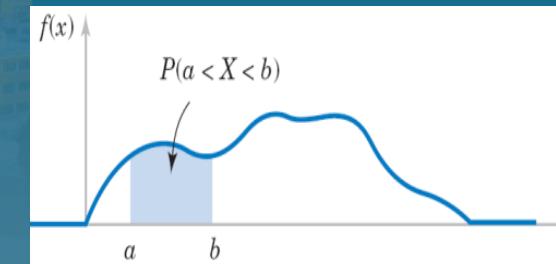




Sandia  
National  
Laboratories

# A Study of Bias-Variance in Variational Inferencing Using Delta Method



Niladri Das & Thomas A. Catanach (P.I.)

July 12, 2022

2022 SIAM Annual Meeting, Pittsburgh, Pennsylvania, USA



Sandia National Laboratories is a multimission laboratory managed and operated by National Technology & Engineering Solutions of Sandia, LLC, a wholly owned subsidiary of Honeywell International Inc., for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-NA0003525.

# A Study of Bias-Variance in Variational Inferencing Using Delta Method

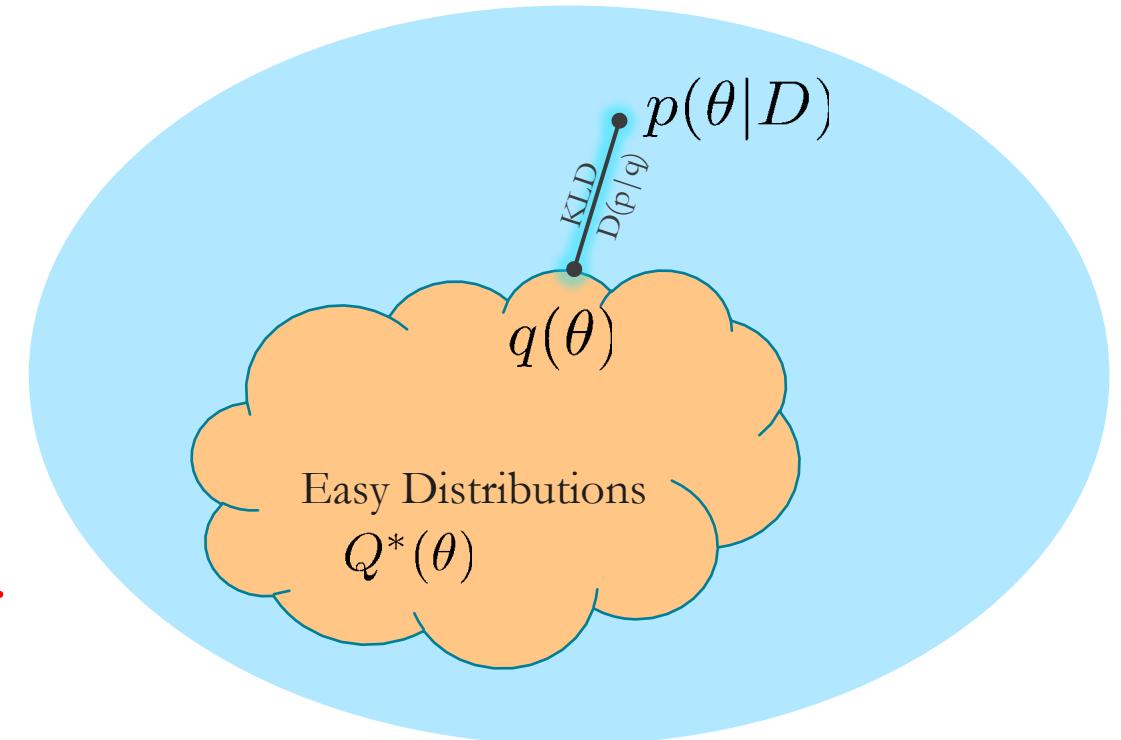
Bayes Rule

$$p(\theta|D) = \frac{p(\theta)p(D|\theta)}{\int_{\theta} p(\theta)p(D|\theta)d\theta}$$

