Uncertainty Quantification for Predictive Models

Eric Nalisnick
University of Amsterdam

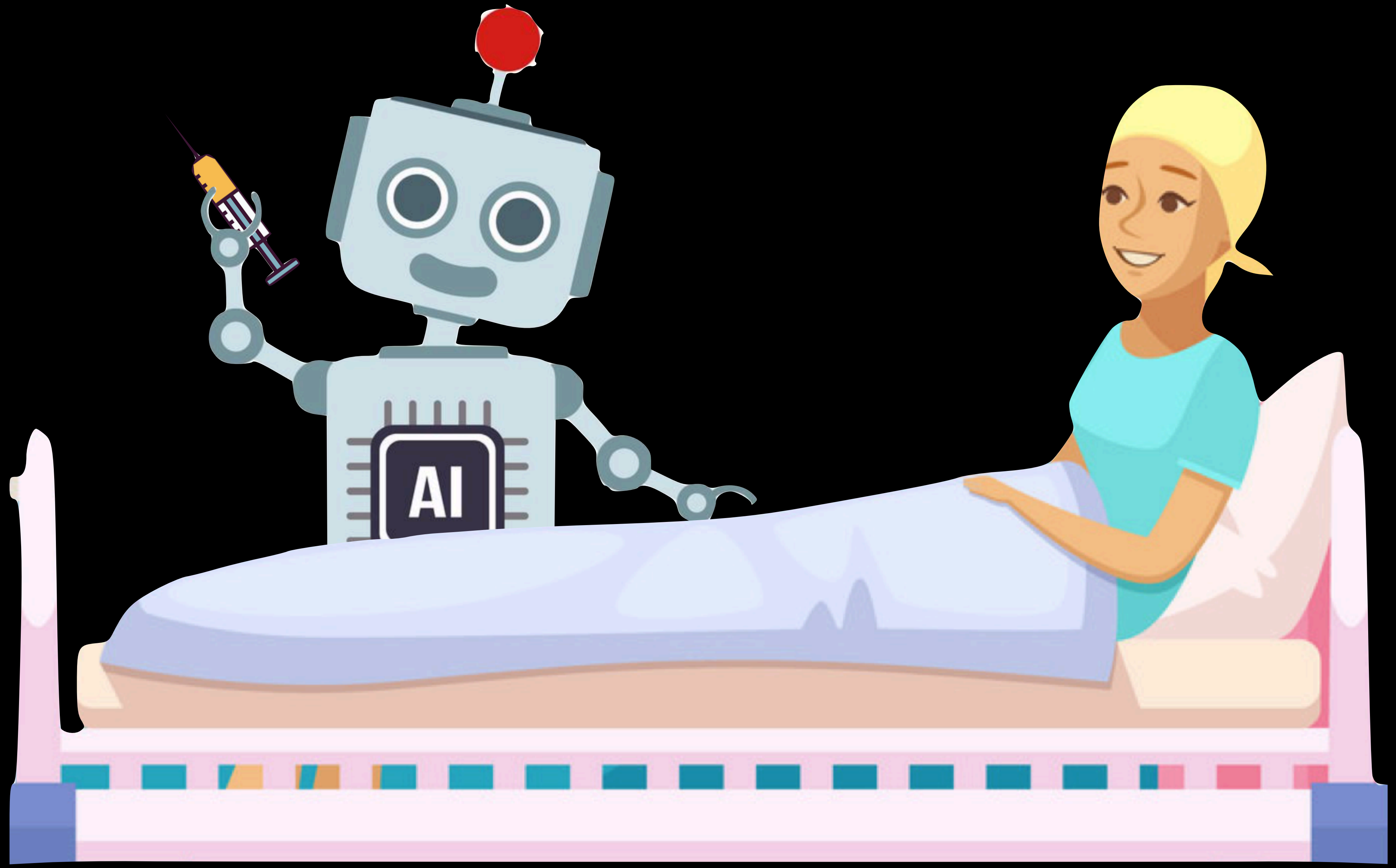
feature
vector

predicted
label

$$f(x) = \hat{y}$$

classifier

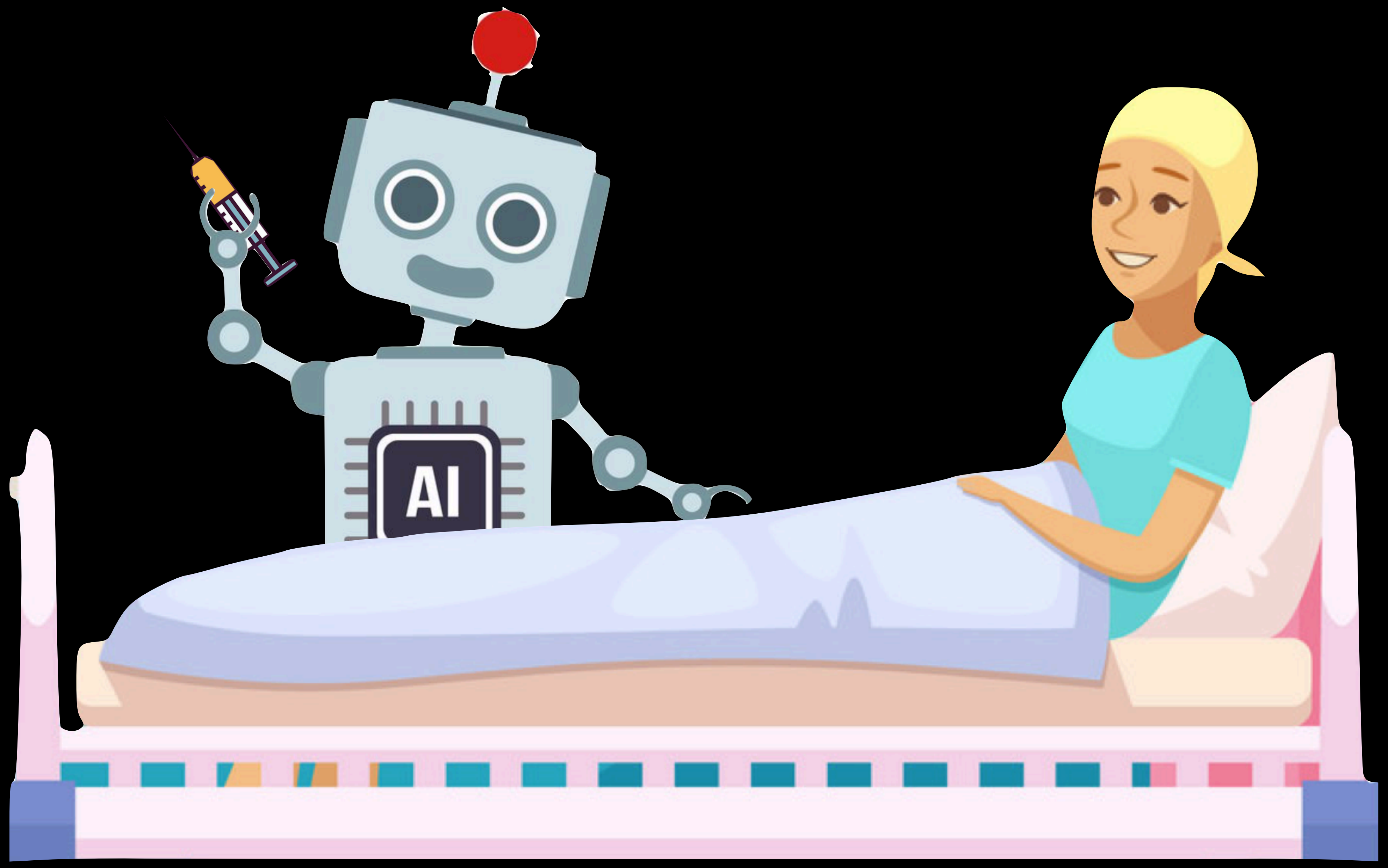
$$f(x) = \hat{y}$$



diagnosis

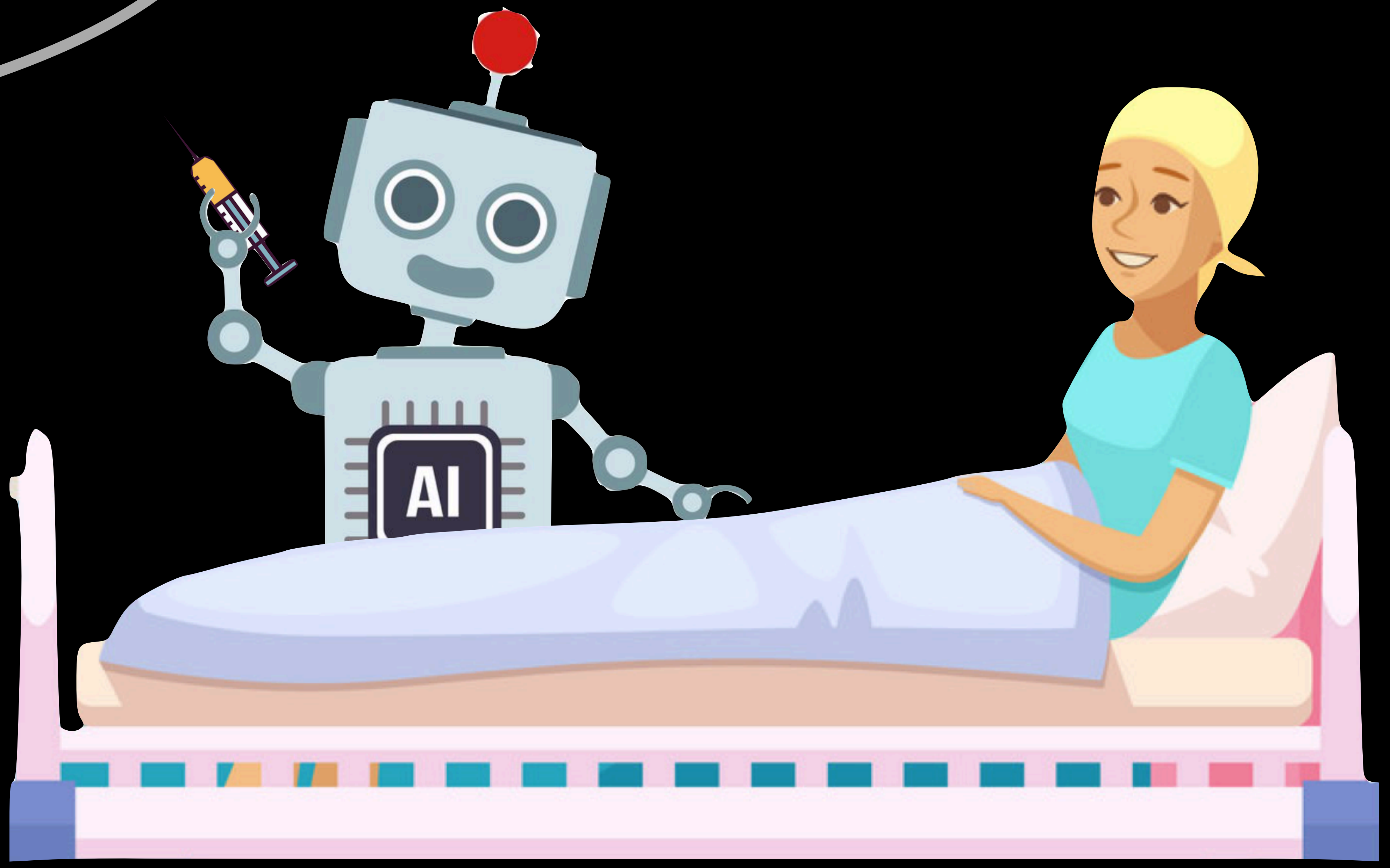
$$f(x) = \hat{y}$$

health measurements



$$f(x) = \hat{y}$$

Wait a minute…How *certain* is the model about its prediction?



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$$f(x) = \hat{y} \quad + \quad ???$$

Wait a minute…How *certain* is the model about its prediction?

$$f(x) = \hat{y} \quad + \quad \mathbb{P}\left(y = \hat{y} \mid x\right)$$

example: *80% confident that the patient has pneumonia*

Wait a minute…How *certain* is the model about its prediction?

$$f(x) = \hat{y} \quad + \quad \mathbb{P}\big(y^* \in \underbrace{C(x)}_{\text{set of labels}}\big) \geq 95\,\%$$

Wait a minute…How *certain* is the model about its prediction?

$$f(x) = \hat{y} \quad + \quad \mathbb{P}\big(y^* \in C(x)\big) \geq 95\,\%$$

example: *95% confident that the patient has pneumonia, tuberculosis, or asthma.*

This talk is about how to know what your model doesn’t know.

I. What is Uncertainty?

Two Types of Uncertainty

- ⊗ Aleatoric
  - fundamental, related to Bayes error rate
  - possibly reduced by collecting more features
- ⊗ Epistemic
  - due to lack of experience / observations
  - always reduced by collecting more data points

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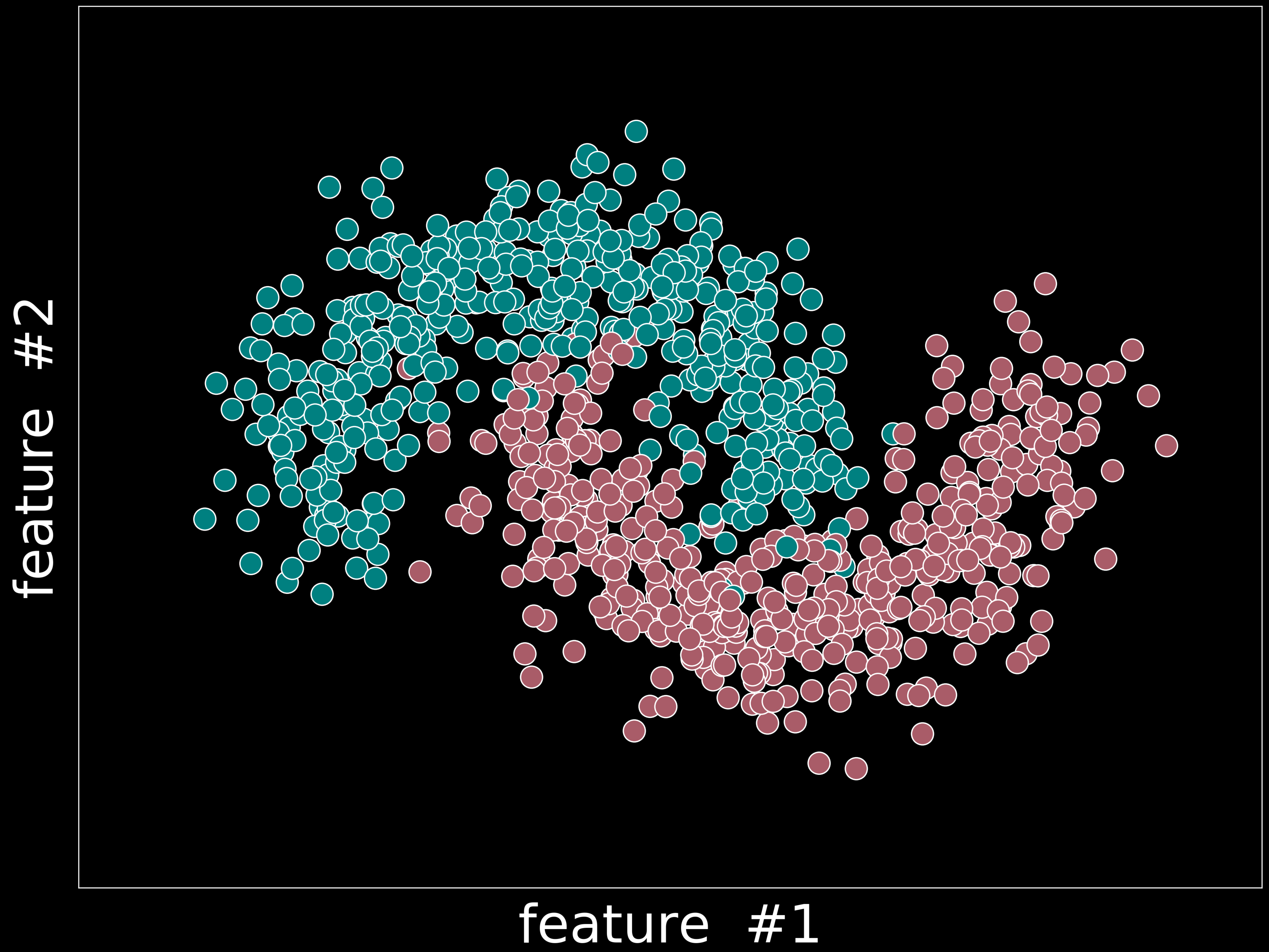
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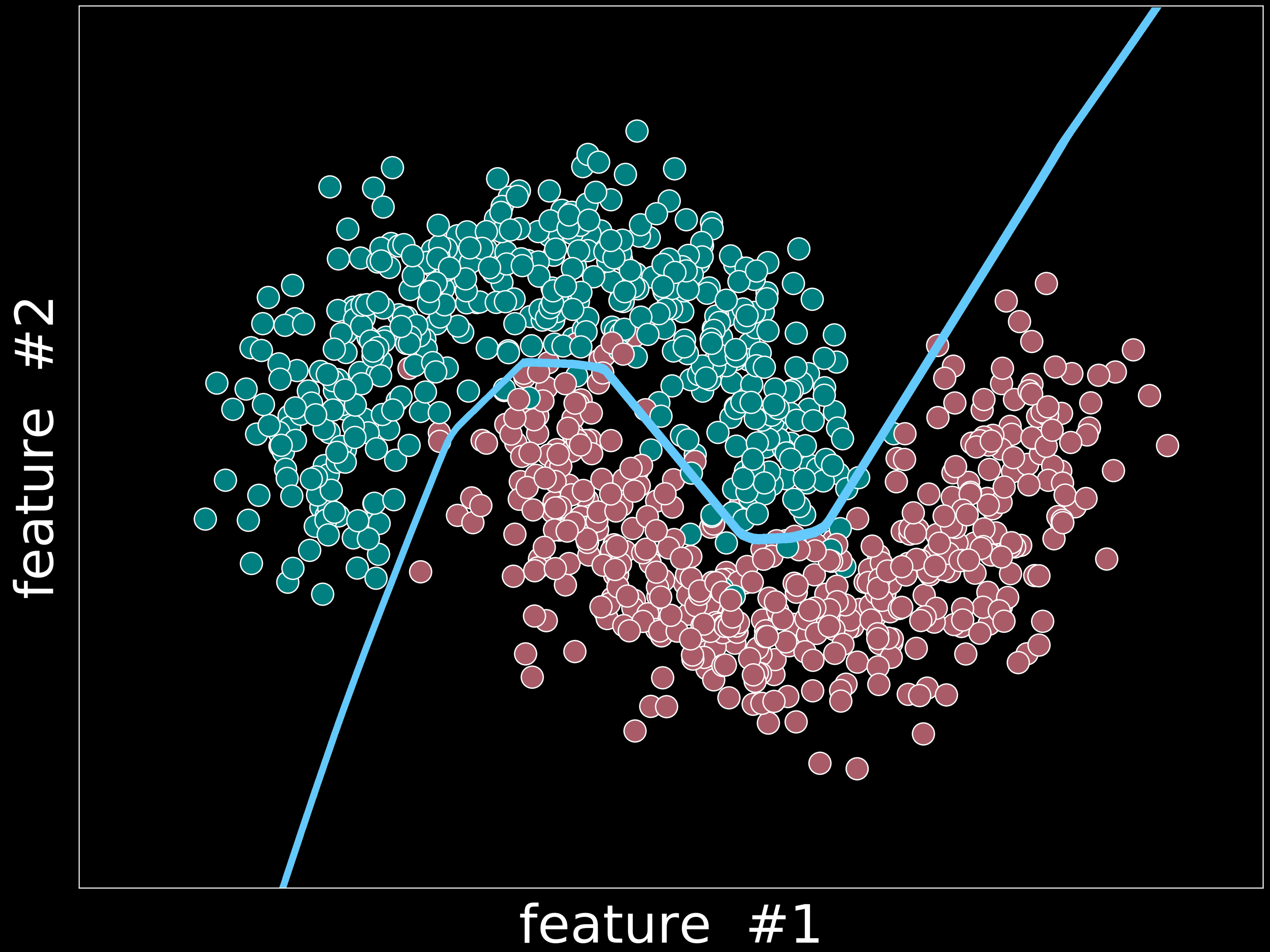
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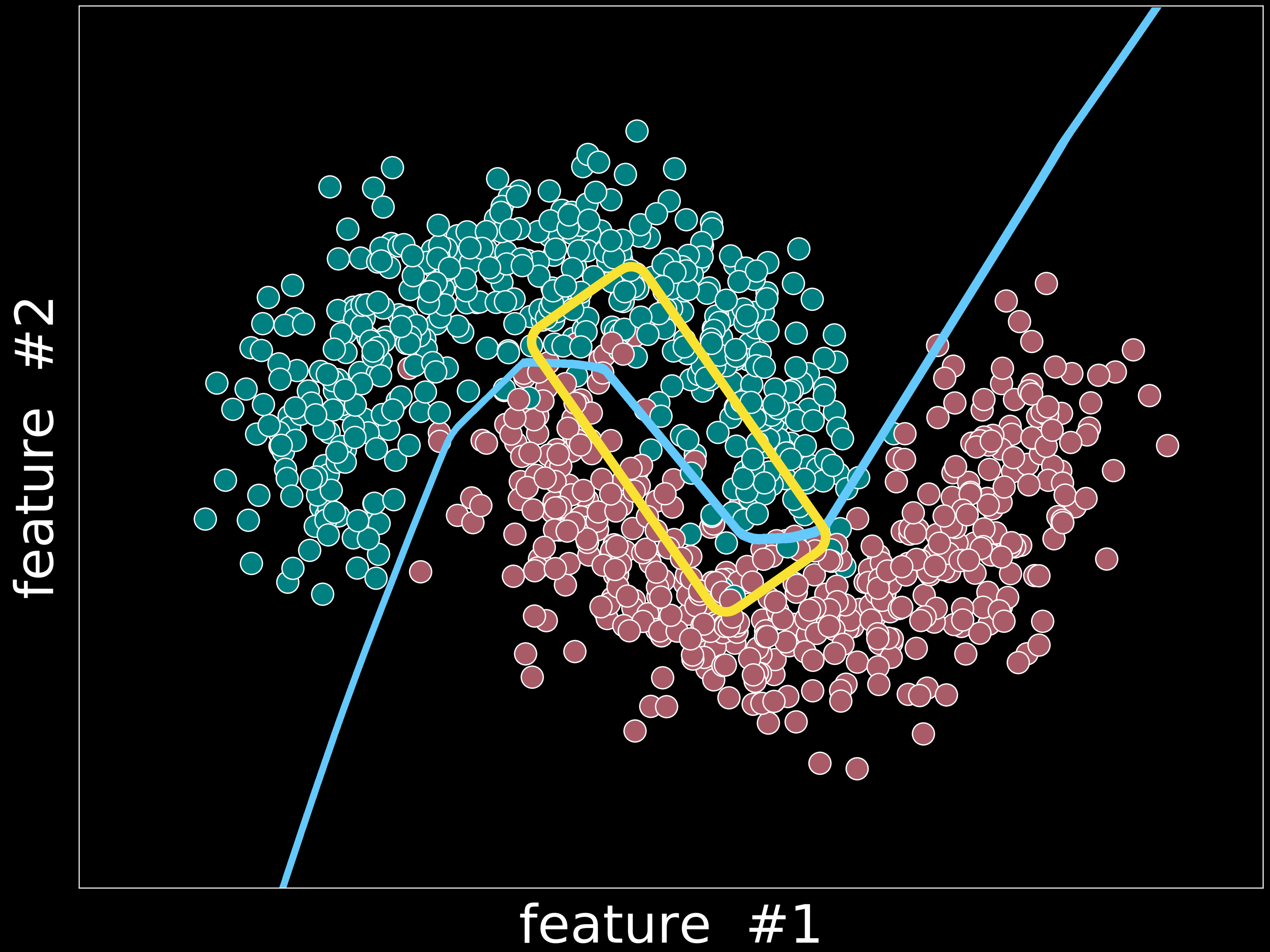
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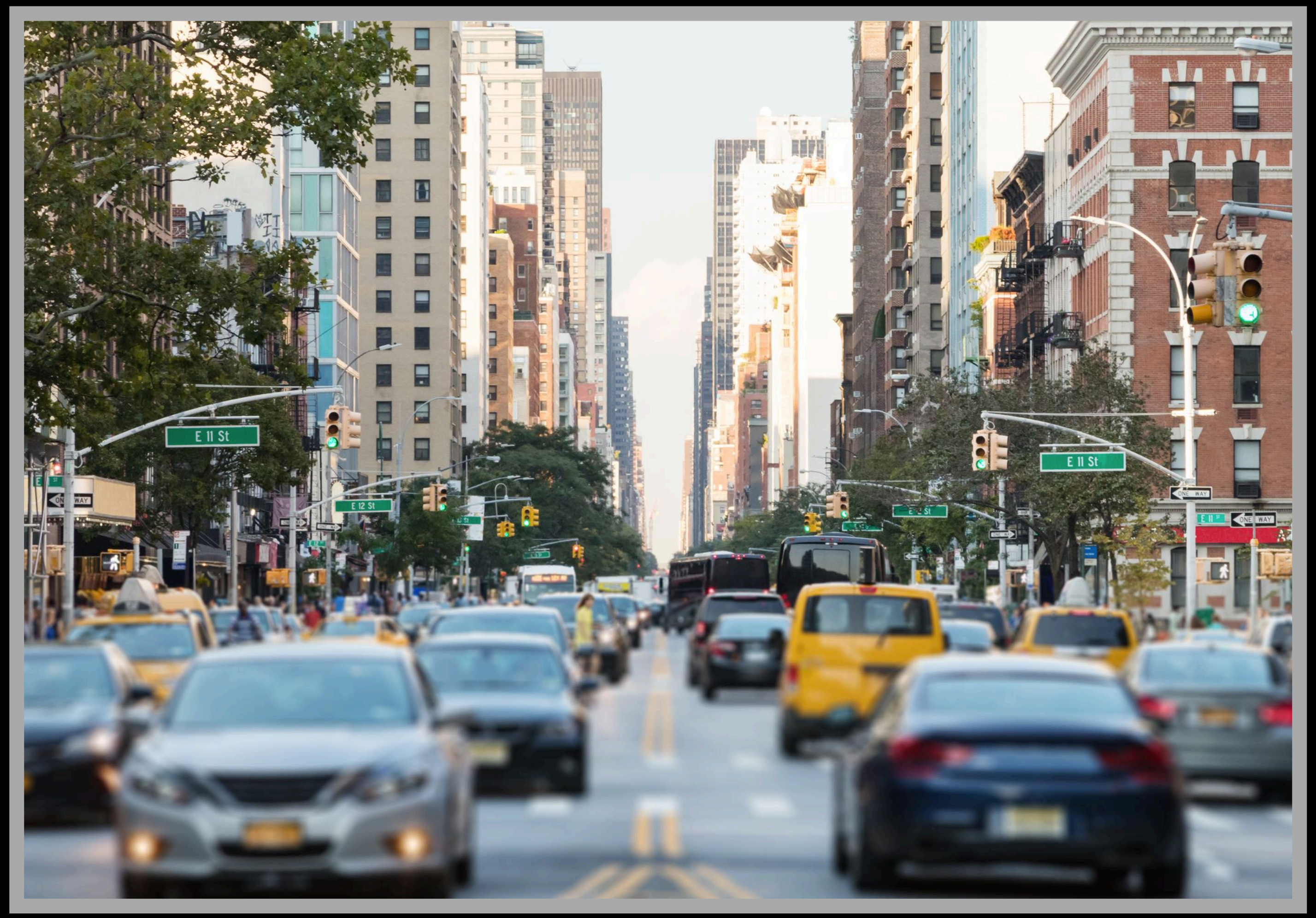
Examples from Autonomous Driving

train in urban environment



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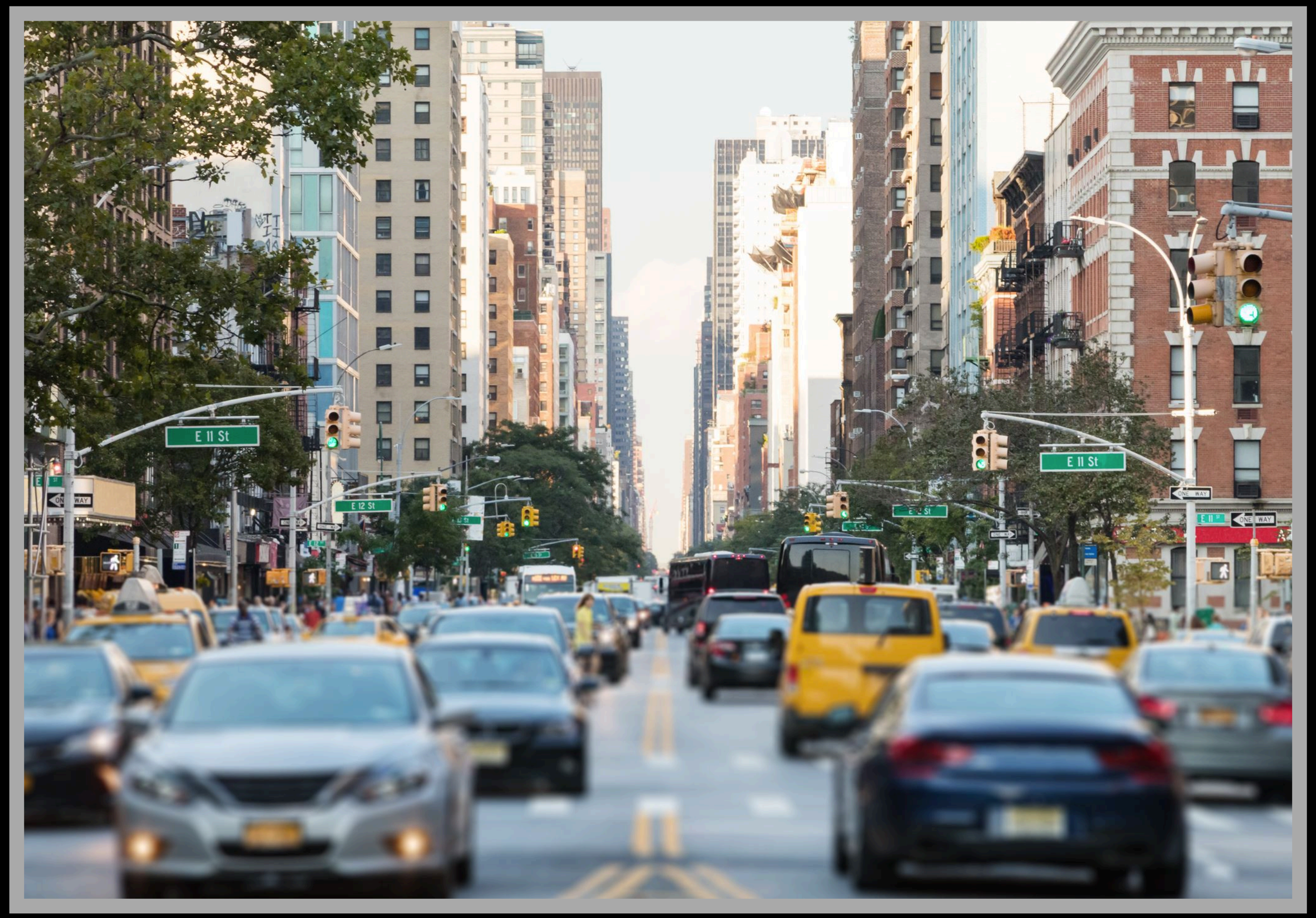

