11-785/ Spring 2019/ Recitation 3

Efficient Deep Learning Optimization Methods

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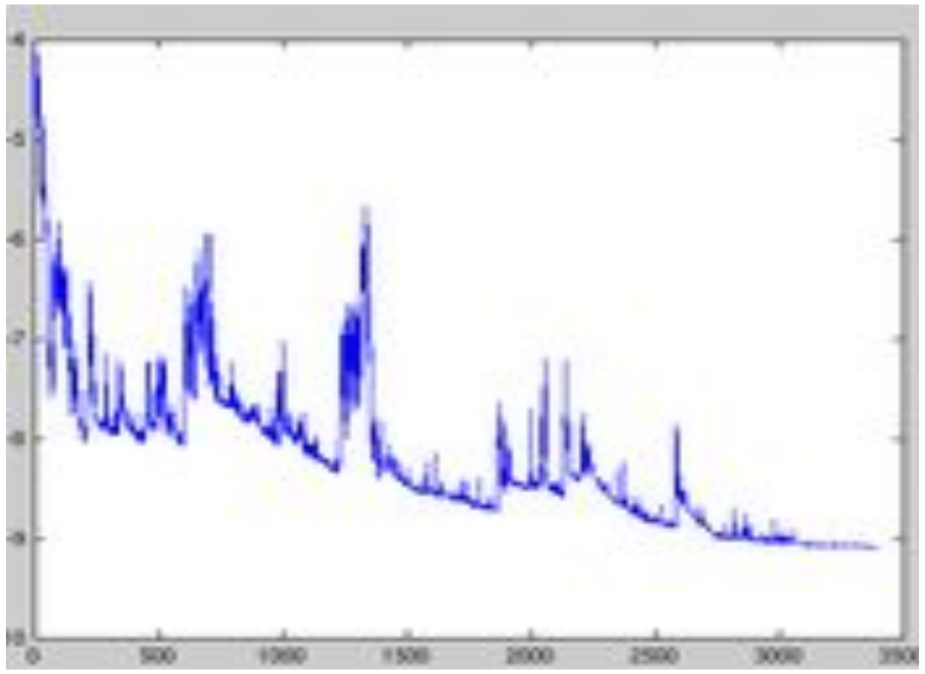
Outline

- 1 Review of optimization
- 2 Optimization practice
- 3 Training tips in PyTorch

1.1 Mini-batch gradient descent

- What is it?
    - Performs update for every mini-batch of data.
- Why mini-batch?
    - Batch gradient descent that uses the whole dataset for one update: slow and intractable for large datasets to fit into memory.
    - Stochastic gradient descent that updates for each data: high variance updates.



SGD fluctuation (Source: wiki)

1.1 Mini-batch gradient descent (continue)

- Update equation
  - Let F be our model, and θ is the parameter: $\hat{y} = F(x;\theta)$
  - The loss function is L, minimize the loss on the dataset:

$$g = \frac{1}{n}\sum_{i=1}^{n} L(y_i, \hat{y}_i)$$

  - Let η be the learning rate, compute the update:

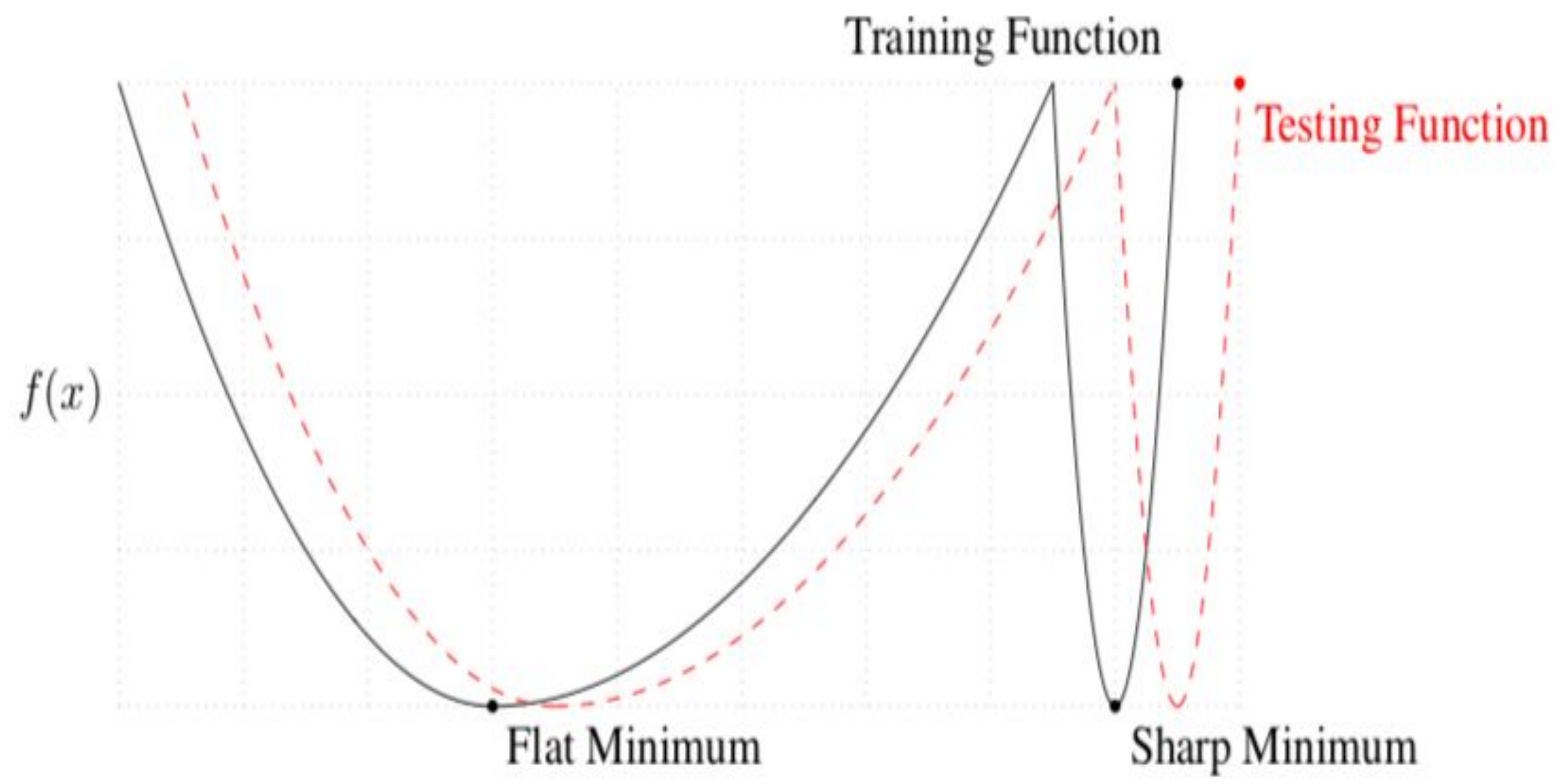
$$\hat{g} = \frac{1}{m}\sum_{i=1}^{m} \nabla_\theta L(y_i, \hat{y}_i), \quad \theta = \theta - \eta \cdot \hat{g}$$

1.1 Mini-batch gradient descent (Continue)

- The good things of mini-batch gradient descent
  - Reduces variance of updates
  - Matrix multiplication is faster
- Have to decide mini-batch size now!
  - The common mini-batch size are 32-256.
  - Too small: Slow and high variance,
    Batch Norm requires a suitable batch size
  - Too big: Harder to escape from local minima.
    Decay in generalization (paper link).

1.1 Mini-batch gradient descent (Continue)

The figure shows why big batch size is not OK:



Y-axis: value of the loss.   X-axis :the parameters.

