# The Amortized Bootstrap

### **Eric Nalisnick**

University of California, Irvine

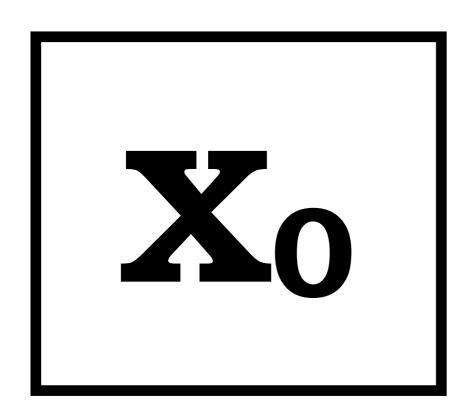
In collaboration with

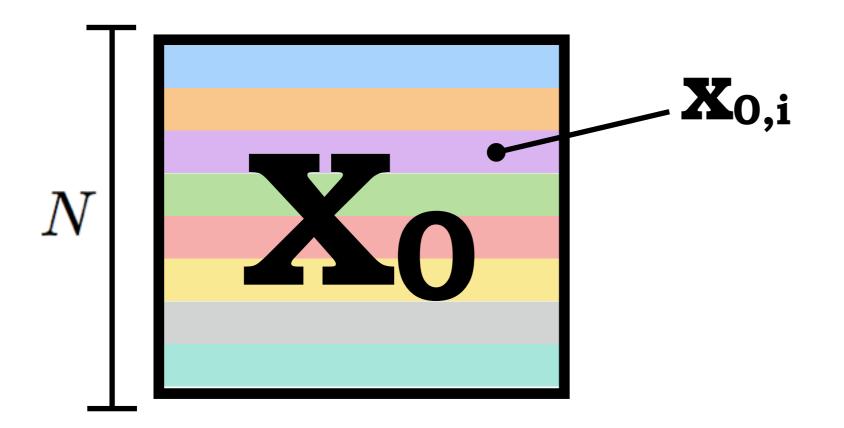


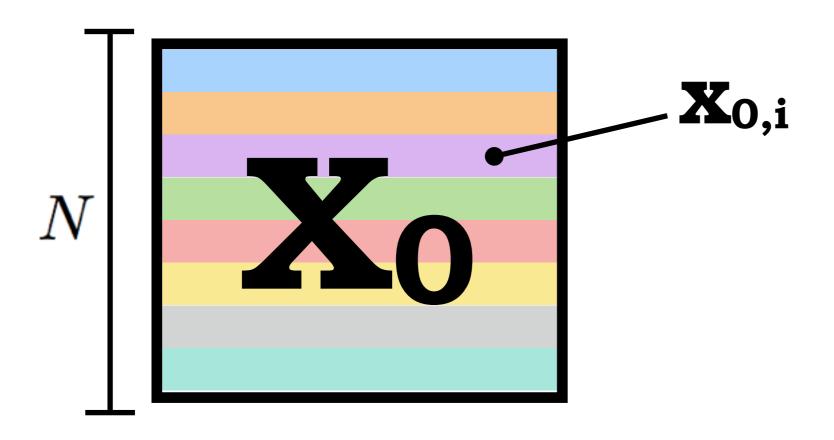
Padhraic Smyth