high aleatoric:
avoiding a head-on collision

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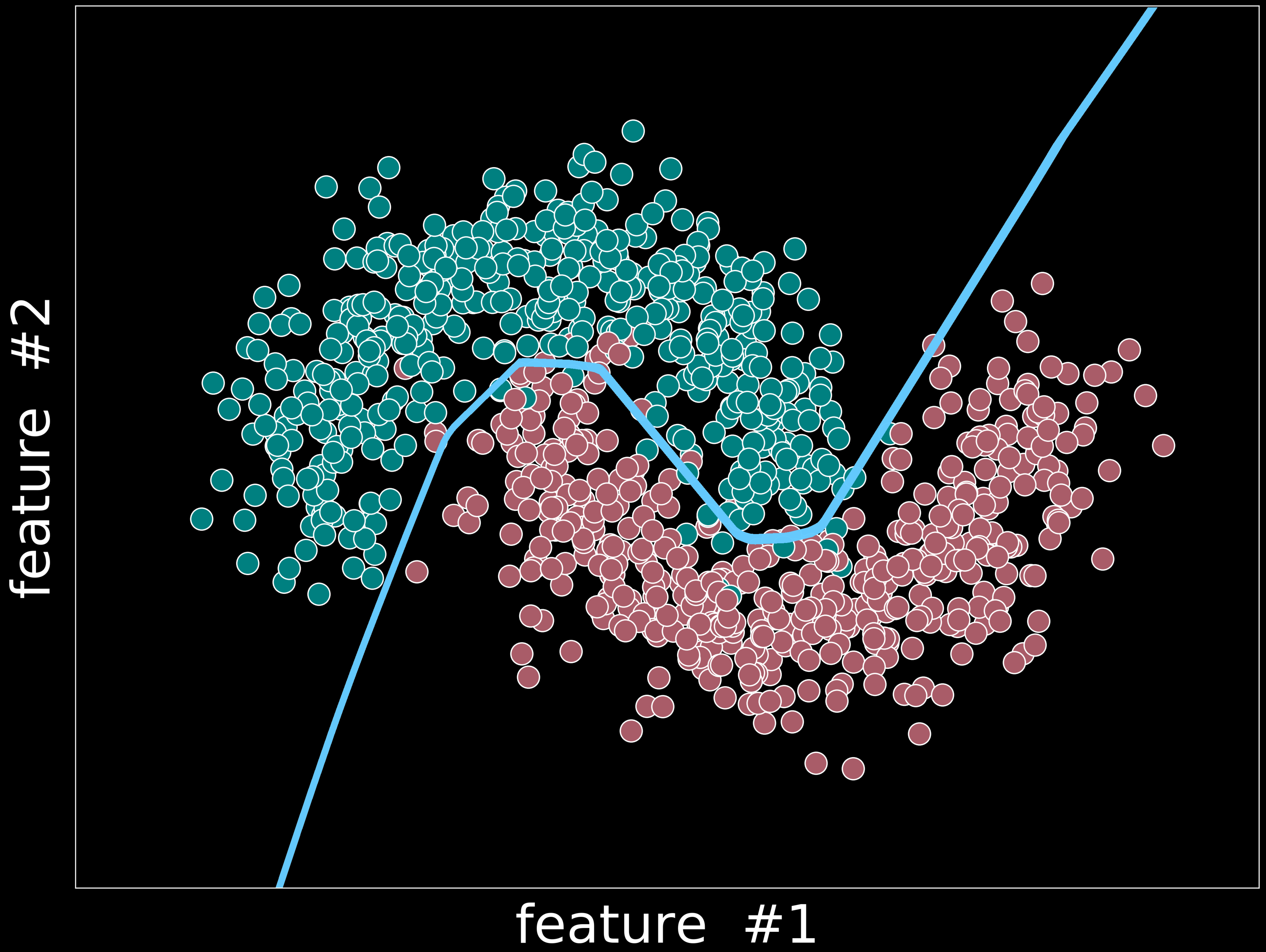
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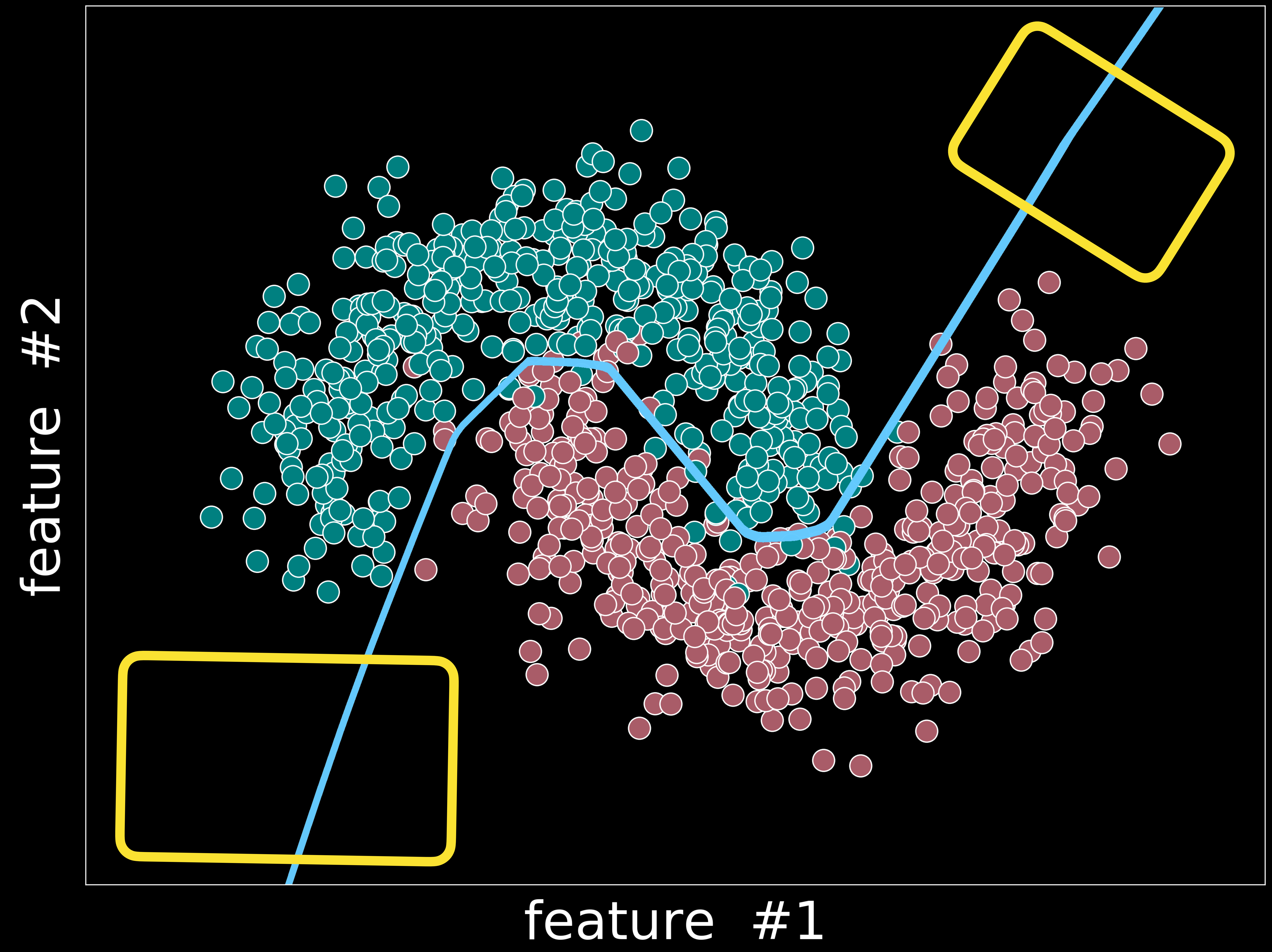
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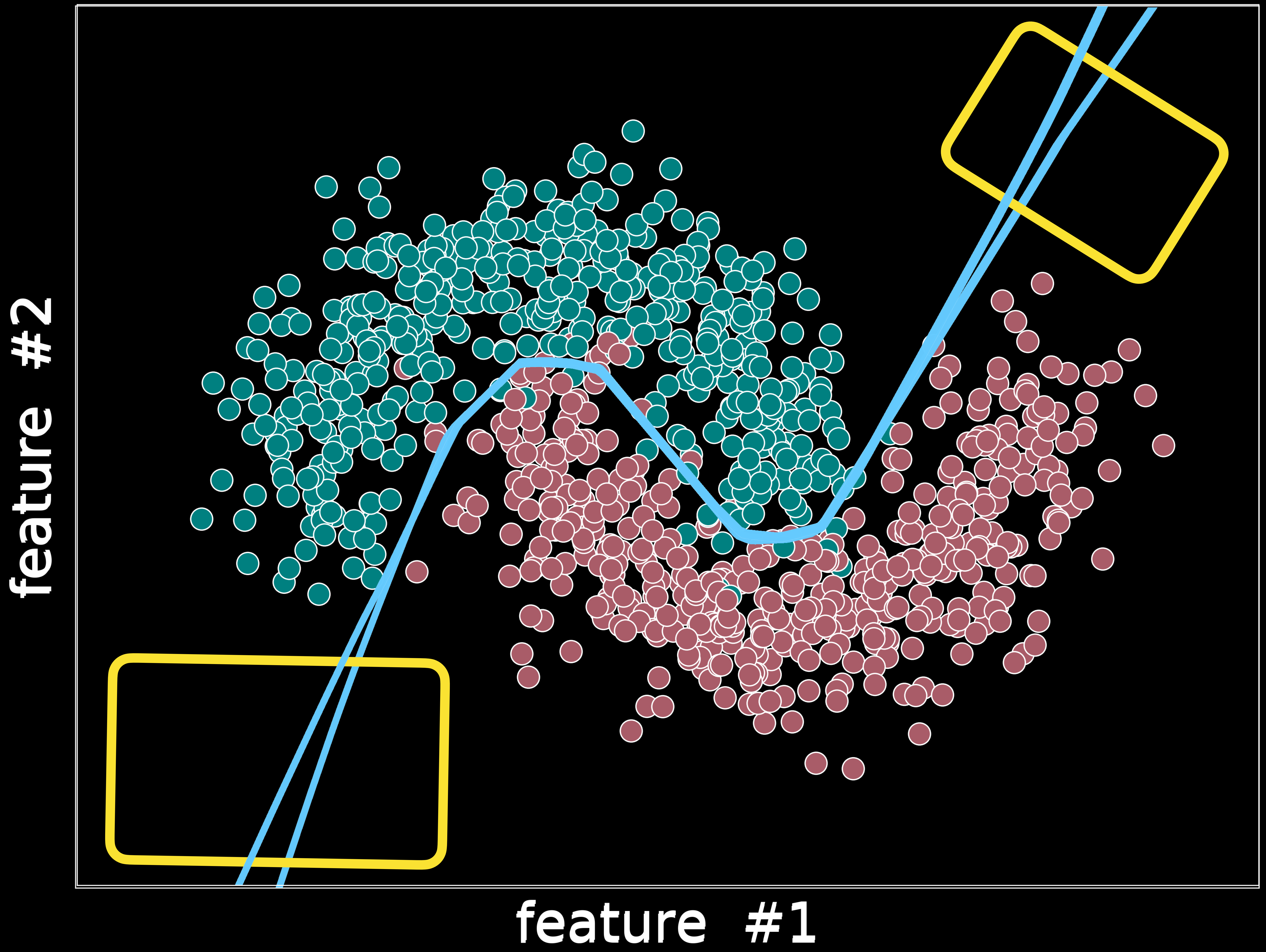
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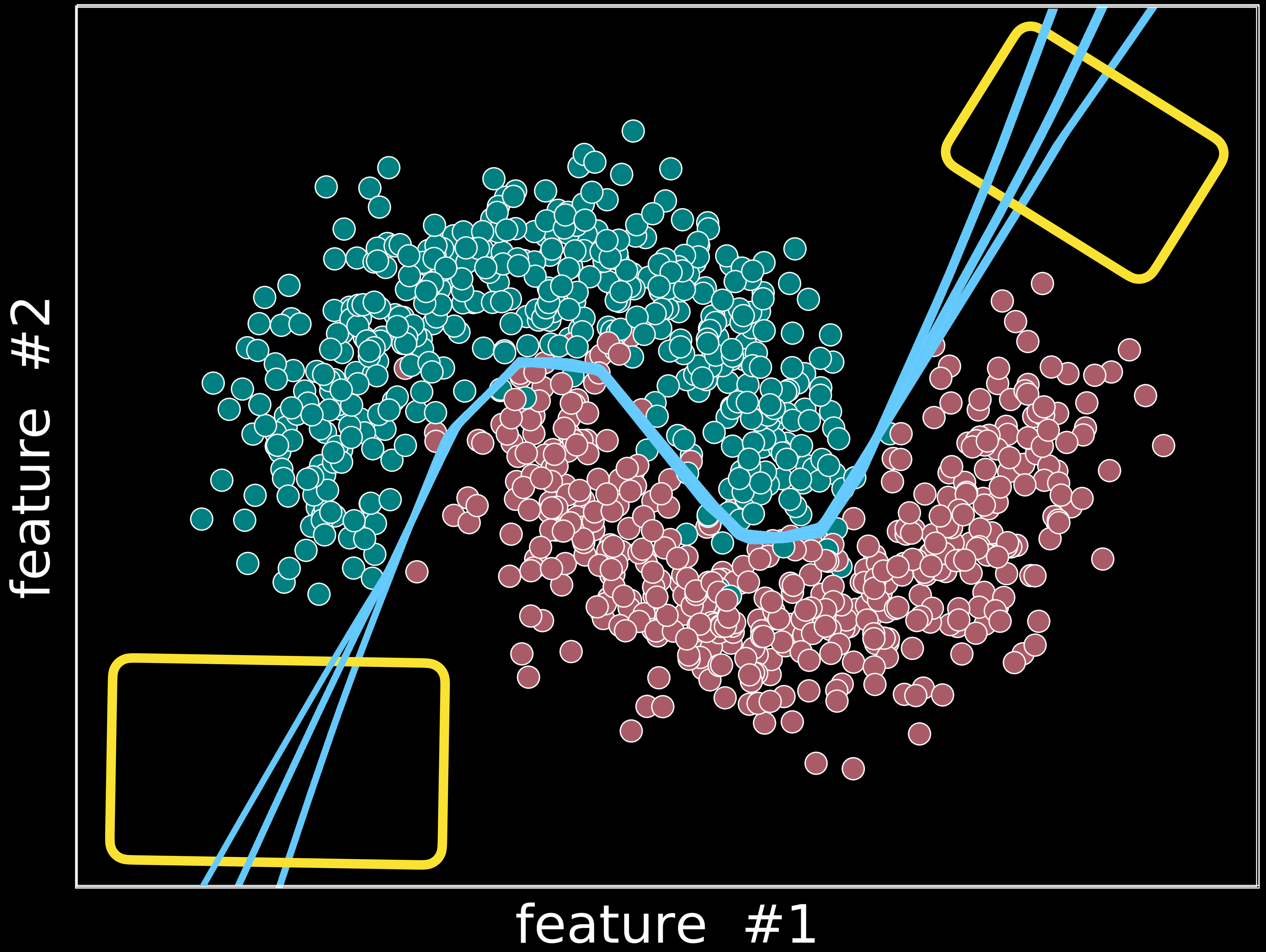
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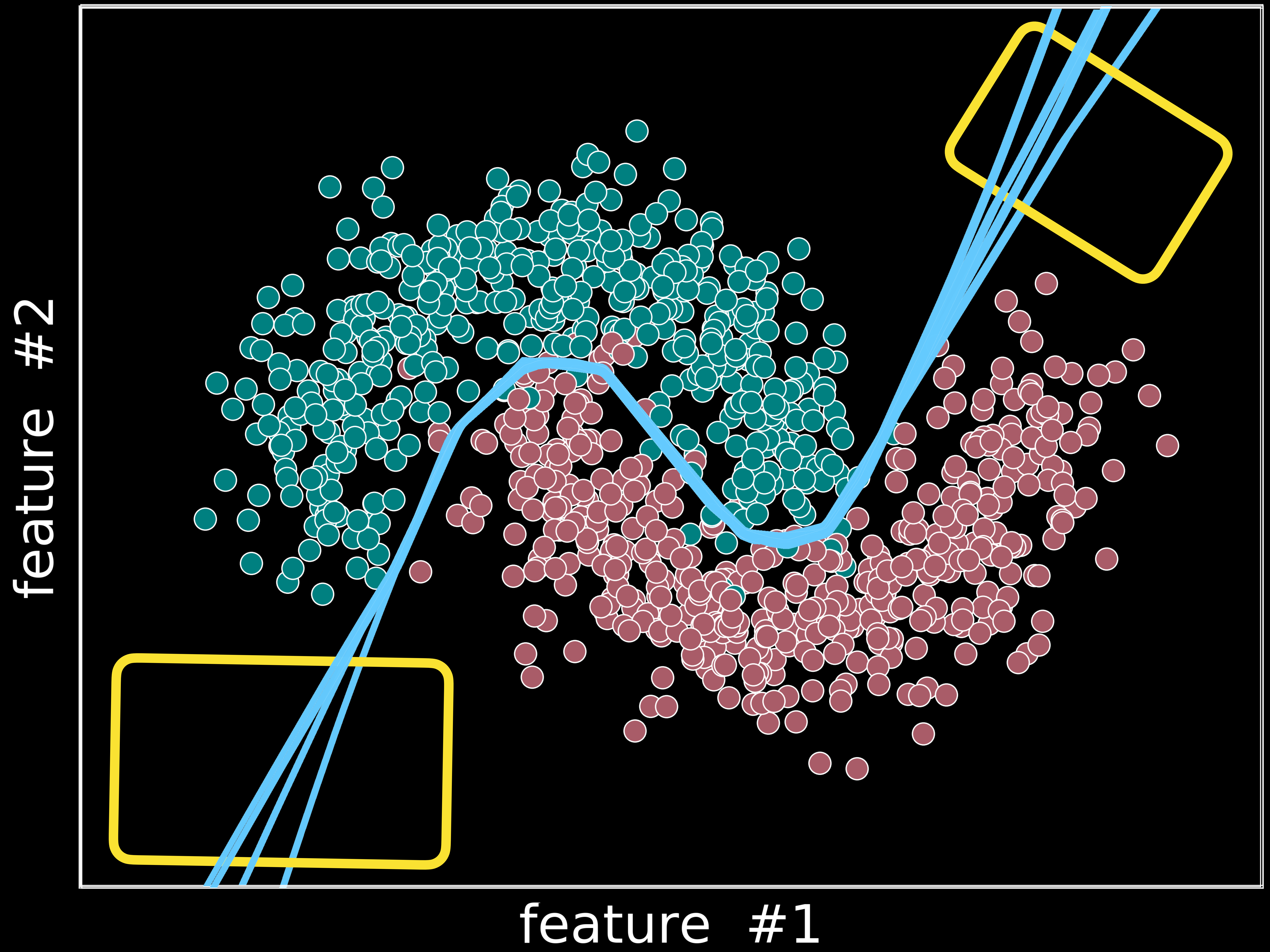
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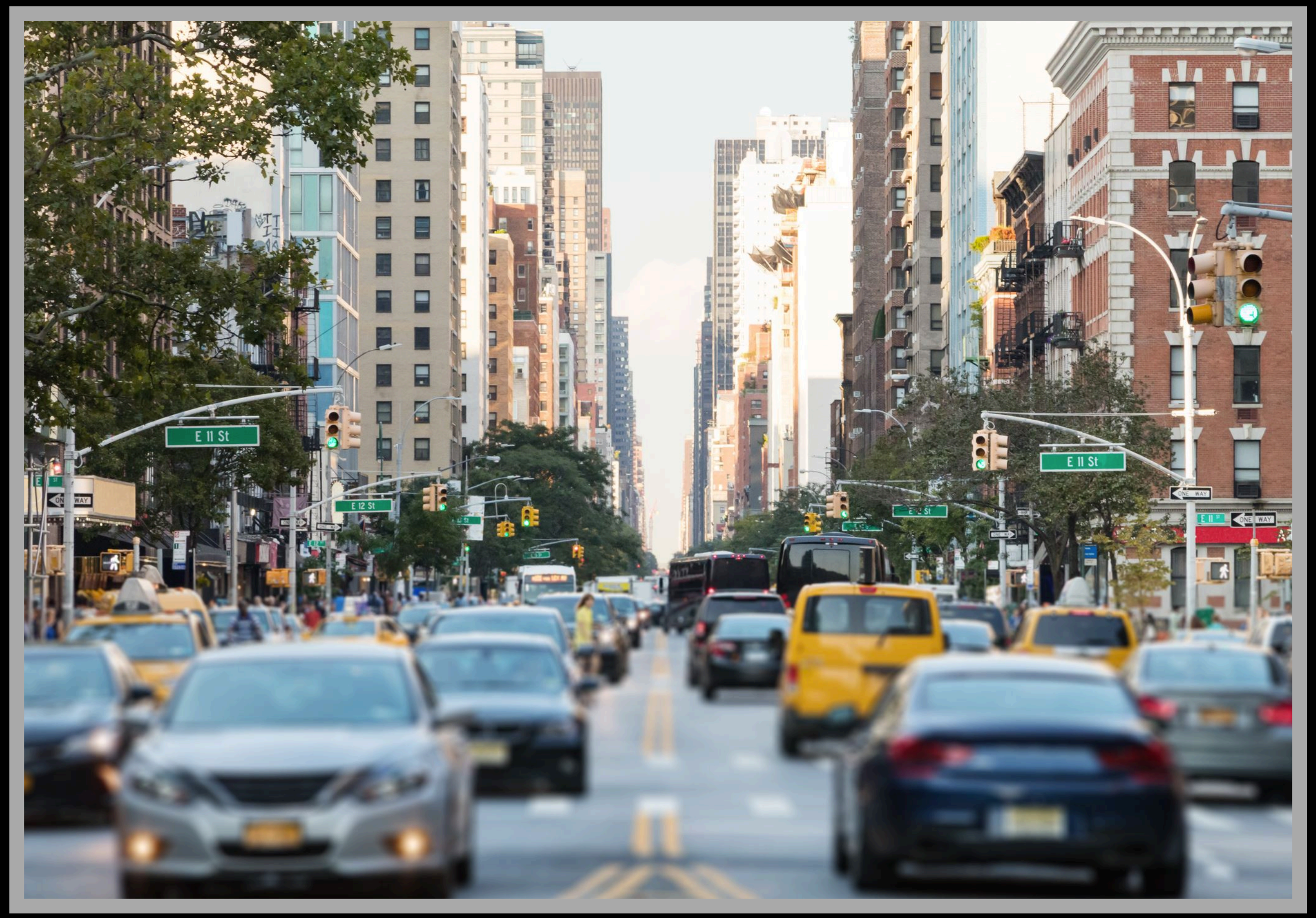

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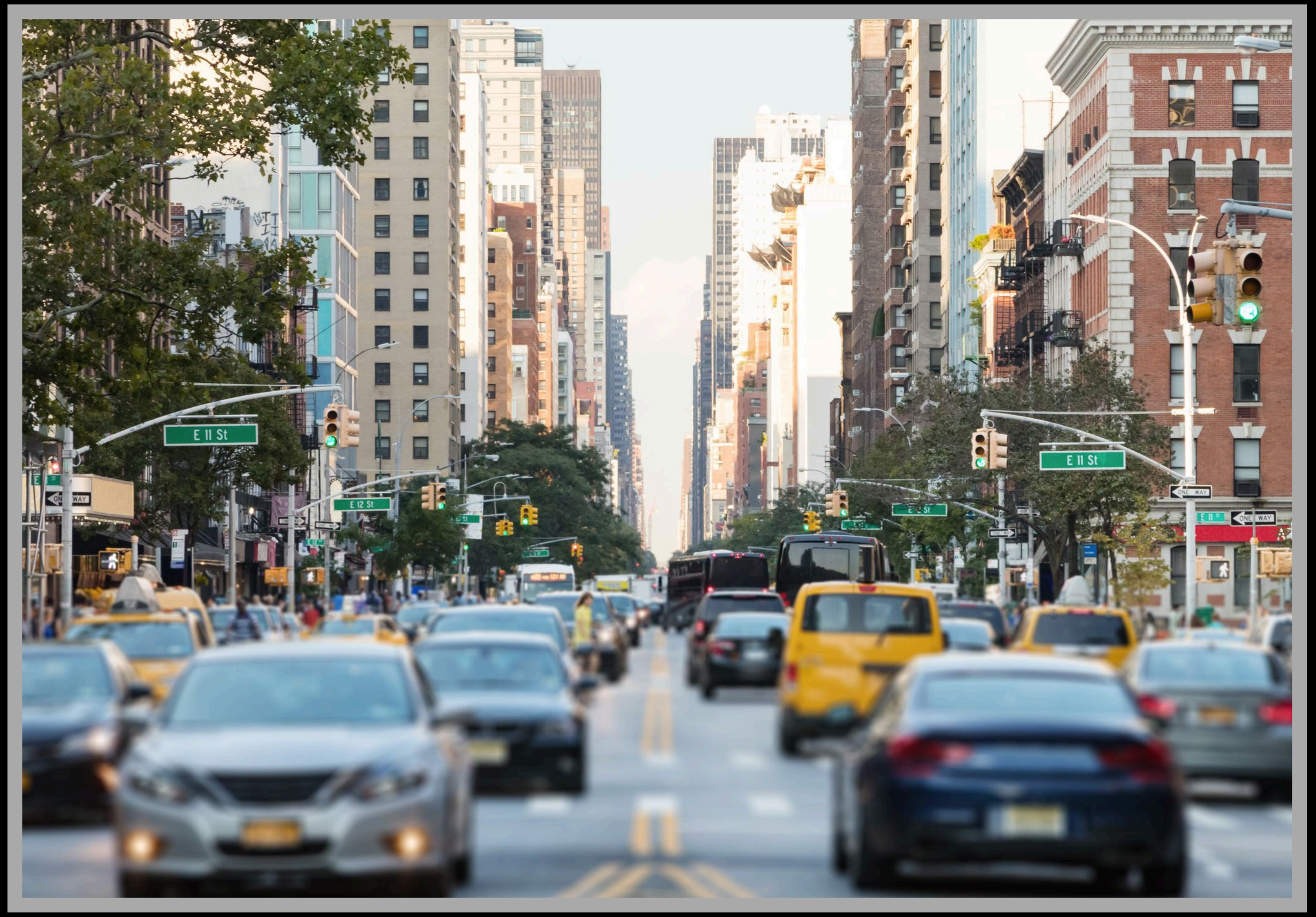

high aleatoric:
avoiding a head-on collision

high epistemic:
driving in the mountains

In practice, distinguishing aleatoric vs epistemic uncertainty is incredibly difficult.

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For the rest of this talk, I’ll ignore the distinction: uncertainty is ‘high’ when either types are ‘high.’

