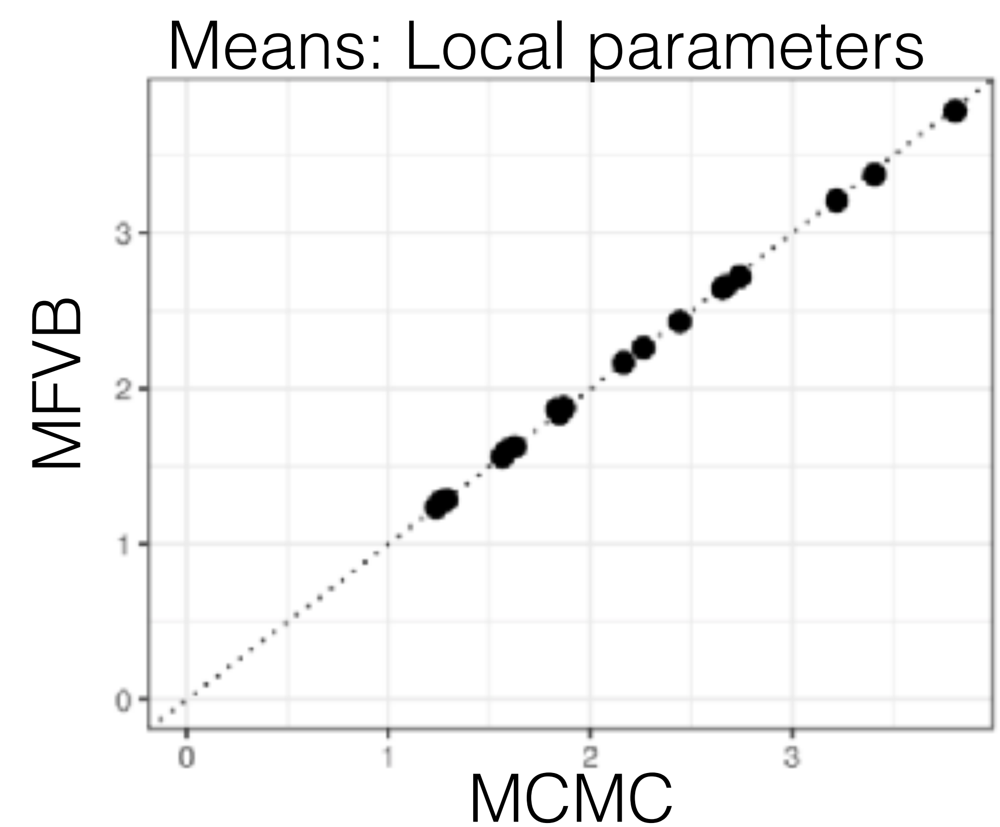

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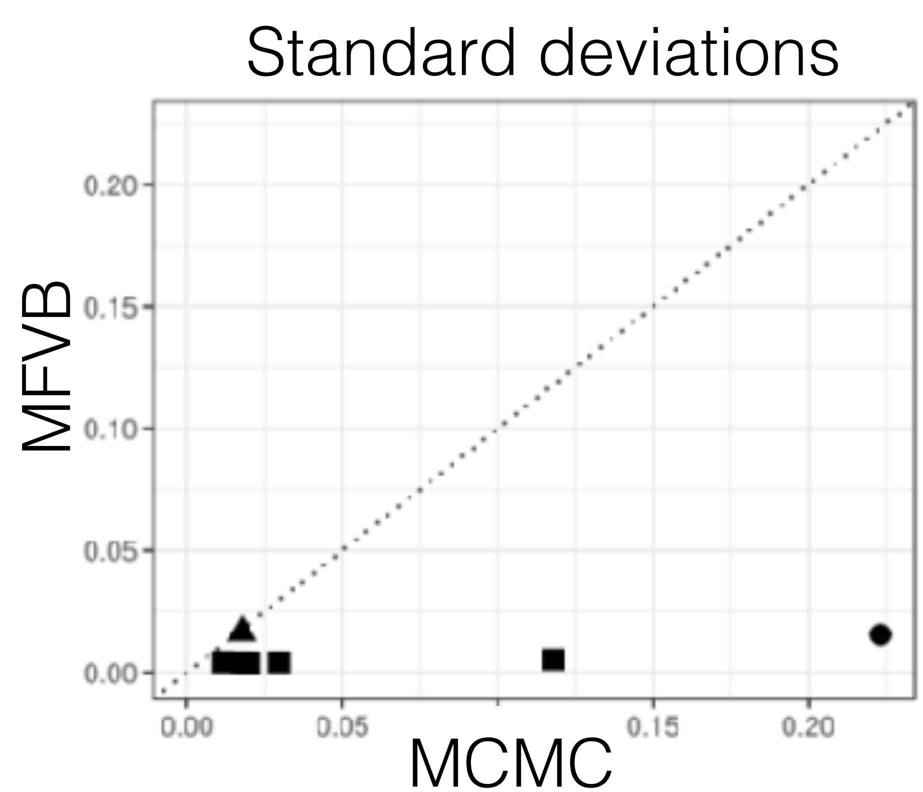
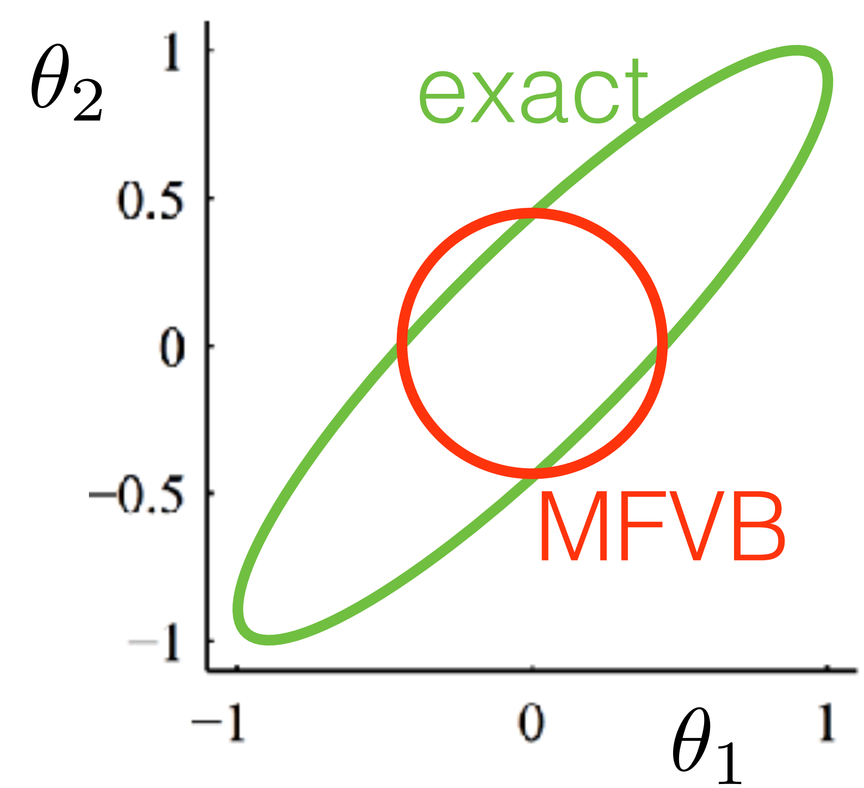
- Posterior means





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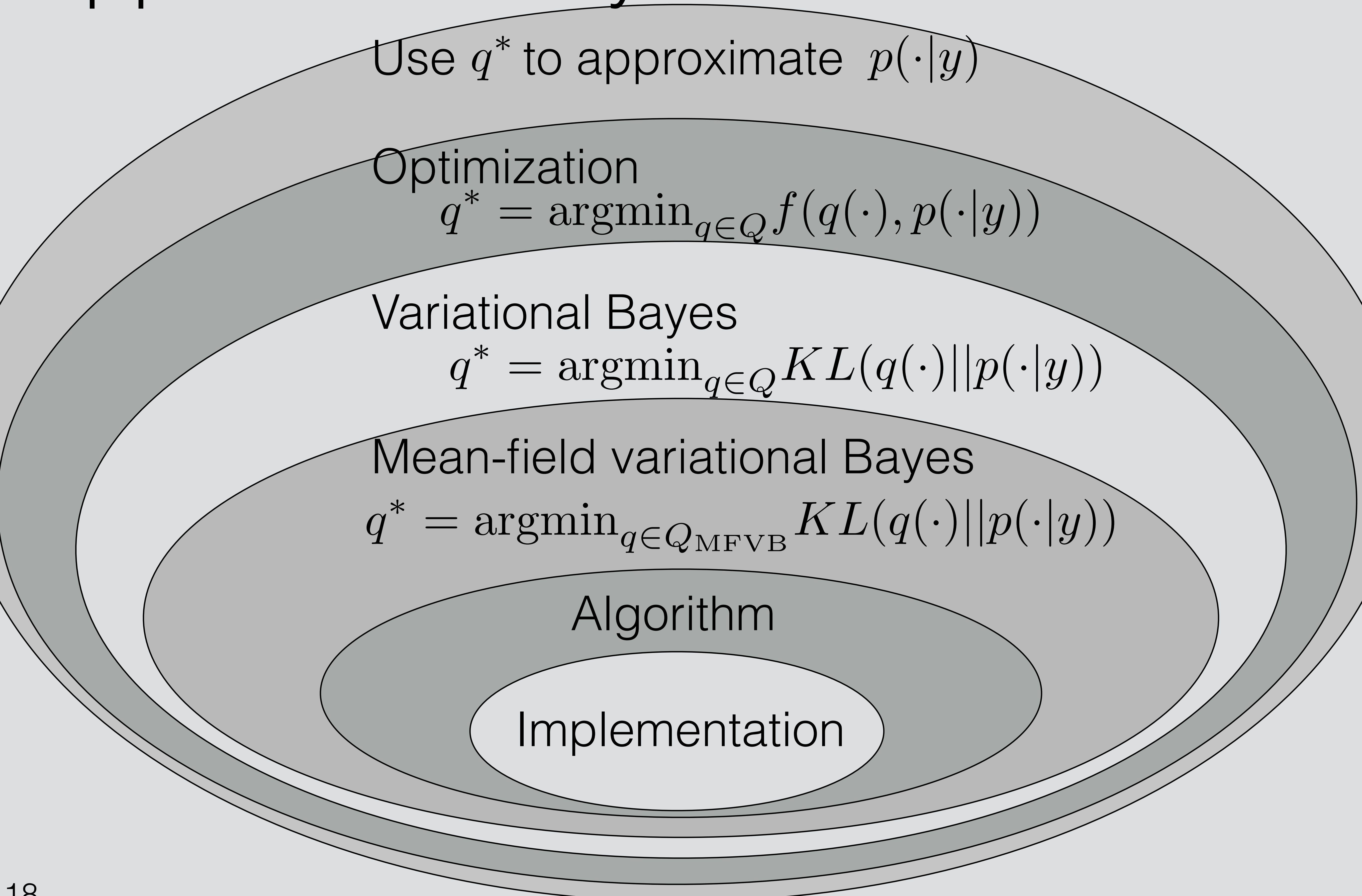
Approximate Bayesian inference



Approximate Bayesian inference

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

Optimization

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

Variational Bayes

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

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

Algorithm

Implementation

How deep is the issue?

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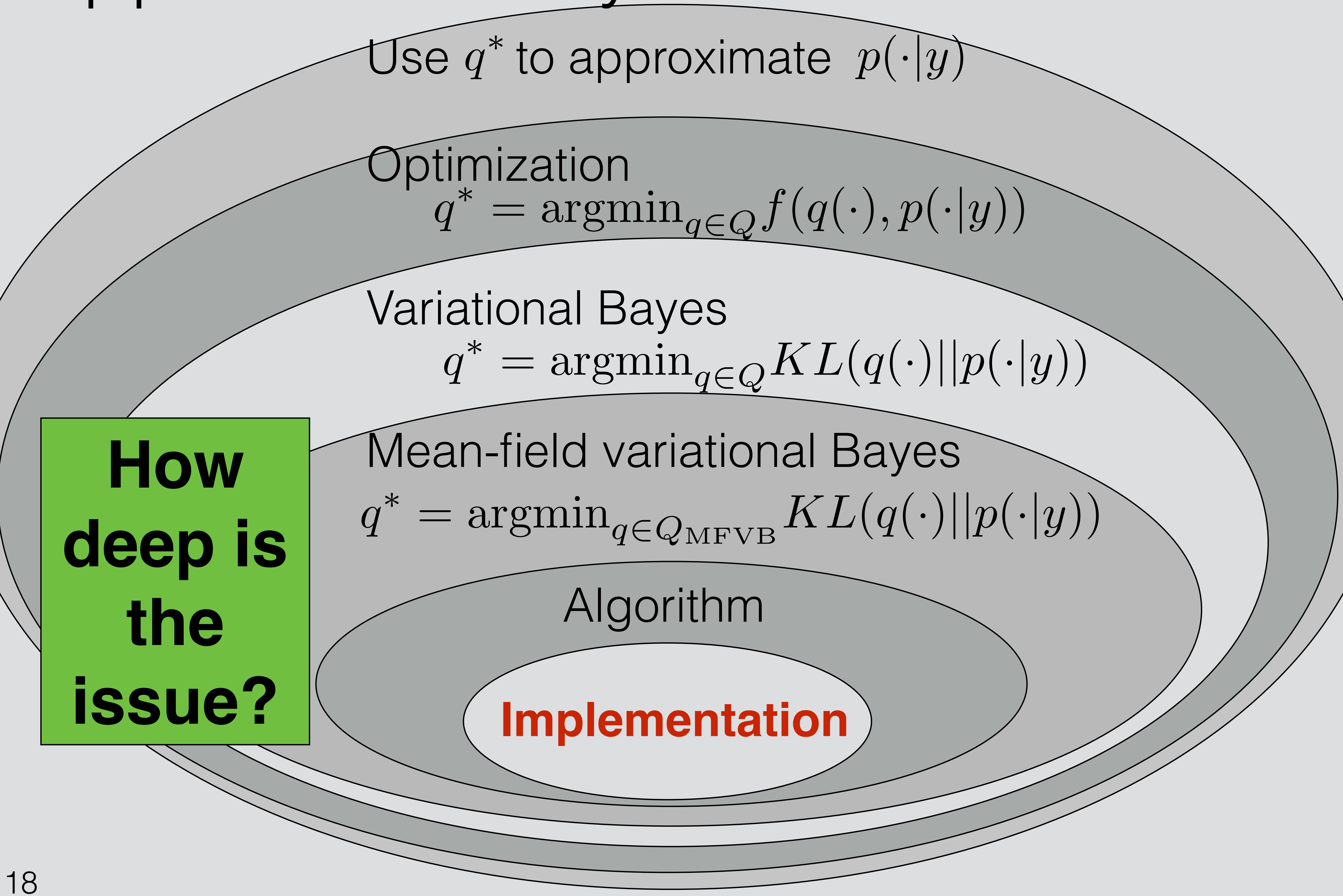

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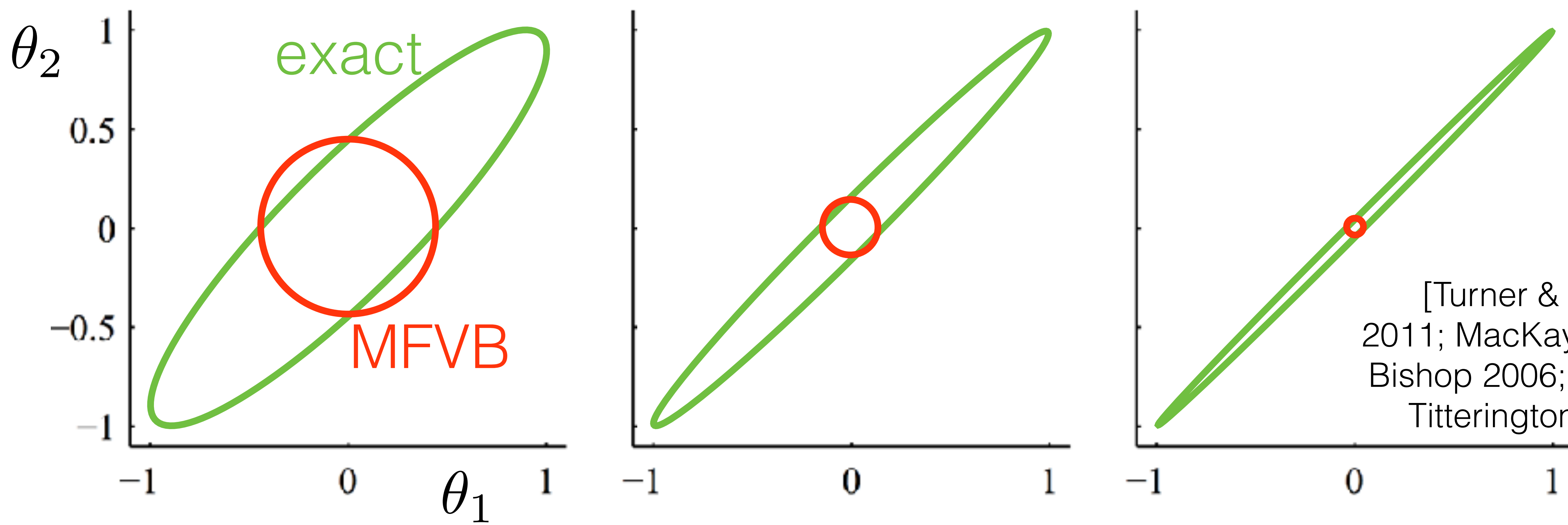
$$KL(q||p(\cdot|y)) = \int_\theta q(\theta) \log \frac{q(\theta)}{p(\theta|y)} d\theta \qquad q(\theta) = \prod_{j=1}^{J} q_j(\theta_j)$$



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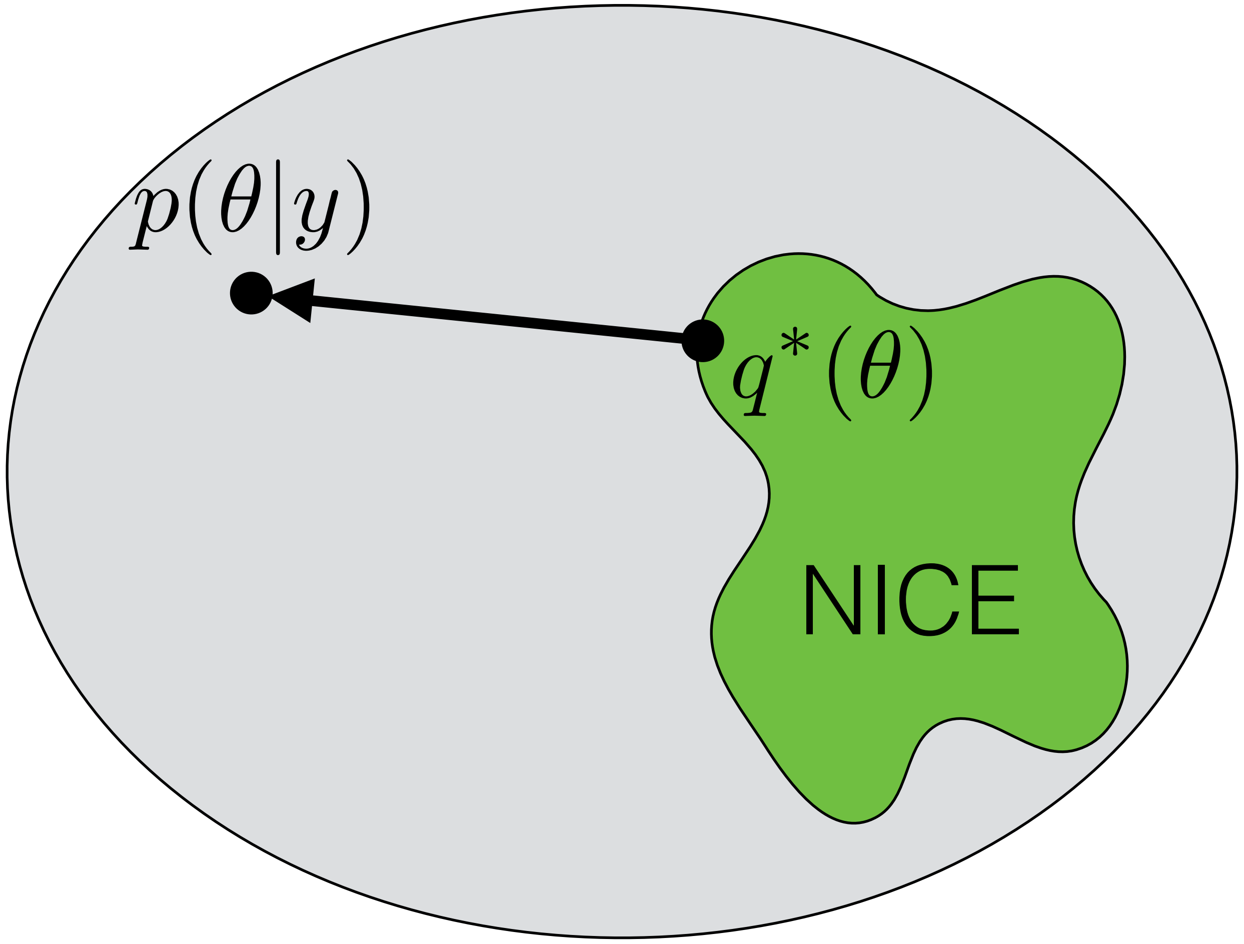

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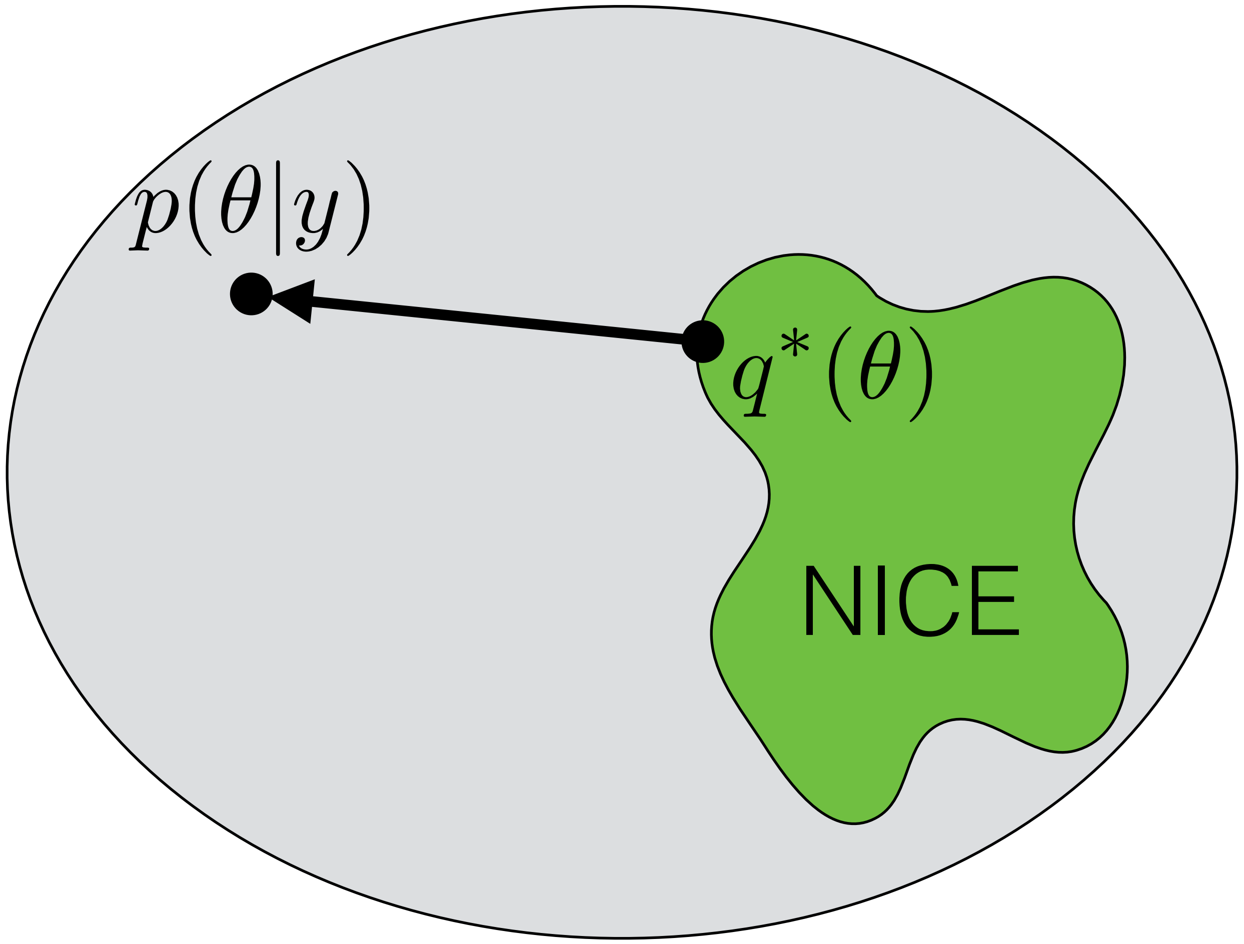

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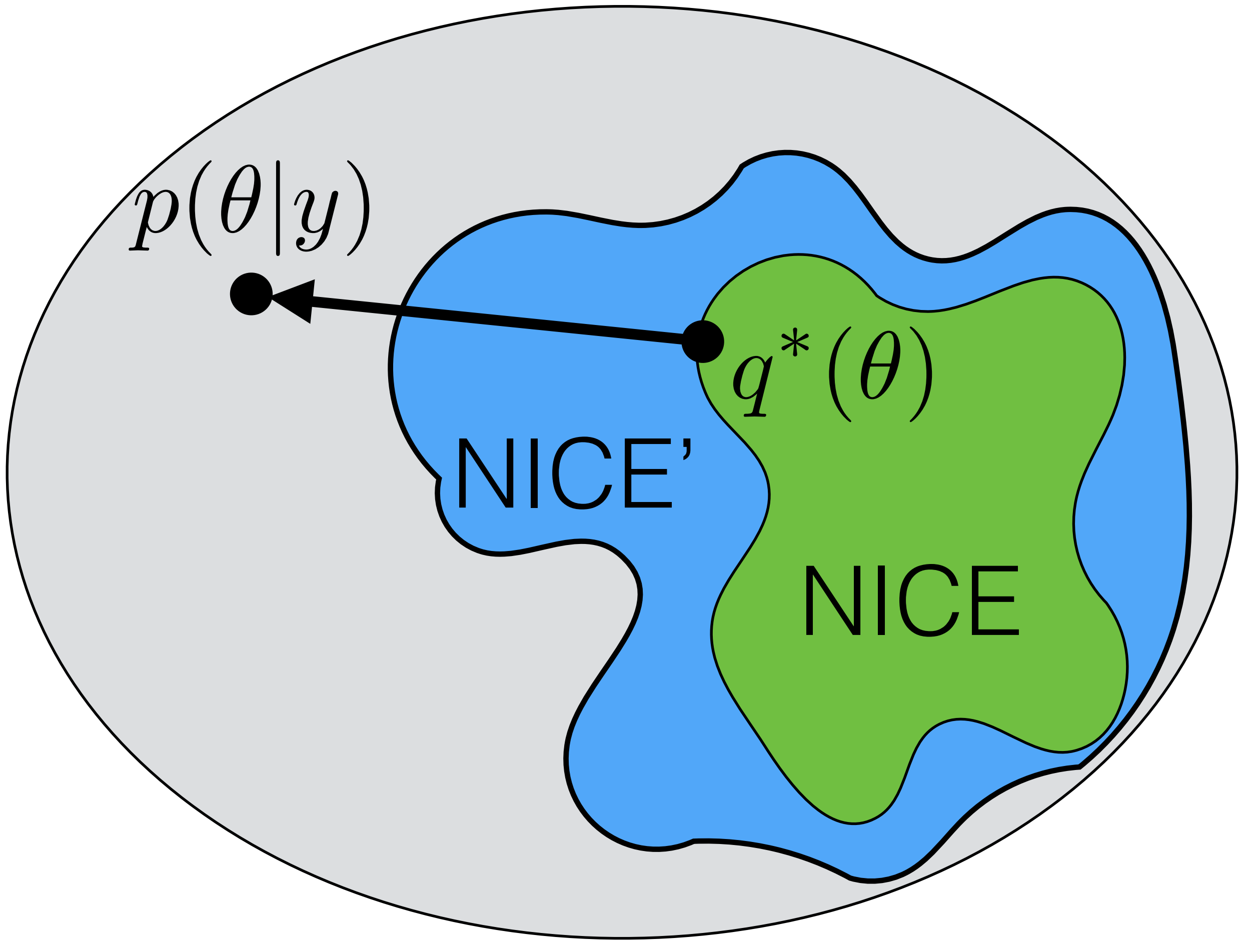

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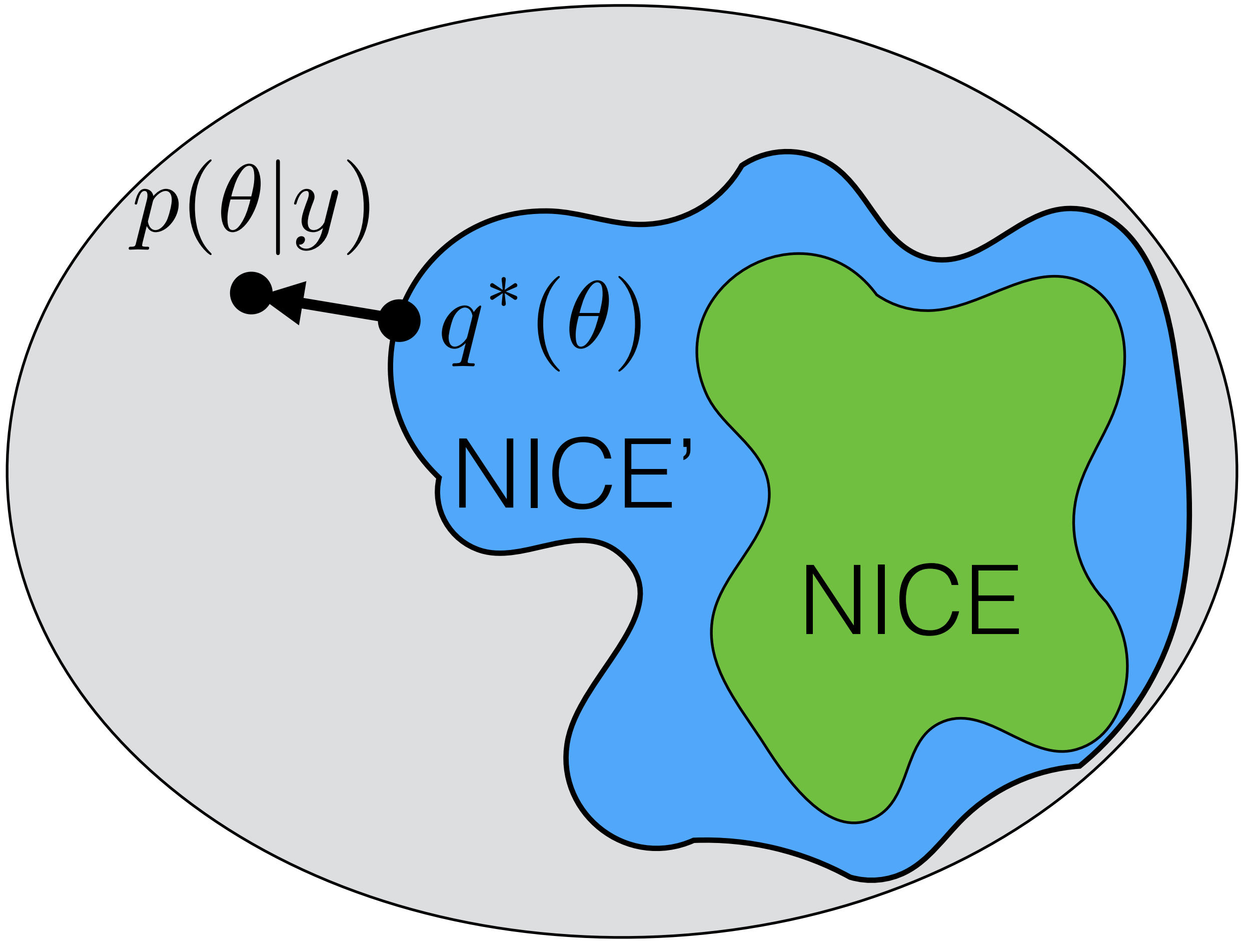

