Approximate Inference for Frequentist Uncertainty Estimation

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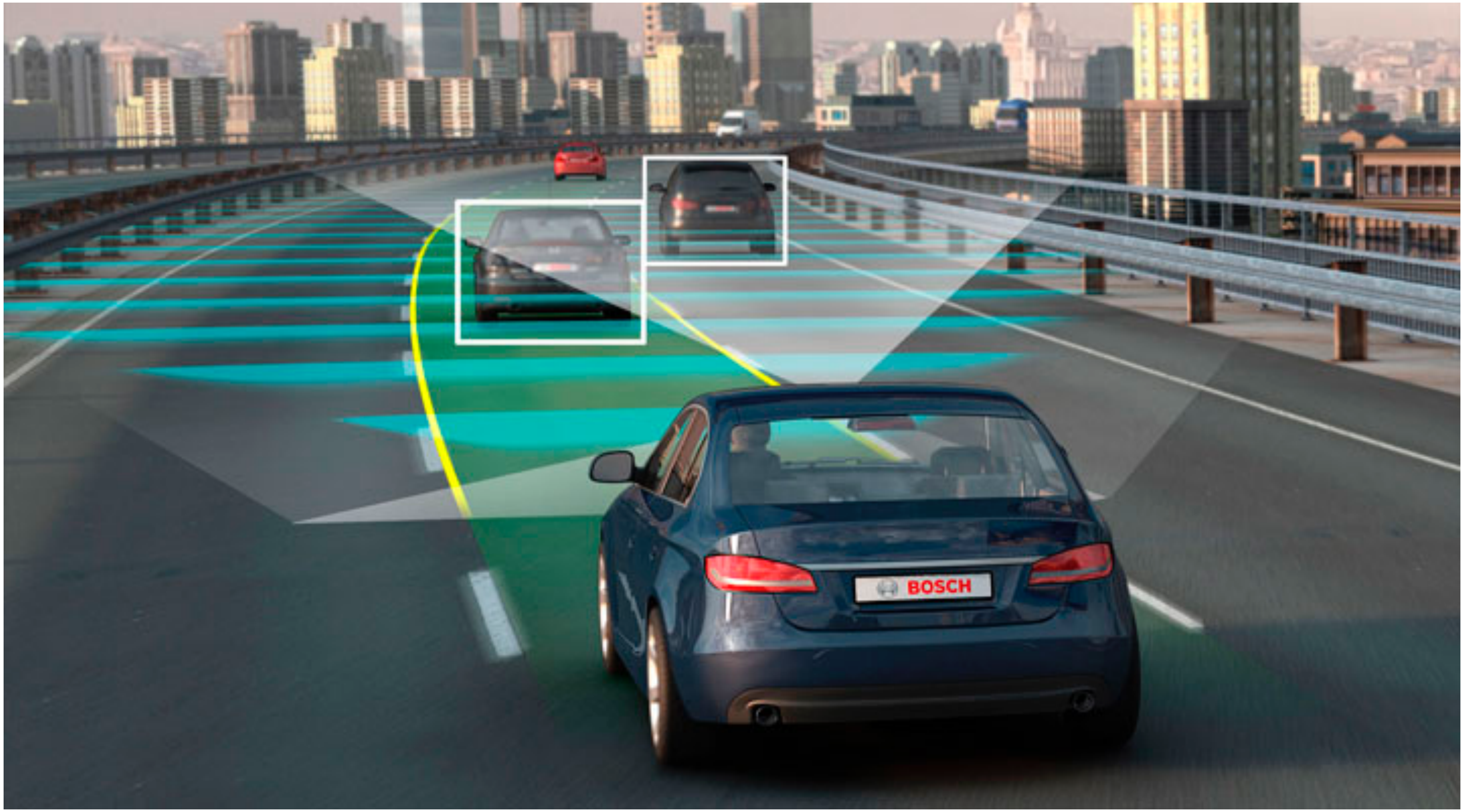
University of California, Irvine

Why should we care about uncertainty estimation?



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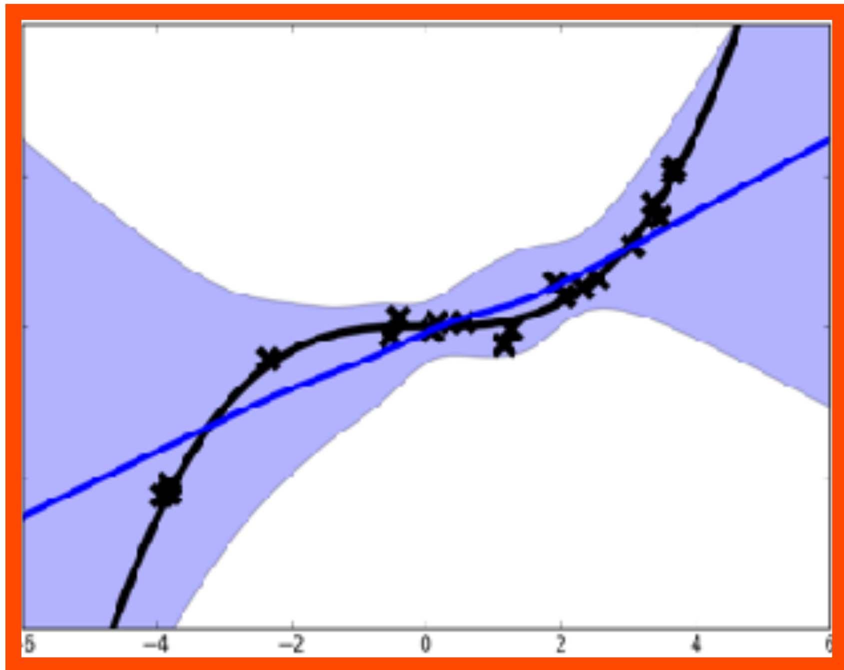

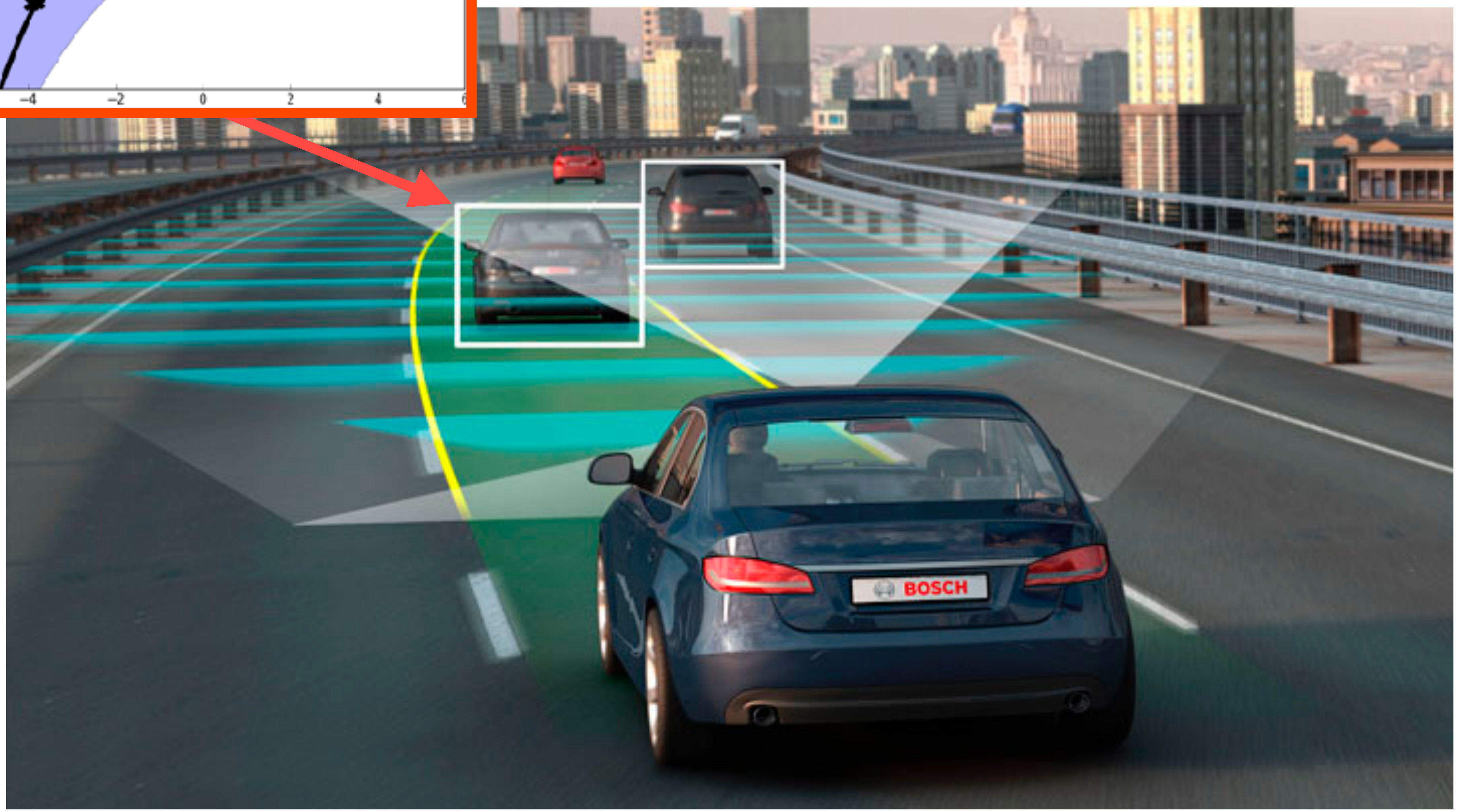

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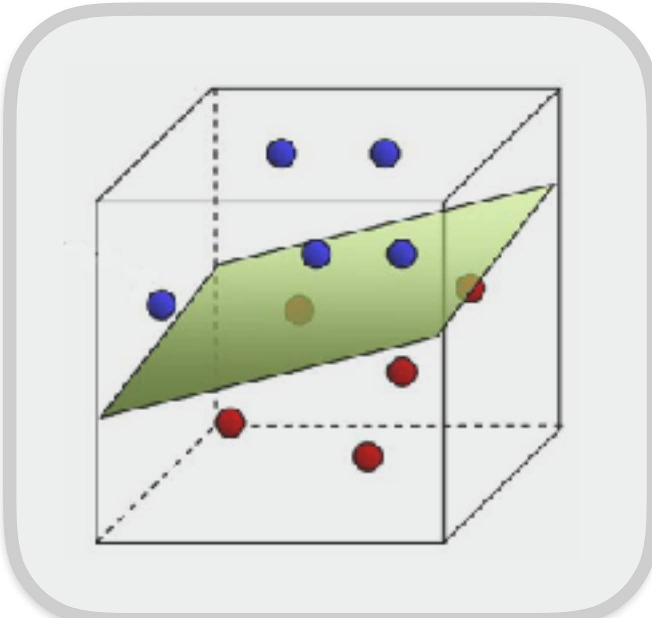
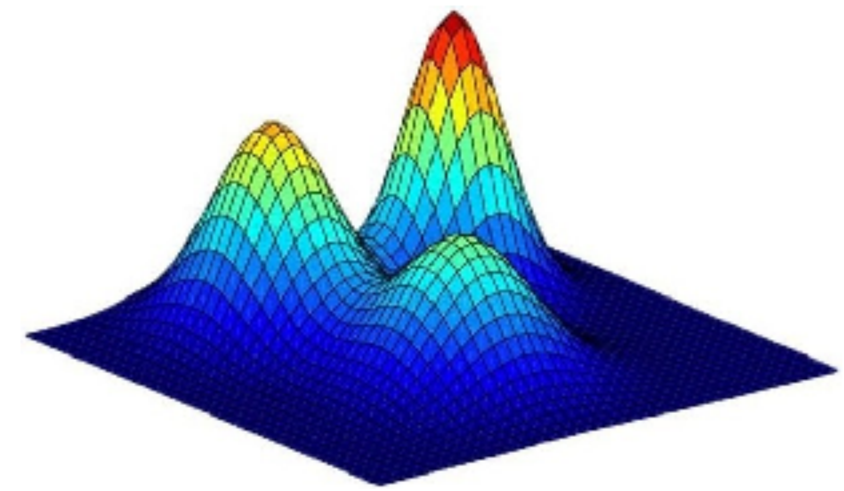
ML MODEL



INFERENCE

$\longrightarrow$



$$p(\mathcal{D}|\boldsymbol{\theta}) \qquad\qquad \pi(\boldsymbol{\theta})$$

PREDICTIVE DISTRIBUTION

$$p(\mathbf{x}^*|\mathcal{D}) = \int_{\boldsymbol{\theta}} \pi(\boldsymbol{\theta})\, p(\mathbf{x}^*|\boldsymbol{\theta})\, d\boldsymbol{\theta}$$

$$p(\boldsymbol{\theta}|\mathcal{D}) = \frac{p(\mathcal{D}|\boldsymbol{\theta})\; p(\boldsymbol{\theta})}{p(\mathcal{D})}$$


THOMAS BAYES

$$p(\boldsymbol{\theta}|\mathcal{D}) = \frac{p(\mathcal{D}|\boldsymbol{\theta})\, p(\boldsymbol{\theta})}{p(\mathcal{D})}$$

THOMAS BAYES

Surge of progress in scalable / approximate Bayesian inference.

