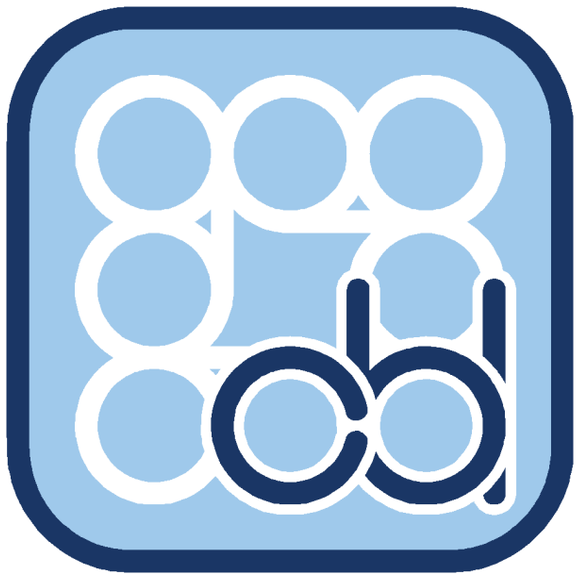
Machine Learning with Objective Priors

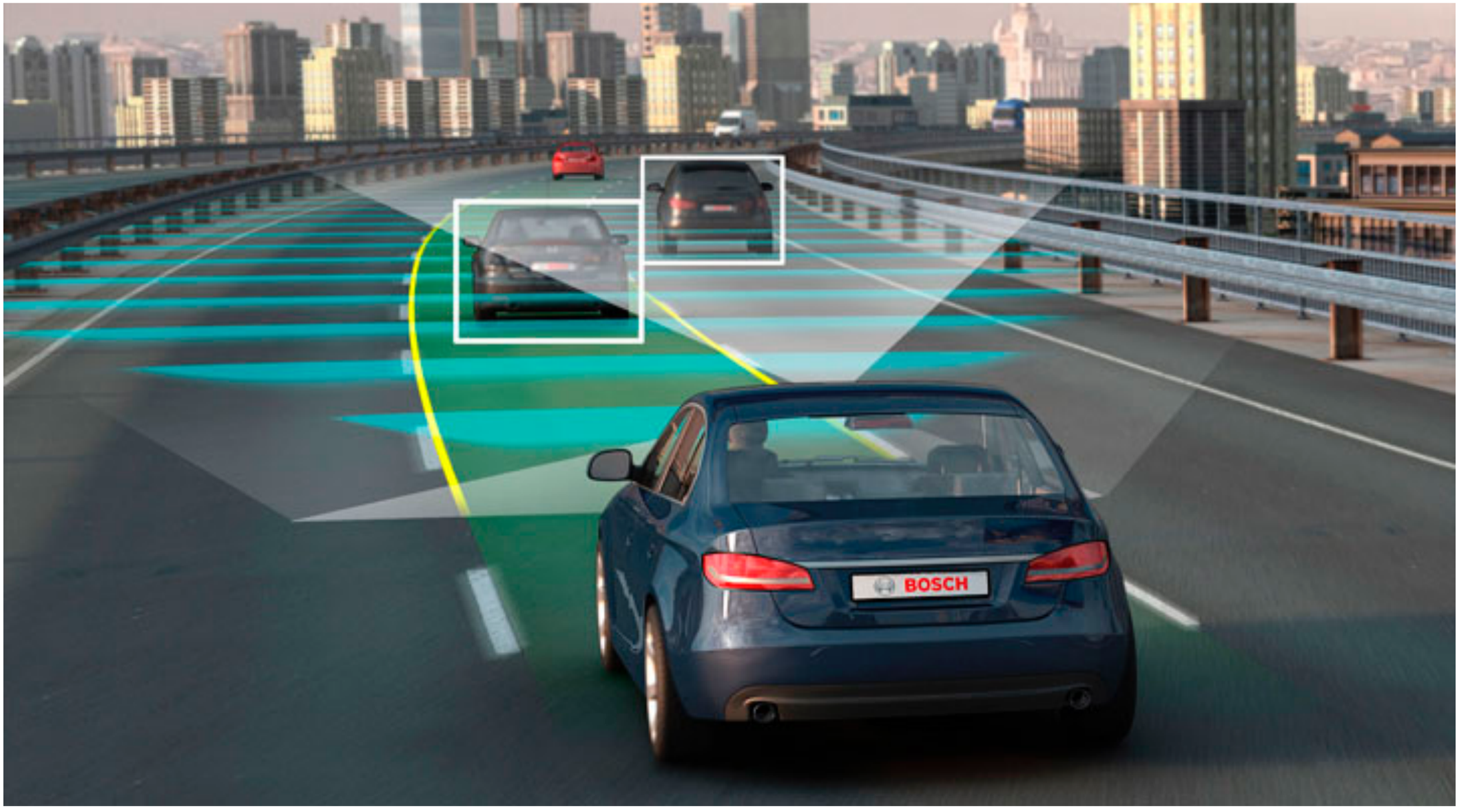
Eric Nalisnick



Computational and Biological Learning
University of Cambridge

Div F Conference
20.3.2019

Modern machine learning requires uncertainty estimation.



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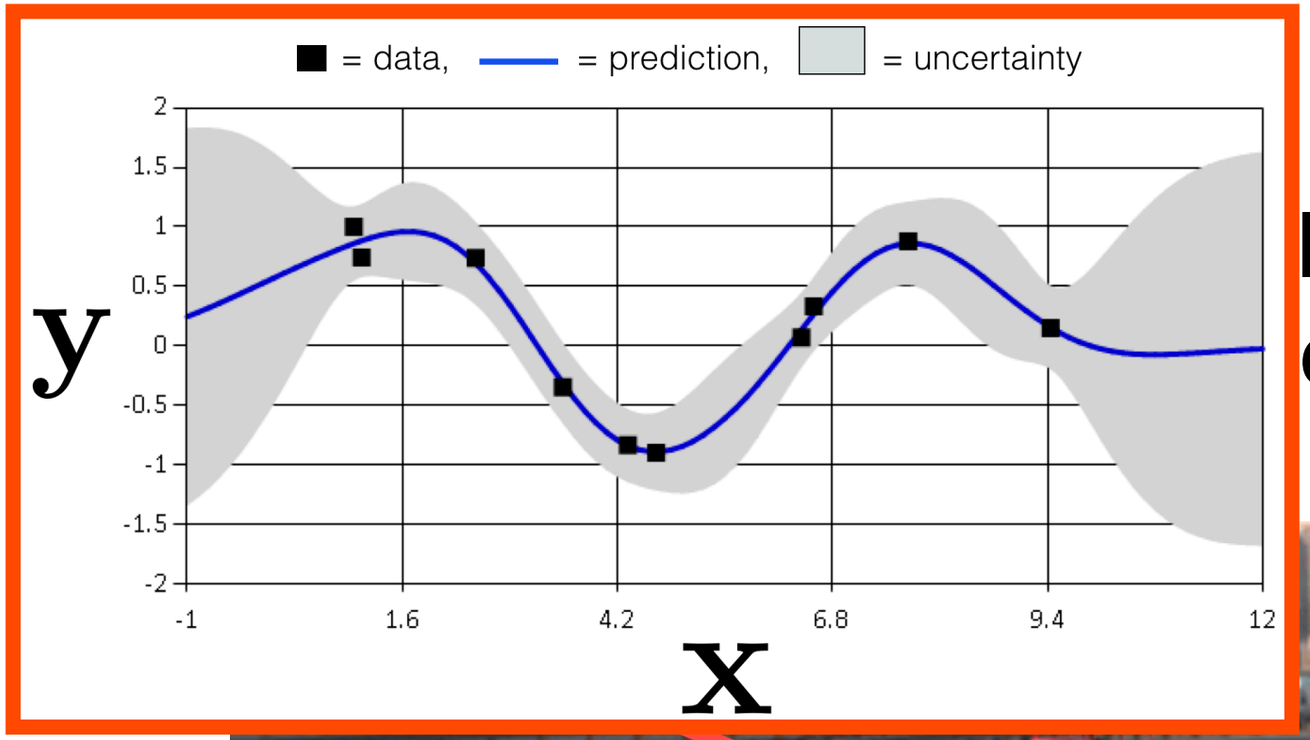
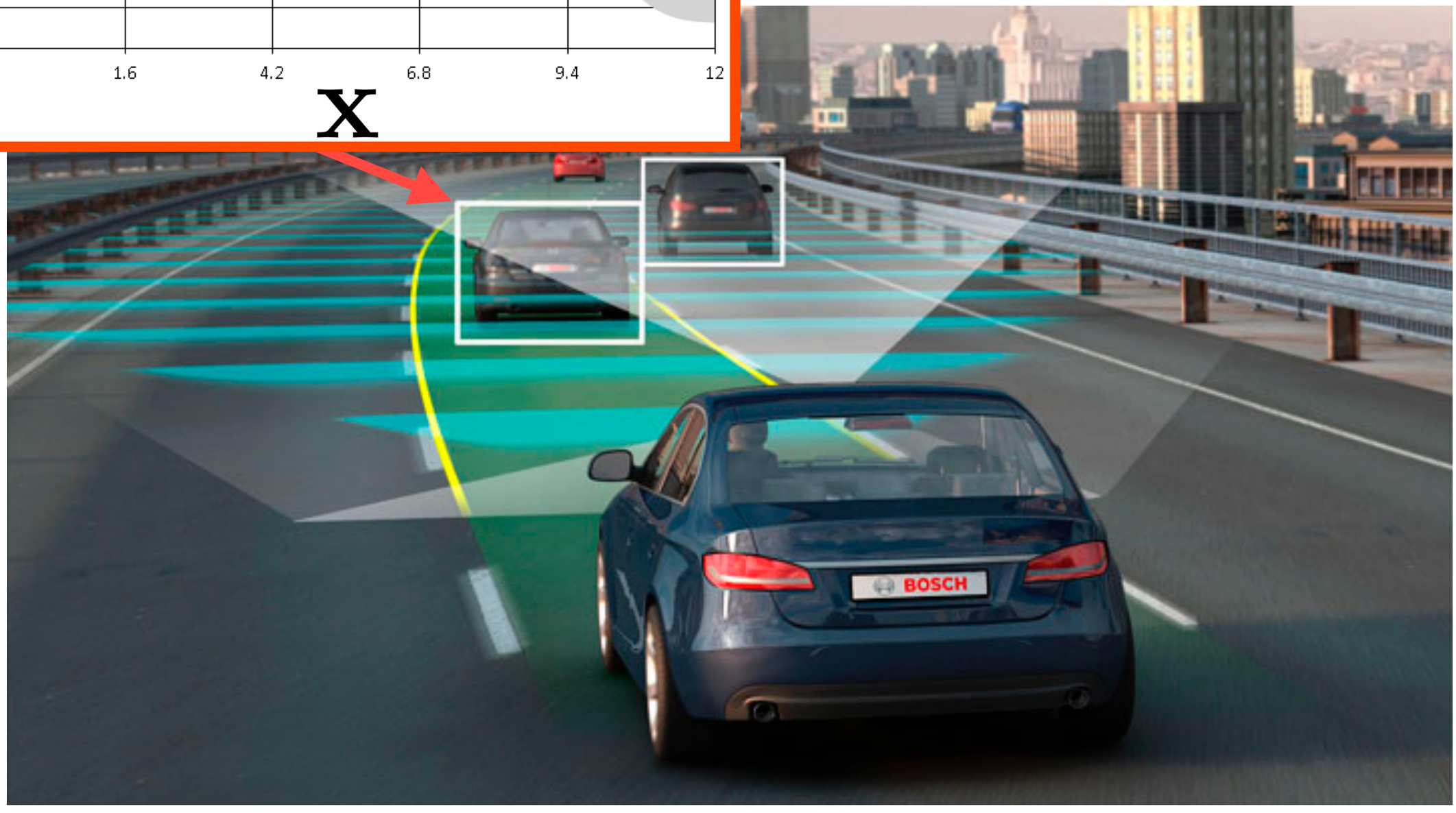


learning requires estimation.