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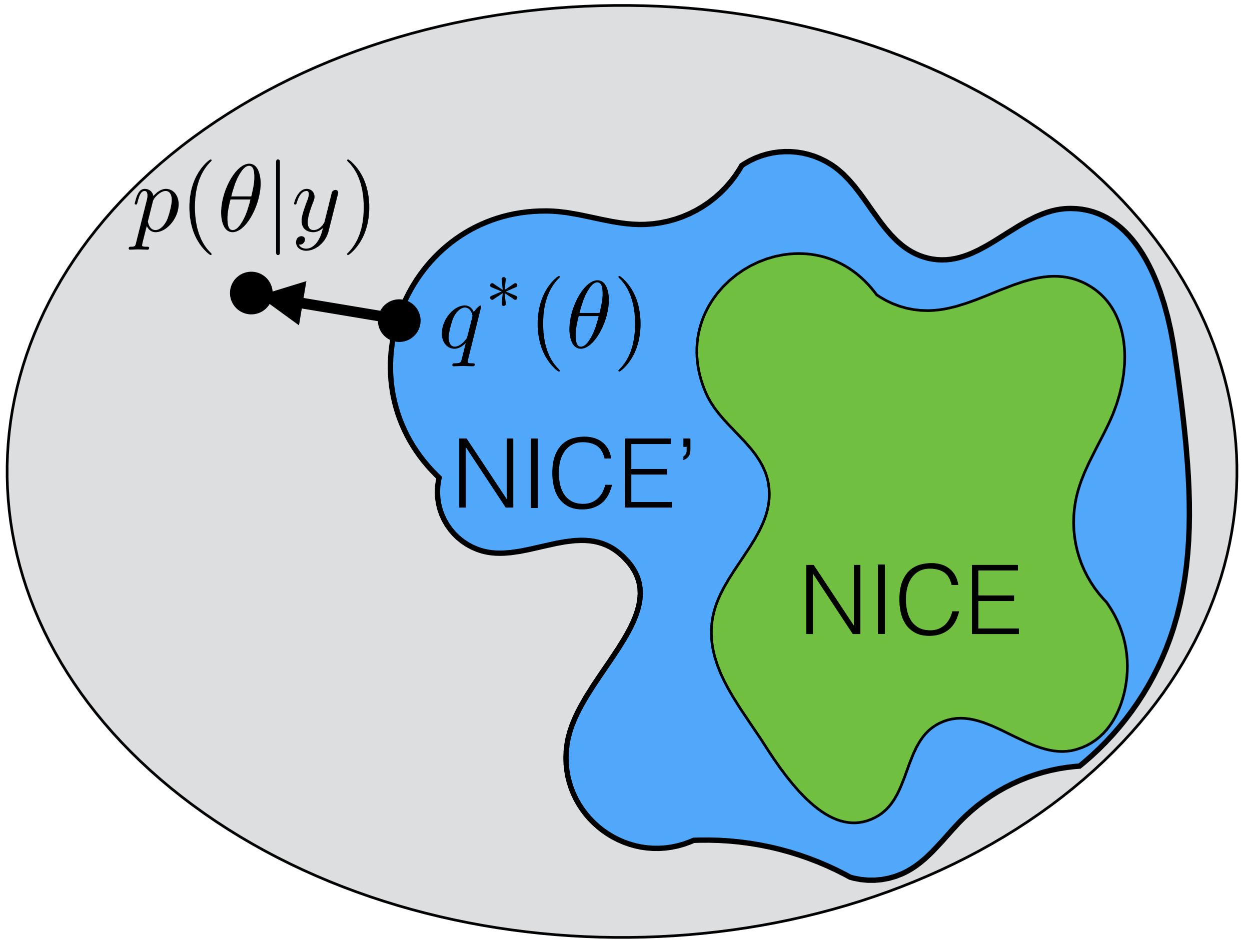

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- Exercise: Show, with a simple example, that a smaller KL does not imply better mean and variance estimates

[Baqué et al 2017; Huggins, Karsprzak, Campbell, Broderick 2020]

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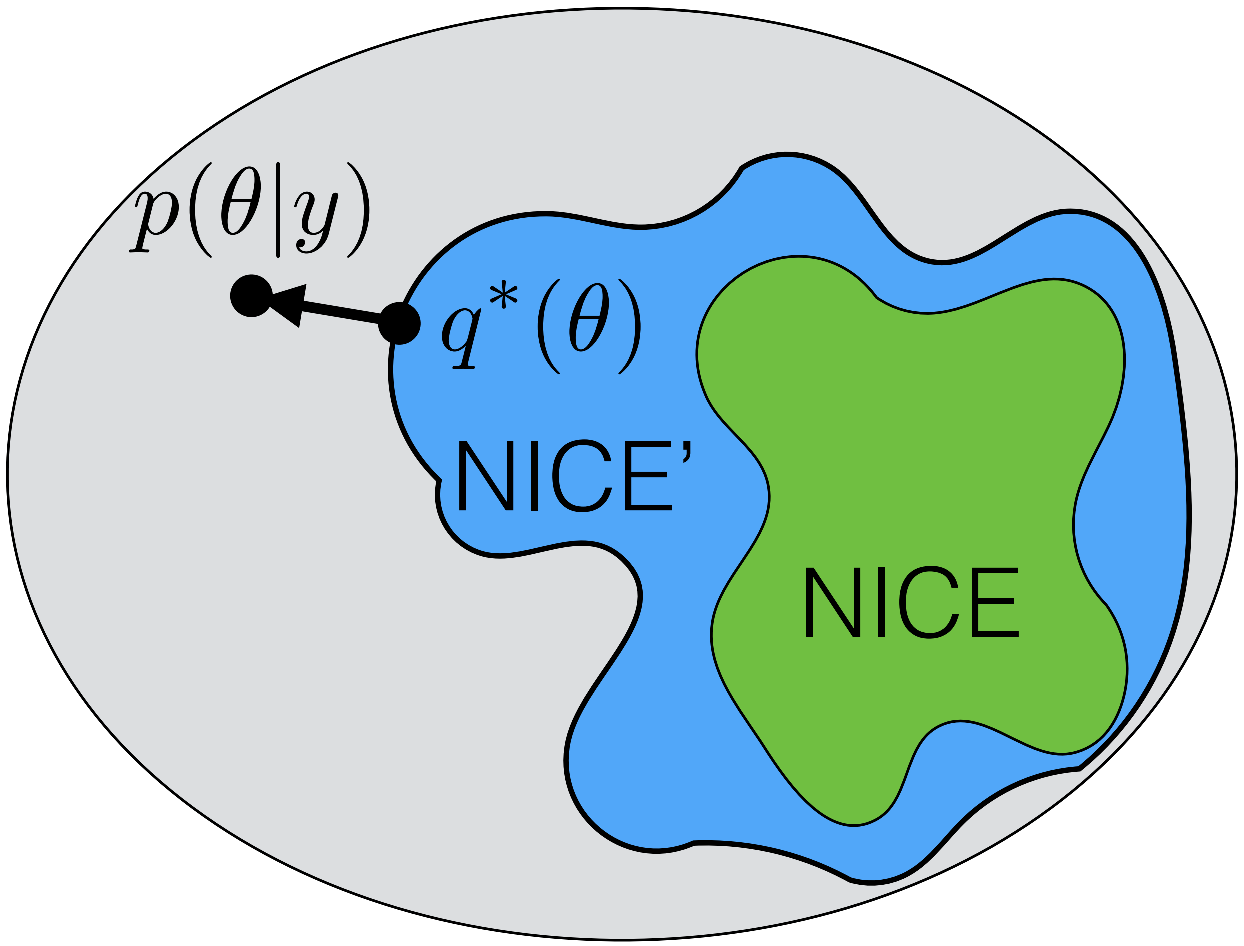

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- Exercise: Show, with a simple example, that a smaller KL does not imply better mean and variance estimates
- But how much worse can the estimates be? And could it have just been the implementation?

[Baqué et al 2017; Huggins, Karsprzak, Campbell, Broderick 2020]

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

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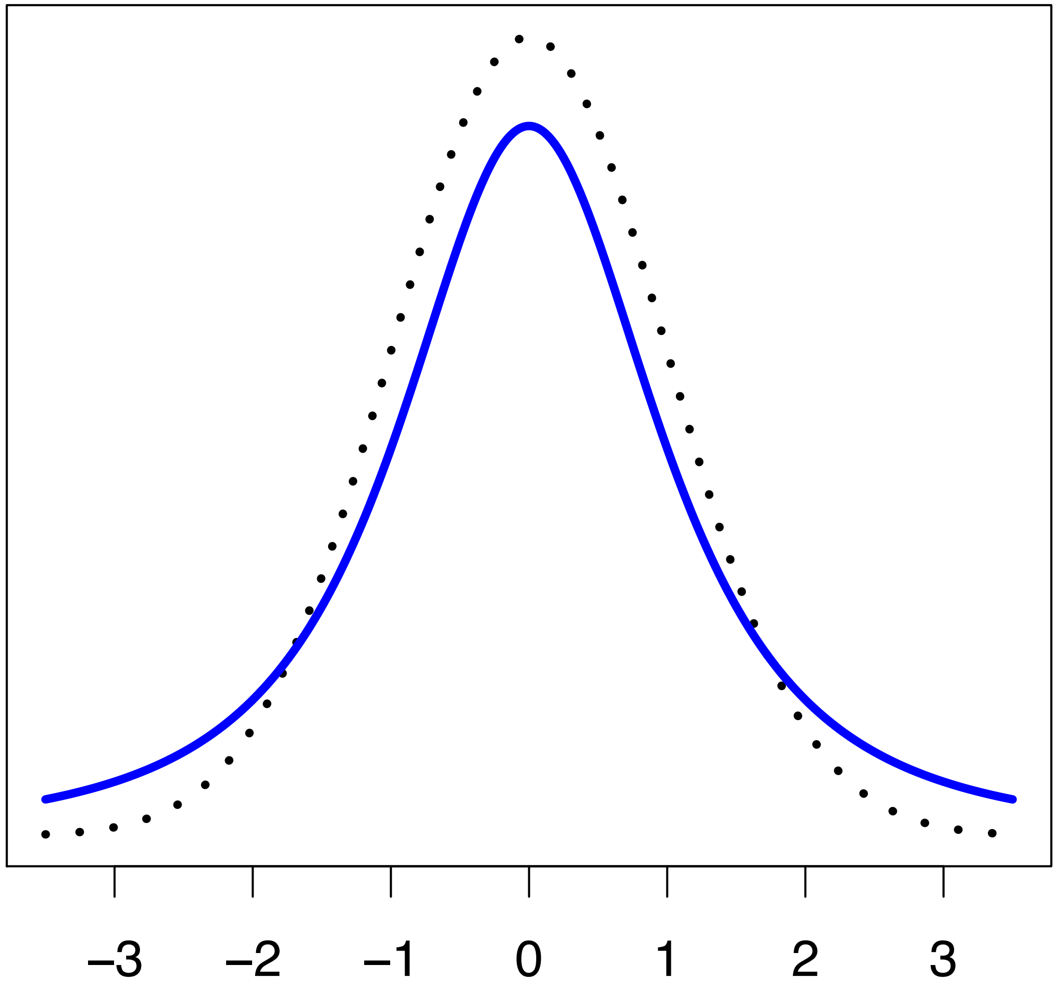

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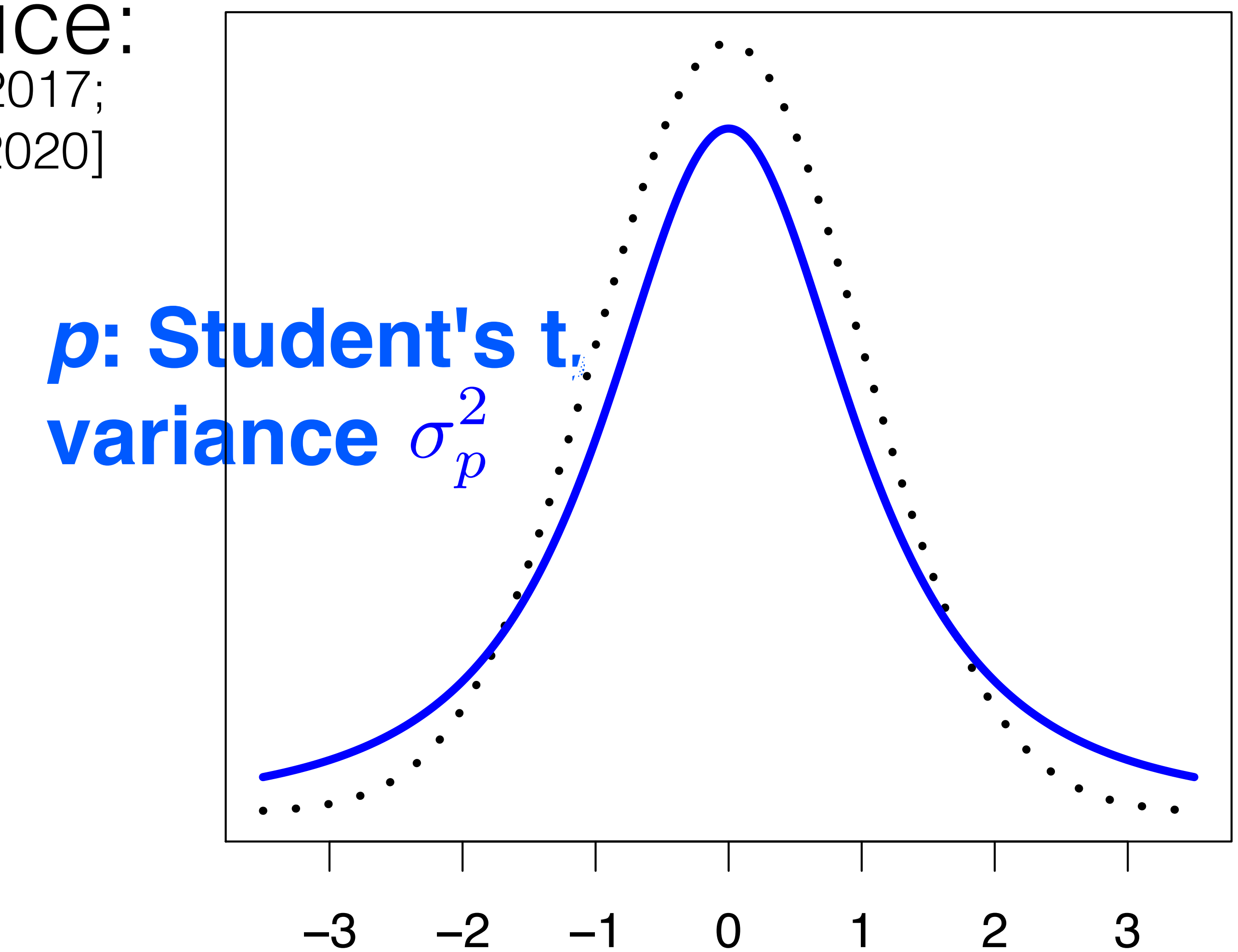

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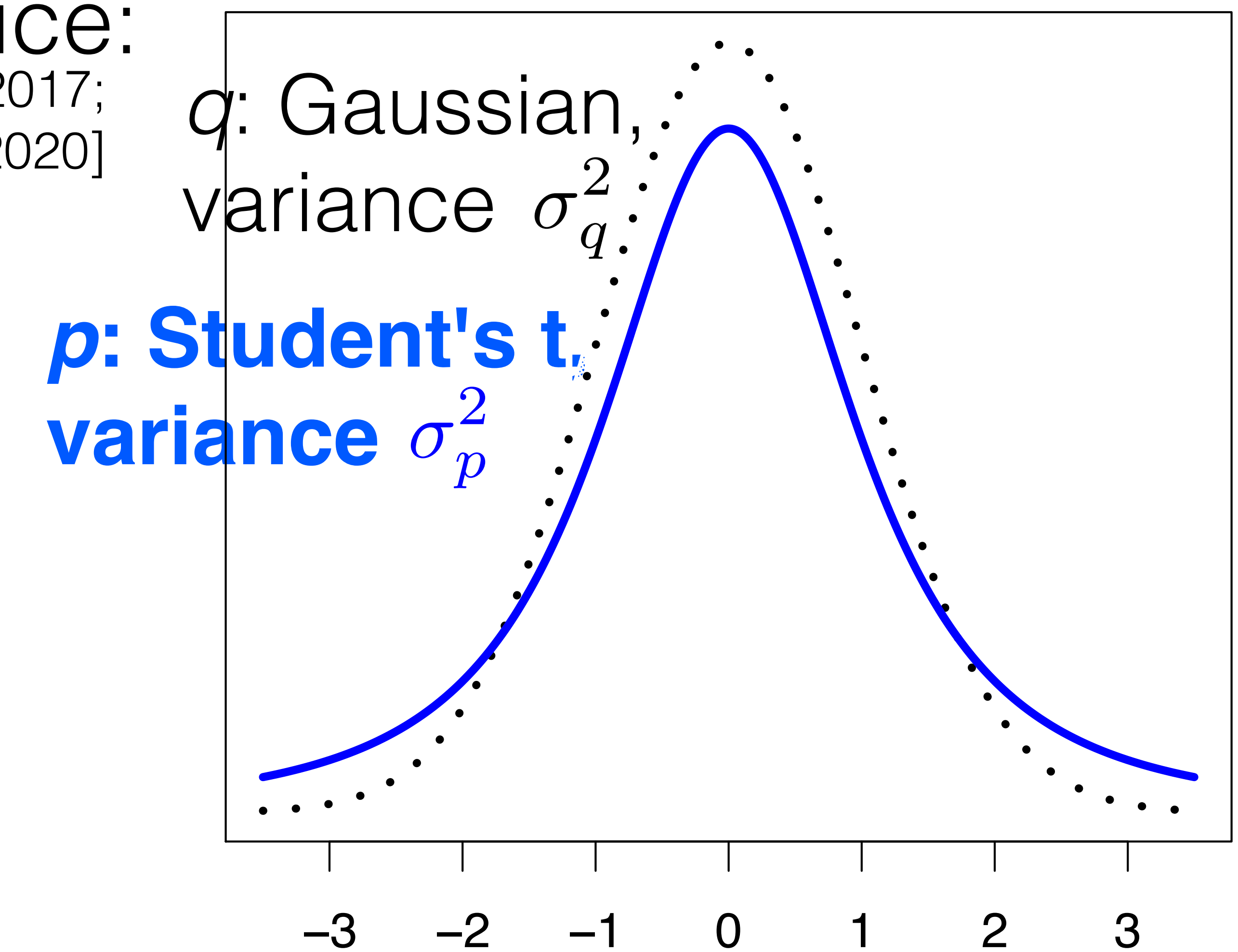

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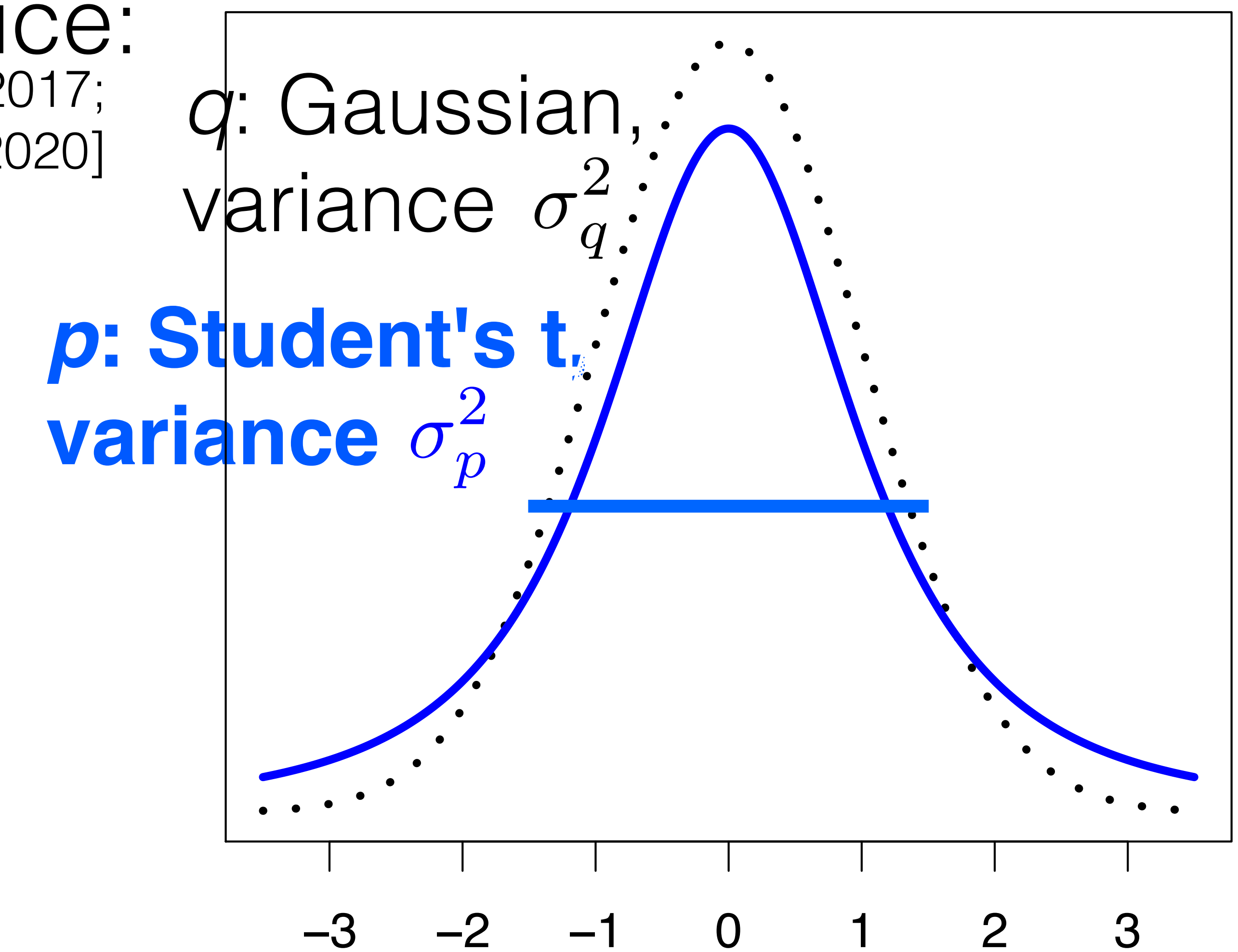

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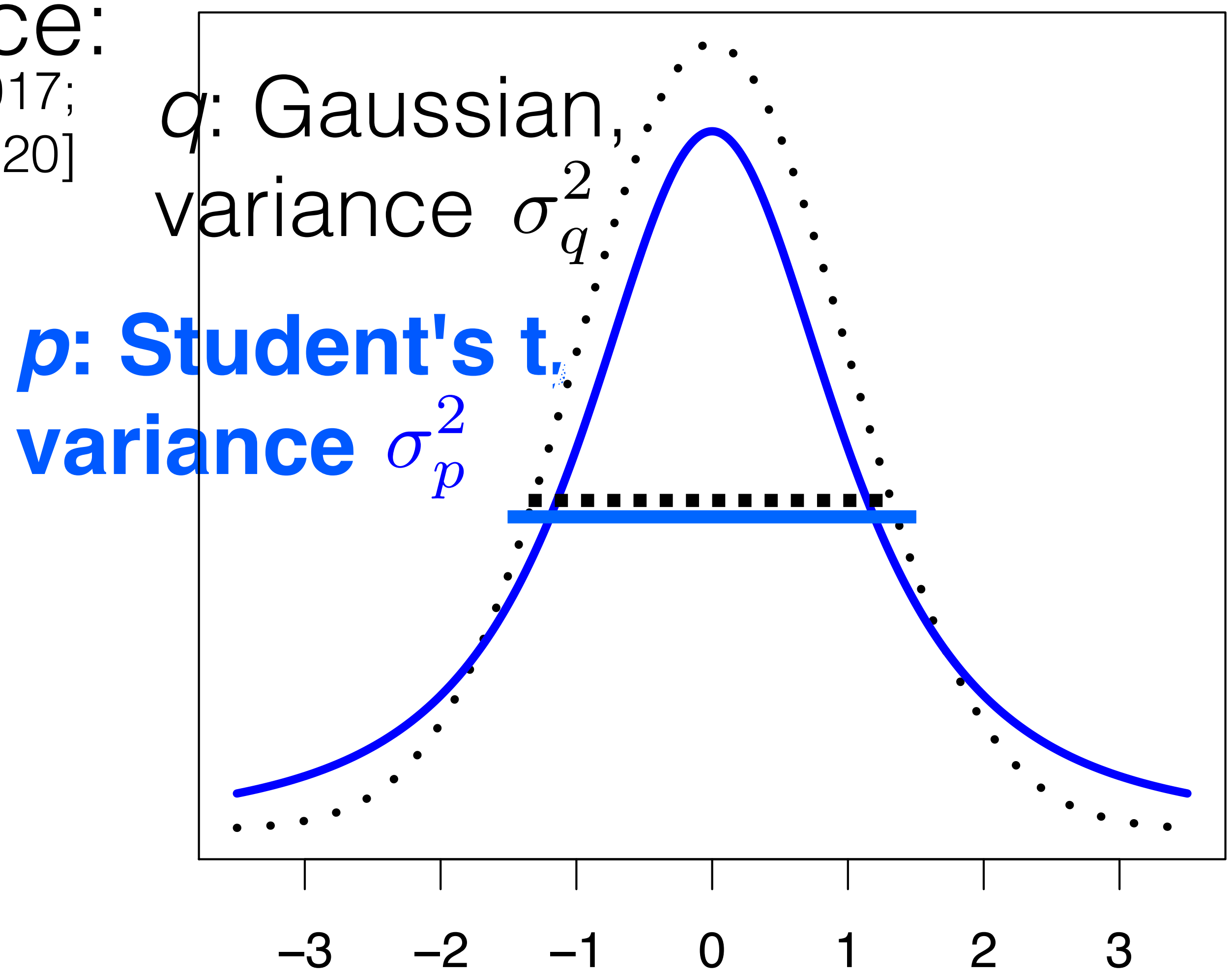

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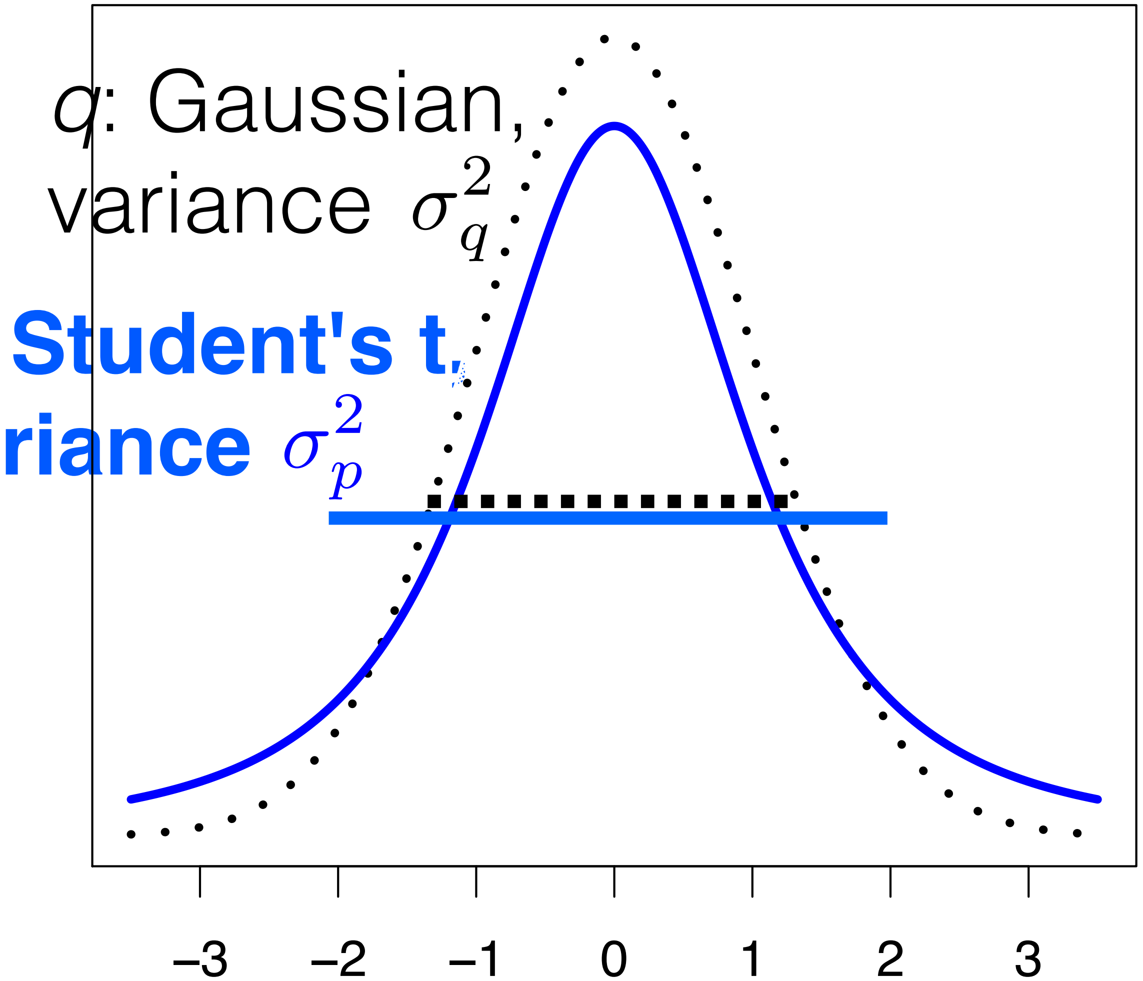

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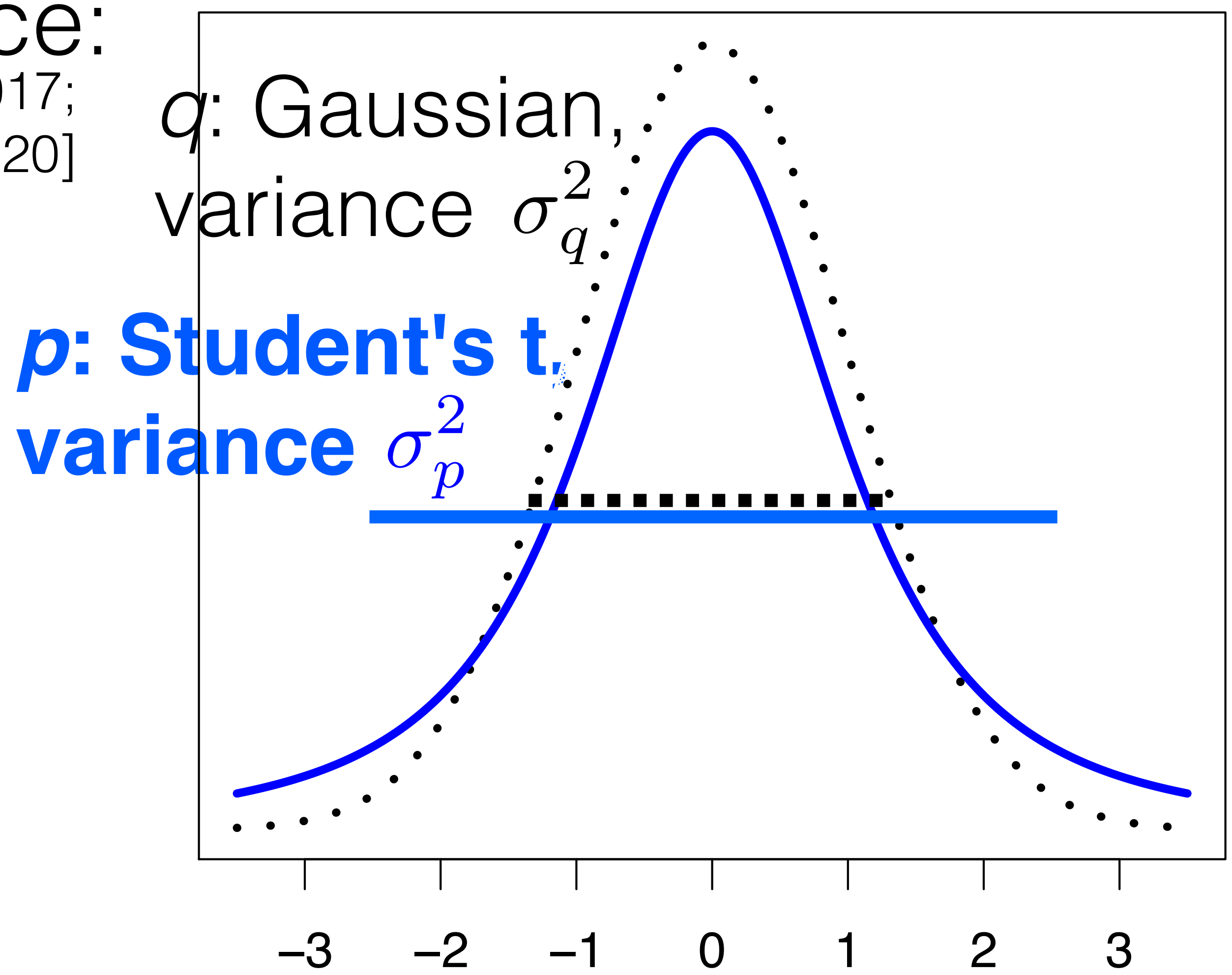