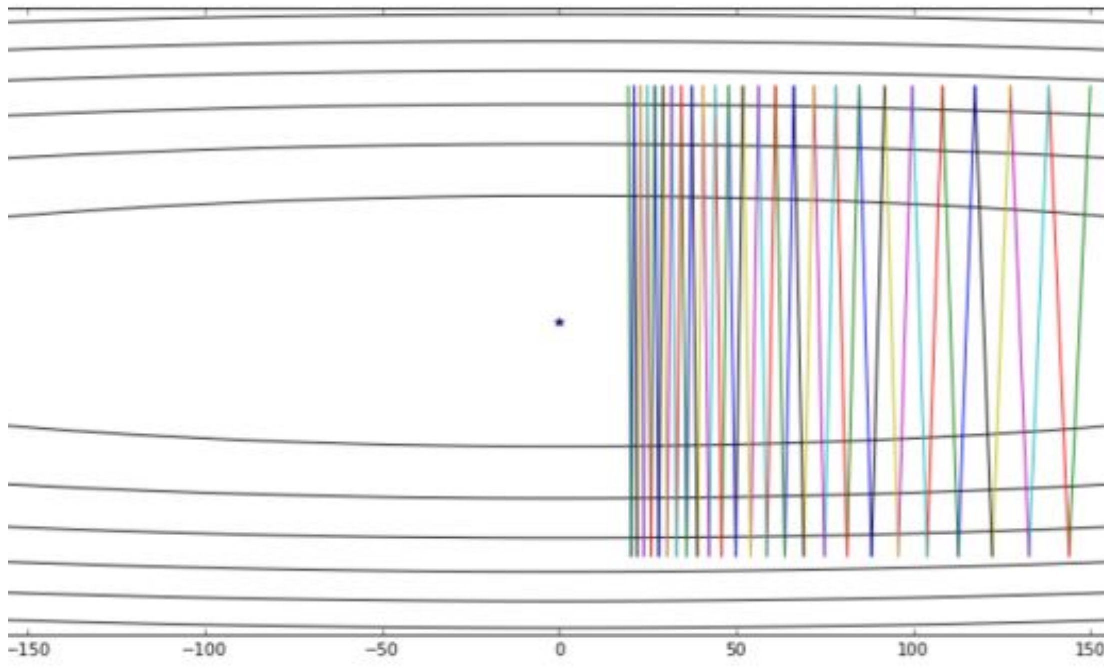
1.2 Momentum

- SGD has trouble navigating ravine. Momentum helps SGD accelerate.
- Adds a fraction γ of the update vector of the past step V_{t-1} to current update vector V_t. Momentum term γ is usually set to 0.9.
- Update: $$v_t = \gamma v_{t-1} + \eta \nabla_\theta L(\theta); \quad \theta = \theta - v_t$$

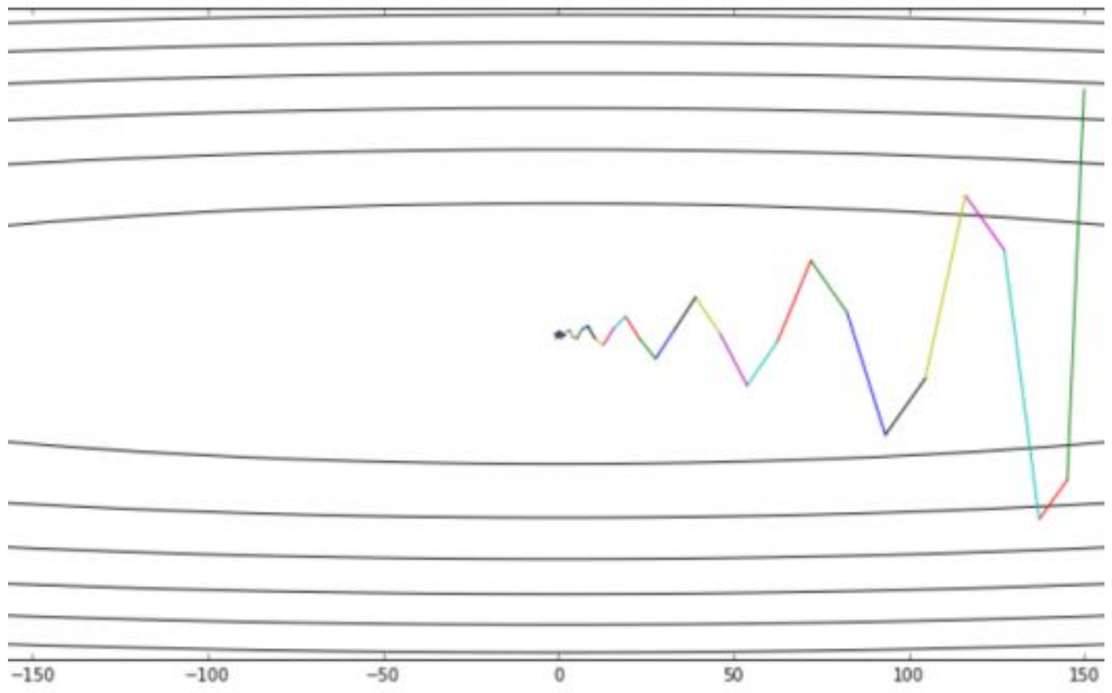
- Example: find the minima of $z = x^2 + 50y^2$