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$$p(\boldsymbol{\theta}|\mathbf{X}) = \frac{p(\mathbf{X}|\boldsymbol{\theta})\ \ p(\boldsymbol{\theta})}{p(\mathbf{X})}$$

THOMAS BAYES

Likelihood

Prior

Posterior

$$p(\boldsymbol{\theta}|\mathbf{X}) = \frac{p(\mathbf{X}|\boldsymbol{\theta})\ p(\boldsymbol{\theta})}{p(\mathbf{X})}$$

Marginal Likelihood

(a.k.a. model evidence)
(a.k.a. normalizing constant)
(a.k.a. partition function)

$$p(\mathbf{X}) = \int_{\boldsymbol{\theta}} p(\mathbf{X}|\boldsymbol{\theta})\ p(\boldsymbol{\theta})\ d\boldsymbol{\theta}$$

THOMAS BAYES

$$p(\boldsymbol{\theta}|\mathbf{X}) = \frac{p(\mathbf{X}|\boldsymbol{\theta})\ \ p(\boldsymbol{\theta})}{p(\mathbf{X})}$$

THOMAS BAYES

$$p(\boldsymbol{\theta}|\mathbf{X}) = \frac{p(\mathbf{X}|\boldsymbol{\theta})\,p(\boldsymbol{\theta})}{p(\mathbf{X})}$$

Garbage in: arbitrary priors
Garbage out: uncontrollable error bars

~ Michael I. Jordan, *MLSS* (2017)

THOMAS BAYES

$$p(\boldsymbol{\theta}|\mathbf{X}) = \frac{p(\mathbf{X}|\boldsymbol{\theta})\,p(\boldsymbol{\theta})}{p(\mathbf{X})}$$

How should we think about priors for machine learning models?

THOMAS BAYES

EXAMPLE

Priors for Modeling Coin Tosses

Priors for Modeling Coin Tosses

$$\mathbf{X} = \{X_n \in \{0, 1\}\}_{n=1}^{N}$$

$$p(\mathbf{X}|\theta) = \texttt{Binomial}(N, \theta)$$

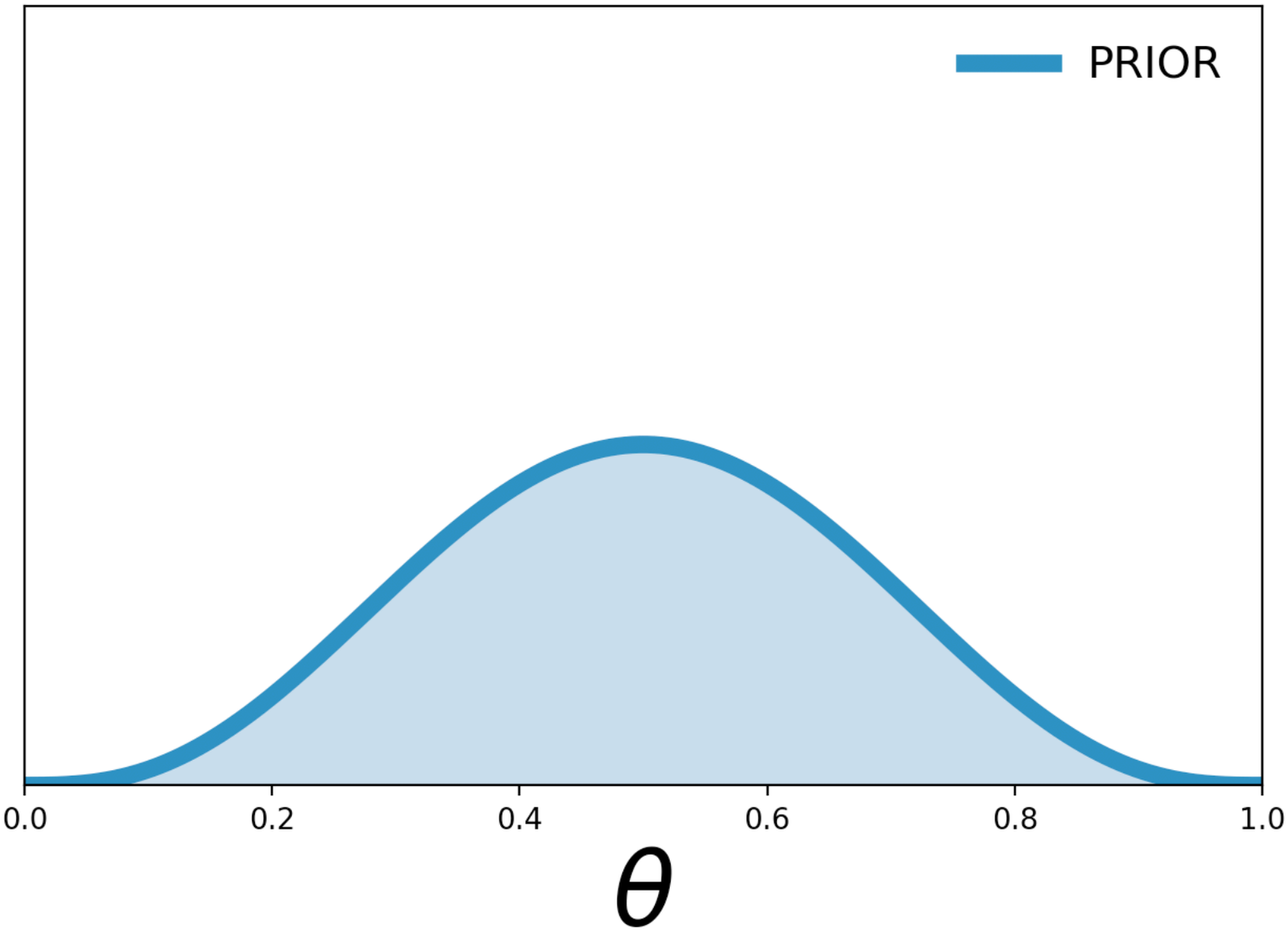
$$p(\theta) = \texttt{Beta}(\alpha_0, \beta_0)$$

Priors for Modeling Coin Tosses

$$p(\theta|\mathbf{X}) \propto \texttt{Binomial}(N, \theta)\ \texttt{Beta}(\alpha_0, \beta_0)$$

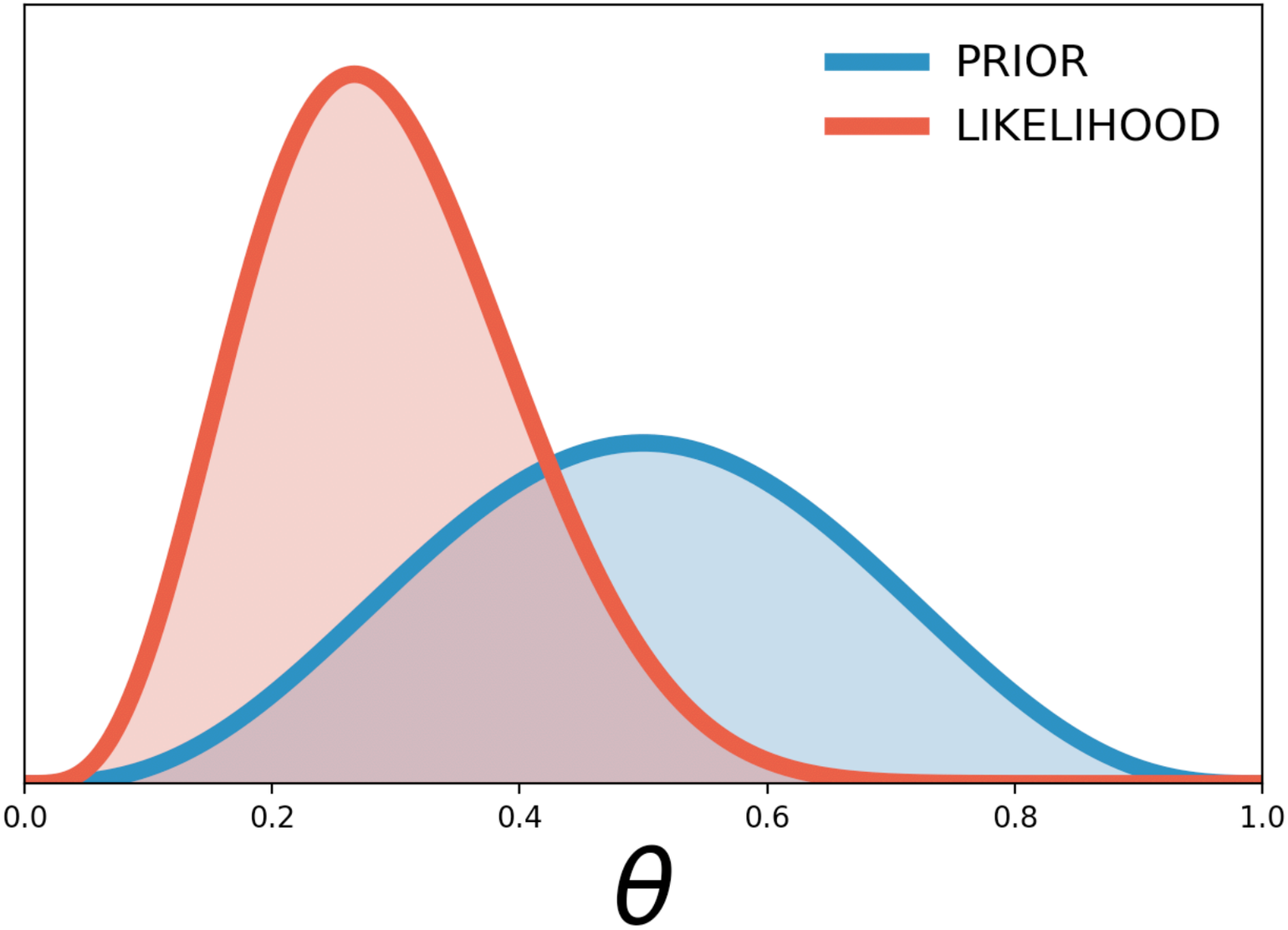
Priors for Modeling Coin Tosses

$$p(\theta|\mathbf{X}) \propto \texttt{Binomial}(N, \theta)\ \texttt{Beta}(4, 4)$$