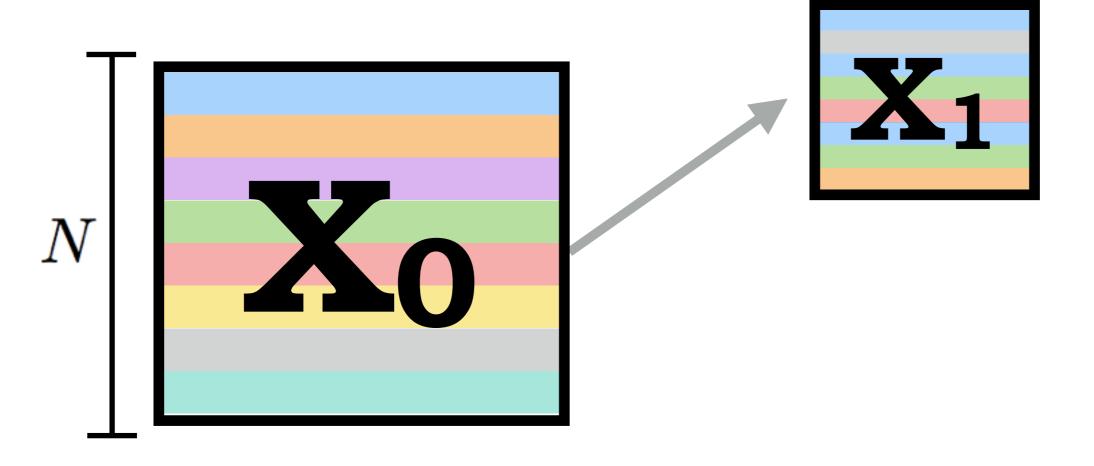
# The Bootstrap



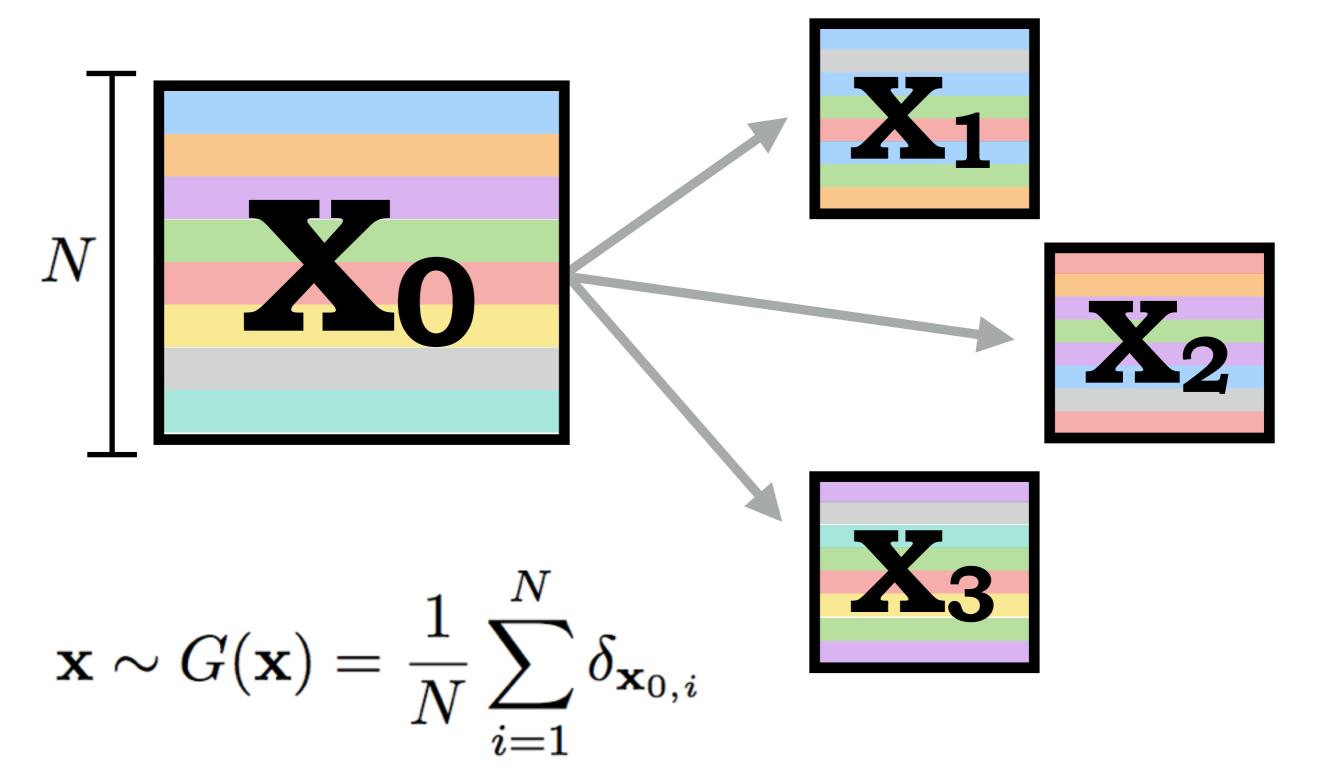




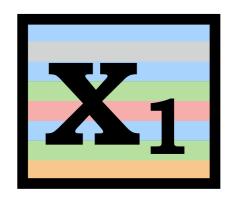
$$\mathbf{x} \sim G(\mathbf{x}) = \frac{1}{N} \sum_{i=1}^{N} \delta_{\mathbf{x}_{0,i}}$$