The function looks like this

1.2 Momentum (Continue)



Use GD



GD + Momentum

- Reduces updates for dimensions whose gradients change directions.
- Increases updates for dimensions whose gradients point in the same directions.

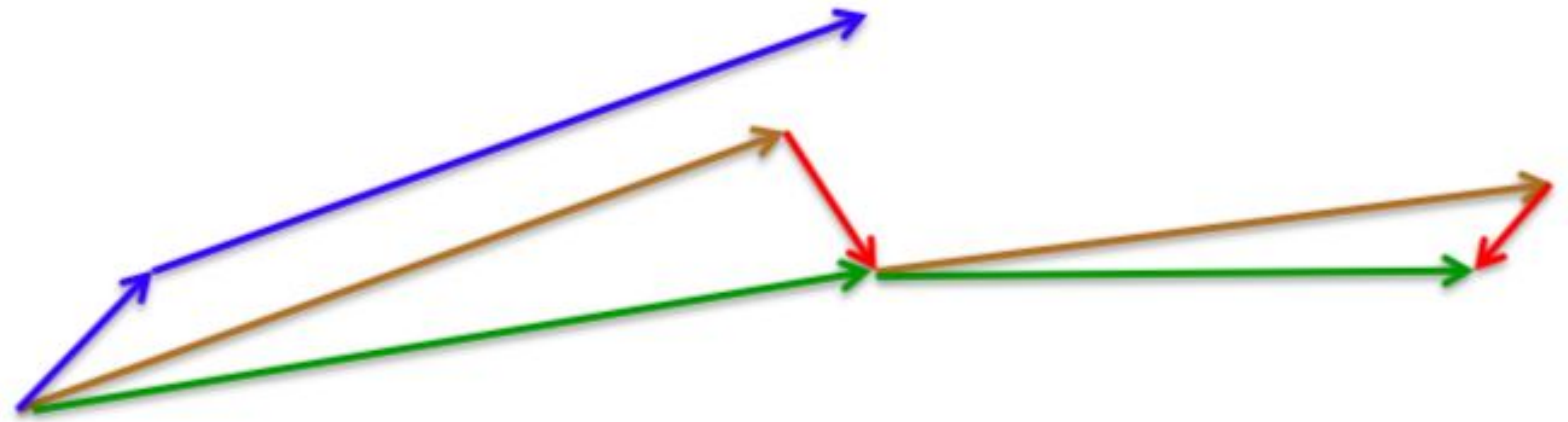
1.3 Nesterov accelerated gradient (NAG)

- The moment uses history information for better update. NAG wants to add some future information.
- Update:

$$v_t = \gamma v_{t-1} + \eta \nabla_\theta L(\theta - \gamma v_{t-1}); \quad \theta = \theta - v_t$$

A picture of the Nesterov method

- First make a big jump in the direction of the previous accumulated gradient.
- Then measure the gradient where you end up and make a correction.



brown vector = jump, red vector = correction, green vector = accumulated gradient

blue vectors = standard momentum

1.4 Adagrad

- The previous methods: same learning rate for all parameters.
- Adagrad adapts the learning rate to the parameters
  large updates for infrequent parameters
  small updates for frequent parameters
- Adagrad divides the learning rate by the square root of the sum of squares of historic gradients.
- Update:

$$r_t = \sum_{i=1}^{t} g_i^2, \quad \theta = \theta - \frac{\eta}{\sqrt{r_t + \epsilon}} * g_t$$

g_t is the sum of the squares of the gradients.