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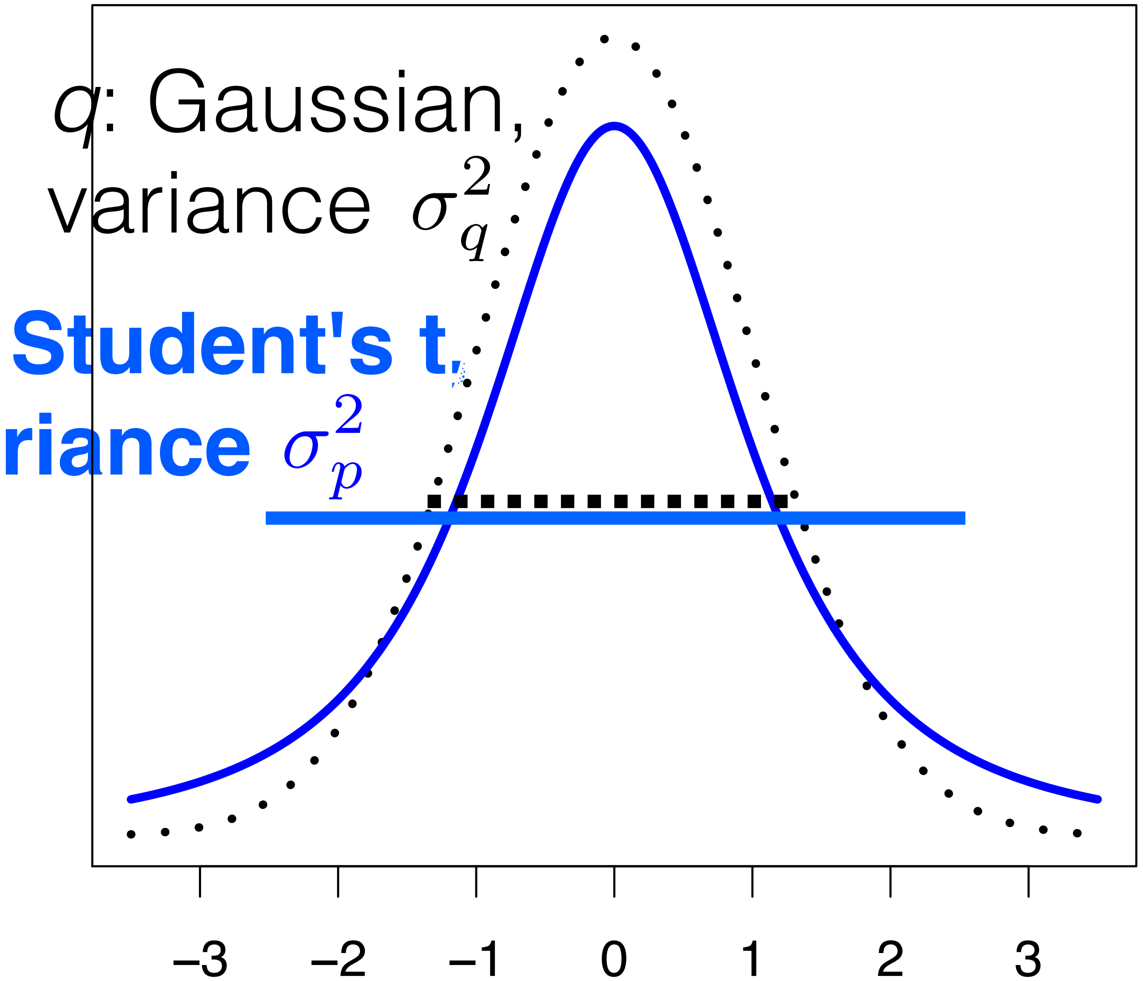

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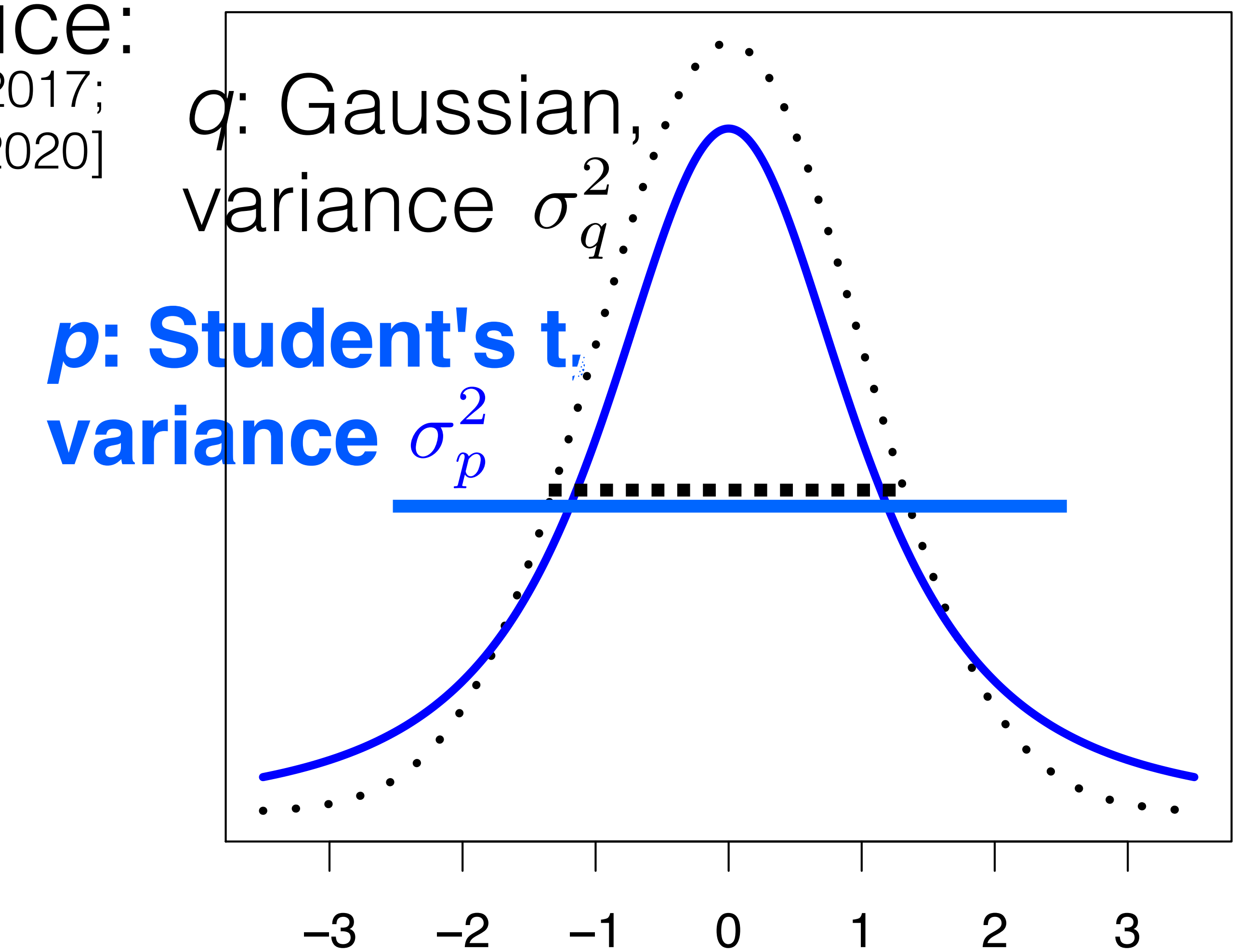

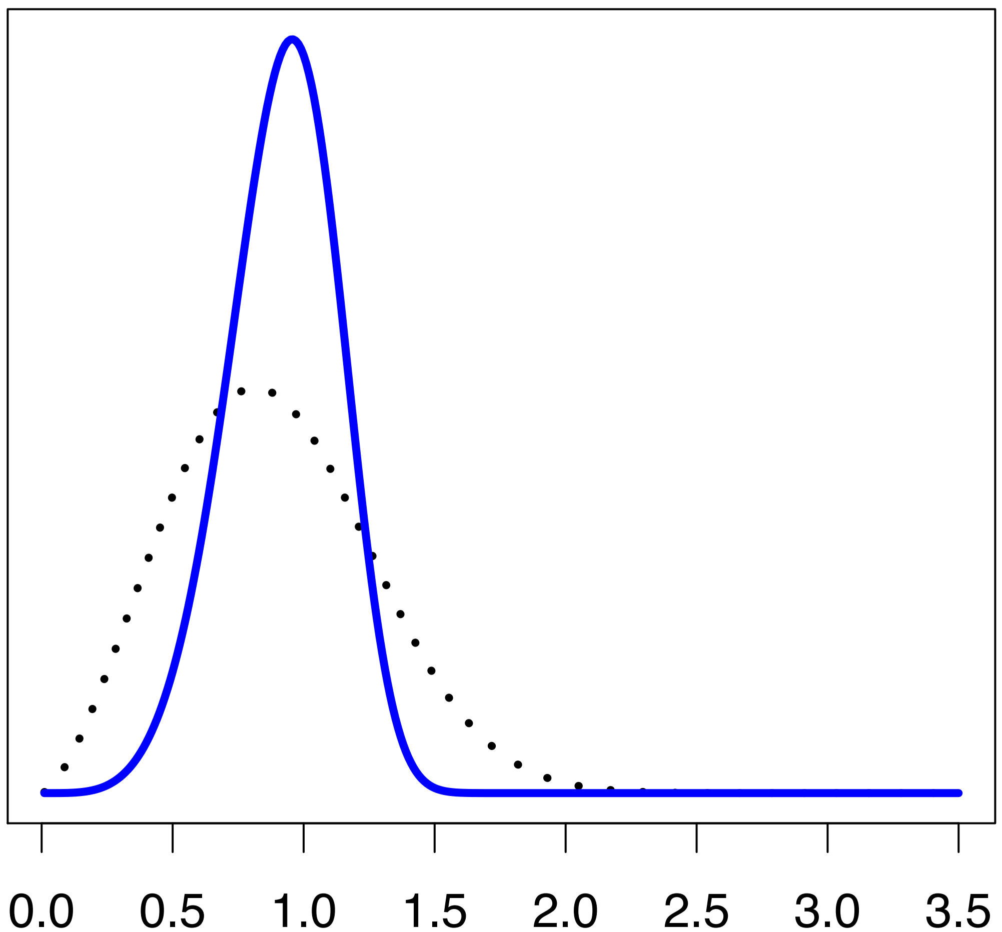

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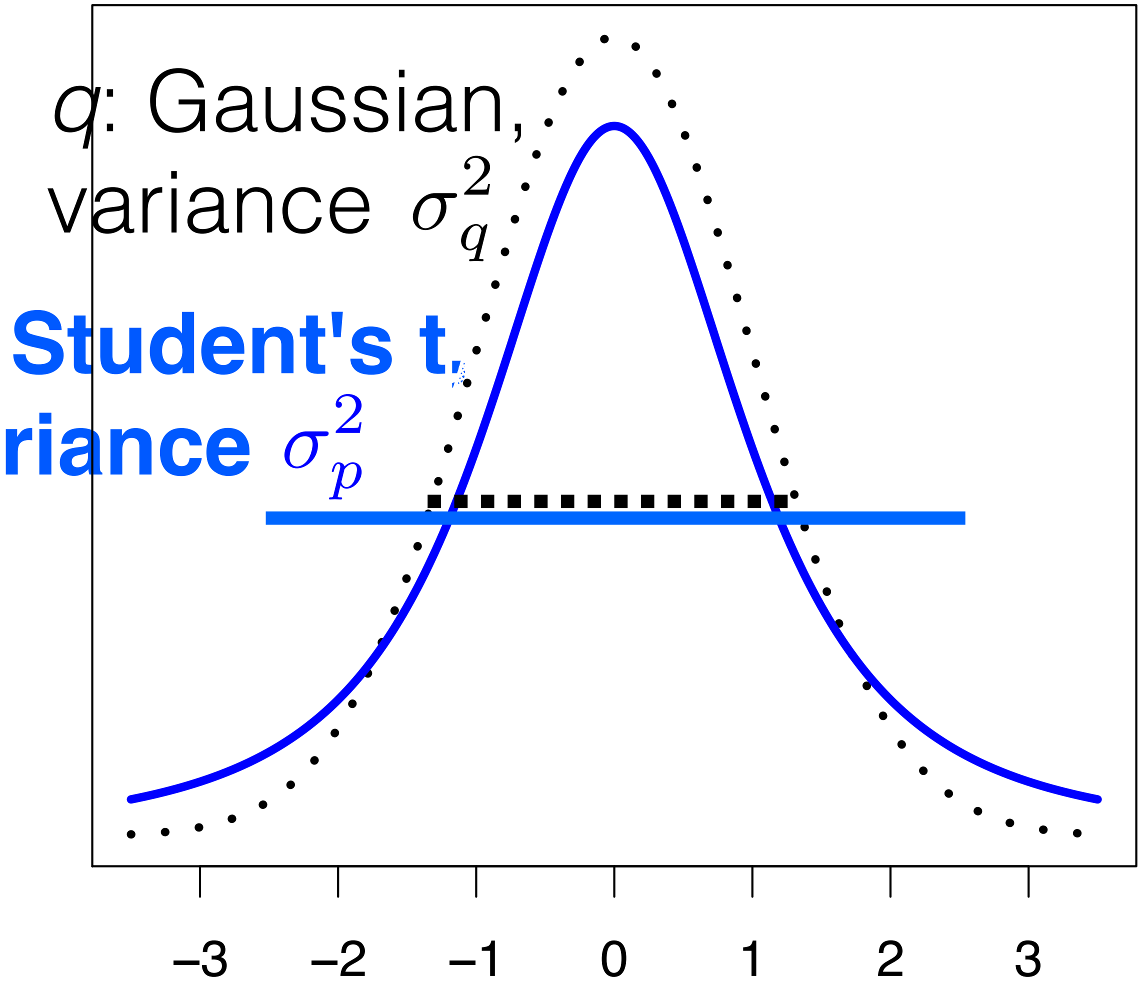

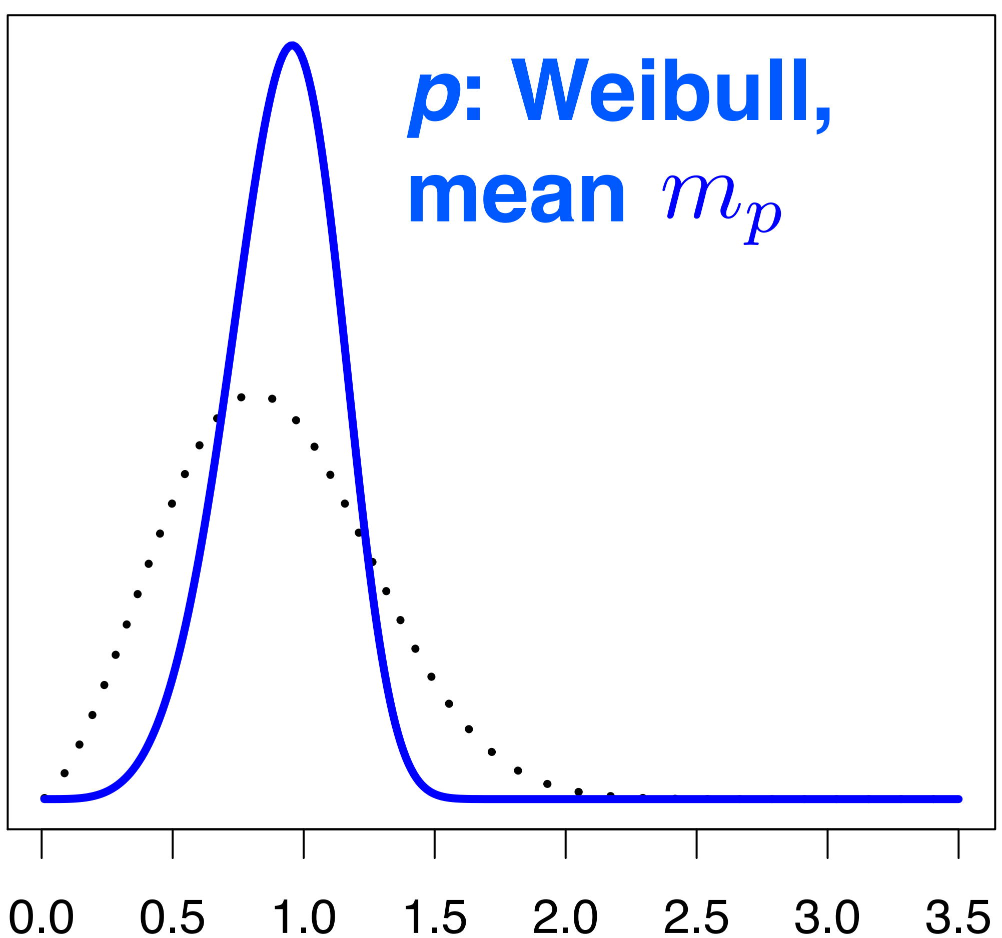

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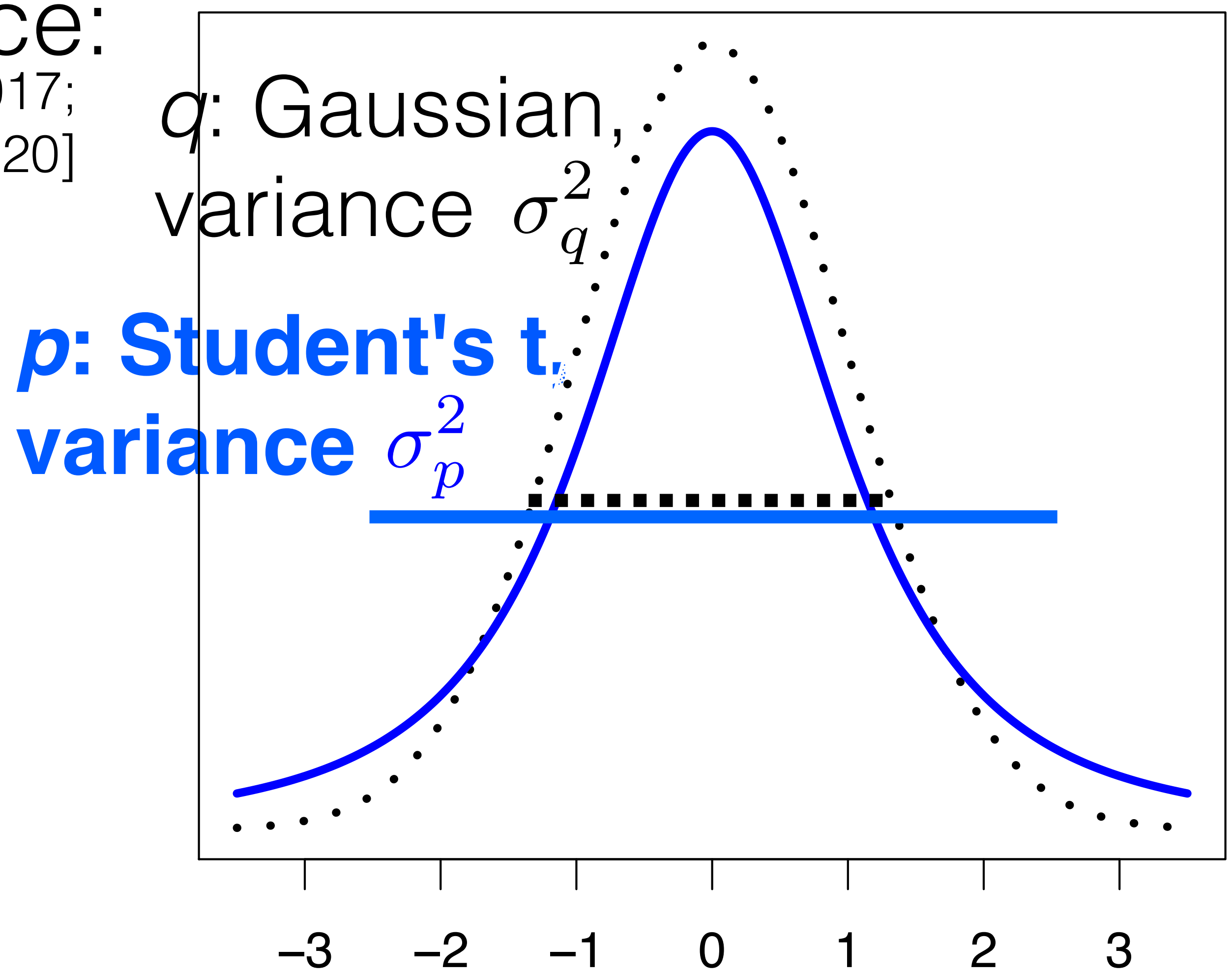

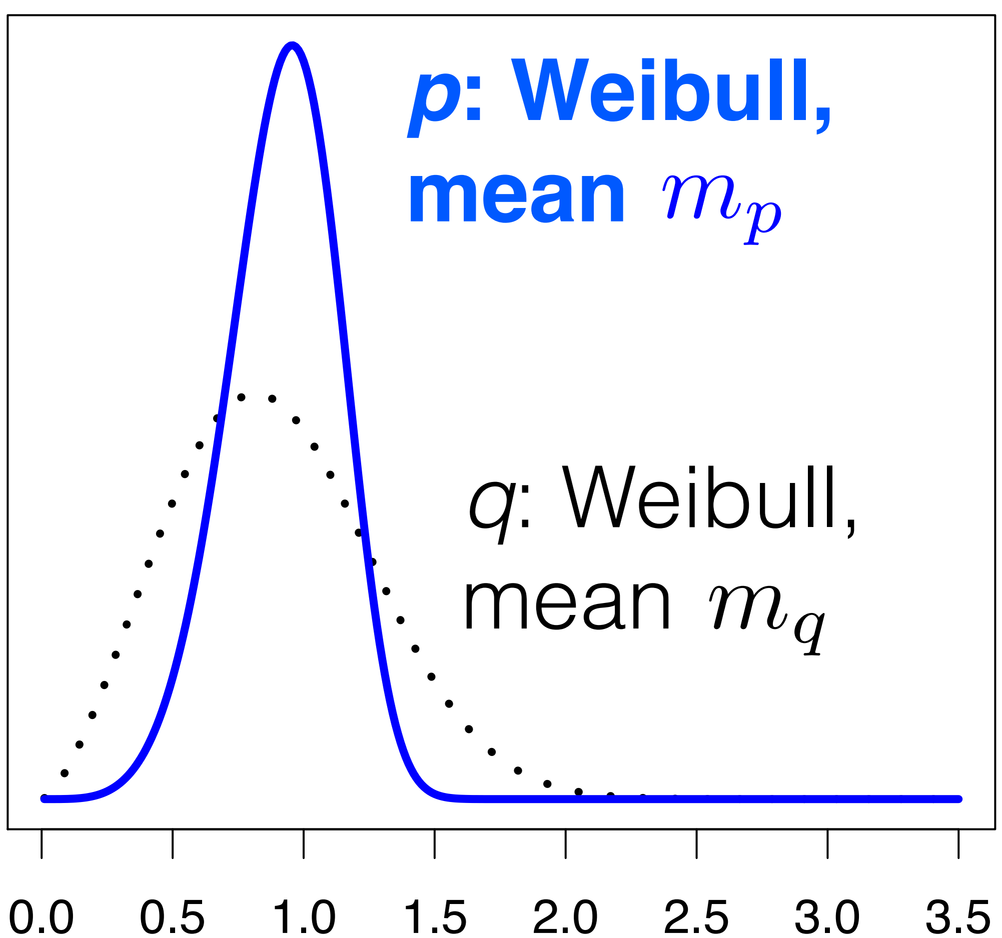

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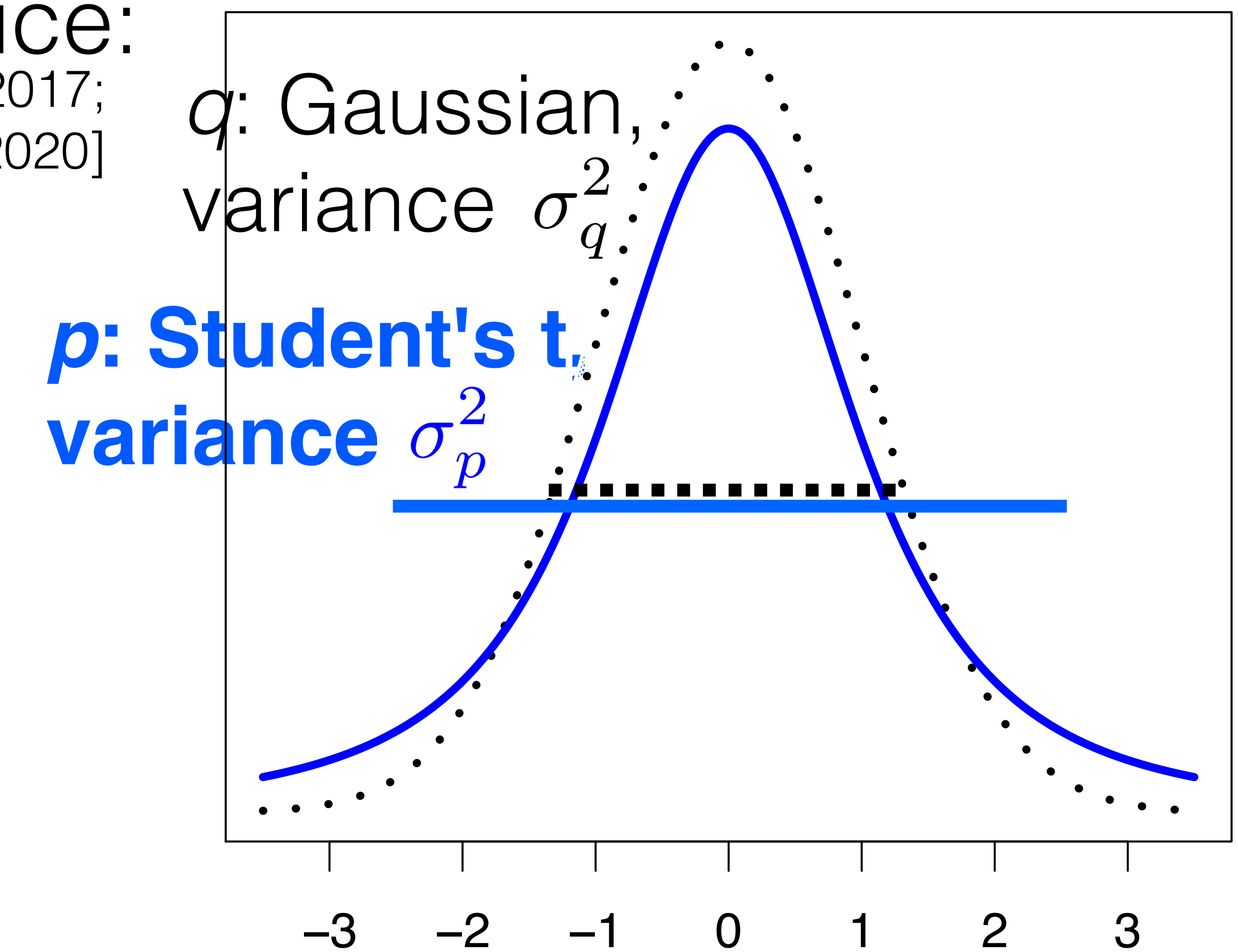

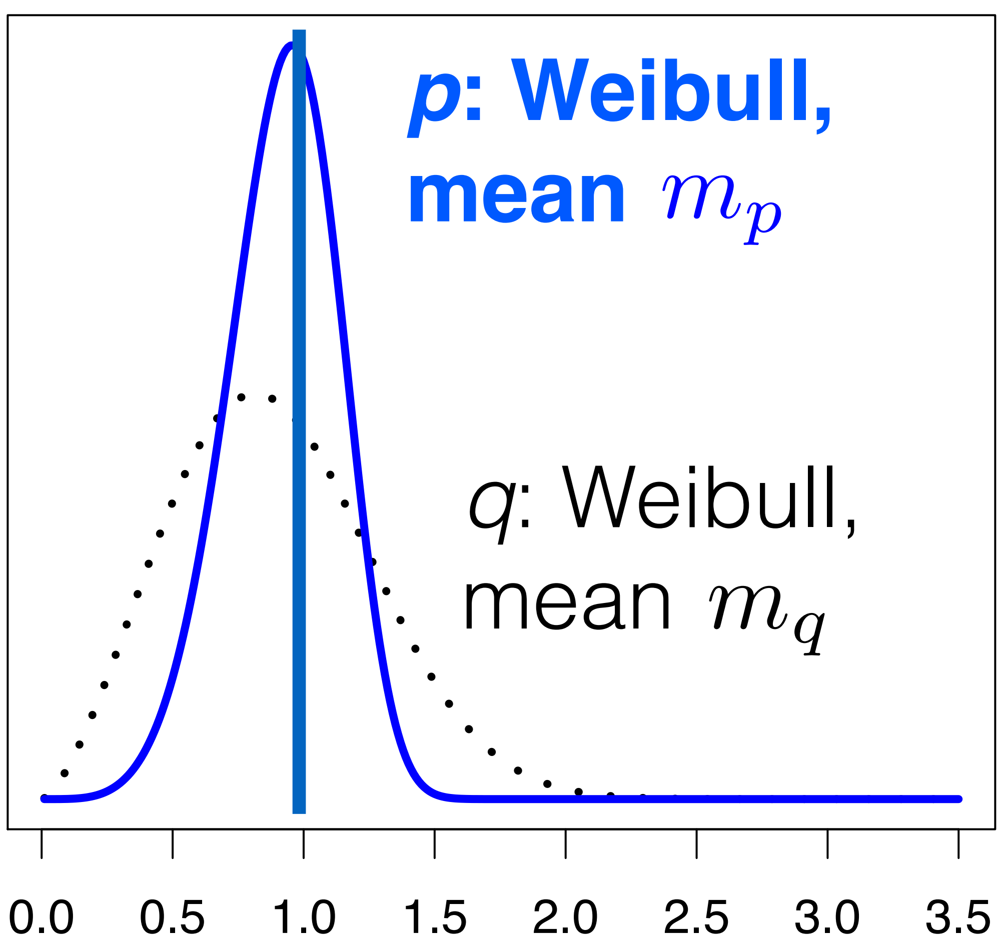

Proposition. Can have small KL (<0.9) and arbitrarily bad mean estimate

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

[Huggins, Karsprzak, Campbell, Broderick 2020]

Is it just MFVB?

