CSC321 Lecture 21: Bayesian Hyperparameter Optimization

Roger Grosse

Why auto-tuning matters

Humans are really bad at

Need good tuning to accurately compare models

Hard to beat state-of-the-art without good tuning

On the State of the Art of Evaluation in Neural Language Models

Gábor Melis[†] **Chris Dyer**[†] **Phil Blunsom**[†‡]
[†]DeepMind [‡]University of Oxford
{melisgl,cdyer,pblunsom}@google.com

Abstract

Ongoing innovations in recurrent neural network architectures have provided a steady influx of apparently state-of-the-art results on language modelling benchmarks. However, these have been evaluated using differing code bases and limited computational resources, which represent uncontrolled sources of experimental variation. We reevaluate several popular architectures and regularisation methods with large-scale automatic black-box hyperparameter tuning and arrive at the somewhat surprising conclusion that standard LSTM architectures, when properly regularised, outperform more recent models. We establish a new state of the art on the Penn Treebank and Wikitext-2 corpora, as well as strong baselines on the Hutter Prize dataset.

Tuning tips

Keep an open-mind (explore the full space from the beginning)

Don’t do grid search

Try and eliminate hyperparameters

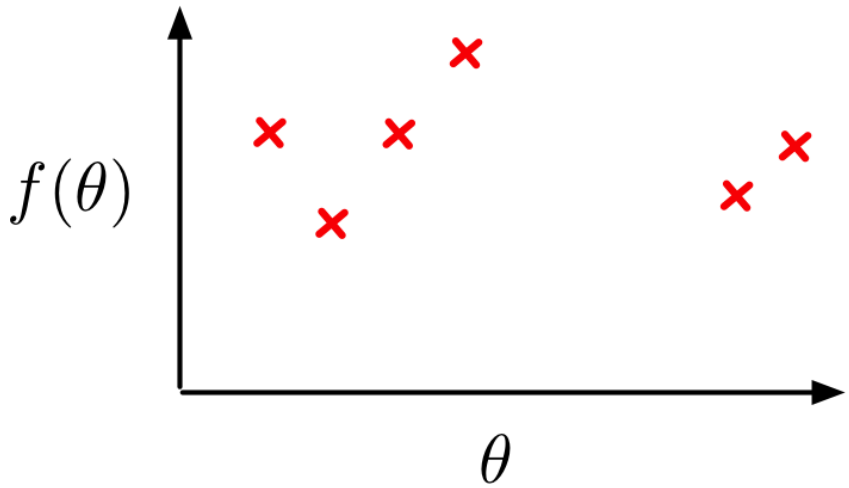
To see a clear pattern it can take way longer than you expect

Overview

- Today's lecture: a neat application of Bayesian parameter estimation to automatically tuning hyperparameters
- Recall that neural nets have certain hyperparmaeters which aren't part of the training procedure
  - E.g. number of units, learning rate, L_2 weight cost, dropout probability
- You can evaluate them using a validation set, but there's still the problem of which values to try
  - Brute force search (e.g. grid search, random search) is very expensive, and wastes time trying silly hyperparameter configurations

Overview

- Hyperparamter tuning is a kind of black-box optimization: you want to minimize a function $f(\theta)$, but you only get to query values, not compute gradients
  - Input θ: a configuration of hyperparameters
  - Function value $f(\theta)$: error on the validation set
- Each evaluation is expensive, so we want to use few evaluations.
- Suppose you've observed the following function values. Where would you try next?

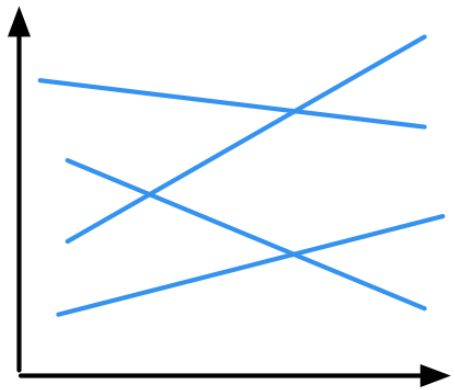


Overview

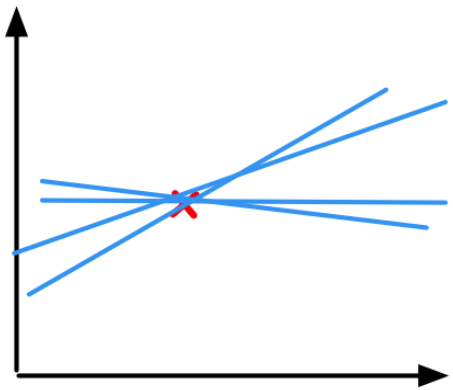
- You want to query a point which:
  - you expect to be good
  - you are uncertain about
- How can we model our uncertainty about the function?
- Bayesian regression lets us predict not just a value, but a distribution. That's what the first half of this lecture is about.

