CSC 561: Neural Networks and Deep Learning

Optimization (part 2)

Marco Alvarez

Department of Computer Science and Statistics
University of Rhode Island

Spring 2025

THINK BIG WE DO℠

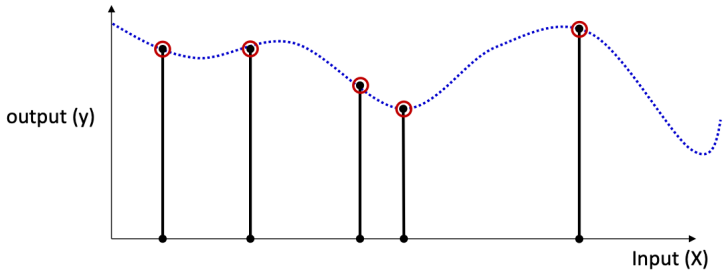
Credit: the following slides are taken from one of the "11-785 Introduction to Deep Learning - CMU" lectures

MLSP MachineLearning For SignalProcessing Group

Training Neural Networks: Optimization

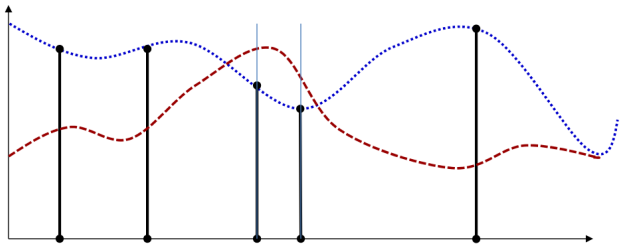
Intro to Deep Learning, Spring 2025

The training formulation



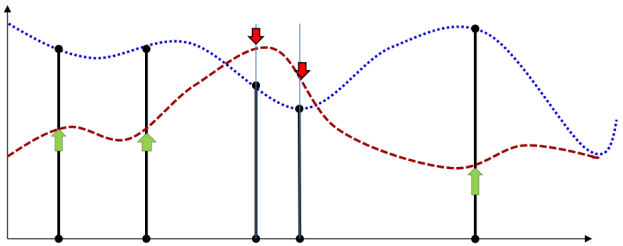
- Given input output pairs at a number of locations, estimate the entire function

Gradient descent



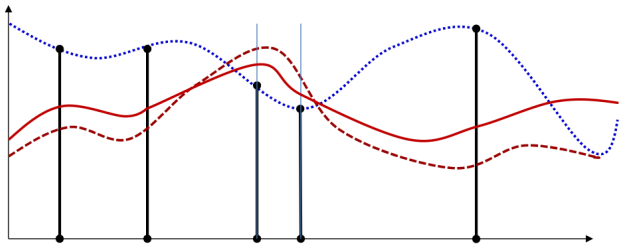
- Start with an initial function

Gradient descent



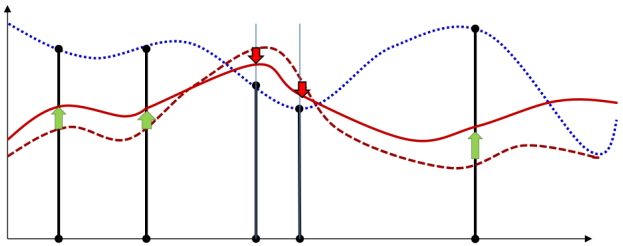
- Start with an initial function
- Adjust its value at *all* points to make the outputs closer to the required value
  - Gradient descent adjusts parameters to adjust the function value at *all* points
  - Repeat this iteratively until we get arbitrarily close to the target function at the training points

Gradient descent



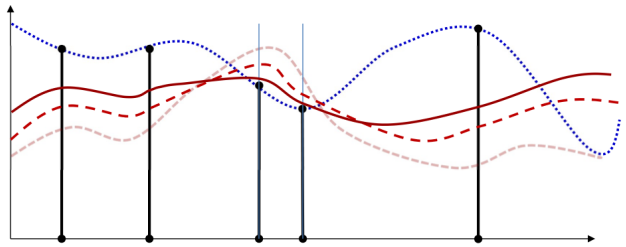
- Start with an initial function
- Adjust its value at *all* points to make the outputs closer to the required value
  - Gradient descent adjusts parameters to adjust the function value at *all* points
  - Repeat this iteratively until we get arbitrarily close to the target function at the training points