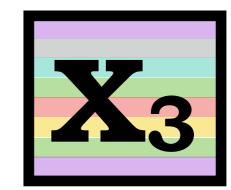
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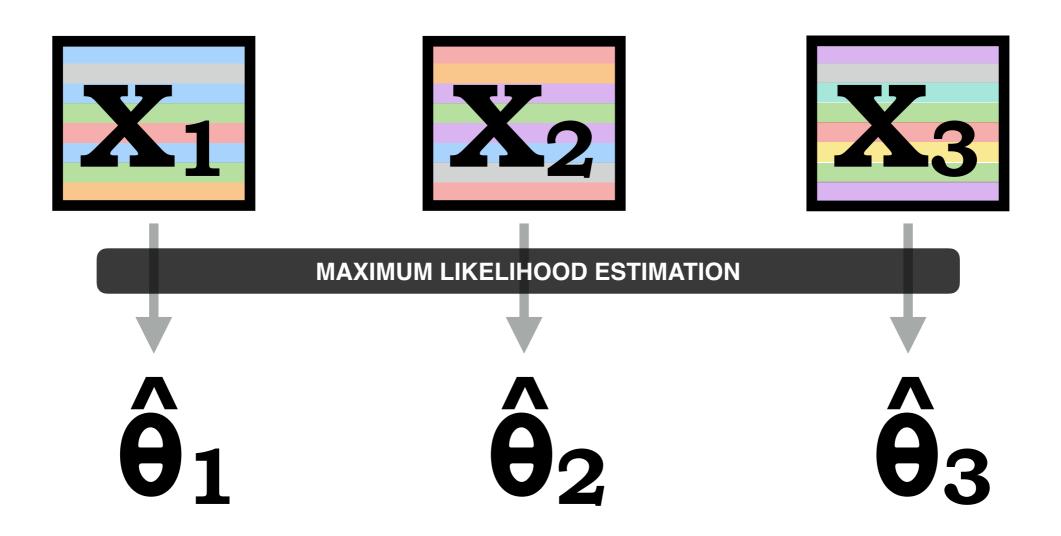
# **Bootstrap Distribution**