Bayesian Linear Regression

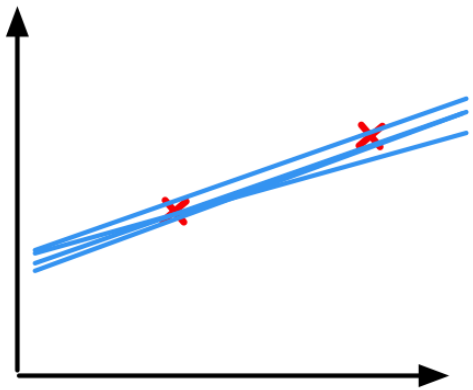
- We're interested in the uncertainty
- Bayesian linear regression considers various plausible explanations for how the data were generated.
- It makes predictions using all possible regression weights, weighted by their posterior probability.



no observations



one observation

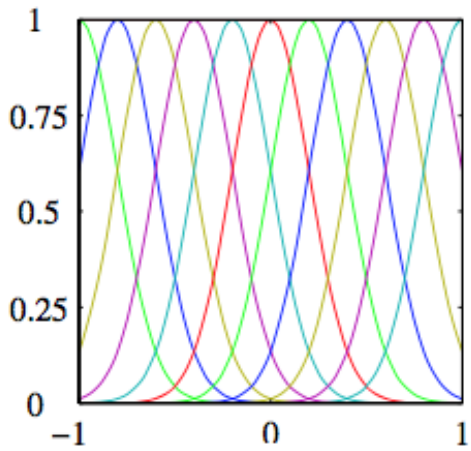


two observations

Bayesian Linear Regression

- We can turn this into nonlinear regression using basis functions.
- E.g., Gaussian basis functions

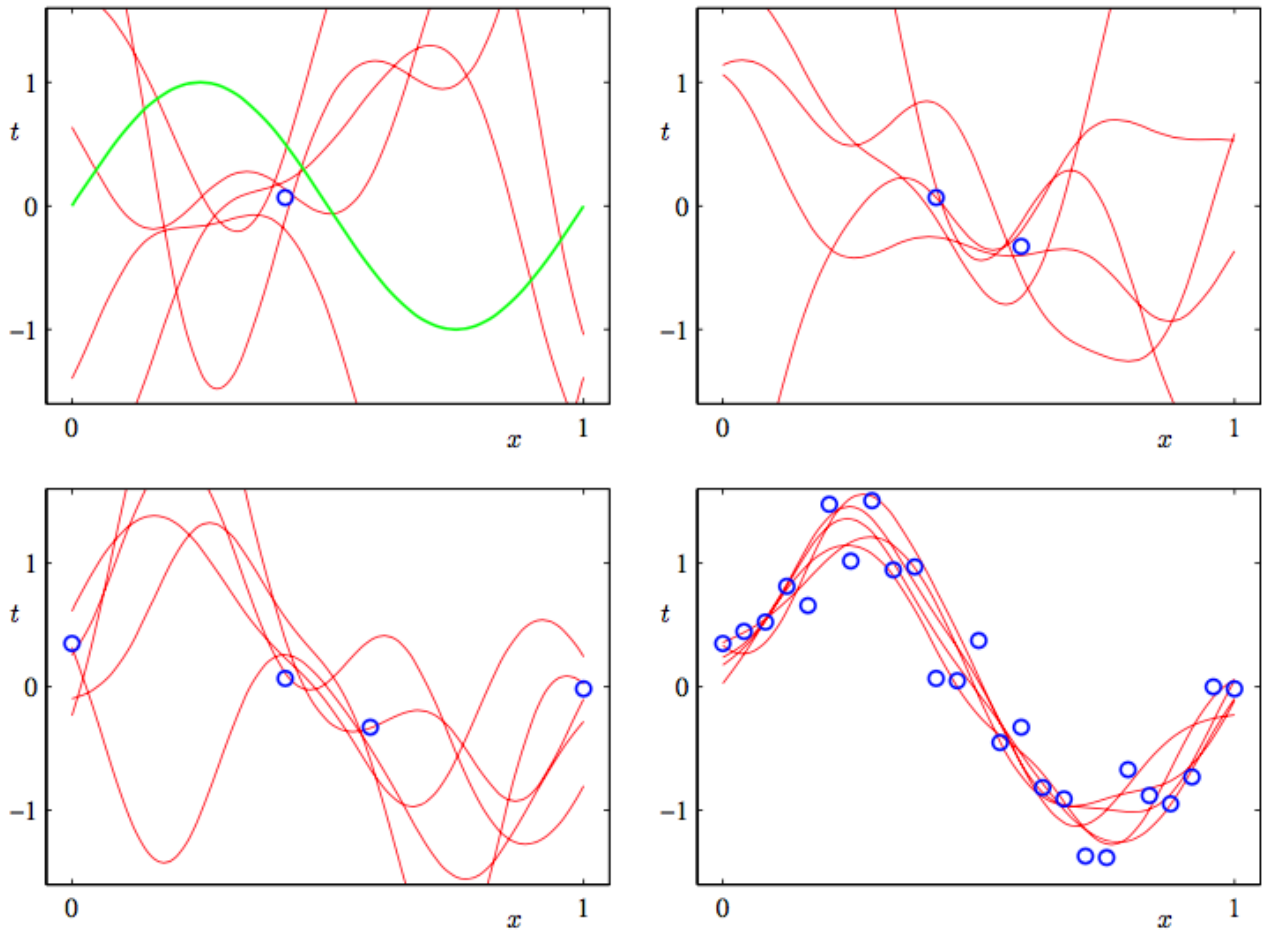
$$\phi_j(x) = \exp\left(-\frac{(x-\mu_j)^2}{2s^2}\right)$$