II. Modeling Paradigms

Assumptions

fixed, unknown distribution generates the data:

$$y \sim \mathbb{P}\left(y \,|\, x\right)$$

we only see samples, i.e. the training set:

$$\mathfrak{D} = \left\{(x_n, y_n)\right\}_{n=1}^{N}$$

fit model to recover the ground-truth distribution:

$$p(y \,|\, x) \;\approx\; \mathbb{P}\left(y \,|\, x\right)$$

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Two Modeling Paradigms

- ⊗ Frequentism: randomness from data's sampling distribution
- ⊗ Bayesianism: randomness from prior distribution over model parameters

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Frequentist Learning: Maximum Likelihood

maximize the log-likelihood of parameters:

$$\hat{\theta} = \underset{\theta \in \Theta}{\operatorname{argmax}} \sum_{n=1}^{N} \log p\left(y_n \mid x_n, \theta\right)$$

(for classification, equivalent to cross-entropy loss)

Frequentist Learning: Ideal UQ

under (near) perfect learning, can quantify uncertainty simply by…

model probability reflects confidence:

$$\mathrm{p}\left(\hat{\mathrm{y}} \,|\, \mathrm{x}; \hat{\theta}\right) \approx \mathbb{P}\left(\mathrm{y} = \hat{\mathrm{y}} \,|\, \mathrm{x}\right)$$

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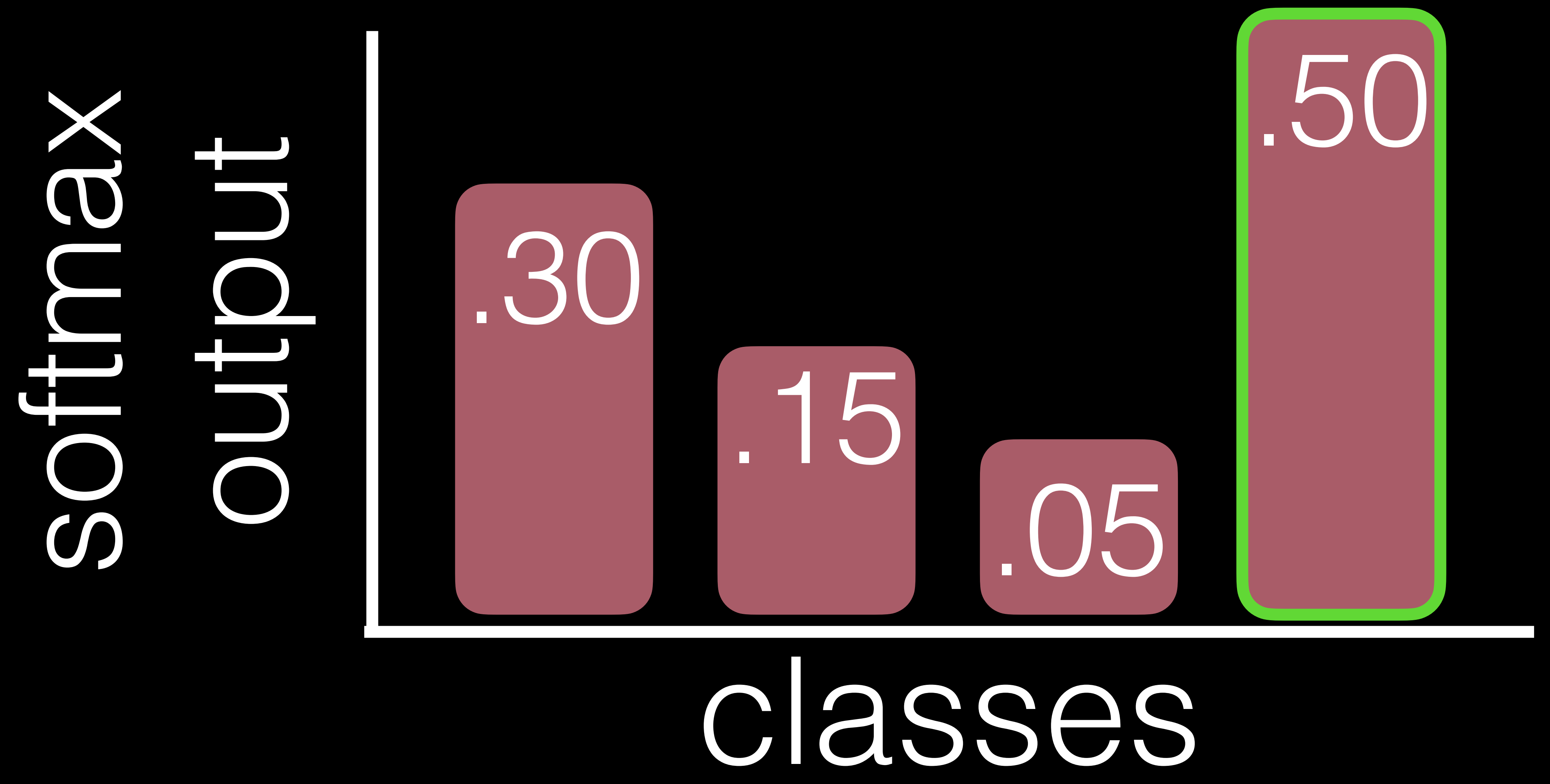

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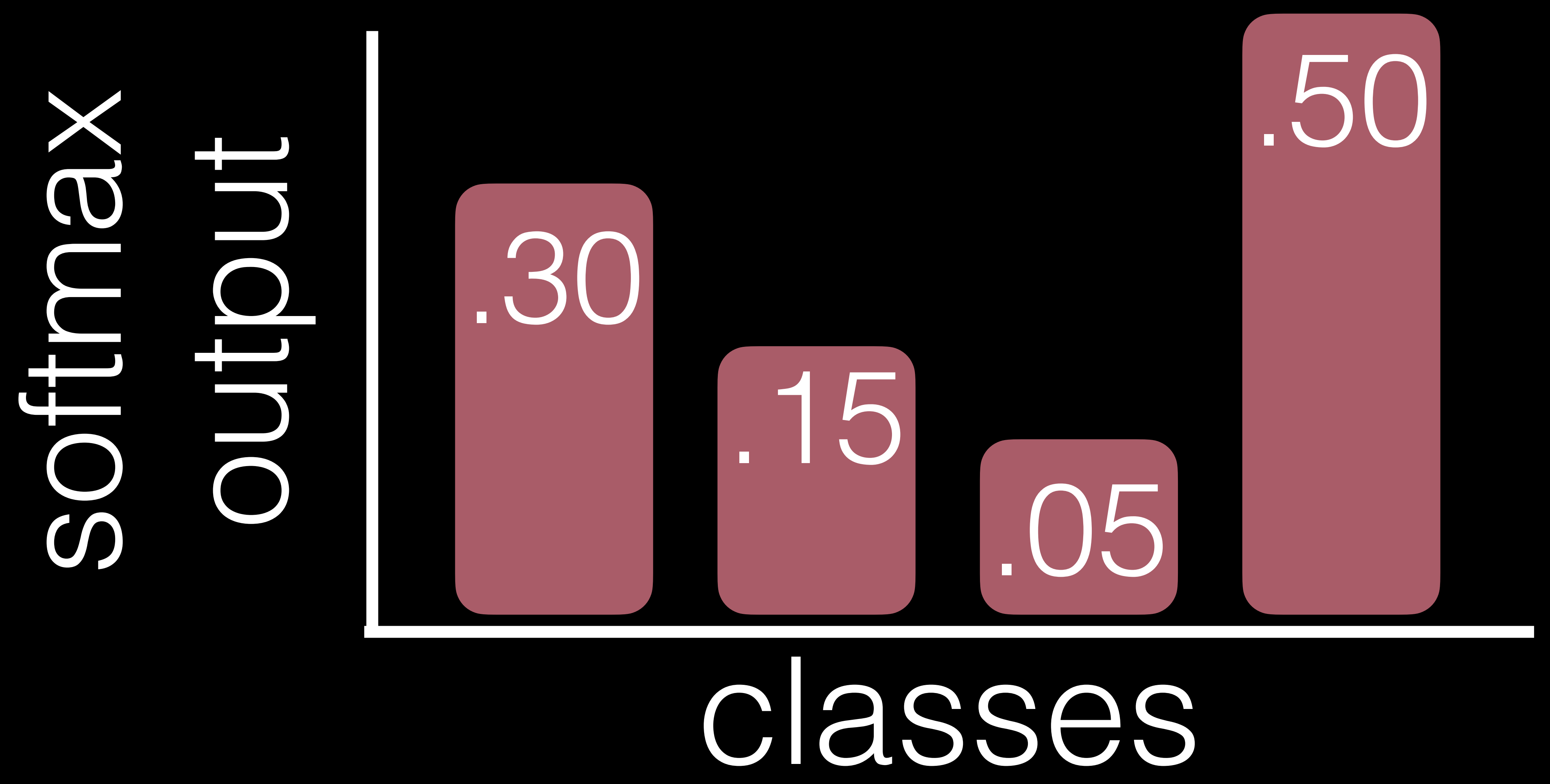

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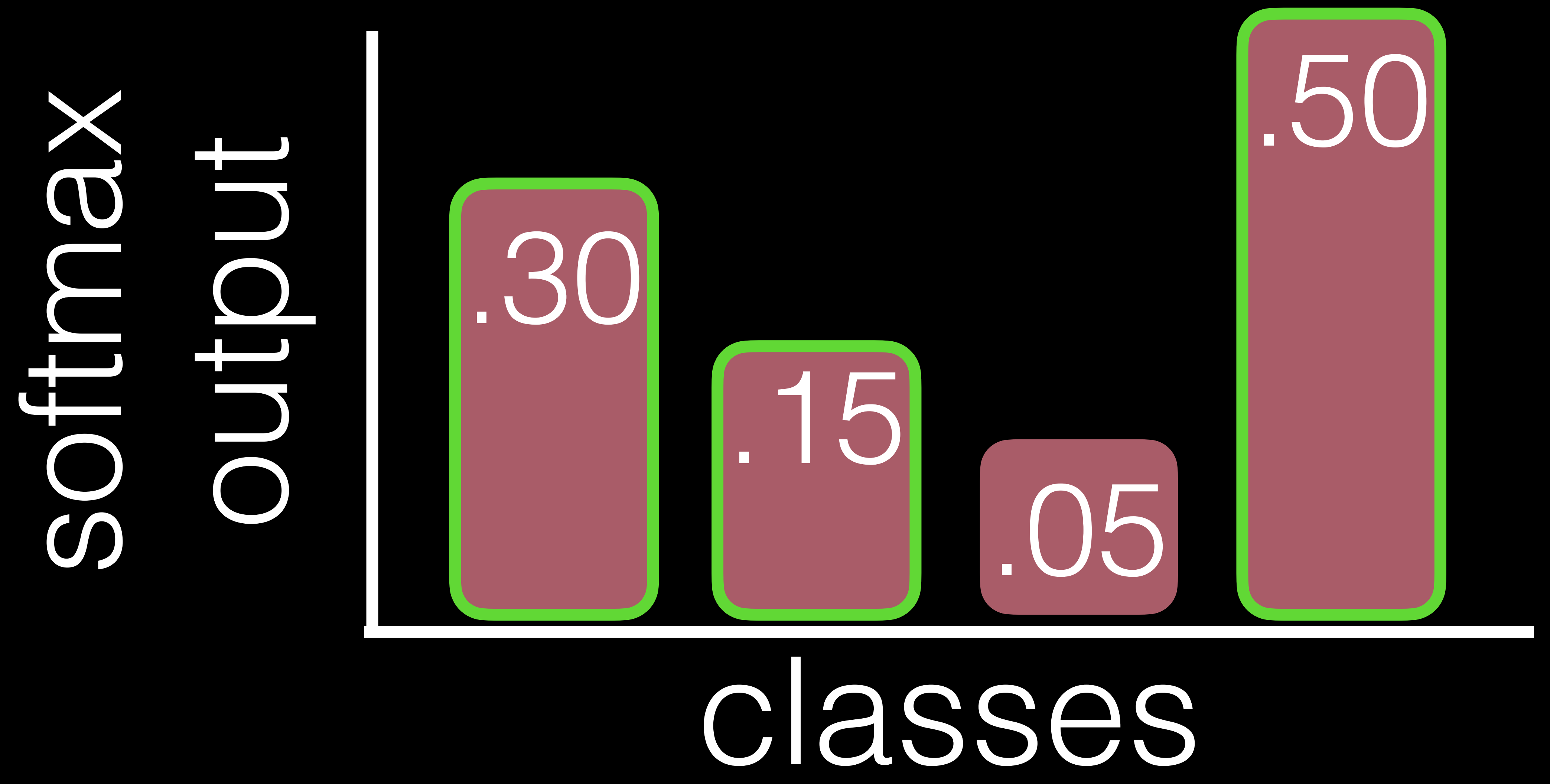
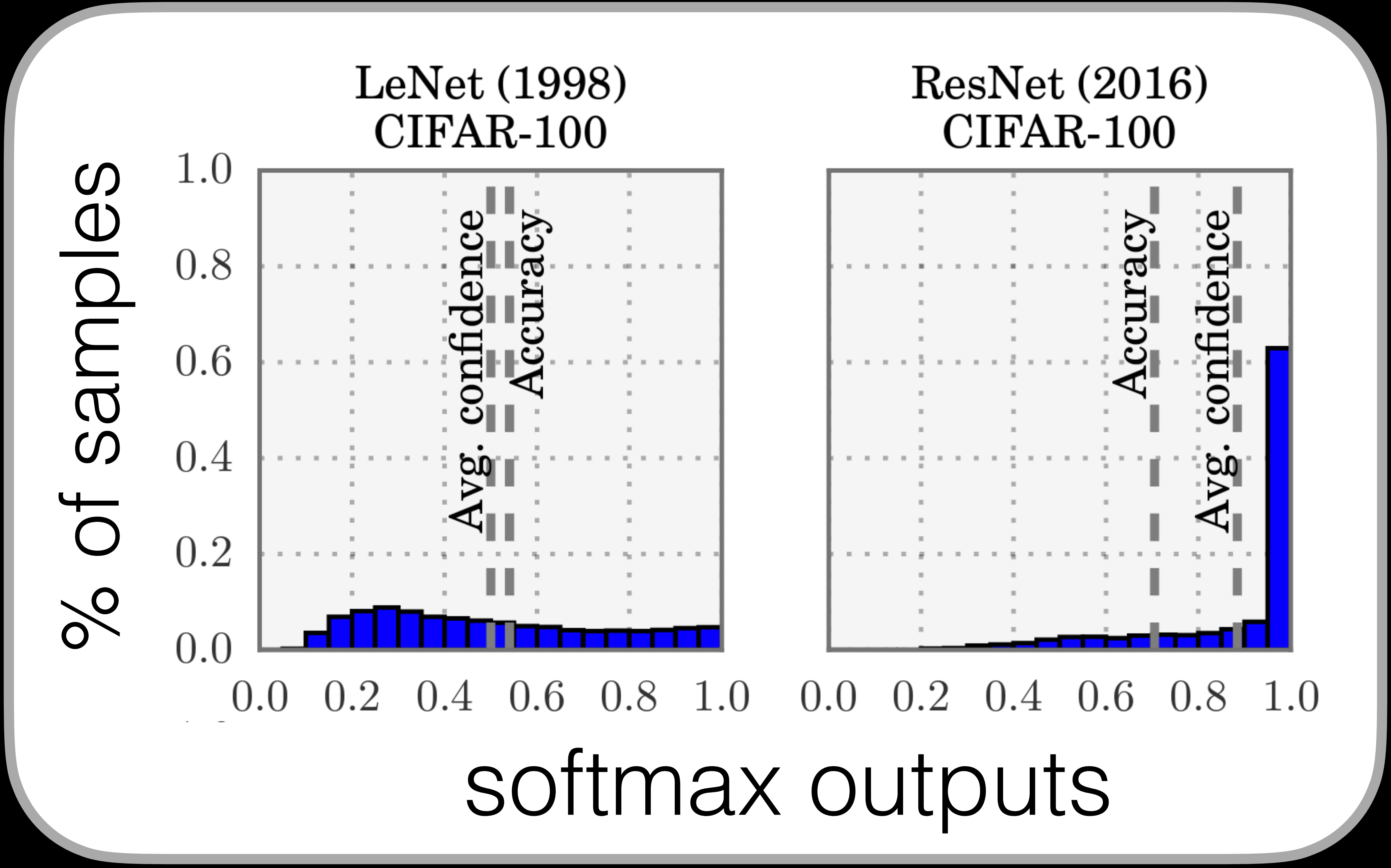


Frequentist Learning: Limitations

well-motivated with large data sets, but models are big and data is often scarce!



[Guo et al., ICML 2017]

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Bayesian Learning: Posterior Distribution

$$p\left(\theta \mid \mathfrak{D}\right) = \frac{p\left(\theta\right) \prod_{n=1}^{N} p\left(y_n \mid x_n, \theta\right)}{p(\mathfrak{D})}$$

posterior distribution

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$$\int_\theta p(\theta) \prod_{n=1}^{N} p\left(y_n \mid x_n, \theta\right) \, d\theta$$

marginal likelihood

Bayesian Learning: Ideal UQ

for new data point $\tilde{\mathrm{x}}$

integrate out posterior distribution:

$$\mathrm{p}\left(\tilde{\mathrm{y}} \,|\, \tilde{\mathrm{x}}, \mathfrak{D}\right) = \int_{\theta} \mathrm{p}\left(\tilde{\mathrm{y}} \,|\, \tilde{\mathrm{x}}, \theta\right) \; \mathrm{p}\left(\theta \,|\, \mathfrak{D}\right) \; \mathrm{d}\theta$$

posterior predictive distribution

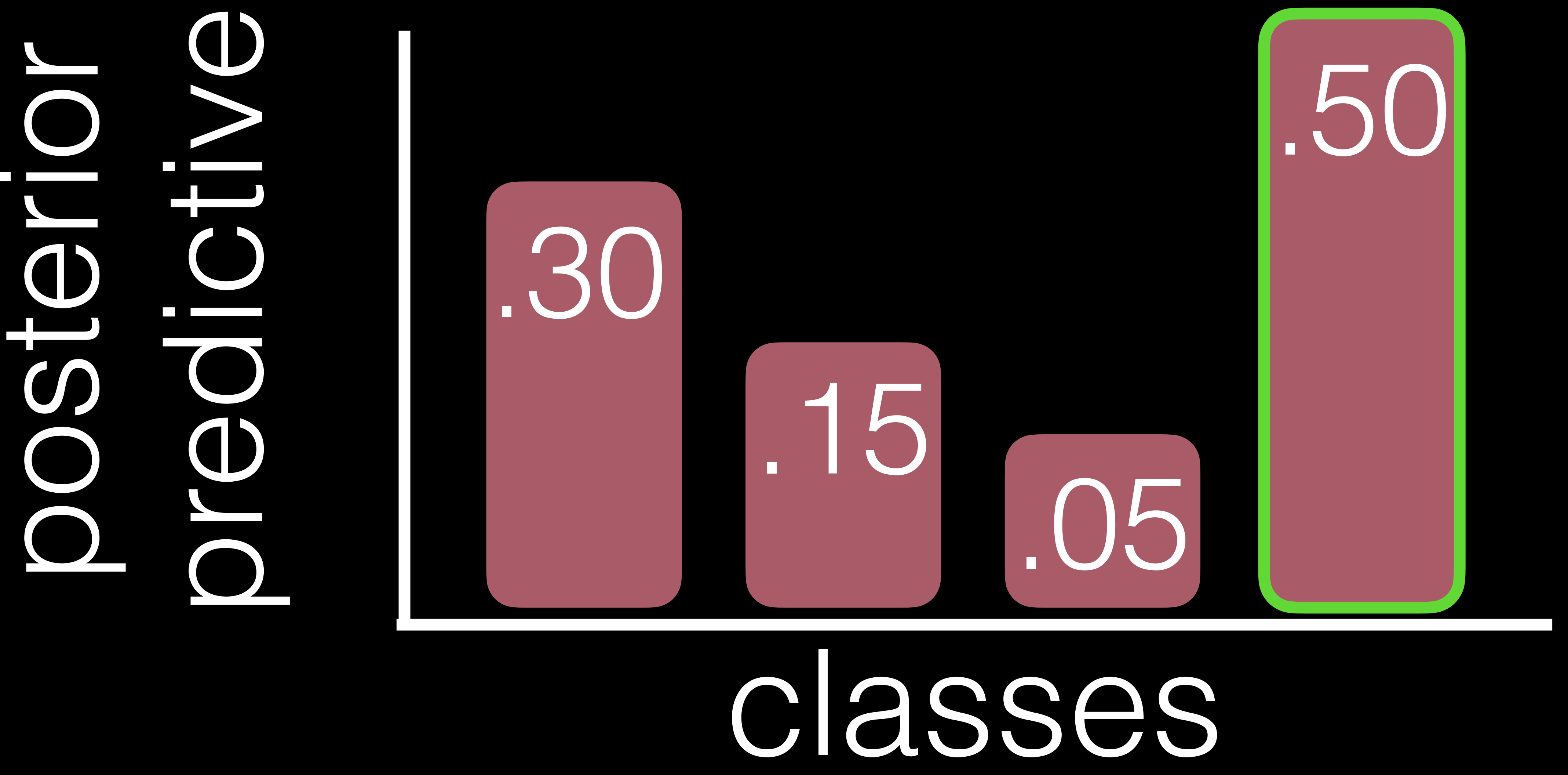
Bayesian Learning: Ideal UQ

under (near) perfect learning, use posterior predictive distribution for ground-truth probabilities

$$p\left(\tilde{y} \,|\, \tilde{x}, \mathfrak{D}\right) \;\approx\; \mathbb{P}\left(y = \tilde{y} \,|\, x\right)$$

Bayesian Learning: Ideal UQ

under (near) perfect learning, use posterior predictive distribution for ground-truth probabilities



Bayesian Learning: Limitations

integrating over the parameters is difficult to even approximate for neural networks.

- ✗ marginal likelihood
- ✗ posterior predictive distribution

Bayesianism vs Frequentism: Summary

- Frequentism
  - 🟩 data-driven, easy computation
  - 🟥 misled by sampling noise if dataset is not large

- Bayesianism
  - 🟩 prior distribution ‘jump starts’ learning
  - 🟥 computation is very, very costly

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III. Uncertainty Quantification in Practice

Practical Methods for UQ

- ⊗ Frequentism
  - bootstrap aggregation (bagging)
  - conformal prediction

- ⊗ Bayesianism
  - sample-then-optimize ensembling
  - variational inference w/ Laplace approximation

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Bootstrap Aggregation

recall that frequentism assumes randomness comes from the data sampling process.

if we could see additional data sets, we could know more about the sampling noise.

$$❌ \; \{\mathfrak{D}_k\}_{k=1}^{K} \sim \mathbb{P}\left(y \,|\, x\right)$$

Bootstrap Aggregation

Bootstrapping synthesizes additional data sets by resampling from the training set.

$$\{\mathfrak{D}_k\}_{k=1}^{K} \sim \frac{1}{N}\sum_{n=1}^{N} \delta\left[(x_n, y_n)\right]$$

sampling with replacement

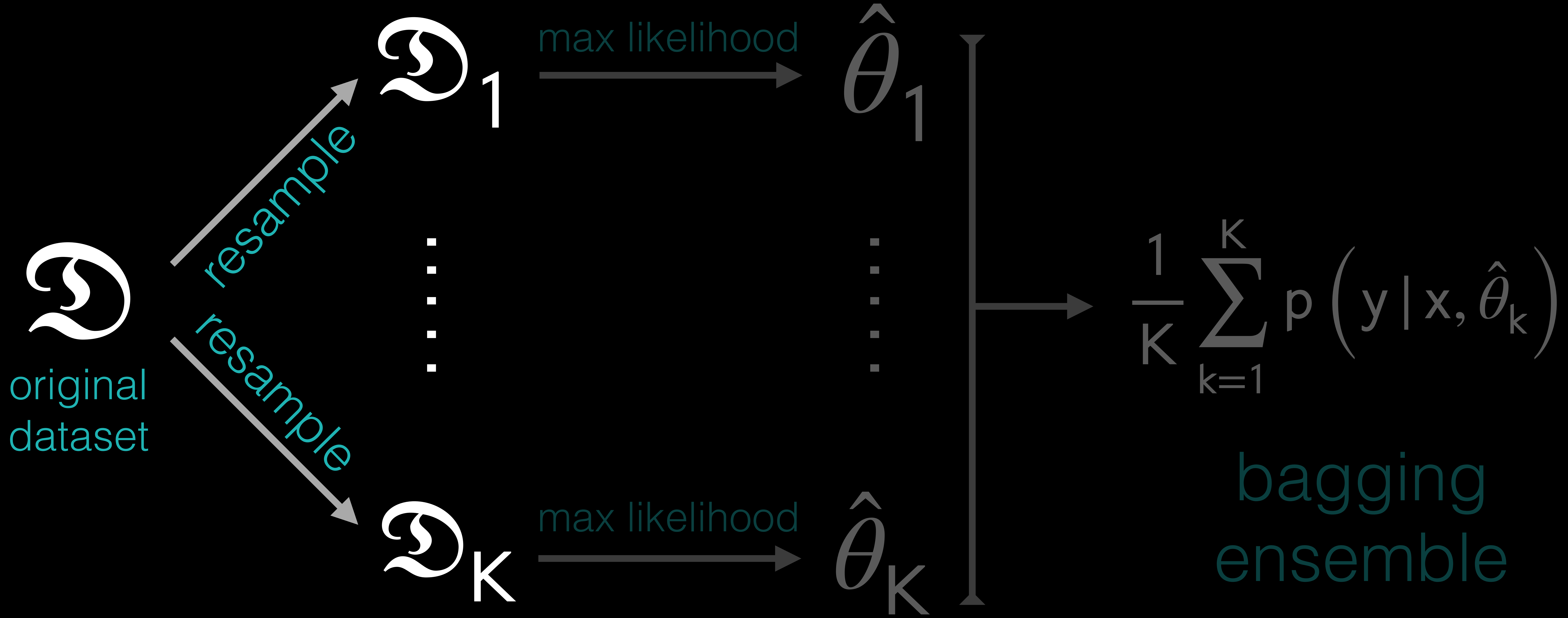
Bootstrap Aggregation

$$\begin{tikzcd}
 & \mathcal{D}_1 \arrow[r, "\text{max likelihood}"] & \hat{\theta}_1 & \\
\mathcal{D} \arrow[ur, "\text{resample}"] \arrow[dr, "\text{resample}"'] & \vdots & \vdots \arrow[r] & \frac{1}{K}\sum_{k=1}^{K} p\left(y \mid x, \hat{\theta}_k\right) \\
 & \mathcal{D}_K \arrow[r, "\text{max likelihood}"] & \hat{\theta}_K &
\end{tikzcd}$$

original dataset

bagging ensemble

Bootstrap Aggregation



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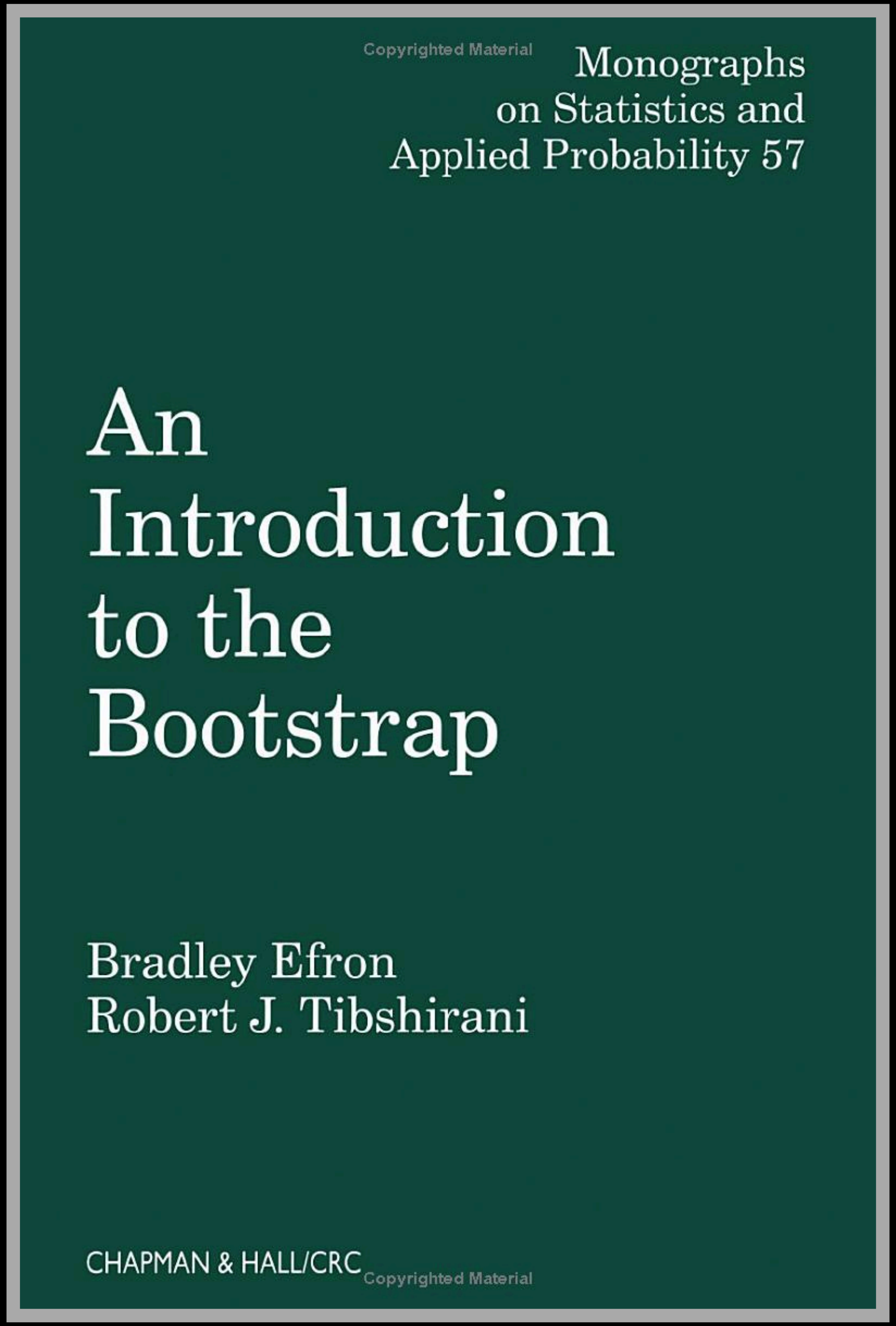
Further Reading



Monographs on Statistics and Applied Probability 57

An Introduction to the Bootstrap

Bradley Efron
Robert J. Tibshirani

CHAPMAN & HALL/CRC

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Sample-then-Optimize Ensemble

recall that Bayesianism assumes randomness comes from the prior.

we perform a bagging-like procedure, but using samples from the prior to initialize training.