VARIATIONAL INFERENCE

Inference Models / Amortization
- Regression (Salimans & Knowles, 2014)
- Neural Networks (Kingma & Welling, 2014) (Rezende et al., 2014)
- Gaussian Processes (Tran et al., 2016)

Approximations via Transformation
- Normalizing Flows (Rezende & Mohamed, 2015)
- Hamiltonian Flow (Salimans et al, 2015)
- Inv. Auto-Regressive (Kingma et al., 2016)

Implicit Posterior Approximations
- Stein Particle Descent (Liu & Wang, 2016)
- Operator VI (Ranganath et al., 2016)
- Adversarial VB (Mescheder et al., 2017)

BAYESIAN NEURAL NETS

Scalable Posterior Inference
- Prob. Backpropagation (Hernández-Lobato & Adams, 2015)
- Bayes by Backprop. (Blundell et al., 2015)
- Matrix Gauss. Approx. (Louizos & Welling, 2016)

Latent Variable Models
- Variational Autoencoders (Kingma & Welling, 2014)
- Structured VAEs (Johnson et al., 2017)
- Bayesian GANs (Saatchi & Wilson, 2017)

"X as Bayesian Inference"
- Dropout as Bayesian Approx. (Gal & Ghahramani, 2016)
- Posterior Distillation (Balan et al., 2015)

What about Frequentism?

Why Be Frequentist?

No priors: choice of prior affects the marginal likelihood, if not the posterior too.

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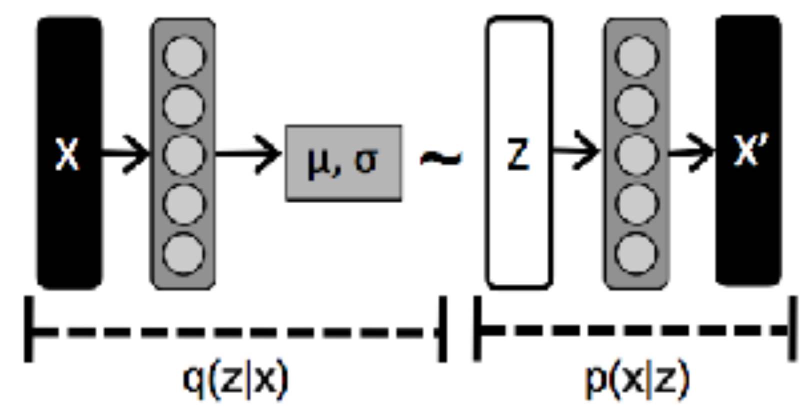

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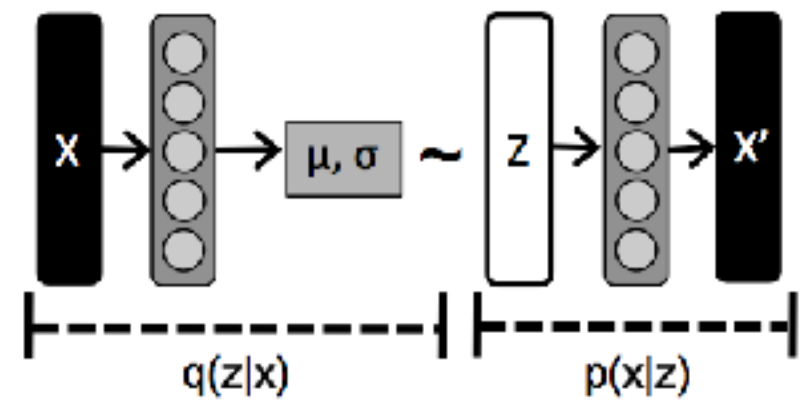

> "…to improve our variational bounds we should improve our priors and not just the encoder and decoder….perhaps we should investigate multimodal priors…"

M. Hoffman & M. Johnson. "ELBO Surgery". NIPS 2016 Workshop on *Advances in Approx. Bayesian Inference*.

Other work showing deficiencies with prior / marginal matching:

(Kingma et al., NIPS 2015), (Chen et al., ICLR 2017), (Tomczak & Welling, ArXiv 2017), (Zhao et al., ArXiv 2017)

Frequentist Methods: Two Routes

1 Knowledge of asymptotic behavior.

Maximum Likelihood: $\hat{\boldsymbol{\theta}}_{\mathrm{MLE}} \rightarrow \mathrm{N}(\boldsymbol{\theta}_0,\ \mathcal{I}(\boldsymbol{\theta}))$

'Objective' Bayesian Priors: $p^*(\boldsymbol{\theta}) = \underset{p(\boldsymbol{\theta})}{\operatorname{argmax}}\, I(\boldsymbol{\theta}, \mathcal{D})$

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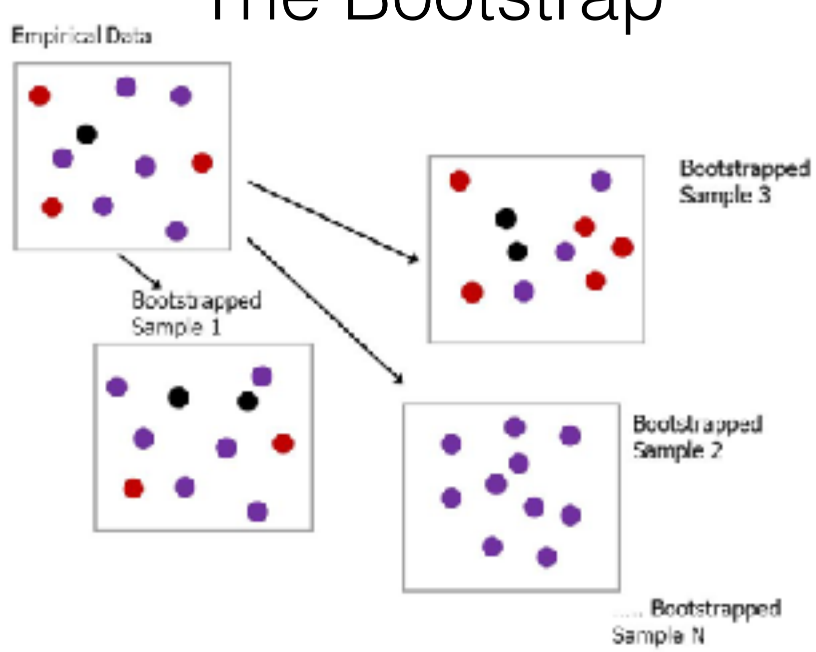
2 Simulation of sampling process.

The Bootstrap



Other examples: jackknife, cross-validation, permutation tests, Monte Carlo tests…

Image from "Resampling Techniques" by Joel Edwards

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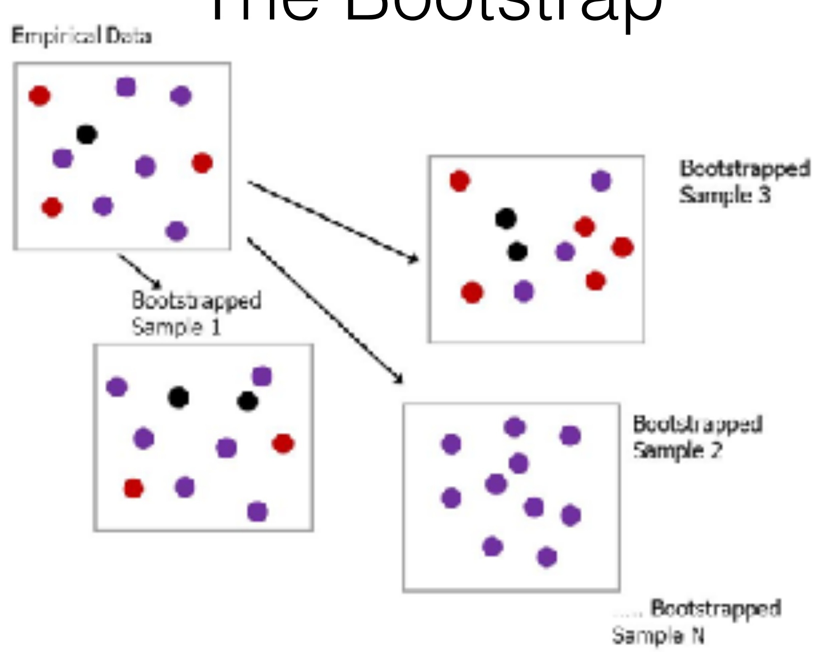

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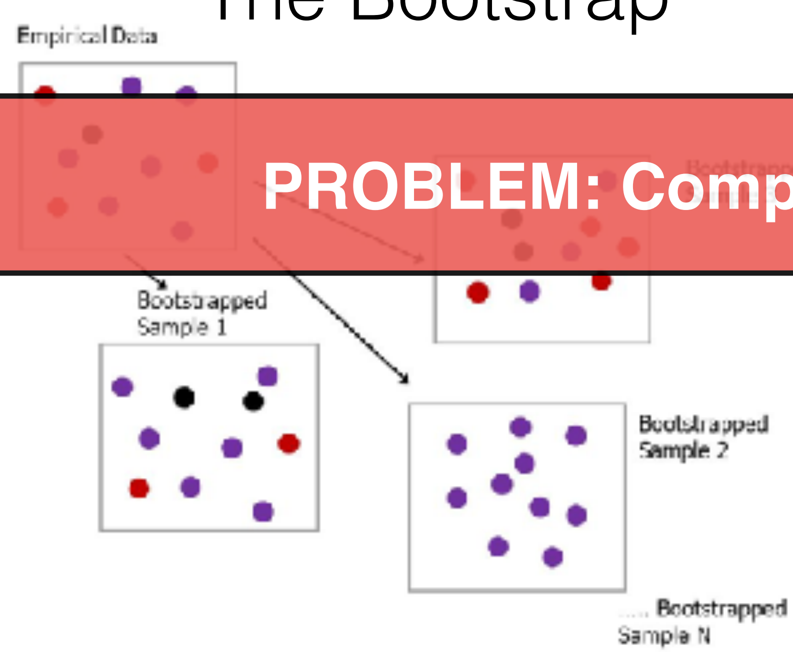

PROBLEM: Computationally Expensive

Other examples: jackknife, cross-validation, permutation tests, Monte Carlo tests…

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Using Advances in Approx. Inference for Frequentism

1 Knowledge of asymptotic behavior.

CONTRIBUTION

Approximating Objective Bayesian Priors

(Nalisnick & Smyth, UAI 2017)

Use variational bound to find an approximate prior.

2 Simulation of sampling process.

CONTRIBUTION

The Amortized Bootstrap

(Nalisnick & Smyth, SoCalML 2017)

Use implicit models to approximate bootstrap distribution.

Approximating Reference Priors

(Nalisnick & Smyth, UAI 2017)

Objective Bayesian Priors

Reference Priors (Bernardo, 1979):

$$p^*(\boldsymbol{\theta}) = \underset{p(\boldsymbol{\theta})}{\operatorname{argmax}}\, I(\boldsymbol{\theta}, \mathcal{D})$$

$$= \underset{p(\boldsymbol{\theta})}{\operatorname{argmax}} \int_{\mathcal{D}} p(\mathcal{D})\mathrm{KLD}[p(\boldsymbol{\theta}|\mathcal{D}) \;||\; p(\boldsymbol{\theta})]d\mathcal{D}.$$

Objective Bayesian Priors

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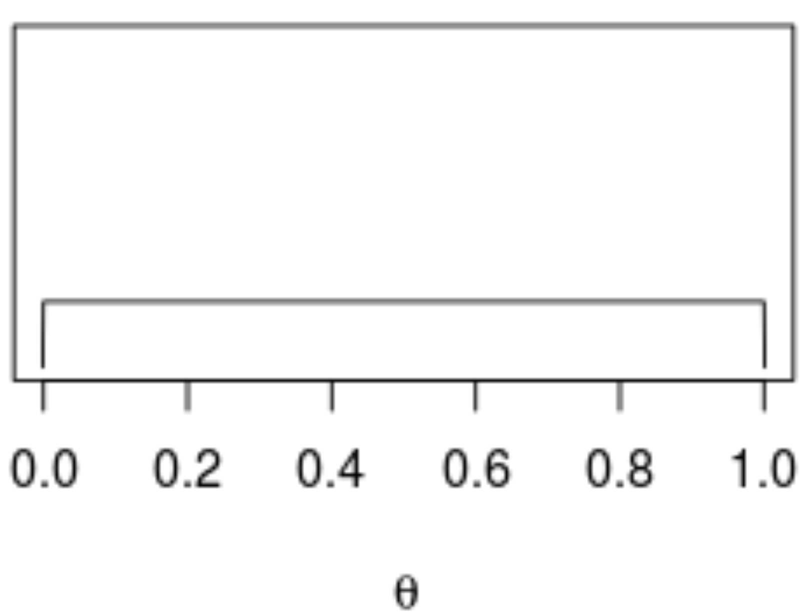
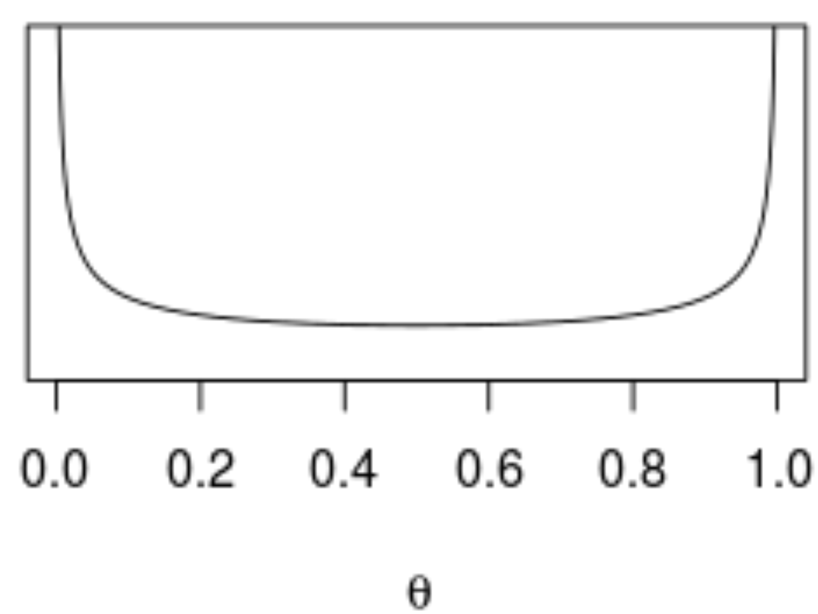
Equivalent to *Jeffreys* priors in one-dimension.