Priors for Modeling Coin Tosses

$$p(\theta|\mathbf{X}) \propto \texttt{Binomial}(15, \theta)\,\texttt{Beta}(4, 4)$$



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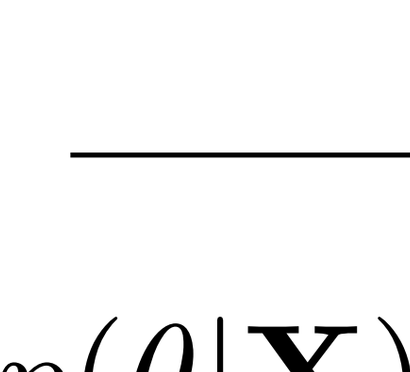
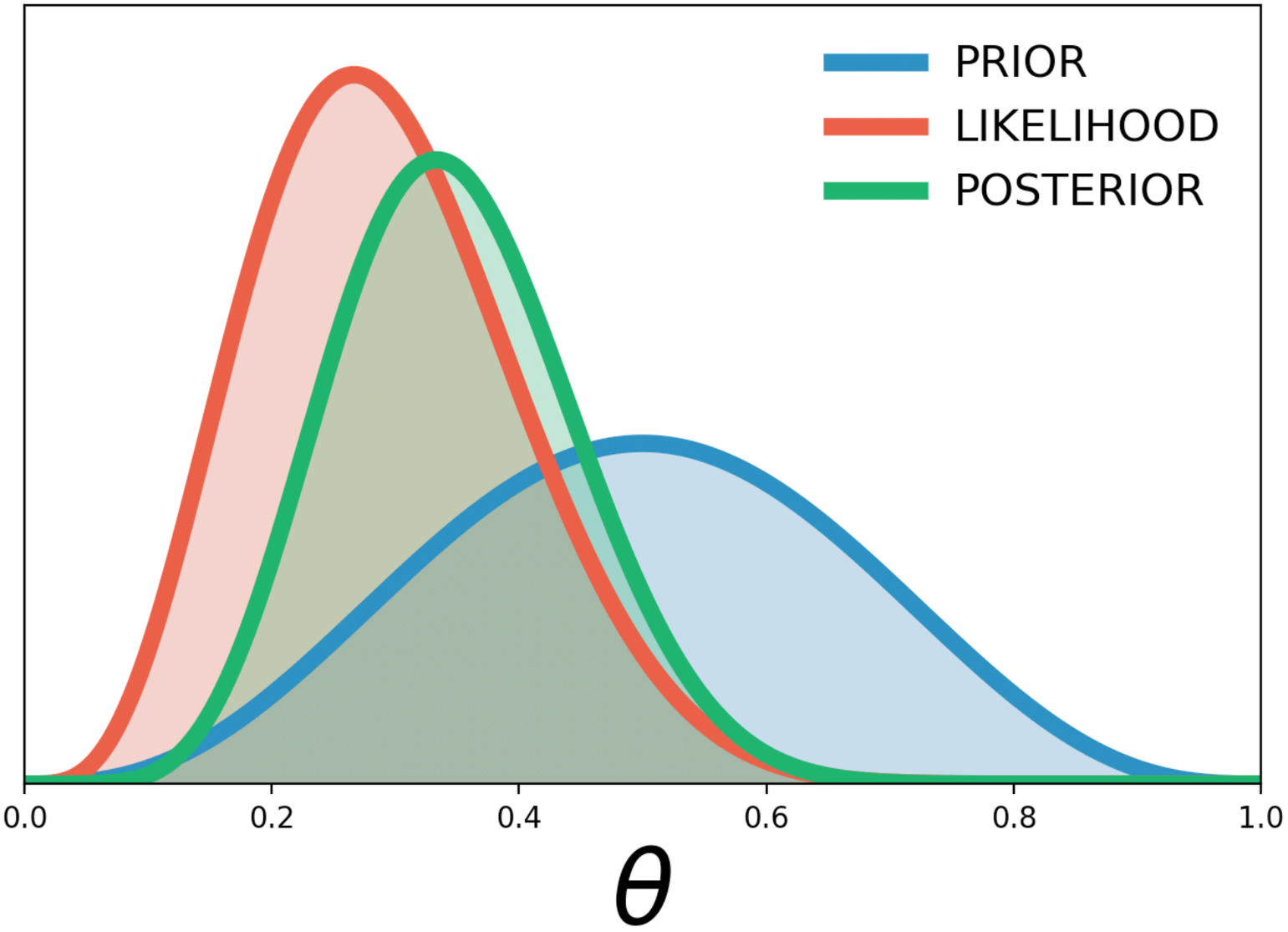




Priors for Modeling Coin Tosses

$$p(\theta|\mathbf{X}) \propto \texttt{Binomial}(N, \theta)\ \texttt{Beta}(\alpha_0, \beta_0)$$

…But what if we have *even stronger* prior information?

Priors for Modeling Coin Tosses

$$p(\theta|\mathbf{X}) \propto \texttt{Binomial}(N, \theta)\ \texttt{Beta}(\alpha_0, \beta_0)$$

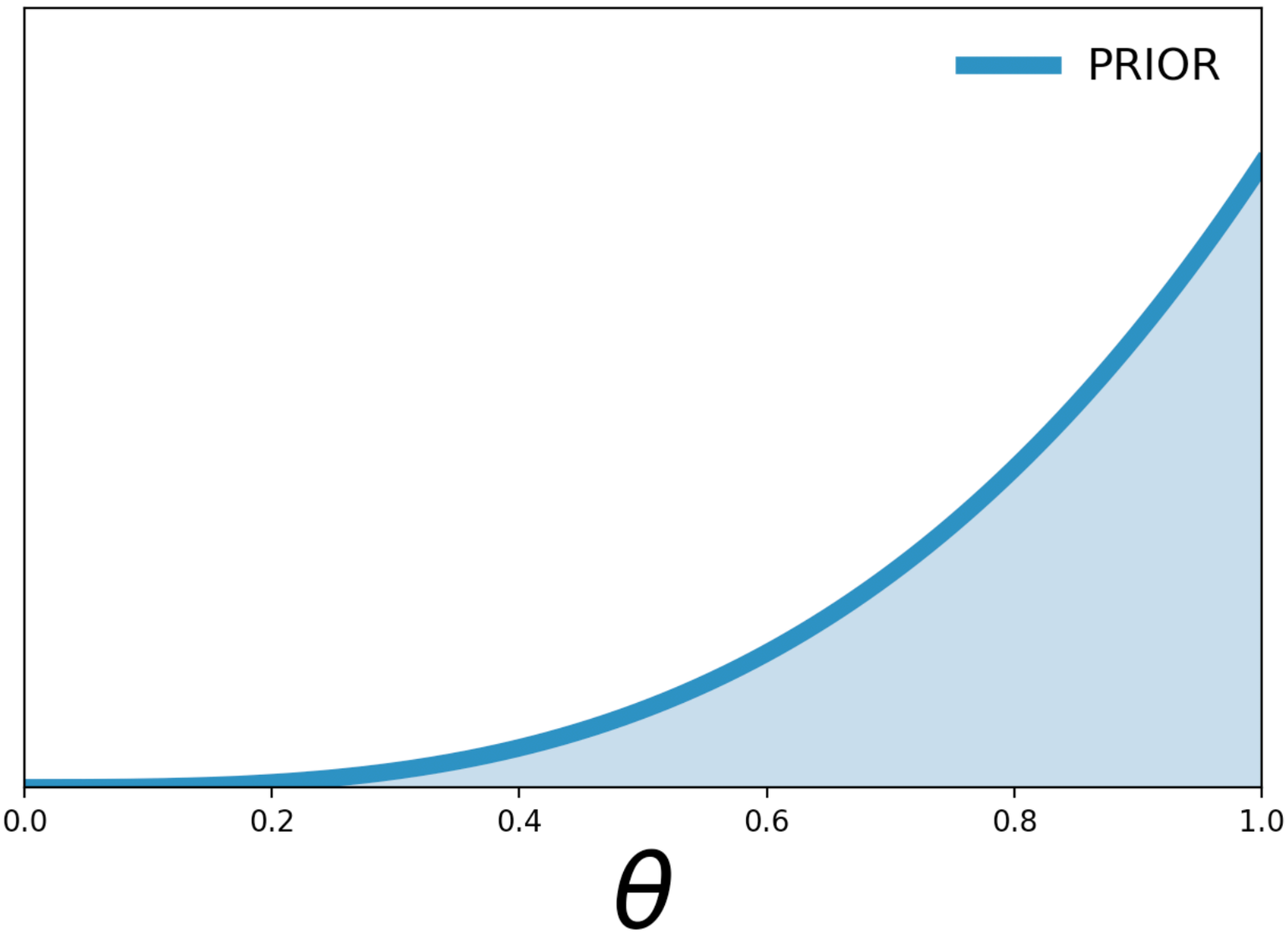
Harvey Dent
aka “Two-Face”
The Dark Knight, 2008

…But what if we have *even stronger* prior information?

Priors for Modeling Coin Tosses

$$p(\theta|\mathbf{X}) \propto \texttt{Binomial}(N, \theta)\ \texttt{Beta}(4, 1)$$

Harvey Dent
aka “Two-Face”
The Dark Knight, 2008



Objective Priors

…But what if we have <u>no</u> information?

Say we are completely agnostic about Θ;
What prior represents a *state of ignorance*?