$$\{\bar{\theta}_k\}_{k=1}^{K} \sim p(\theta)$$

Sample-then-Optimize Ensemble

$$\begin{tikzcd}
 & \bar{\theta}_1 \arrow[r, "\text{max likelihood}"] & \hat{\theta}_1 & \\
p(\theta) \arrow[ur, "\text{sample}"] \arrow[dr, "\text{sample}"'] & \vdots & \vdots \arrow[r] & \frac{1}{K}\sum_{k=1}^{K} p\left(y \,|\, x, \hat{\theta}_k\right) \\
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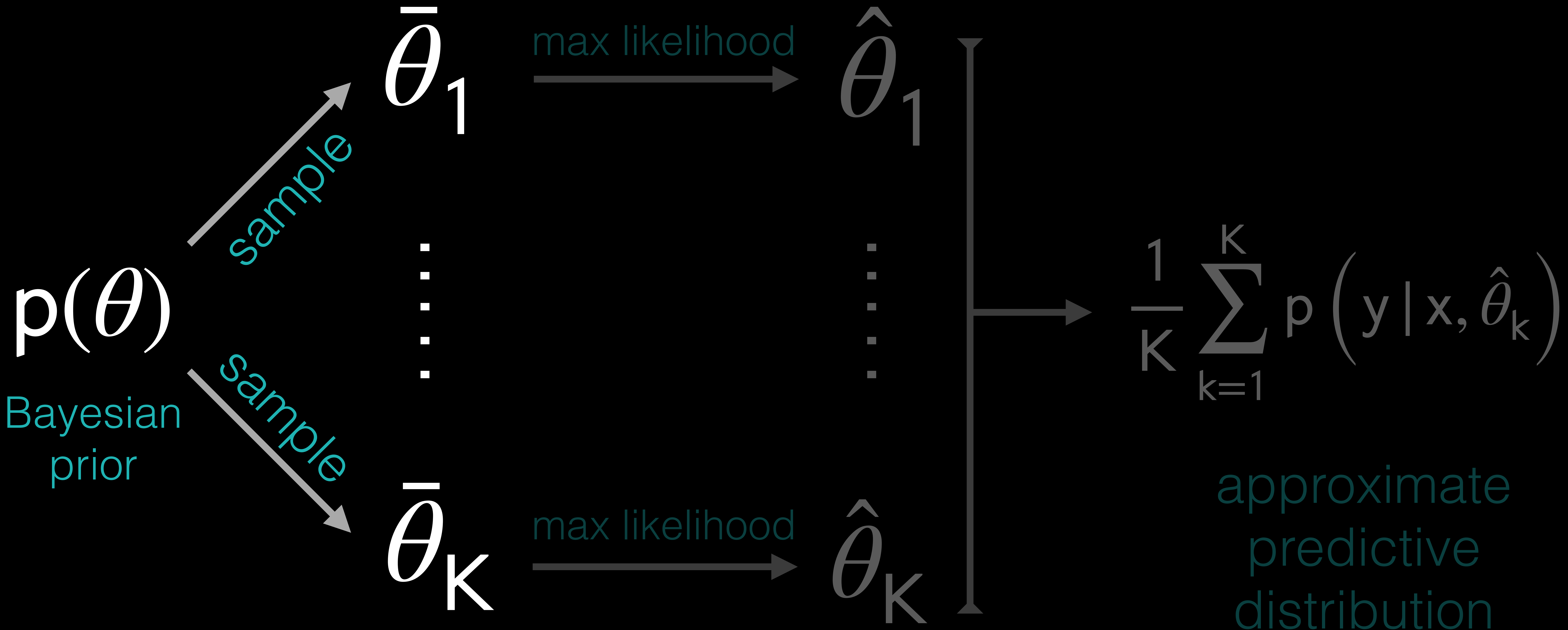
Bayesian prior

approximate predictive distribution

Sample-then-Optimize Ensemble



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Bayesian prior

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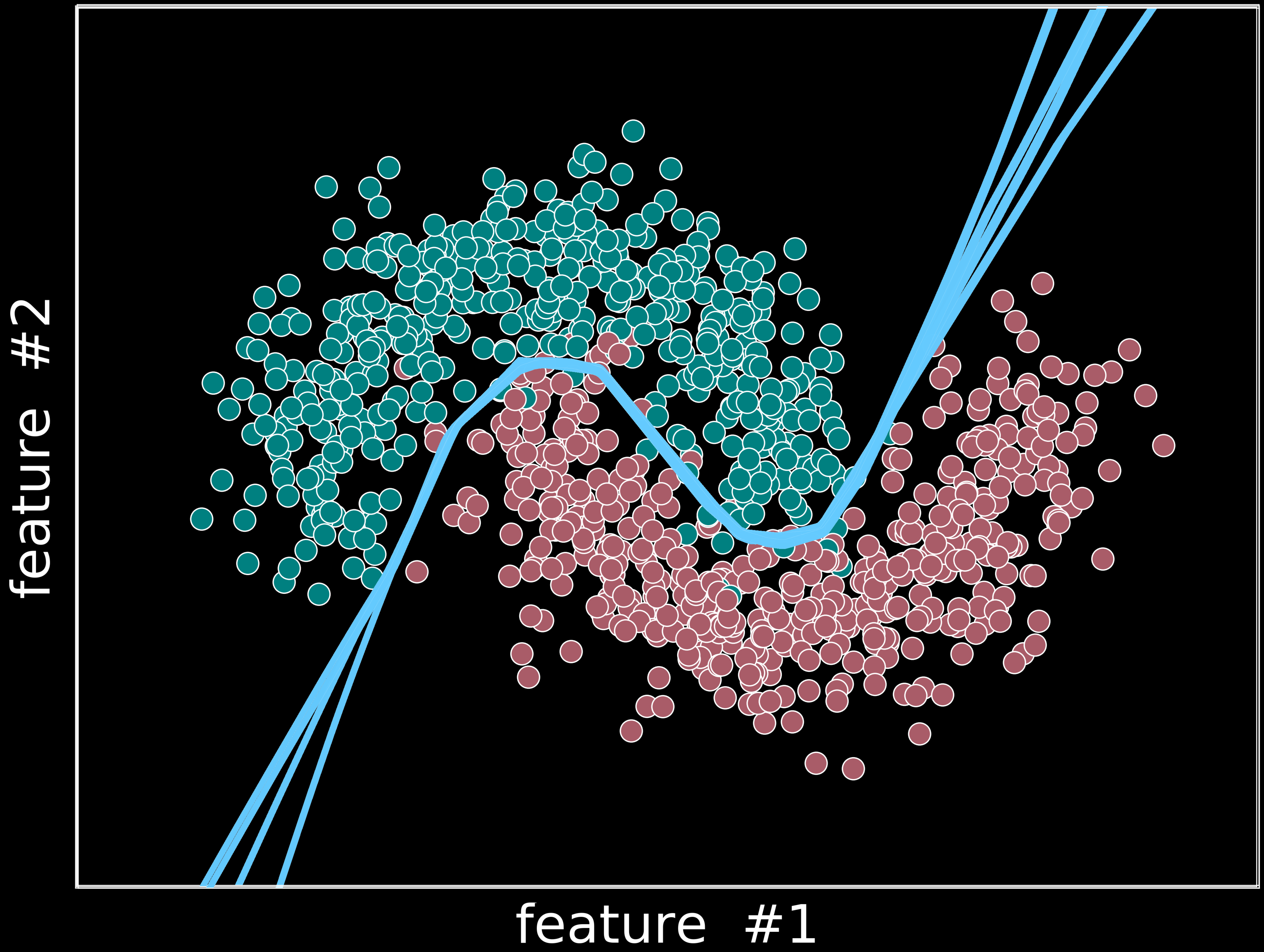
Sample-then-Optimize Ensemble

[Matthews et al., 2017] show the procedure
(very nearly) recovers the posterior in linear models.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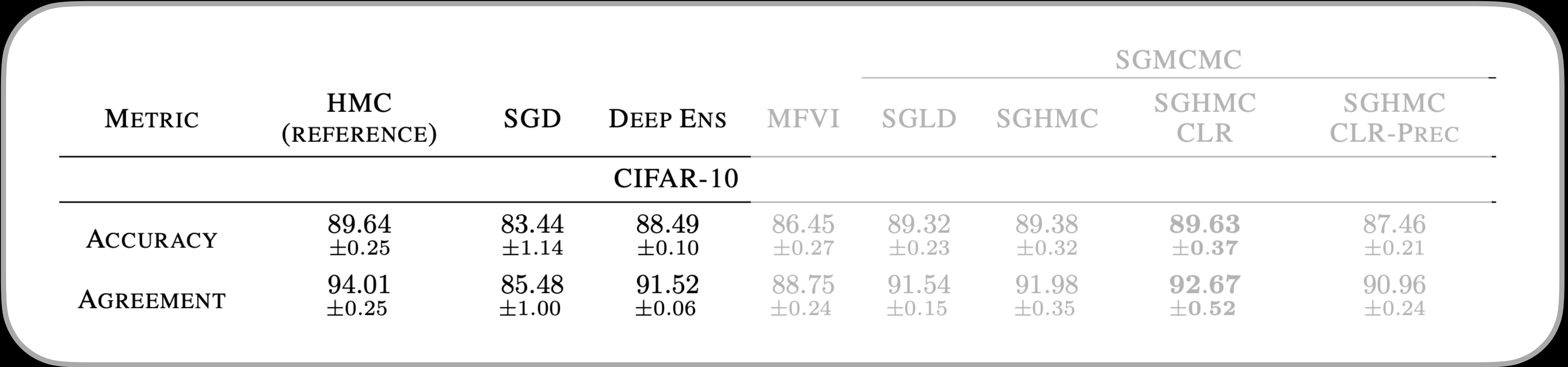
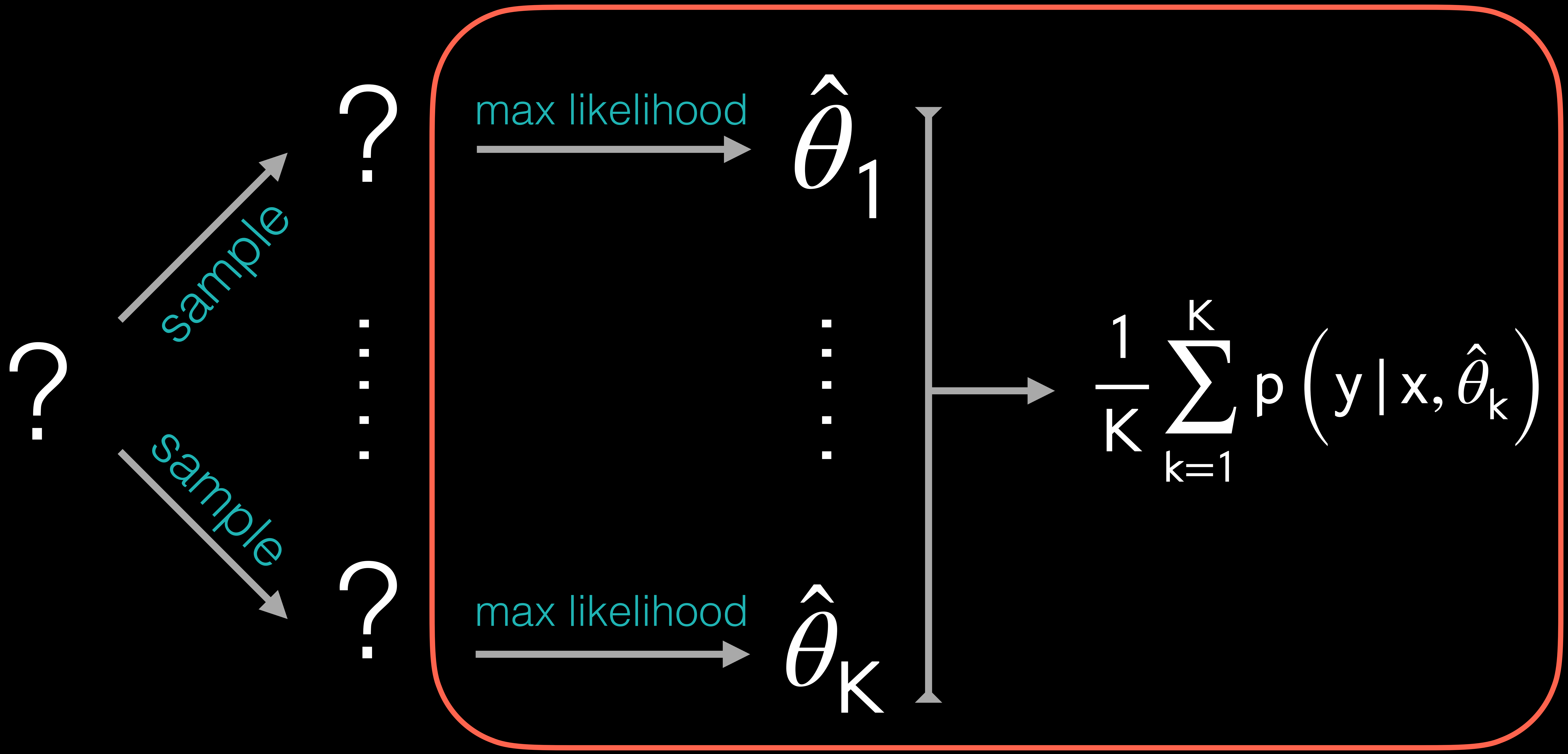


					SGMCMC			
Metric	HMC (reference)	SGD	Deep Ens	MFVI	SGLD	SGHMC	SGHMC CLR	SGHMC CLR-Prec
			CIFAR-10					
Accuracy	89.64 ±0.25	83.44 ±1.14	88.49 ±0.10	86.45 ±0.27	89.32 ±0.23	89.38 ±0.32	**89.63 ±0.37**	87.46 ±0.21
Agreement	94.01 ±0.25	85.48 ±1.00	91.52 ±0.06	88.75 ±0.24	91.54 ±0.15	91.98 ±0.35	**92.67 ±0.52**	90.96 ±0.24

surprisingly comparable to high-fidelity Bayesian inference (performed on 512 TPUs).

[Izmailov et al., ICML 2021]

Bayesian vs Frequentist Ensembles



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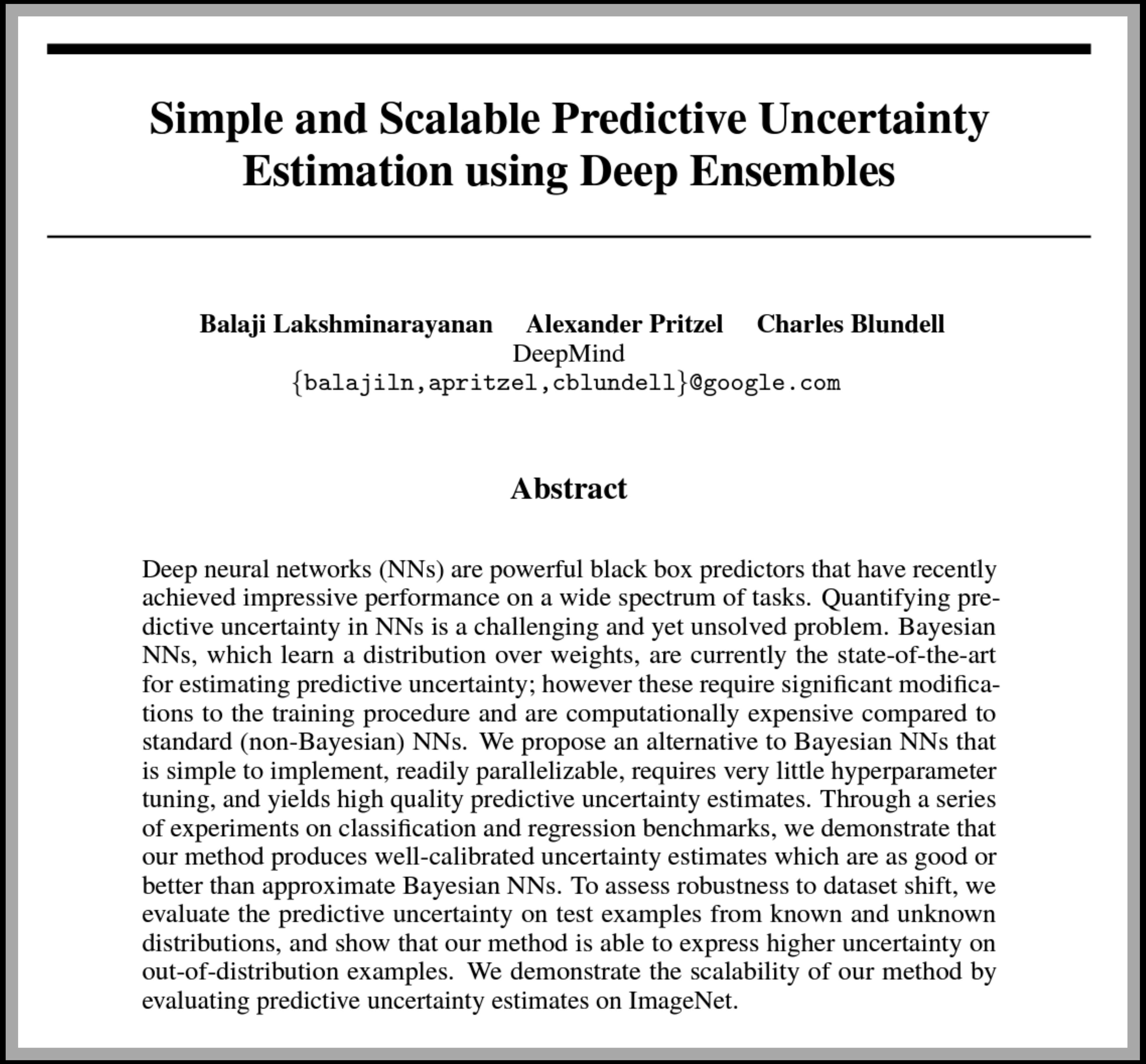
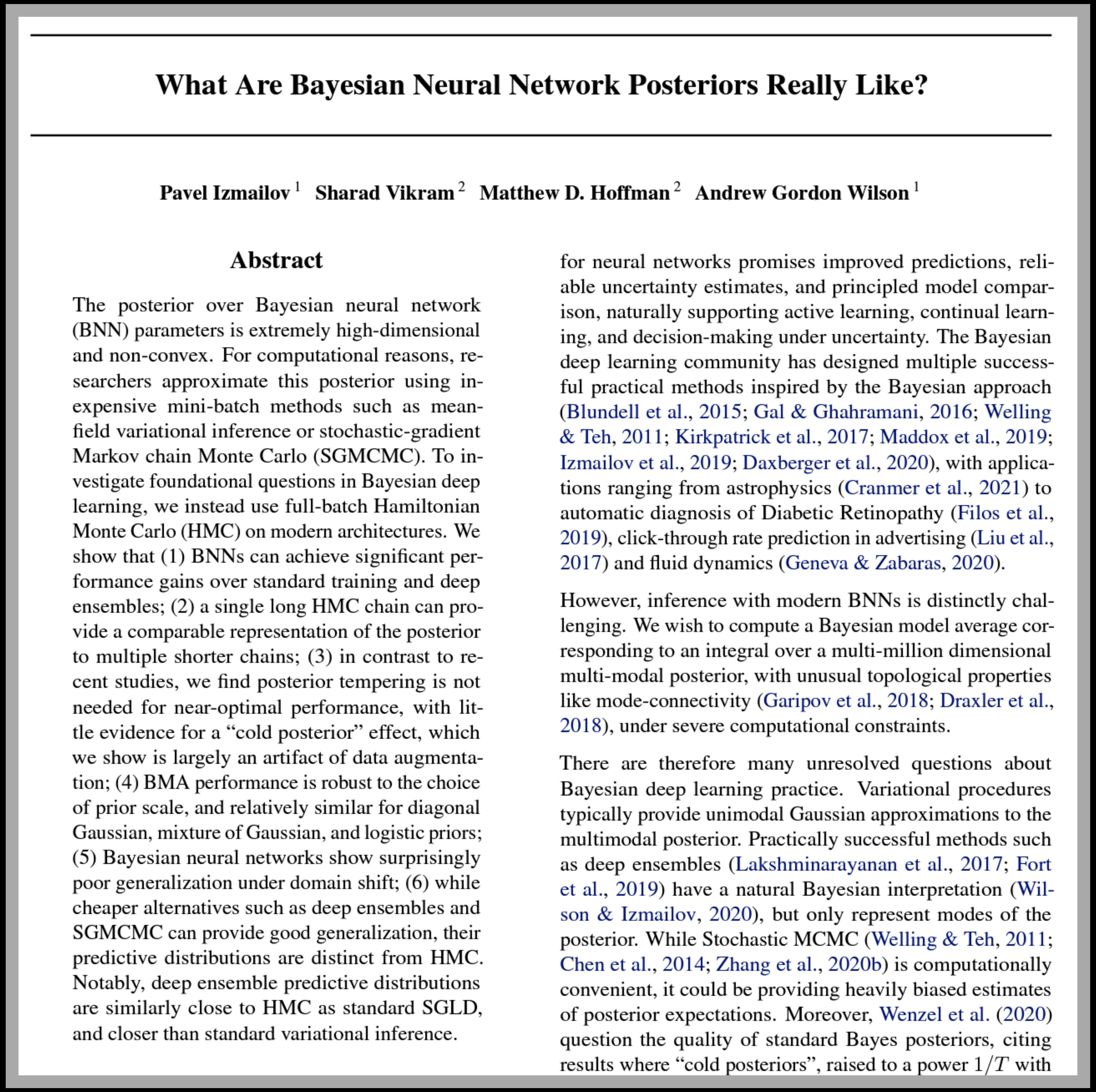


Simple and Scalable Predictive Uncertainty Estimation using Deep Ensembles

Balaji Lakshminarayanan **Alexander Pritzel** **Charles Blundell**
DeepMind
{balajiln,apritzel,cblundell}@google.com

Abstract

Deep neural networks (NNs) are powerful black box predictors that have recently achieved impressive performance on a wide spectrum of tasks. Quantifying predictive uncertainty in NNs is a challenging and yet unsolved problem. Bayesian NNs, which learn a distribution over weights, are currently the state-of-the-art for estimating predictive uncertainty; however these require significant modifications to the training procedure and are computationally expensive compared to standard (non-Bayesian) NNs. We propose an alternative to Bayesian NNs that is simple to implement, readily parallelizable, requires very little hyperparameter tuning, and yields high quality predictive uncertainty estimates. Through a series of experiments on classification and regression benchmarks, we demonstrate that our method produces well-calibrated uncertainty estimates which are as good or better than approximate Bayesian NNs. To assess robustness to dataset shift, we evaluate the predictive uncertainty on test examples from known and unknown distributions, and show that our method is able to express higher uncertainty on out-of-distribution examples. We demonstrate the scalability of our method by evaluating predictive uncertainty estimates on ImageNet.



What Are Bayesian Neural Network Posteriors Really Like?

Pavel Izmailov [1] **Sharad Vikram** [2] **Matthew D. Hoffman** [2] **Andrew Gordon Wilson** [1]

Abstract

The posterior over Bayesian neural network (BNN) parameters is extremely high-dimensional and non-convex. For computational reasons, researchers approximate this posterior using inexpensive mini-batch methods such as mean-field variational inference or stochastic-gradient Markov chain Monte Carlo (SGMCMC). To investigate foundational questions in Bayesian deep learning, we instead use full-batch Hamiltonian Monte Carlo (HMC) on modern architectures. We show that (1) BNNs can achieve significant performance gains over standard training and deep ensembles; (2) a single long HMC chain can provide a comparable representation of the posterior to multiple shorter chains; (3) in contrast to recent studies, we find posterior tempering is not needed for near-optimal performance, with little evidence for a "cold posterior" effect, which we show is largely an artifact of data augmentation; (4) BMA performance is robust to the choice of prior scale, and relatively similar for diagonal Gaussian, mixture of Gaussian, and logistic priors; (5) Bayesian neural networks show surprisingly poor generalization under domain shift; (6) while cheaper alternatives such as deep ensembles and SGMCMC can provide good generalization, their predictive distributions are distinct from HMC. Notably, deep ensemble predictive distributions are similarly close to HMC as standard SGLD, and closer than standard variational inference.

for neural networks promises improved predictions, reliable uncertainty estimates, and principled model comparison, naturally supporting active learning, continual learning, and decision-making under uncertainty. The Bayesian deep learning community has designed multiple successful practical methods inspired by the Bayesian approach (Blundell et al., 2015; Gal & Ghahramani, 2016; Welling & Teh, 2011; Kirkpatrick et al., 2017; Maddox et al., 2019; Izmailov et al., 2019; Daxberger et al., 2020), with applications ranging from astrophysics (Cranmer et al., 2021) to automatic diagnosis of Diabetic Retinopathy (Filos et al., 2019), click-through rate prediction in advertising (Liu et al., 2017) and fluid dynamics (Geneva & Zabaras, 2020).

However, inference with modern BNNs is distinctly challenging. We wish to compute a Bayesian model average corresponding to an integral over a multi-million dimensional multi-modal posterior, with unusual topological properties like mode-connectivity (Garipov et al., 2018; Draxler et al., 2018), under severe computational constraints.

There are therefore many unresolved questions about Bayesian deep learning practice. Variational procedures typically provide unimodal Gaussian approximations to the multimodal posterior. Practically successful methods such as deep ensembles (Lakshminarayanan et al., 2017; Fort et al., 2019) have a natural Bayesian interpretation (Wilson & Izmailov, 2020), but only represent modes of the posterior. While Stochastic MCMC (Welling & Teh, 2011; Chen et al., 2014; Zhang et al., 2020b) is computationally convenient, it could be providing heavily biased estimates of posterior expectations. Moreover, Wenzel et al. (2020) question the quality of standard Bayes posteriors, citing results where "cold posteriors", raised to a power $1/T$ with

Practical Methods for UQ

- ⊗ Frequentism
  - bootstrap aggregation (bagging)
  - conformal prediction
- ⊗ Bayesianism
  - sample-then-optimize ensembling
  - variational inference w/ Laplace approximation

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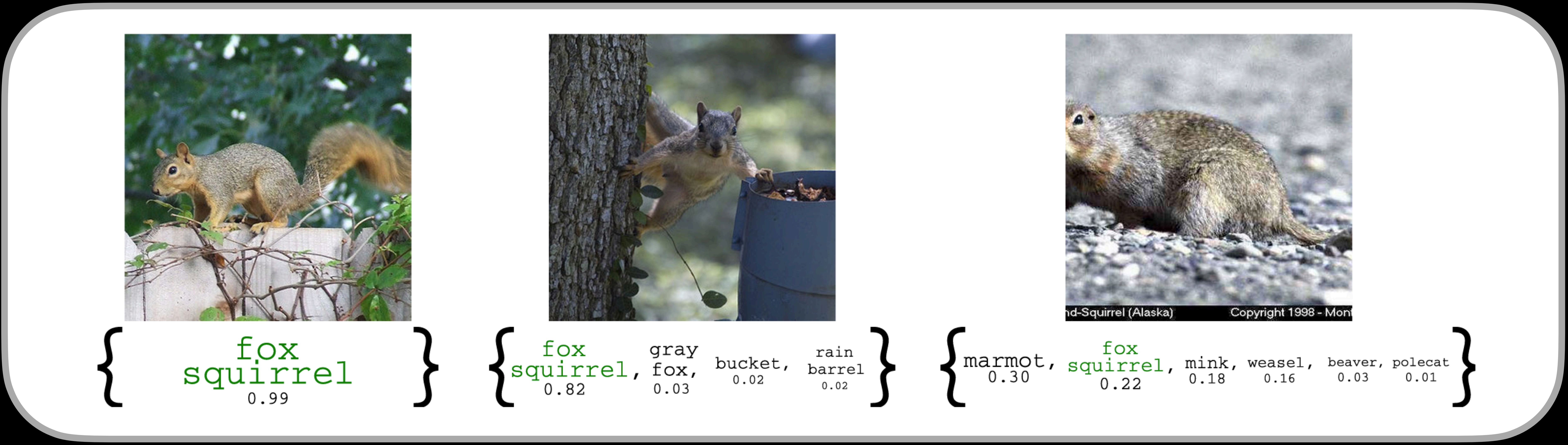
Conformal Prediction

The aim of conformal prediction is to construct uncertainty sets with guaranteed validity.