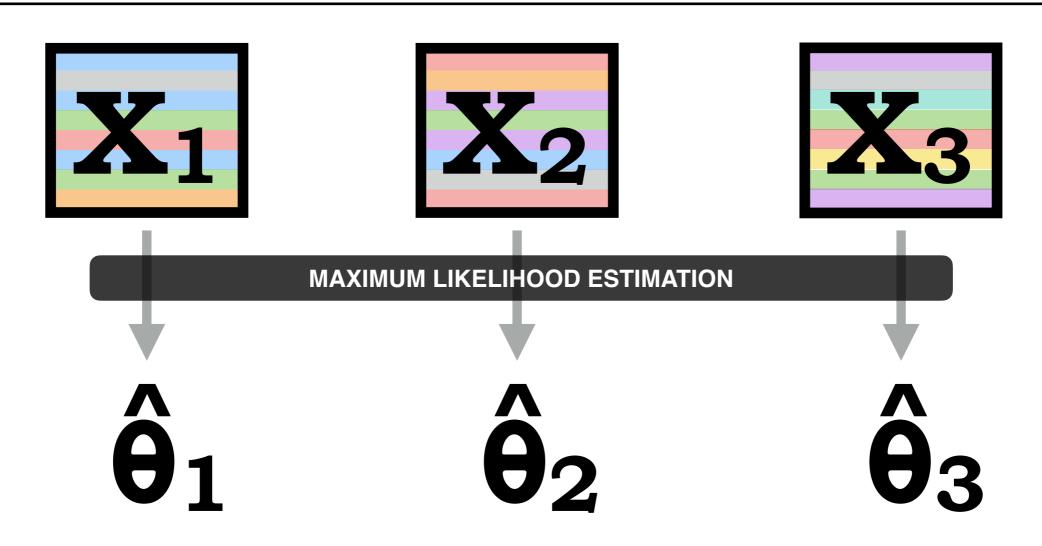




## **Bootstrap Distribution**



### **Bootstrap Distribution**



$$\boldsymbol{\theta} \sim F(\boldsymbol{\theta}) = \frac{1}{K} \sum_{k=1}^{K} \delta_{\hat{\boldsymbol{\theta}}_k}$$

# The Amortized Bootstrap

**QUESTION**: Can we approximate the bootstrap distribution  $F(\theta)$  with a model (like in variational inference for Bayesian posteriors)?

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**IDEA**: Use an *implicit model* to approximate  $F(\theta)$ .

$$\hat{\boldsymbol{\theta}} = f_{\boldsymbol{\phi}}(\boldsymbol{\xi}), \quad \boldsymbol{\xi} \sim p_0$$

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**PROS** 

- **Amortized Inference:** share statistical strength across dataset replications / generate unlimited samples.
- Results in bootstrap smoothing (Efron & Tibshirani, 1997).

**IDEA**: Use an *implicit model* to approximate  $F(\theta)$ .

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- Amortized Inference: share statistical strength across dataset replications / generate unlimited samples.
- Results in bootstrap smoothing (Efron & Tibshirani, 1997).
- Breaks bootstrap theory. Can recover only an approximation.
- Can't distribute computation.

$$\mathcal{J}(\mathbf{X}_0, \boldsymbol{\phi}) = \mathbb{E}_{F_{\boldsymbol{\phi}}(\boldsymbol{\theta})} \mathbb{E}_{G(\mathbf{x})}[\log p(\mathbf{X}|\boldsymbol{\theta})]$$

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Regular bootstrap update

$$\mathcal{J}(\mathbf{X}_0, \boldsymbol{\phi}) = \mathbb{E}_{F_{\boldsymbol{\phi}}(\boldsymbol{\theta})} \mathbb{E}_{G(\mathbf{x})}[\log p(\mathbf{X}|\boldsymbol{\theta})]$$

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Regular bootstrap Shared update params.

$$\mathcal{J}(\mathbf{X}_0, \boldsymbol{\phi}) = \mathbb{E}_{F_{\boldsymbol{\phi}}(\boldsymbol{\theta})} \mathbb{E}_{G(\mathbf{x})}[\log p(\mathbf{X}|\boldsymbol{\theta})]$$

$$\mathcal{L}_{\text{ELBO}} = \mathbb{E}_{q(\boldsymbol{\theta})}[\log p(\mathbf{X}|\boldsymbol{\theta})] - \text{KLD}[q(\boldsymbol{\theta})||p(\boldsymbol{\theta})]$$

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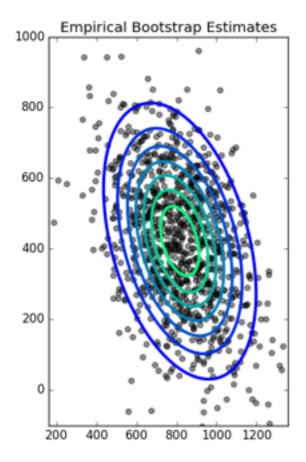


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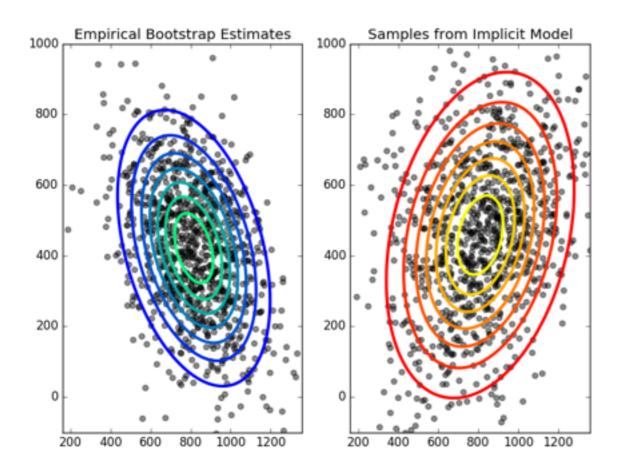
Data-driven uncertainty as opposed to arbitrary priors that can hinder performance (Hoffman & Johnson, 2016).