FLAT PRIOR



REFERENCE / JEFFREYS PRIOR



Reference Priors

- Prior that results in the data having max affect on the posterior.
- Posterior credible intervals match the corresponding confidence intervals*.
- Called ‘reference’ because they serve as a point of comparison for subjective priors.

* conditions apply

Reference Priors

We can lower-bound the mutual information with the following Monte Carlo objective:

$$I(\boldsymbol{\theta}, \mathcal{D}) \geq \mathcal{J}_{\text{RP}}(\boldsymbol{\lambda})$$

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where $\hat{\theta}_s \sim p_{\boldsymbol{\lambda}}(\boldsymbol{\theta})$

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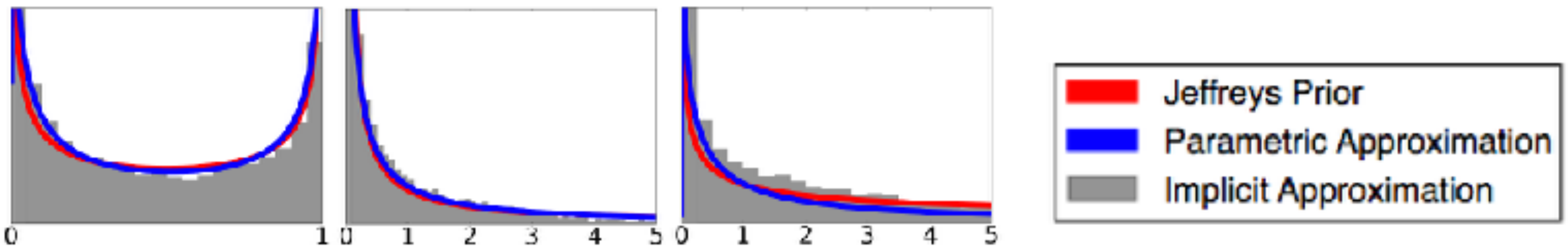
$$= \frac{1}{S} \sum_{s=1}^{S} \text{KLD}[p(\mathcal{D}|\hat{\boldsymbol{\theta}}_s) \mid\mid p(\mathcal{D}|\hat{\boldsymbol{\theta}}_{\max})]$$

where $\hat{\theta}_s \sim p_{\boldsymbol{\lambda}}(\boldsymbol{\theta})$

Reference Priors

Recovering Jeffreys priors:



(a) Bernoulli (b) Gaussian Scale (c) Poisson

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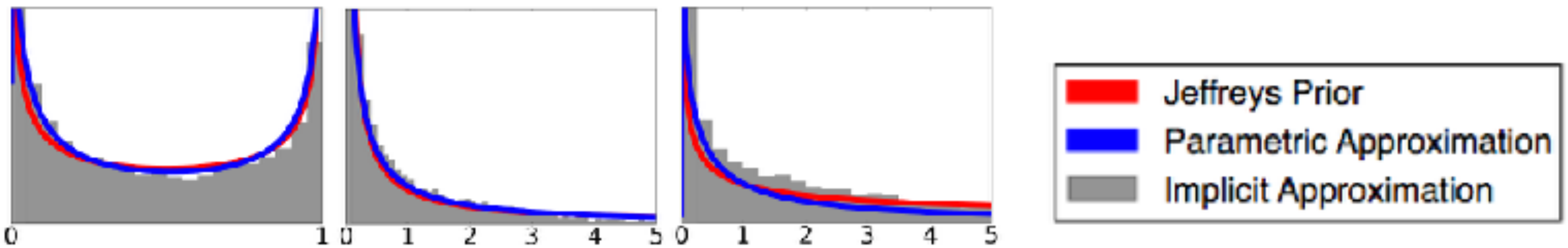

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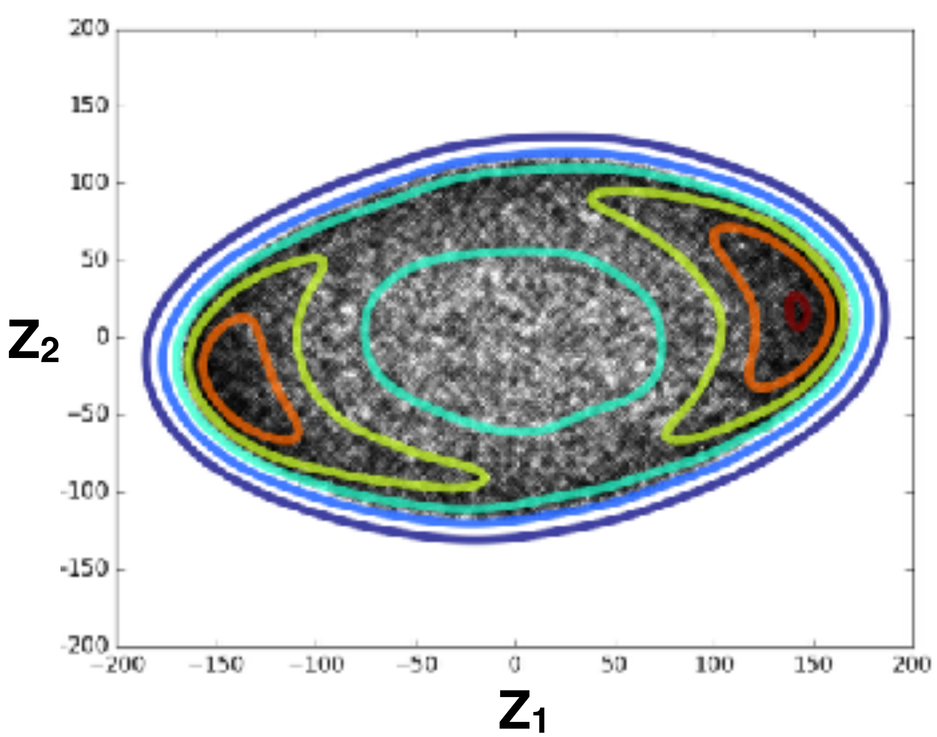
Variational Autoencoder's reference prior:



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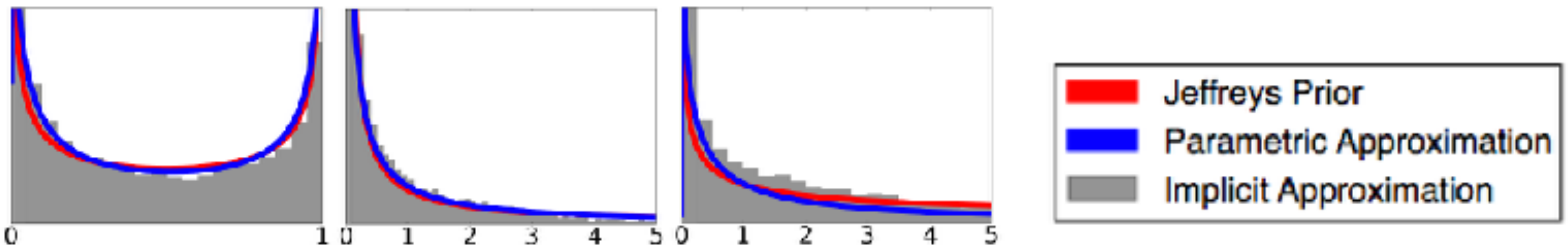

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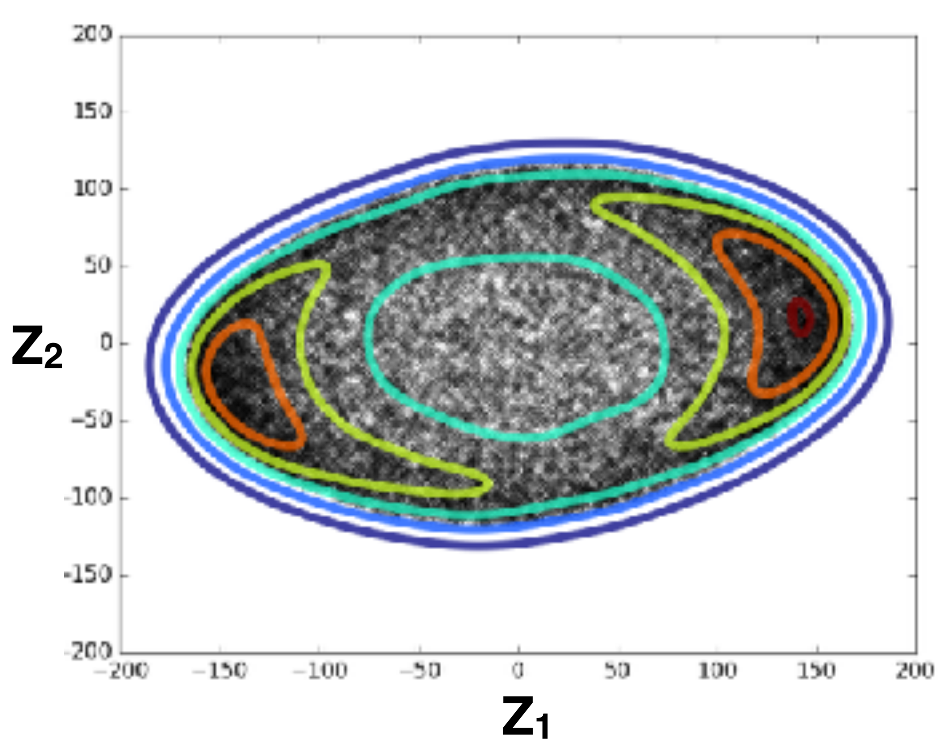


Improves performance for low-dimensional (< 15) latent spaces but gives (approx.) identical performance for 50 dims, the size commonly used.

The Amortized Bootstrap

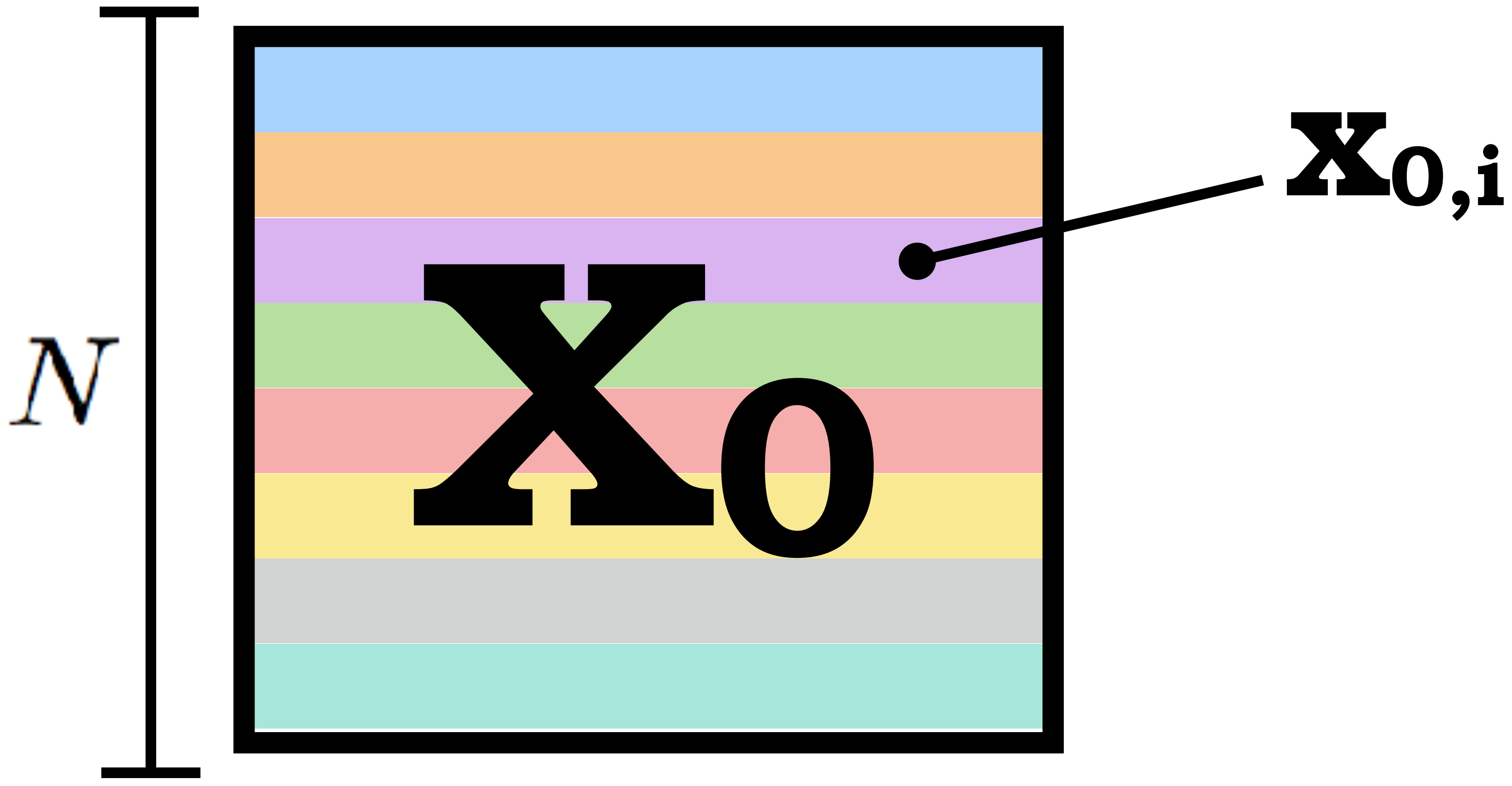
(Nalisnick & Smyth, SoCalML 2017)