{fox squirrel 0.99}
{fox squirrel 0.82, gray fox 0.03, bucket 0.02, rain barrel 0.02}
nd-Squirrel (Alaska) Copyright 1998 - Mon
{marmot 0.30, fox squirrel 0.22, mink 0.18, weasel 0.16, beaver 0.03, polecat 0.01}

$$\mathbb{P}\left(y^{*}_{N+1} \in C(x_{N+1})\right) \geq 1 - \alpha$$

[Angelopoulos & Bates, 2022]

Conformal Prediction

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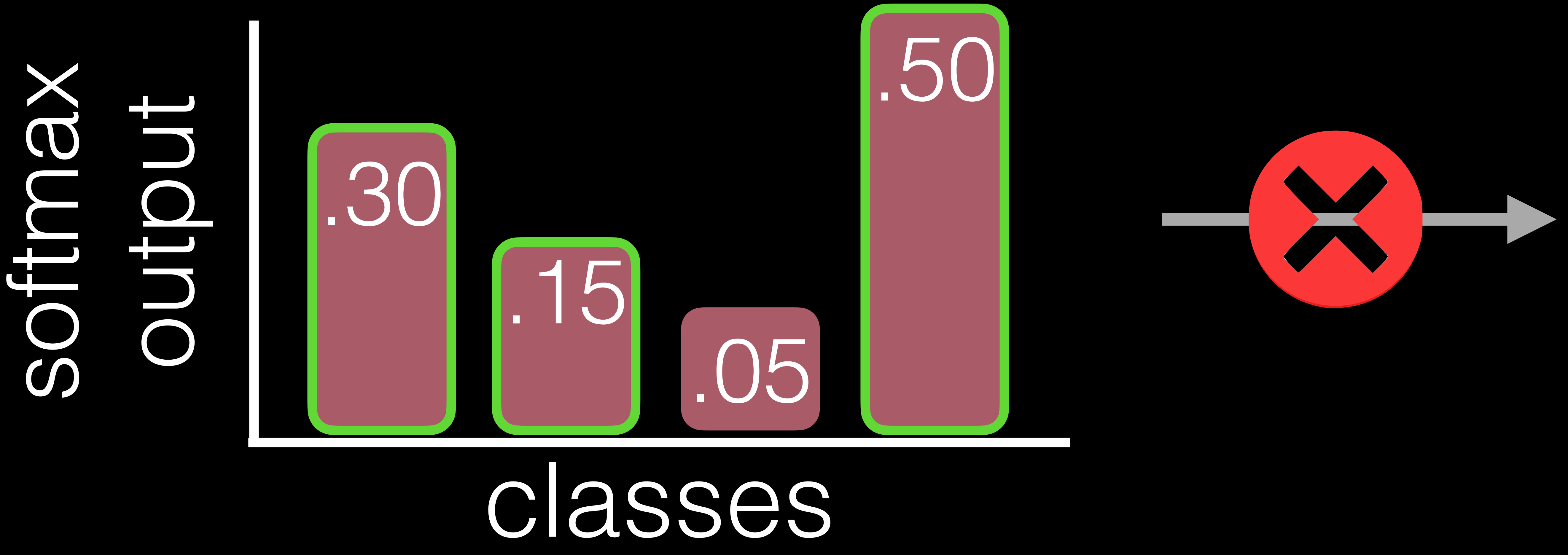

$$\mathbb{P}\left(y^* \in C(x)\right) = 95\,\%$$

Conformal Prediction

instead of using raw outputs as the confidence level, use held-out data to adapt the threshold

theoretical guarantee stems from the assumption of exchangeability:

$$\mathbb{P}\left(y_1, y_2, y_3\right) = \mathbb{P}\left(y_{\pi(1)}, y_{\pi(2)}, y_{\pi(3)}\right)$$

for any permutation π

Conformal Prediction: Train-Time

$p(y = 1 | x)$ $p(y = 2 | x)$ $p(y = 3 | x)$

i) for every point in the held-out set, sort the model probabilities in decreasing order.

Conformal Prediction: Train-Time

$$p(y = 2 \mid x) > p(y = 1 \mid x) > p(y = 3 \mid x)$$

i) for every point in the held-out set, sort the model probabilities in decreasing order.

Conformal Prediction: Train-Time

$$p(y = 2 \mid x) \quad > \quad p(y = 1 \mid x) \quad > \quad p(y = 3 \mid x)$$

ii) sum the probabilities (decreasing order) until the true-class is included.

Conformal Prediction: Train-Time

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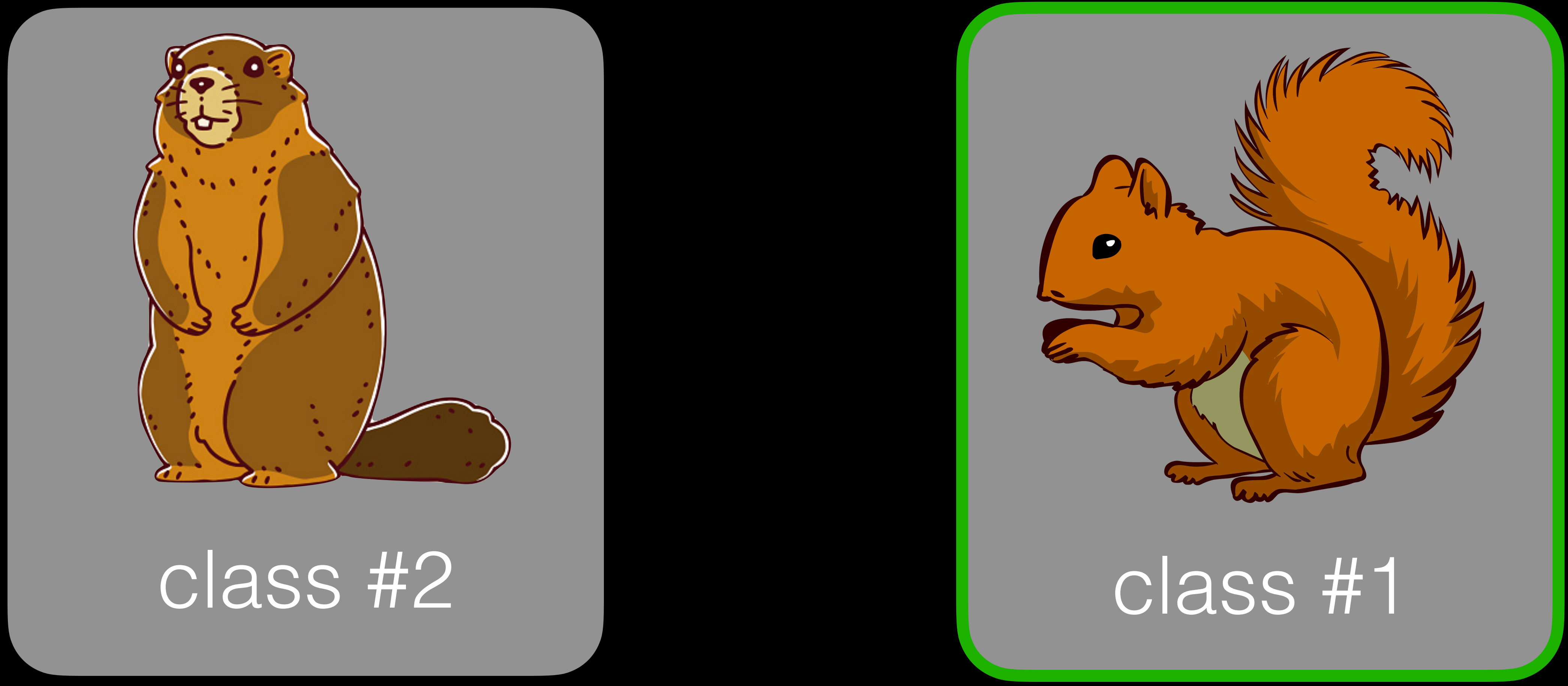
Conformal Prediction: Train-Time



$$s(x) = p(y = 2 \mid x) + p(y = 1 \mid x)$$

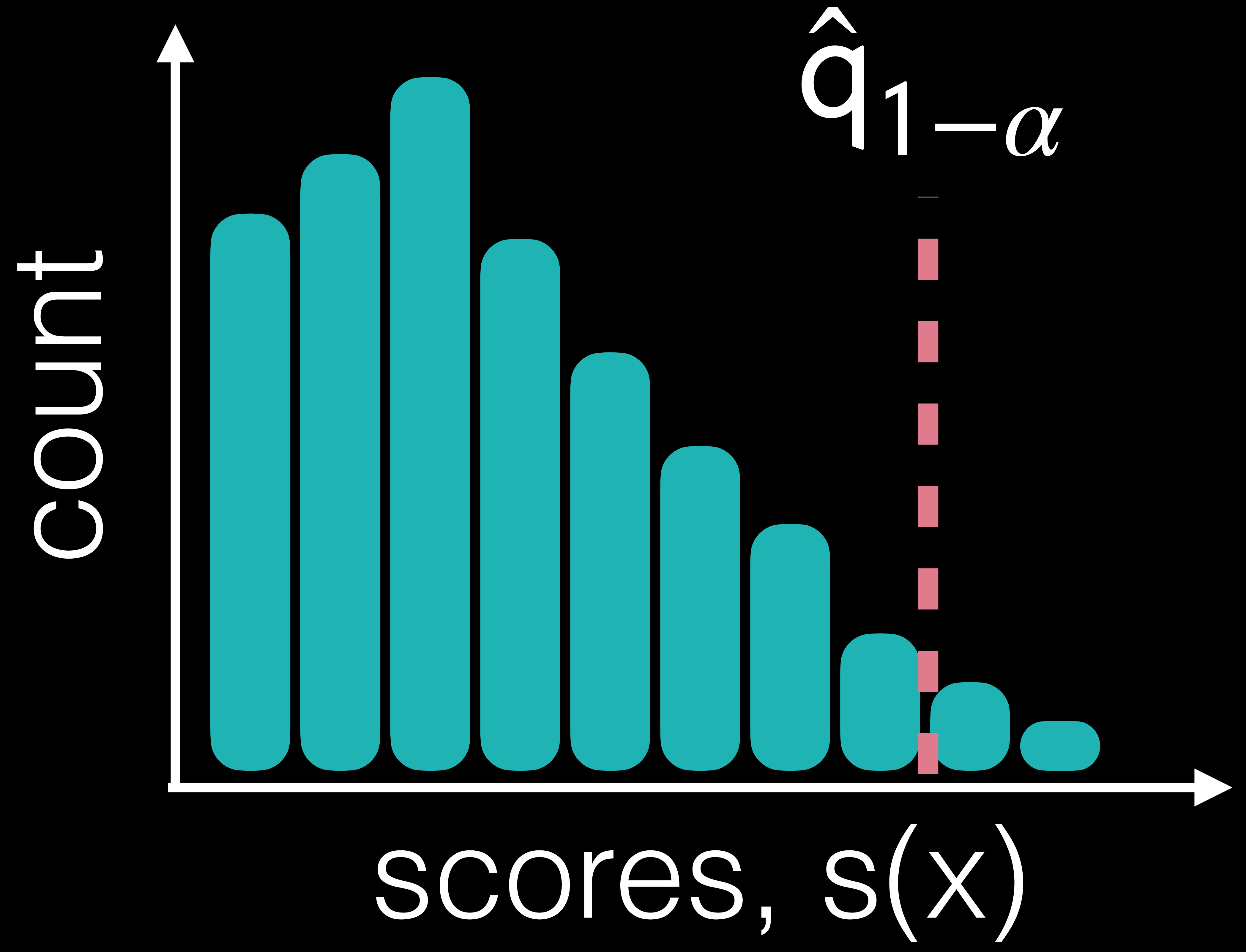
ii) sum the probabilities (decreasing order) until the true-class is included.

Conformal Prediction: Train-Time

$$s(x) = p(y = 2 \mid x) + p(y = 1 \mid x)$$

iii) compute the (1-α)-quantile of the scores across the held-out set.

Conformal Prediction: Train-Time



iv) compute the (1-α)-quantile of the scores.

Conformal Prediction: Test-Time

$p(y = 1 \mid x)$ $p(y = 2 \mid x)$ $p(y = 3 \mid x)$

i) rank classes by model probabilities.

Conformal Prediction: Test-Time

$$p(y = 3 \mid x) > p(y = 2 \mid x) > p(y = 1 \mid x)$$

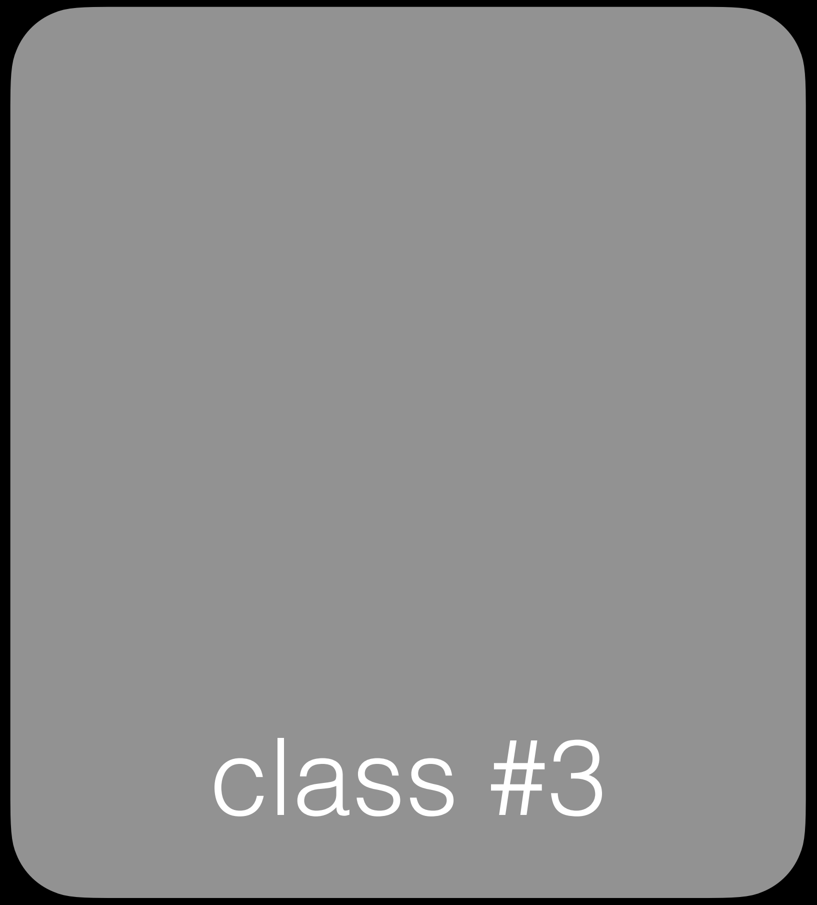
i) rank classes by model probabilities.

Conformal Prediction: Test-Time

$$p(y = 3 \mid x) > p(y = 2 \mid x) > p(y = 1 \mid x)$$

ii) $C(x) = \left\{ \qquad\qquad \right\}$ checking if $\sum_{y \in C(x)} p(y \mid x) \overset{?}{\geq} \hat{q}_{1-\alpha}$

Conformal Prediction: Test-Time



$$p(y = 3 | x) > p(y = 2 | x) > p(y = 1 | x)$$

ii) $C(x) = \{$ $\}$ checking if $\sum_{y \in C(x)} p(y | x) \overset{?}{\geq} \hat{q}_{1-\alpha}$

Conformal Prediction: Test-Time

class #3

class #2

Class #1

$$p(y = 3 \mid x) > p(y = 2 \mid x) > p(y = 1 \mid x)$$

ii) $C(x) = \{$ $\}$ checking if $\sum_{y \in C(x)} p(y \mid x) \geq \hat{q}_{1-\alpha}$ ✗

Conformal Prediction: Test-Time

class #3

class #2

Class #1

$$p(y = 3 \mid x) > p(y = 2 \mid x) > p(y = 1 \mid x)$$

ii) $C(x) = \Big\{$ $\Big\}$ checking if $\sum_{y \in C(x)} p(y \mid x) \overset{?}{\geq} \hat{q}_{1-\alpha}$

Conformal Prediction: Test-Time

class #3
class #2
Class #1

$$p(y = 3 \mid x) > p(y = 2 \mid x) > p(y = 1 \mid x)$$

ii) $C(x) = \{$ $\}$ checking if $\sum_{y \in C(x)} p(y \mid x) \geq \hat{q}_{1-\alpha}$ ✓

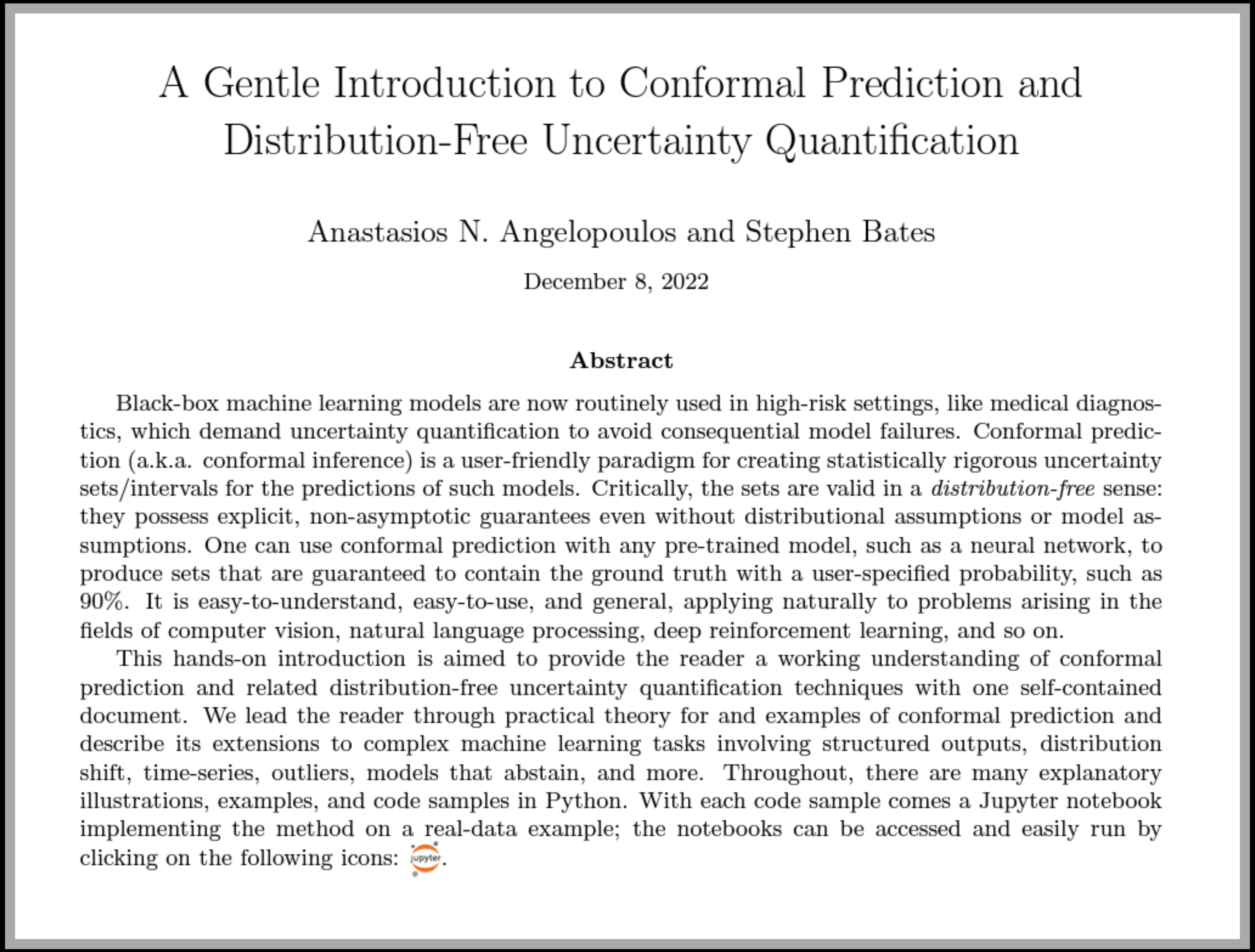
Conformal Prediction: Test-Time

$C(x) = \{$ $\}$

$y = 3$ $y = 2$

true label is guaranteed to be in this set (1-α)% of the time, on average over the test set.

Further Reading



A Gentle Introduction to Conformal Prediction and Distribution-Free Uncertainty Quantification

Anastasios N. Angelopoulos and Stephen Bates

December 8, 2022

Abstract

Black-box machine learning models are now routinely used in high-risk settings, like medical diagnostics, which demand uncertainty quantification to avoid consequential model failures. Conformal prediction (a.k.a. conformal inference) is a user-friendly paradigm for creating statistically rigorous uncertainty sets/intervals for the predictions of such models. Critically, the sets are valid in a *distribution-free* sense: they possess explicit, non-asymptotic guarantees even without distributional assumptions or model assumptions. One can use conformal prediction with any pre-trained model, such as a neural network, to produce sets that are guaranteed to contain the ground truth with a user-specified probability, such as 90%. It is easy-to-understand, easy-to-use, and general, applying naturally to problems arising in the fields of computer vision, natural language processing, deep reinforcement learning, and so on.

This hands-on introduction is aimed to provide the reader a working understanding of conformal prediction and related distribution-free uncertainty quantification techniques with one self-contained document. We lead the reader through practical theory for and examples of conformal prediction and describe its extensions to complex machine learning tasks involving structured outputs, distribution shift, time-series, outliers, models that abstain, and more. Throughout, there are many explanatory illustrations, examples, and code samples in Python. With each code sample comes a Jupyter notebook implementing the method on a real-data example; the notebooks can be accessed and easily run by clicking on the following icons: .

Practical Methods for UQ

- ⊗ Frequentism
  - bootstrap aggregation (bagging)
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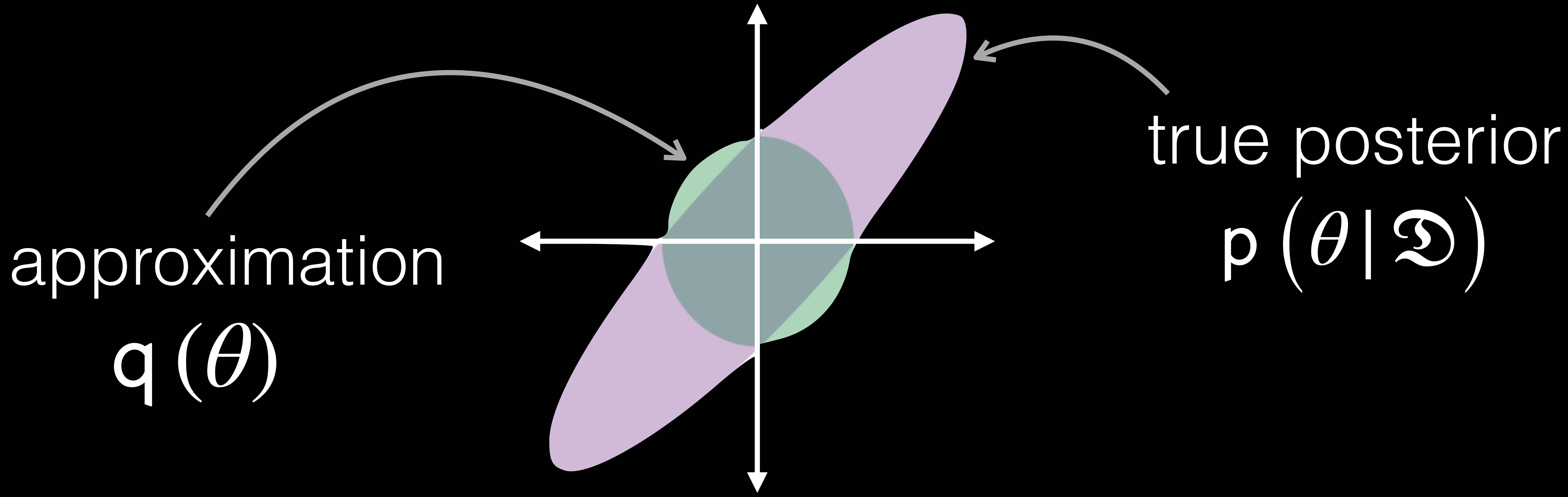
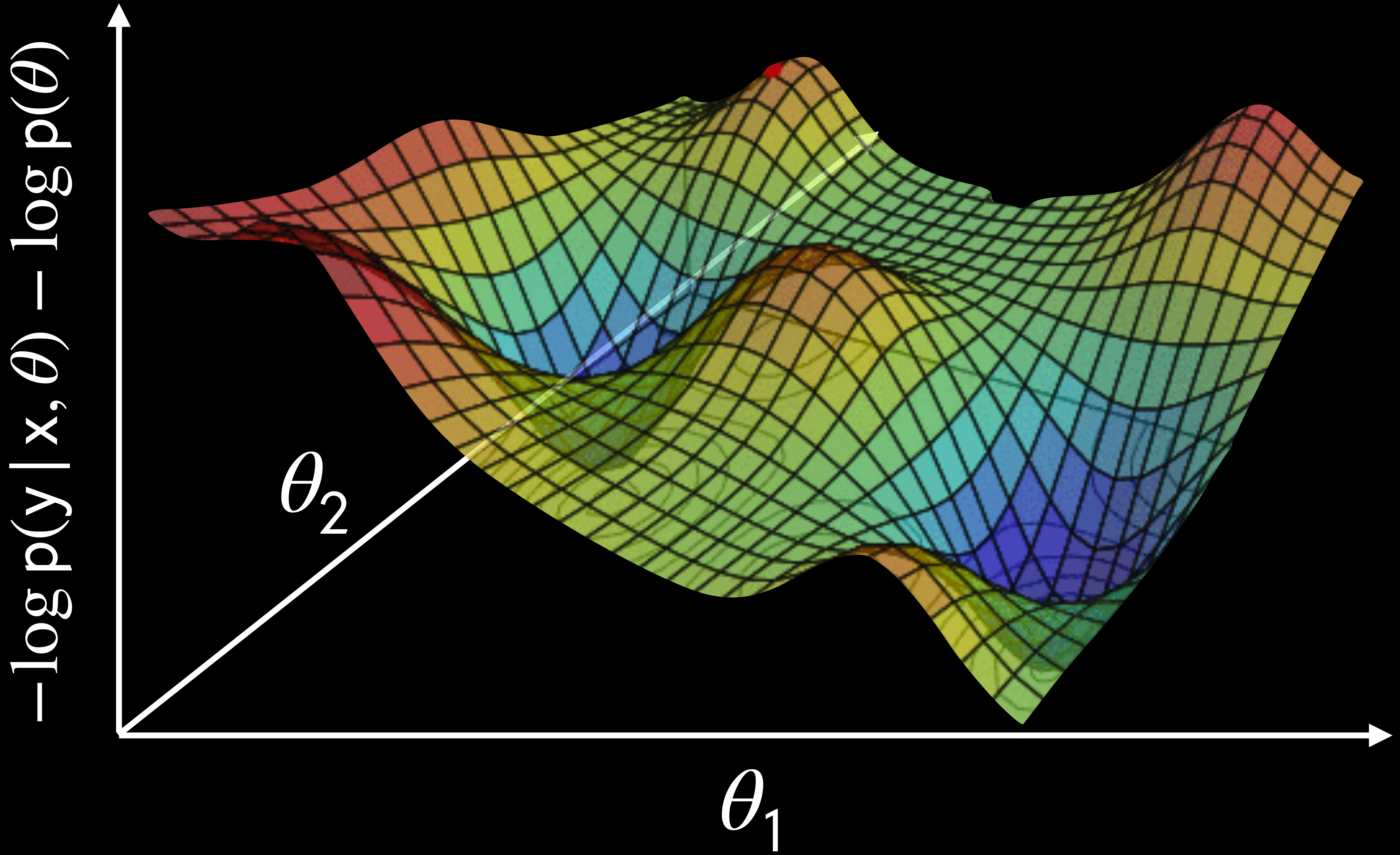
Variational Inference

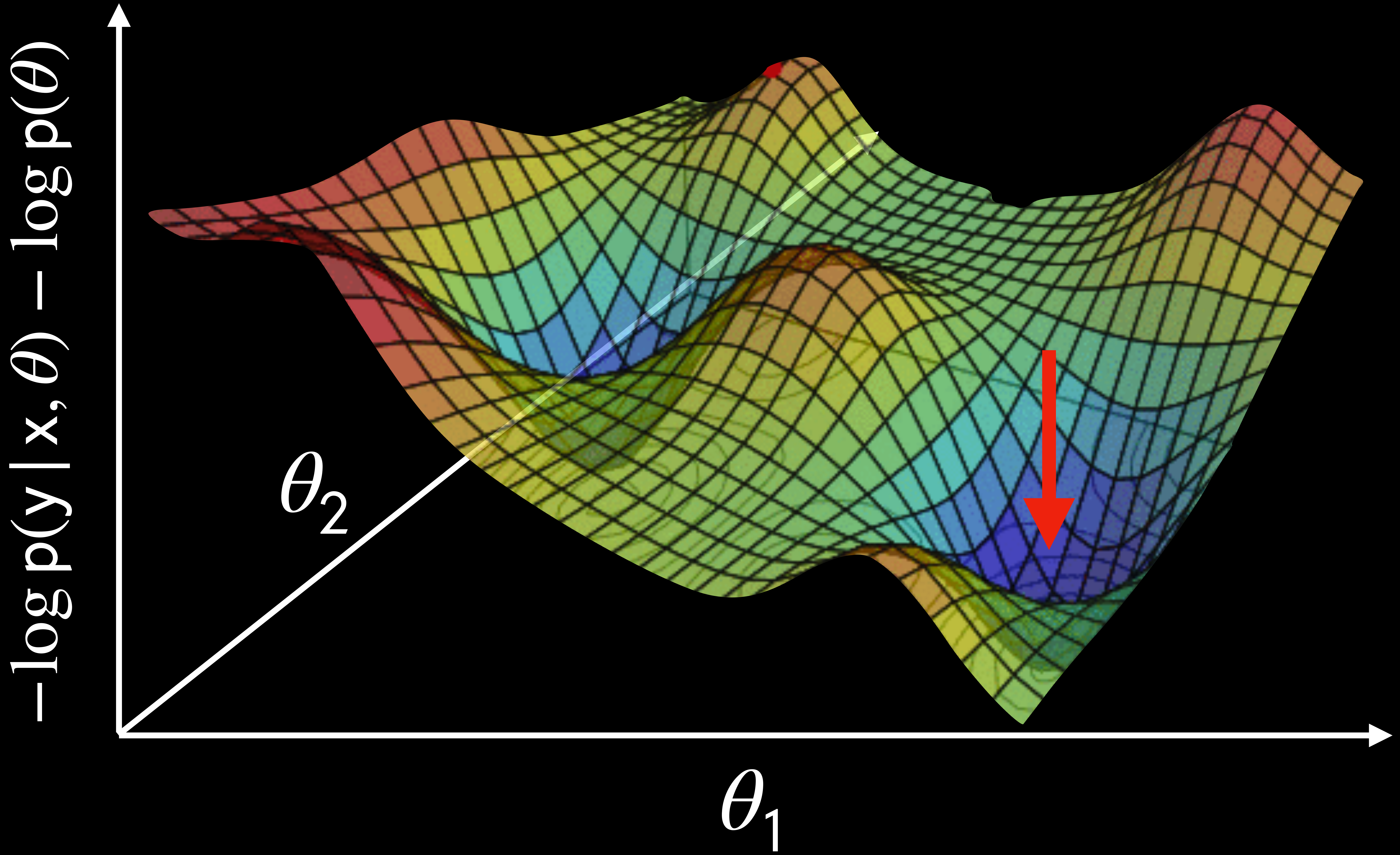
construct a tractable approximation to the Bayesian posterior distribution.