Posterior      Prior      Likelihood

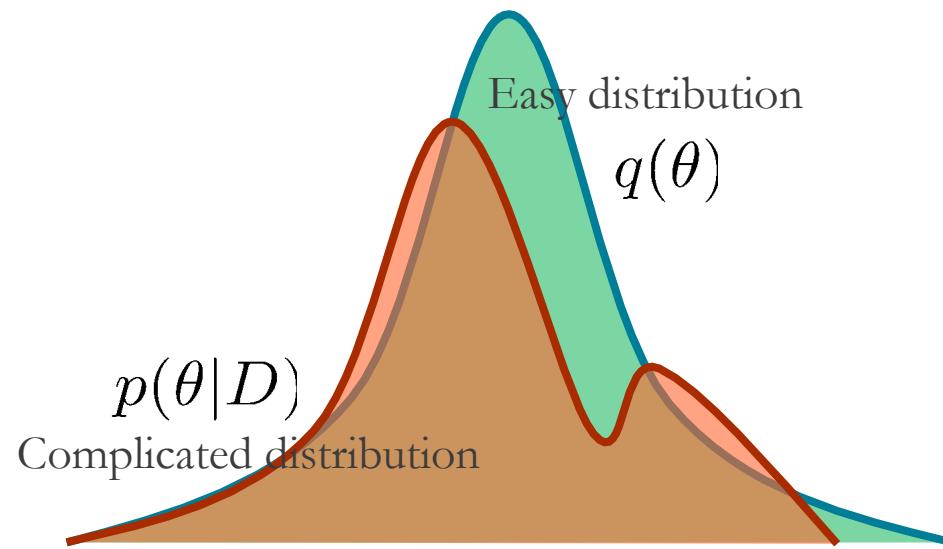
$\mathbb{R}^{100\dots}$

At even moderately high dimensions of the  $\theta$  amount numerical operations **explode**.



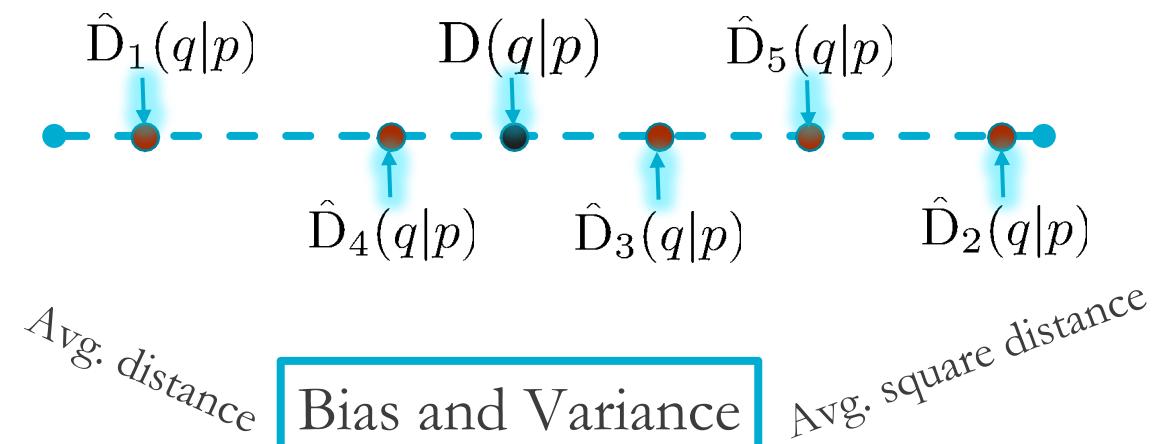
$q(\theta)$  : Variational Distribution

# A Study of Bias-Variance in Variational Inferencing Using Delta Method



$$D(p|q) = \text{KLD}$$

Sample Estimate





# A Study of Bias-Variance in Variational Inferencing Using Delta Method

$$D(q|p) = \int q(\theta | \phi) \log \frac{q(\theta | \phi)}{p(\theta)} d\theta - \int q(\theta | \phi) \log p(\mathcal{D} | \theta) d\theta + \log \int p(\mathcal{D} | \theta) p(\theta) d\theta$$

**Minimize**



Log Evidence , independent  
of VI params.  $\phi$

$$\text{ELBO} = - \int q(\theta | \phi) \log \frac{q(\theta | \phi)}{p(\theta)} d\theta + \int q(\theta | \phi) \log p(\mathcal{D} | \theta) d\theta$$

**Maximize**

$$= -\frac{1}{N} \Sigma(\dots) + \frac{1}{N} \Sigma(\dots)$$



# A Study of Bias-Variance in Variational Inferencing Using Delta Method

$$D(q|p) = \int q(\theta | \phi) \log \frac{q(\theta | \phi)}{p(\theta)} d\theta - \int q(\theta | \phi) \log p(\mathcal{D} | \theta) d\theta + \log \int p(\mathcal{D} | \theta) p(\theta) d\theta$$