The Bootstrap

Bootstrap Resampling

$$\boxed{X_0}$$

Bootstrap Resampling



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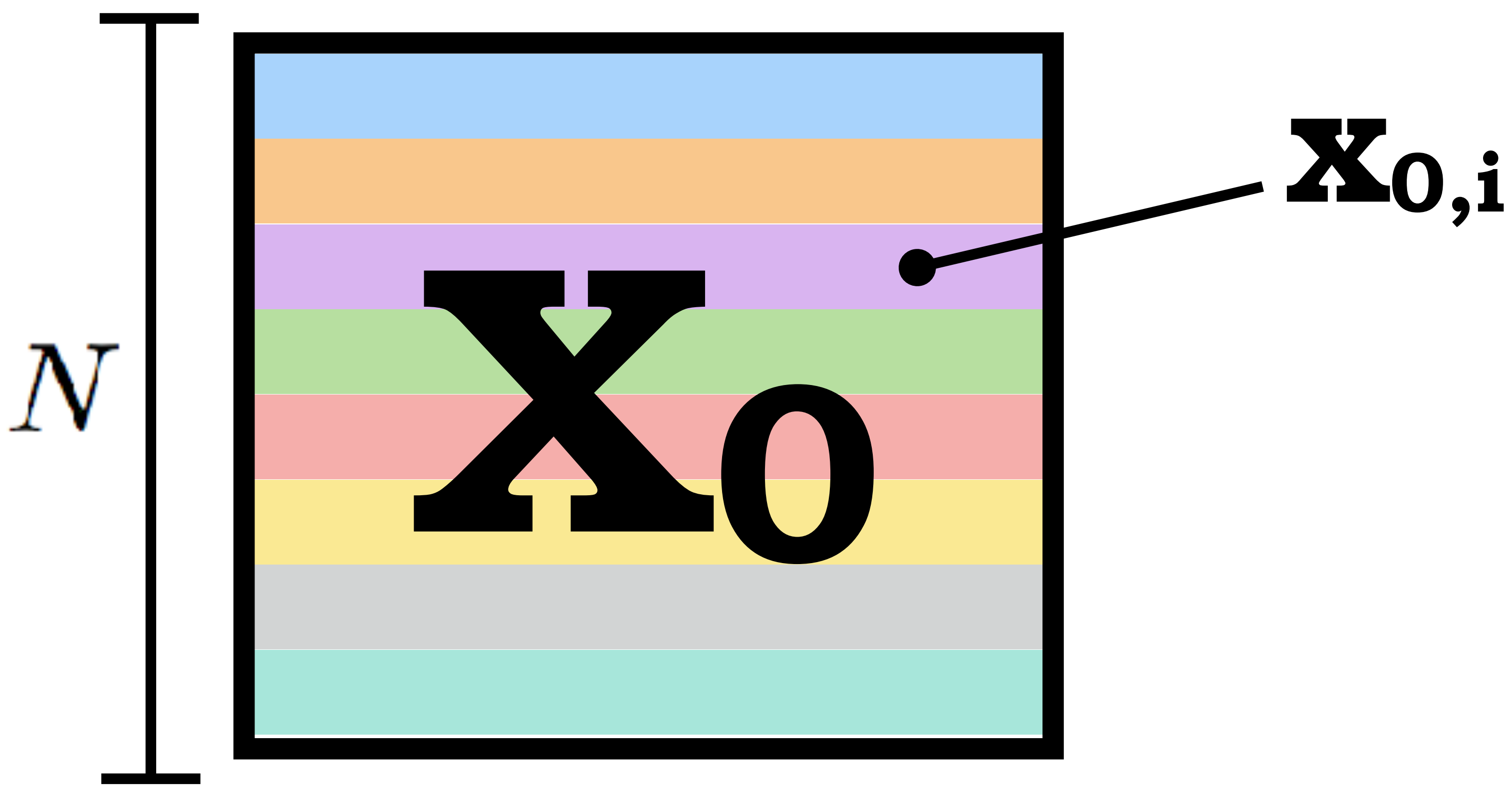

$$\mathbf{x} \sim G(\mathbf{x}) = \frac{1}{N} \sum_{i=1}^{N} \delta_{\mathbf{x}_{0,i}}$$

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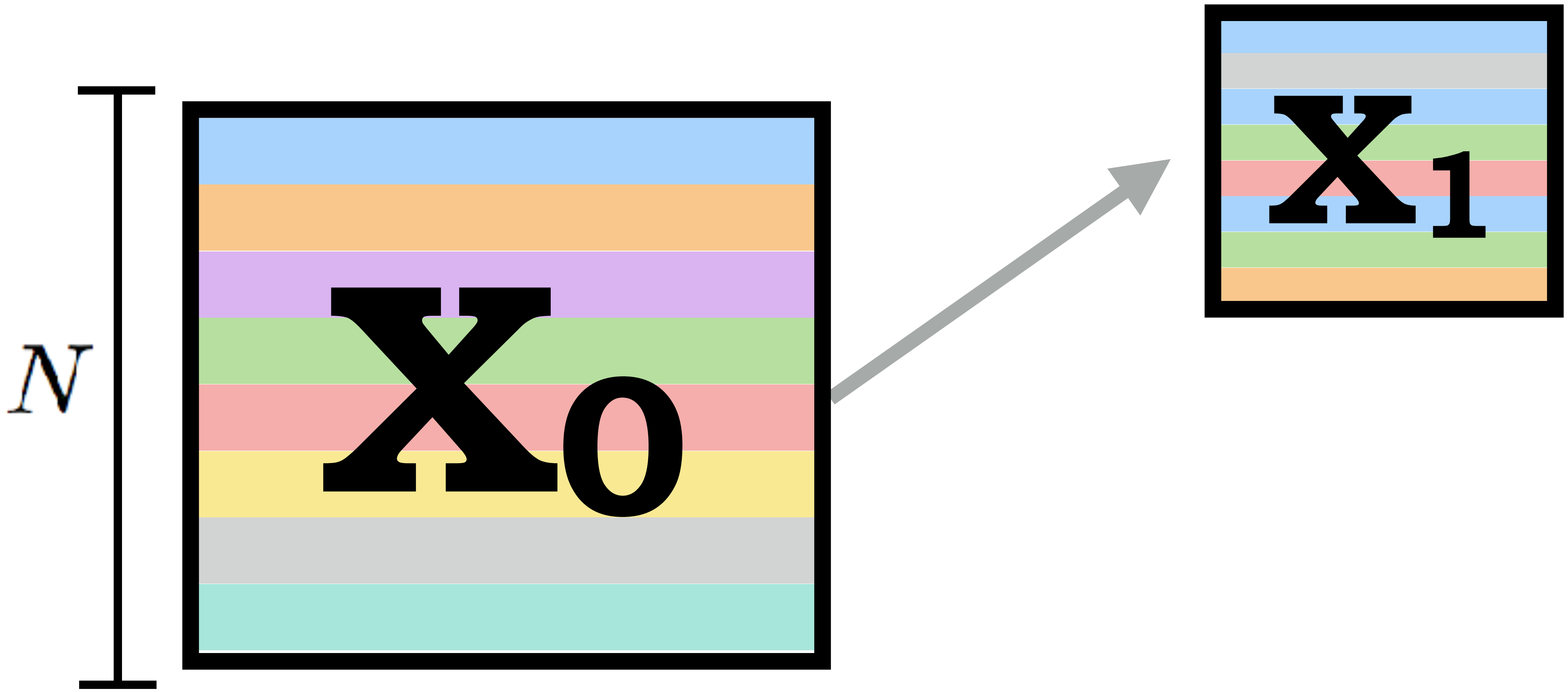

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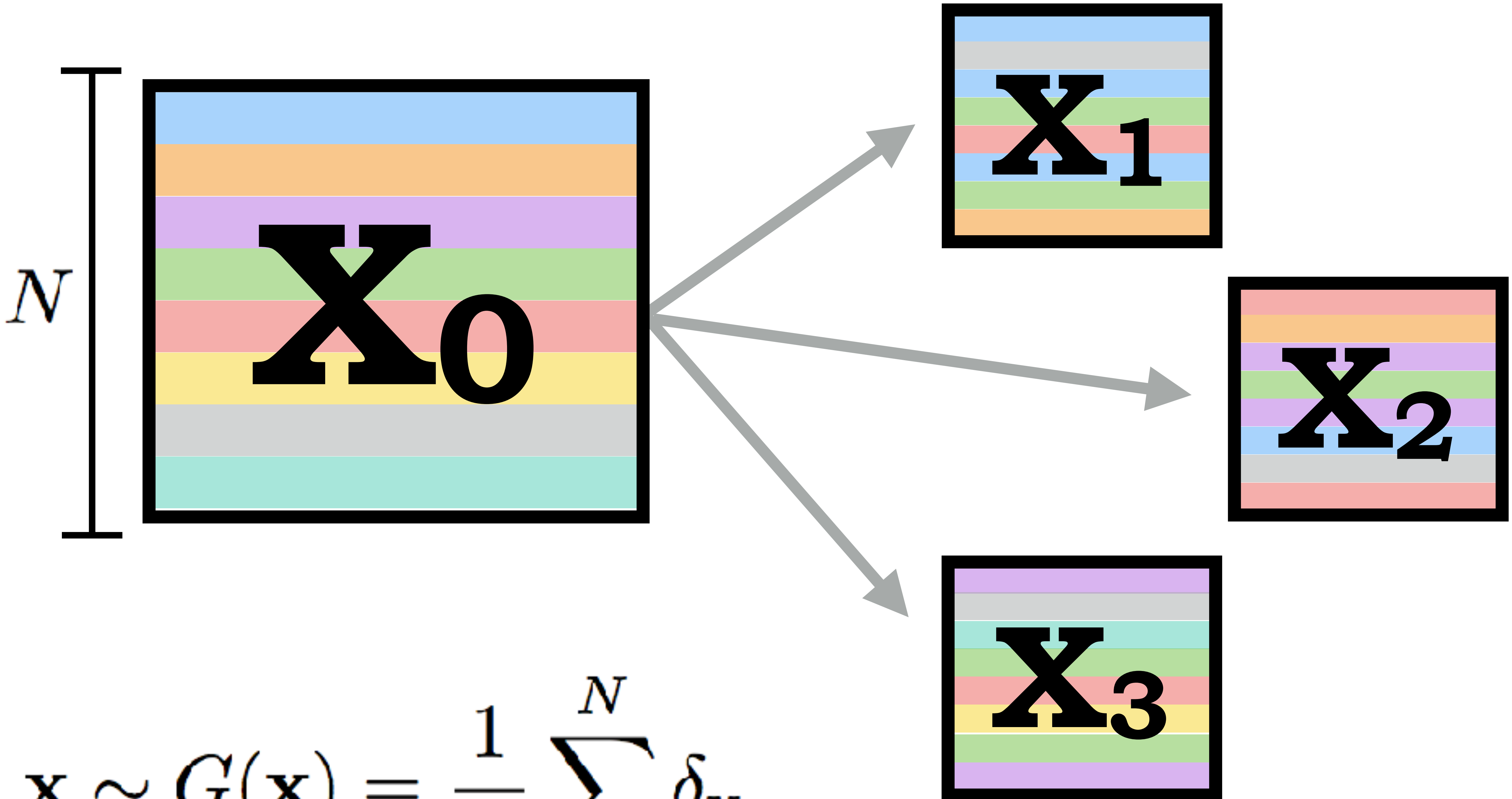

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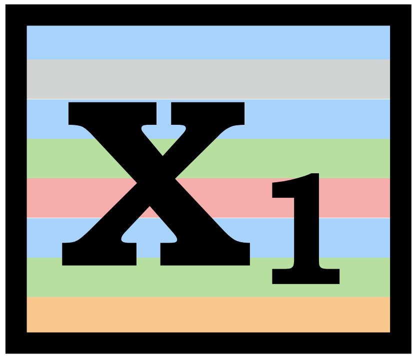
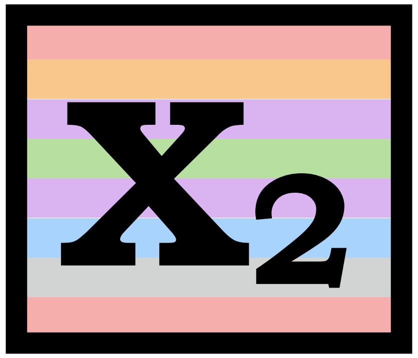
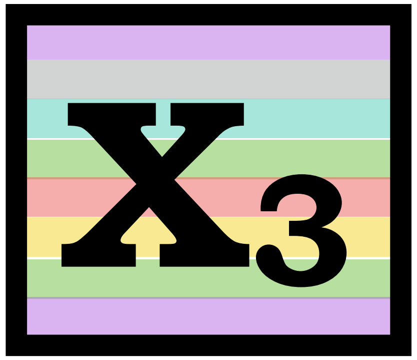
Bootstrap Distribution