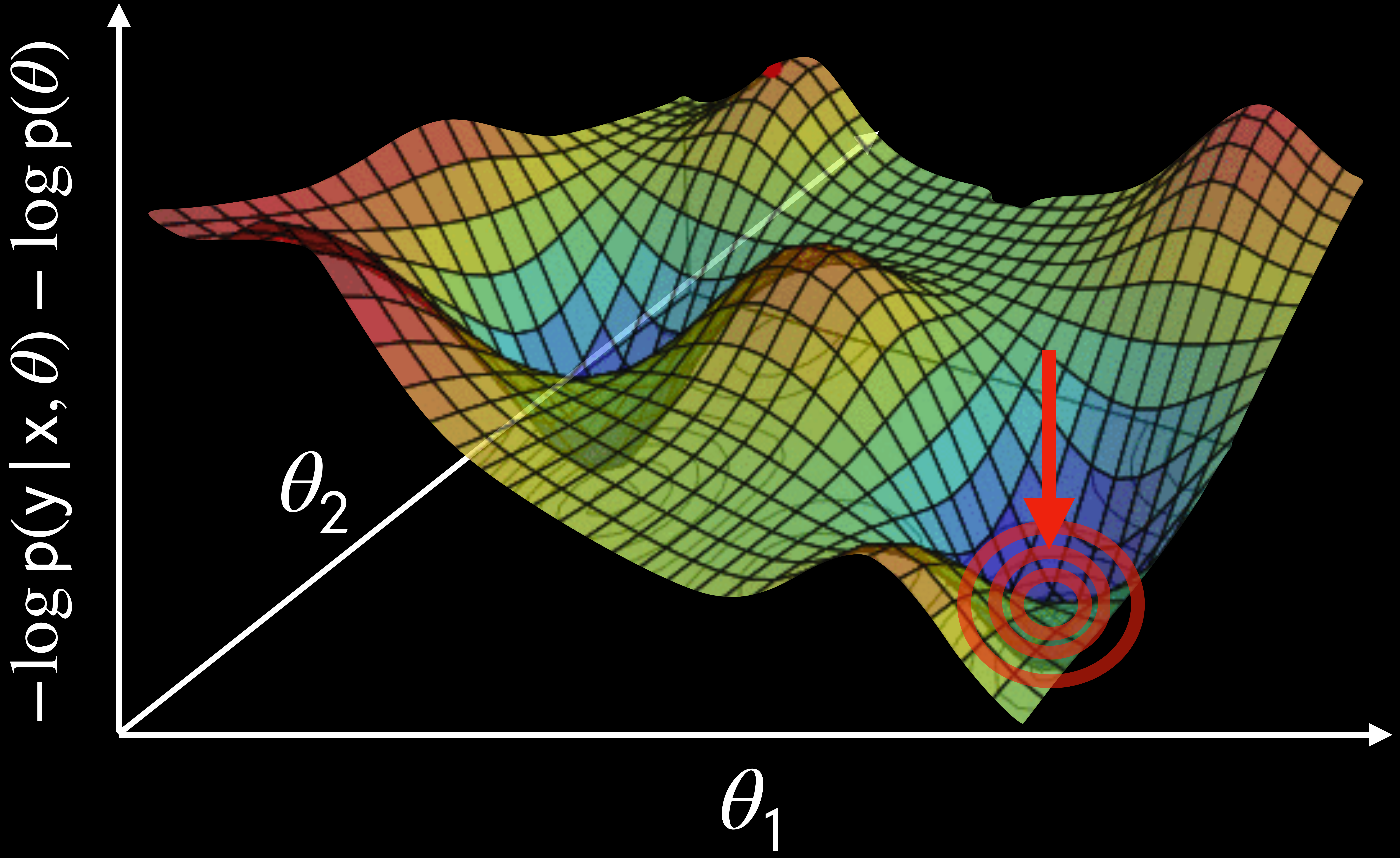
Laplace Approximation



Laplace Approximation



Laplace Approximation



Laplace Approximation

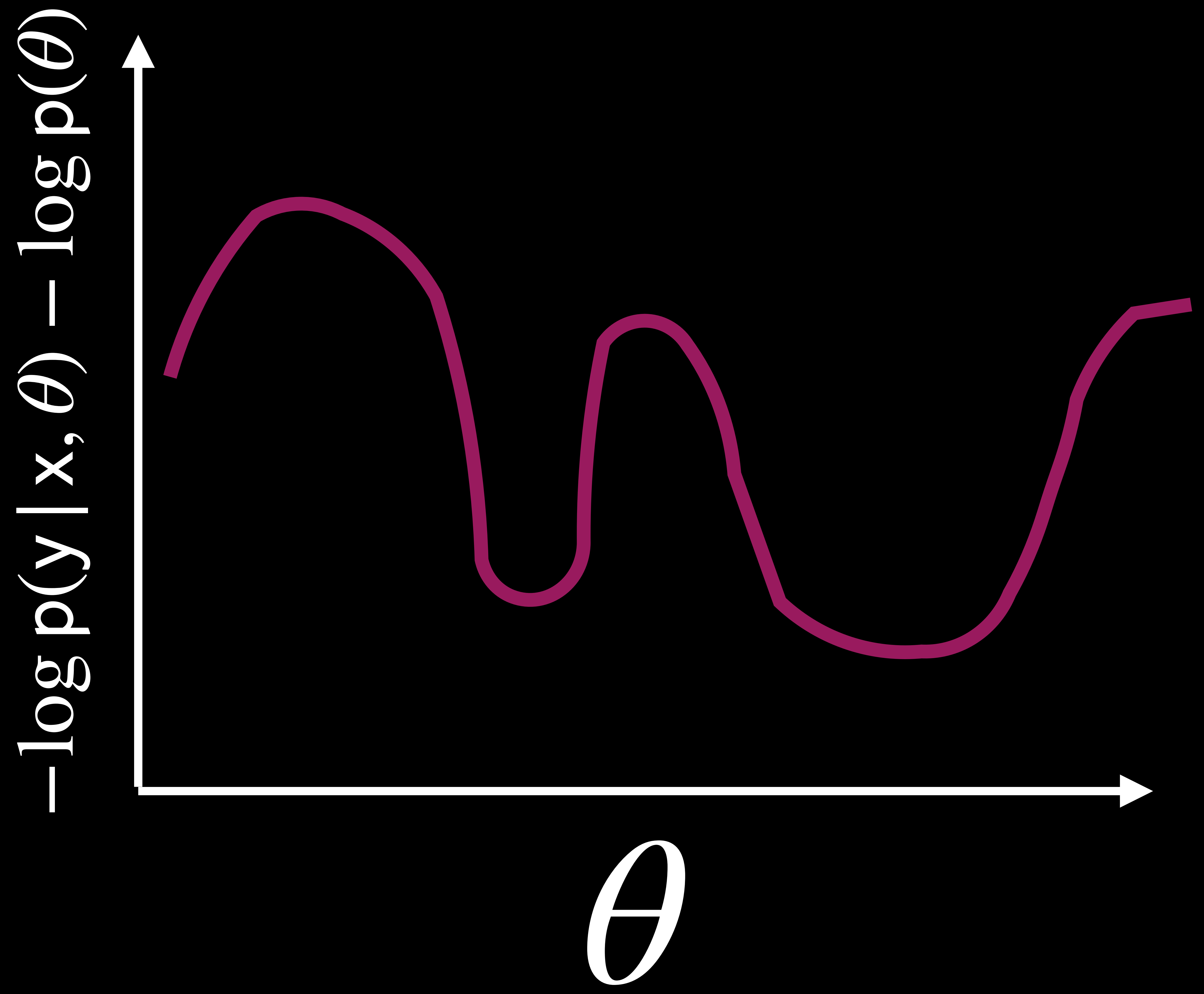
$$\mathsf{p}\left(\theta \,|\, \mathfrak{D}\right) \approx \mathsf{N}\left(\hat{\theta}_{\mathsf{MAP}}, \mathsf{H}^{-1}(\hat{\theta}_{\mathsf{MAP}})\right)$$

Laplace Approximation

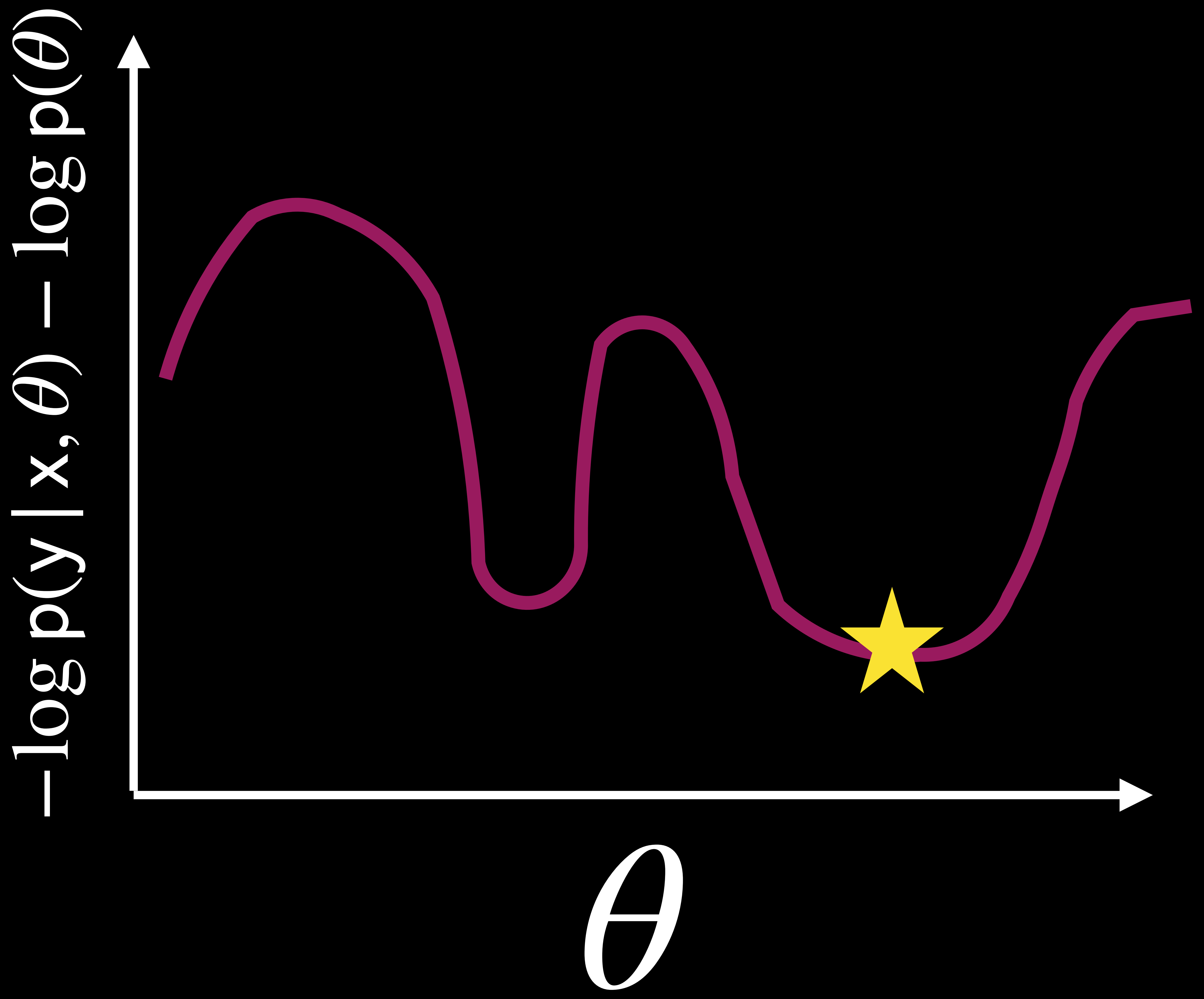
$$\mathsf{p}\left(\theta \,|\, \mathfrak{D}\right) \approx \mathsf{N}\left(\hat{\theta}_{\mathsf{MAP}}, \mathsf{H}^{-1}(\hat{\theta}_{\mathsf{MAP}})\right)$$

$$\mathsf{H}(\theta) = -\sum_{n=1}^{N} \frac{\partial^2 \left\{\log \mathsf{p}(\mathsf{y}_n \,|\, \mathsf{x}_n, \theta) + \log p(\theta)\right\}}{\partial\, \theta^2}$$

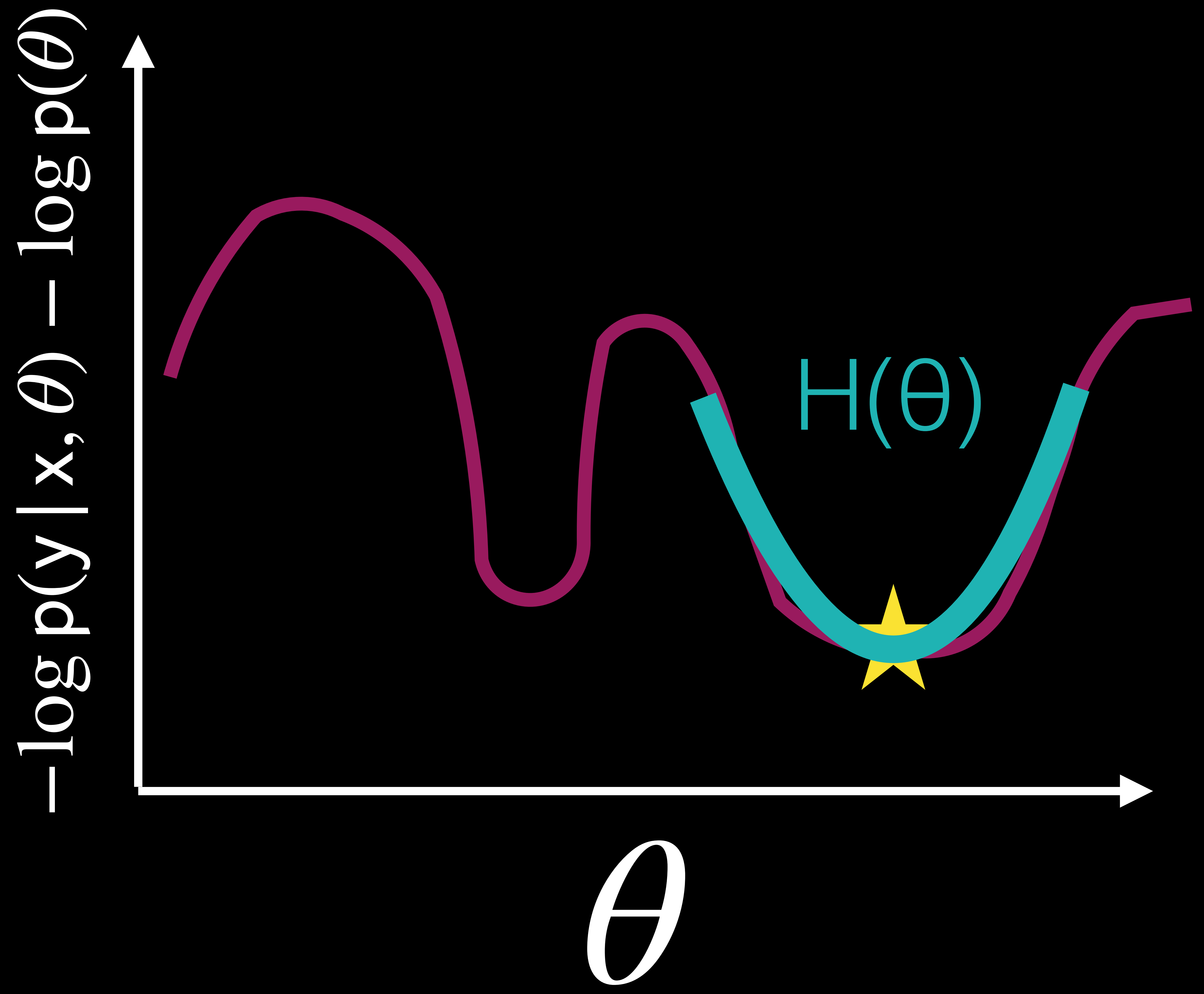
Laplace Approximation



Laplace Approximation



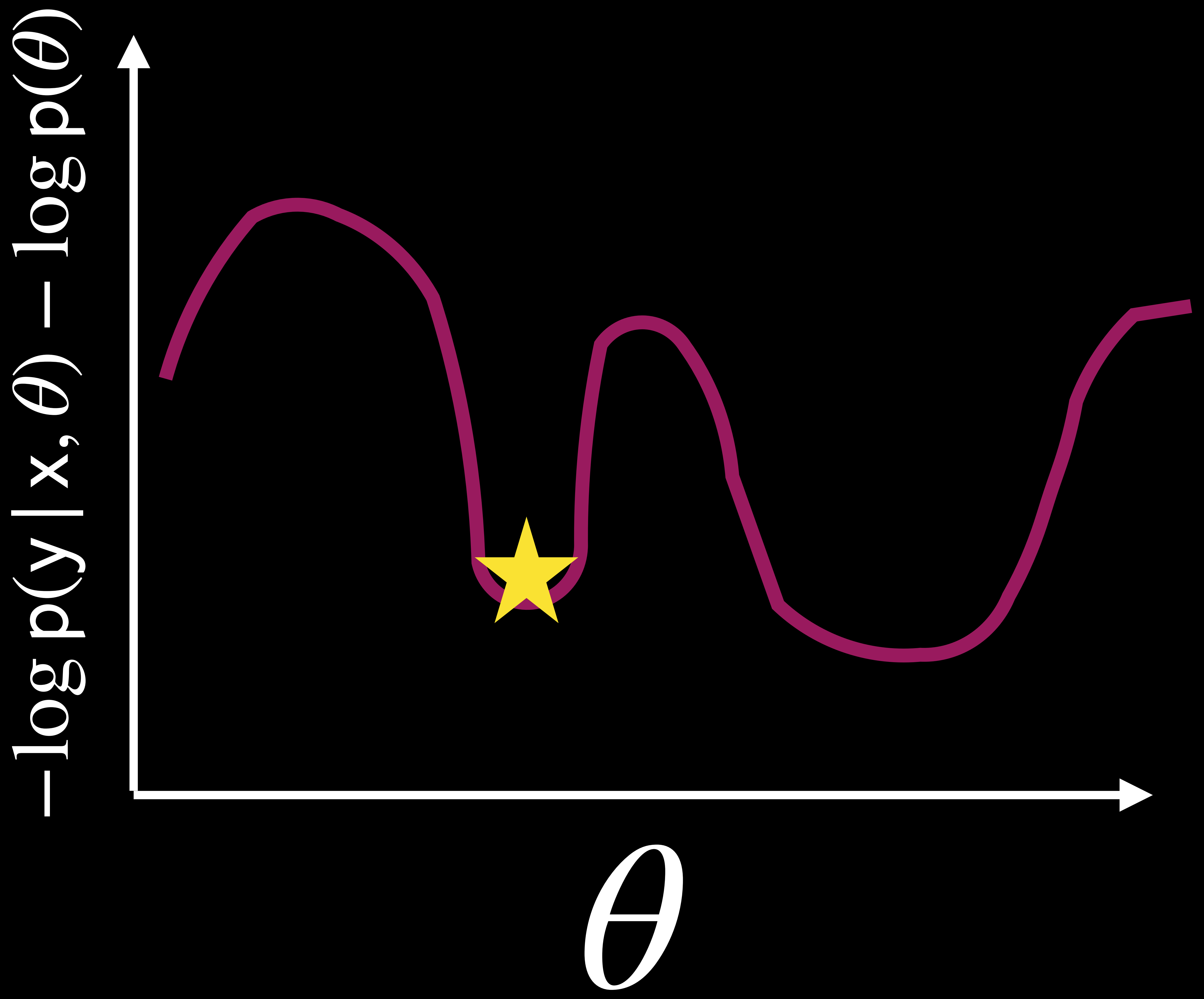
Laplace Approximation



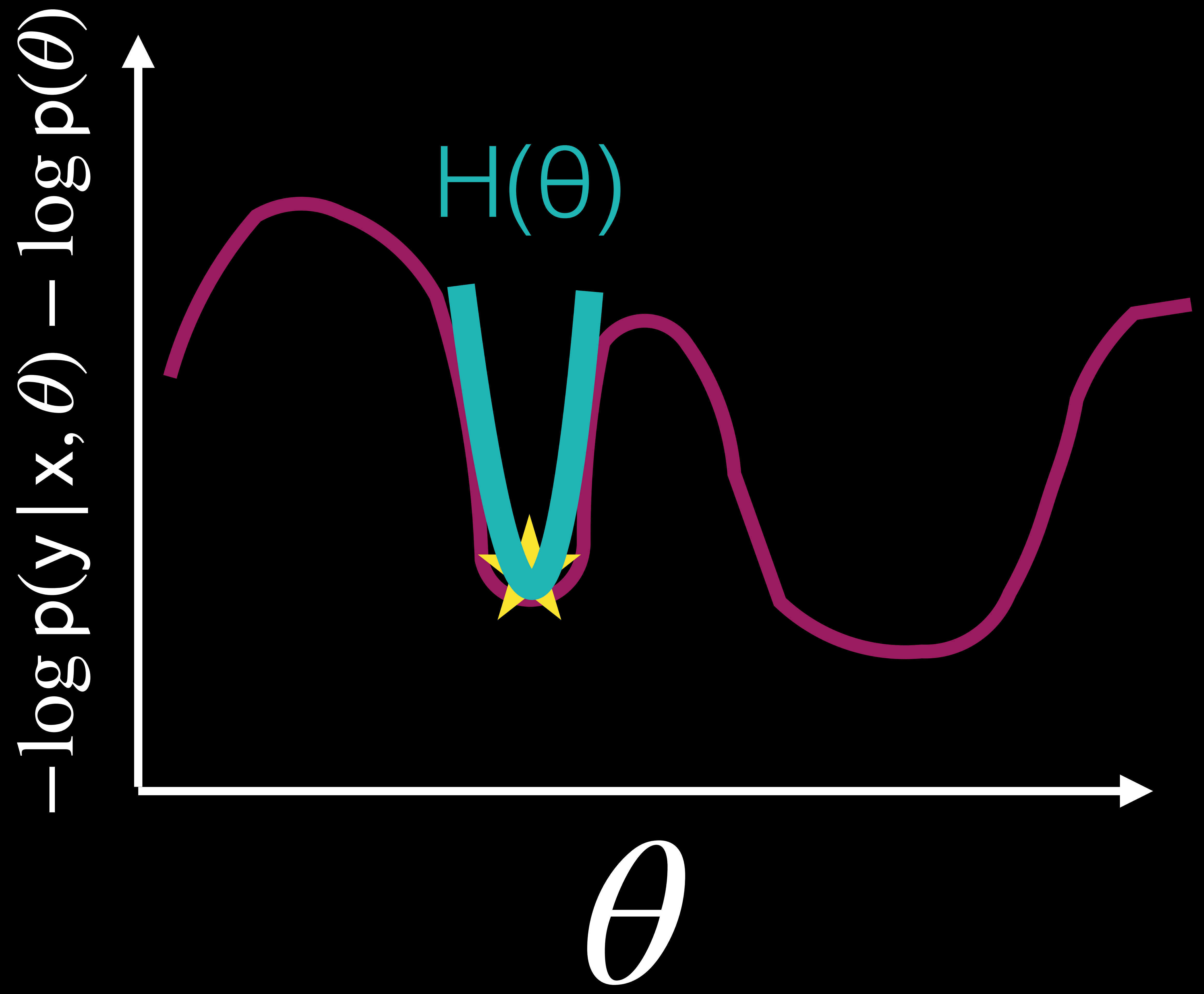
small curvature,
large posterior variance

$$N\left(\hat{\theta}_{\text{MAP}}, H^{-1}(\hat{\theta}_{\text{MAP}})\right)$$

Laplace Approximation



Laplace Approximation



large curvature,
small posterior variance

$$N\left(\hat{\theta}_{\mathrm{MAP}}, H^{-1}(\hat{\theta}_{\mathrm{MAP}})\right)$$

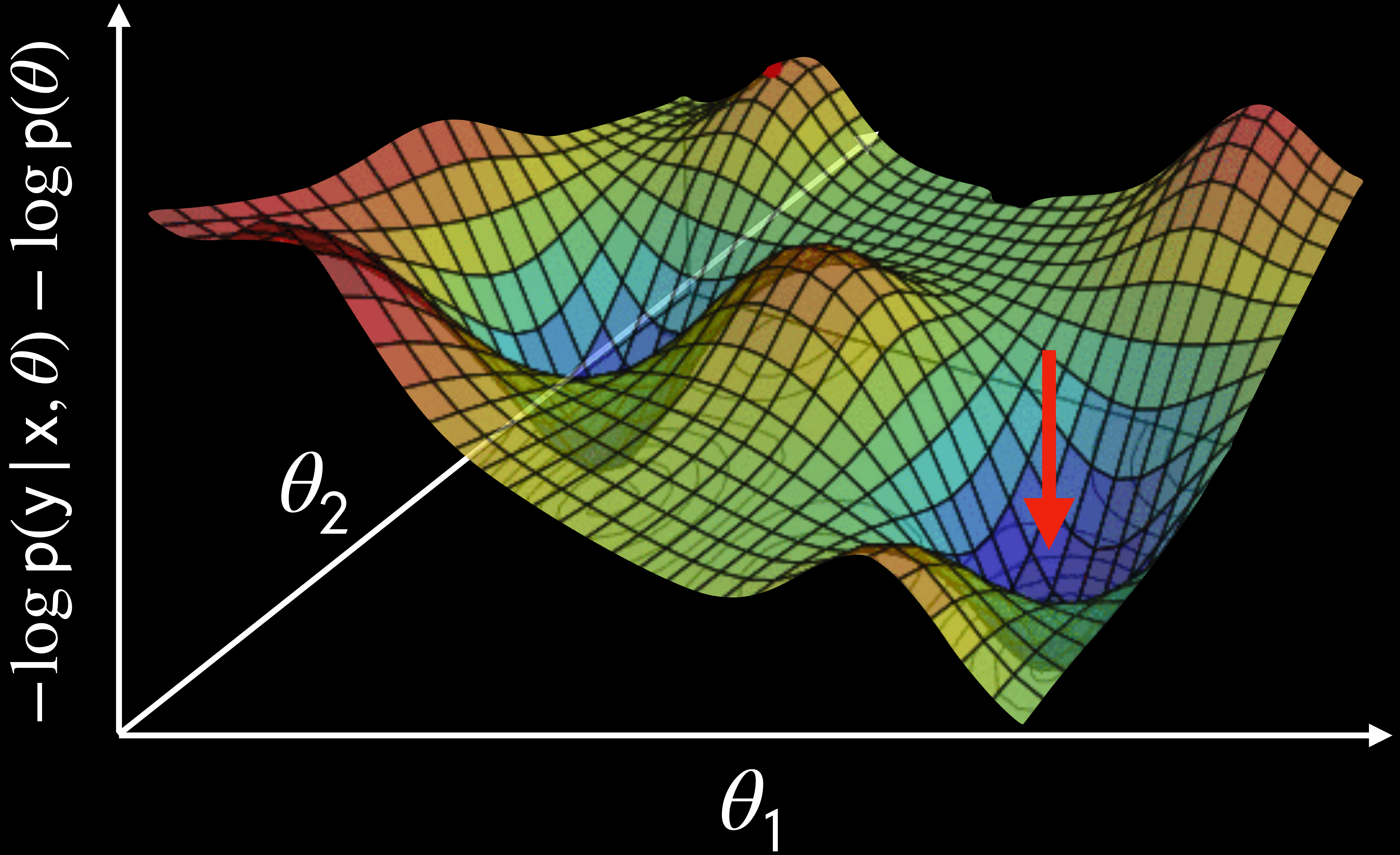
Laplace Approximation

compute predictive distribution using posterior approximation

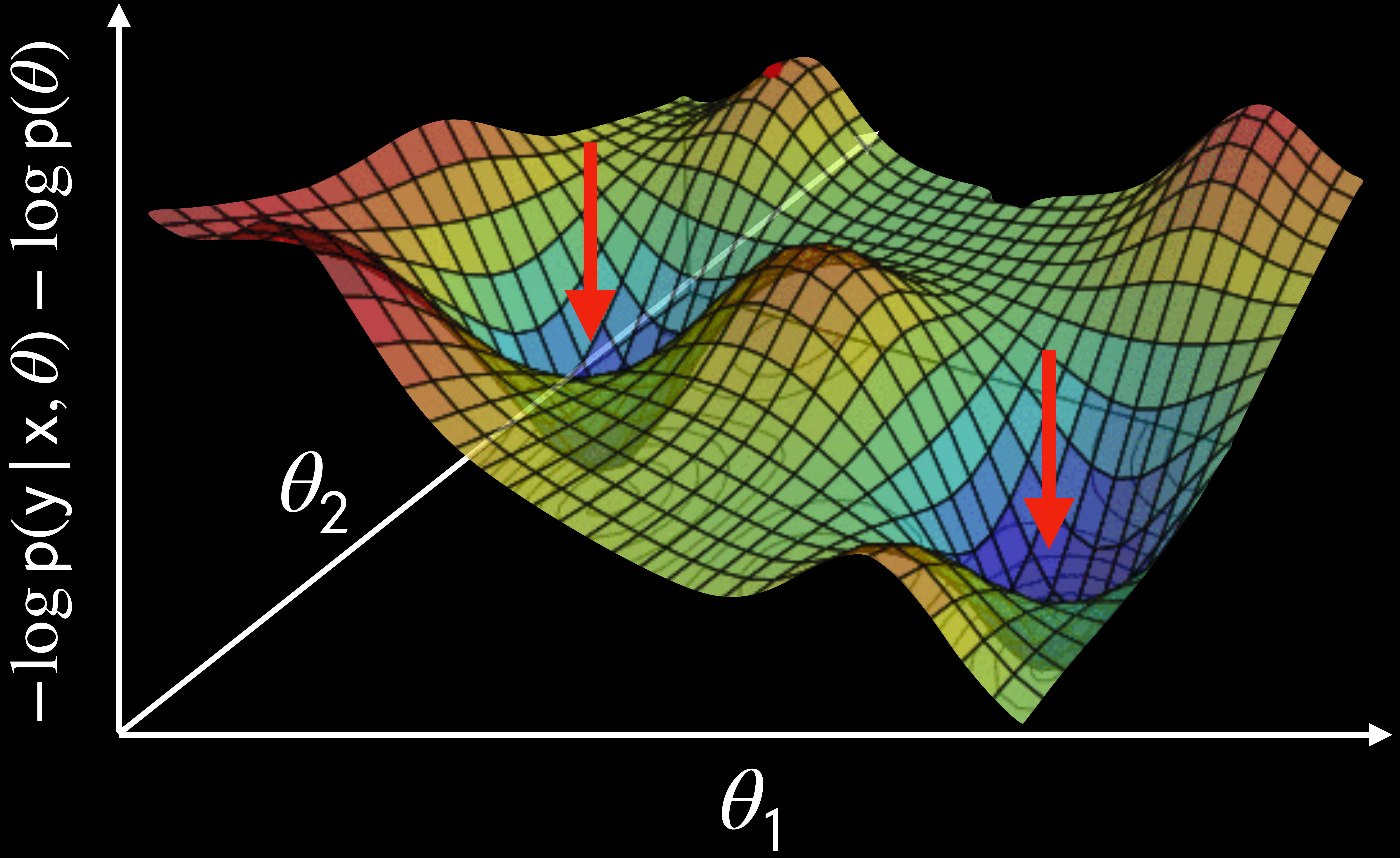
$$\mathrm{p}\left(\tilde{\mathrm{y}}\,|\,\tilde{\mathrm{x}},\mathfrak{D}\right) \approx \int_\theta \mathrm{p}\left(\tilde{\mathrm{y}}\,|\,\tilde{\mathrm{x}},\theta\right)\ \mathrm{N}\left(\hat{\theta}_{\mathrm{MAP}},\ \mathrm{H}^{-1}(\hat{\theta}_{\mathrm{MAP}})\right)\ \mathrm{d}\theta$$