# Experiment #1: Sanity Check

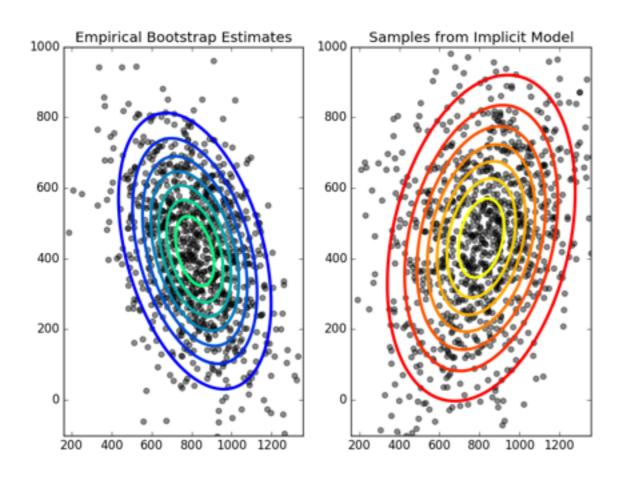
#### **2D Diabetes Dataset**

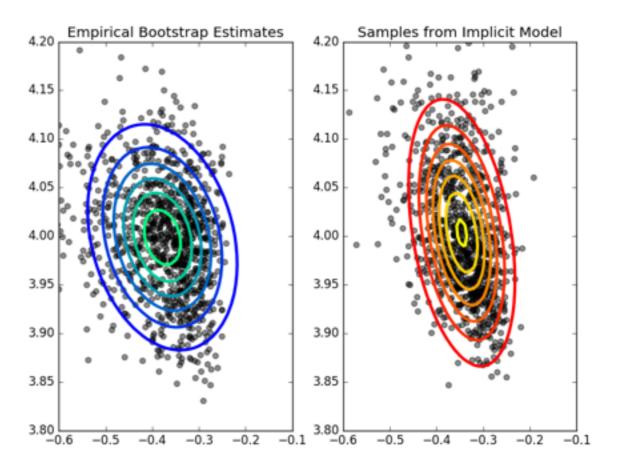