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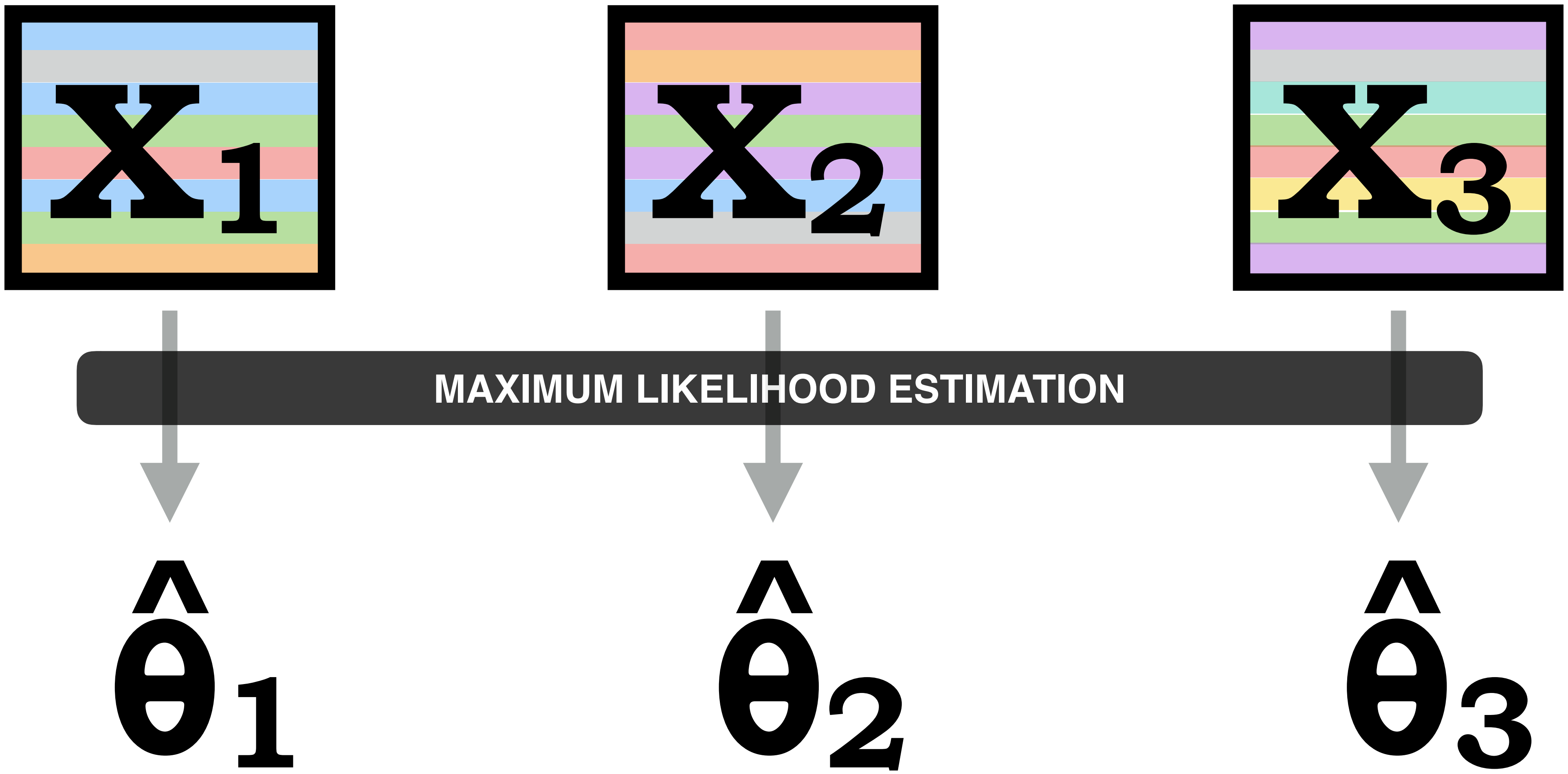

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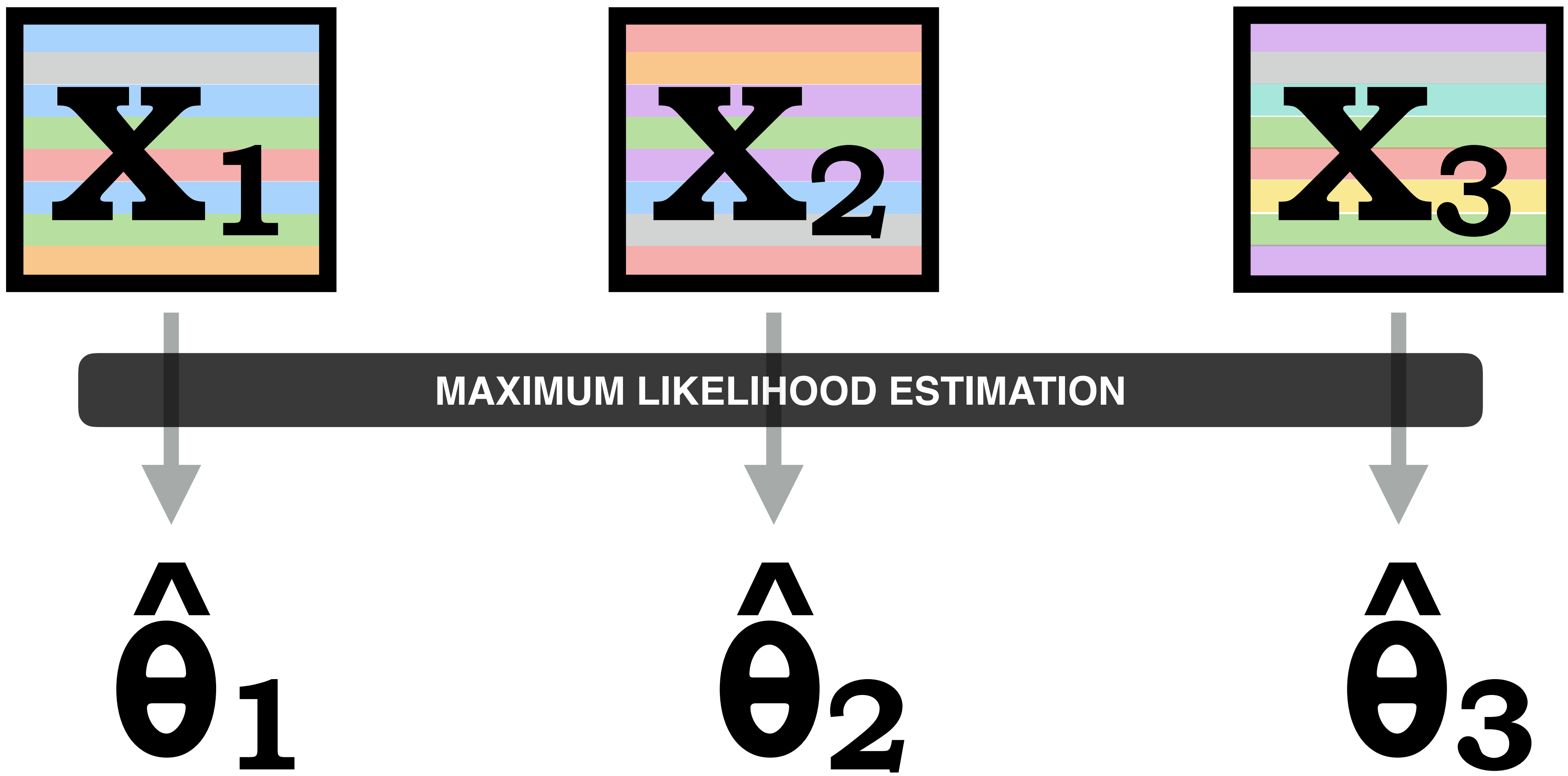

$$\boldsymbol{\theta} \sim F(\boldsymbol{\theta}) = \frac{1}{K} \sum_{k=1}^{K} \delta_{\hat{\boldsymbol{\theta}}_k}$$

The Amortized Bootstrap

Modeling the Bootstrap Distribution

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

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

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CONS

- Breaks bootstrap theory. Can recover only an approximation.
- Can't distribute computation.

Learning the Bootstrap Model

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

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$$\frac{\partial \mathcal{J}(\mathbf{X}_0, \phi)}{\partial \boldsymbol{\phi}} = \frac{1}{K}\sum_{k=1}^{K} \frac{\partial \log p(\mathbf{X}_k|\hat{\boldsymbol{\theta}}_{\boldsymbol{\phi},k})}{\partial \hat{\boldsymbol{\theta}}_{\boldsymbol{\phi},k}} \frac{\partial \hat{\boldsymbol{\theta}}_{\boldsymbol{\phi},k}}{\partial \boldsymbol{\phi}}$$

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

Learning the Bootstrap Model

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

Regularization preventing collapse to ML point estimate.

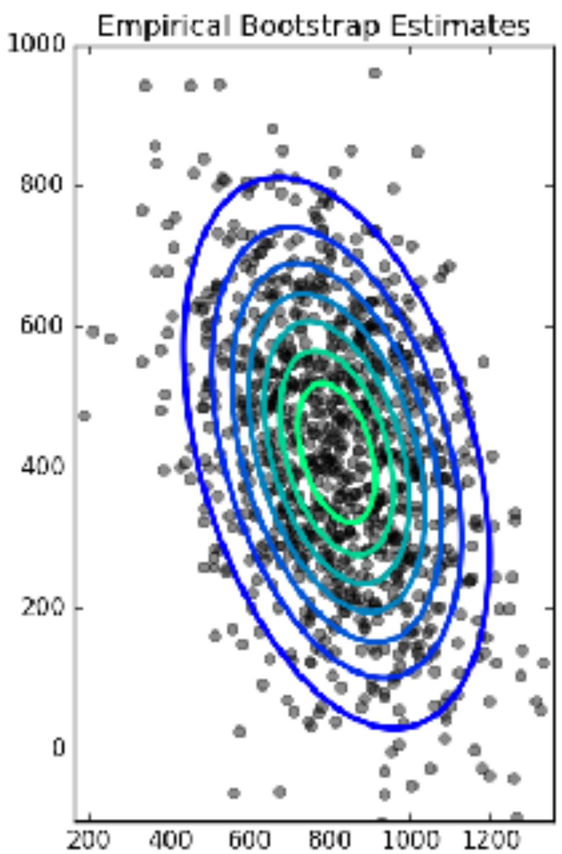
$$\mathcal{L}_{\text{ELBO}} = \mathbb{E}_{q(\boldsymbol{\theta})}[\log p(\mathbf{X}|\boldsymbol{\theta})] - \mathbf{KLD}[q(\boldsymbol{\theta})||p(\boldsymbol{\theta})]$$

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

Experiment #1: Diagnostics

Linear Regression

2D Diabetes Dataset



2D Boston Housing Dataset

Linear Regression

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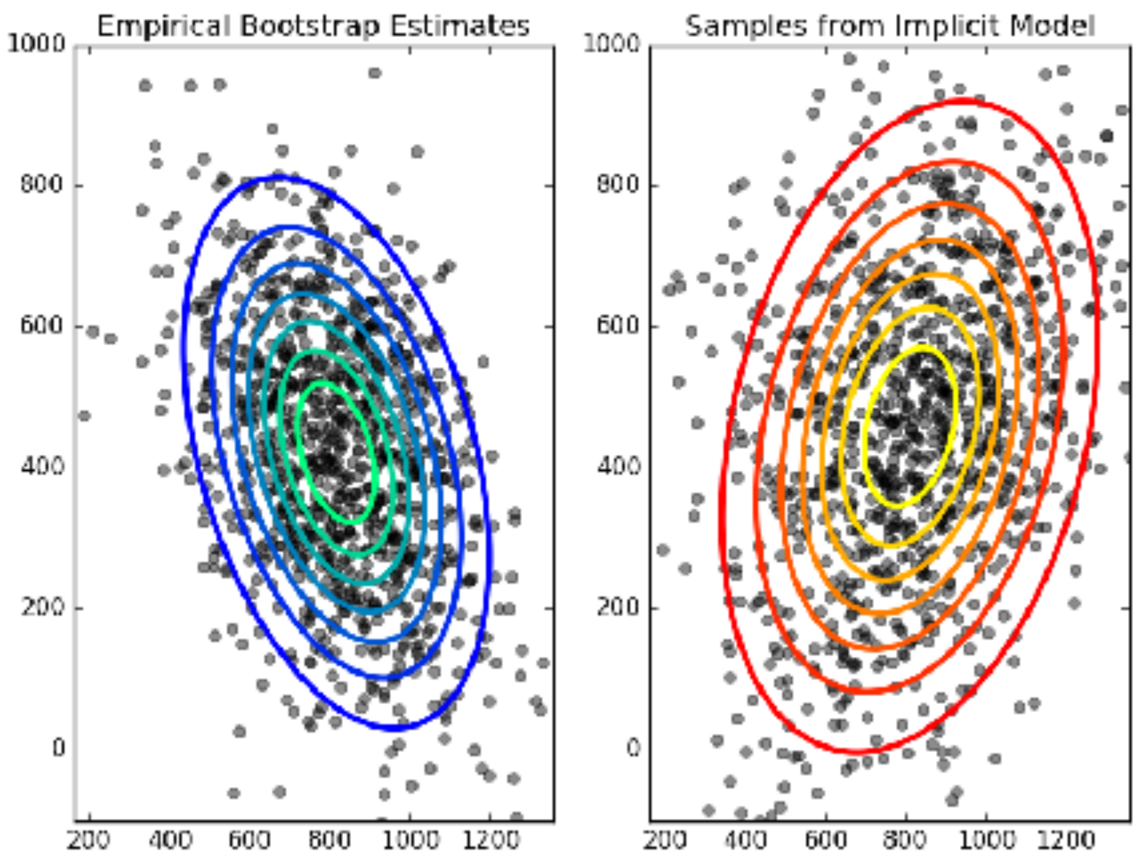