Gradient descent



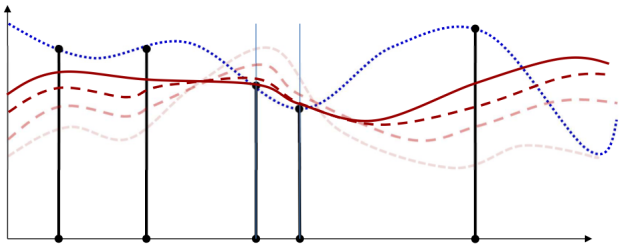
- Start with an initial function
- Adjust its value at *all* points to make the outputs closer to the required value
  - Gradient descent adjusts parameters to adjust the function value at *all* points
  - Repeat this iteratively until we get arbitrarily close to the target function at the training points

Gradient descent



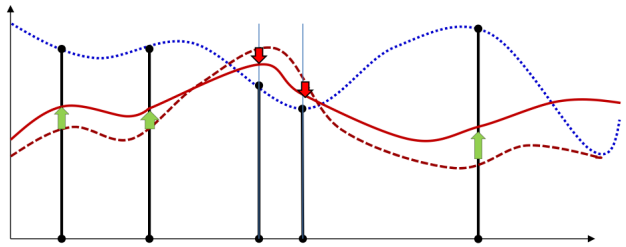
- Start with an initial function
- Adjust its value at *all* points to make the outputs closer to the required value
  - Gradient descent adjusts parameters to adjust the function value at *all* points
  - Repeat this iteratively until we get arbitrarily close to the target function at the training points

Gradient descent



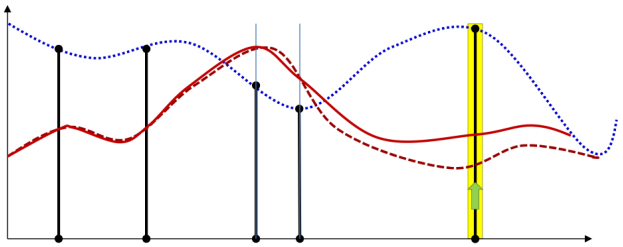
- Start with an initial function
- Adjust its value at *all* points to make the outputs closer to the required value
  - Gradient descent adjusts parameters to adjust the function value at *all* points
  - Repeat this iteratively until we get arbitrarily close to the target function at the training points

Effect of number of samples



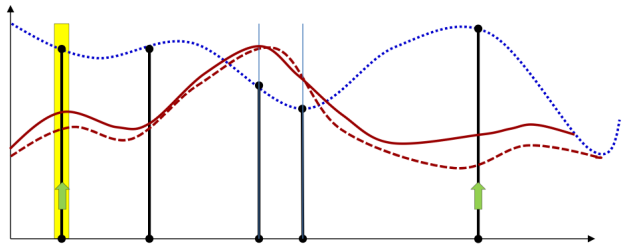
- Problem with conventional gradient descent: we try to simultaneously adjust the function at *all* training points
  - We must process *all* training points before making a single adjustment
  - **"Batch"** update

Alternative: Incremental update



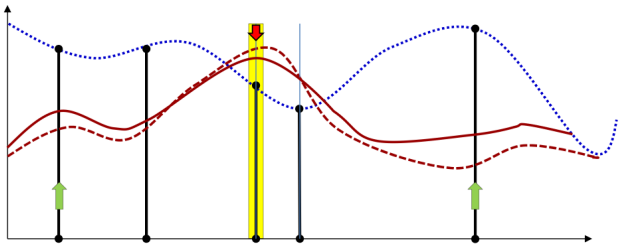
- Alternative: adjust the function at one training point at a time
  - Keep adjustments small

Alternative: Incremental update



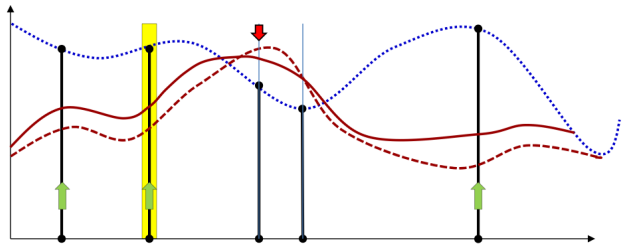
- Alternative: adjust the function at one training point at a time
  - Keep adjustments small

Alternative: Incremental update



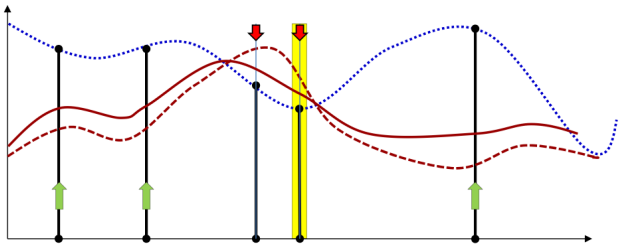
- Alternative: adjust the function at one training point at a time
  - Keep adjustments small