- Some KL values seen in practice: ~1 to ~70, 0.5 to 3 [Baqué et al 2017; Huggins et al 2020]
- Take any constant c

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

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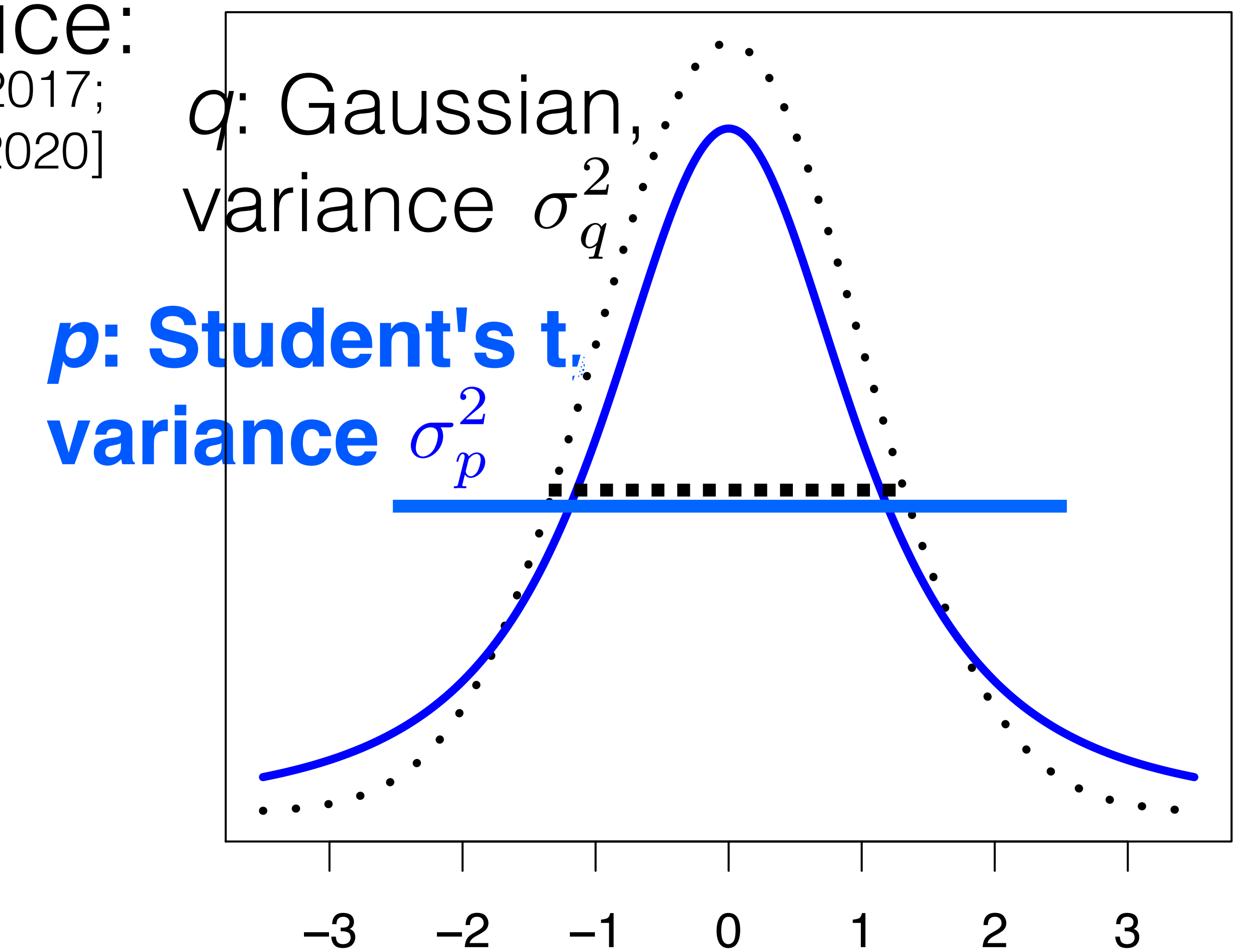

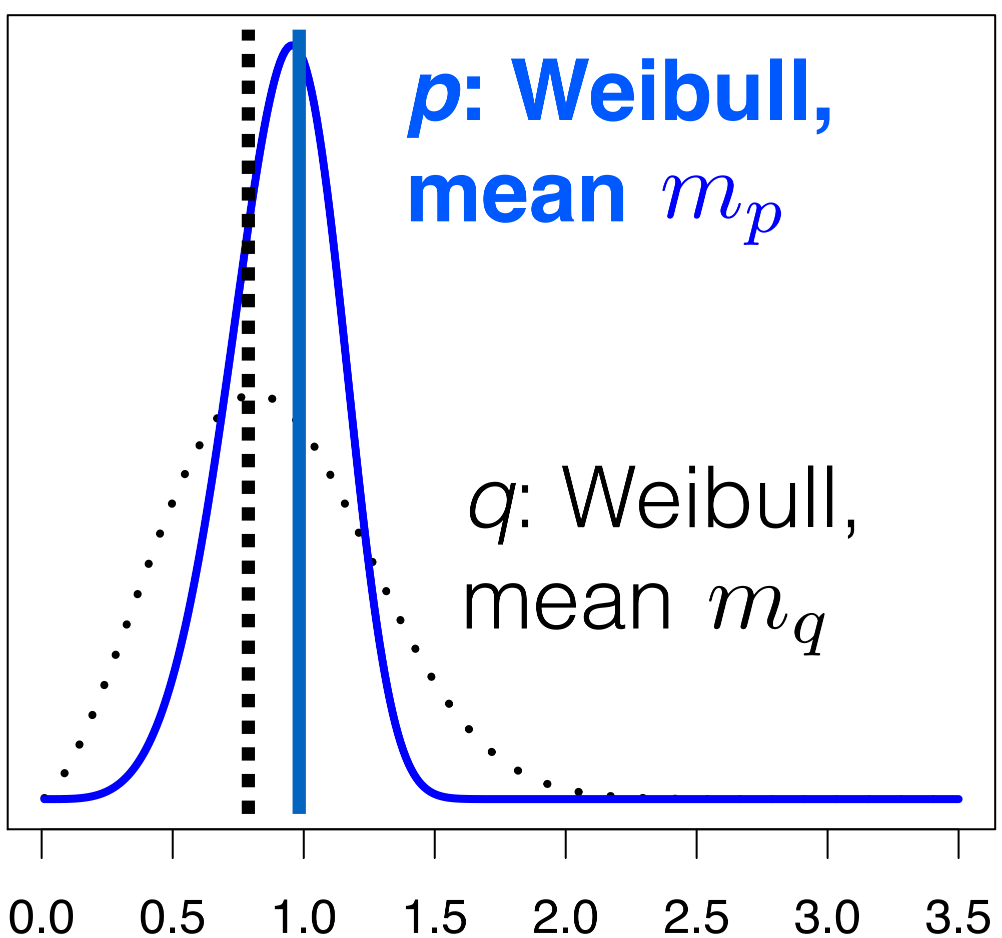

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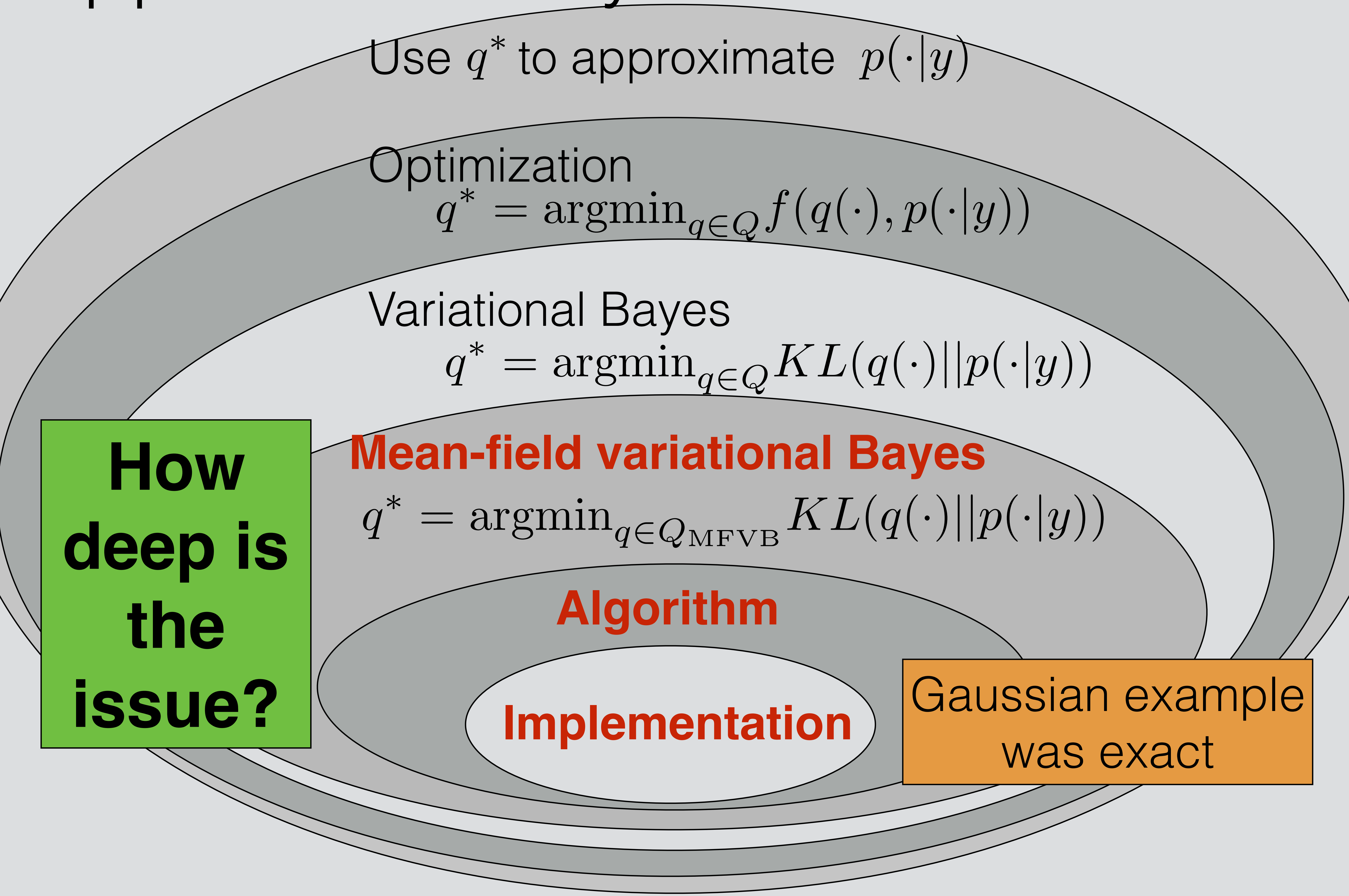

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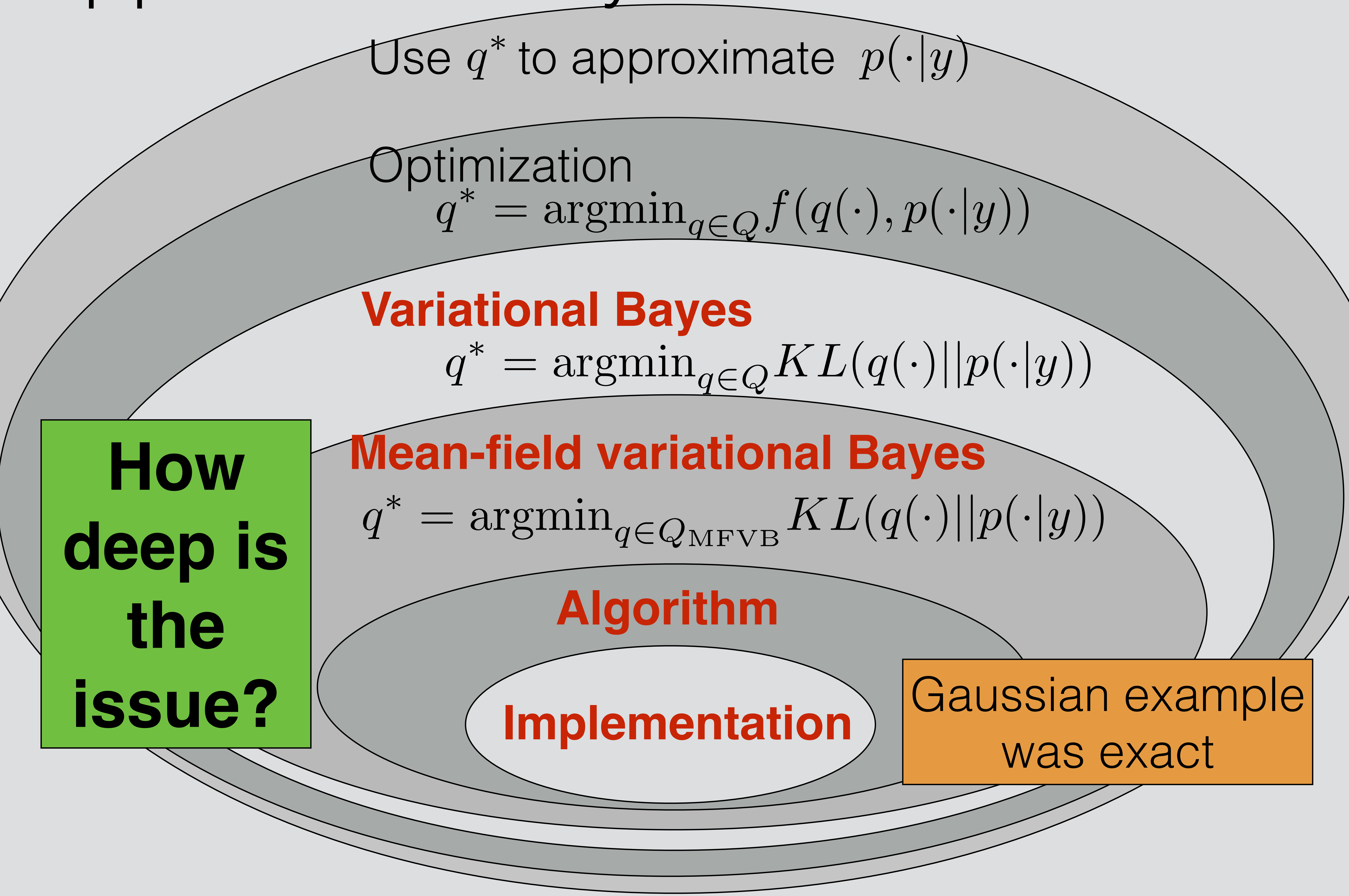

Roadmap

- 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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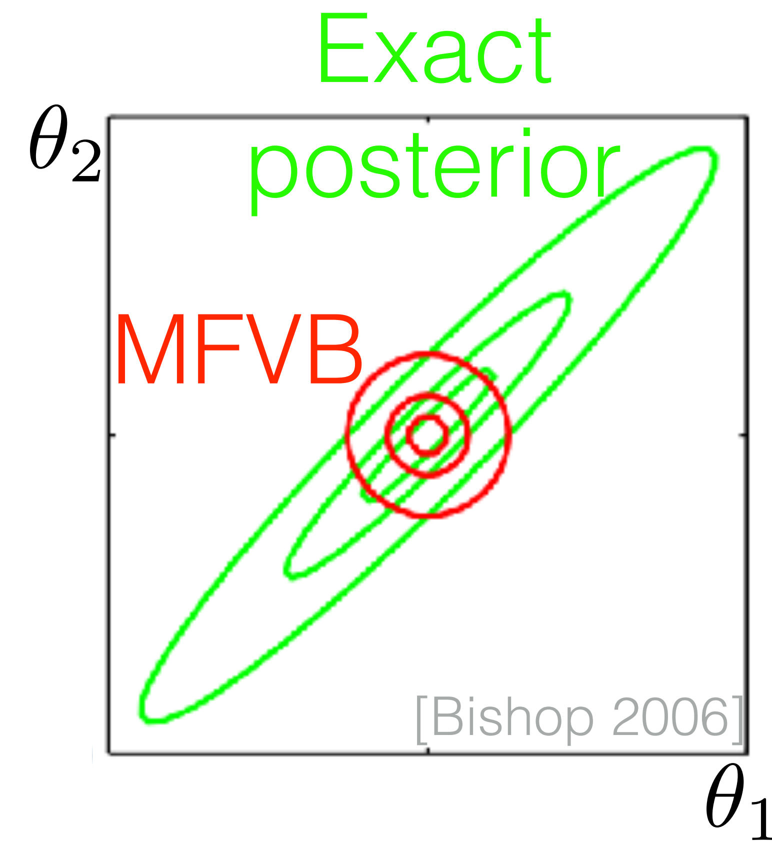

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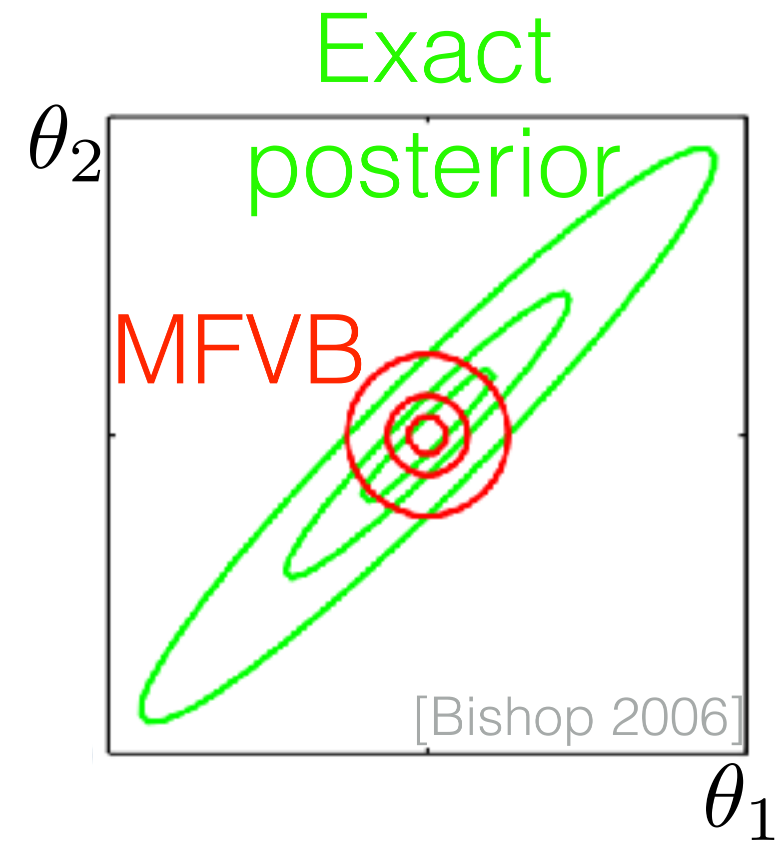

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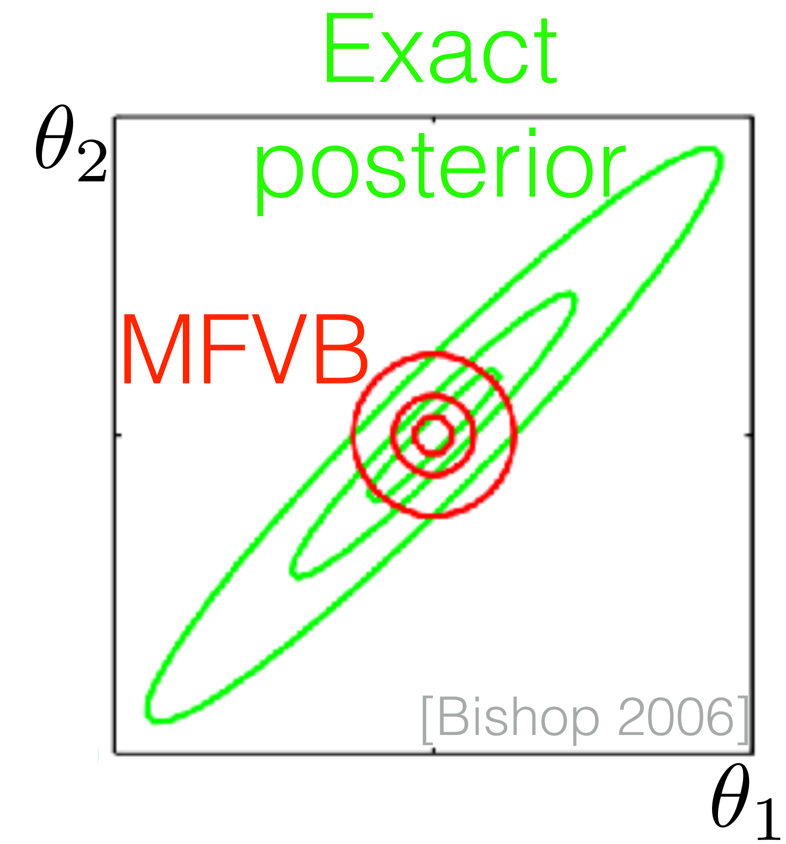

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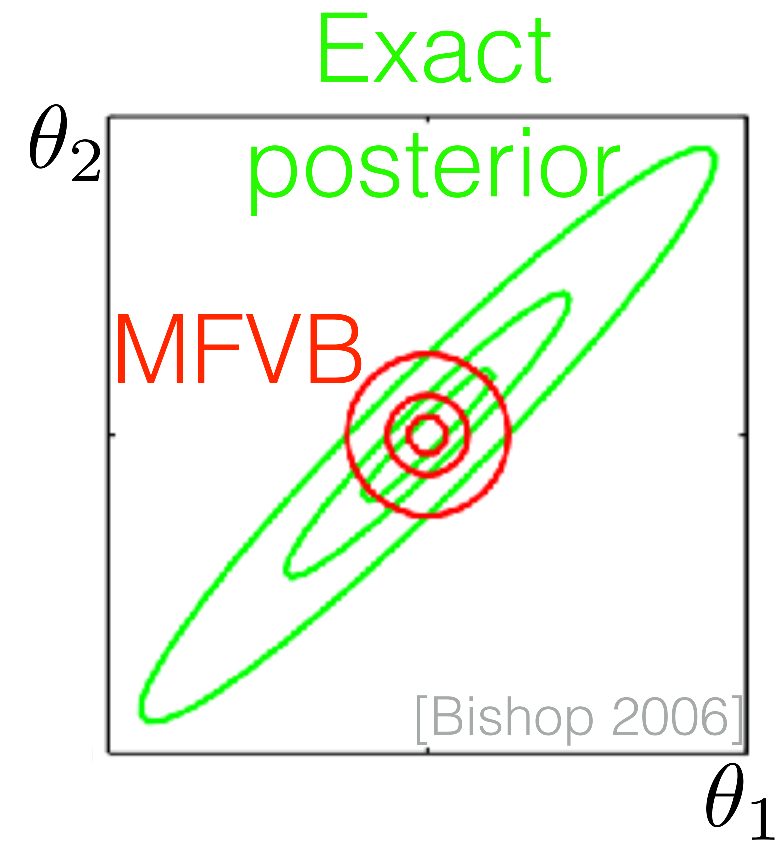

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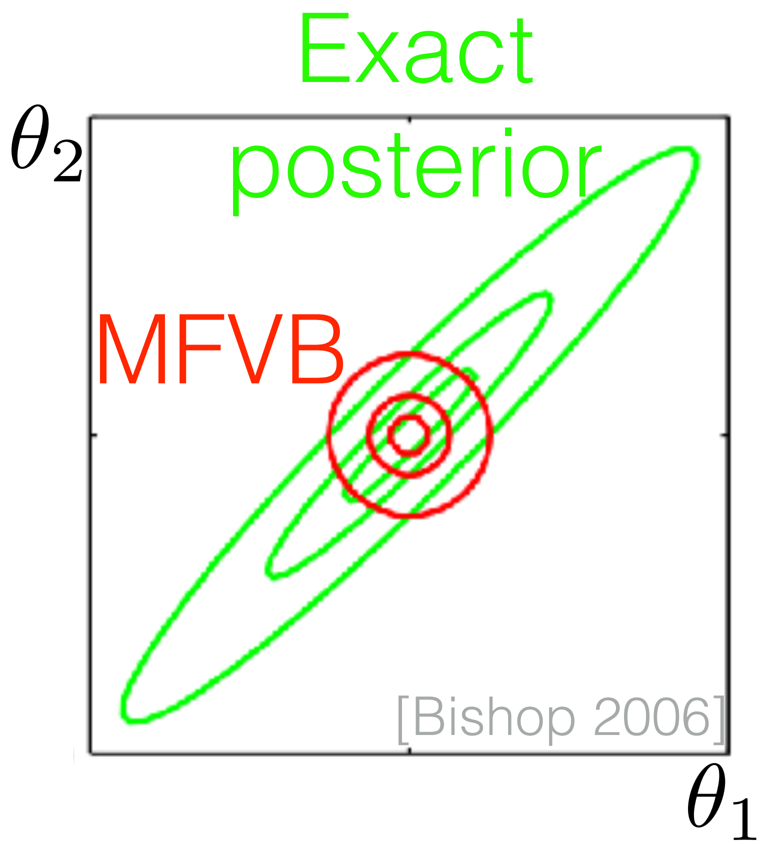

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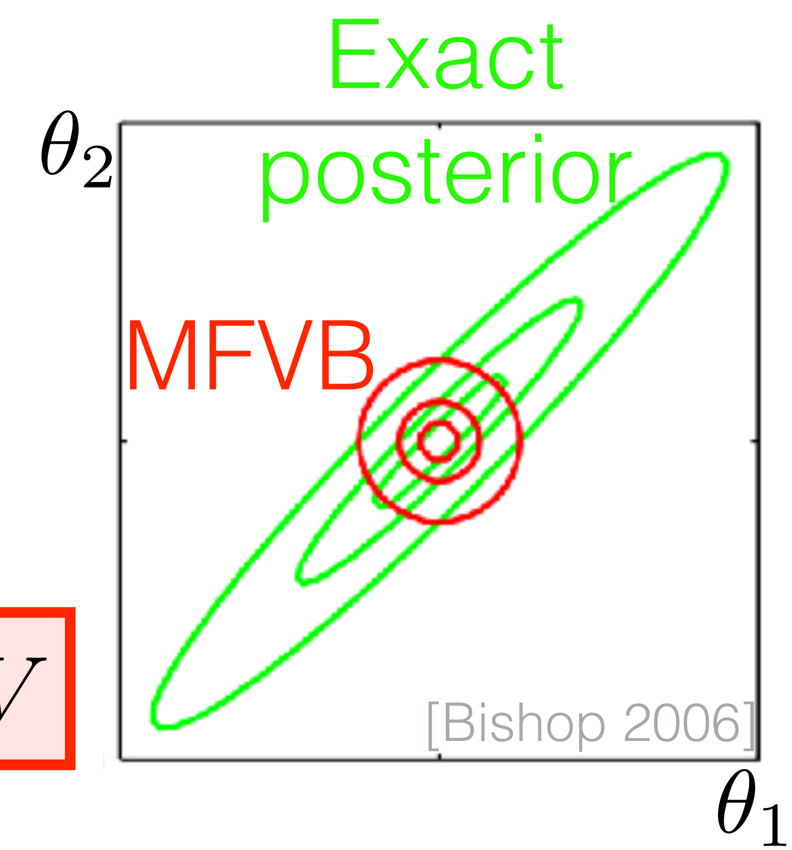

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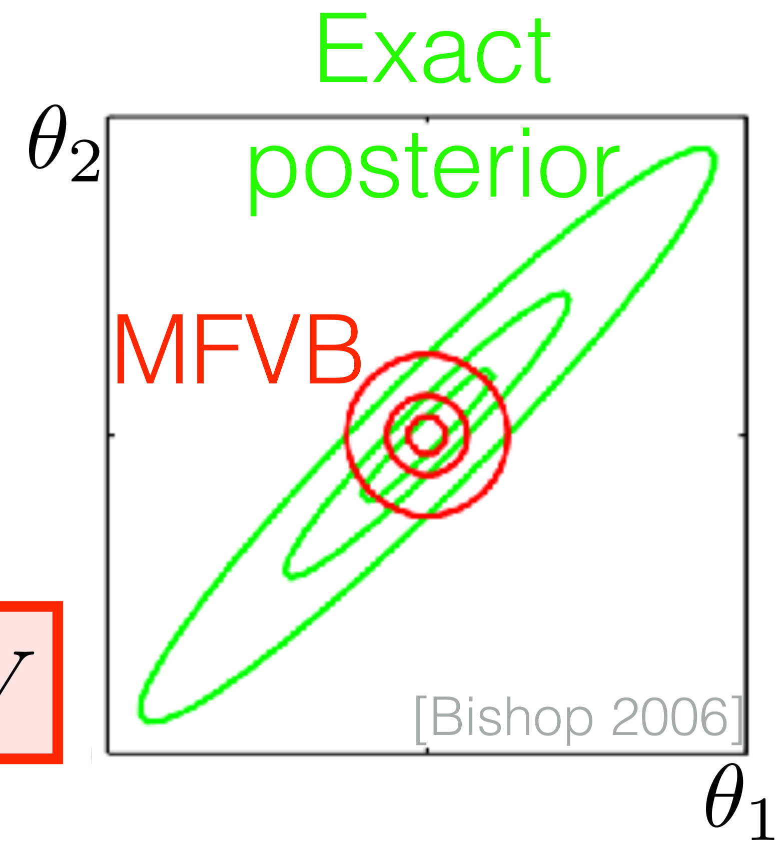

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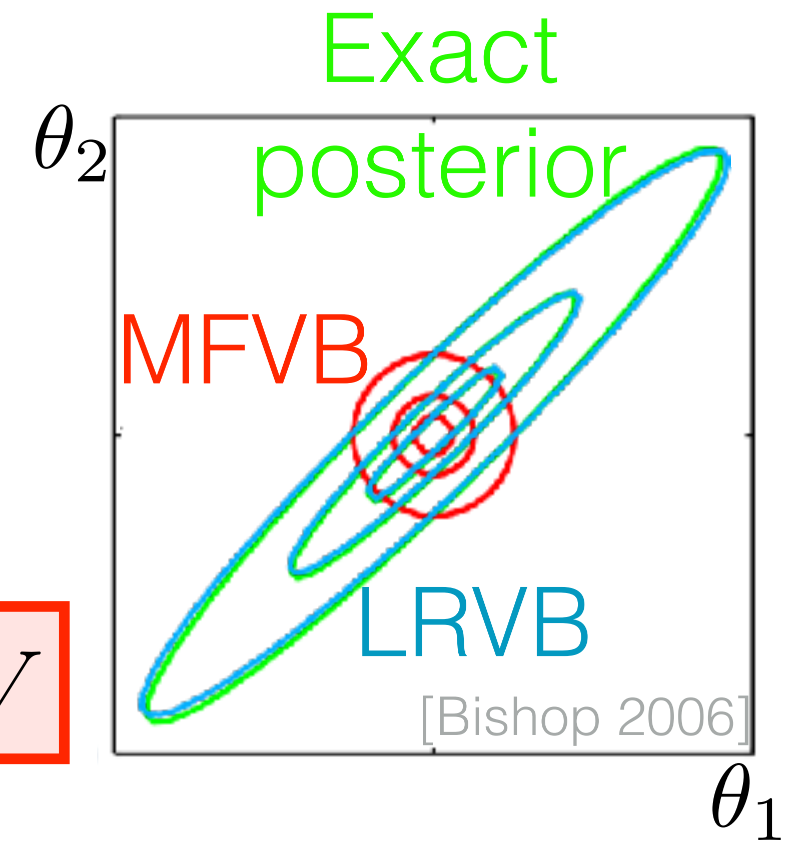

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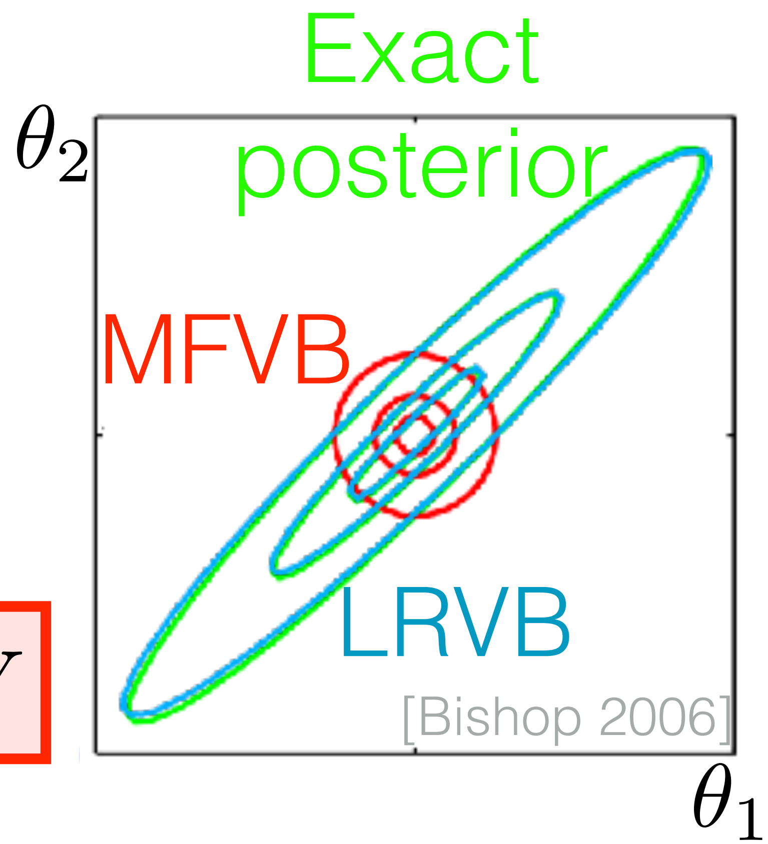

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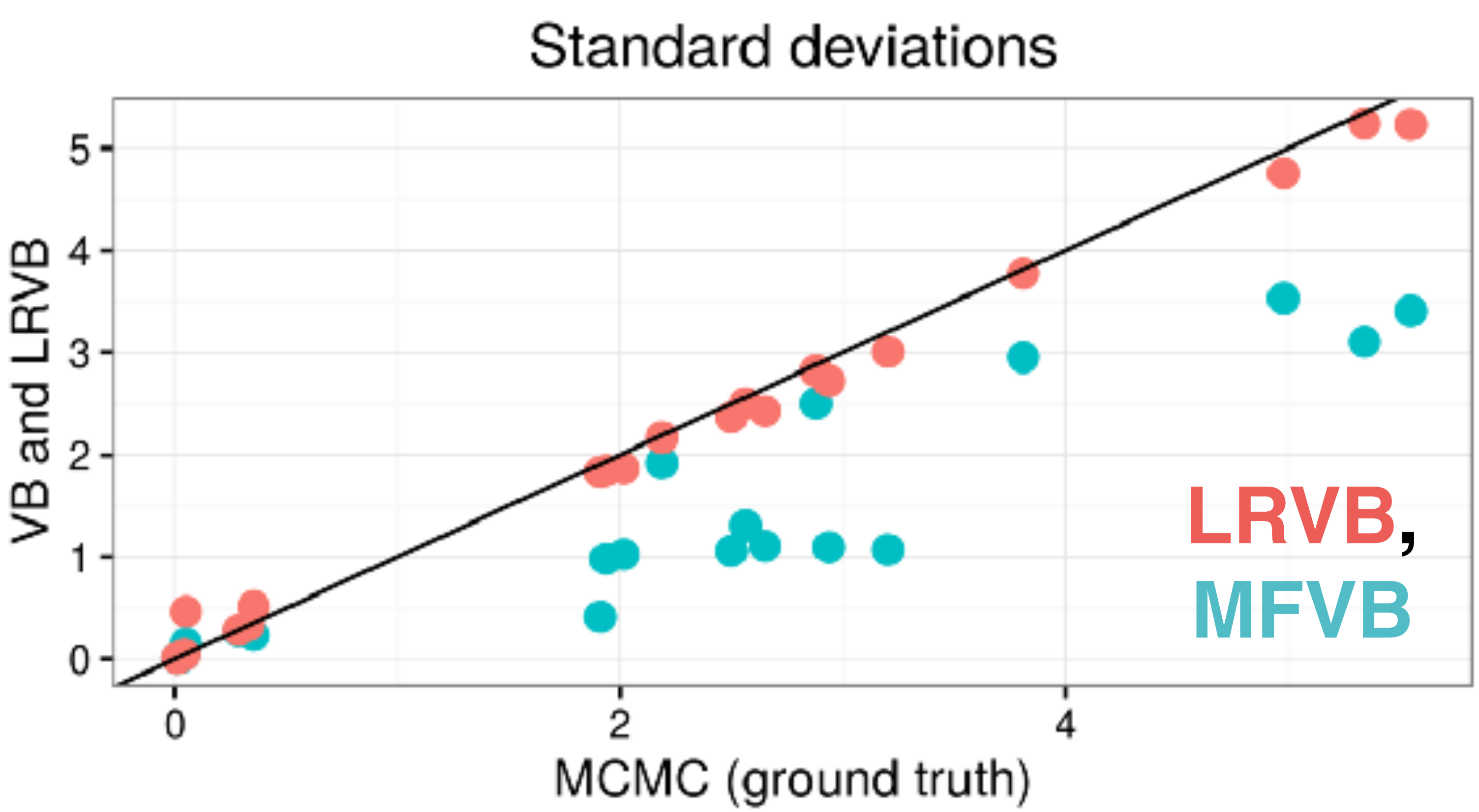