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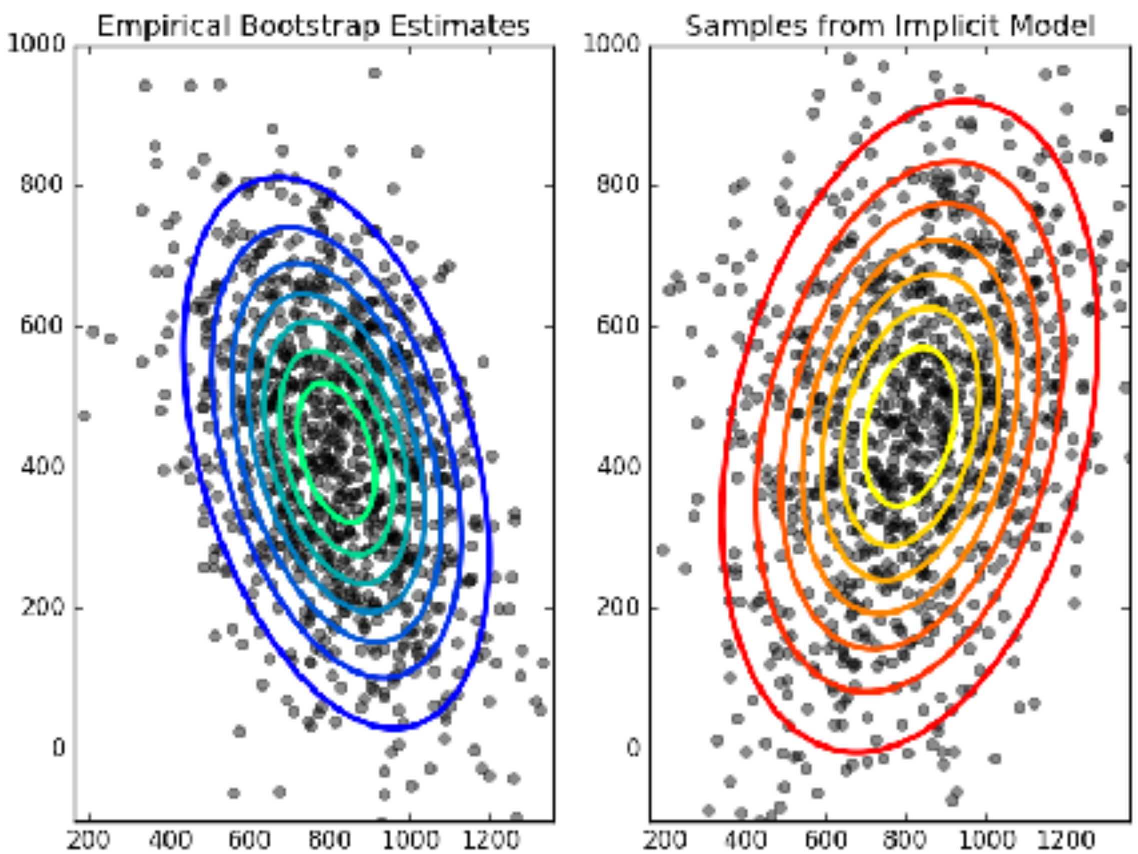

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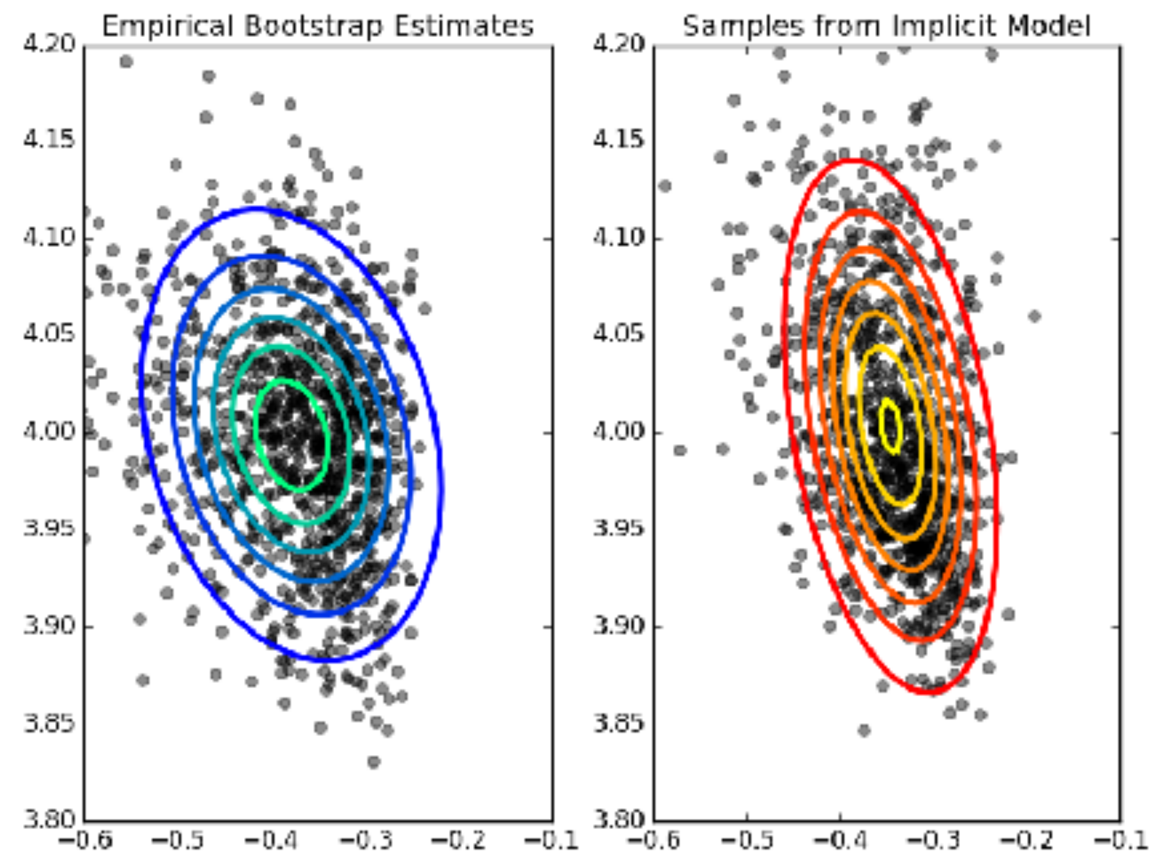

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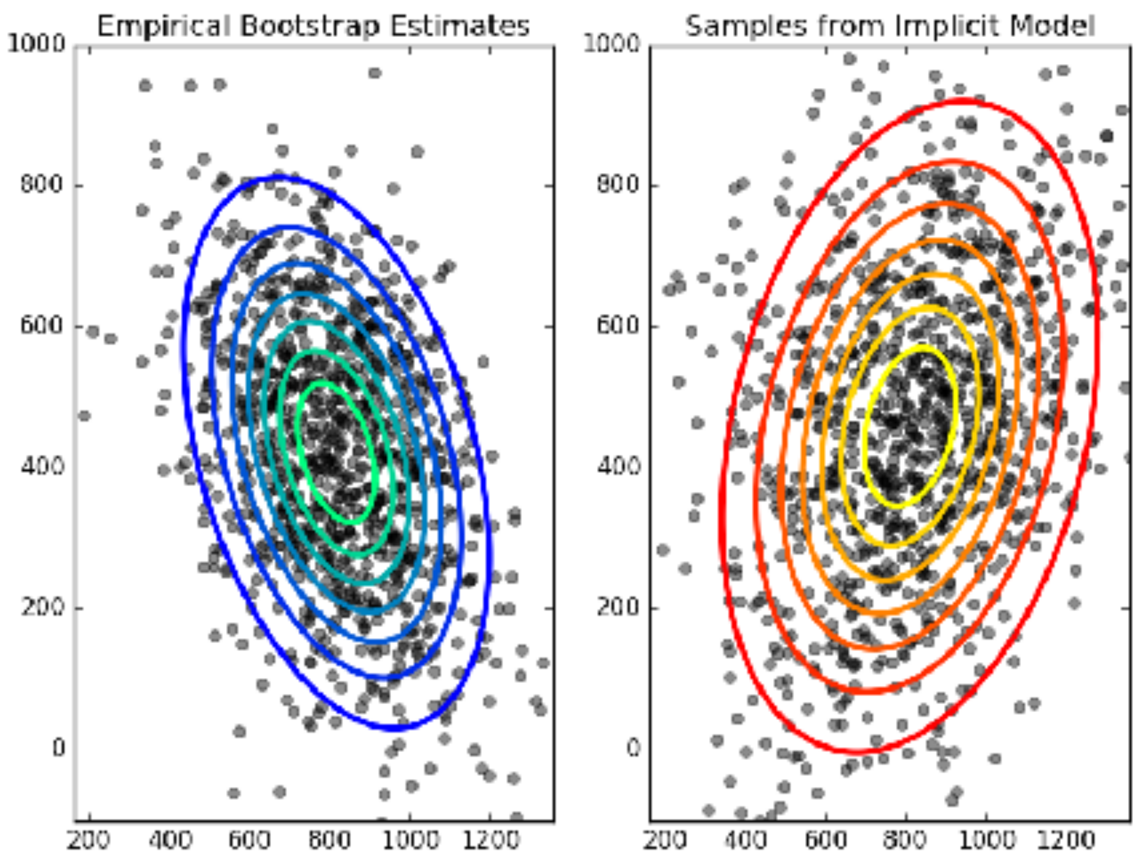