#### **2D Diabetes Dataset**

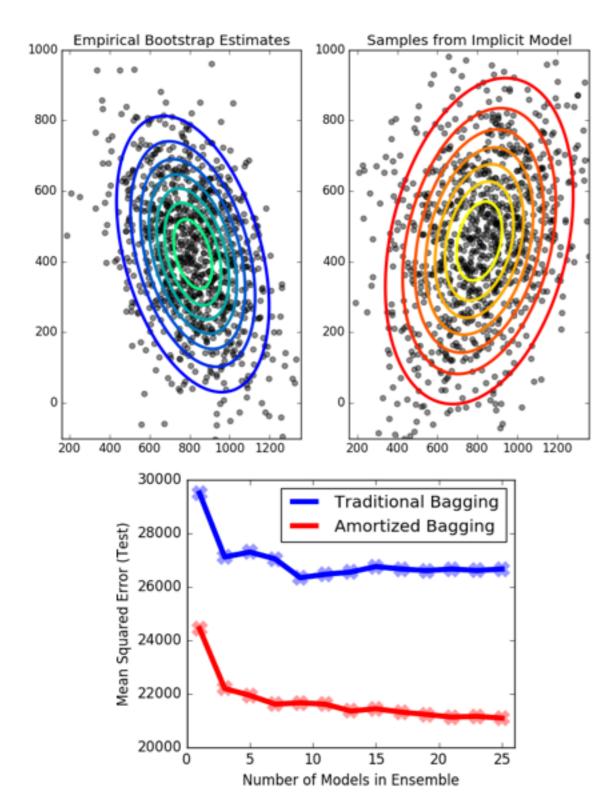


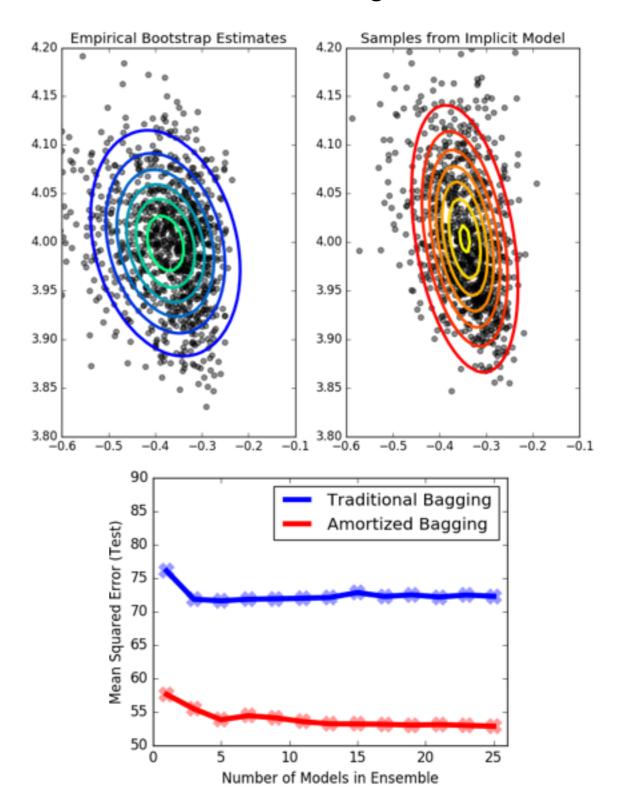
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