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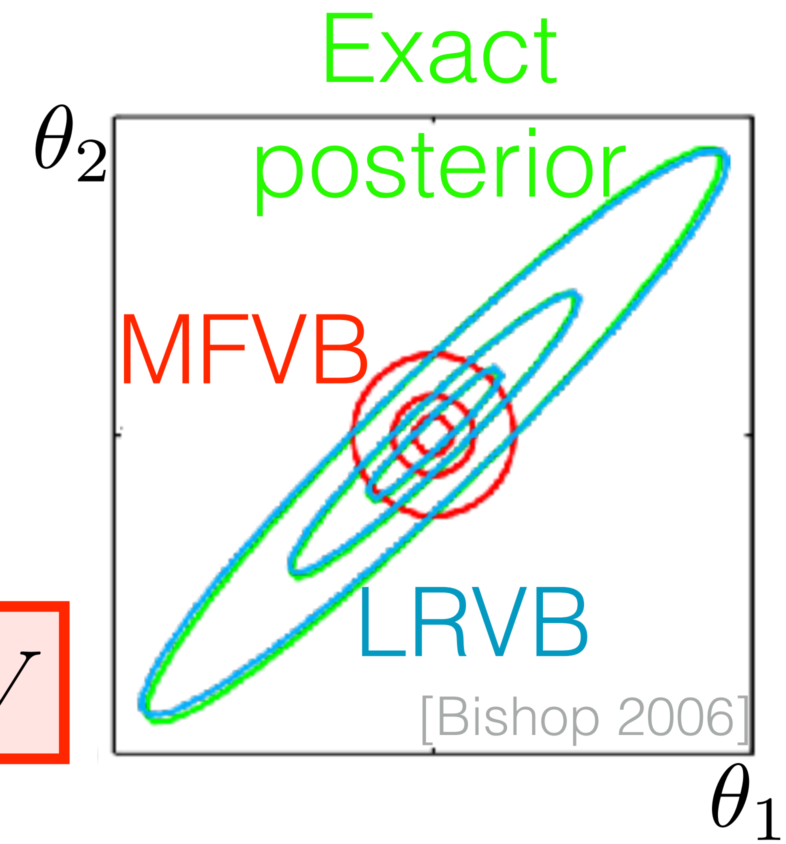

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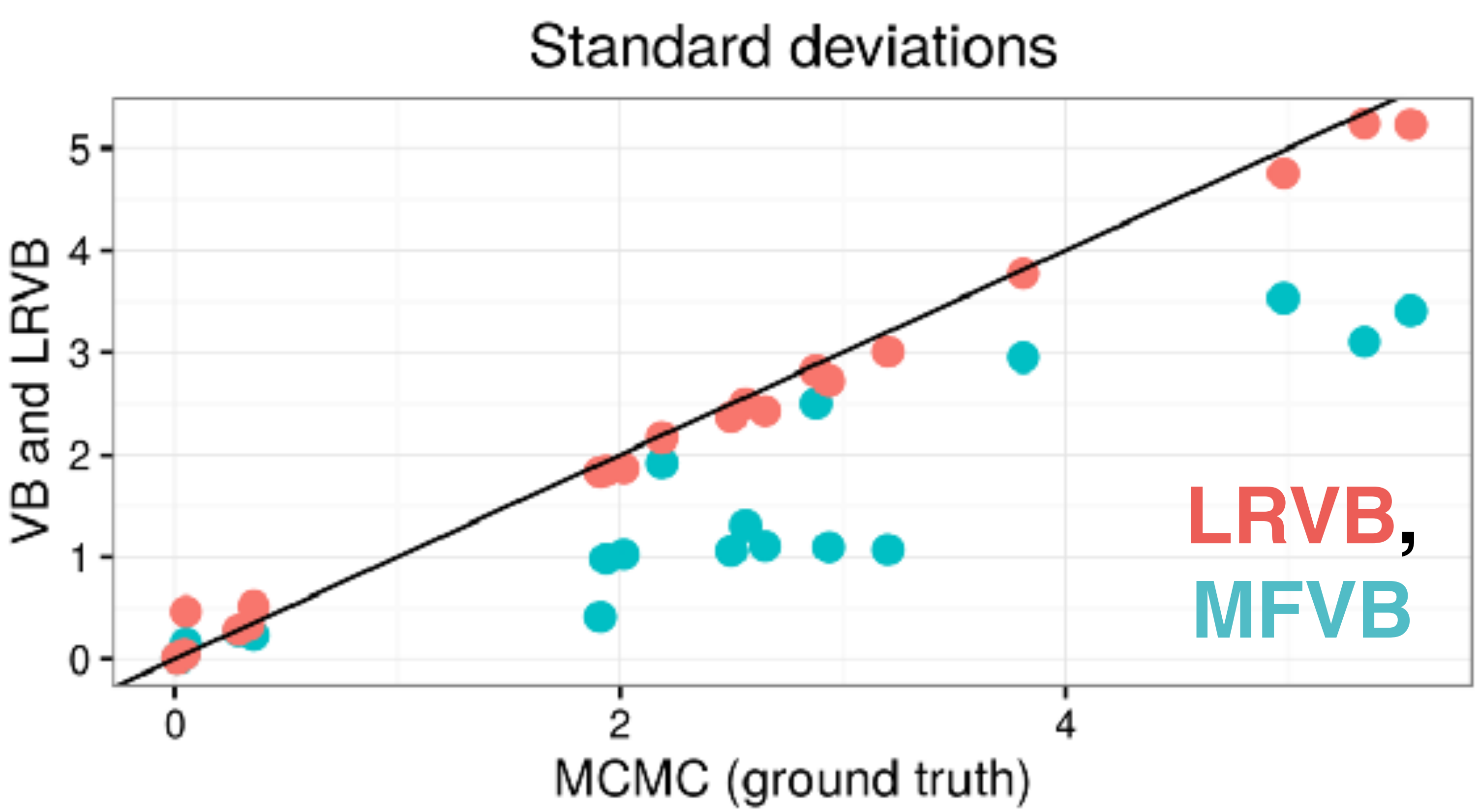

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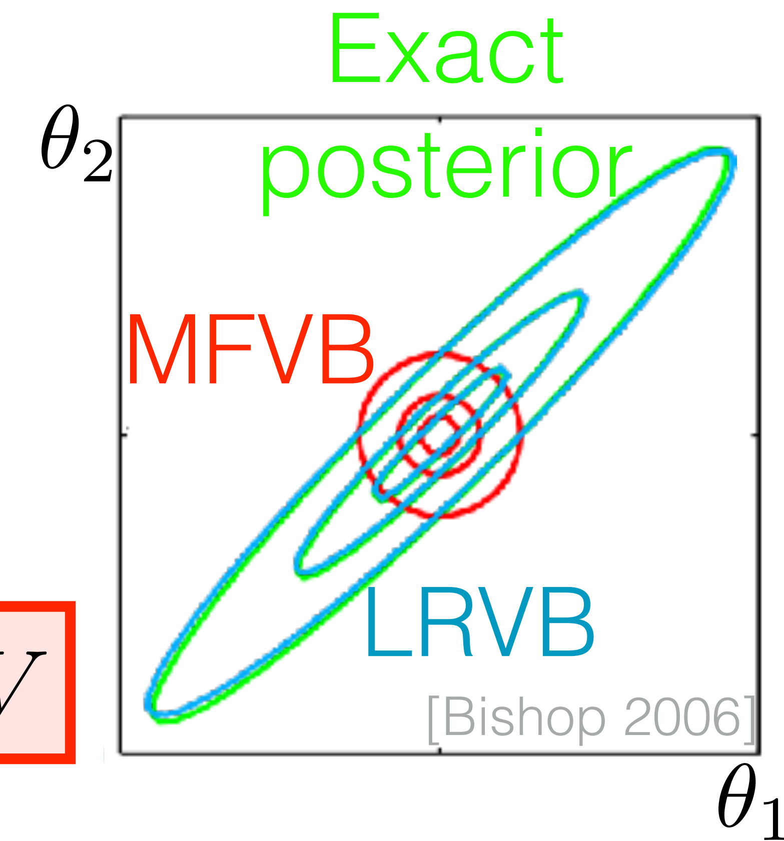

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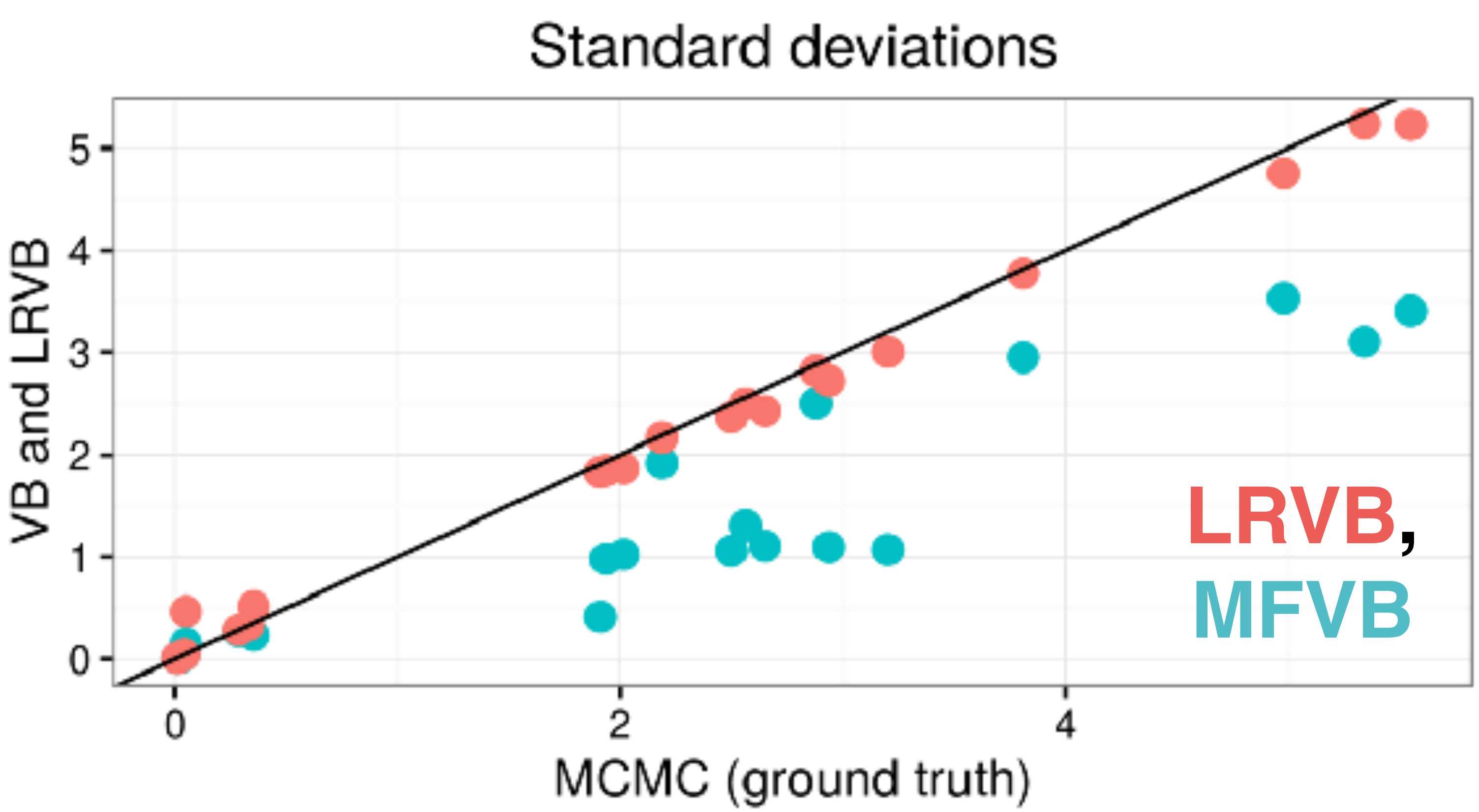

- Exact for Gaussians
- Needs good posterior mean approximation in practice

[Giordano, Broderick, Jordan 2015, 2018]

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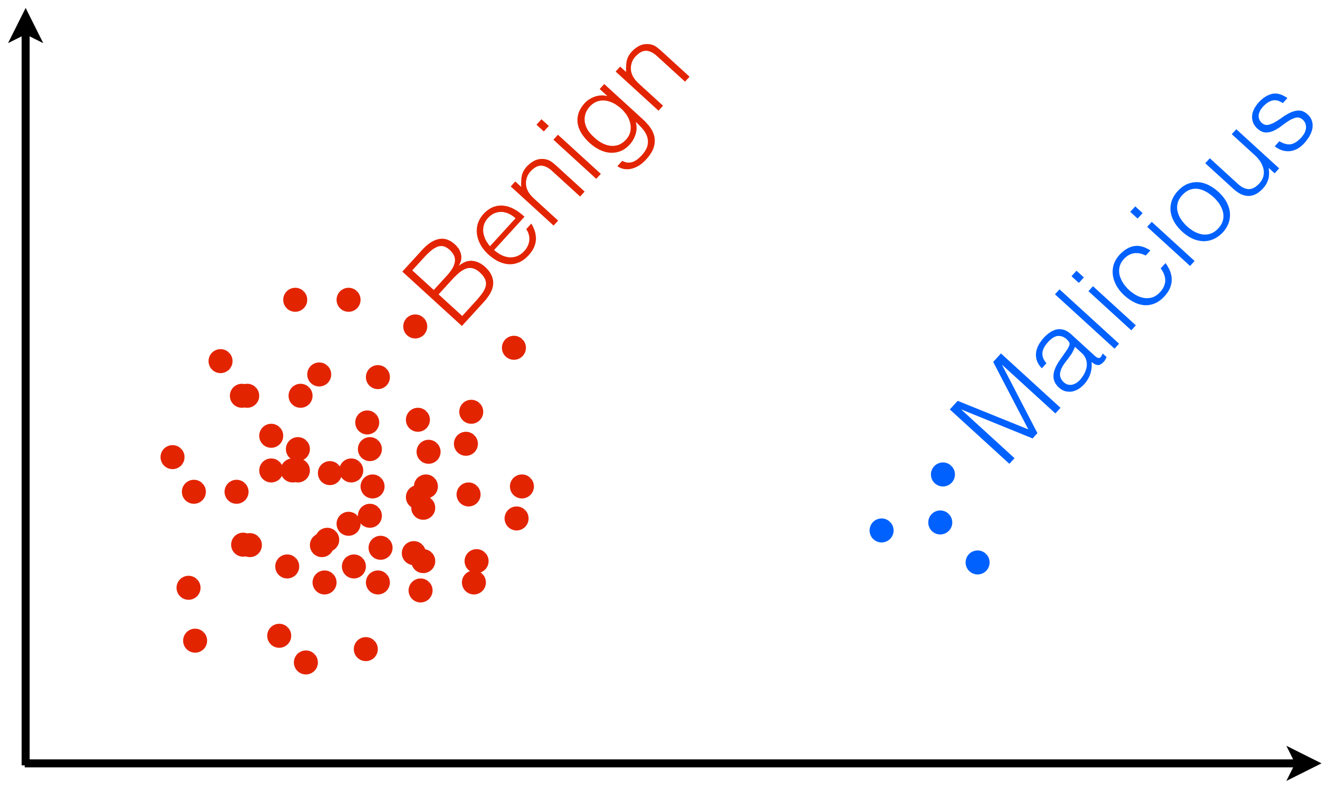

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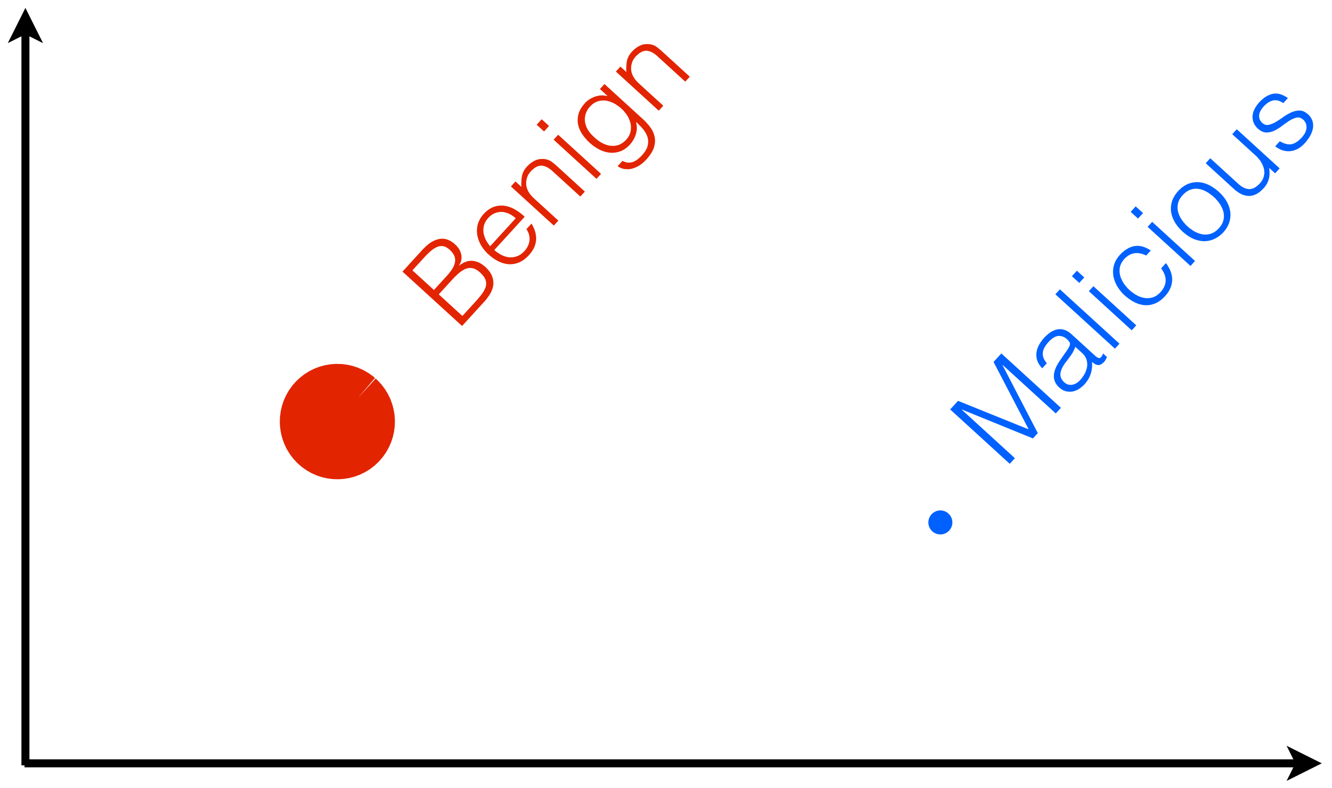

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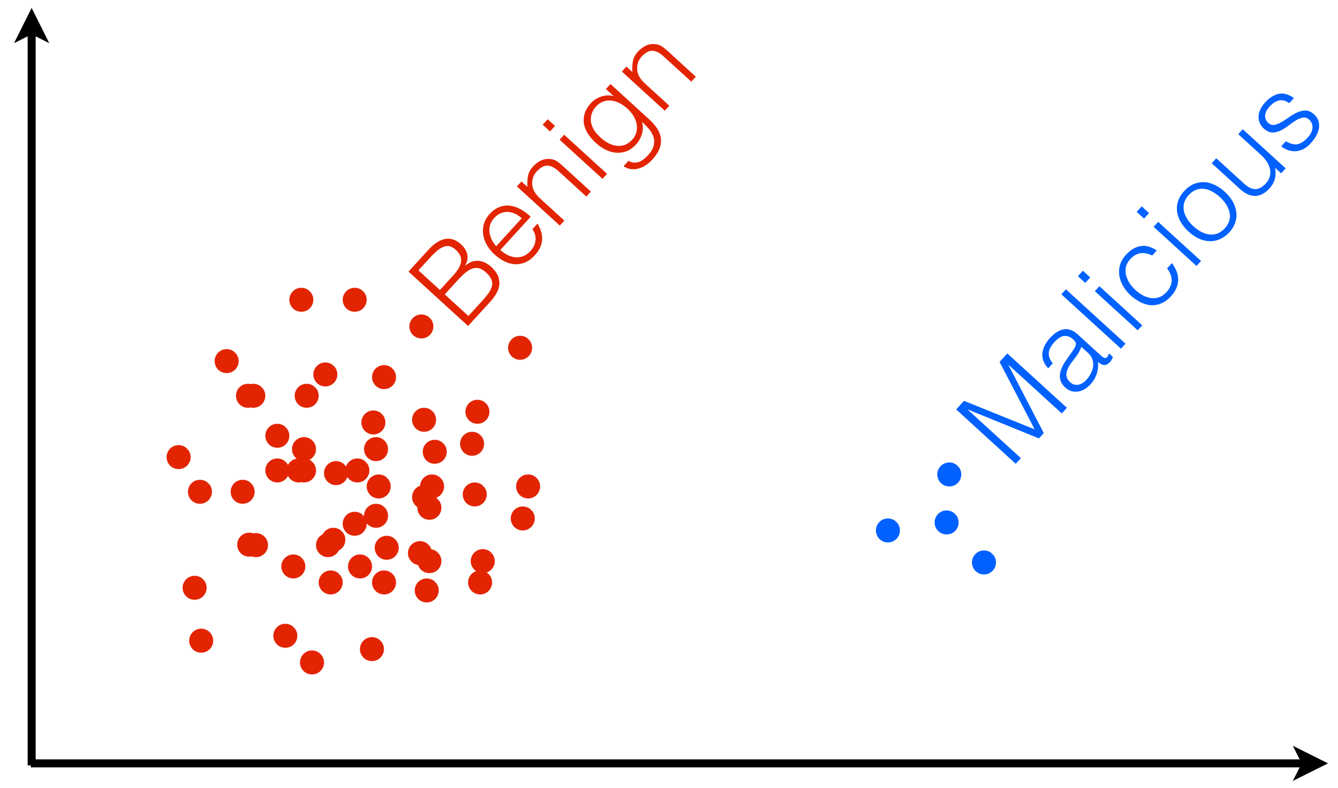

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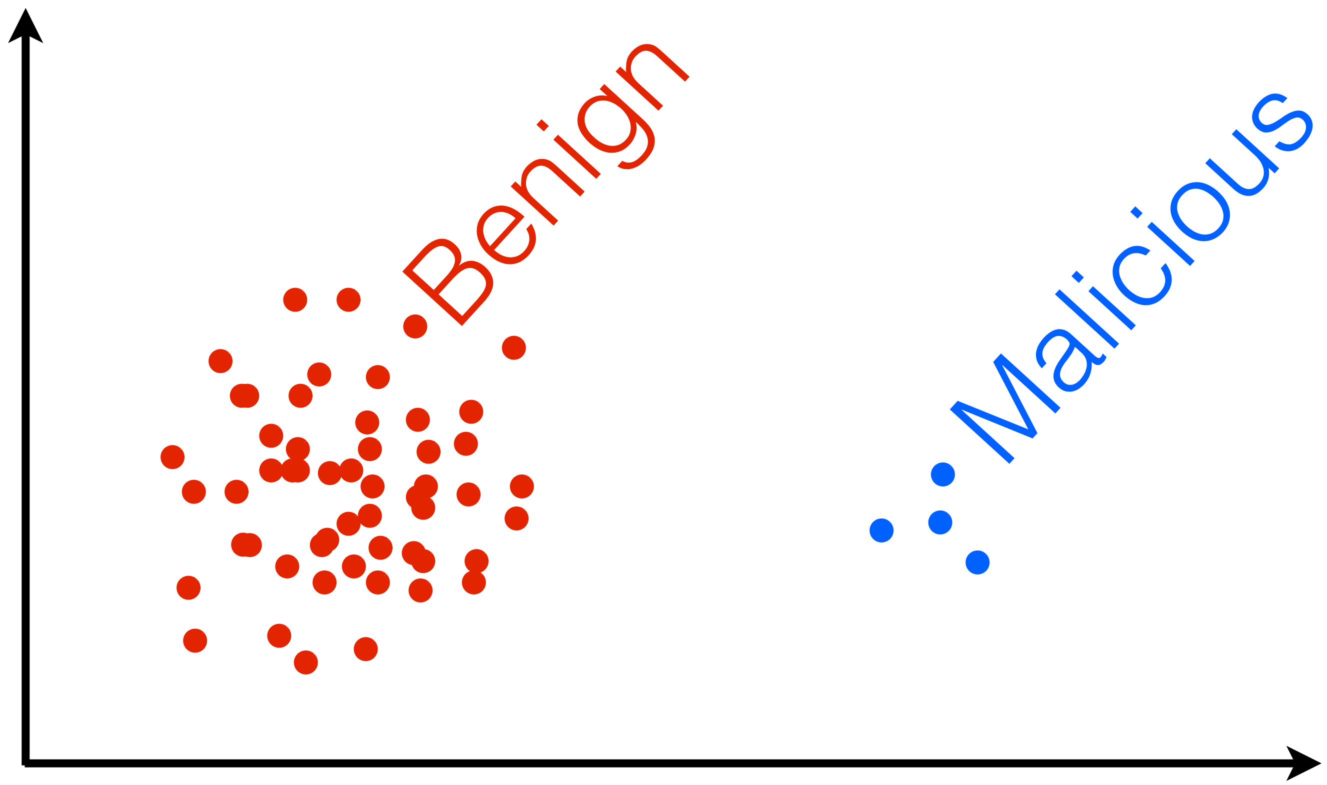

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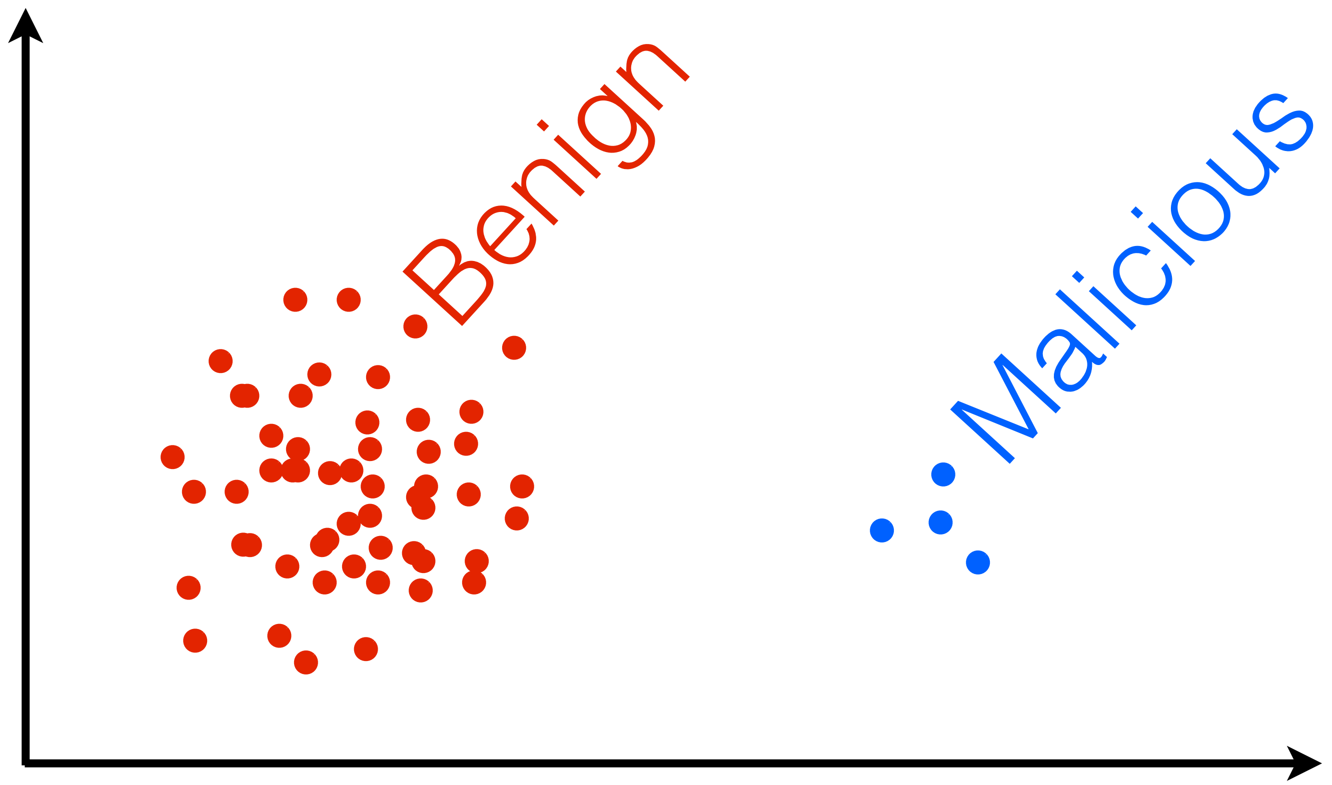

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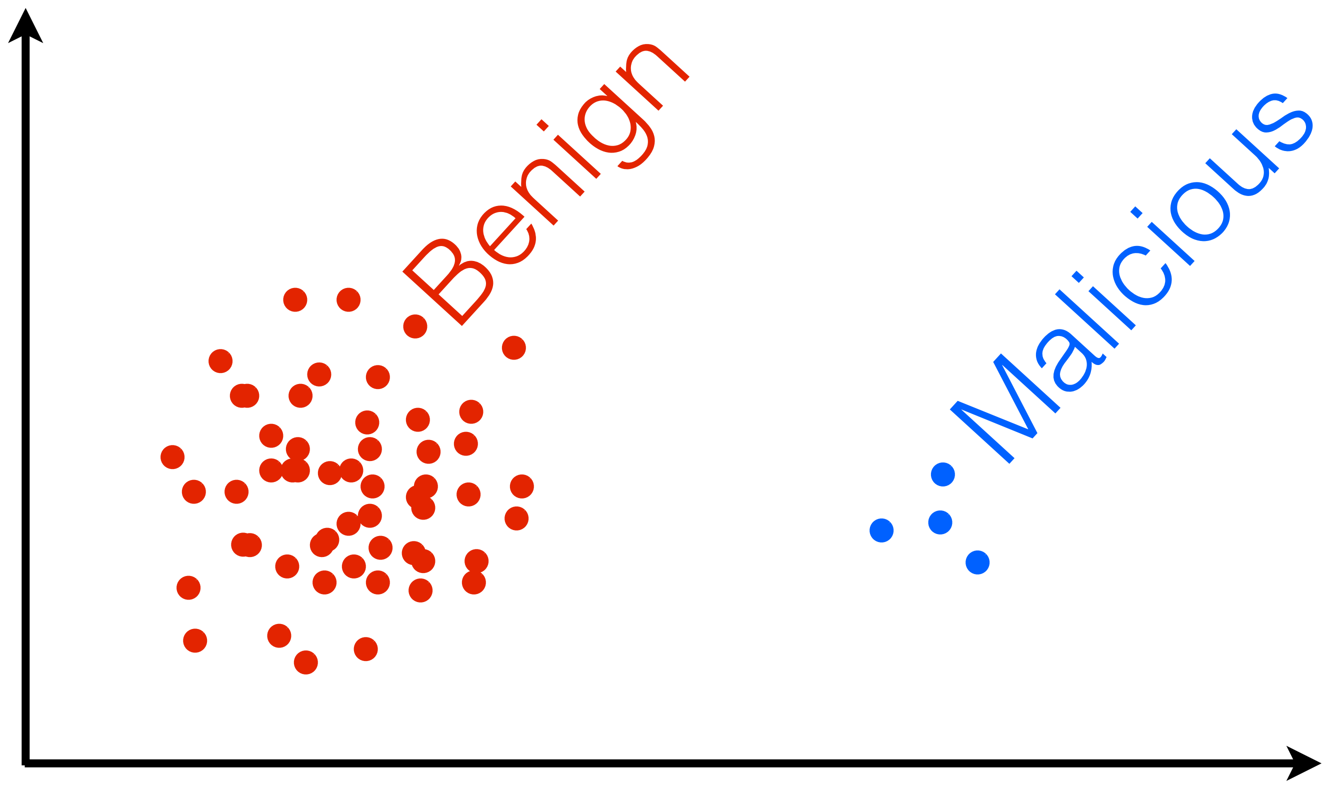

- Theoretical guarantees on quality
- How to develop **coresets for Bayes**?

