Hyperparameter optimization

CS6787 Lecture 6 — Fall 2017

Review — We've covered many methods

- Stochastic gradient descent
  - **Step size/learning rate, how long to run**
- Mini-batching
  - **Batch size**
- Momentum
  - **Momentum parameter**
- Kernel trick/feature extraction
  - **How many features to extract**
- Variance reduction
  - **Step size, epoch length**

How do we set these parameters?

So Far: Theory

- Theoretical analysis of convex problems gives us a **recipe** for assigning hyperparameters
    - Also gives **guarantees** that the algorithm will converge with some optimal rate

- Often based on strong-convexity/Lipschitz constants **μ**, **L**, etc.
    - Parameters that we can **bound analytically**, regardless of the data

- This is usually enough to get an **asymptotically optimal rate**
    - Certainly in the worst case

The Worst-Case Perspective

- Essentially, the theory I showed you is doing

$$\arg \min_{\text{parameters}} \max_{\text{data}} (\text{objective})$$

- We're **not using the training data** at all to set the parameters
  - Or if we are, we're only using it to compute constants like μ and $\mathbf{L}$

- Question: **can we use the data to improve our choice of parameters over what the theory gives us?**

Demo

What happened?

- Theory only **minimizes an upper bound** on the objective.
- But actual algorithm can **do much better than the bound**.
  - As we saw in the demo.
- Problem: in the demo, to find the best parameter setting, we had to first solve the problem exactly, then run the algorithm many times.
  - **Computationally intractable** in practice!
- **Can we use a cheaper heuristic to set the parameters?**

Hyperparameter Optimization

Hyperparameter Optimization

- Also called **metaparameter optimization**
  - I am more used to this term so you will hear me using it more often
- Also called **tuning**
- Any system that chooses hyperparameters automatically
- **What's the difference between the model parameters, and the hyperparameters?**

Many Settings; Many Strategies

- In some settings, just care about the model accuracy
  - Just want to set things like the learning rate
- In other settings, also want to make the hardware fast
  - Want to choose what hardware to run on, how many cores, etc.
- In all settings, there's **many ways to do hyperparameter optimization**

Simplest Strategy: The Null Hyperparameter Optimizer

- Simplest thing to do is to **just set the parameters based on folklore**.
- **Minibatch size:** $\mathbf{b} = \boxed{?}$
- **Momentum:** $\beta = \boxed{?}$
- **SVRG: epoch length =** $\boxed{?}$ **x Training Set Size**

The Effect of Using Folklore

- **Folklore can lead you astray**!
  - Can actually find **simple cases where the folklore settings are wrong**.
  - This is a good way to start a research paper.

- …but **folklore is folklore for a reason**!
  - It exists where people have found empirically that they get good results.
  - So when you try something new, the **first thing to compare to is folklore**.

- To be honest, the results you get from just using the folklore settings are really not that bad for a lot of practical purposes.

From the simplest strategy to…
The Most Complicated Strategy

- Spend **twenty-five years training a Strong AI on custom hardware**, then have it set your hyperparameters.

- …more explicitly, just **get a human to set your hyperparameters**.

- Fortunately, we happen to have a lot of humans
  - But human effort, particularly expert human effort, doesn't scale.

Tuning By Hand

- Just fiddle with the parameters until you get the results you want
- Probably **the most common type of hyperparameter optimization**
- Upsides: the results are generally pretty good…
- Downsides: **lots of effort**, and no theoretical guarantees
  - Although there's nothing fundamental that prevents us from having theory here

Demo

Grid Search

- Define some grid of parameters you want to try
- Try all the parameter values in the grid
  - By **running the whole system** for each setting of parameters
- Then **choose the setting with the best result**
- Essentially a **brute force method**

Downsides of Grid Search

- As the number of parameters increases, the cost of grid search **increases exponentially**!
  - **Why?**
- Still need some way to choose the grid properly
  - Something this can be as hard as the original hyperparameter optimization
- Can't take advantage of any **insight** you have about the system!

Making Grid Search Fast

- **Early stopping to the rescue**
  - Can run all the grid points for one epoch, then discard the half that performed worse, then run for another epoch, discard half, and continue.

- Can **take advantage of parallelism**
  - Run all the different parameter settings independently on different servers in a cluster.
  - An **embarrassingly parallel task**.
  - Downside: **doesn’t reduce the energy cost**.

