Hyperparameter optimization

CS6787 Lecture 6 — Fall 2021
But First...

Final Project Parameters

CS 6787 — Fall 2021
Overview

• **Implement a machine learning system** to solve a problem

• Use one or more of the **techniques we discussed in class**

• To achieve an **improvement over some baseline method**
  • Measuring both statistical performance and hardware performance
  • Or at least evaluate and attempt to achieve such a speedup

• Otherwise, very **open-ended**
  • **Groups of up to three**
Project proposals due in four weeks

• The main body should be about one page in length.
• It should describe the project you intend to do.
• It should contain at least one citation of a relevant paper that we did not cover in class.
• It should include some preliminary or exploratory work you've already done, that helps to support the idea that your project is feasible.
  • Don’t need a lot of work, just a nonzero amount of work supporting feasibility.
• In addition to the one-page text proposal, one short experiment plan per person
Experiment plan

• The hypothesis

• The proxy

• The protocol

• Expected results
In-class project feedback activity

• On **Monday, October 18**

• Basically, breakout sessions to discuss your project ideas with your peers.
  • You are not committing to work on the specific project you present during the feedback activity. You can always change your ideas as a result of the feedback.

• Prepare a **two-minute verbal pitch** of your ideas.

• And try not to sit with others in your group.
  • To get a wider variety of feedback.
Questions?
Hyperparameter optimization

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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 $\mu, L$, 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 $\mu$ and $L$

• 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*

• 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: $b = ?$

• Momentum: $\beta = ?$

• SVRG: epoch length = $? \times$ 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 hyperparameter 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!
Questions?

• Upcoming things
  • Paper review 3a or 3b due on Monday
  • Paper Presentation #4 on Monday