[Bădoiu, Har-Peled, Indyk 2002; Agarwal et al 2005; Feldman & Langberg 2011; Huggins, Campbell, Broderick 2016; Campbell, Broderick 2019; Campbell, Broderick 2018; Agrawal, Campbell, Huggins, Broderick 2019]

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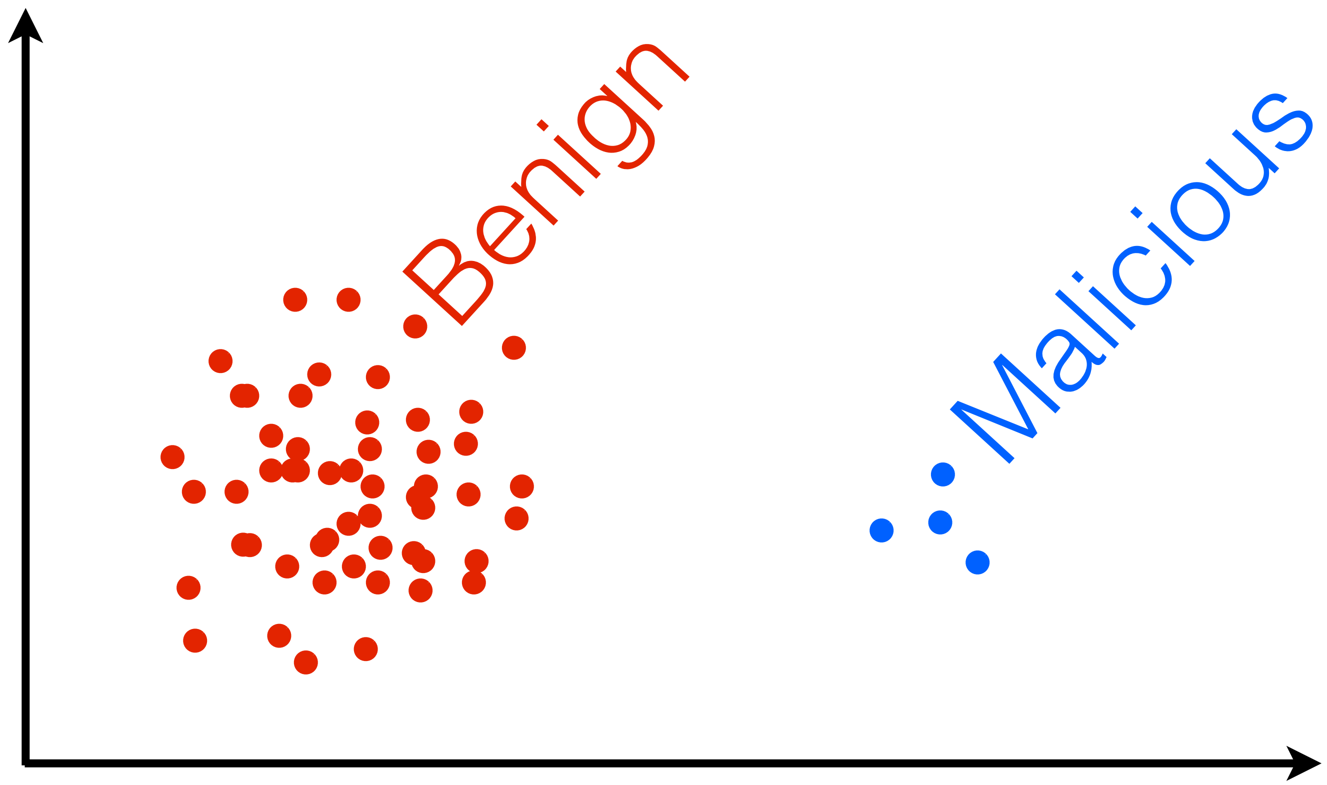

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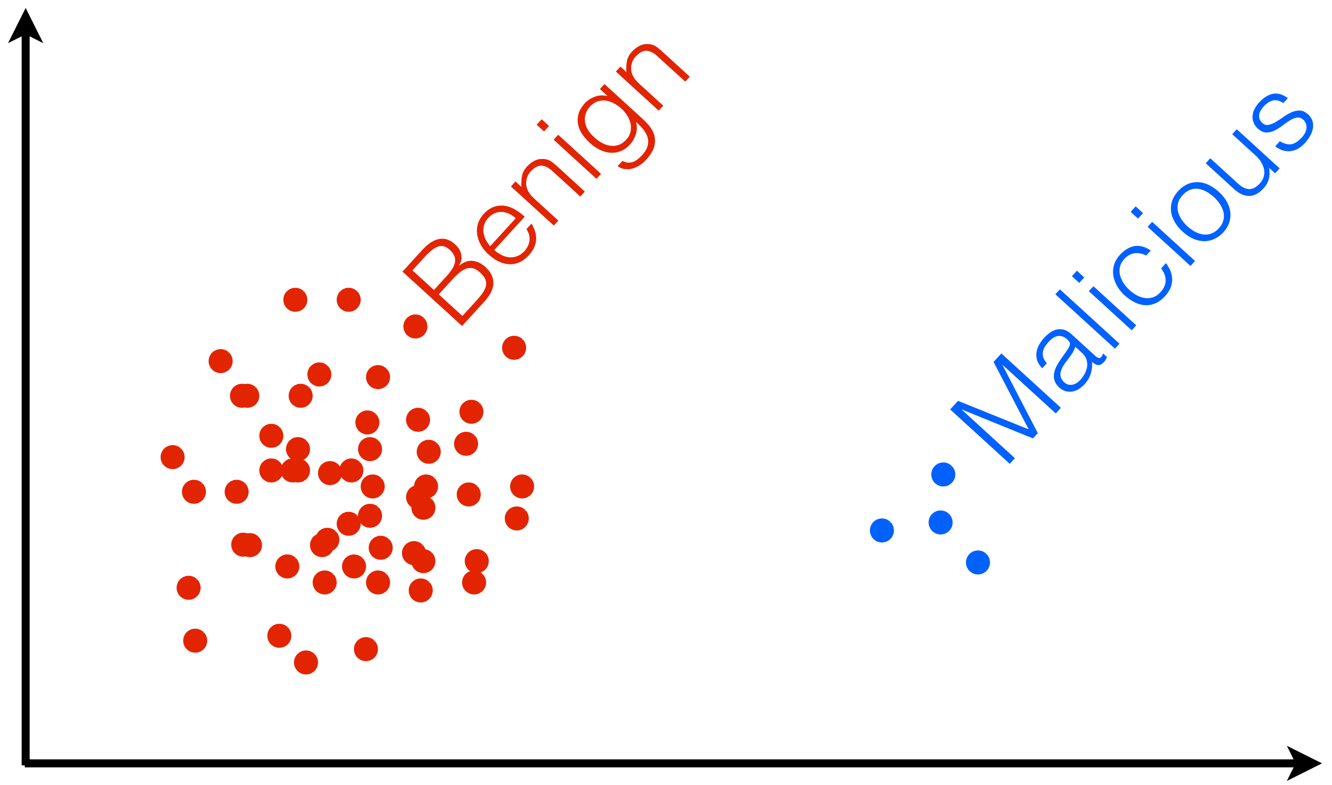

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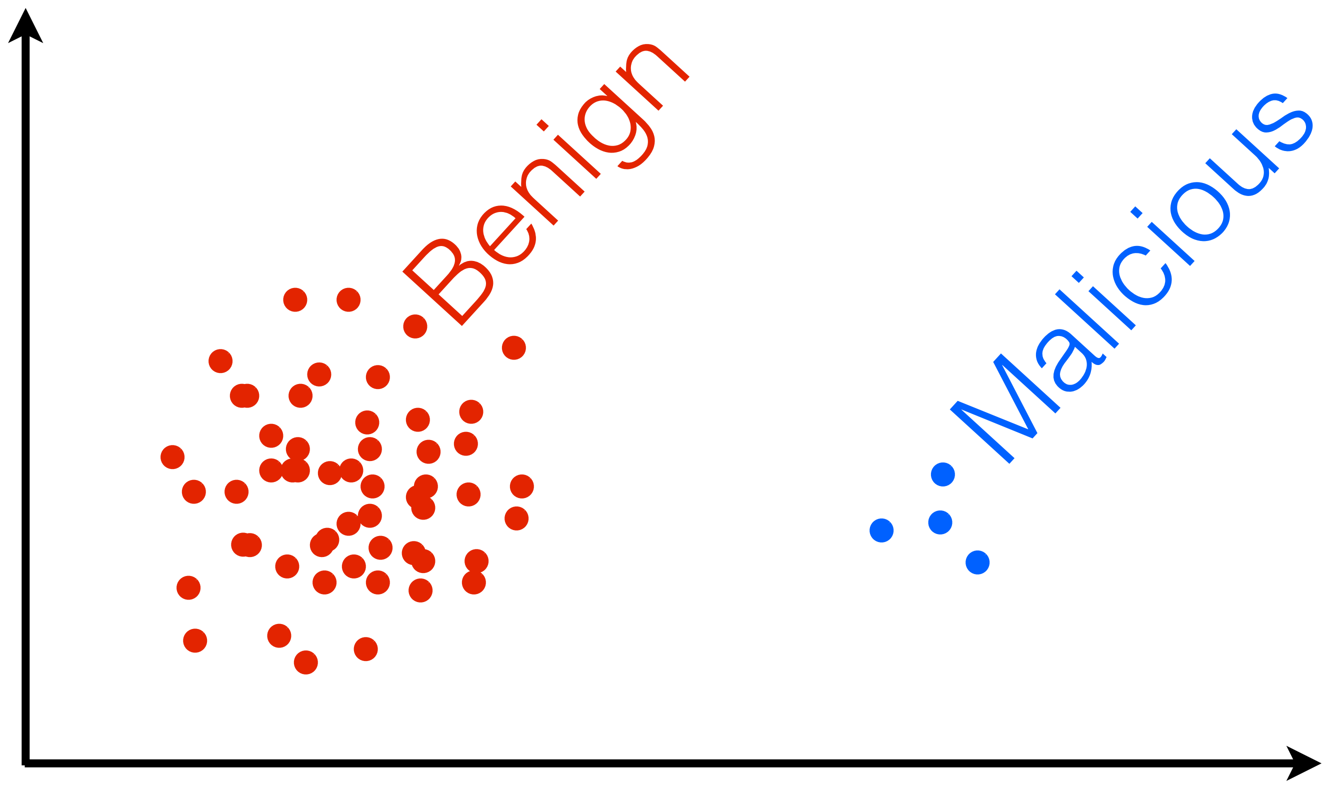

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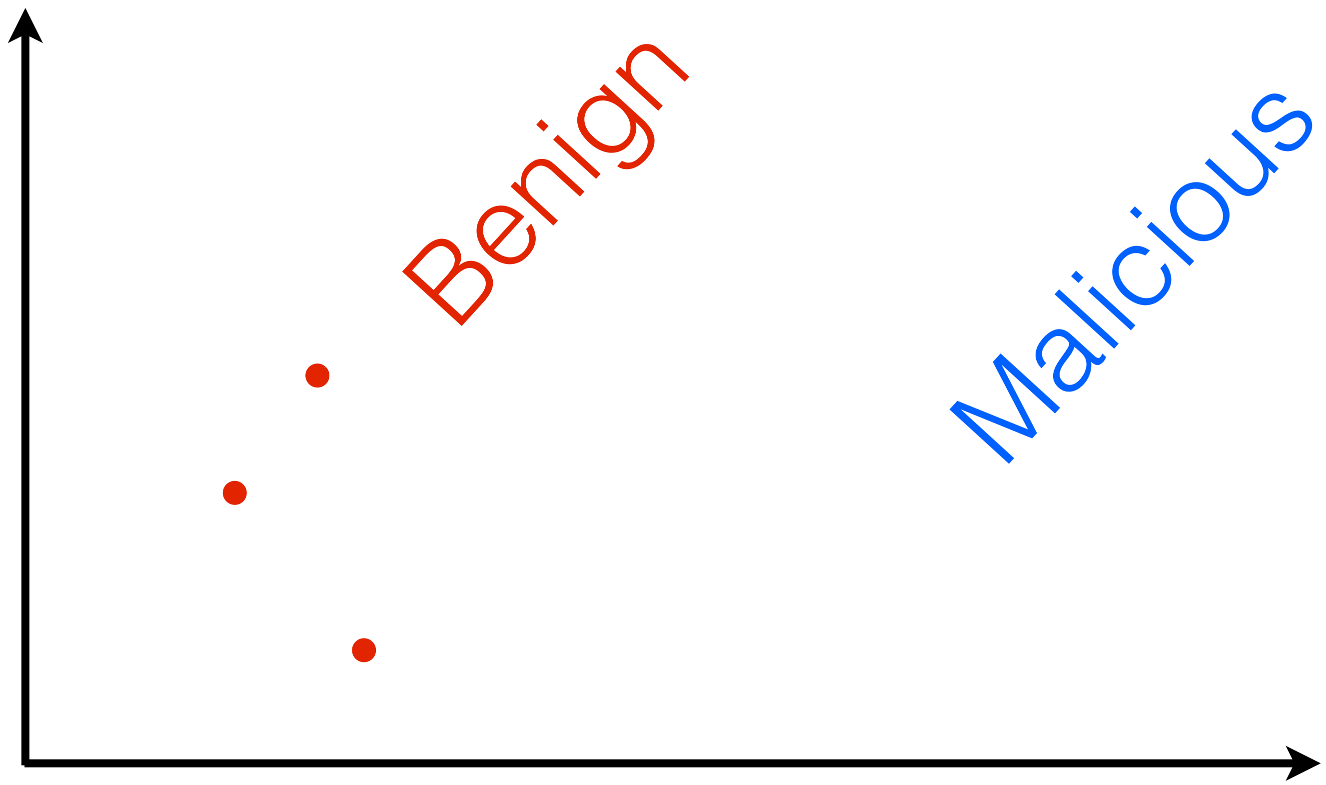

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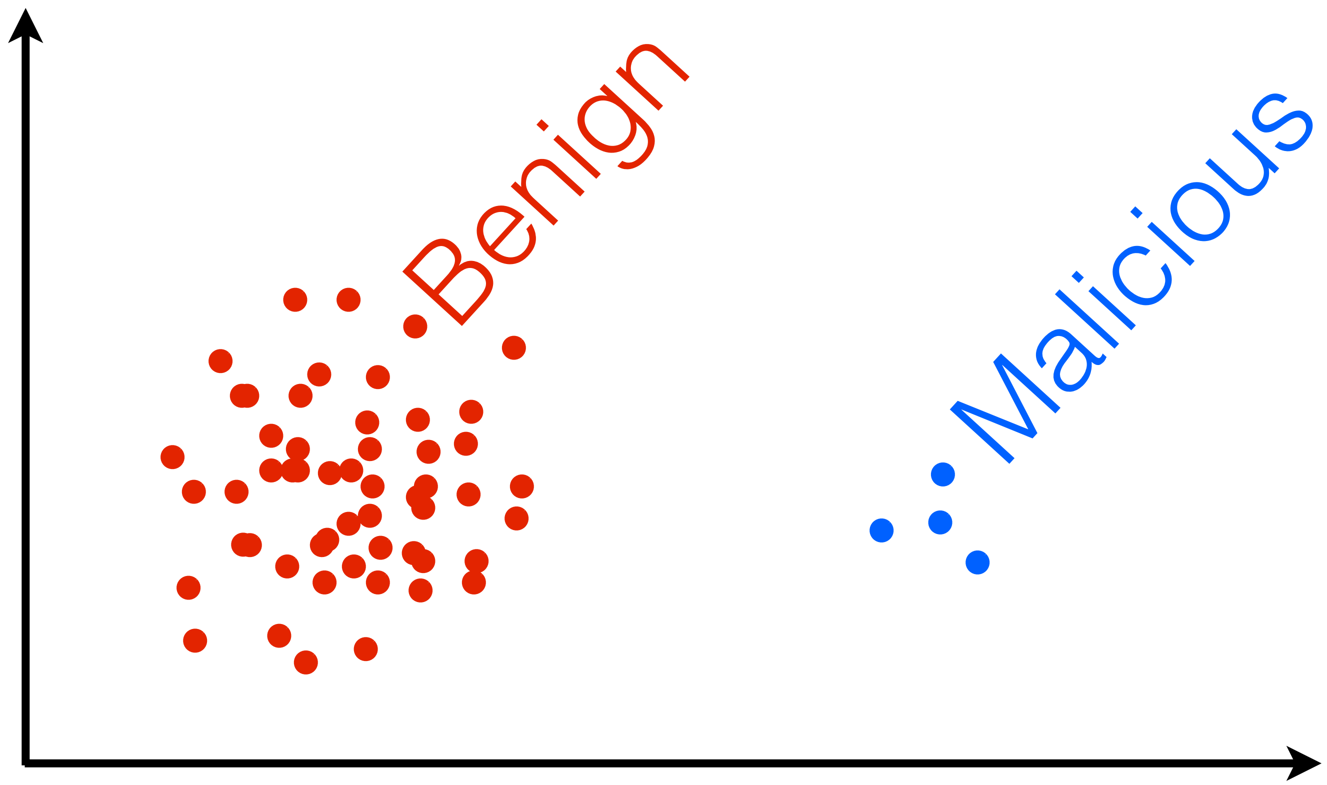

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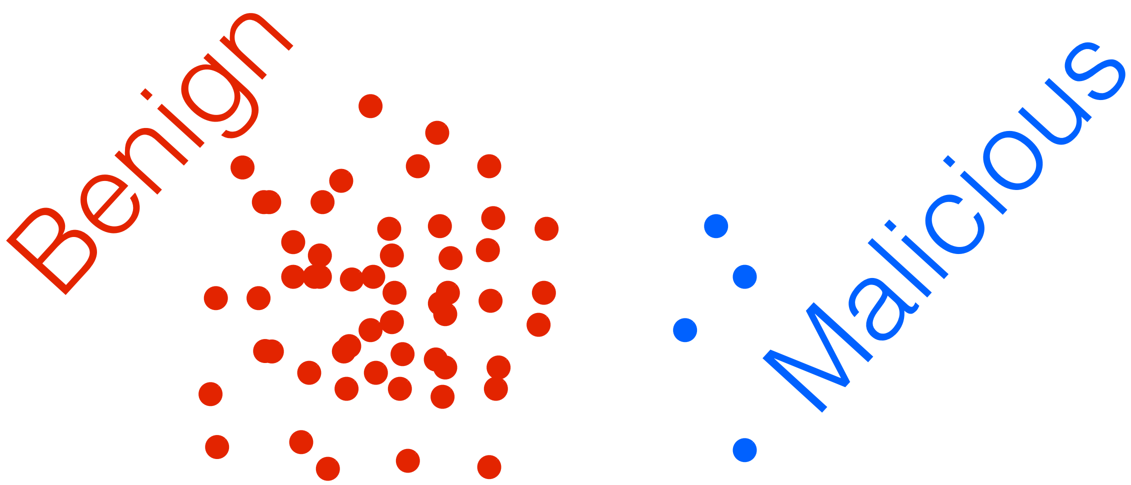

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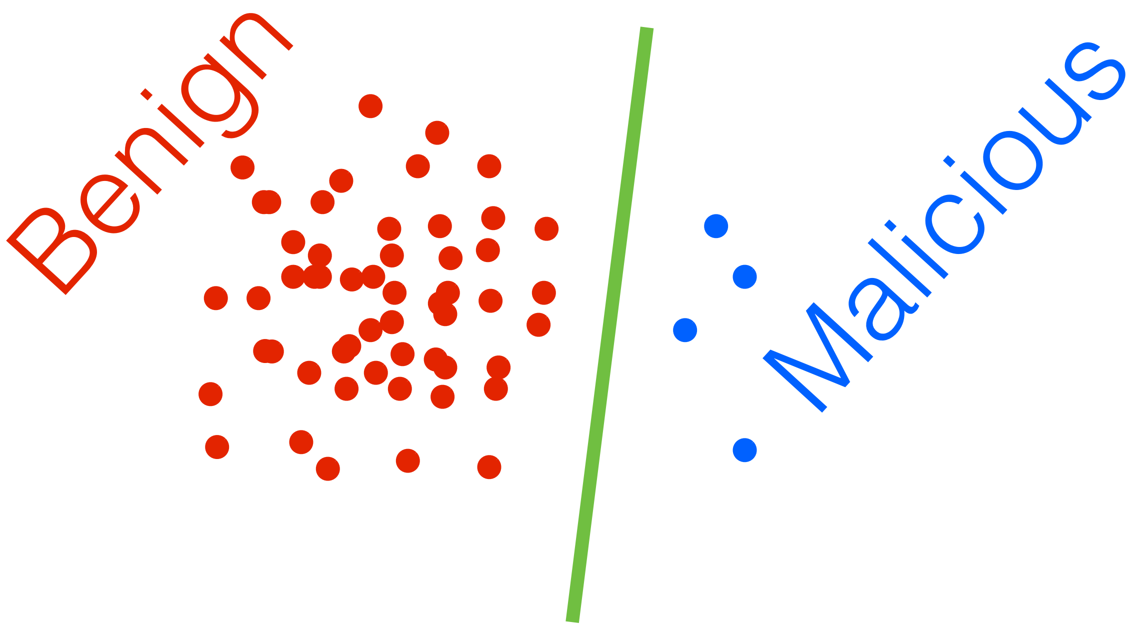

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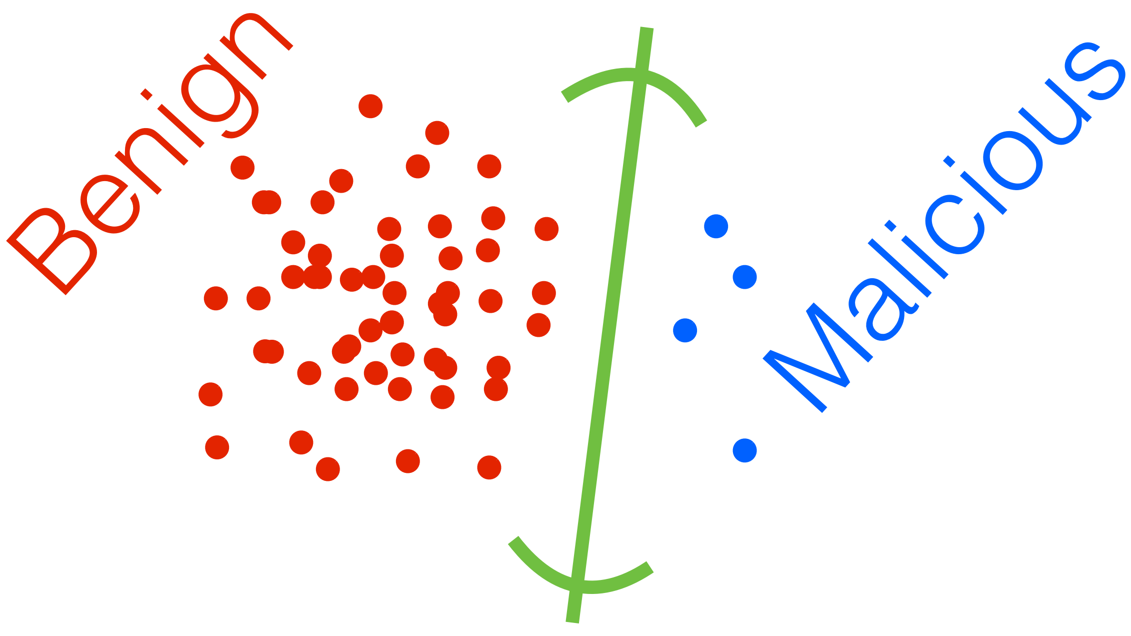

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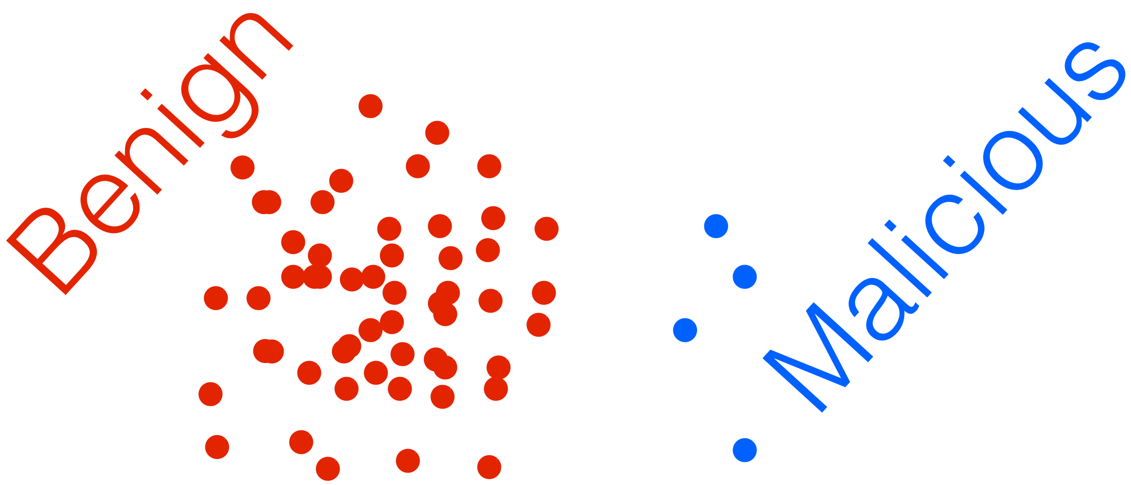

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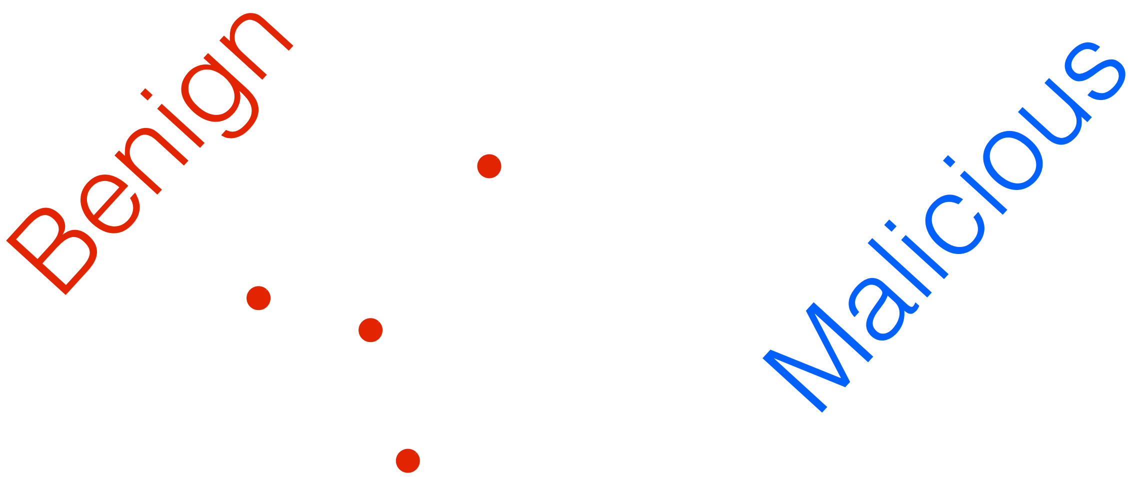

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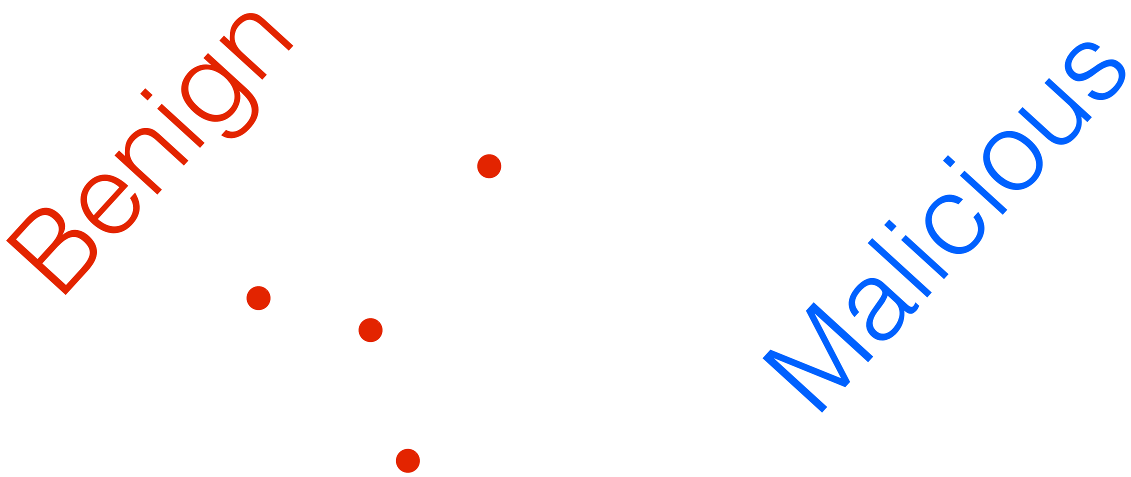

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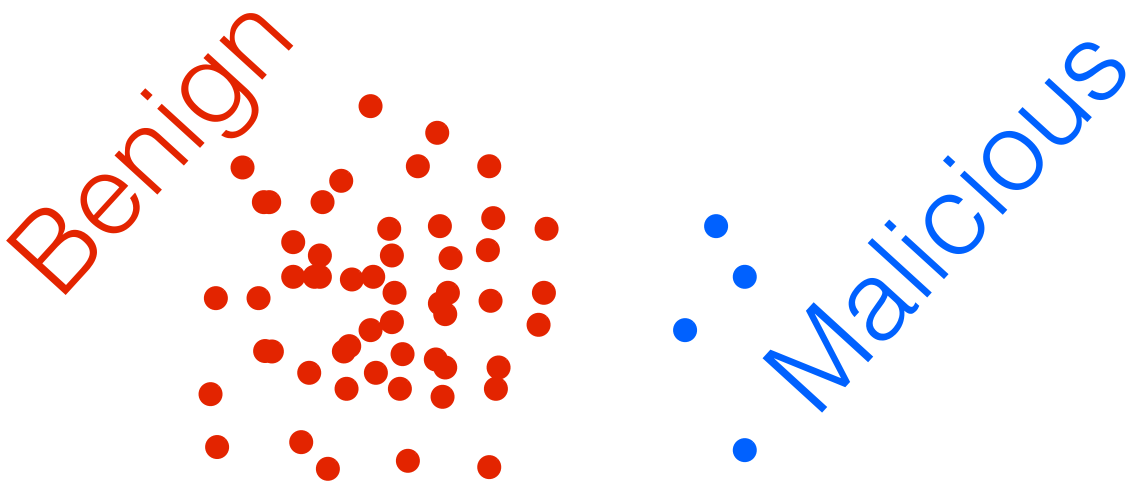

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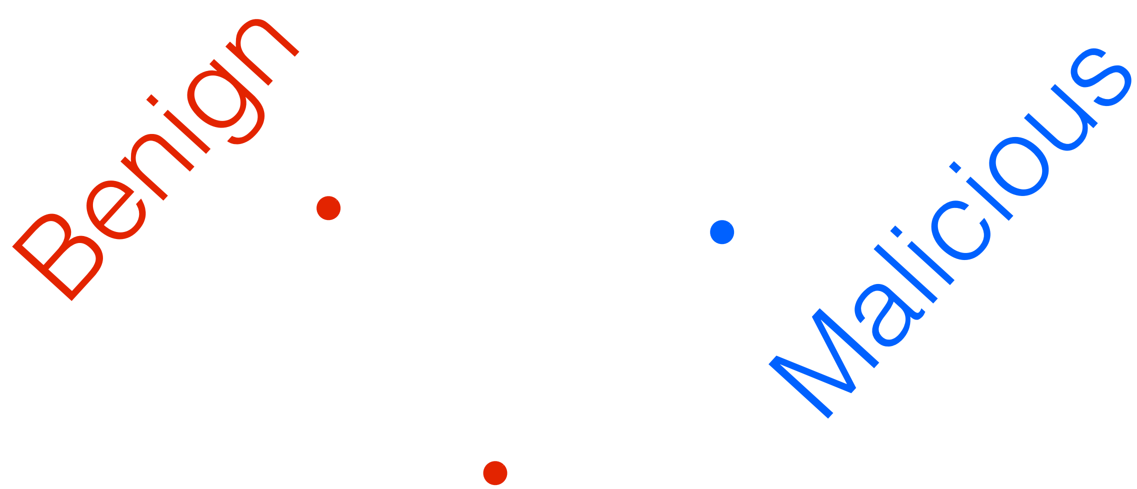