— Bishop, Pattern Recognition and Machine Learning

Bayesian Linear Regression

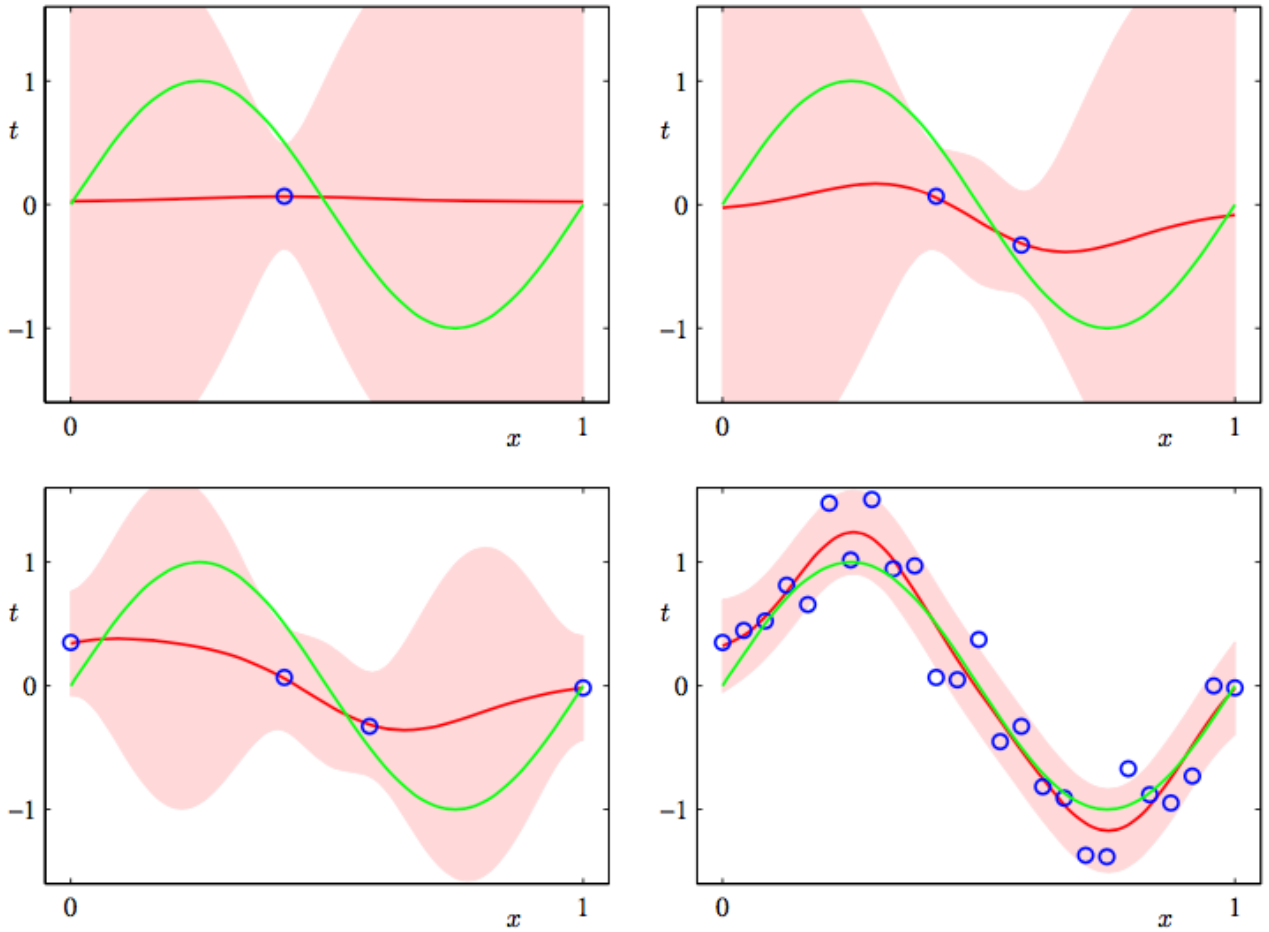
Functions sampled from the posterior:



— Bishop, Pattern Recognition and Machine Learning

Bayesian Linear Regression

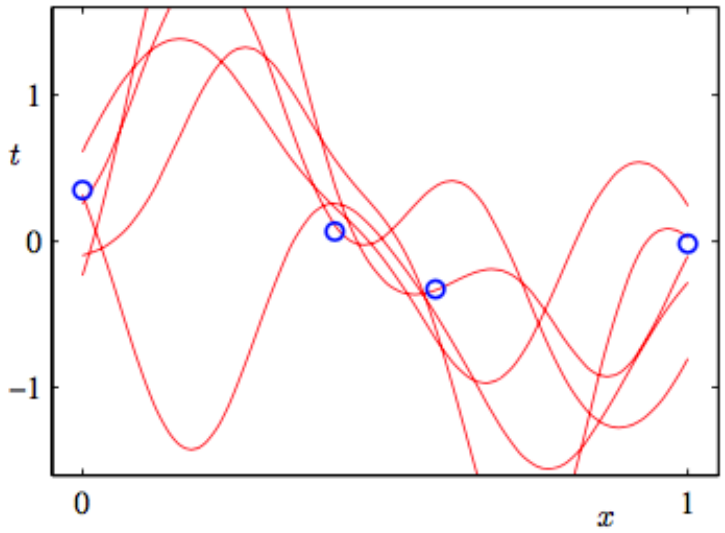
Posterior predictive distribution:



— Bishop, Pattern Recognition and Machine Learning

Bayesian Optimization

- Now let's apply all of this to black-box optimization. The technique we'll cover is called Bayesian optimization.
- The actual function we're trying to optimize (e.g. validation error as a function of hyperparameters) is really complicated. Let's approximate it with a simple function, called the surrogate function.
- After we've queried a certian number of points, we can condition on these to infer the posterior over the surrogate function using Bayesian linear regression.