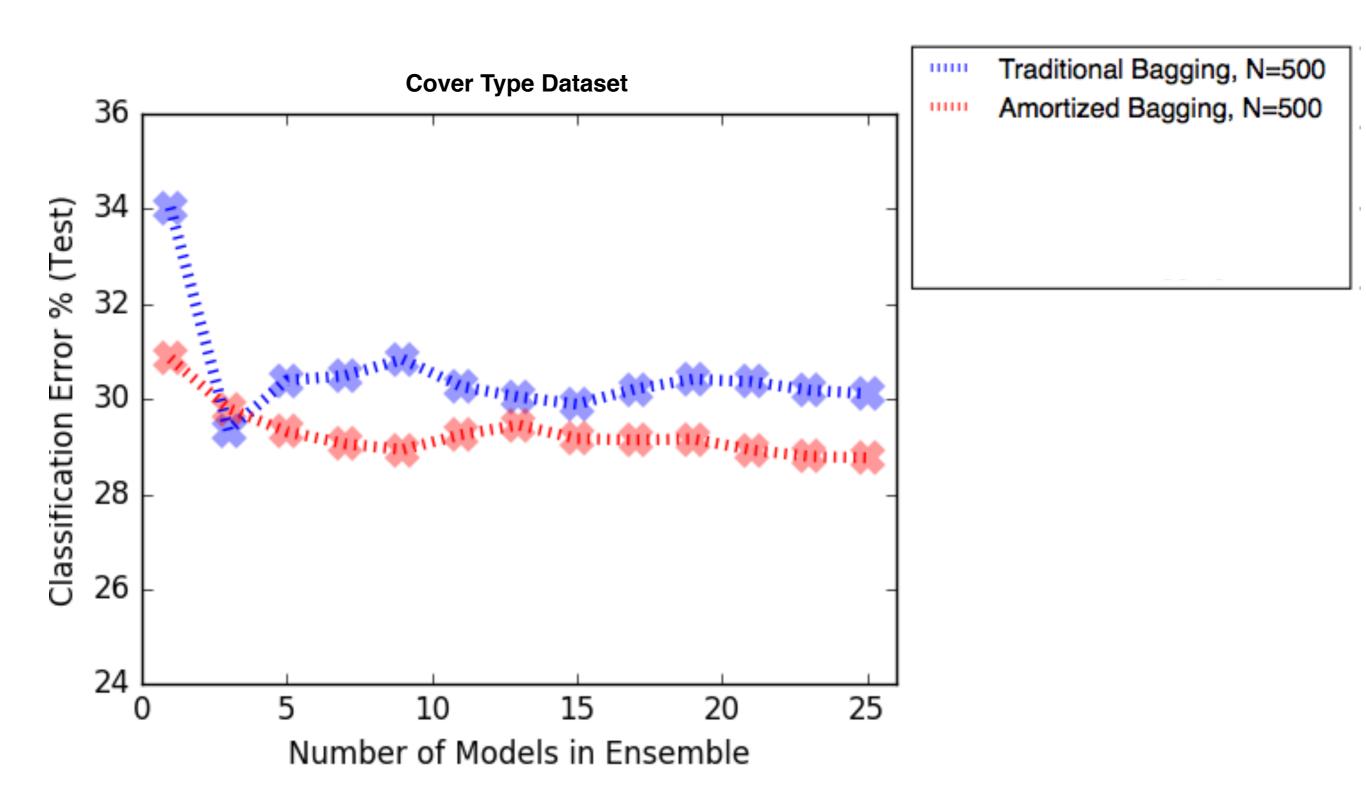
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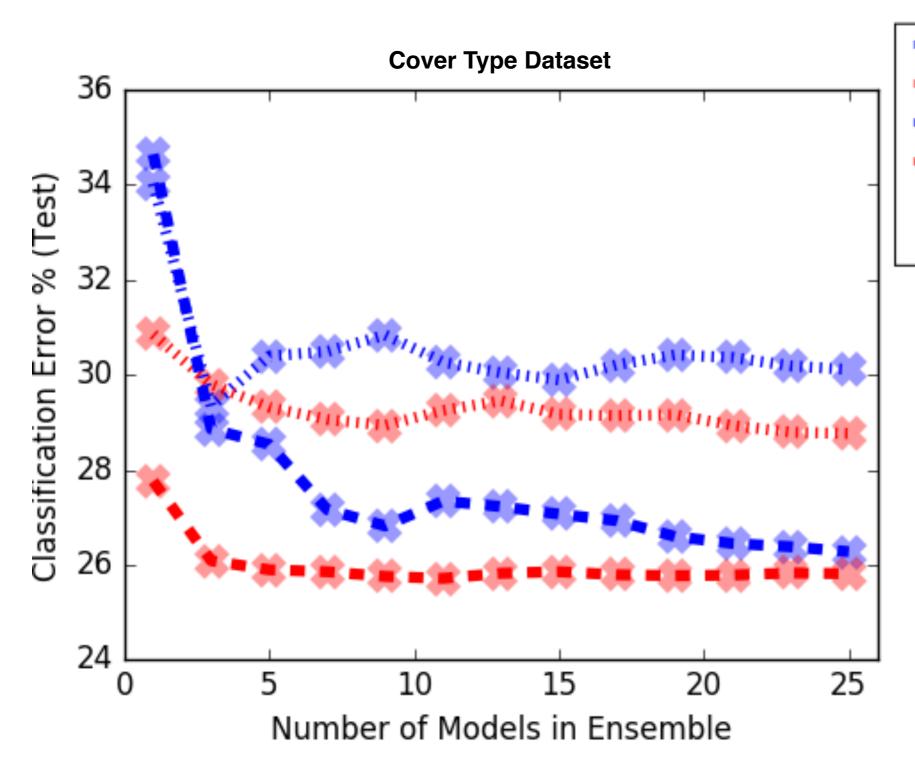