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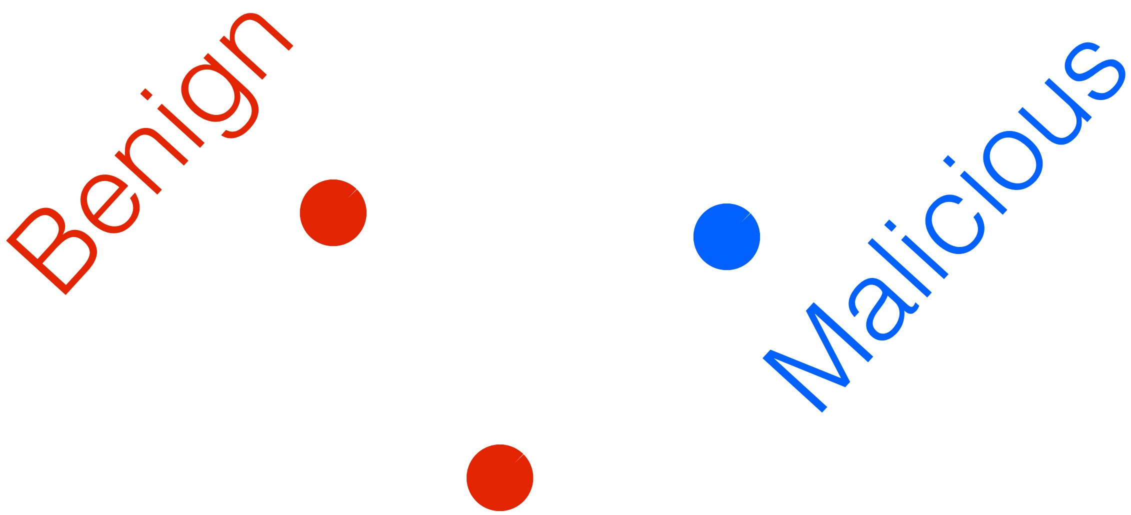

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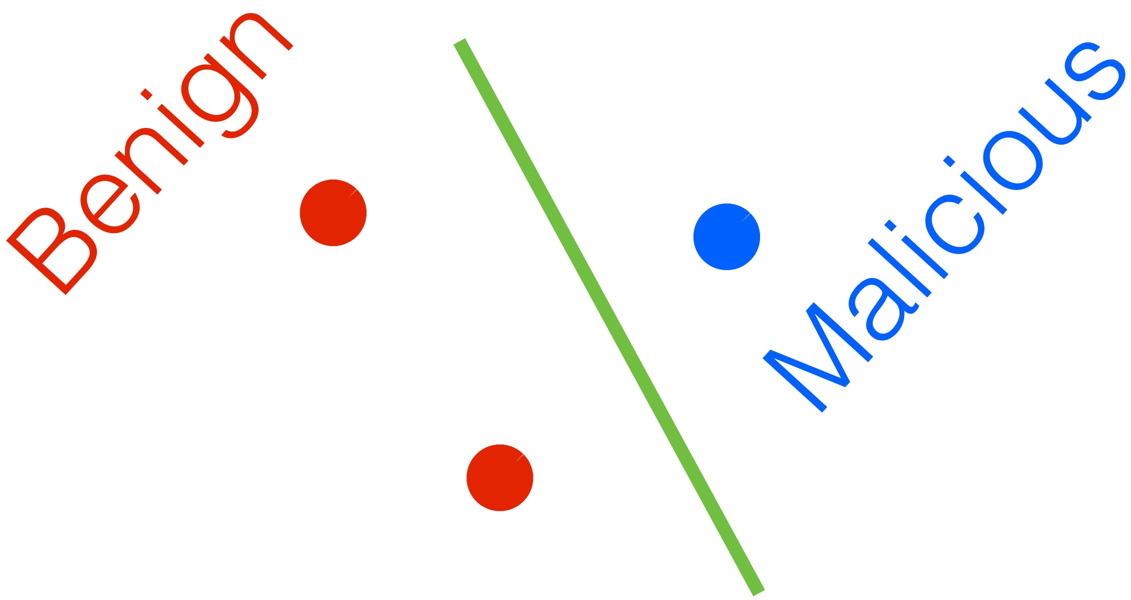

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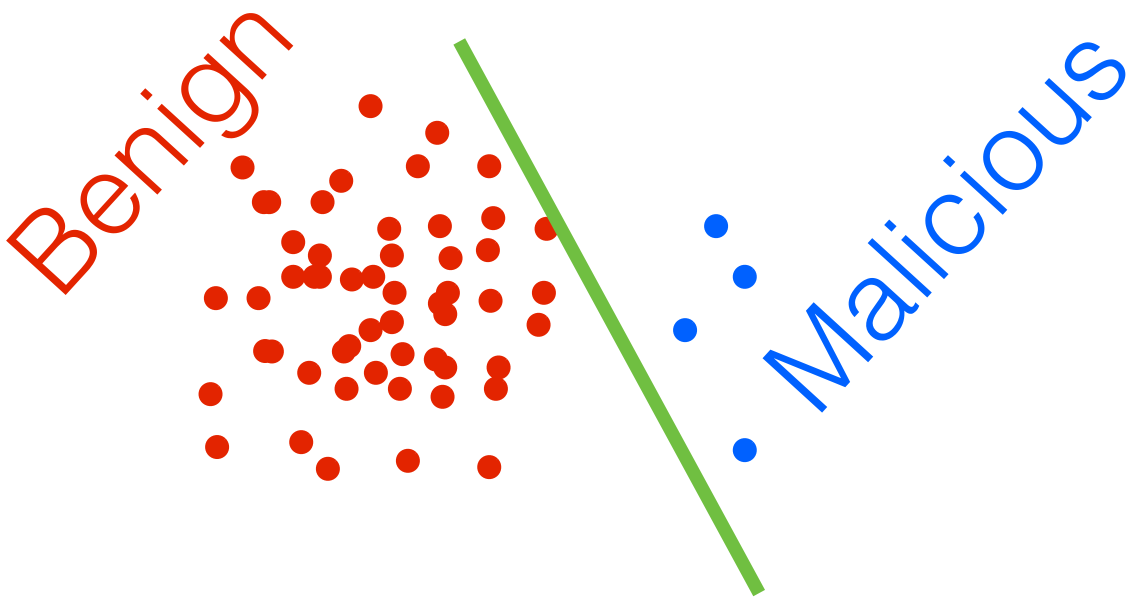

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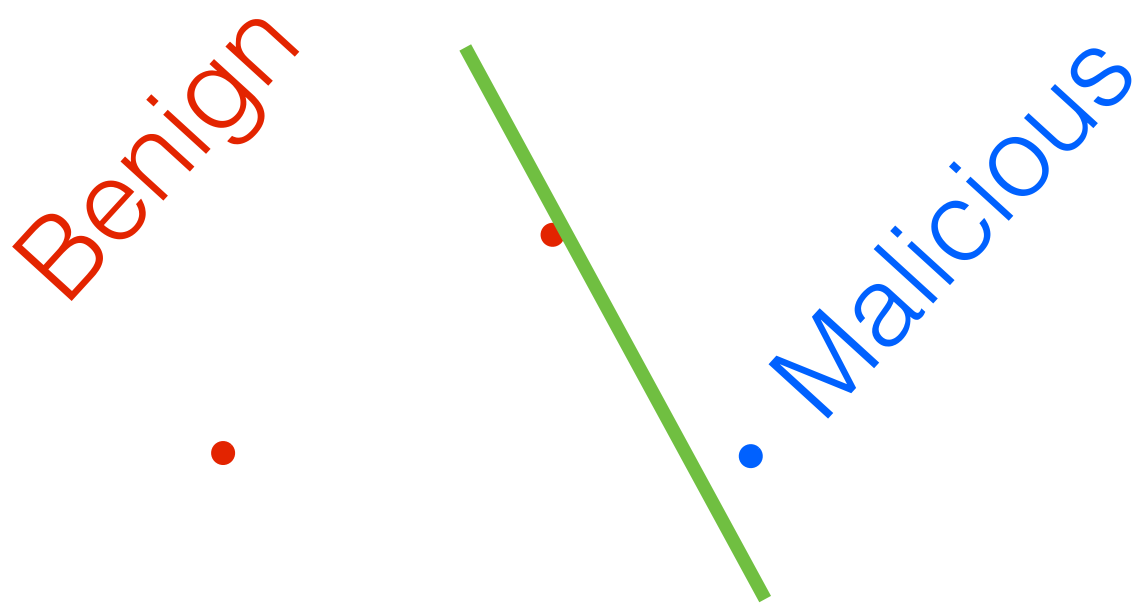

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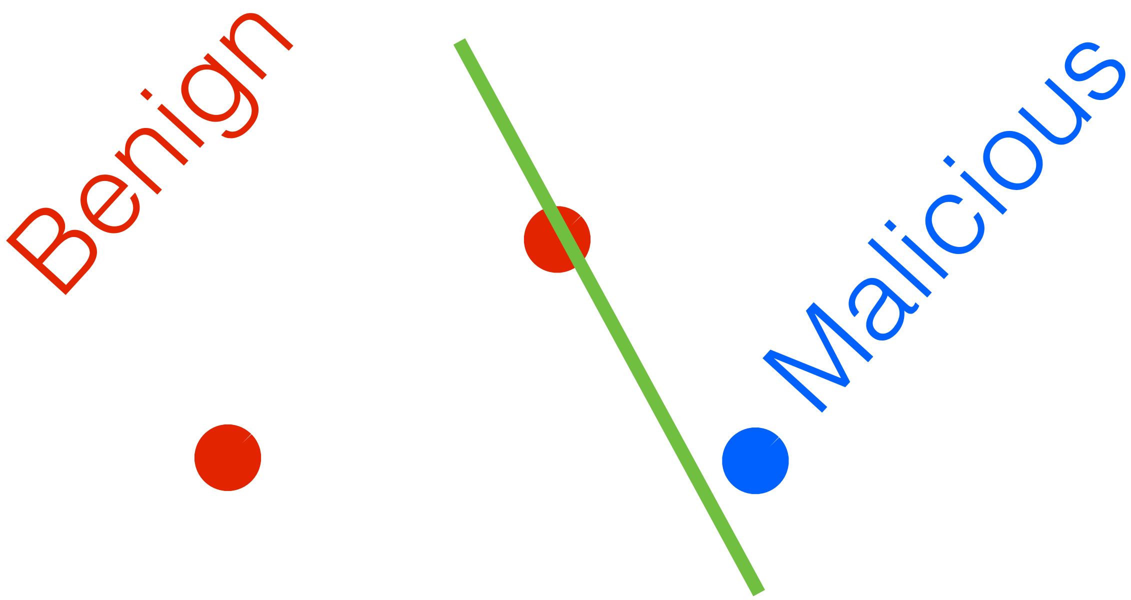

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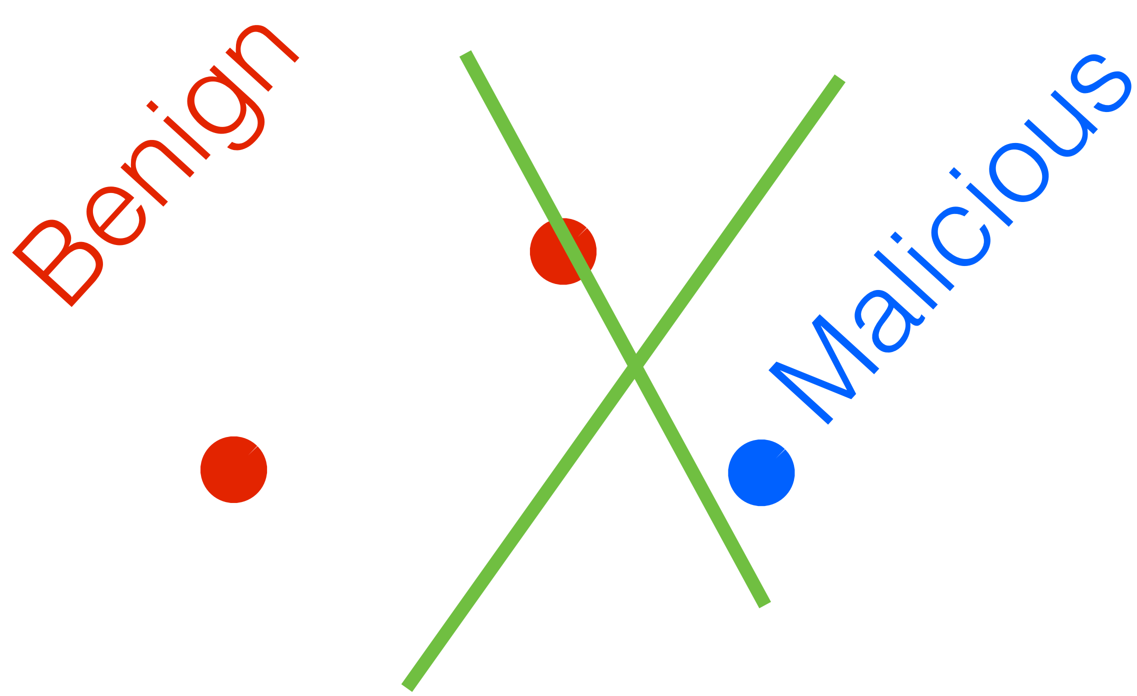

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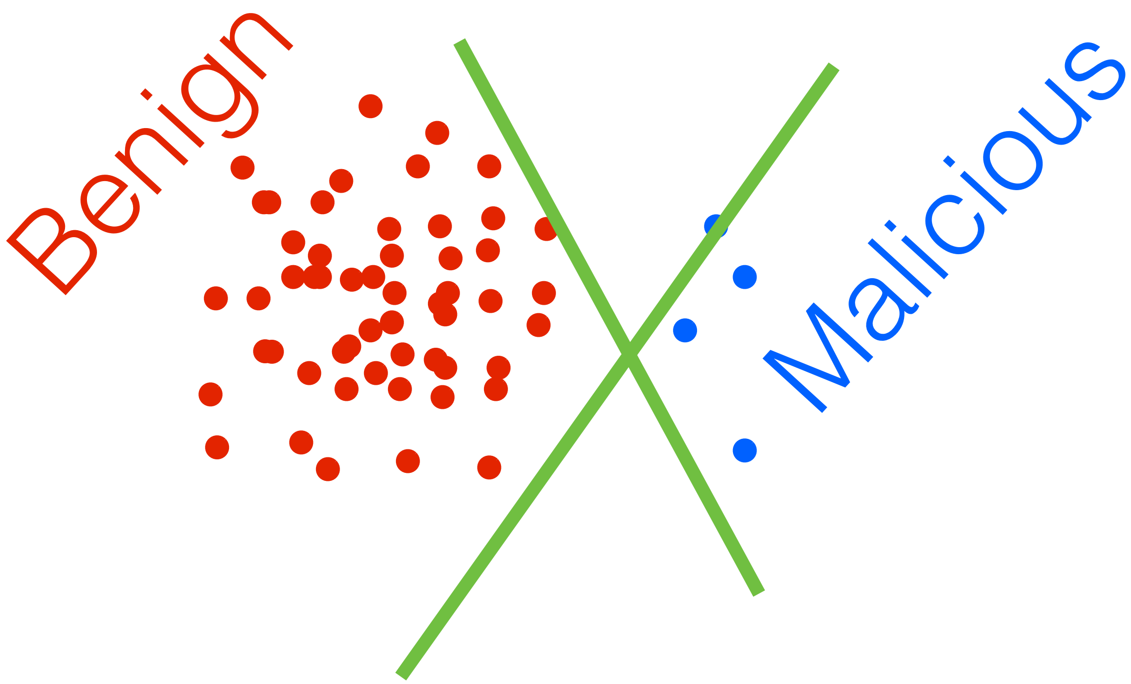

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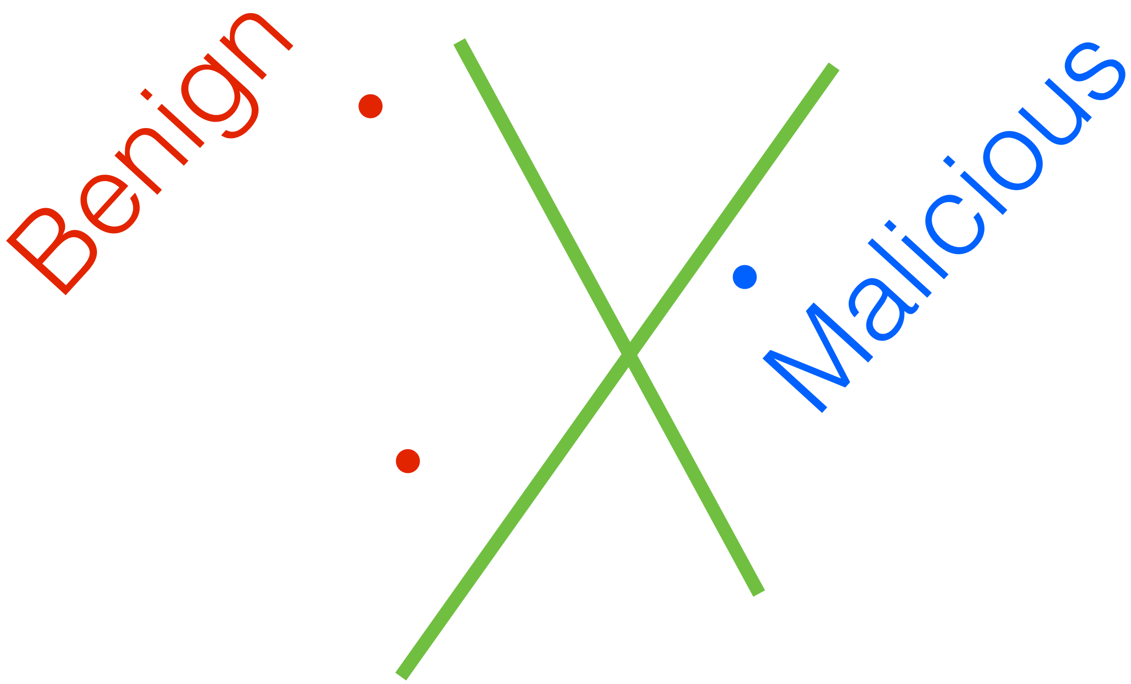

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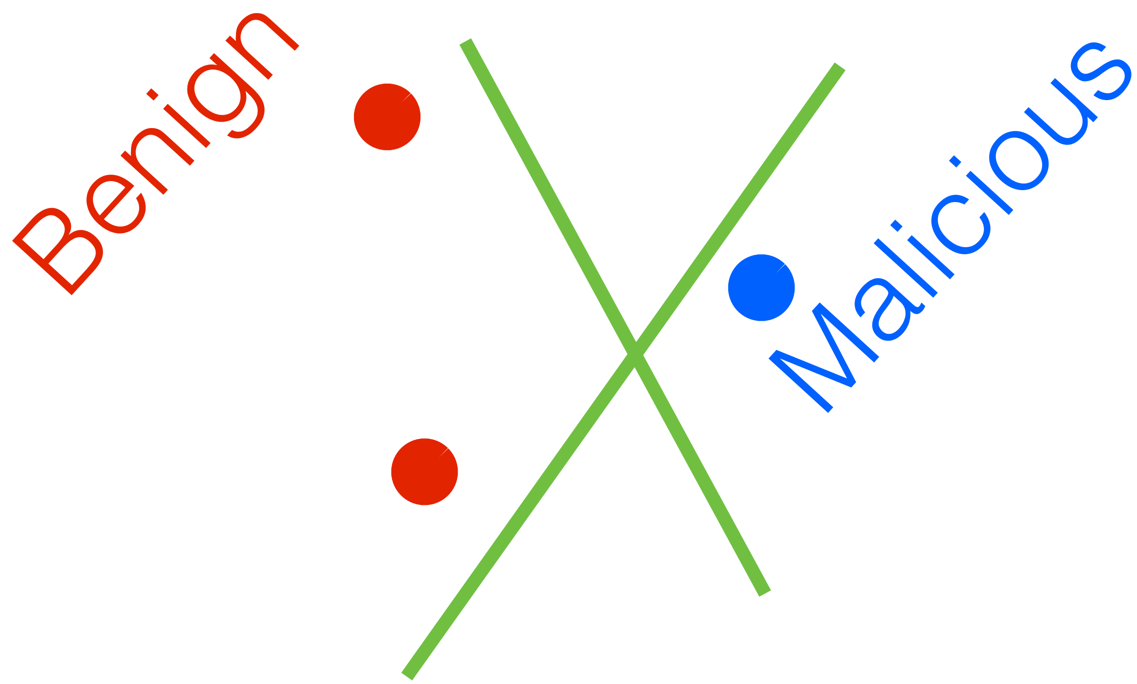

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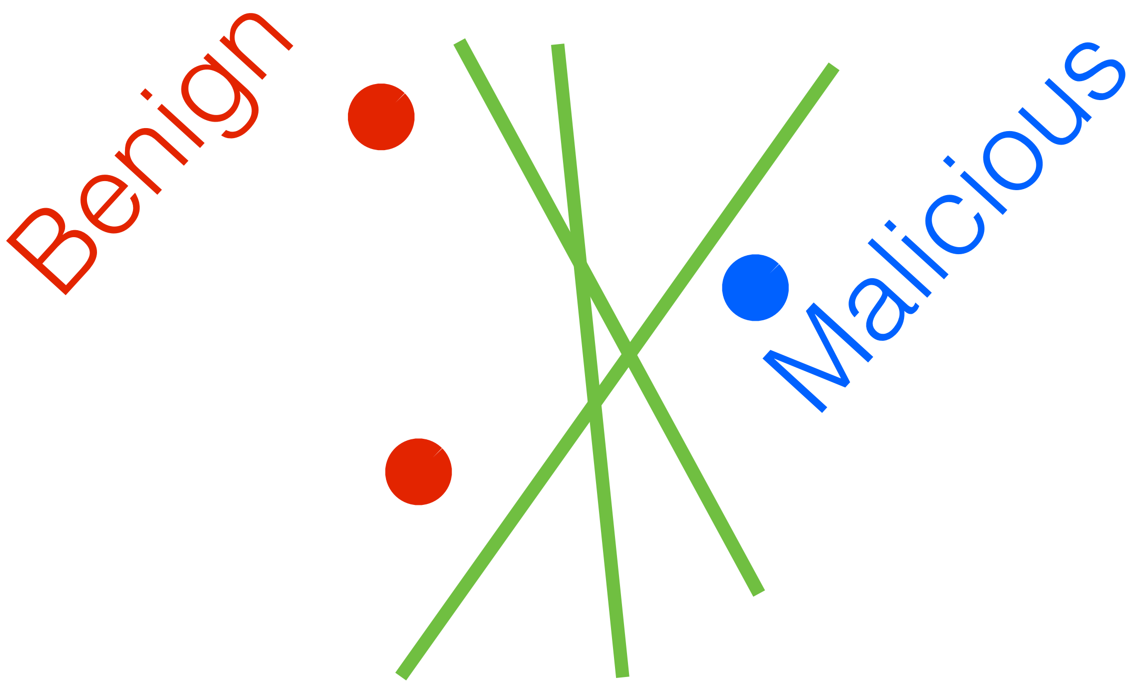

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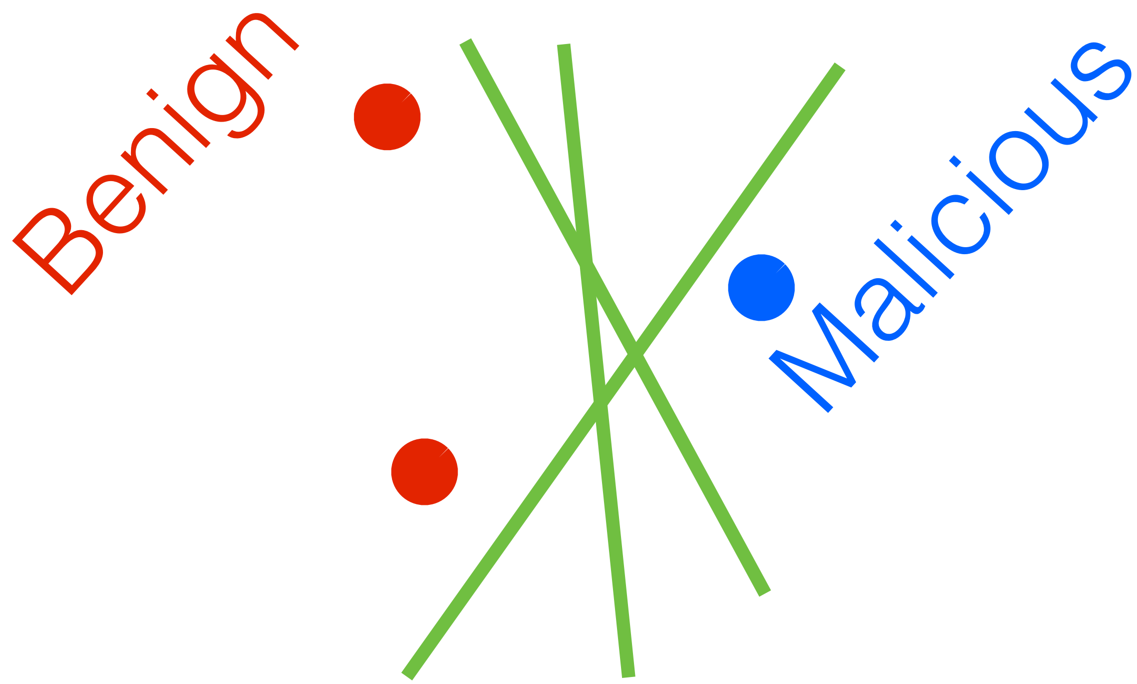

- Might miss important data
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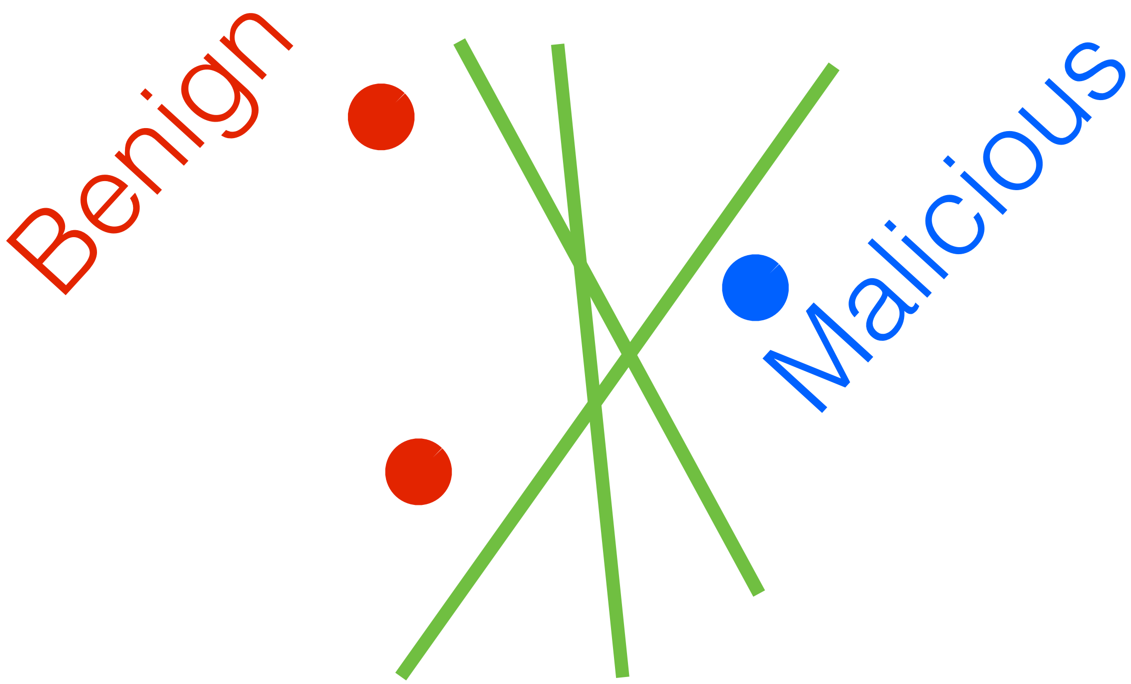
Uniform subsampling



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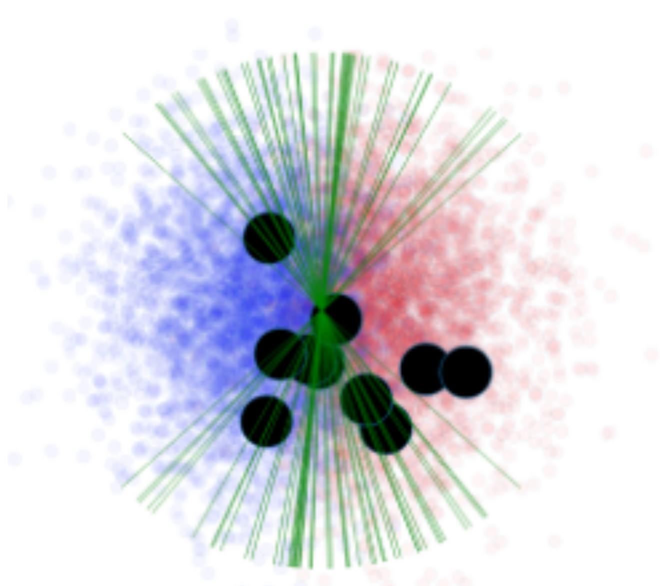
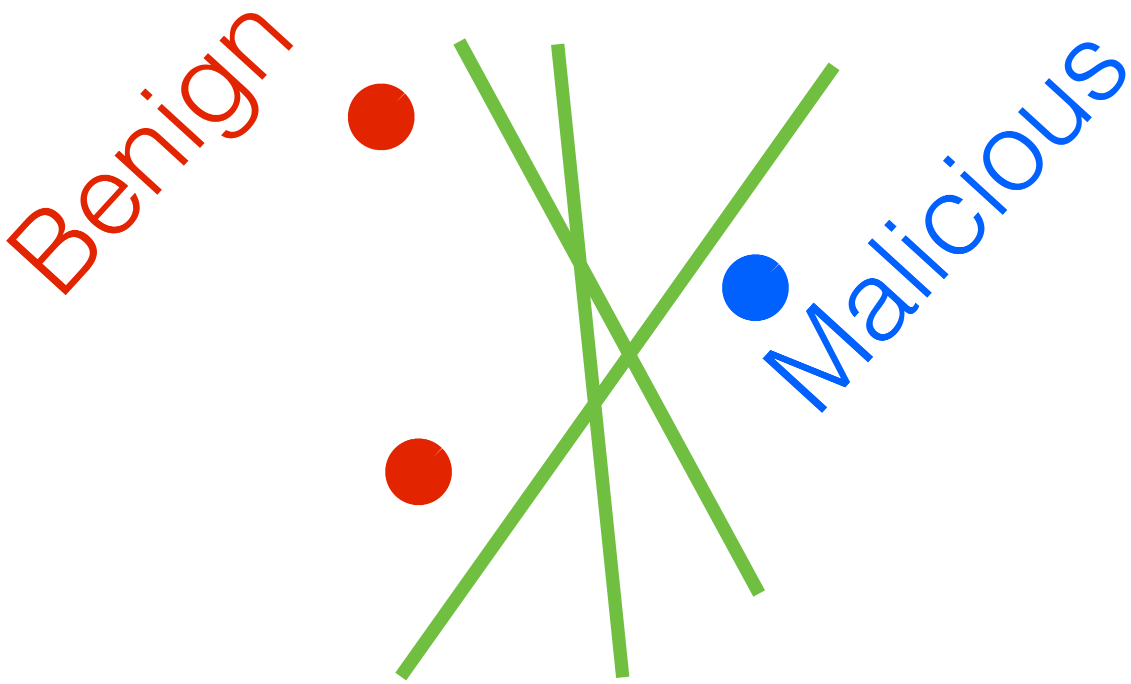
- Noisy estimates



$M = 10$

[Campbell, Broderick 2018, 2019]