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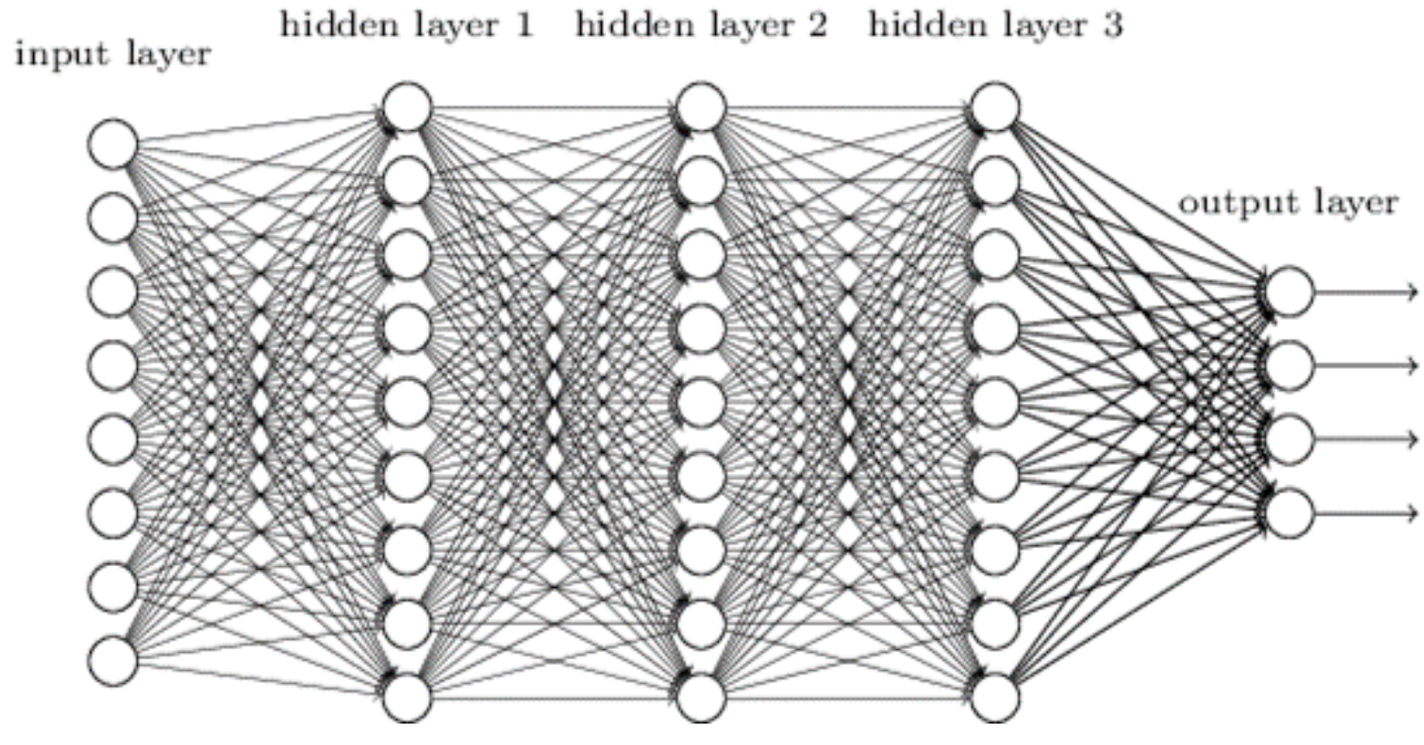

Objective Priors

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Say we are completely agnostic about Θ;
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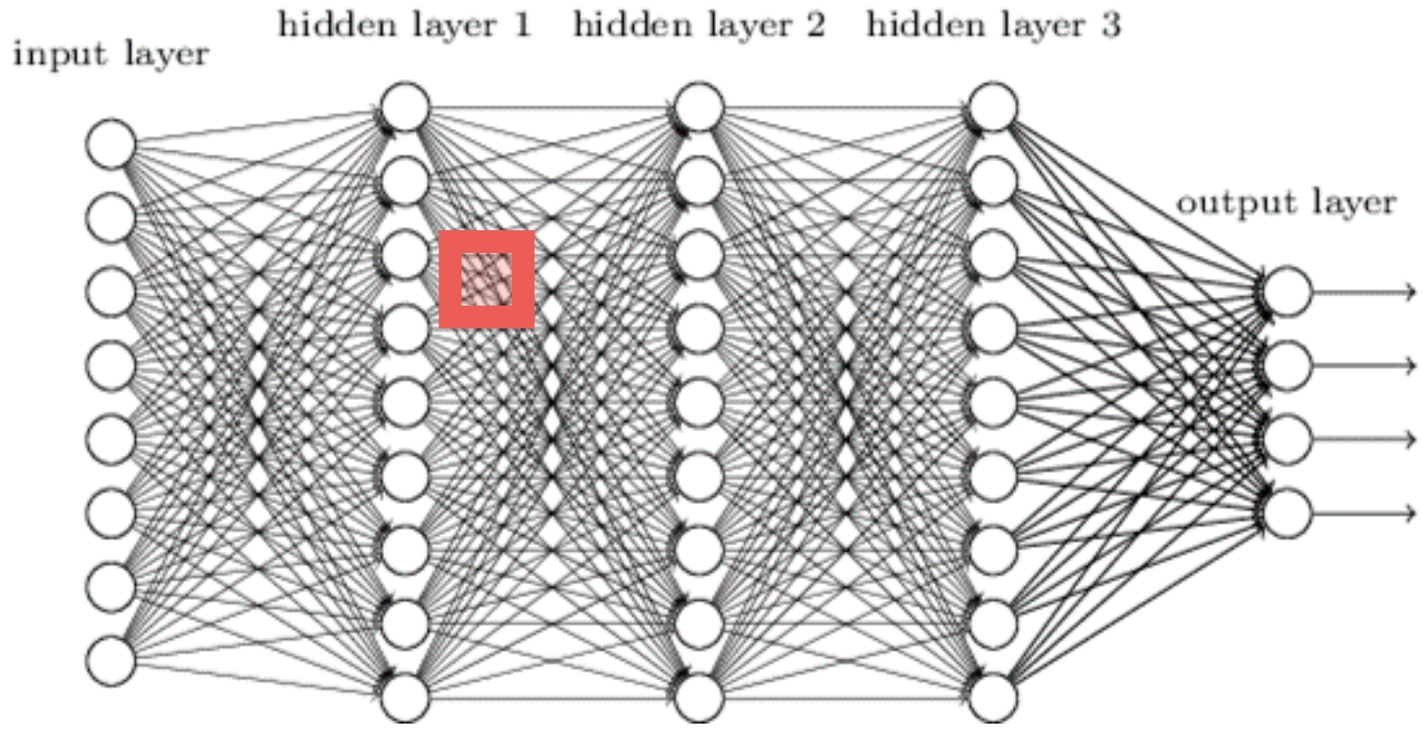
What prior beliefs do I have about the 341st weight?

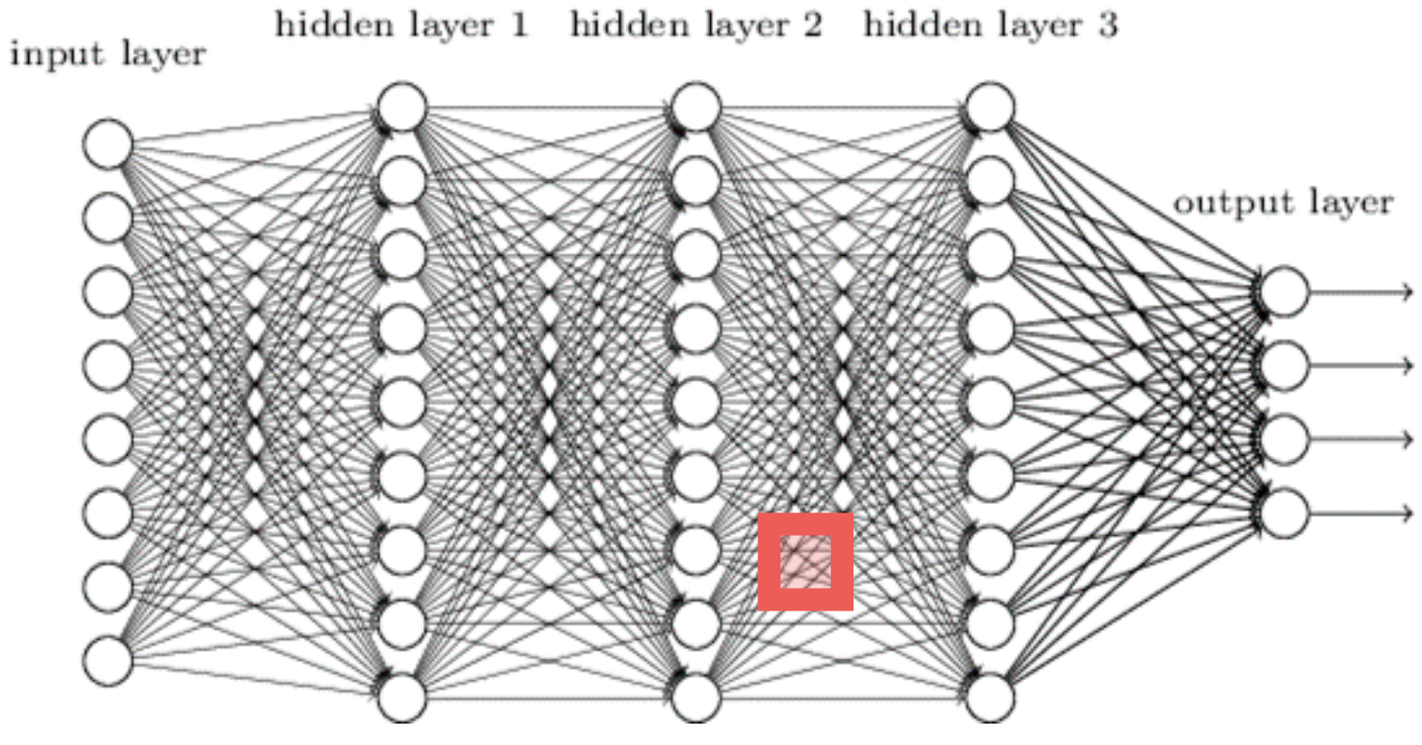


Objective Priors

…But what if we have <u>no</u> information?

Say we are completely agnostic about Θ;
What prior represents a *state of ignorance*?