**Minimize**

↓

Accurate Calculation

↓

$\mathcal{X}$

↓

$\log(\mathcal{Y})$

$= \frac{1}{N} \Sigma(\dots)$

$= \frac{1}{N} \Sigma(\dots)$

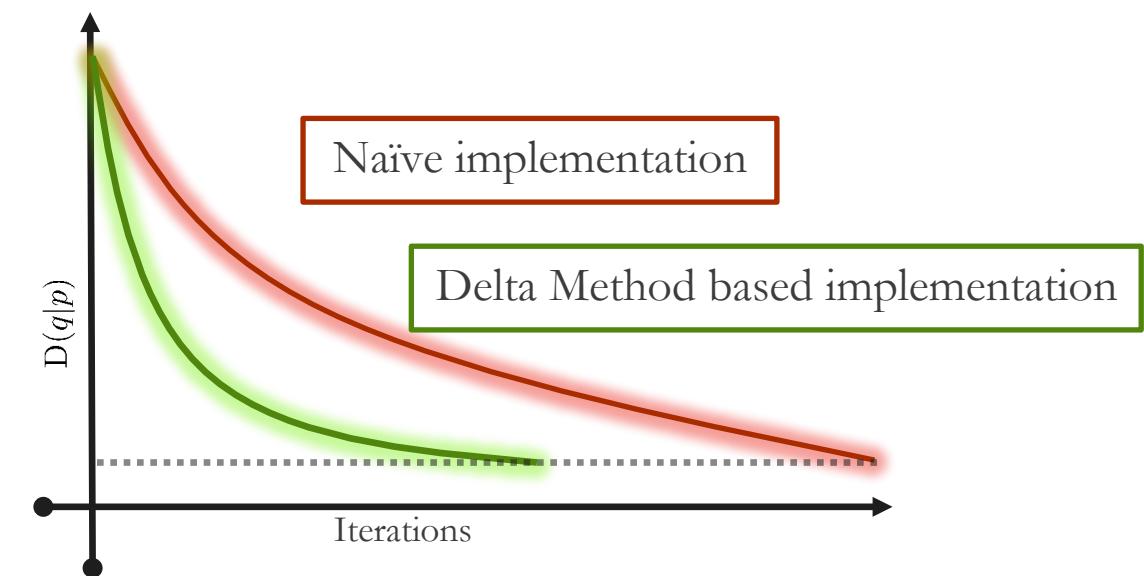
$$Var(\hat{\mathcal{X}} + \log(\hat{\mathcal{Y}})) = \frac{\Sigma_{\mathcal{X}}}{N} + \frac{\Sigma_{\mathcal{Y}}}{N\mathcal{Y}^2} + 2\frac{\Sigma_{\mathcal{X}\mathcal{Y}}}{N\mathcal{Y}}$$

# A Study of Bias-Variance in Variational Inferencing Using Delta Method

**Delta Method** : Approx. probability distribution of  $D(q|p)$

**Technique** : Reduce variance in approx. of  $D(q|p)$

**Performance** : Faster convergence to  $q(\theta)$





# A Study of Bias-Variance in Variational Inferencing Using Delta Method

$$D(q|p) = \int q(\theta | \phi) \log \frac{q(\theta | \phi)}{p(\theta)} d\theta - \int q(\theta | \phi) \log p(\mathcal{D} | \theta) d\theta + \log \int \frac{p(\mathcal{D} | \theta) p(\theta)}{q(\theta | \phi)} q(\theta | \phi) d\theta$$

$$= f(\phi) - \int \frac{q(\theta(\zeta) | \phi)}{r(\theta(\zeta) | \varphi)} \log p(\mathcal{D} | \theta(\zeta)) p(\zeta) d\zeta + \log \int \frac{p(\mathcal{D} | \theta(\zeta)) p(\theta(\zeta))}{r(\theta(\zeta) | \varphi)} p(\zeta) d\zeta$$