Uniform subsampling



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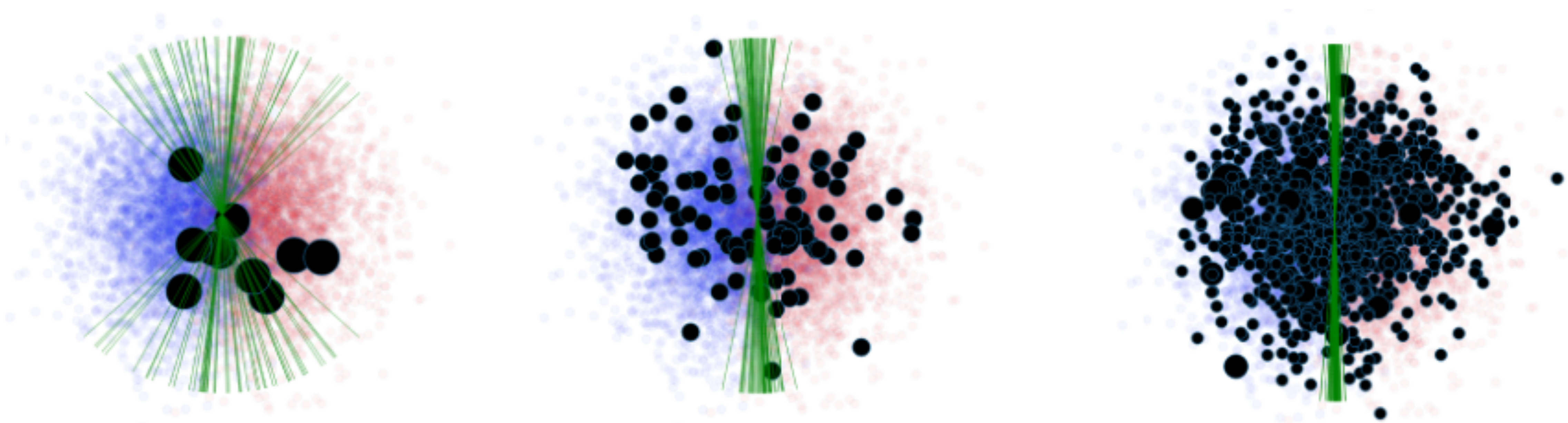
- Noisy estimates

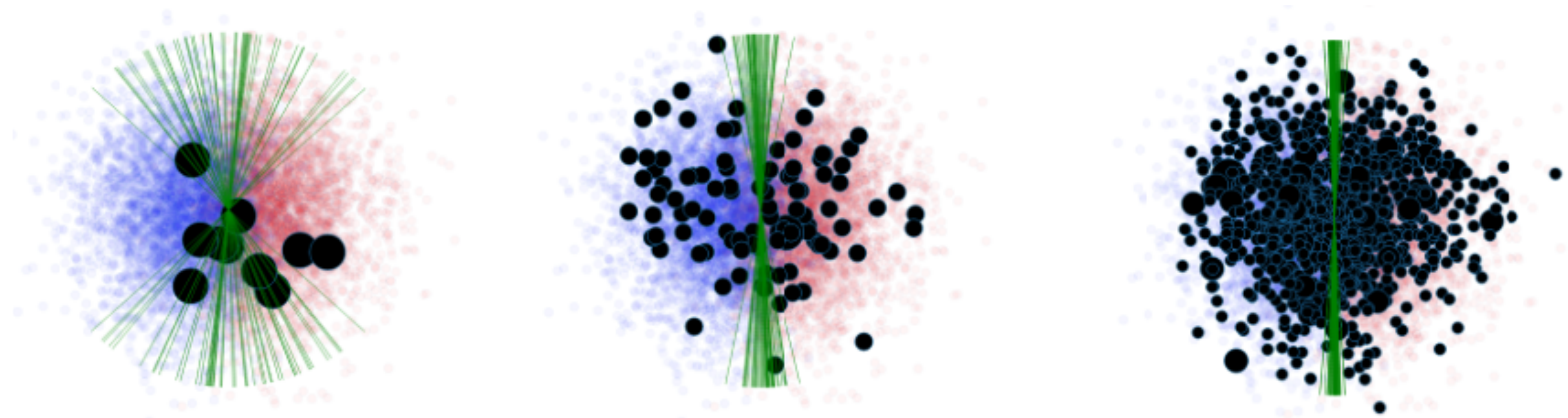


$M = 10$ $M = 100$ $M = 1000$

[Campbell, Broderick 2018, 2019]

Data summarization alternatives

Uniform subsampling



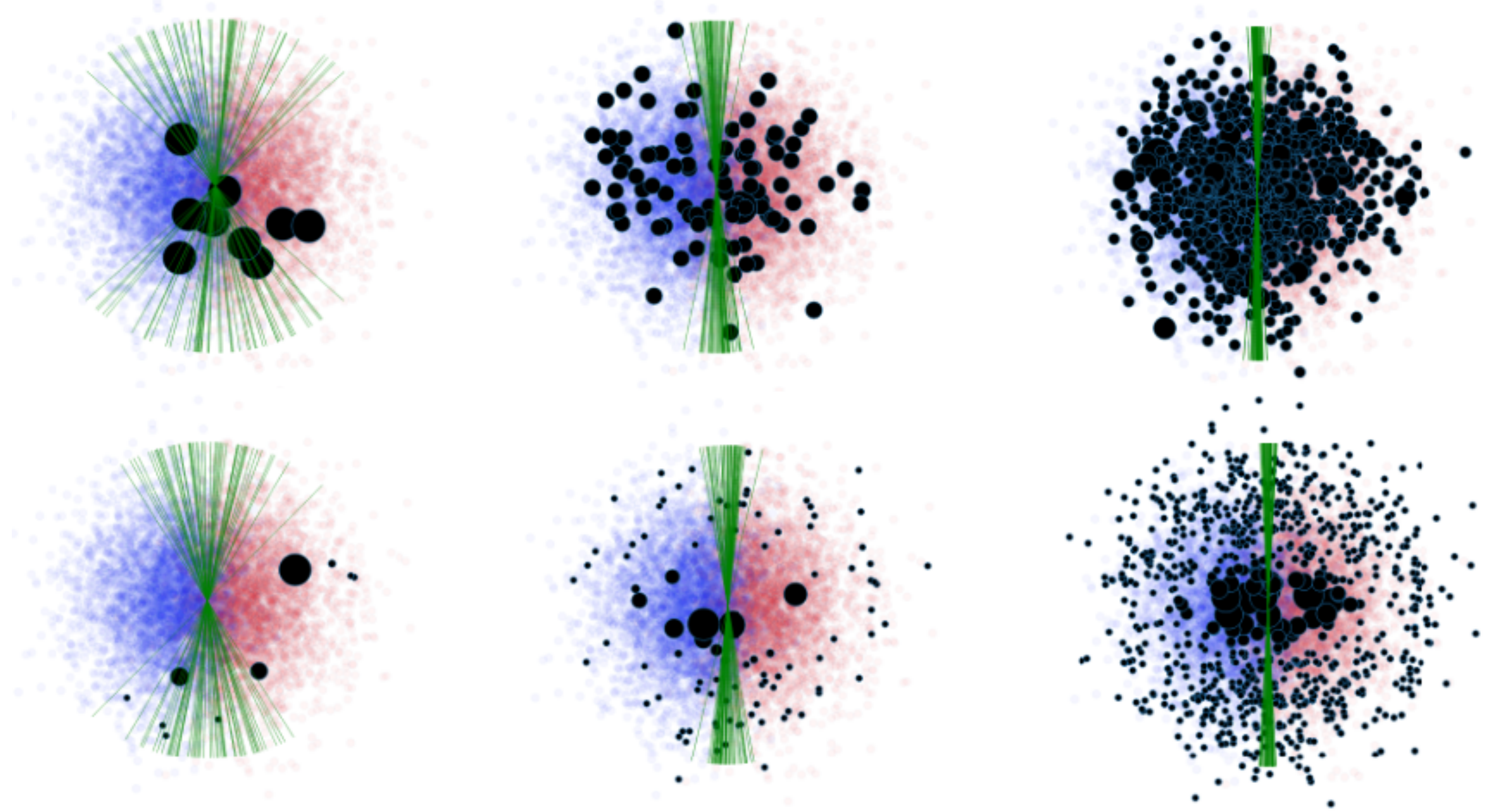
$M = 10$ $M = 100$ $M = 1000$

[Campbell, Broderick 2018, 2019]

Data summarization alternatives

Uniform subsampling

Importance sampling



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

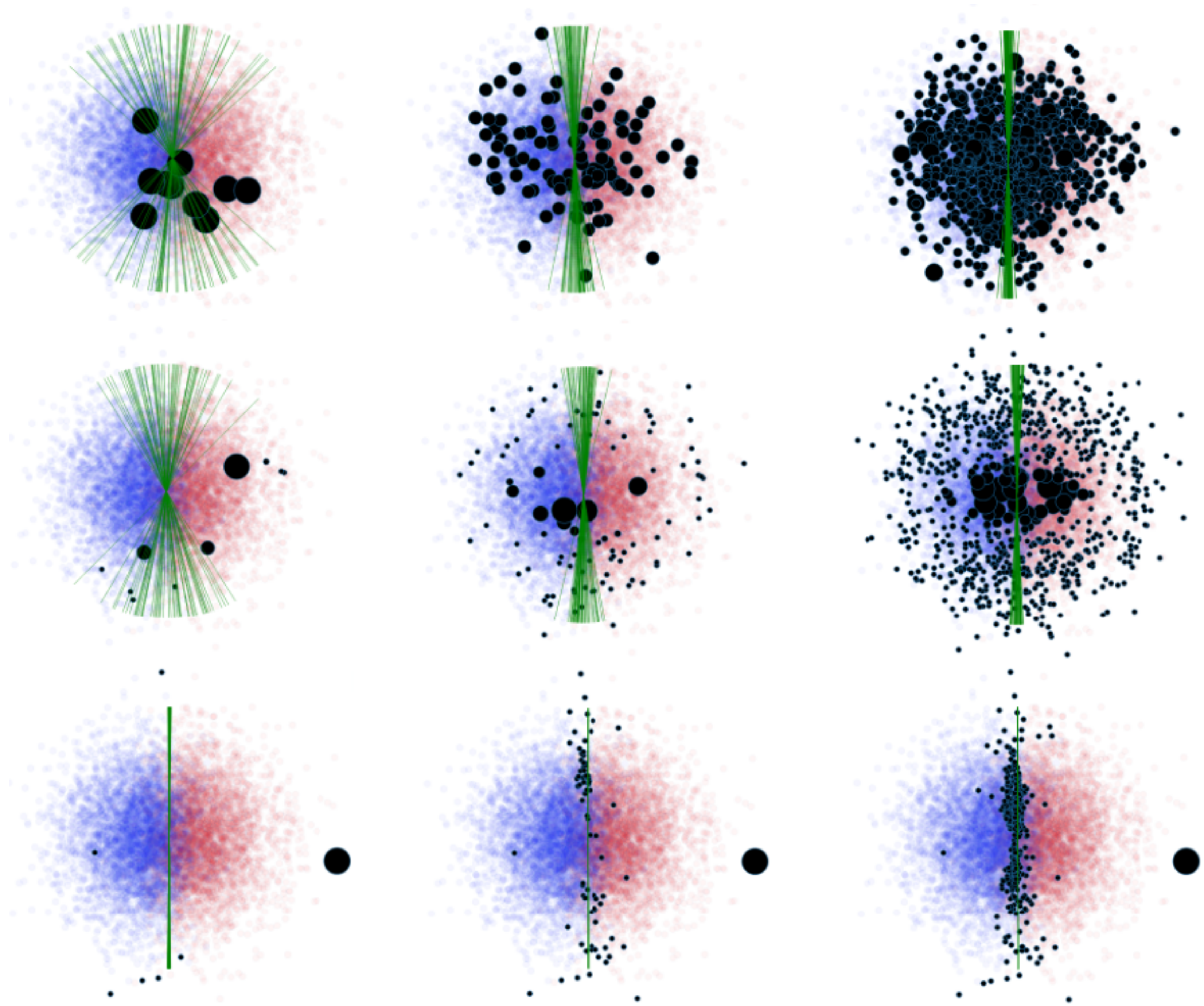
[Campbell, Broderick 2018, 2019]

Data summarization alternatives

Uniform subsampling

Importance sampling

Bayesian/Hilbert coresets



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

[Campbell, Broderick 2018, 2019]

Reliable diagnostics

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- ELBO or KL alone isn't enough

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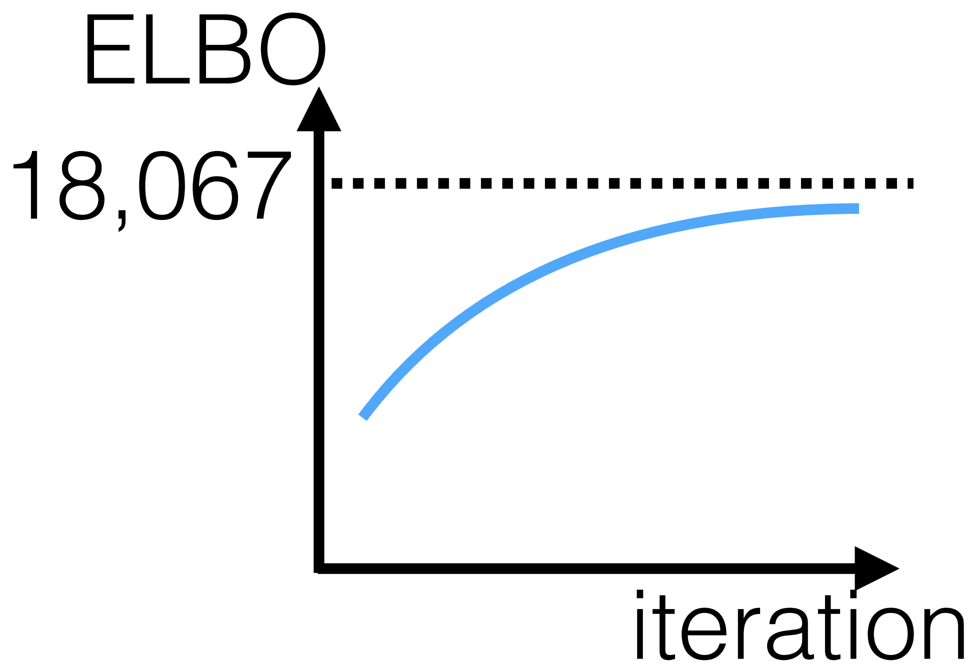

Reliable diagnostics

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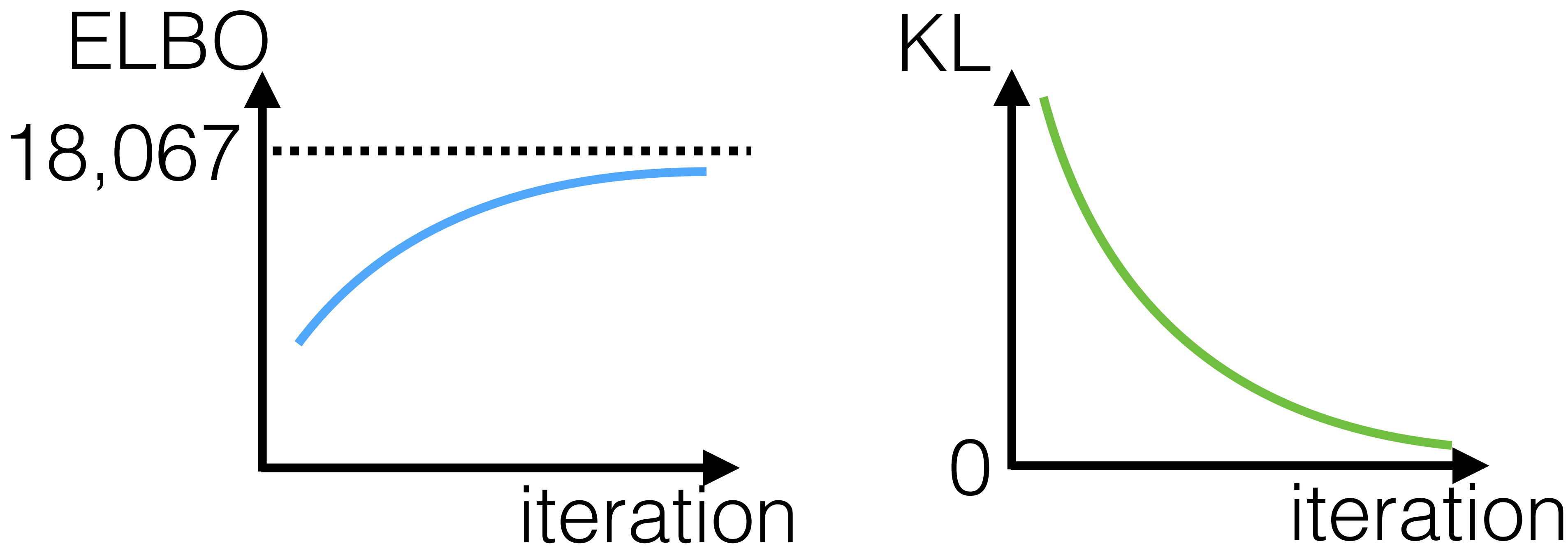

Reliable diagnostics

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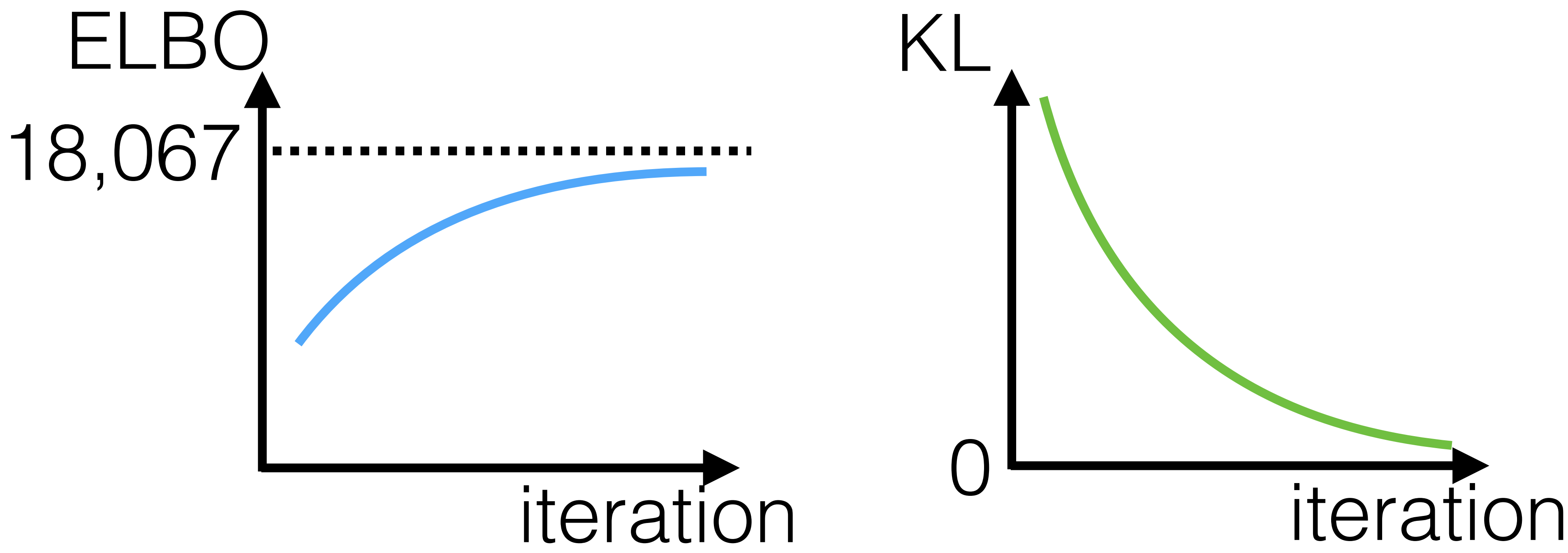

- Instead: easy-to-compute bound on Wasserstein [Huggins, Kasprzak, Campbell, Broderick, 2020]
  - Wasserstein bounds error in posterior mean and variance

Reliable diagnostics

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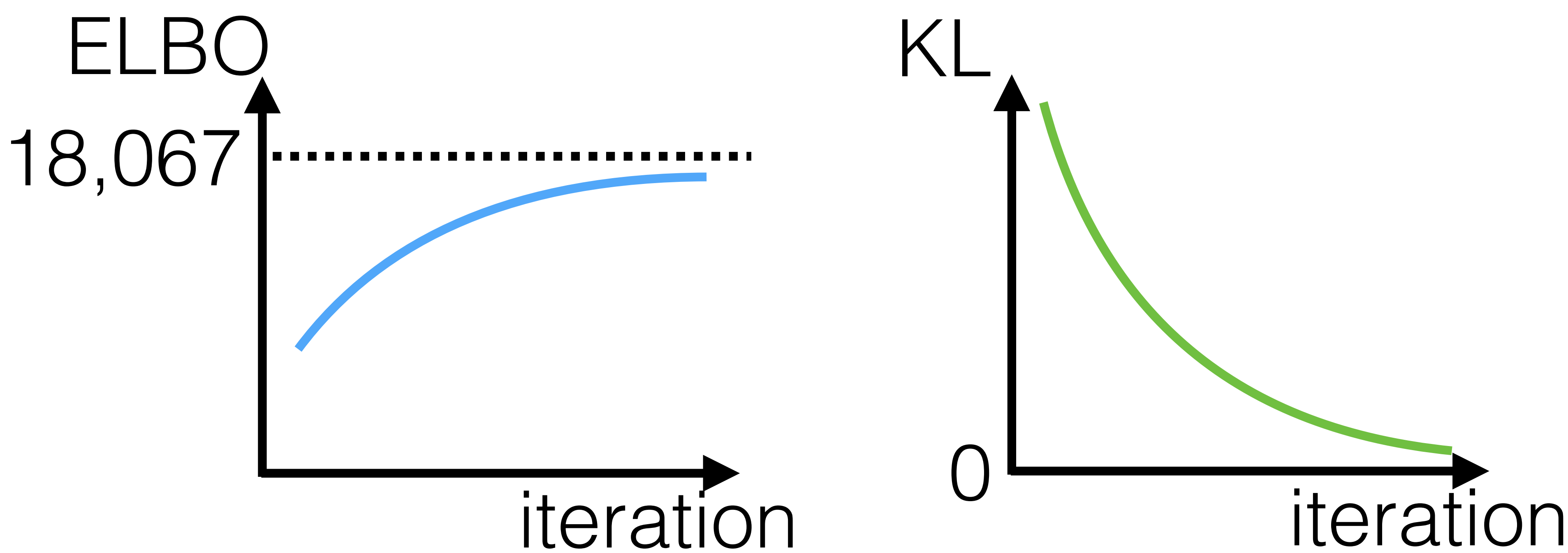

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- Part of a validated workflow for VB [Huggins, Kasprzak, Campbell, Broderick, 2020]

Reliable diagnostics

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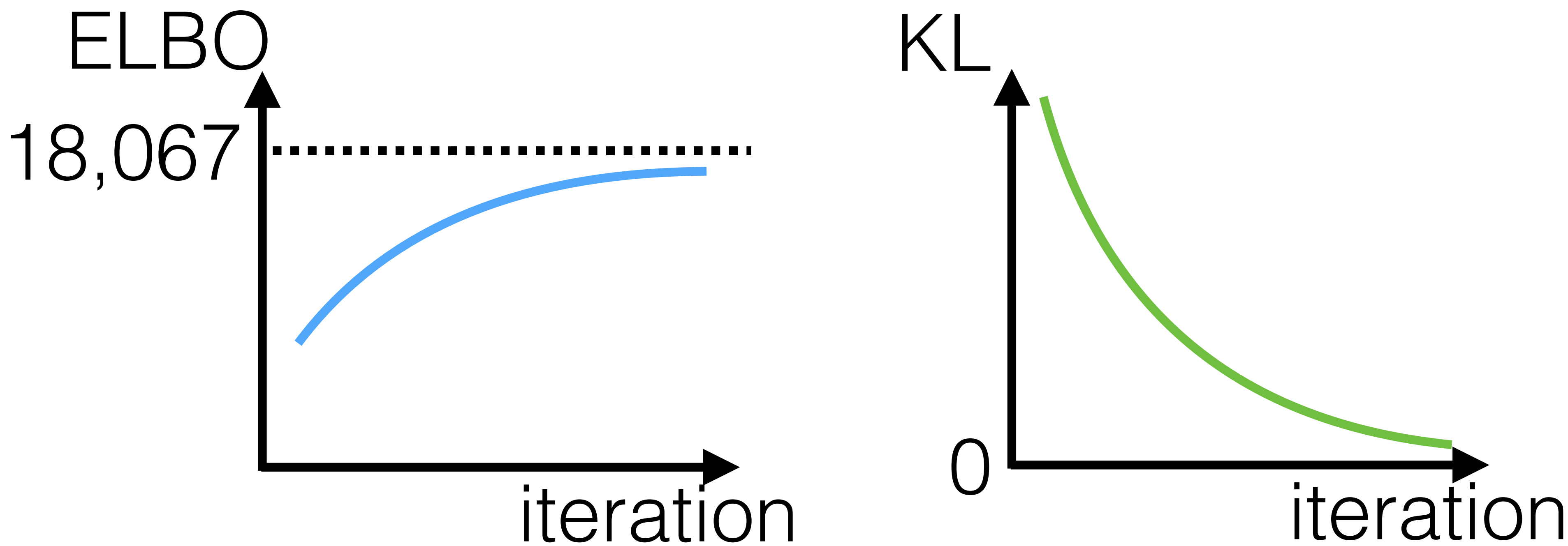

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  - Builds on e.g. [Dieng et al 2017; Yao et al 2018]

Reliable diagnostics

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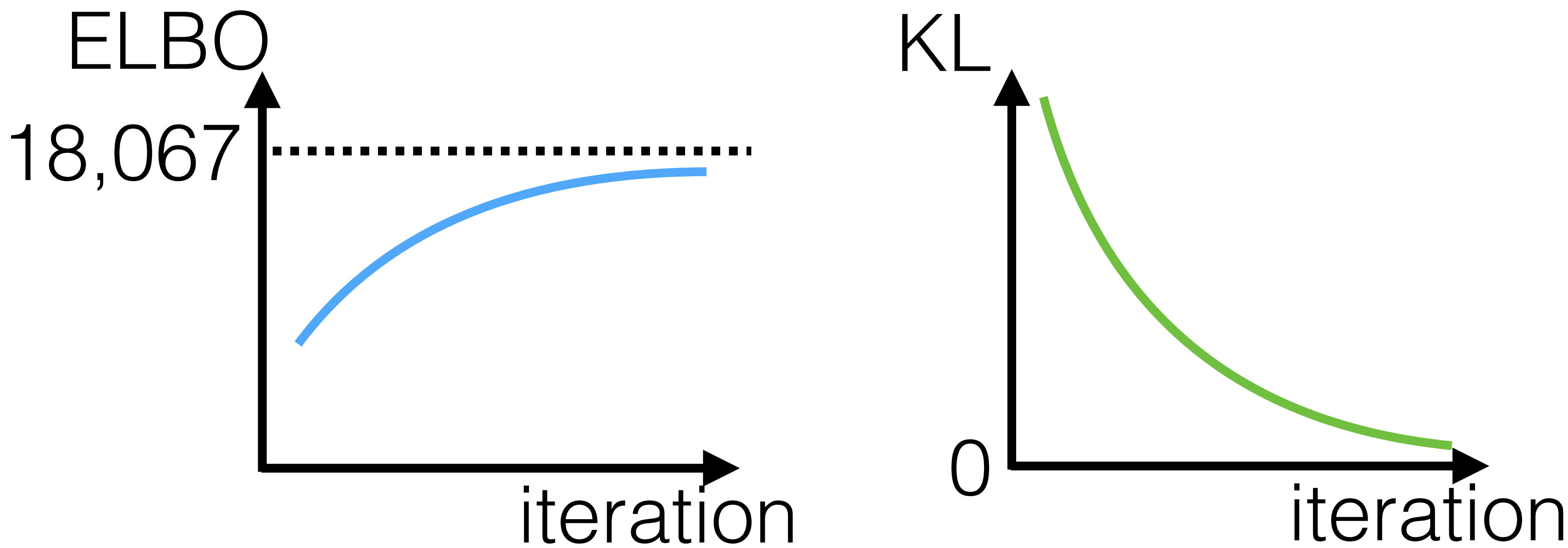

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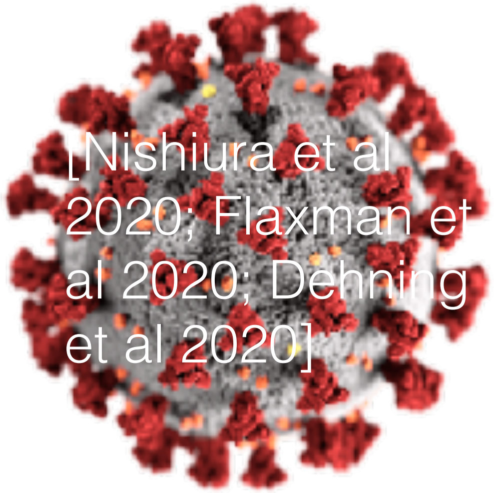
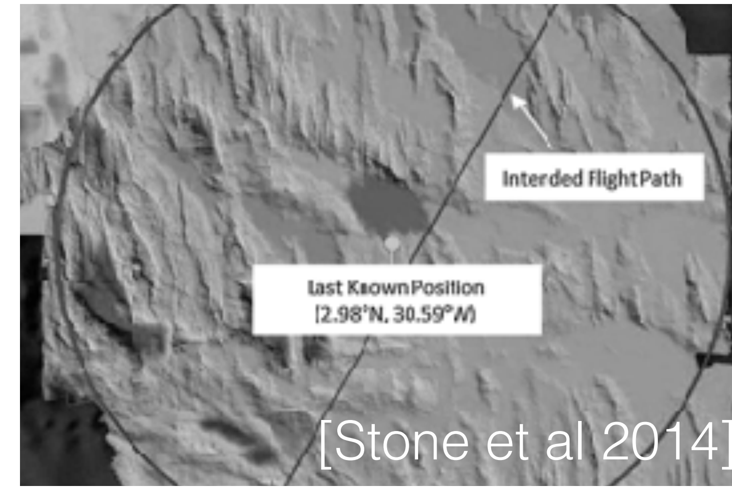
  - Builds on e.g. [Dieng et al 2017; Yao et al 2018]
- See also [Gorham, Mackey 2015, 2017; Chwialkowski, Strathmann, Gretton 2016; Jitkrittum et al 2017; Talts et al 2018, etc.]

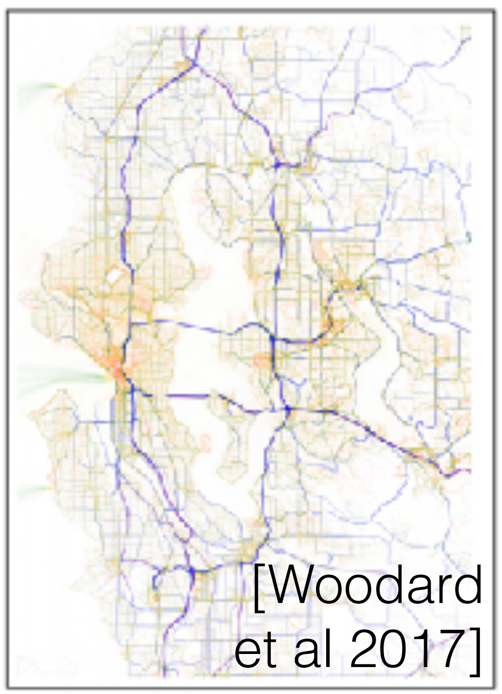
Roadmap

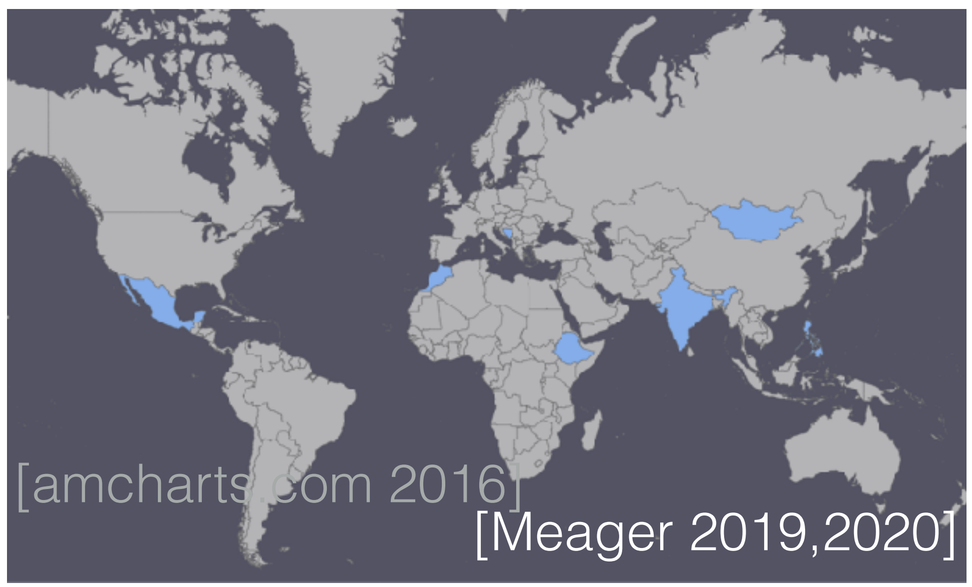
- Bayes & Approximate Bayes review
- What is:
  - Variational Bayes (VB)
  - Mean-field variational Bayes (MFVB)
- Why use VB?
- When can we trust VB?
- Where do we go from here?

Bayesian inference









[mc-stan.org]

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

What to read next

Textbooks and Reviews

- Bishop. *Pattern Recognition and Machine Learning*, Ch 10. 2006.
- Blei, Kucukelbir, McAuliffe. Variational inference: A review for statisticians, *JASA* 2016.
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