What prior beliefs do I have about the 833rd weight? etc…



Objective Priors for Coin Tosses

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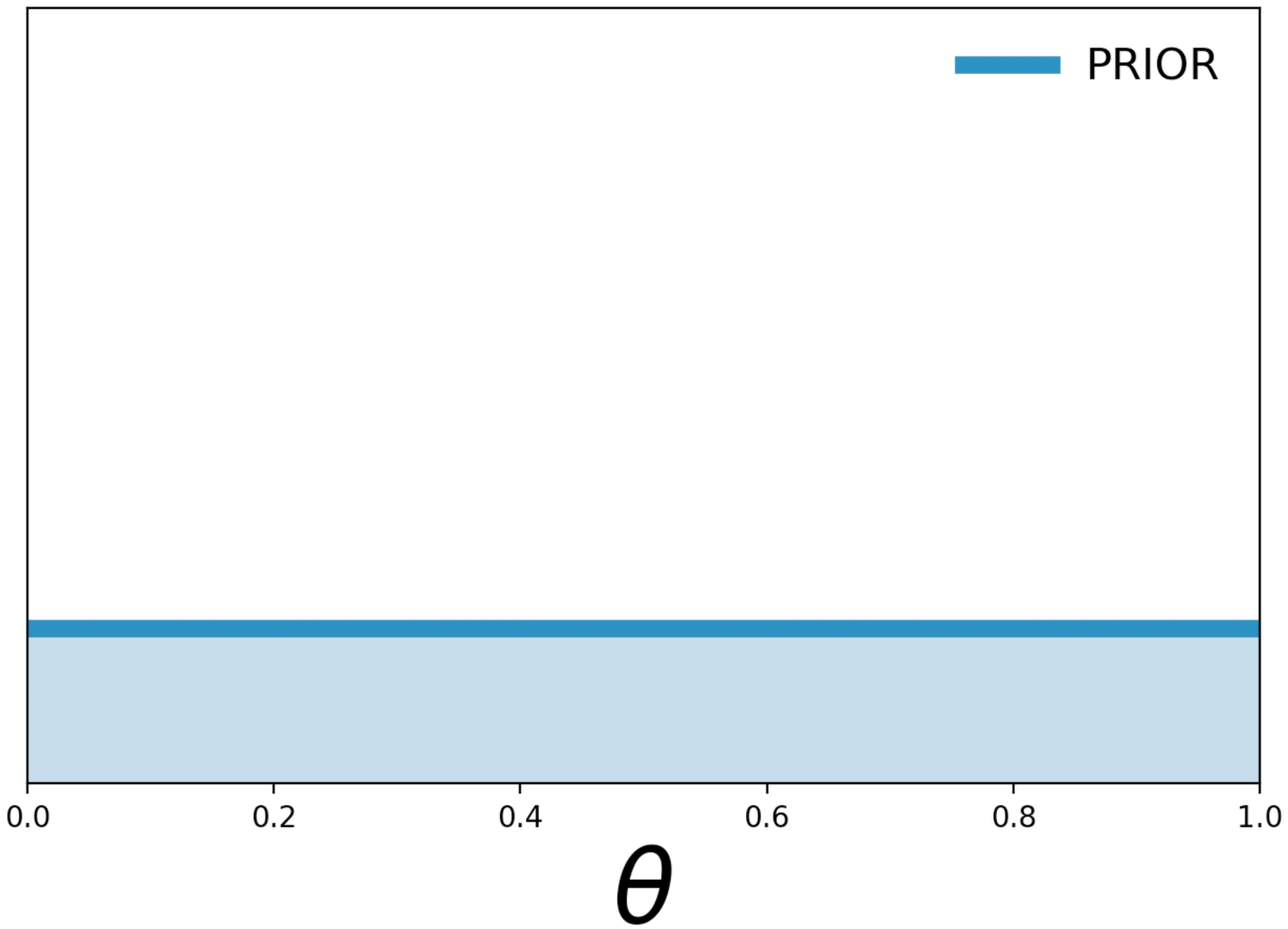
Objective Priors for Coin Tosses

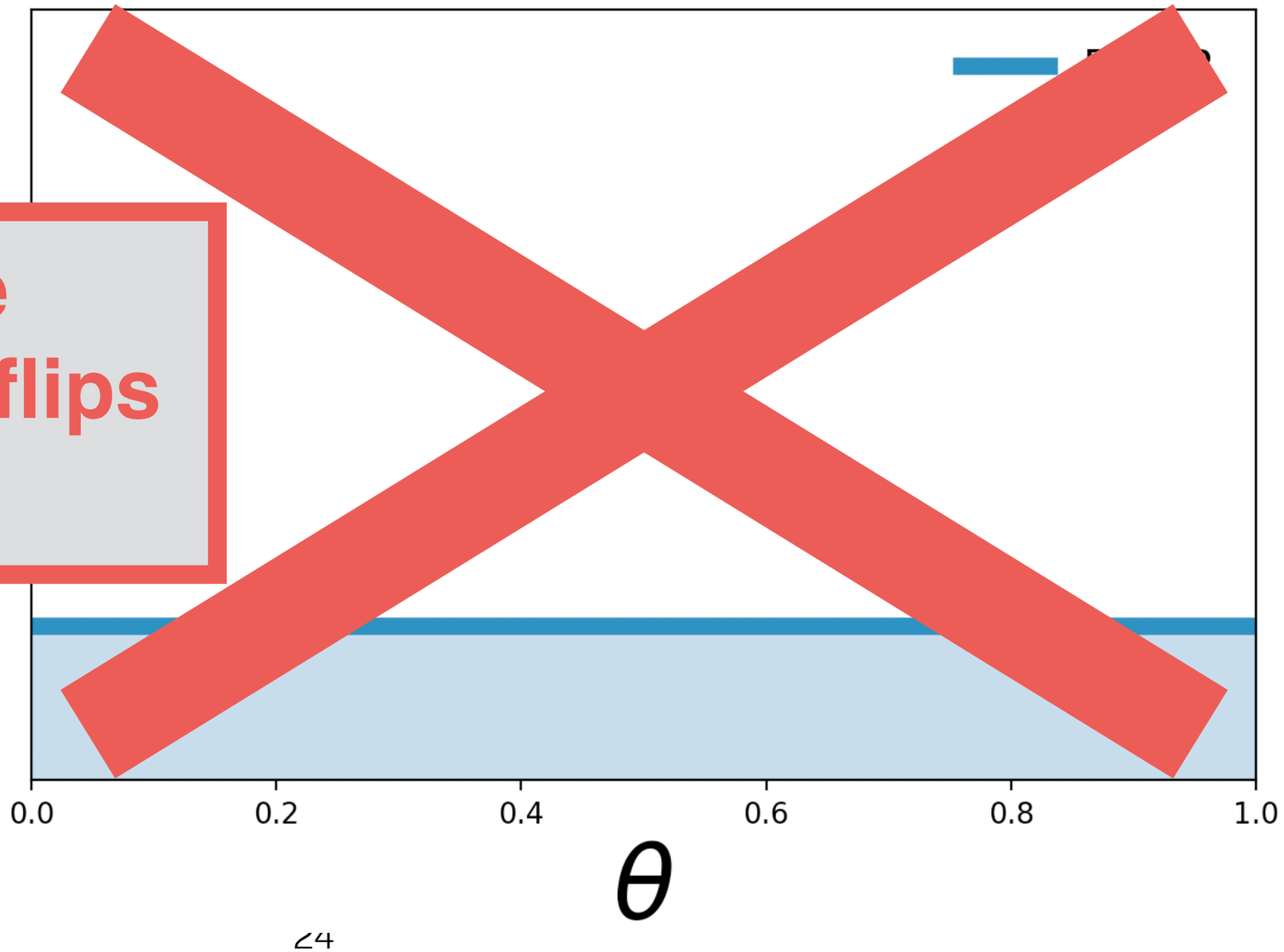
$$p(\theta|\mathbf{X}) \propto \texttt{Binomial}(N, \theta)\ \texttt{Beta}(1, 1)$$



Objective Priors for Coin Tosses

$$p(\theta|\mathbf{X}) \propto \texttt{Binomial}(N, \theta)\ \texttt{Beta}(1, 1)$$

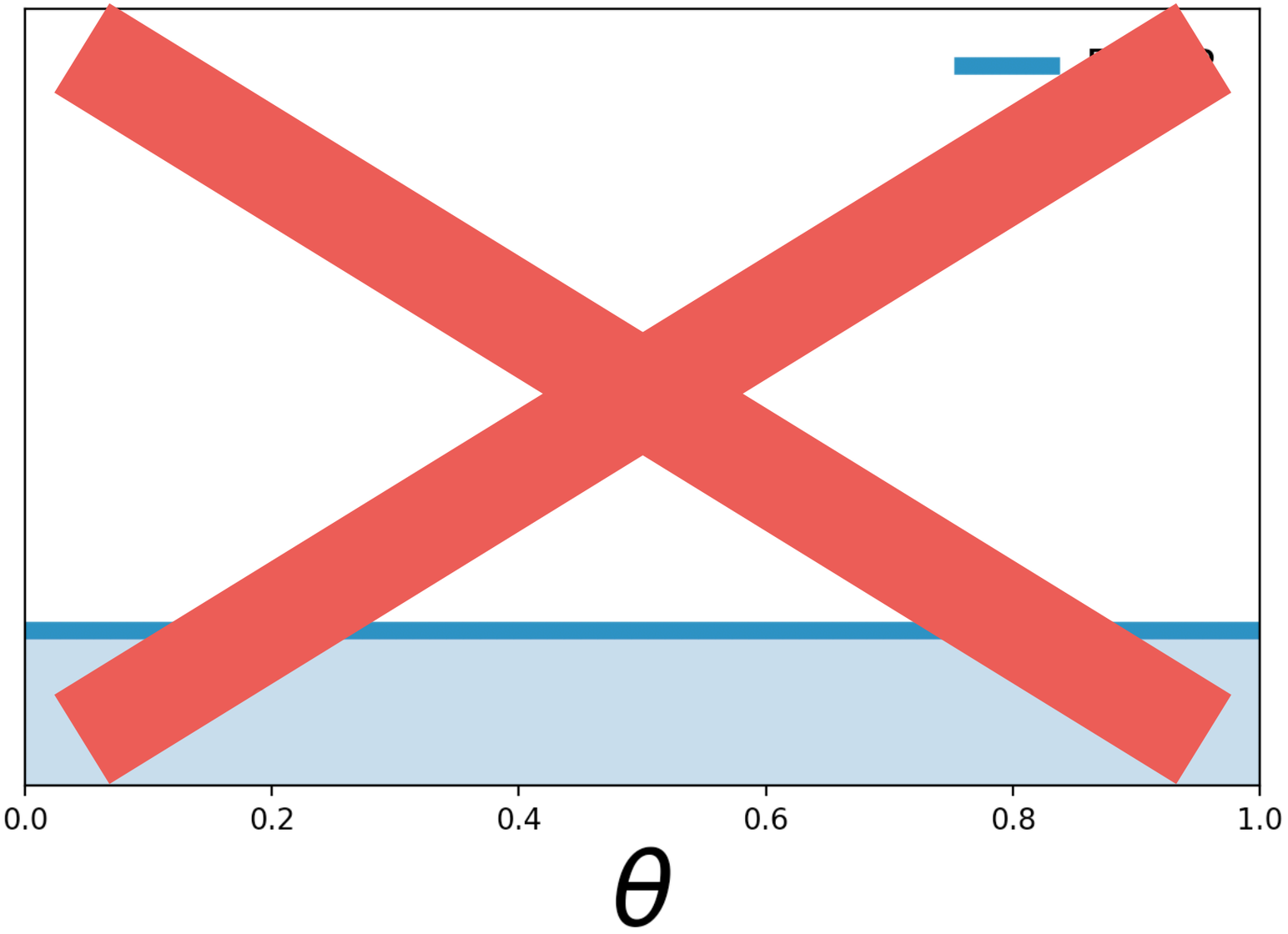
Implies that we've already seen two flips
one heads, one tails.