* is element-wise multiplication.

1.4 Adagrad (Continue)

- Pros

  1) Good when dealing with sparse data.

  2) Lesser need to manually tune learning rate.

- Cons

  Recall that the update is:

$$\theta = \theta - \frac{\eta}{\sqrt{\sum_{i=1}^{t} g_i^2 + \epsilon}} * g_t$$

Accumulates squared gradients in denominator.

Causes the learning rate to shrink and become infinitesimally small.

1.5 Adadelta

- In adagrad, the learning rate may become infinitesimally small.
- Adadelta was designed to solve this problem. It replaces the denominator
  by the running average of squared gradients:

$$\mathbb{E}[g^2]_t = \gamma \mathbb{E}[g^2]_{t-1} + (1-\gamma) g_t^2$$

- Preliminary Adadelta update (Also named RMSprop):

$$\theta = \theta - \frac{\eta}{\sqrt{\mathbb{E}[g^2]_t + \epsilon}} * g_t$$

- Compare with adagrad:

$$\theta = \theta - \frac{\eta}{\sqrt{\sum_{i=1}^{t} g_i^2 + \epsilon}} * g_t$$

1.5 Adadelta (Continue)

- Denominator is called root mean squared (RMS) error of gradient, we can write the update as:

$$\Delta\theta_t = -\eta \frac{g_t}{RMS[g]_t}$$

- The units do not match!
- Define the running average of squared parameter updates and RMS:

$$\mathbb{E}[\Delta\theta^2]_t = \gamma \mathbb{E}[\Delta\theta^2]_{t-1} + (1-\gamma)\Delta\theta_t^2$$

- Now we can replace η with $RMS[\theta]_{t-1}$ for the final update:

$$\Delta\theta_t = -RMS[\theta]_{t-1} \frac{g_t}{RMS[g]_t}$$

1.6 Adam

- Now we have two kinds of ideas for improving SGD:
  1) Momentum and Nesterov: use more gradients
  2) Adagrad and Adadelta: different LR for different parameters.
- Combine the two ideas. Adam!
- Update. First store the mean and uncentered variance of gradients:

$$m_t = \beta_1 m_{t-1} + (1-\beta_1) g_t$$

$$v_t = \beta_2 v_{t-1} + (1-\beta_2) g_t^2$$

- m_t is the running mean of gradients and v_t is the running uncentered variance of gradients

1.6 Adam (Continue)

- m_t and v_t are initializes as zero vectors. So they are biased estimation and we want to correct them as:

$$\hat{m}_t = \frac{m_t}{1-\beta_1^t}, \quad \hat{v}_t = \frac{v_t}{1-\beta_2^t}$$

- The update rule is:

$$\theta = \theta - \frac{\eta}{\sqrt{\hat{v}_t + \epsilon}} \hat{m}_t$$

- Question: Adam looks like RMS with Momentum, what are the differences?

2.1 Parameter Initialization

- Can we start with zero initial weights?
- Can we have equal initial weights?
- Methods to initialize
    - Random (typically gaussian)
    - Xavier
    - He initialization with ReLU
    - Pretraining

2.1 Parameter Initialization (Continue)

- Xavier: Uniform distribution from [-a, a].
- You want the variance of Input and Output to be the same:

$$y = \sum_{i=1}^{n} w_i x_i$$

- If you work out the math, Var(w_i) = 1/n
- But you do not have only one output, you may have m outputs:

$$var(w_i) = \frac{2}{n+m}$$

- The variance of Uniform distribution from [a, b] is

$$\frac{(b-a)^2}{12}$$

- Solve for a

2.1 Parameter Initialization (Continue)

- He Initialization for ReLU
  Uniform distribution from [-a, a].