Bayesian Optimization

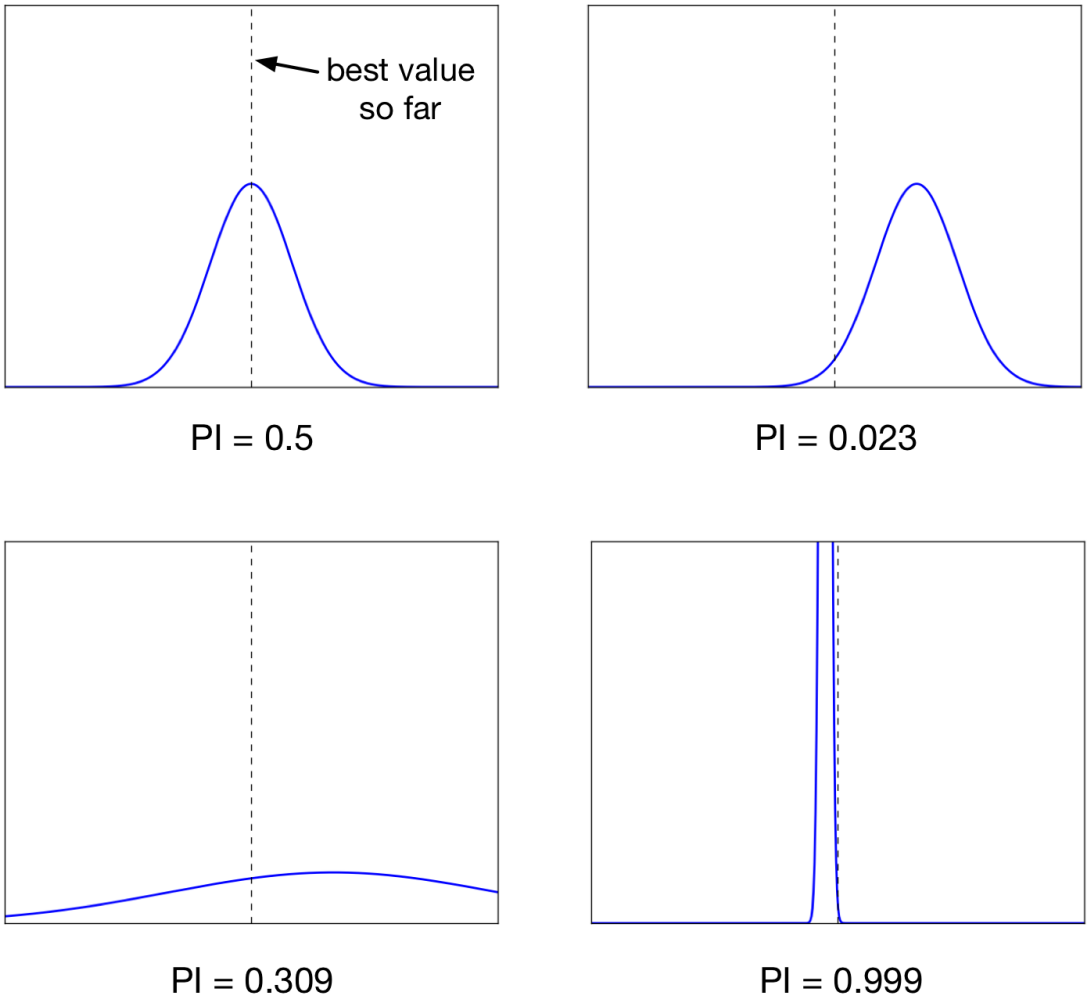
- To choose the next point to query, we must define an acquisition function, which tells us how promising a candidate it is.
- What's wrong with the following acquisition functions:
  - posterior mean: $-\mathbb{E}[f(\boldsymbol{\theta})]$
  - posterior variance: $\mathrm{Var}(f(\boldsymbol{\theta}))$
- Desiderata:
  - high for points we expect to be good
  - high for points we're uncertain about
  - low for points we've already tried
- Candidate 1: probability of improvement (PI)

$$\mathrm{PI} = \Pr(f(\theta) < \gamma - \epsilon),$$

where γ is the best value so far, and ϵ is small.

Bayesian Optimization

Examples:



- Plots show the posterior predictive distribution for $f(\theta)$.

Bayesian Optimization

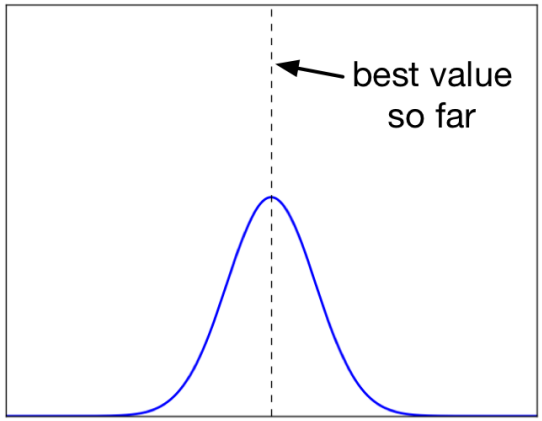
- The problem with Probability of Improvement (PI): it queries points it is highly confident will have a small imporvement
  - Usually these are right next to ones we've already evaluated
- A better choice: Expected Improvement (EI)

$$\mathrm{EI} = \mathbb{E}[\max(\gamma - f(\boldsymbol{\theta}), 0)]$$

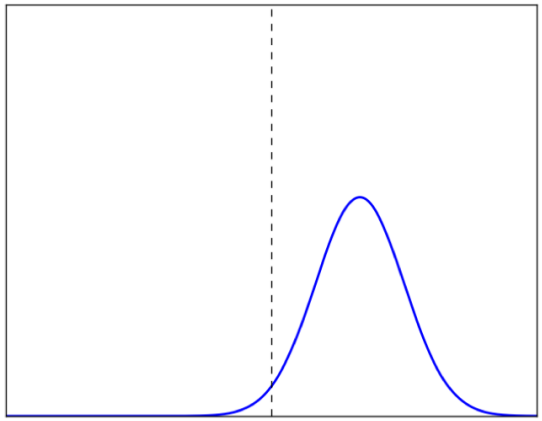
  - The idea: if the new value is much better, we win by a lot; if it's much worse, we haven't lost anything.
  - There is an explicit formula for this if the posterior predictive distribution is Gaussian.