Objective Priors for Coin Tosses

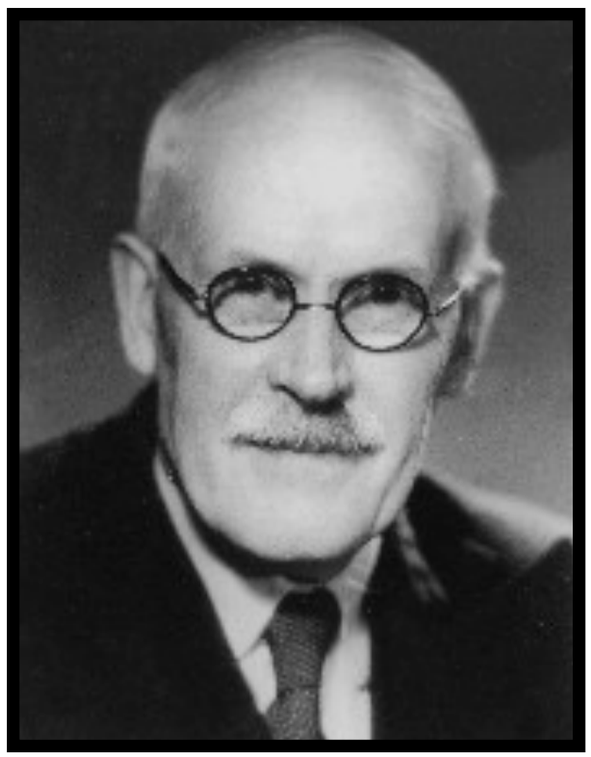
$$p(\theta|\mathbf{X}) \propto \texttt{Binomial}(N, \theta)\ \texttt{Beta}(1, 1)$$

Pierre-Simon Laplace
(1814)

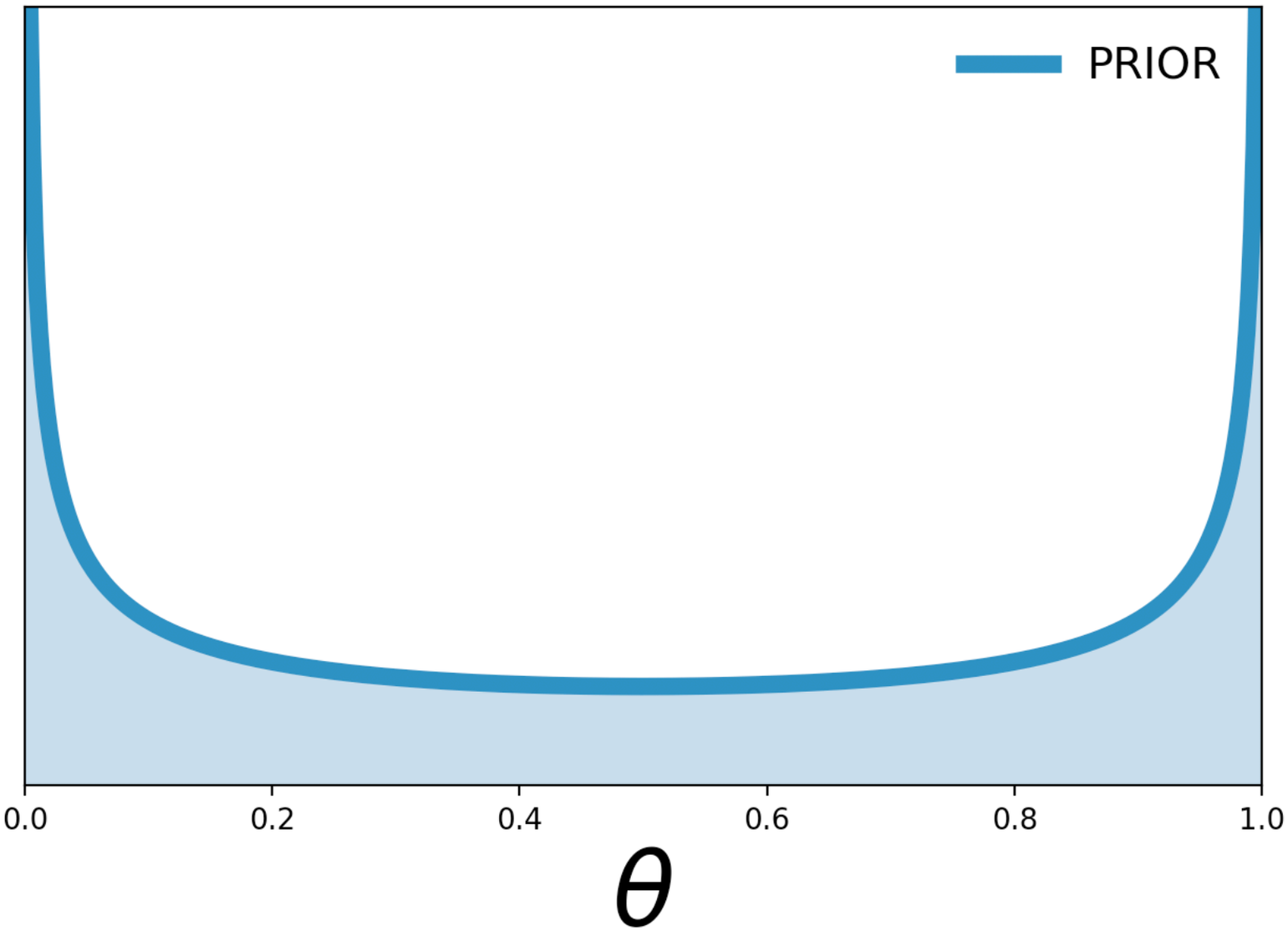


Objective Priors for Coin Tosses

$$p(\theta|\mathbf{X}) \propto \texttt{Binomial}(N, \theta)\, \texttt{Beta}(0.5, 0.5)$$



Sir Harold Jeffreys
(1946)



Objective Priors

[Bernardo, 1979]

$$p^*(\boldsymbol{\theta}) = \underset{p(\boldsymbol{\theta})}{\operatorname{argmax}}\ \mathbb{I}[\boldsymbol{\theta}, \mathbf{X}]$$

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$$= \underset{p(\boldsymbol{\theta})}{\operatorname{argmax}} \int_{\mathbf{X}} p(\mathbf{X})\ \mathrm{KLD}[p(\boldsymbol{\theta}|\mathbf{X})||p(\boldsymbol{\theta})]\ d\mathbf{X}$$

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Maximize **divergence between posterior and prior**

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Averaged over marginal likelihood

Maximize **divergence between posterior and prior**

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More Examples

$$p(\theta) \propto 1$$

Gaussian Mean

$$p(\theta) \propto \frac{1}{\sigma}$$

Gaussian Scale

$$p(\theta) \propto \frac{1}{\sqrt{\lambda}}$$

Poisson Rate

Objective Priors

[Bernardo, 1979]

$$p^*(\boldsymbol{\theta}) = \underset{p(\boldsymbol{\theta})}{\operatorname{argmax}}\ \mathbb{I}[\boldsymbol{\theta}, \mathbf{X}]$$

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Properties

- ☐ **Invariant** to model reparametrization.
- ☐ **Credible intervals** nearly match **confidence intervals**.*

* Under certain conditions

Objective Priors

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Problems / Obstacles

- [ ]
- [ ]

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Problems / Obstacles

- [ ] **Calculus of variations problem:** Solve for function
- [ ]

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Problems / Obstacles

- [ ] **Calculus of variations problem:** Solve for function
- [ ] **Need posterior in closed-form**

CONTRIBUTION

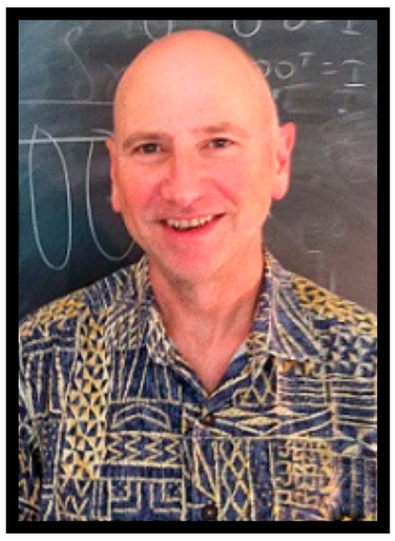
Approximating Objective Priors

Can we approximate objective priors so as to expand their use in machine learning?

Previous Work

Markov Chain Monte Carlo [Lafferty & Wasserman, 2001]**:**
Use MCMC to draw samples from the objective prior.

$$p^*(\theta) \approx \frac{1}{S} \sum_{s=1}^{S} \delta[\hat{\theta}_s]$$



Iterative Markov Chain Monte Carlo Computation of Reference Priors and Minimax Risk

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John Lafferty Larry Wasserman

UAI 2001

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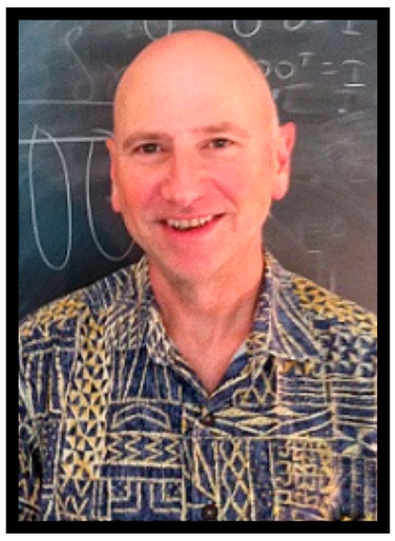
Use MCMC to draw samples from the objective prior.

$$p^*(\theta) \approx \frac{1}{S} \sum_{s=1}^{S} \delta[\hat{\theta}_s]$$

Drawback: Have to perform a second modeling step in order to evaluate the prior's density.



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UAI 2001

A Parametric Approach

We propose optimizing a **parametric approximation**.

$$p^*(\theta) \approx p(\theta; \underline{\lambda}^*)$$

Optimize w.r.t. $\boldsymbol{\lambda}$ instead of function itself.

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$$p^*(\theta) \approx p(\theta; \underline{\lambda^*})$$

Optimize w.r.t. $\boldsymbol{\lambda}$ instead of function itself.