Alternative: Incremental update



- Alternative: adjust the function at one training point at a time
  - Keep adjustments small

Alternative: Incremental update



- Alternative: adjust the function at one training point at a time
  - Keep adjustments small
  - Eventually, when we have processed all the training points, we will have adjusted the entire function
    - With *greater* overall adjustment than we would if we made a single "Batch" update

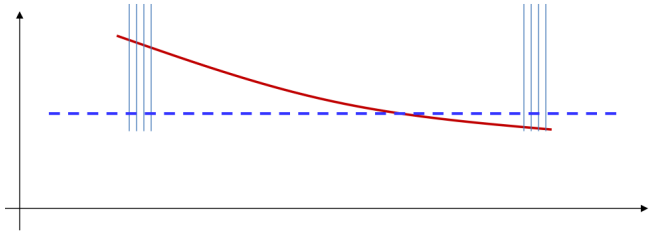
Incremental Updates

- The iterations can make multiple passes over the data
- A single pass through the entire training data is called an "epoch"
  - An epoch over a training set with T samples results in T updates of parameters

Incremental Update

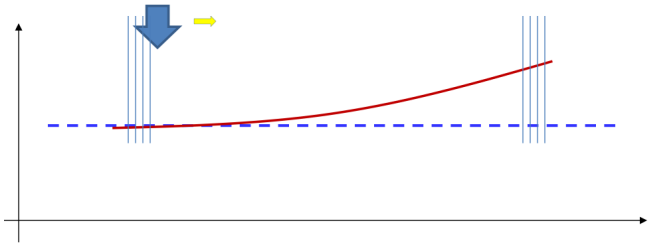
- Given (X_1, d_1), (X_2, d_2),…, (X_T, d_T)
- Initialize all weights $W_1, W_2, \ldots, W_K$
- Do: (Over multiple epochs)
  - For all $t = 1:T$ (One epoch)
    - For every layer k:
      - Compute $\nabla_{W_k} \boldsymbol{Div}(\boldsymbol{Y_t}, \boldsymbol{d_t})$
      - Update
        $W_k = W_k - \eta \nabla_{W_k} \boldsymbol{Div}(\boldsymbol{Y_t}, \boldsymbol{d_t})^T$ (One update)
- Until $Loss$ has converged

Caveats: order of presentation



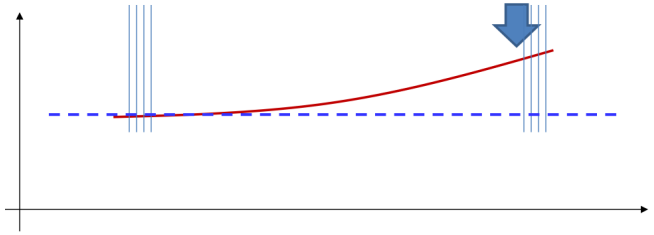
- If we loop through the samples in the same order, we may get *cyclic* behavior

Caveats: order of presentation



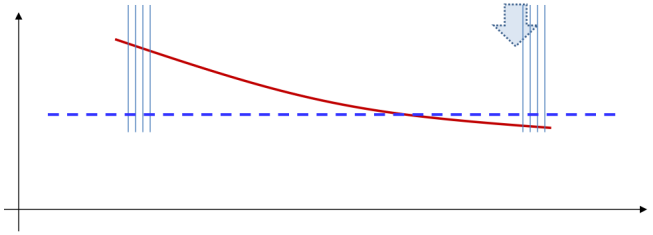
- If we loop through the samples in the same order, we may get *cyclic* behavior

Caveats: order of presentation



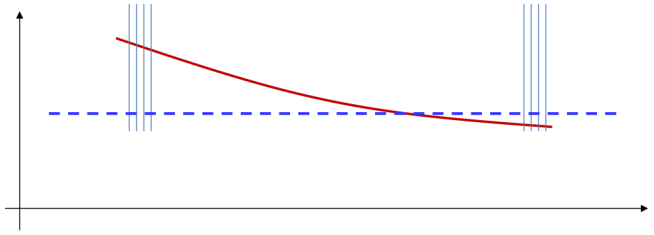
- If we loop through the samples in the same order, we may get *cyclic* behavior