One Variant: Random Search

- This is just grid search, but with randomly chosen points instead of points on a grid.

- **This solves the curse of dimensionality**
  - Don't need to increase the number of grid points exponentially as the number of dimensions increases.

- Problem: with random search, **not necessarily going to get anywhere near the optimal parameters** in a finite sample.

One Variant: Best Ball

- Works with epochs.

- At each epoch, do a small grid search **around the current hyperparameter settings**

- Then evaluate the objective and choose the **"best ball"**
  - The choice of parameters that gave the best objective for that epoch

- And repeat until a solution of desired quality is achieved.

An Alternative: Bayesian Optimization

- Statistical approach for **minimizing noisy black-box functions**.

- Idea: **learn a statistical model** of the function from hyperparameter values to the loss function
  - Then choose parameters to minimize the loss under this model

- Main benefit: choose the hyperparameters to test not at random, but in a way that gives the **most information about the model**
  - This lets it learn faster than grid search

Effect of Bayesian Optimization

- Downside: it's a pretty **heavyweight method**
  - The updates are not as simple-to-implement as grid search

- Upside: empirically it has been demonstrated to **get better results in fewer experiments**
  - Compared with grid search and random search

- Pretty widely used method
  - Lots of research opportunities here.

A related method: DFO

- **Derivative-free optimization**
- Also called **zeroth-order optimization**
- These methods optimize a function using only evaluations, no derivatives
- Ideal for use with metaparameter optimization
  - Also ideal for **reinforcement learning**

The opposite of DFO
Gradient-based optimization

- These strategies say: **"I'm doing SGD to learn, I may as well use it to optimize my hyperparameters."**

- When we can efficiently differentiate with respect to the hyperparameters, this strategy actually works pretty well.

- But generally, we **can't do it**.

Methods that Look at the Data

- Many methods look at curvature/variance info to decide how to set hyperparameters, and update their settings throughout the algorithm

- Example: **ADAGRAD**

- Example: **Adam**
  - Which you will be reading in a few weeks.

Evaluating the Hyperparameter Optimization

How to evaluate the hyperparameters?

- Unlike the model parameters, we're **not given a loss function**
- **Can't we just use the training loss?**
- **Not always**: we don't want to **overfit the hyperparameters**
  - Especially not when they are things that affect the model

Cross-Validation

- Partition part of the available data to create an **validation dataset** that we don't use for training.

- Then **use that set to evaluate the hyperparameters**.

- Typically, **multiple rounds of cross-validation** are performed using different partitions
  - Can get a very good sense of how good the hyperparameters are
  - But at a **significant computational cost**!

Evaluating the System Cost

- In practice we **don't just care about the statistics**
  - Not just about the accuracy after a fixed number of iterations
- We care about wall-clock **time**, and we care about **energy**
  - How much did solving this problem **actually cost**?
- The parameters we chose can affect these systems properties
  - As we saw with our SVRG demo!
- Need to **include systems cost as part of the metric**!

Hardware efficiency

- **How long does an iteration take, on average?**
- Hardware efficiency measures the systems cost of doing a single update.
- Key point: many hyperparameters do not affect hardware efficiency
  - **Which ones?**
- **Which hyperparameters do affect hardware efficiency?**

Statistical Efficiency

- **How many iterations do we need to get to a specified level of accuracy?**

- Statistical efficiency measures how many updates we need to get an answer of the quality that we want.

- **Which hyperparameters affect statistical efficiency?**
  - And which ones don't?

Total performance

- Total cost of running the algorithm is:

HARDWARE EFFICIENCY x STATISTICAL EFFICIENCY

- We can estimate these quantities separately, then use their product to evaluate our hyperparameters.
- For example, we can use theory to evaluate statistical efficiency and a hardware model to evaluate hardware efficiency.

Benefits of Looking at Both

- Looking at **both statistical and hardware efficiency together** has some important benefits!

- Many times the **optimal parameter settings are different** than if you set the parameters to optimize hardware efficiency or statistical efficiency individually.

- There's a lot of **open research opportunities** here!

Recent example: YellowFin Tuner

- System that among other things tunes the **momentum**
  - As well as using **asynchronous parallelism**, which we'll talk about later.