Objective is a **lower bound** on the mutual information.

$$\mathbb{I}[\boldsymbol{\theta}, \mathbf{X}] \geq \mathbb{E}_{\boldsymbol{\theta}_{\boldsymbol{\lambda}}, \mathbf{X}} \left[\log p(\mathbf{X}|\boldsymbol{\theta}) \; - \; \max_{\boldsymbol{\theta}_{\boldsymbol{\lambda}}} \; \log p(\mathbf{X}|\boldsymbol{\theta}) \right]$$

$$\approx \frac{1}{S} \sum_{s=1}^{S} \mathrm{KLD} \left[p(\mathbf{X}|\hat{\boldsymbol{\theta}}_s) \; || \; p(\mathbf{X}|\hat{\boldsymbol{\theta}}_{\max}) \right]$$

Samples depend on $\boldsymbol{\lambda}$.

A Parametric Approach

BENEFITS

A Parametric Approach

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- **Comparison to Lafferty & Wasserman's [2001] MCMC**: No need to perform a second modeling step to evaluate the prior.

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Gaussian mean:

$$p^*(\boldsymbol{\mu}) \propto 1$$

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Parametric Approximation:

$$\mathrm{N}(\boldsymbol{\mu}_\lambda, \boldsymbol{\sigma}_\lambda)$$

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Gaussian mean:	**Parametric Approximation**:	**Optimization Objective**:
$p^*(\boldsymbol{\mu}) \propto 1$	$\mathrm{N}(\boldsymbol{\mu}_\lambda, \boldsymbol{\sigma}_\lambda)$	$\mathcal{J}(\boldsymbol{\lambda}) = \|\|\boldsymbol{\sigma}_\lambda\|\|_2^2$

A Parametric Approach

BENEFITS

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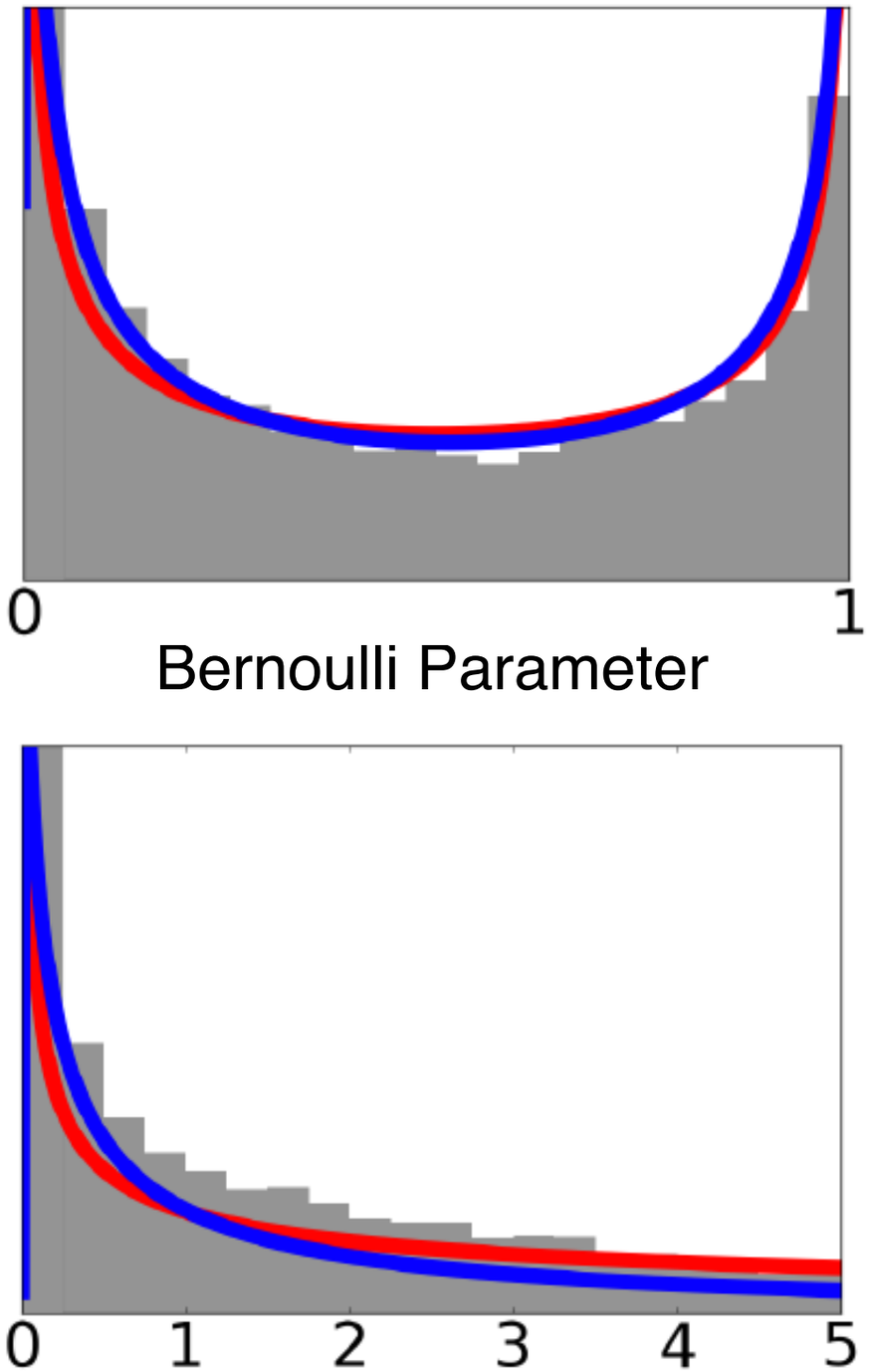
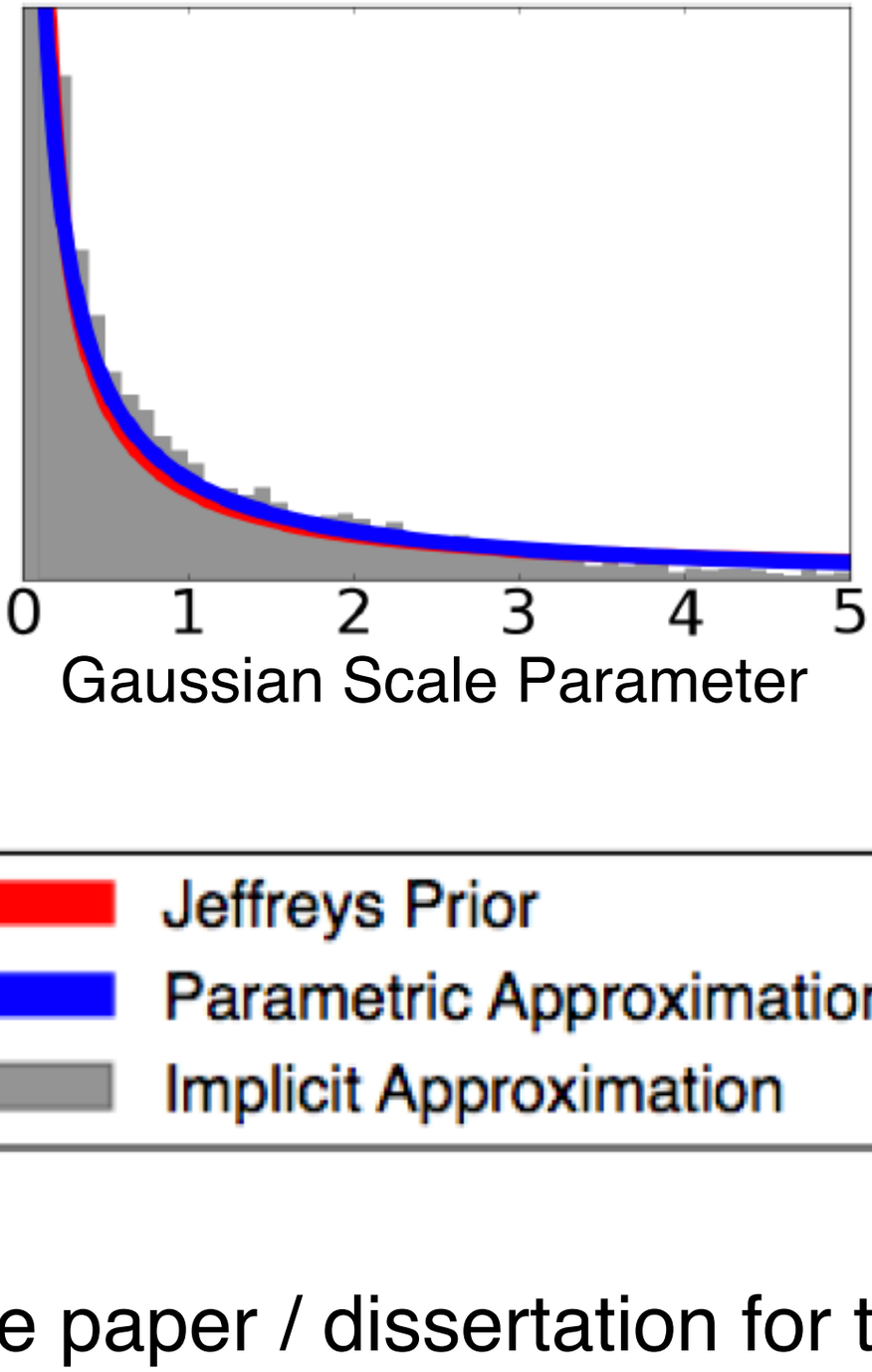
$p^*(\boldsymbol{\mu}) \propto 1$	$\mathrm{N}(\boldsymbol{\mu}_\lambda, \boldsymbol{\sigma}_\lambda)$	$\mathcal{J}(\boldsymbol{\lambda}) = \|\|\boldsymbol{\sigma}_\lambda\|\|_2^2$