# Experiment #2: Varying Dataset Size

# **Logistic Regression**



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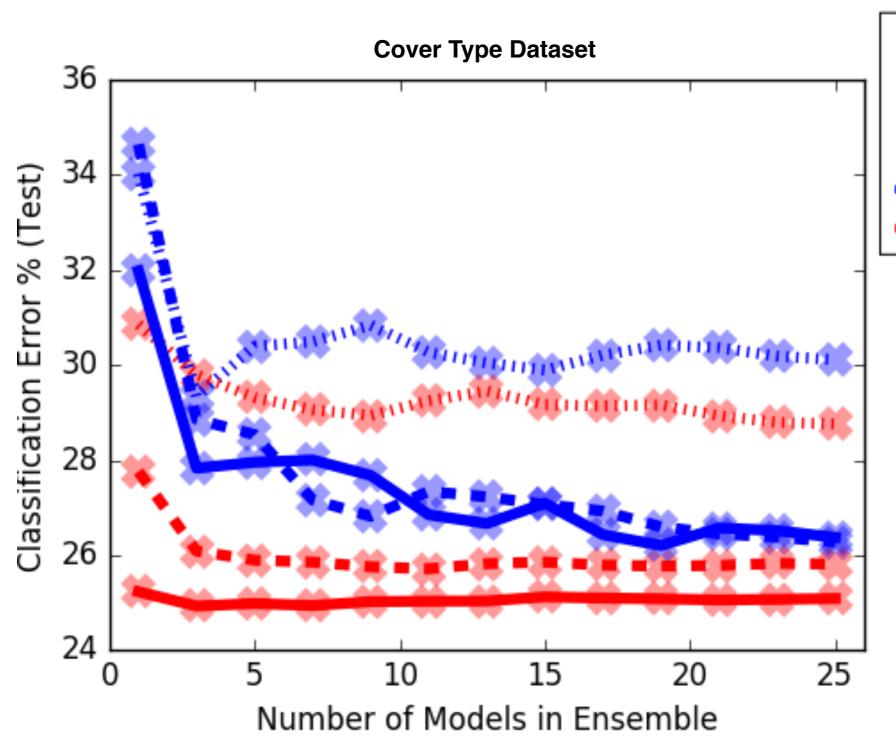


Traditional Bagging, N=500
Amortized Bagging, N=500

Traditional Bagging, N=1500

Amortized Bagging, N=1500

## **Logistic Regression**



Traditional Bagging, N=500
Amortized Bagging, N=500
Traditional Bagging, N=1500
Amortized Bagging, N=1500
Traditional Bagging, N=2500
Amortized Bagging, N=2500
Amortized Bagging, N=2500

# Experiment #3: Classification with NN

## **Neural Networks**

	Test Error for Ensemble of Size $K$		
	K = 1	K = 5	K = 25
Bagged NNs, Traditional	22.57	19.68	18.57
Bagged NNs, Amortized	17.03	16.82	16.18

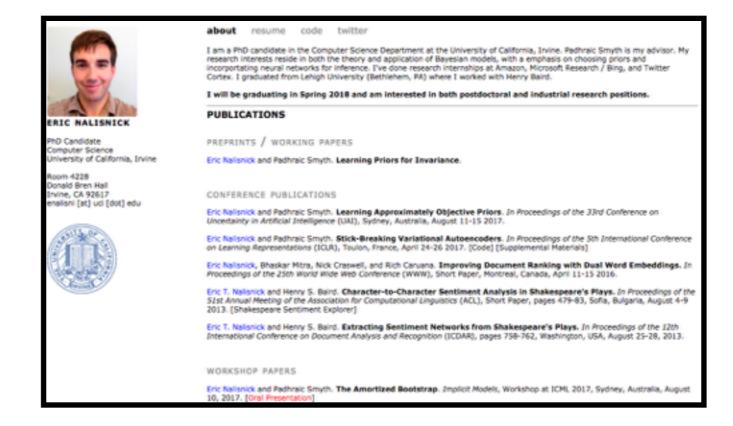
**Rotated MNIST Dataset** 

### **Conclusions**

Model-based bootstrap results in superior bagging performance due (ostensibly) to smoothing and amortization.

Future work: larger-scale experiments, theoretical analysis, uncertainty quantification.

# Thank you. Questions?



**Acknowledgements** 



http://www.ics.uci.edu/~enalisni/