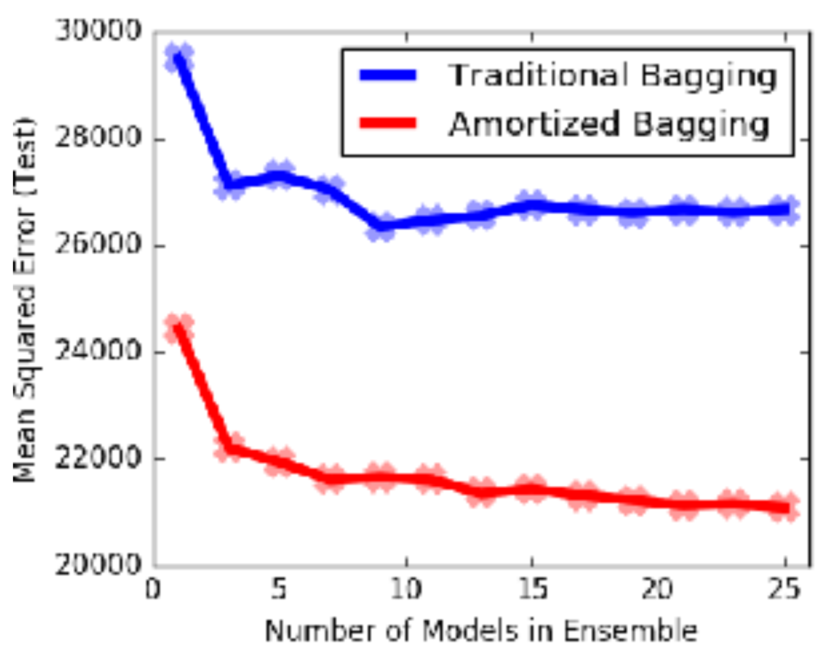

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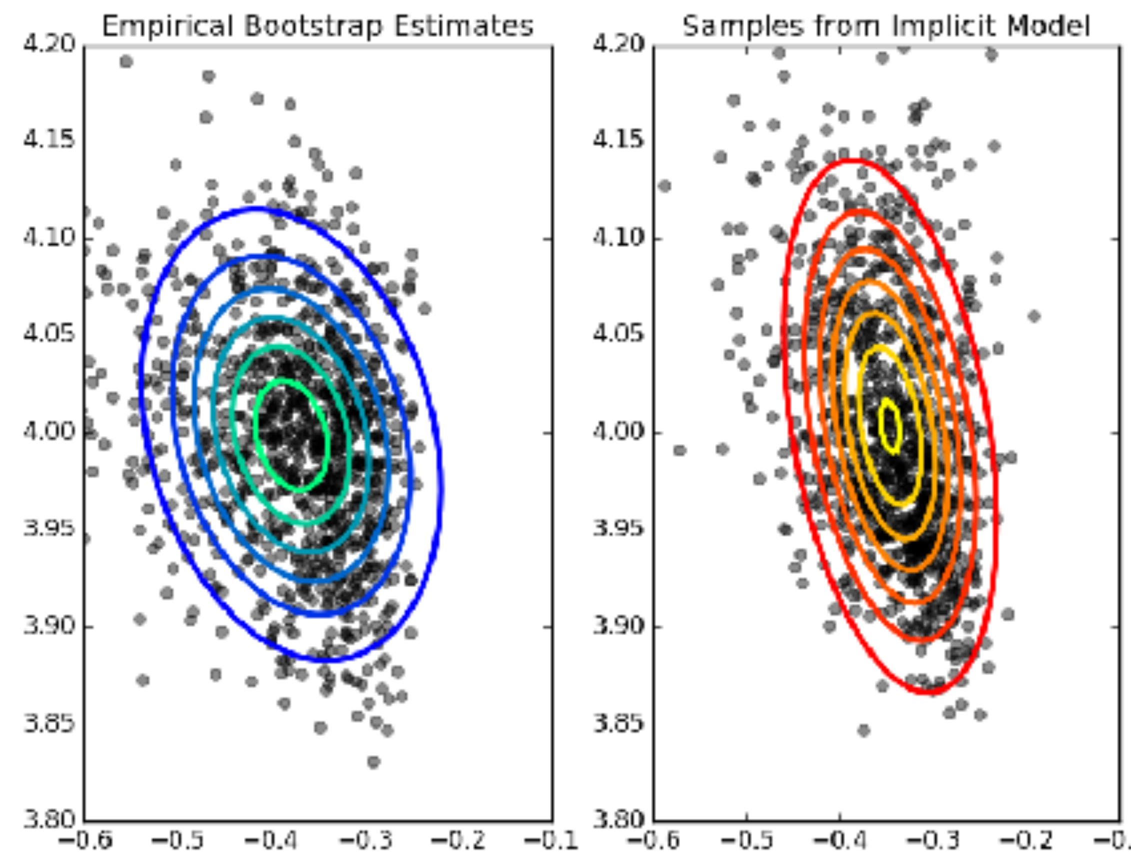
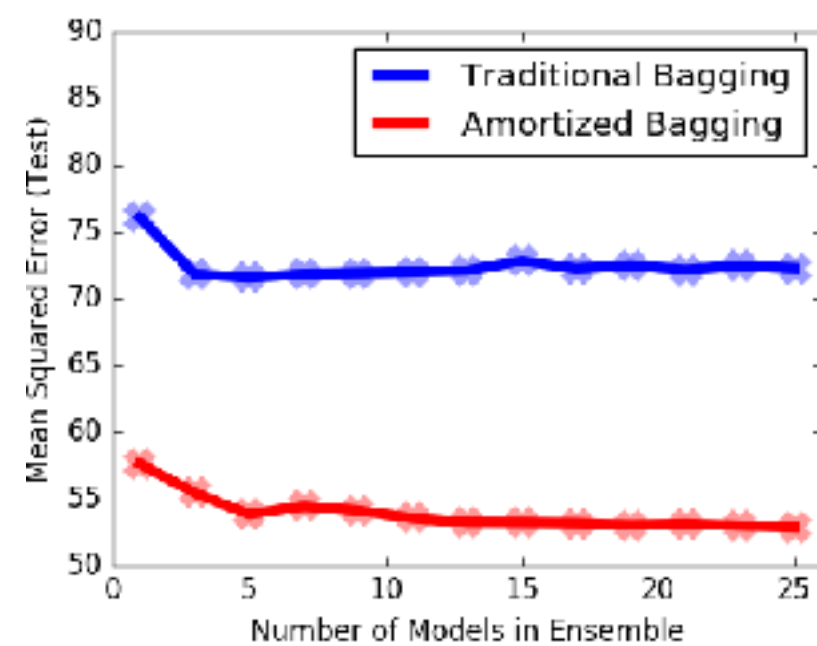
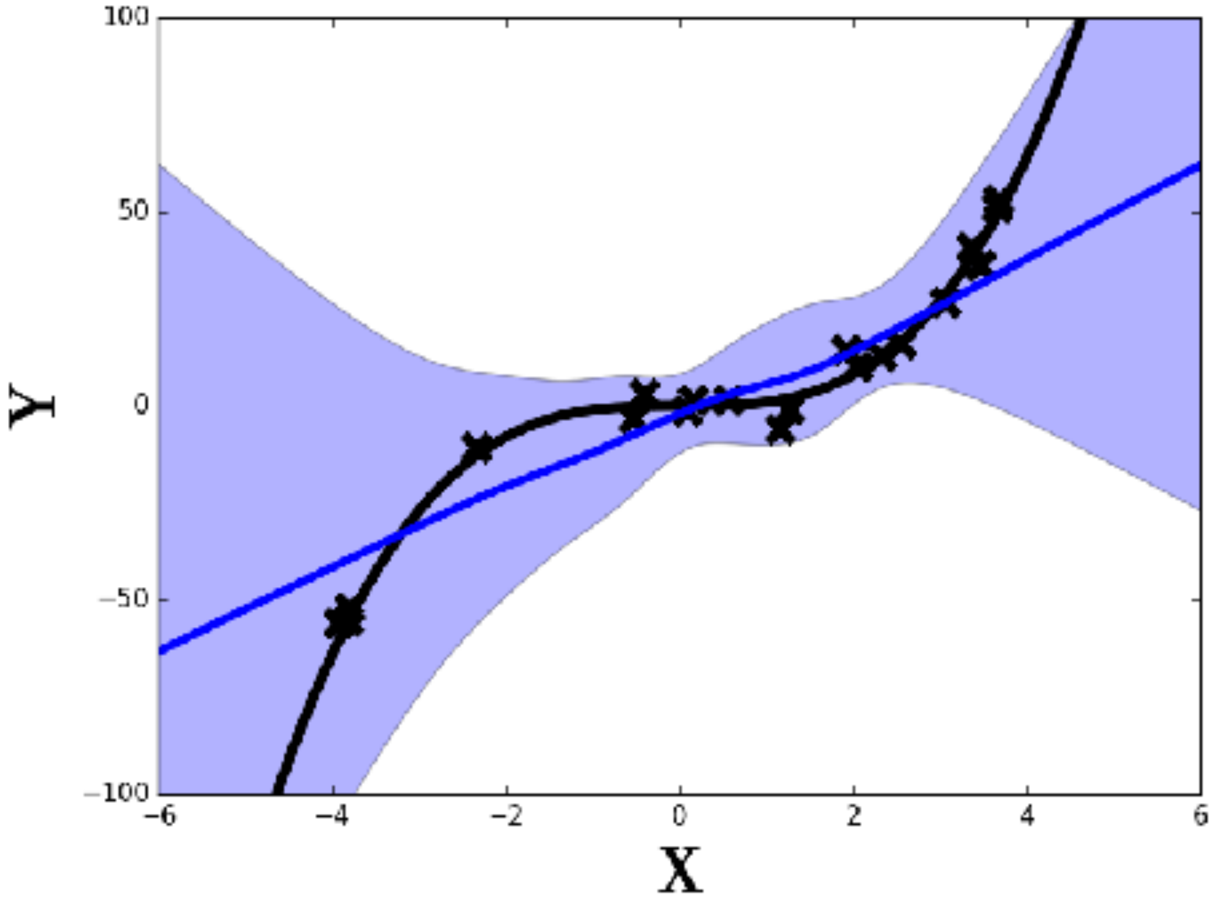