- About half output will return zero after ReLU

$$y = ReLU(\sum_{i=1}^{n} w_i x_i)$$

- The variance changes to Var(w_i) = 2/n
- Re-solve for a

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2.2 Annealing the learning rate

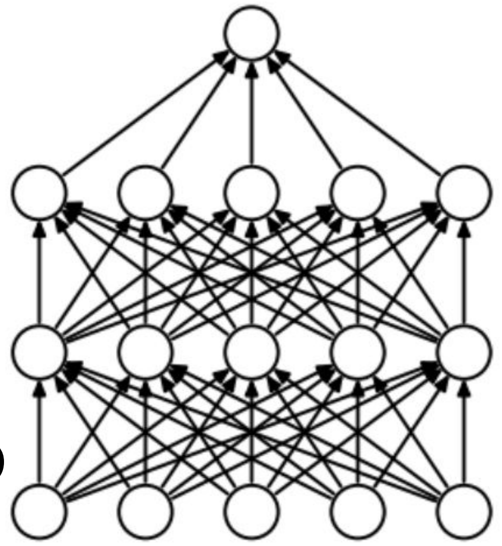
- Usually helpful to anneal the learning rate over time
- High learning rates can cause the parameter vector to bounce around chaotically, unable to settle down into deeper, but narrower parts of the loss function
- **Step decay**: Reduce the learning rate by some factor after some number of epochs (i.e. reduce by a half every 5 epochs, or by 0.1 every 20 epochs).
- **Plateau decay**: Watch the validation error or loss while training with a fixed learning rate, and reduce the learning rate by a constant factor whenever the validation performance stops improving
- **Exponential decay**: It has the mathematical form lr = lr0 * e^(−kt), where lr0, k are hyperparameters and t is the iteration number

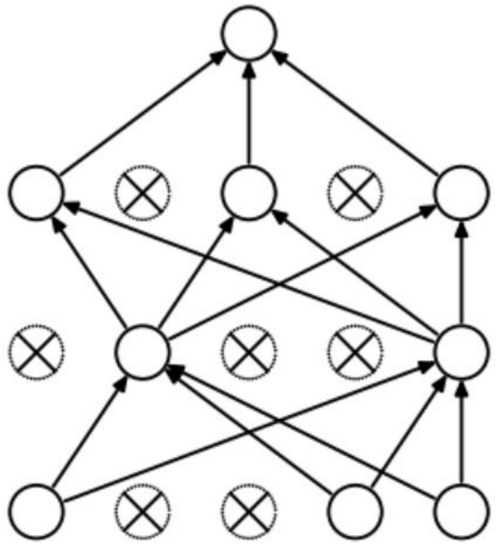
2.2 Annealing the learning rate (Continue)

- Learning rate schedulers in PyTorch

- torch.optim.lr_scheduler.<StepLR|ExponentialLR|ReduceLROnPlateau>
- Each type of scheduler requires hyperparameters unique to it on initialization – read the docs
- scheduler.step(val_loss)
    - At end of each epoch – maintains history of epoch loss to determine when to decay the learning rate

2.3 Random Dropout


(a) Standard Neural Net


(b) After applying dropout.

- Implementation

  Dropout each unit with probability p

  No parameters dropped at test time
- Results

  Network is forced to learn a distributed representation

  Improves generalization by eliminating neuron co-dependencies within a layer
- In PyTorch

  nn.Dropout(p = _)

  Typical dropout probability is around 0.1 to 0.5

2.4 Others:

- Shuffle the dataset
  If not shuffle, the network will remember the data order!
  In hw1p2, it is a frame-level task, so you need to shuffle in frames.
- Weight decay:
  L2 regularization for (not) overfitting:

$$loss = \sum_{i=1}^{n} L(y_i, \hat{y}_i) + \frac{1}{2} w\theta^2$$

$$\theta = \theta - \Delta\theta - w\theta$$

- Early Stopping for (not) overfitting