RESULT: $p^* \propto 1 \approx \mathrm{N}(\cdot, \infty)$

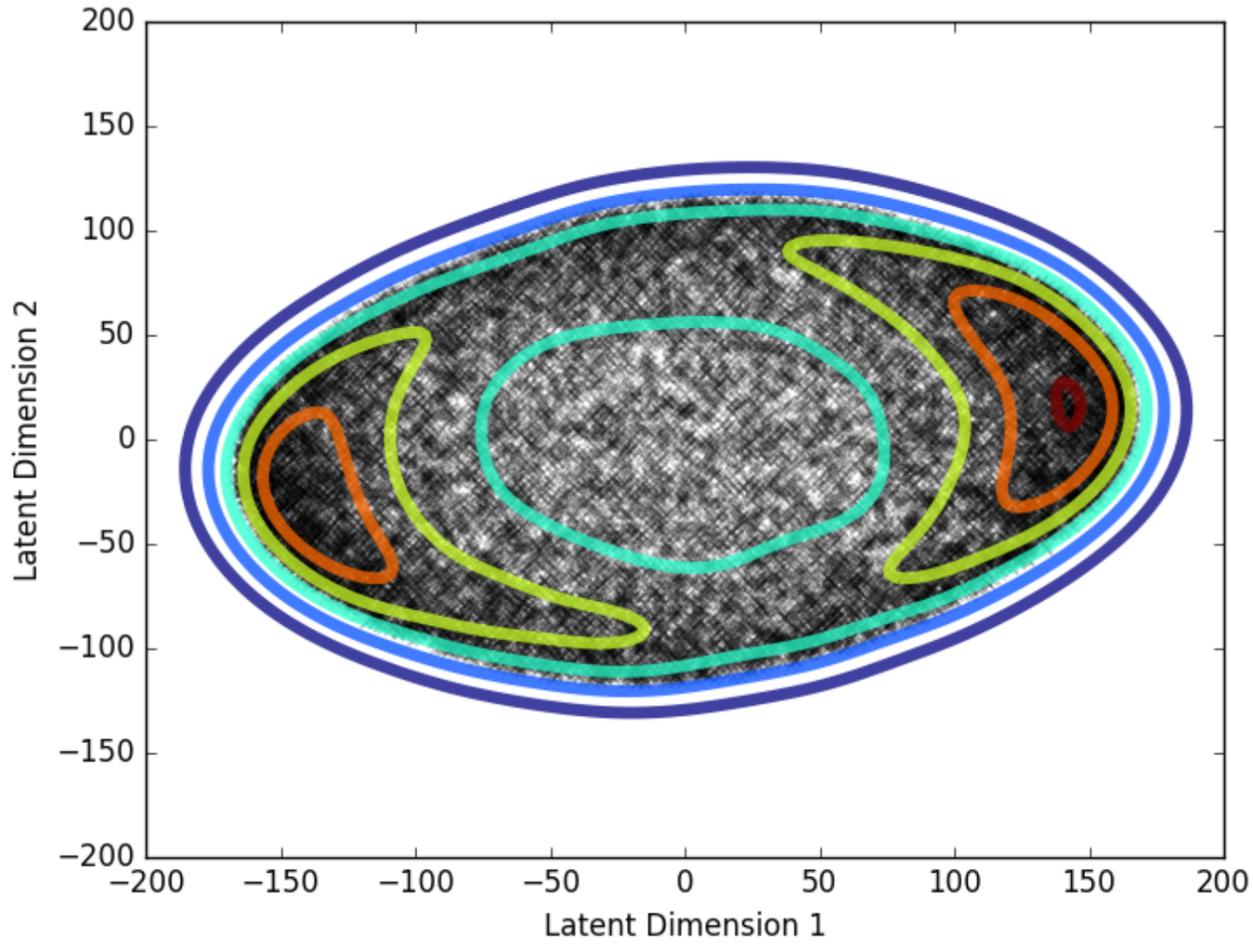
Recovering Jeffreys Priors





See paper / dissertation for two-sample tests comparing approximation methods.

Finding the Variational Autoencoder's Objective Prior



p(**z**)

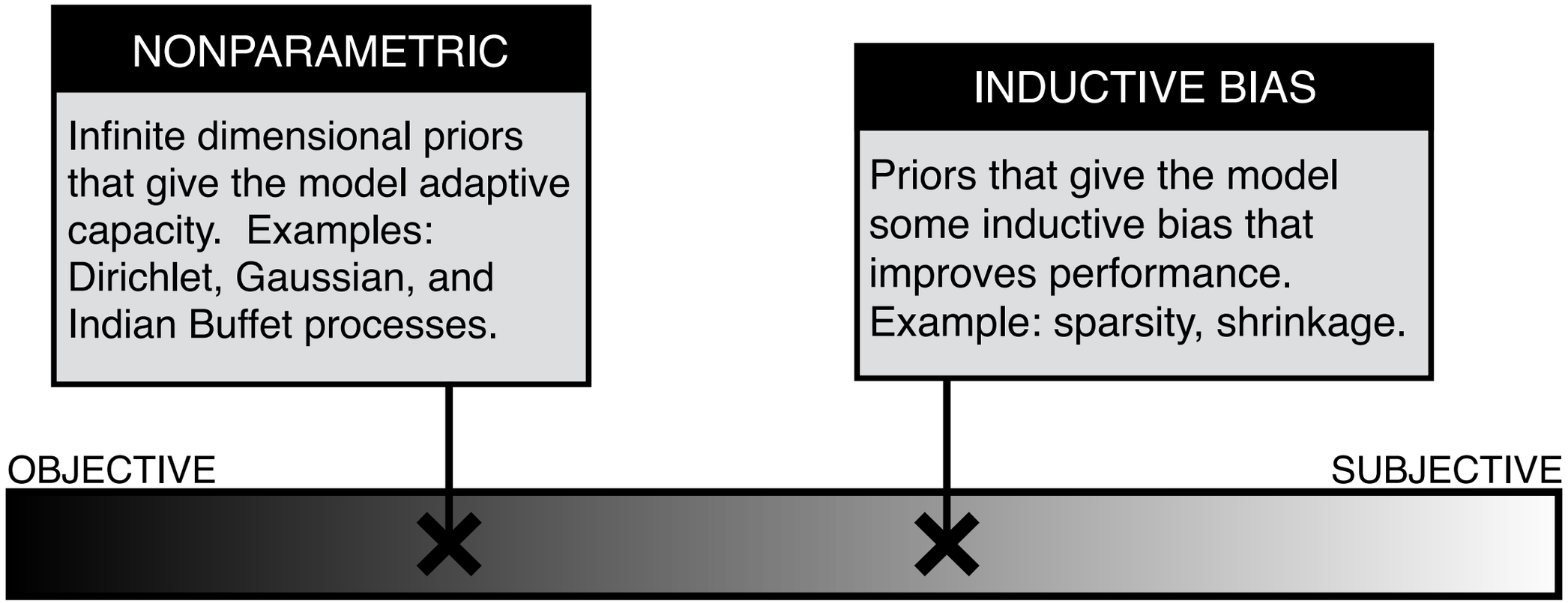
Conclusions

Priors for Machine Learning

A SPECTRUM OF PRIORS

Priors for Machine Learning

A SPECTRUM OF PRIORS



Priors for Machine Learning

A SPECTRUM OF PRIORS

NONPARAMETRIC

Infinite dimensional priors that give the model adaptive capacity. Examples: Dirichlet, Gaussian, and Indian Buffet processes.

INDUCTIVE BIAS

Priors that give the model some inductive bias that improves performance. Example: sparsity, shrinkage.

OBJECTIVE

SUBJECTIVE

SUBJECTIVE

Priors determined by intuition, previous experiments, or expert knowledge.

Priors for Machine Learning

A SPECTRUM OF PRIORS

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OBJECTIVE ← → SUBJECTIVE

Published as a conference paper at ICLR 2019

FUNCTIONAL VARIATIONAL BAYESIAN NEURAL NETWORKS

Shengyang Sun*†, **Guodong Zhang***†, **Jiaxin Shi***‡, **Roger Grosse**†
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SUBJECTIVE

Priors determined by intuition, previous experiments, or expert knowledge.

Priors for Machine Learning

A SPECTRUM OF PRIORS

NONPARAMETRIC

Infinite dimensional priors that give the model adaptive capacity. Examples: Dirichlet, Gaussian, and Indian Buffet processes.

INDUCTIVE BIAS

Priors that give the model some inductive bias that improves performance. Example: sparsity, shrinkage.

OBJECTIVE

SUBJECTIVE

THIS TALK

OBJECTIVE

Priors that 'follow the data,' perhaps having frequentist properties. Examples: diffuse, Jeffreys, reference, empirical Bayes.

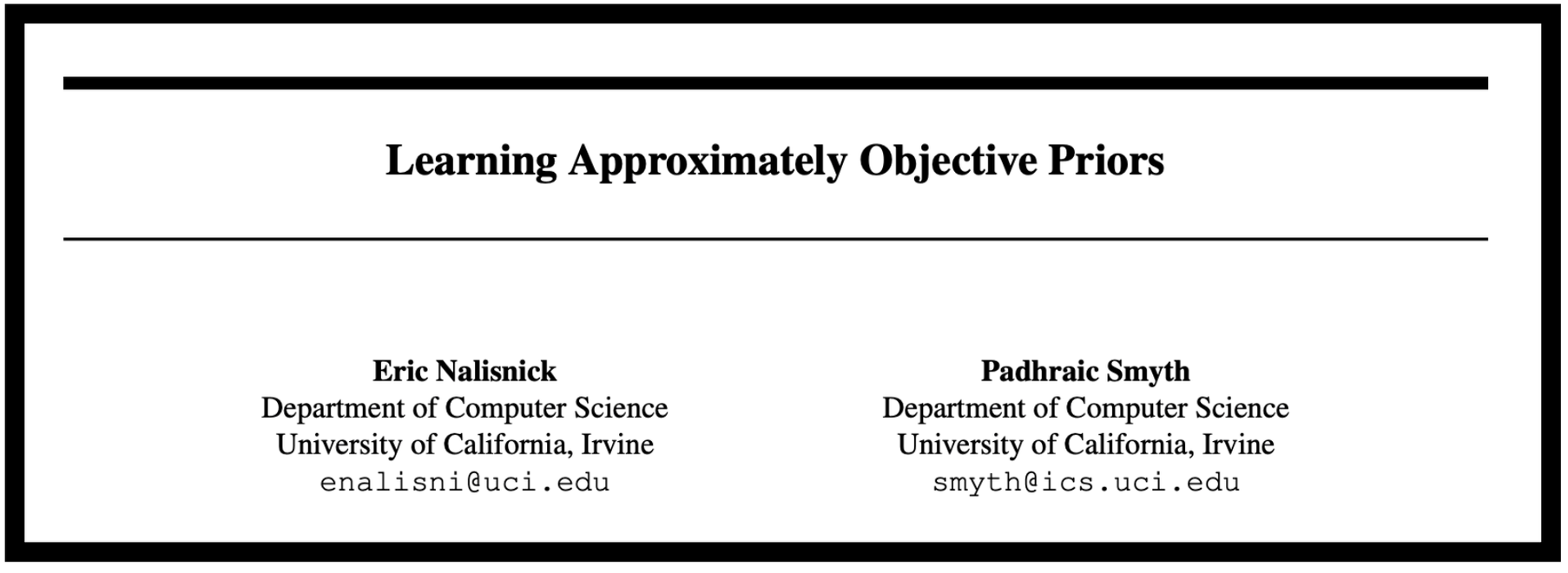
SUBJECTIVE

Priors determined by intuition, previous experiments, or expert knowledge.

Thank you. Questions?

In collaboration with…

Padhraic Smyth



Learning Approximately Objective Priors

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