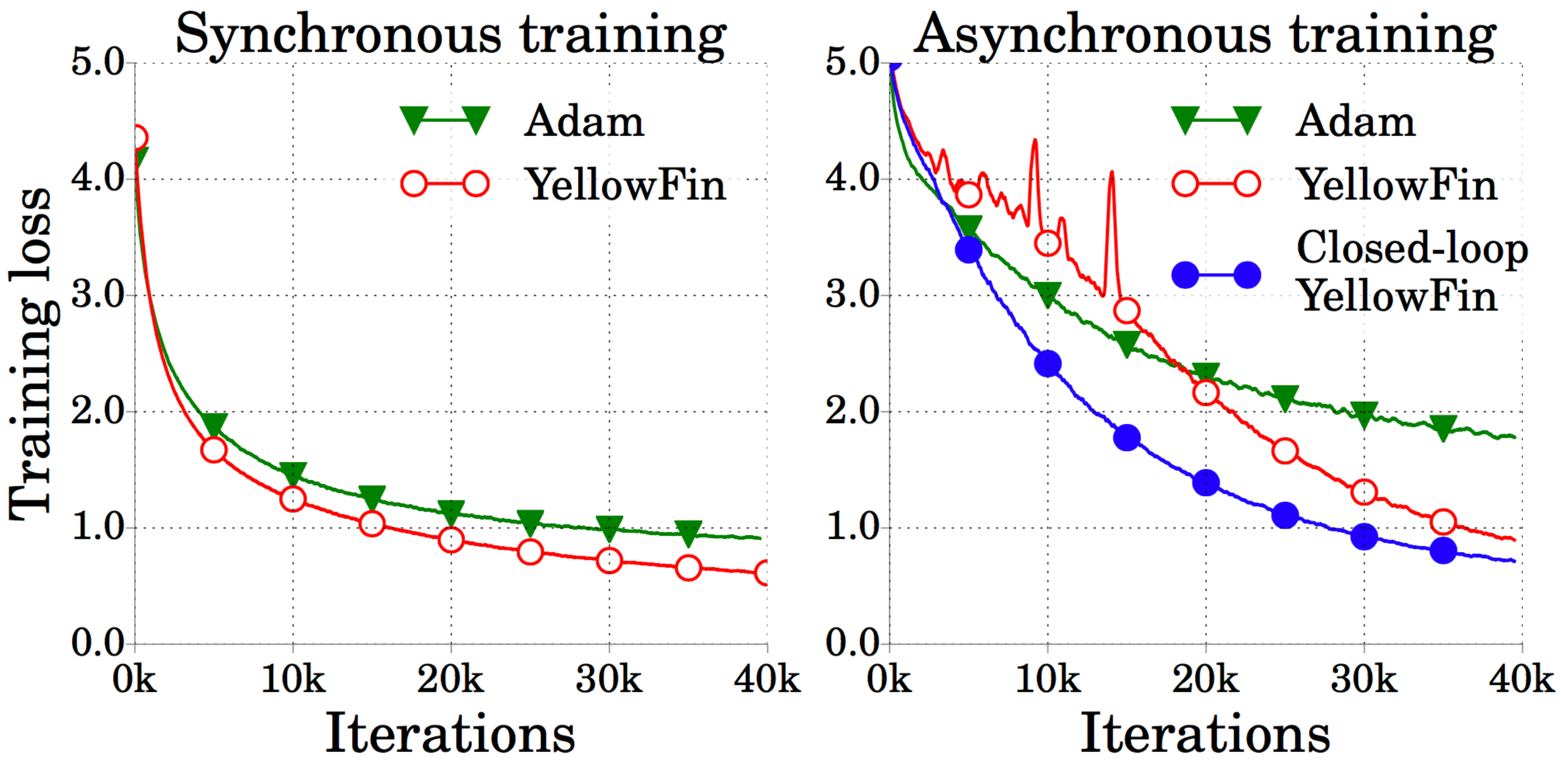

Figure 1 from *"YellowFin and the Art of Momentum Tuning"* Zhang et al, 2017.

Questions?

- Upcoming things
  - Fall break next Monday — **no lecture**
  - Paper review #4 **due Today**
  - Paper Presentation #5 **on Wednesday** — read paper before class
  - Paper Presentation #6 **the following Wednesday**