might need to approximate integral with sampling

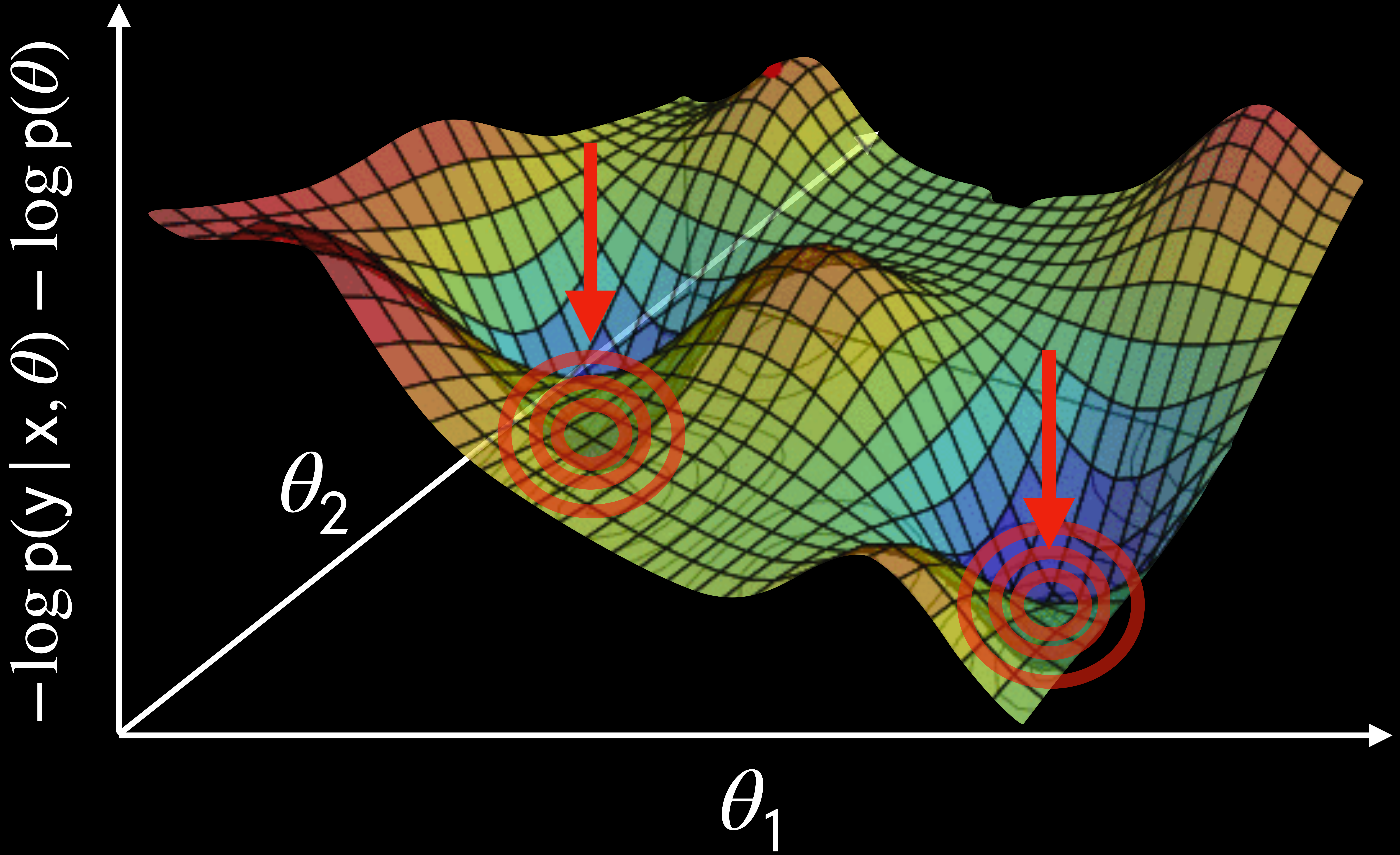
Laplace Approximation



Laplace Approximation



Laplace Approximation

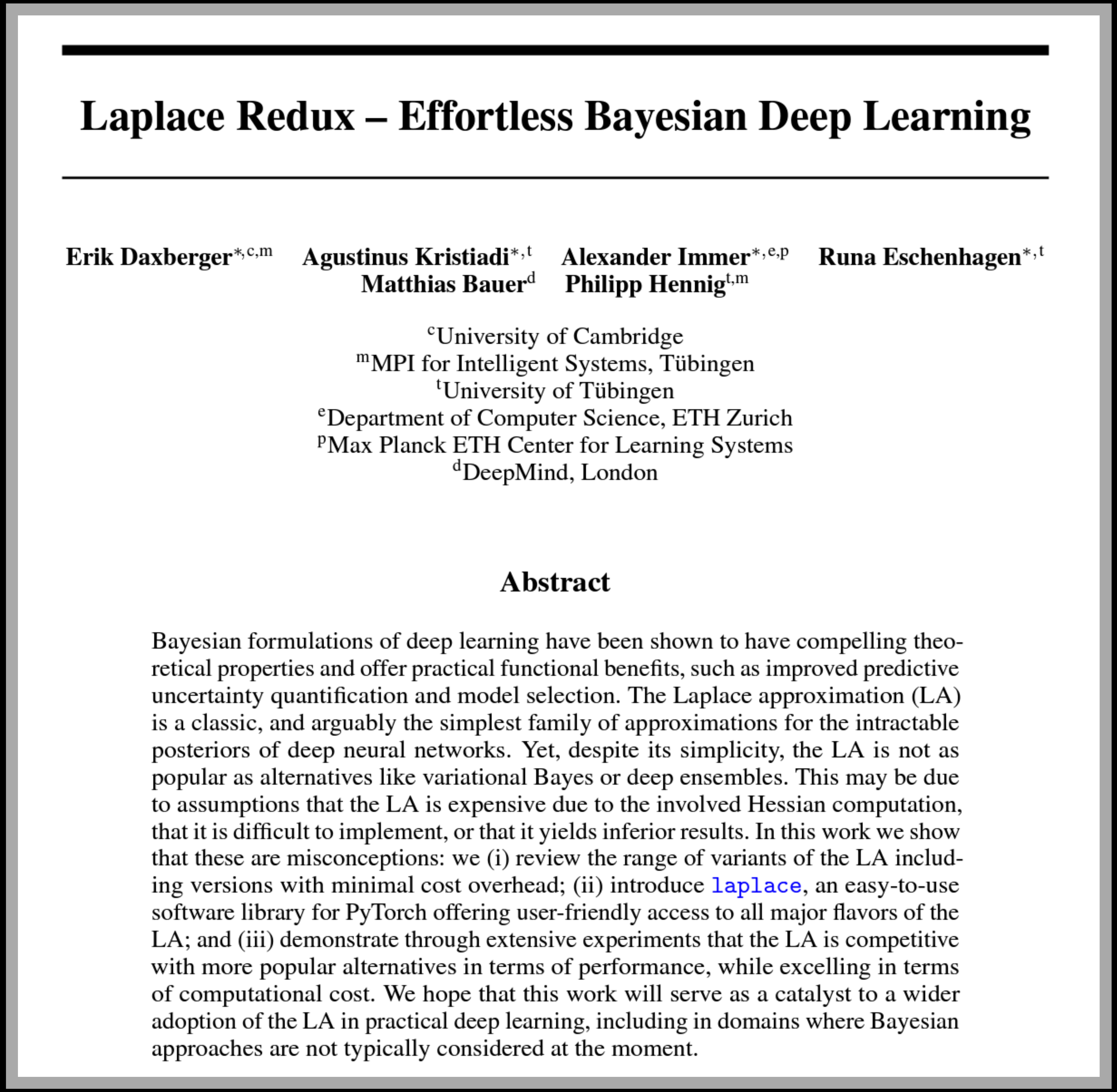


Sample-then-Optimize Laplace Approximation

$$\begin{tikzcd}
 & \bar{\theta}_1 \arrow[r, "\text{optimize}"] & \hat{\theta}_1 & \\
p(\theta) \arrow[ur, "\text{sample}"] \arrow[dr, "\text{sample}"'] & \vdots & \vdots & p(\theta \mid \mathfrak{D}) \approx \frac{1}{K}\sum_{k=1}^{K} N\left(\hat{\theta}_k, H^{-1}(\hat{\theta}_k)\right) \\
 & \bar{\theta}_K \arrow[r, "\text{optimize}"] & \hat{\theta}_K &
\end{tikzcd}$$

Bayesian prior

Further Reading



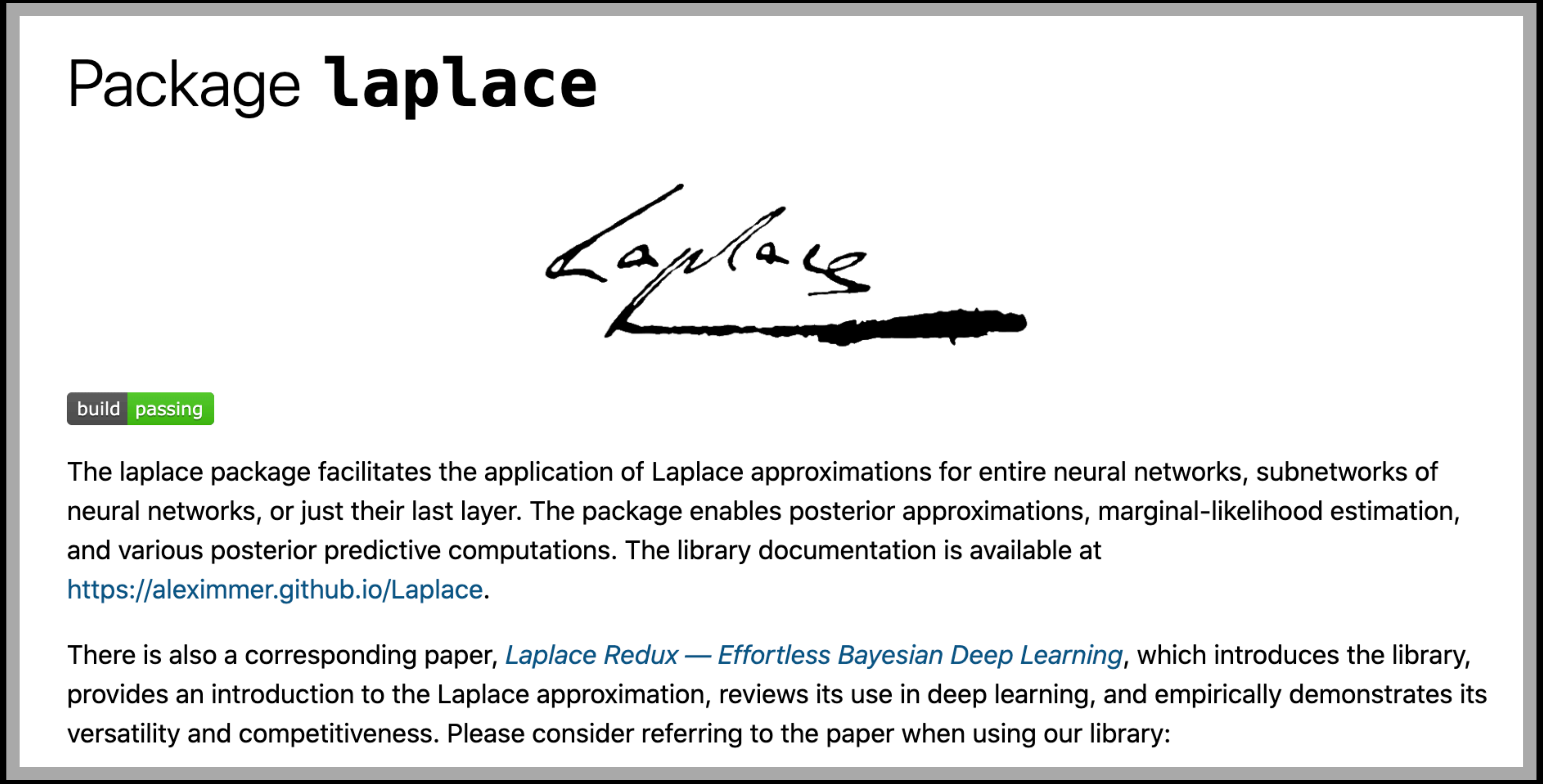
Laplace Redux – Effortless Bayesian Deep Learning

Erik Daxberger[*,c,m] Agustinus Kristiadi[*,t] Alexander Immer[*,e,p] Runa Eschenhagen[*,t]
Matthias Bauer[d] Philipp Hennig[t,m]

[c]University of Cambridge
[m]MPI for Intelligent Systems, Tübingen
[t]University of Tübingen
[e]Department of Computer Science, ETH Zurich
[p]Max Planck ETH Center for Learning Systems
[d]DeepMind, London

Abstract

Bayesian formulations of deep learning have been shown to have compelling theoretical properties and offer practical functional benefits, such as improved predictive uncertainty quantification and model selection. The Laplace approximation (LA) is a classic, and arguably the simplest family of approximations for the intractable posteriors of deep neural networks. Yet, despite its simplicity, the LA is not as popular as alternatives like variational Bayes or deep ensembles. This may be due to assumptions that the LA is expensive due to the involved Hessian computation, that it is difficult to implement, or that it yields inferior results. In this work we show that these are misconceptions: we (i) review the range of variants of the LA including versions with minimal cost overhead; (ii) introduce `laplace`, an easy-to-use software library for PyTorch offering user-friendly access to all major flavors of the LA; and (iii) demonstrate through extensive experiments that the LA is competitive with more popular alternatives in terms of performance, while excelling in terms of computational cost. We hope that this work will serve as a catalyst to a wider adoption of the LA in practical deep learning, including in domains where Bayesian approaches are not typically considered at the moment.



Package **`laplace`**

build passing

The laplace package facilitates the application of Laplace approximations for entire neural networks, subnetworks of neural networks, or just their last layer. The package enables posterior approximations, marginal-likelihood estimation, and various posterior predictive computations. The library documentation is available at https://aleximmer.github.io/Laplace.

There is also a corresponding paper, *Laplace Redux — Effortless Bayesian Deep Learning*, which introduces the library, provides an introduction to the Laplace approximation, reviews its use in deep learning, and empirically demonstrates its versatility and competitiveness. Please consider referring to the paper when using our library:

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- conformal prediction

⊗ Bayesianism

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Practical Methods for UQ: Summary

⊗ Frequentism
- need to do more than maximum likelihood
- extra data: synthesized or from held-out set

⊗ Bayesianism
- need to do less for the sake of computation
- construct approximations localized to areas of high posterior density.

Hybrid Methods for UQ

can mix Bayesian and frequentist procedures!

- ⊗ data augmentation: sampling new data by applying bespoke transformations to original dataset.

- ⊗ apply conformal prediction to posterior predictive distribution: frequentist correction to a Bayesian model

IV. Evaluating Uncertainty Quantification

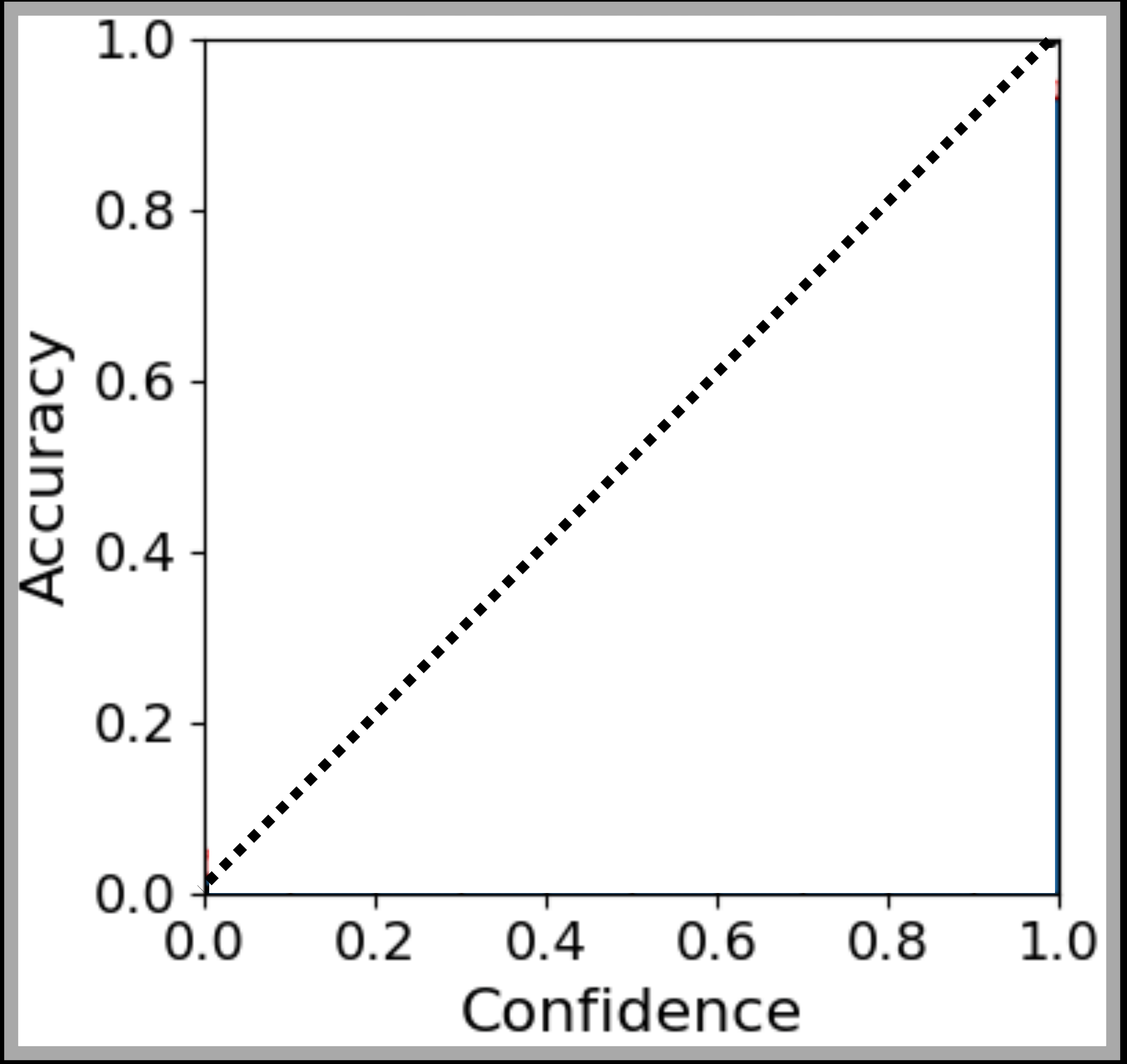
Evaluating UQ

- ⊗ Calibration: can the model forecast its own performance?
- ⊗ Coverage: does the model meet the given error level?

Calibration

does the model confidence reflect its empirical accuracy?

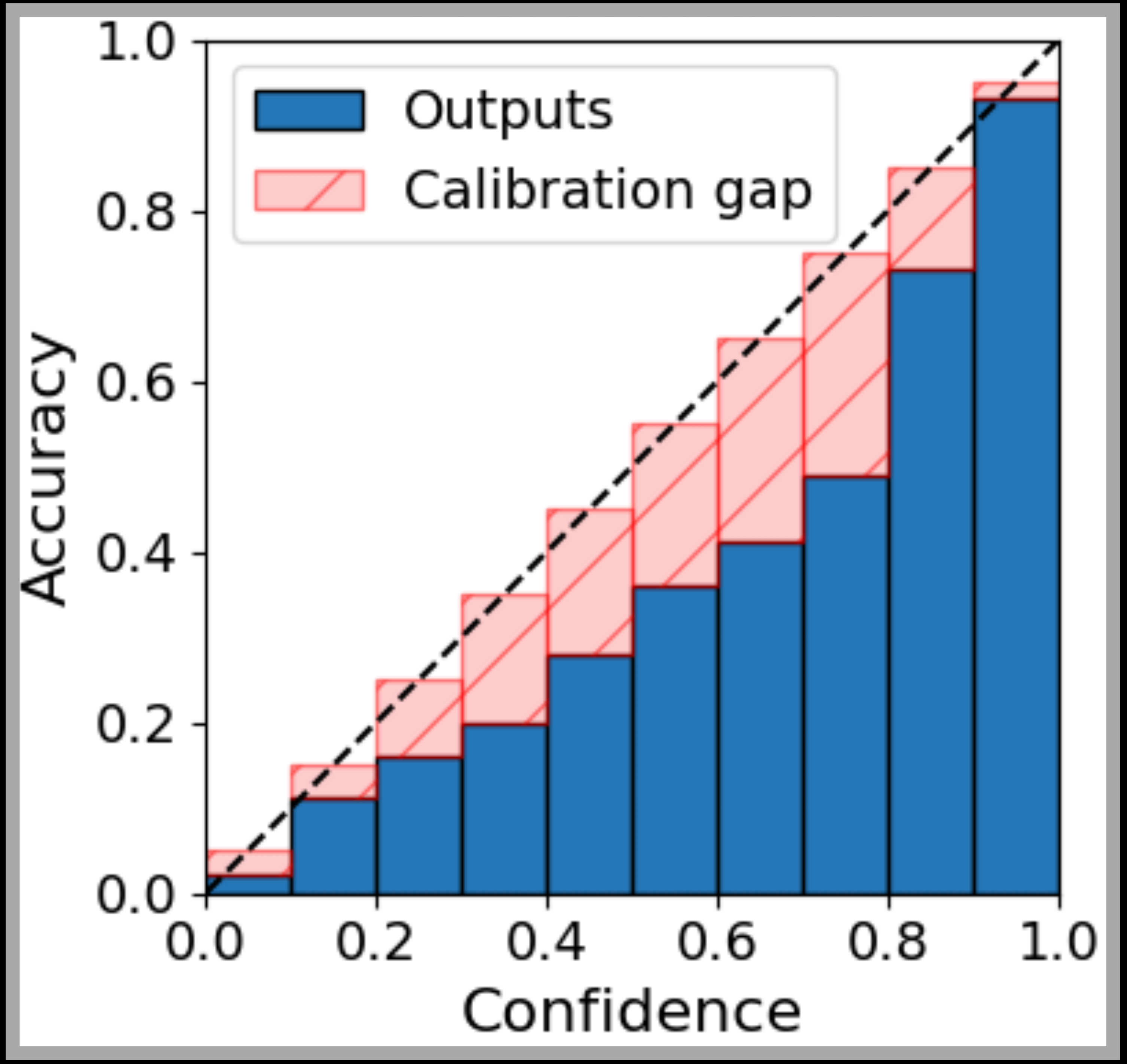
reliability diagram



Calibration

does the model confidence reflect its empirical accuracy?

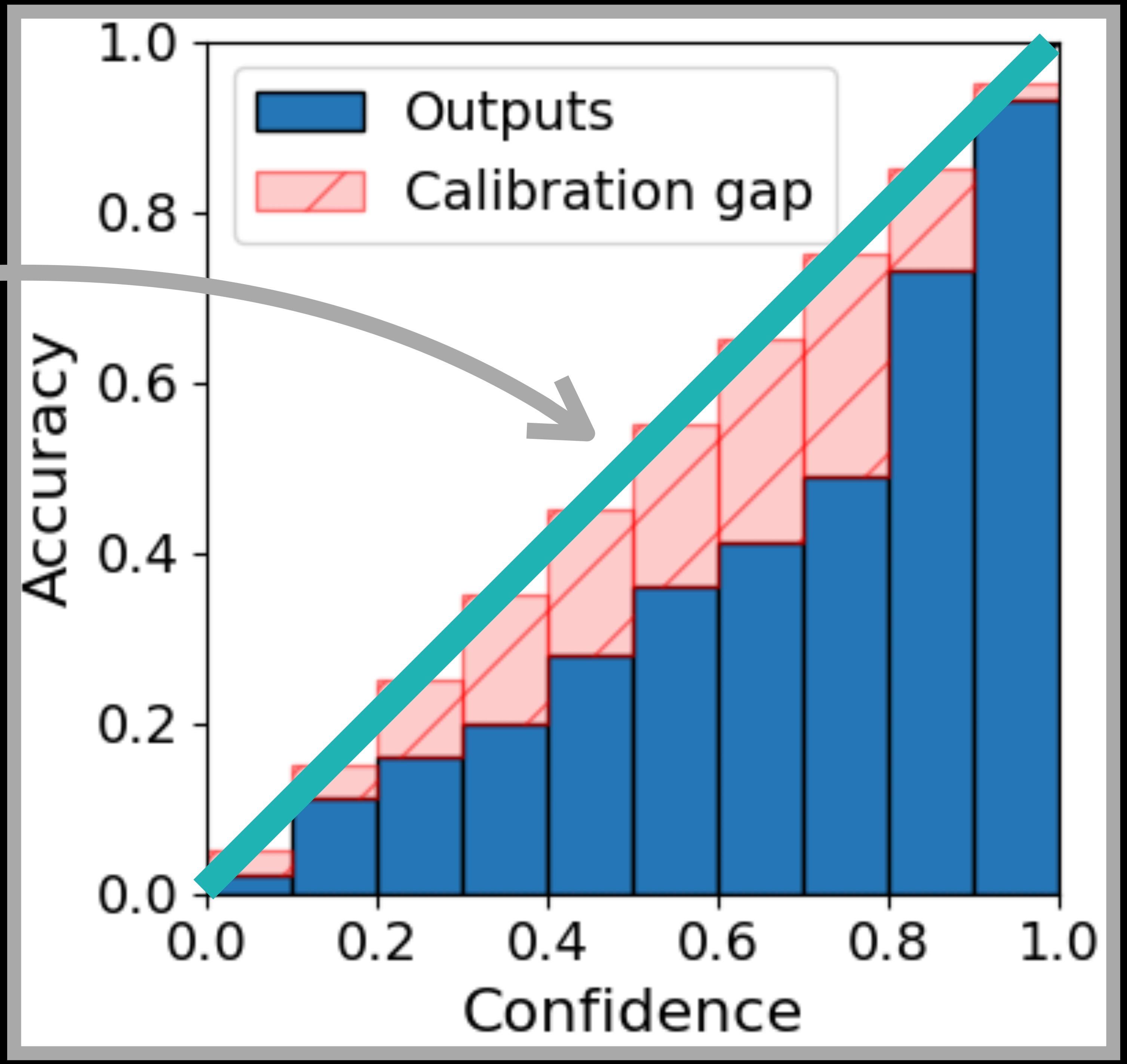
reliability diagram



Calibration

does the model confidence reflect its empirical accuracy?