Bayesian Optimization

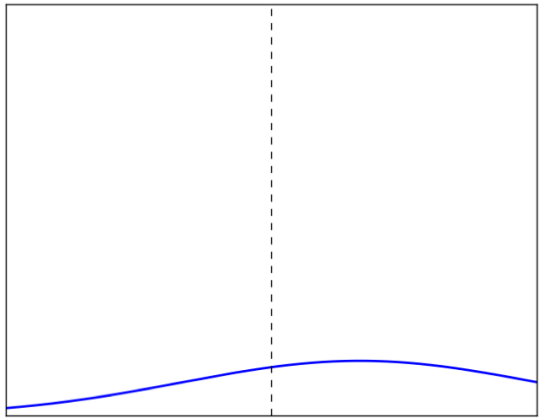
Examples:



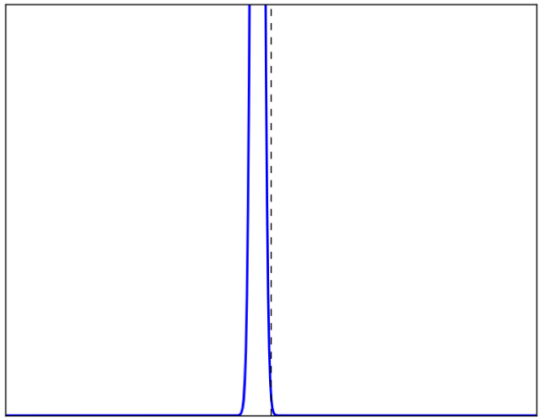
EI = 0.199



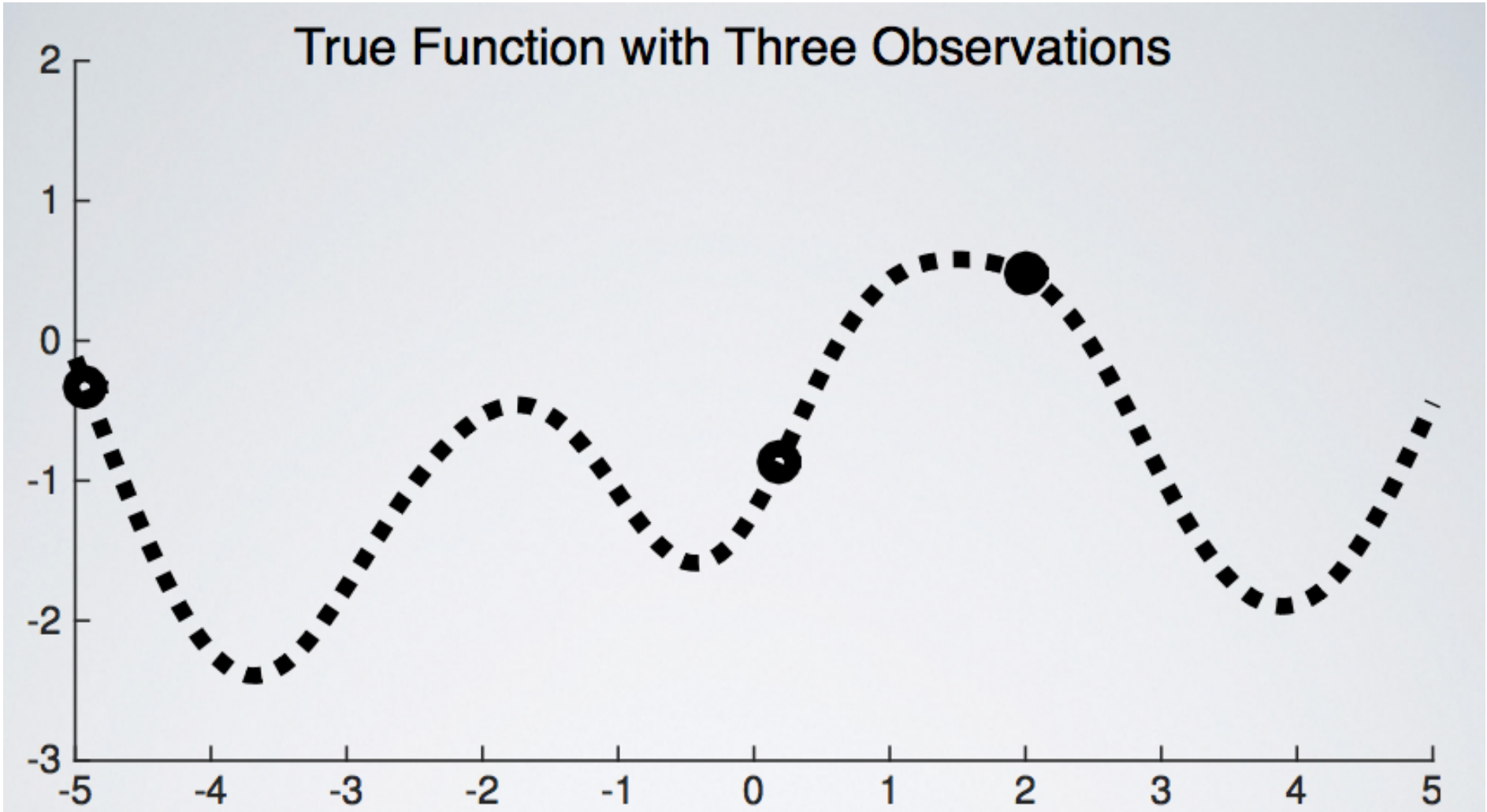
EI = 0.004

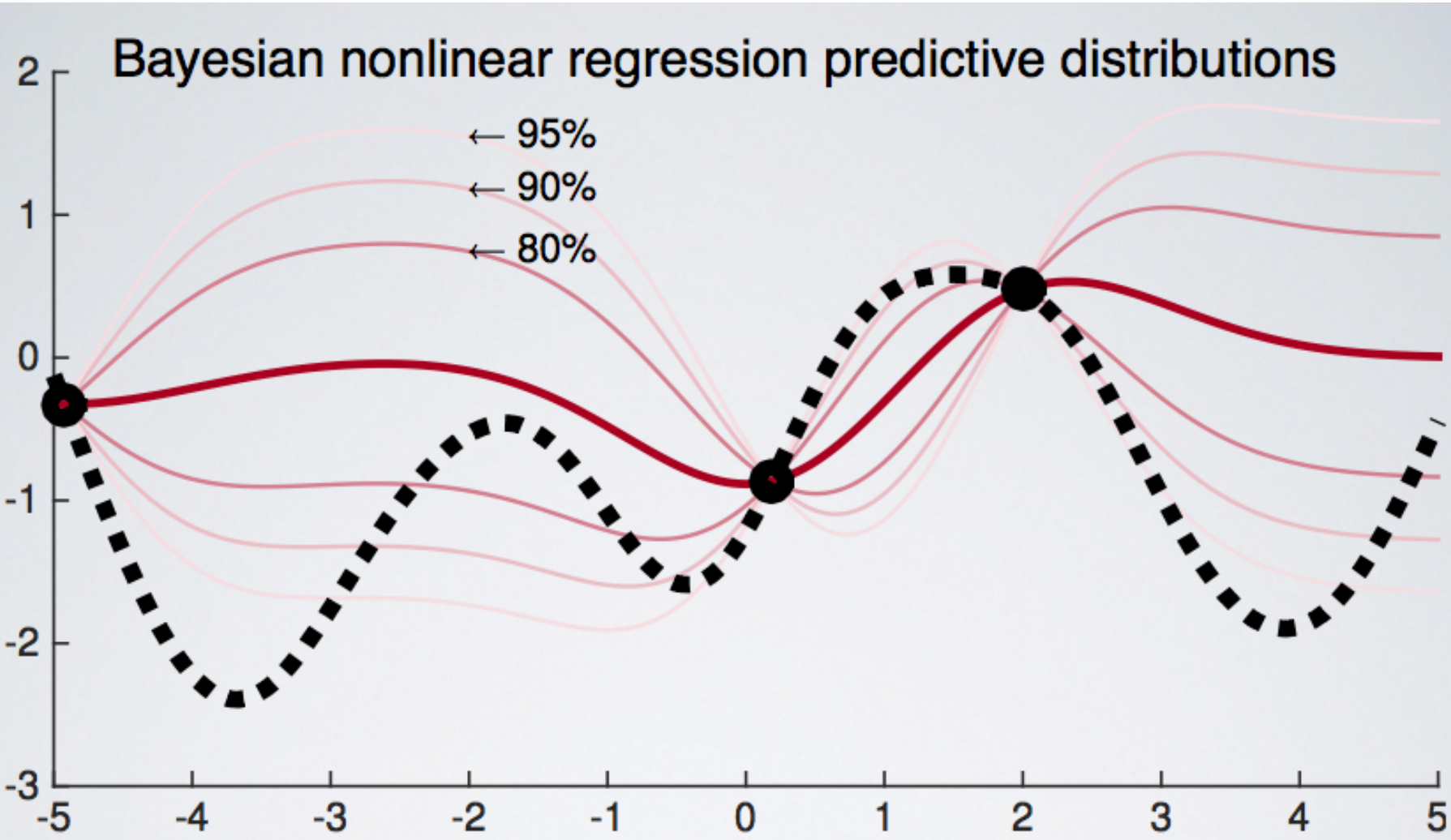


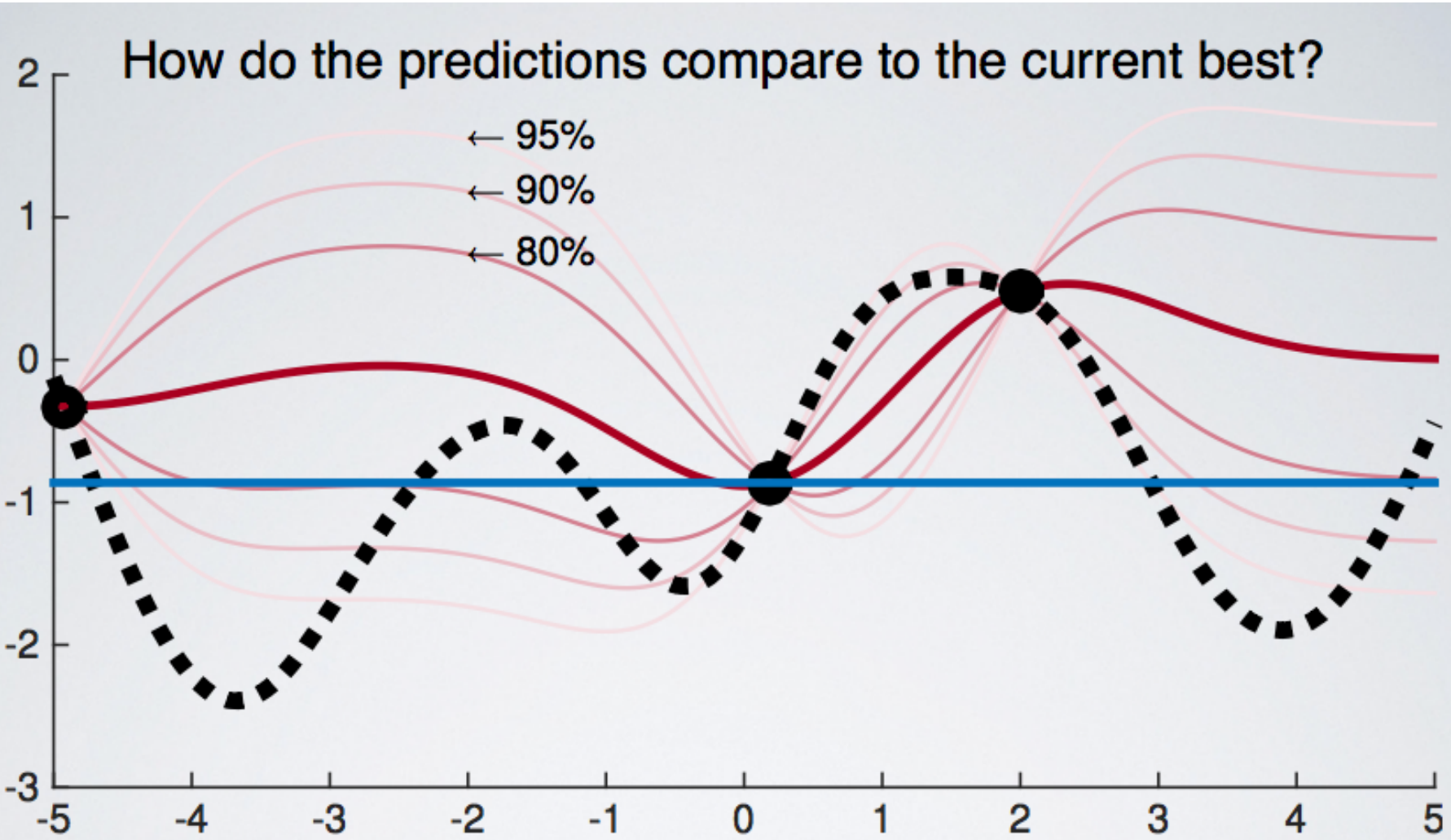
EI = 0.396

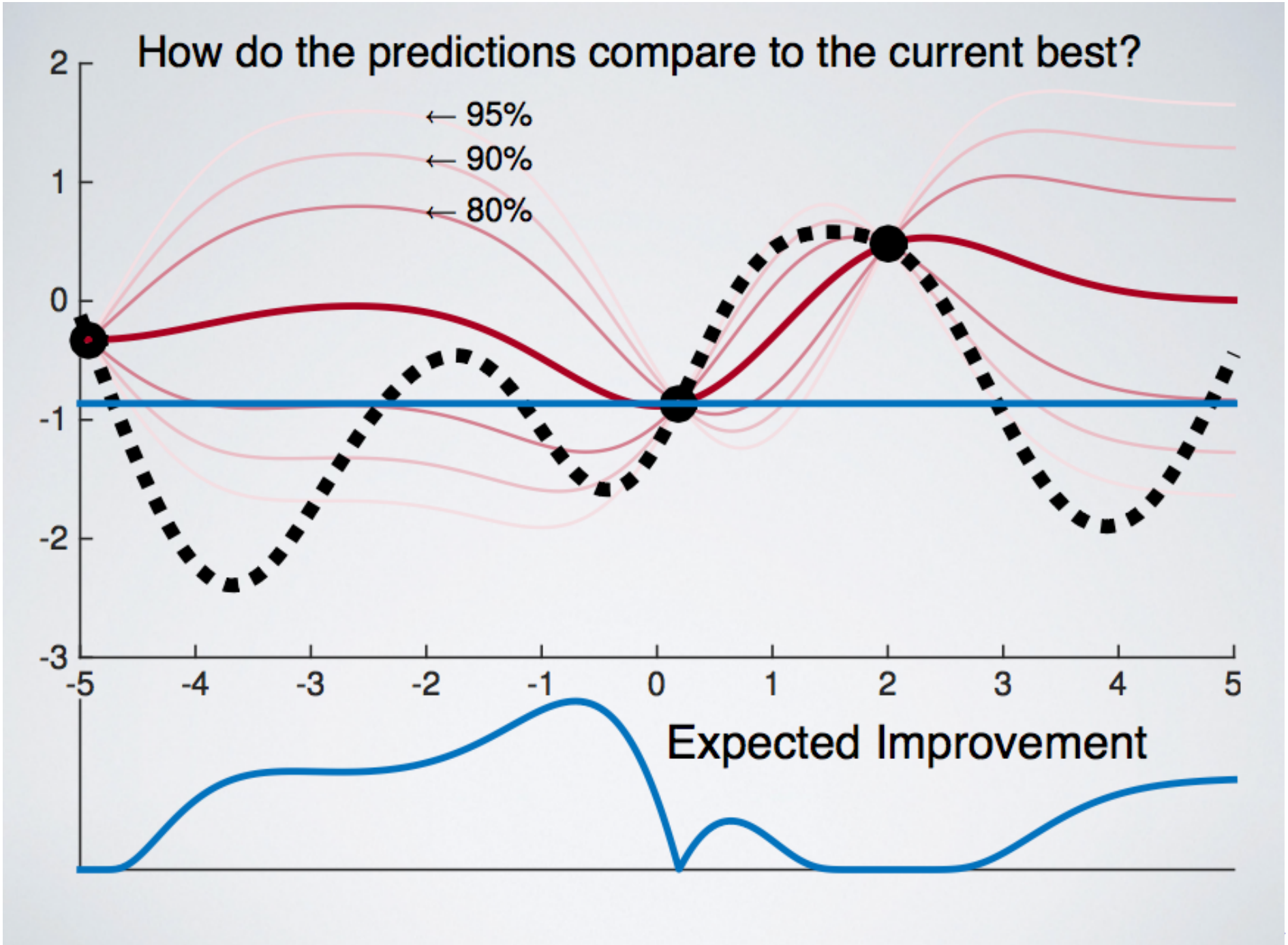


EI = 0.15


True Function with Three Observations
2
1
0
-1
-2
-3
-5
-4
-3
-2
-1
0
1
2
3
4
5


Bayesian nonlinear regression predictive distributions
← 95%
← 90%
← 80%
2
1
0
-1
-2
-3
-5
-4
-3
-2
-1
0
1
2
3
4
5


How do the predictions compare to the current best?
← 95%
← 90%
← 80%
2
1
0
-1
-2
-3
-5
-4
-3
-2
-1
0
1
2
3
4
5