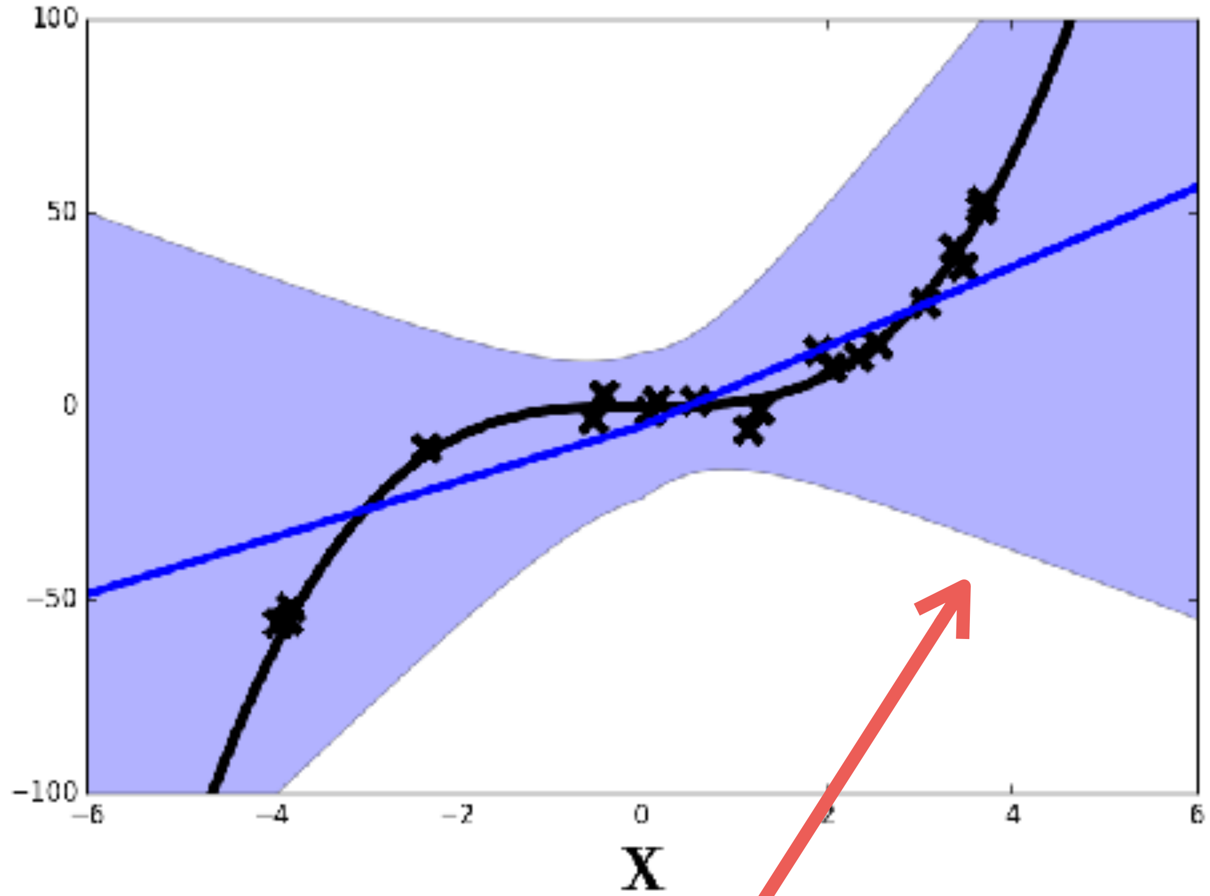


Predictive Uncertainty

TRADITIONAL BOOTSTRAP



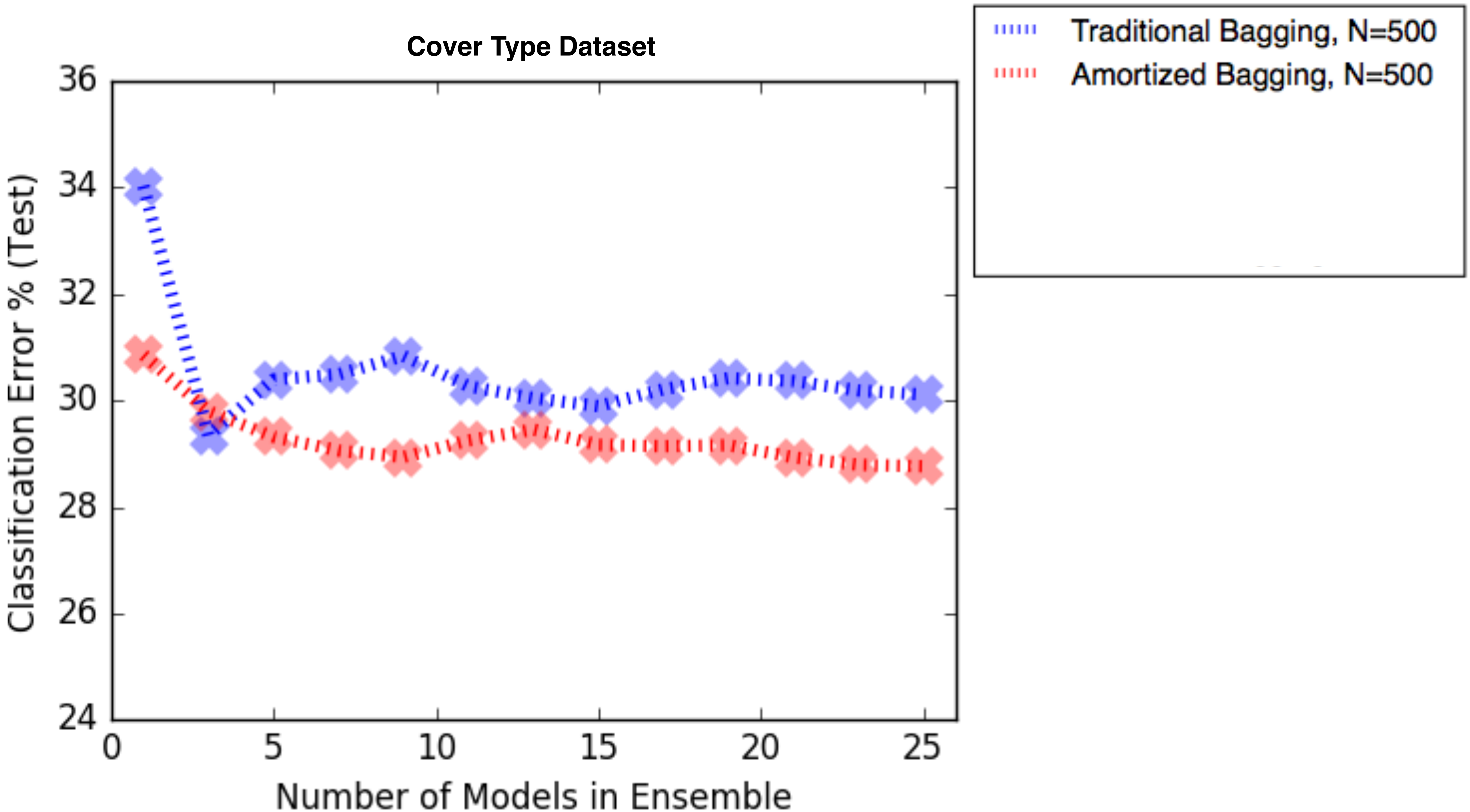
AMORTIZED BOOTSTRAP



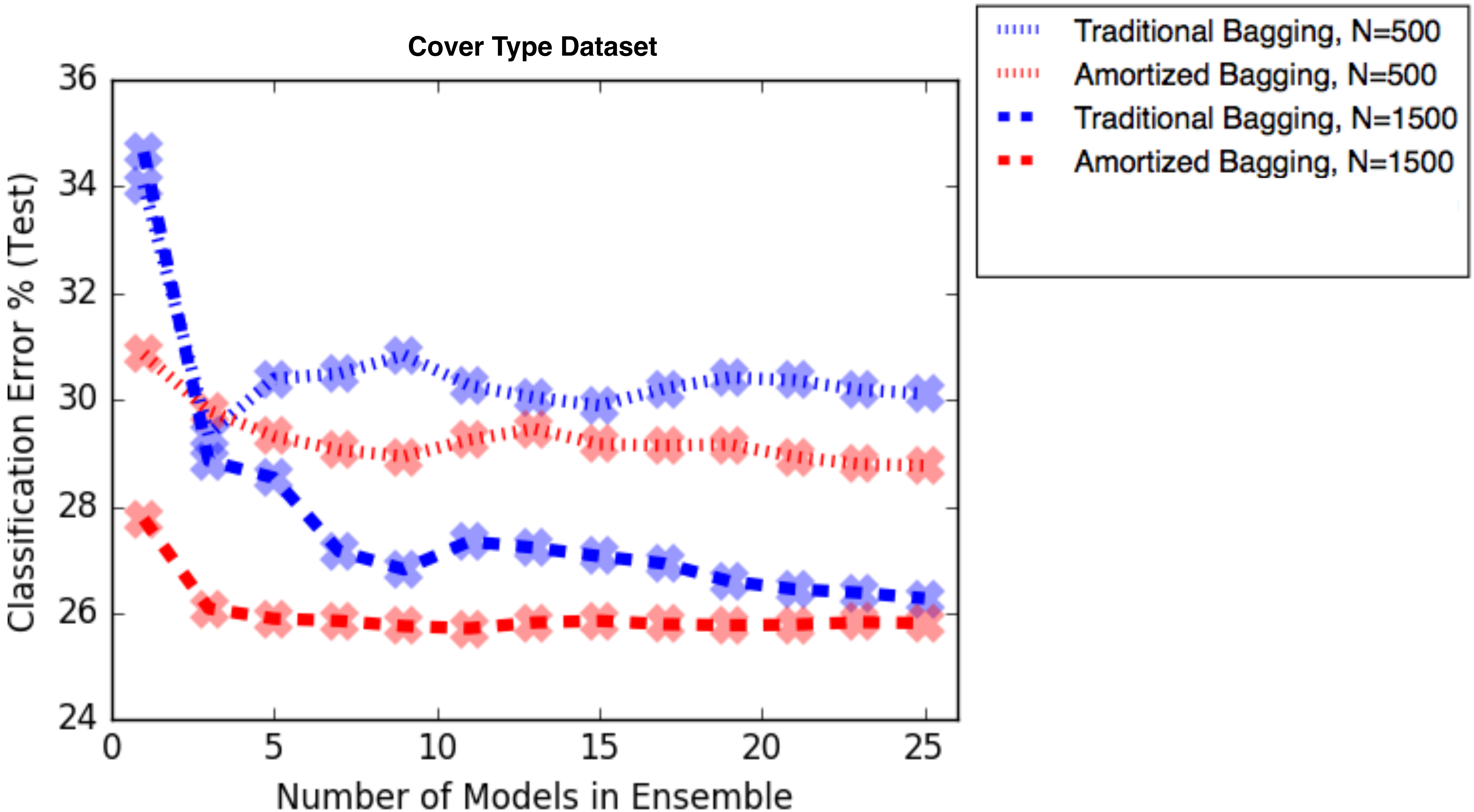
Smooth uncertainty bands, which will likely help in high-dimensions.

Experiment #2: Varying Dataset Size

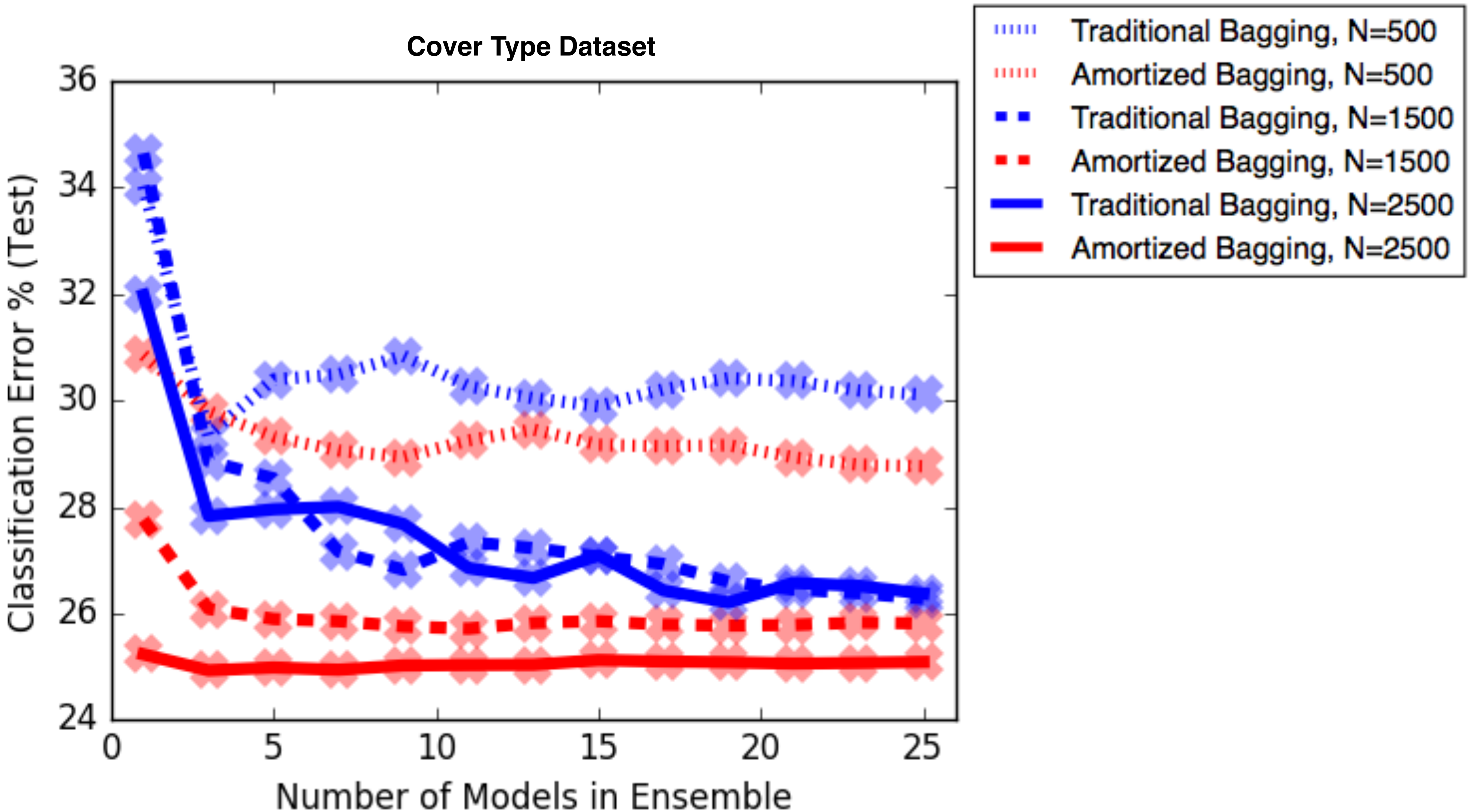
Logistic Regression



Logistic Regression



Logistic Regression



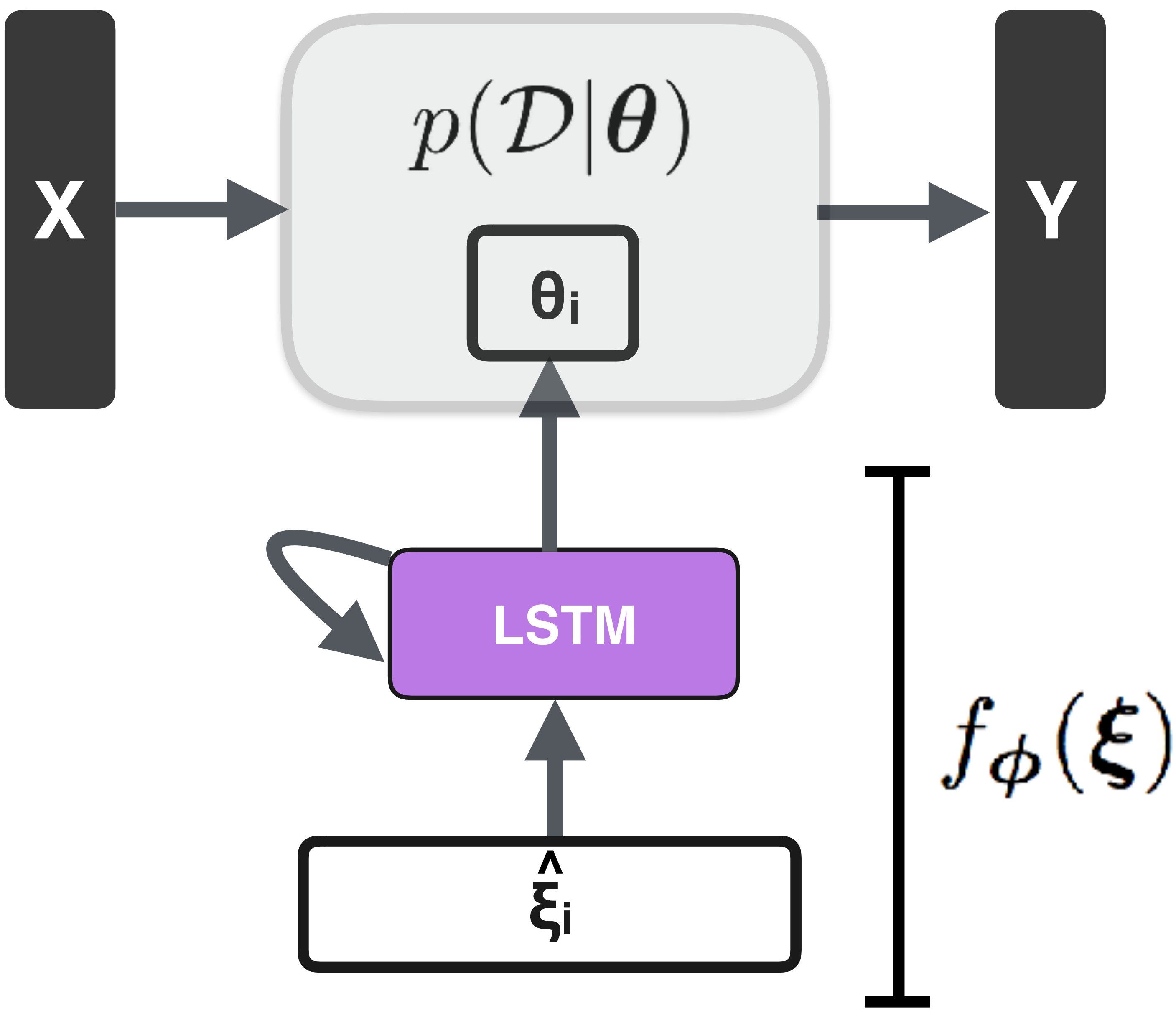
Experiment #3: Classification with NN

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

In-Progress Work: Use RNN Implicit Model



Improve scalability with RNN implicit model.

— NN parameters exhibit low-dim. structure (Denil et al., 2013)

Conclusion: Approx. Inference for Frequentist Tools

- Approximating 'Frequentist-esque' priors.

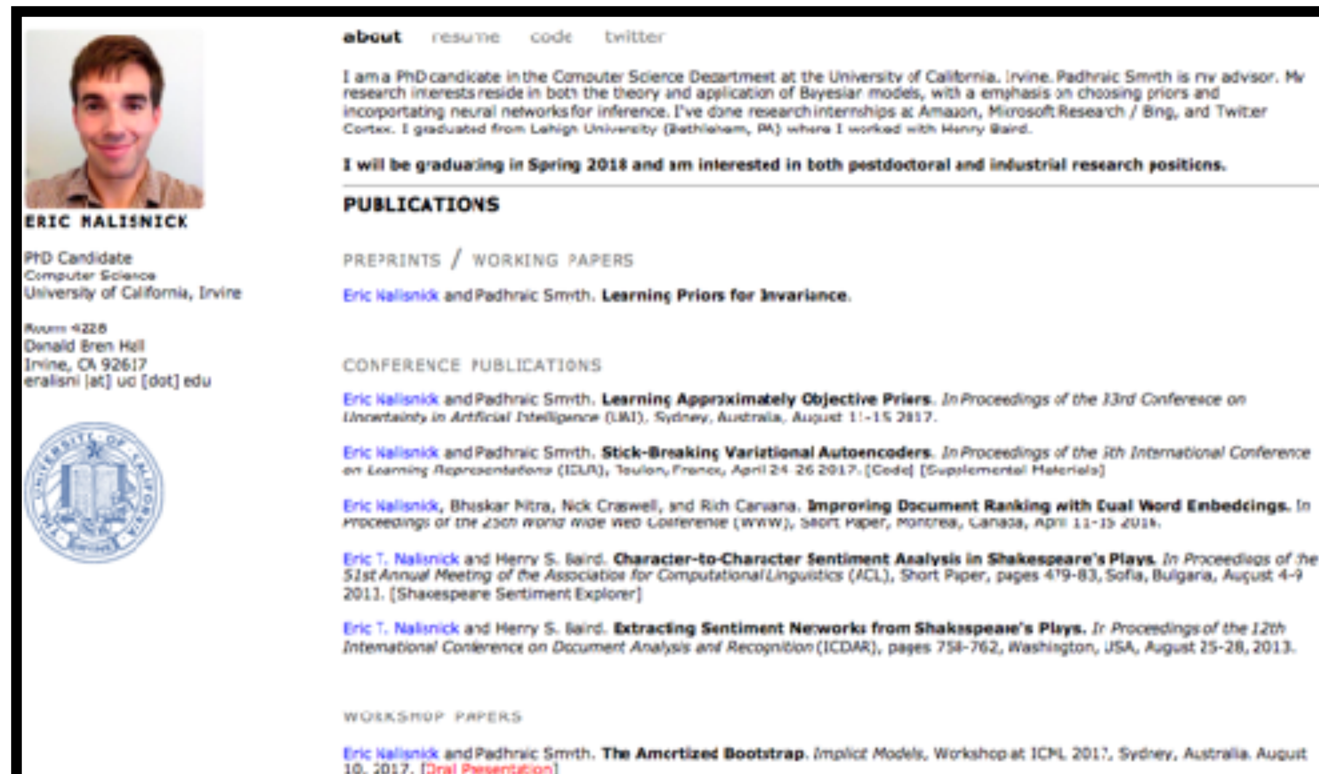
  Obtain data-driven posteriors for complex, formerly intractable models.

- **Amortized bootstrap:** model-based approximation of the bootstrap distribution.

  Results in **superior bagging** performance due (ostensibly) to smoothing and amortization.

Thank you. Questions?

See me at posters #6 and #9.



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

In collaboration with

Padhraic Smyth

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