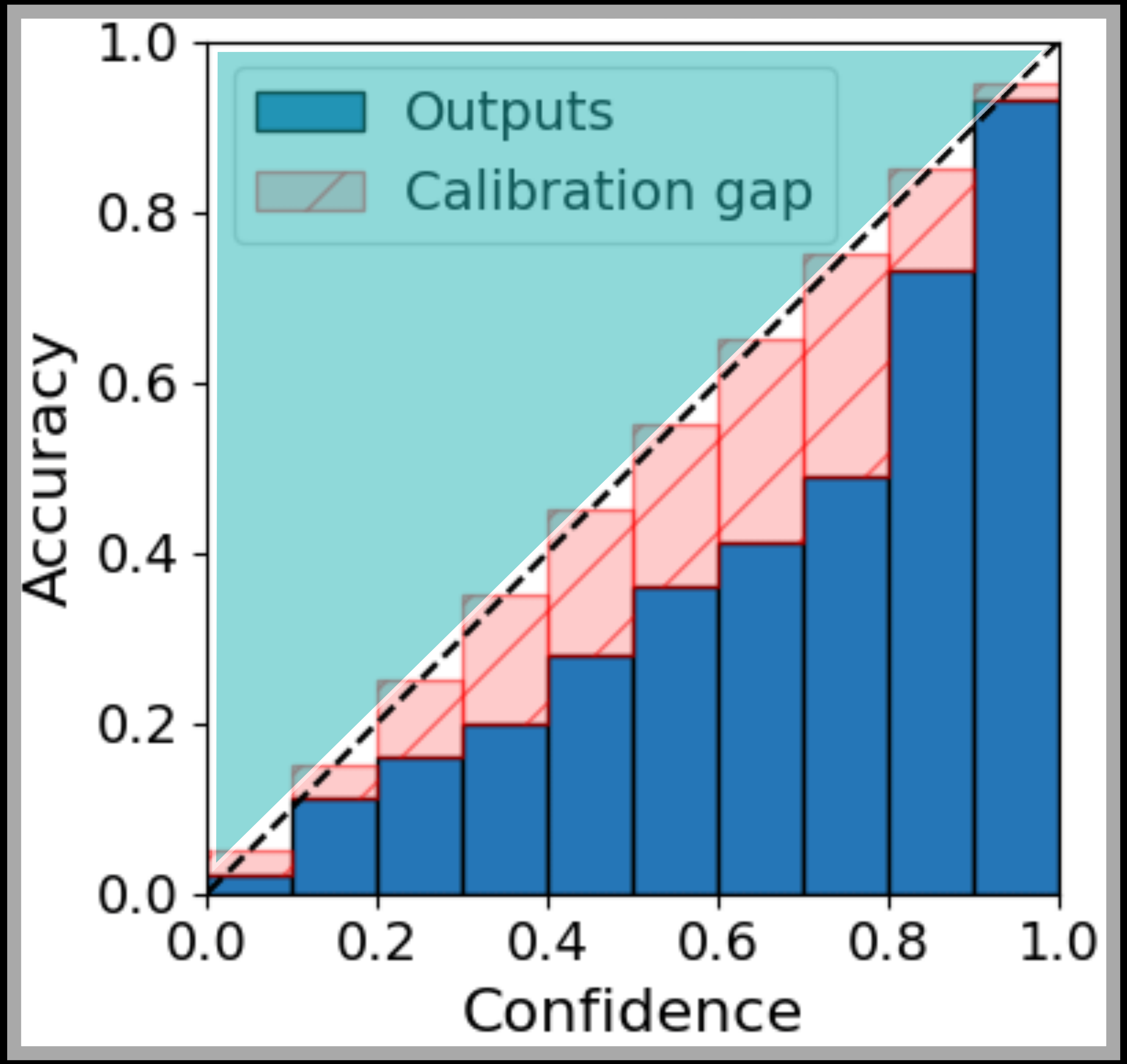
perfect calibration



Calibration

does the model confidence reflect its empirical accuracy?

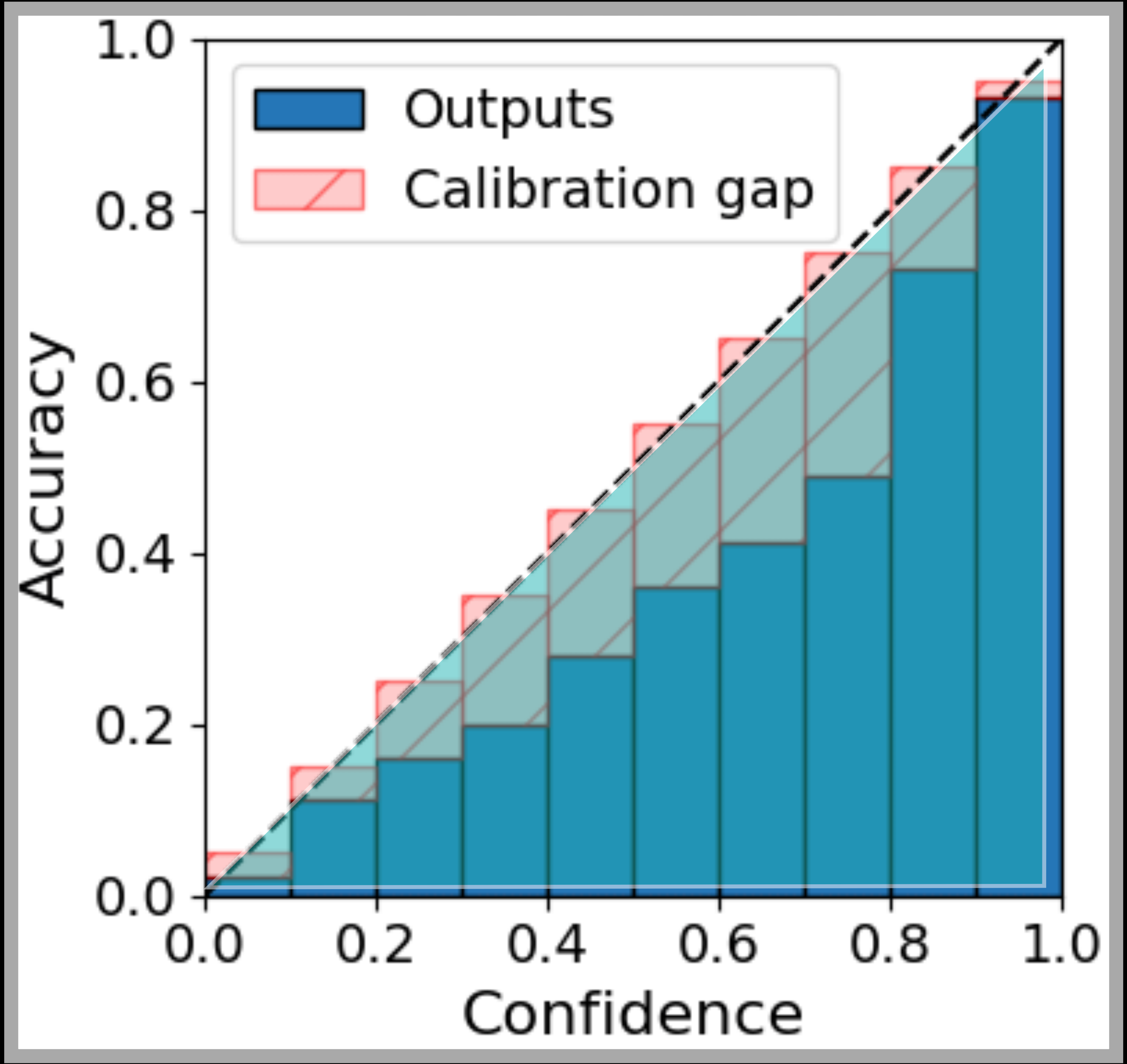
under-confident



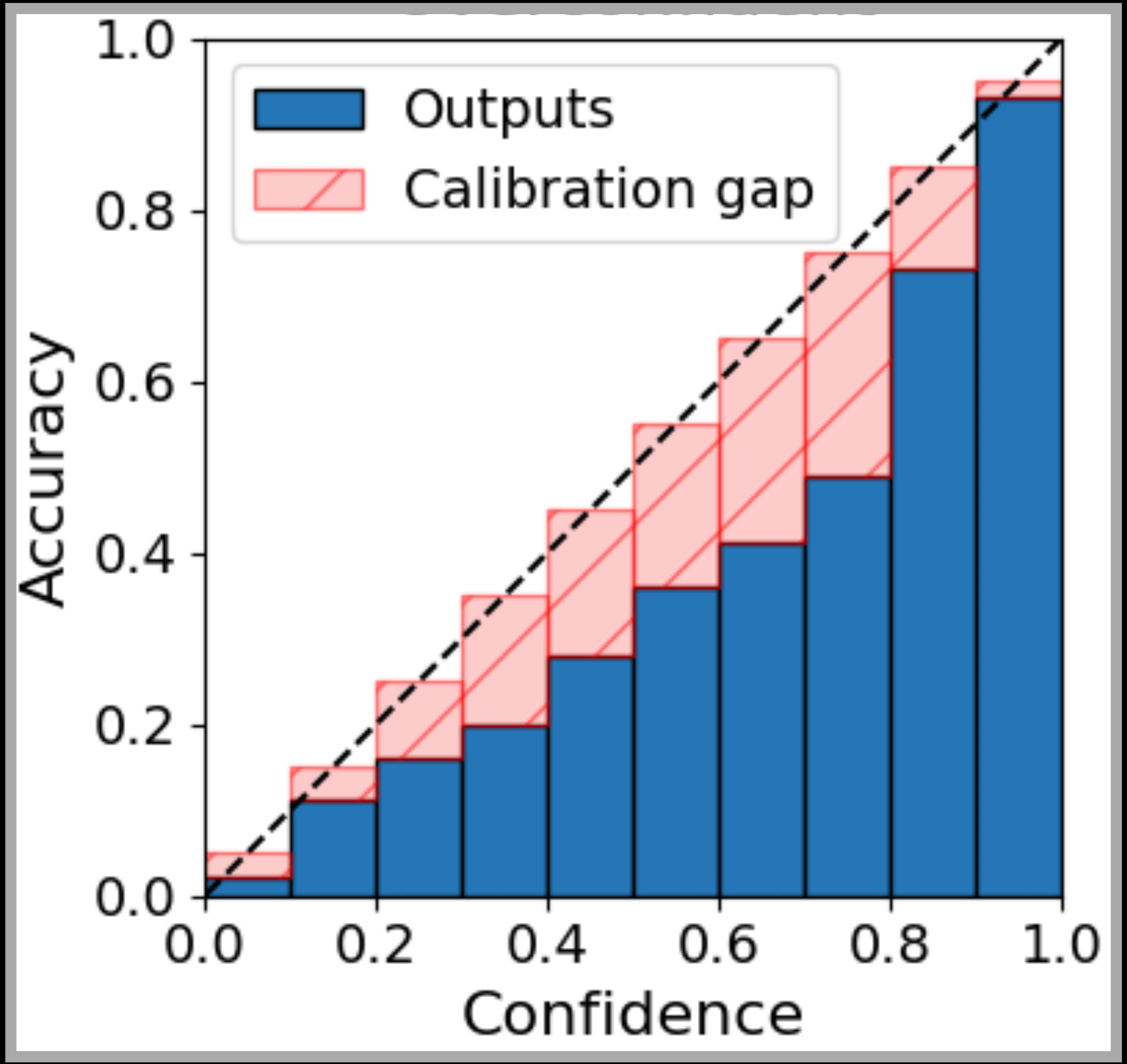
Calibration

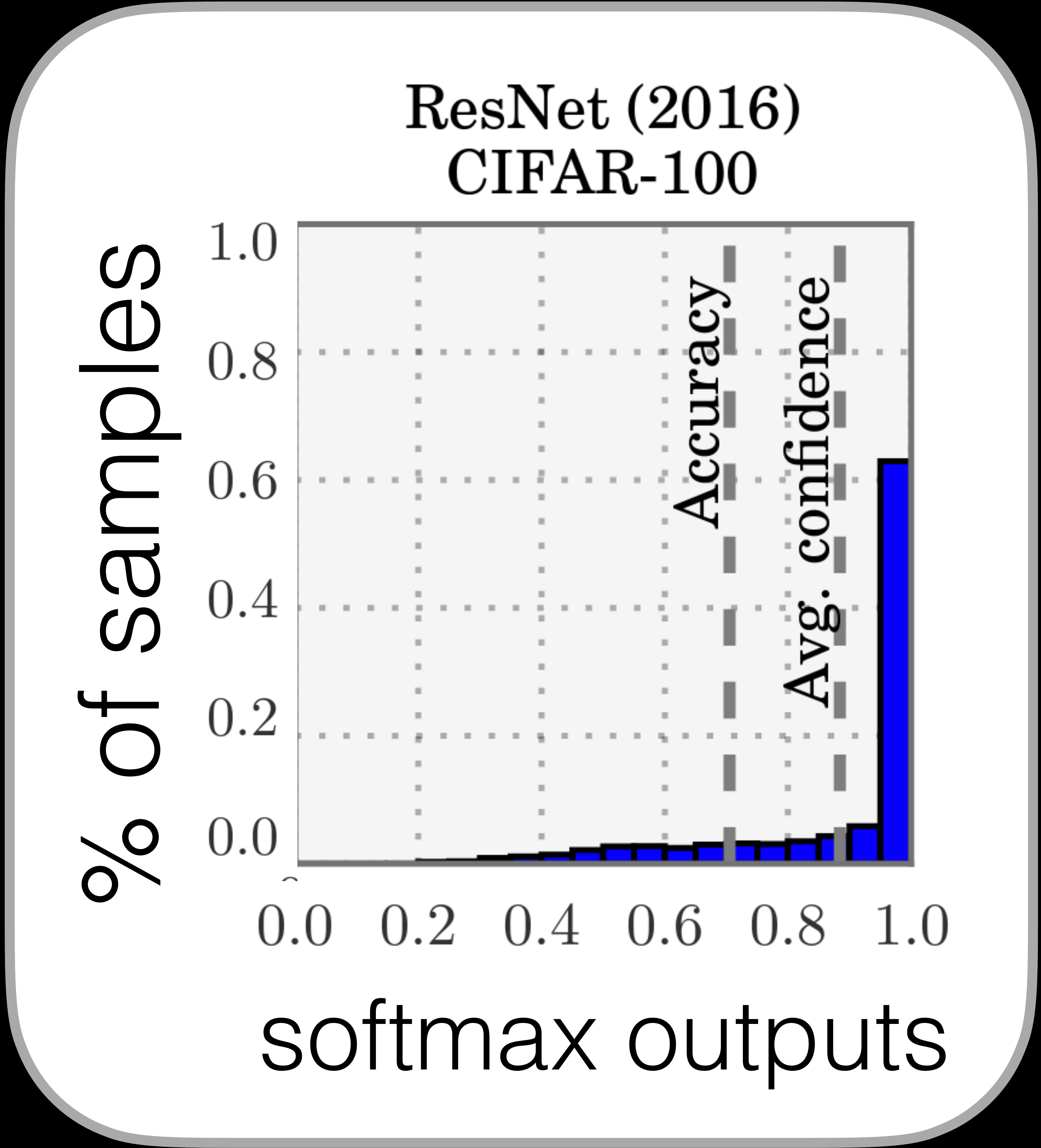
does the model confidence reflect its empirical accuracy?

over-confident



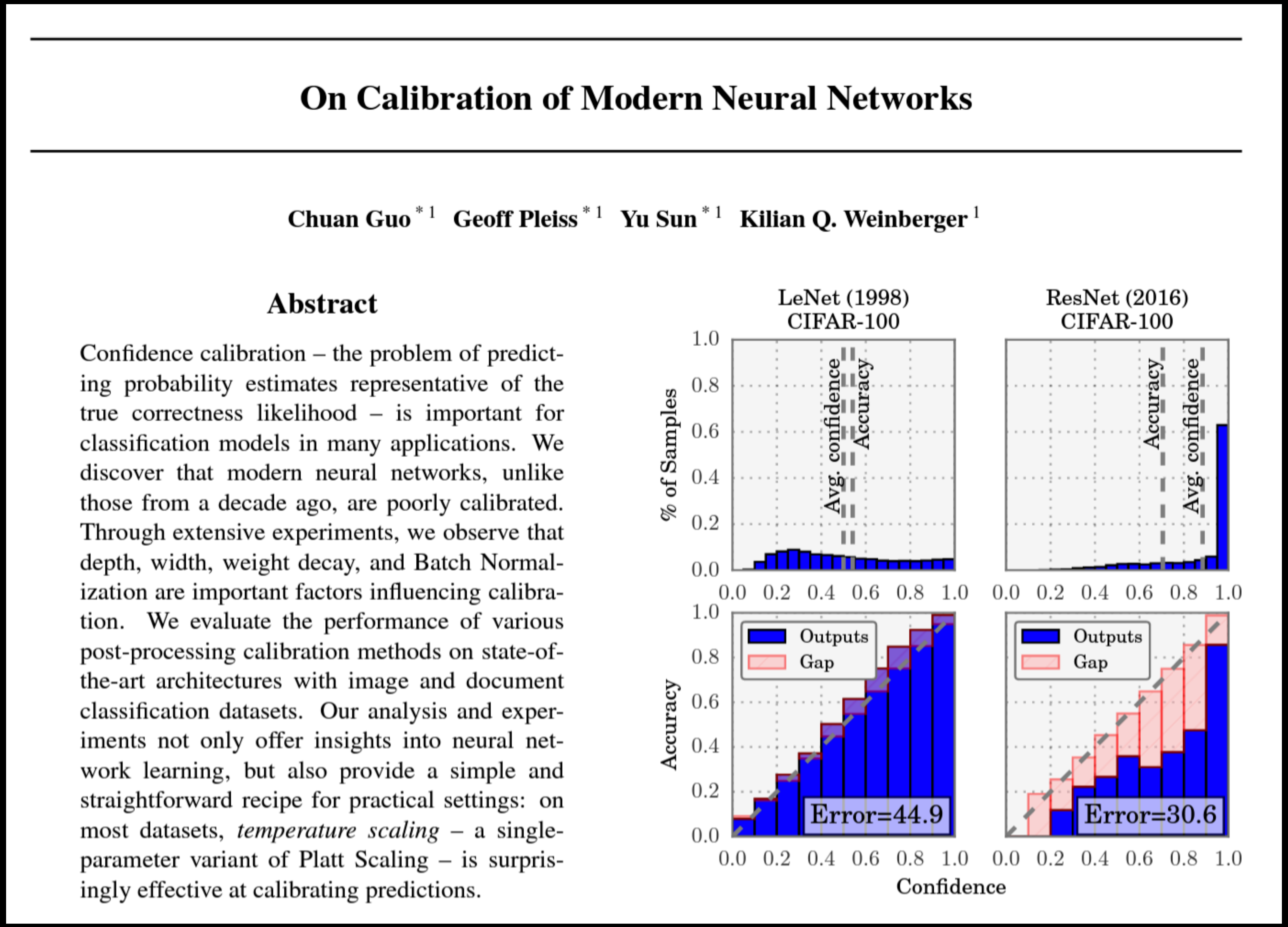
Calibration: Over-Confidence





[Guo et al., ICML 2017]

Further Reading

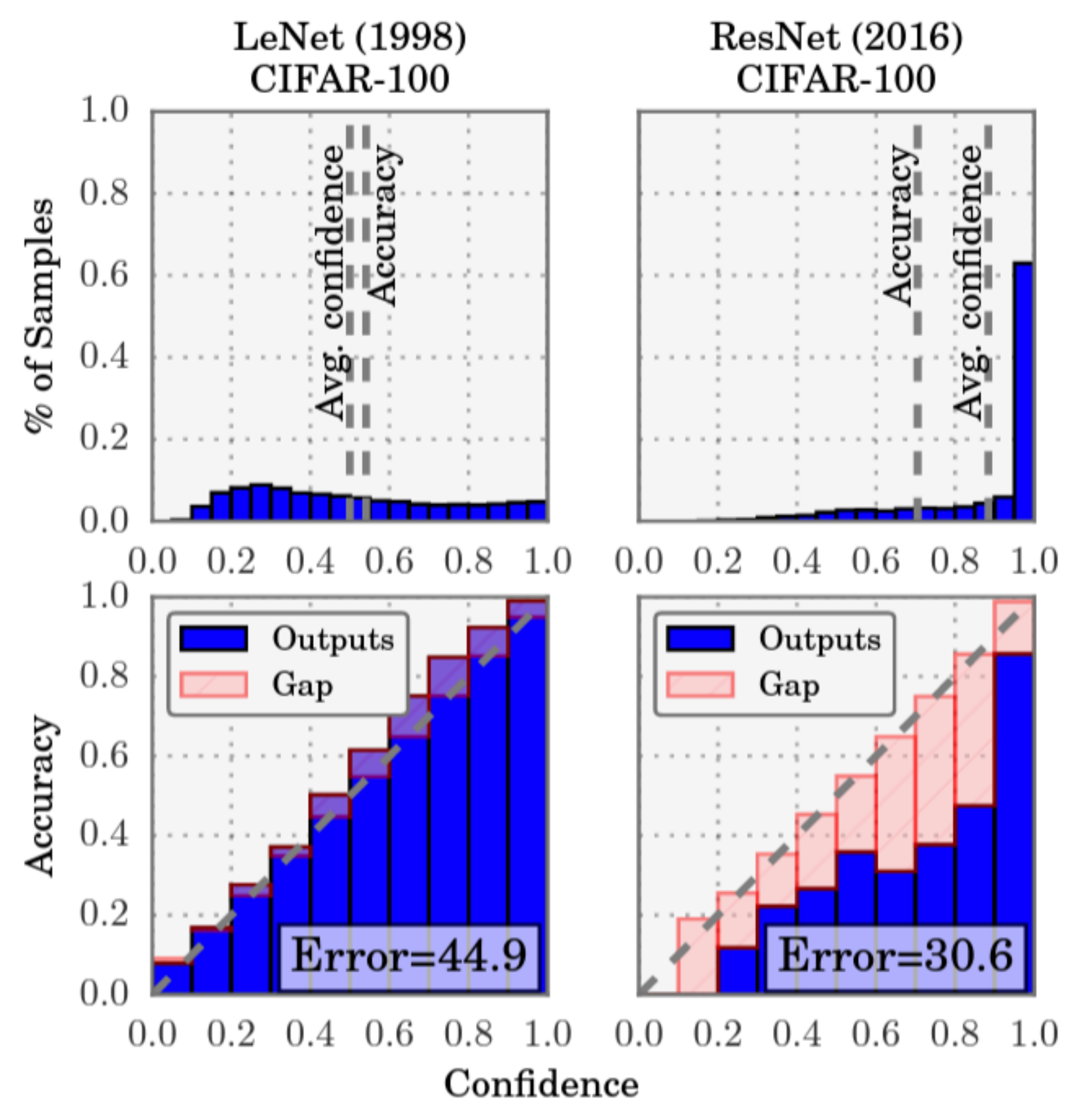


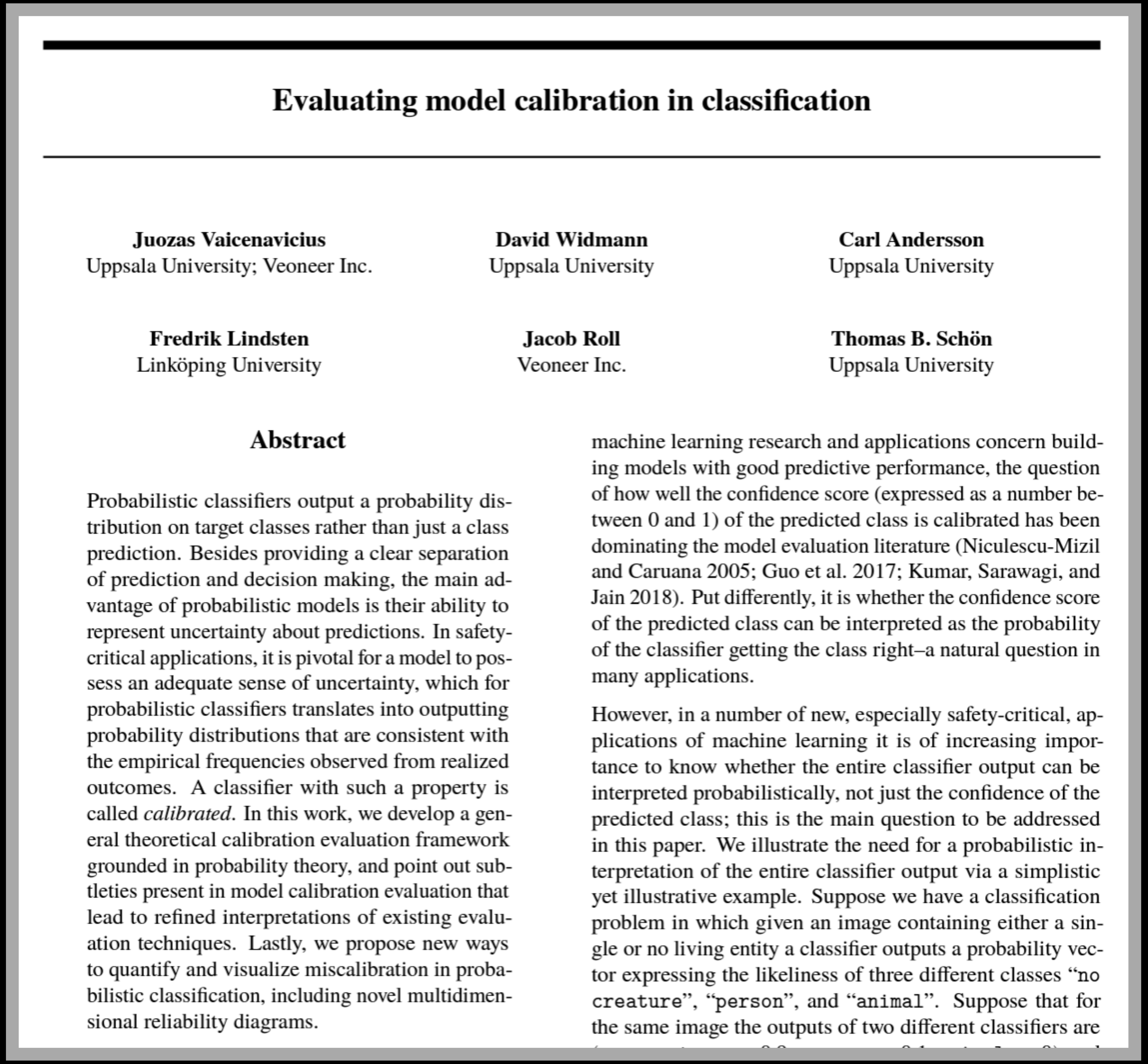
On Calibration of Modern Neural Networks

Chuan Guo [*1] Geoff Pleiss [*1] Yu Sun [*1] Kilian Q. Weinberger [1]

Abstract

Confidence calibration – the problem of predicting probability estimates representative of the true correctness likelihood – is important for classification models in many applications. We discover that modern neural networks, unlike those from a decade ago, are poorly calibrated. Through extensive experiments, we observe that depth, width, weight decay, and Batch Normalization are important factors influencing calibration. We evaluate the performance of various post-processing calibration methods on state-of-the-art architectures with image and document classification datasets. Our analysis and experiments not only offer insights into neural network learning, but also provide a simple and straightforward recipe for practical settings: on most datasets, *temperature scaling* – a single-parameter variant of Platt Scaling – is surprisingly effective at calibrating predictions.





Evaluating model calibration in classification

Juozas Vaicenavicius
Uppsala University; Veoneer Inc.

David Widmann
Uppsala University

Carl Andersson
Uppsala University

Fredrik Lindsten
Linköping University

Jacob Roll
Veoneer Inc.

Thomas B. Schön
Uppsala University

Abstract

Probabilistic classifiers output a probability distribution on target classes rather than just a class prediction. Besides providing a clear separation of prediction and decision making, the main advantage of probabilistic models is their ability to represent uncertainty about predictions. In safety-critical applications, it is pivotal for a model to possess an adequate sense of uncertainty, which for probabilistic classifiers translates into outputting probability distributions that are consistent with the empirical frequencies observed from realized outcomes. A classifier with such a property is called *calibrated*. In this work, we develop a general theoretical calibration evaluation framework grounded in probability theory, and point out subtleties present in model calibration evaluation that lead to refined interpretations of existing evaluation techniques. Lastly, we propose new ways to quantify and visualize miscalibration in probabilistic classification, including novel multidimensional reliability diagrams.

machine learning research and applications concern building models with good predictive performance, the question of how well the confidence score (expressed as a number between 0 and 1) of the predicted class is calibrated has been dominating the model evaluation literature (Niculescu-Mizil and Caruana 2005; Guo et al. 2017; Kumar, Sarawagi, and Jain 2018). Put differently, it is whether the confidence score of the predicted class can be interpreted as the probability of the classifier getting the class right–a natural question in many applications.

However, in a number of new, especially safety-critical, applications of machine learning it is of increasing importance to know whether the entire classifier output can be interpreted probabilistically, not just the confidence of the predicted class; this is the main question to be addressed in this paper. We illustrate the need for a probabilistic interpretation of the entire classifier output via a simplistic yet illustrative example. Suppose we have a classification problem in which given an image containing either a single or no living entity a classifier outputs a probability vector expressing the likeliness of three different classes "`no creature`", "`person`", and "`animal`". Suppose that for the same image the outputs of two different classifiers are

Coverage

on what fraction of the data do the confidence / credible sets cover the true label?

$$\frac{\sum_{m=1}^{M} \mathbb{I}\left[y_m^* \in C(x_m)\right]}{M} \overset{?}{\geq} (1-\alpha)$$

Coverage

on what fraction of the data do the confidence / credible sets cover the true label?

$$\frac{\sum_{m=1}^{M} \mathbb{1}\left[y_m^* \in C(x_m)\right]}{M} \overset{?}{\geq} (1-\alpha)$$

average size of the set is measured as well, since we want sets to be efficient

Evaluating UQ

- ⊗ Calibration: can the model forecast its own performance?
- ⊗ Coverage: does the model meet the given error level?

V. Summary

⊗ Types of Uncertainty

⊗ Modeling Paradigms

- Frequentism: random data
- Bayesianism: random parameters

⊗ Practical Methods

- Frequentism: use ‘extra’ data, possibly synthesized
- Bayesianism: reduce computation with local approximations

⊗ Evaluation

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Open Problems

- ⊗ better methods for Bayesian computations
- ⊗ guarantees in the era of deep learning
- ⊗ setting more informative Bayesian priors
- ⊗ quantifying uncertainty in structured, multi-step, or otherwise correlated tasks.

Thank You!   Questions?