Importance Distribution  
 $r(\theta(\zeta) | \varphi)$

Re-parameterization params.  
 $\zeta$

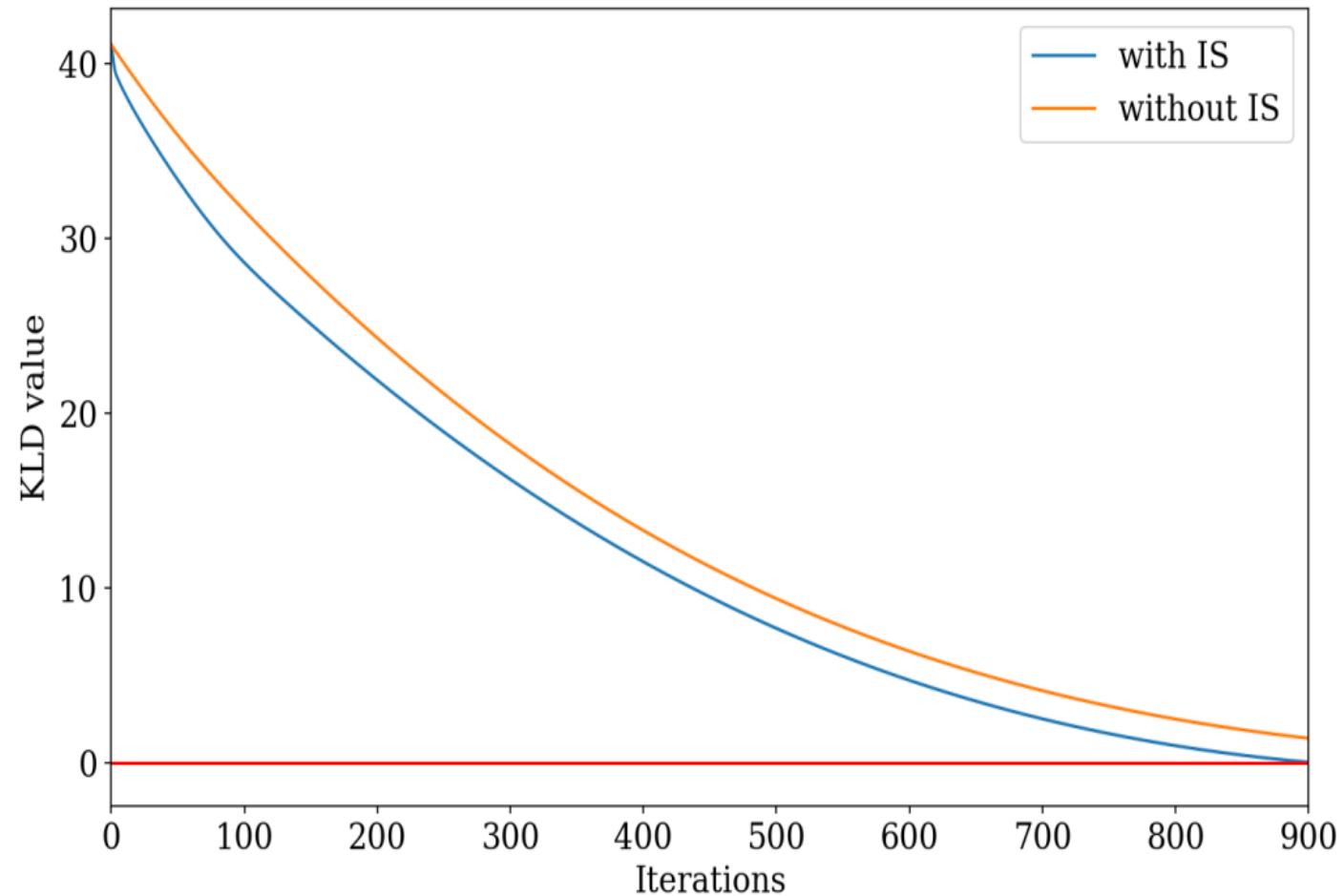
Two Step Optimization:

VI params. Optimization  
 $\phi$

IS params. Optimization  
 $\varphi$

# A Study of Bias-Variance in Variational Inferencing Using Delta Method

- Dimension of the problem : 5
- Linear model :=  $\mathcal{Y} = X + \nu$
- $\nu$  : Zero mean Gaussian noise
- Importance distribution is Gaussian, initialized as the initial variational distribution.
- The VI parameters  $(\mu, L)$  where  $LL^T = \Sigma$
- Sample size 1000 for both VI and IS.





## Contact Information

**Niladri Das** | Postdoctoral Appointee | [ndas@sandia.gov](mailto:ndas@sandia.gov)

**Thomas A. Catanach** | P.I. | [tacatan@sandia.gov](mailto:tacatan@sandia.gov)

08739 | Extreme-scale DS & Analytics

Thank You