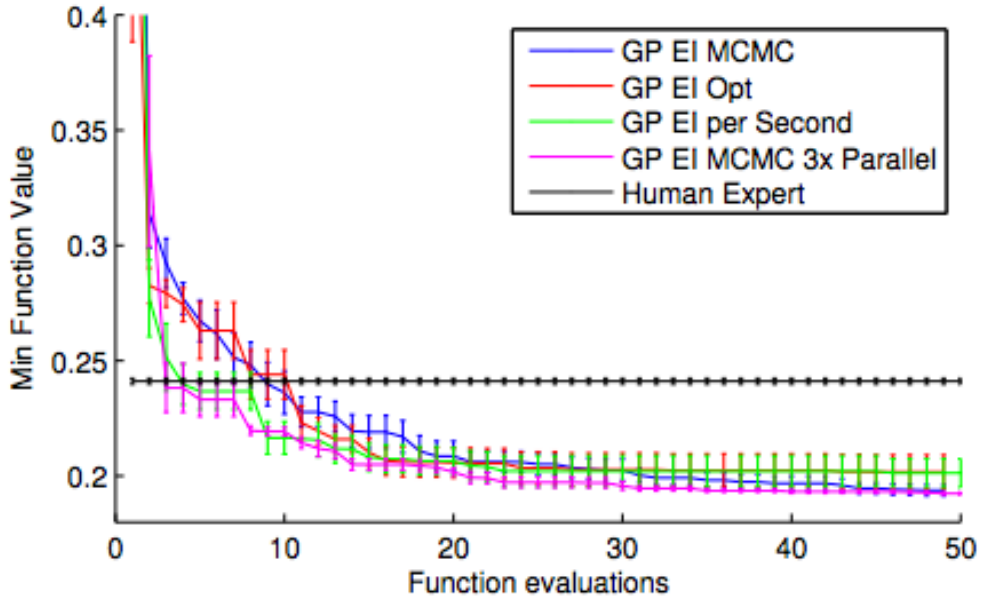

How do the predictions compare to the current best?
← 95%
← 90%
← 80%
2
1
0
-1
-2
-3
-5
-4
-3
-2
-1
0
1
2
3
4
5
Expected Improvement

Bayesian Optimization

- I showed one-dimensional visualizations, but the higher-dimensional case is conceptually no different.
  - Maximize the acquisition function using gradient descent
  - Use lots of random restarts, since it is riddled with local maxima
  - BayesOpt can be used to optimize tens of hyperparameters.
- I've described BayesOpt in terms of Bayesian linear regression with basis functions learned by a neural net.
  - In practice, it's typically done with a more advanced model called Gaussian processes, which you learn about in CSC 412.
  - But Bayesian linear regression is actually useful, since it scales better to large numbers of queries.
- One variation: some configurations can be much more expensive than others
  - Use another Bayesian regression model to estimate the computational cost, and query the point that maximizes expected improvement per second

Bayesian Optimization

- BayesOpt can often beat hand-tuned configurations in a relatively small number of steps.
- Results on optimizing hyperparameters (layer-specific learning rates, weight decay, and a few other parameters) for a CIFAR-10 conv net:



- Each function evaluation takes about an hour
- Human expert = Alex Krizhevsky, the creator of AlexNet

Bayesian Optimization

- Spearmint is an open-source BayesOpt software package that optimizes hyperparameters for you:

  `https://github.com/JasperSnoek/spearmint`

- Much of this talk was taken from the following two papers:
  - J. Snoek, H. Larochelle, and R. P. Adams. Practical Bayesian optimization of machine learning algorithms. NIPS, 2012.

    `http://papers.nips.cc/paper/4522-practical-bayesian-optimization-of-machine-learning-algorithms`
  - J. Snoek et al. Scalable Bayesian optimization using deep neural networks. ICML, 2015.

    `http://www.jmlr.org/proceedings/papers/v37/snoek15.pdf`