Caveats: order of presentation



- If we loop through the samples in the same order, we may get *cyclic* behavior

Caveats: order of presentation



- If we loop through the samples in the same order, we may get *cyclic* behavior
- We must go through them *randomly* to get more convergent behavior

Incremental Update: Stochastic Gradient Descent

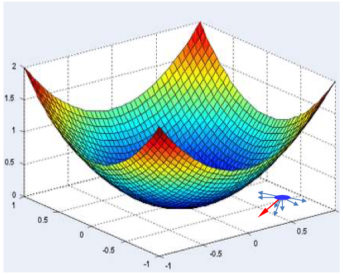
- Given (X_1, d_1), (X_2, d_2),…, (X_T, d_T)
- Initialize all weights $W_1, W_2, \ldots, W_K$
- Do:
  - Randomly permute (X_1, d_1), (X_2, d_2),…, (X_T, d_T)
  - For all $t = 1:T$
    - For every layer k:
      - Compute $\nabla_{W_k} \boldsymbol{Div}(\boldsymbol{Y_t}, \boldsymbol{d_t})$
      - Update

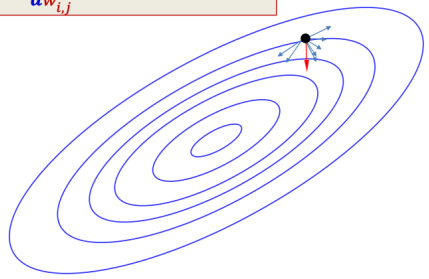
$$W_k = W_k - \eta \nabla_{W_k} \boldsymbol{Div}(\boldsymbol{Y_t}, \boldsymbol{d_t})^T$$

- Until $Loss$ has converged

The expected behavior of the gradient

$$\frac{dE(W^{(1)}, W^{(2)}, \ldots, W^{(K)})}{dw_{i,j}^{(k)}} = \frac{1}{T}\sum_{i} \frac{dDiv(Y(X_i), d_i; W^{(1)}, W^{(2)}, \ldots, W^{(K)})}{dw_{i,j}^{(k)}}$$





- The individual training instances contribute different directions to the overall gradient
  - The final gradient points is the average of individual gradients
  - It points towards the *net* direction

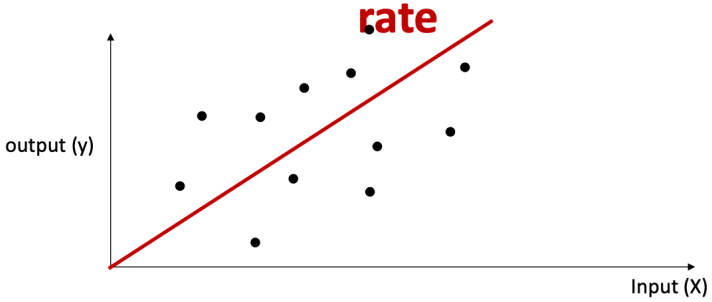
When does it work

- What are the considerations?
- And how well does it work?

Incremental learning runs the risk of always chasing the latest input

- **Incremental learning:** Update the model to always minimize the error on the latest instance
  - It will never converge
  - **Solution?**

Incremental learning caveat: learning rate



- **Incremental learning:** Update the model to always minimize the error on the latest instance
  - **Caveat:** We must *shrink* the learning rate with iterations for convergence
    - Correction for individual instances with the eventual miniscule learning rates will not modify the function

Incremental Update: Stochastic Gradient Descent

- Given $(X_1, d_1), (X_2, d_2), \ldots, (X_T, d_T)$
- Initialize all weights $W_1, W_2, \ldots, W_K$; $j = 0$
- Do:
  - Randomly permute $(X_1, d_1), (X_2, d_2), \ldots, (X_T, d_T)$
  - For all $t = 1:T$
    - $j = j + 1$
    - For every layer k:
      - Compute $\nabla_{W_k} Div(Y_t, d_t)$
      - Update

$$W_k = W_k - \eta_j \nabla_{W_k} Div(Y_t, d_t)^T$$

Randomize input order

Learning rate reduces with j

- Until $Loss$ has converged

SGD convergence

- SGD converges "almost surely" to a global or local minimum for most functions
  - Sufficient condition: step sizes follow the following conditions (Robbins and Munro 1951)

$$\sum_k \eta_k = \infty$$

    - Eventually the entire parameter space can be searched

$$\sum_k \eta_k^2 < \infty$$

    - The steps shrink
  - The fastest converging series that satisfies both above requirements is

$$\eta_k \propto \frac{1}{k}$$

    - This is the optimal rate of shrinking the step size for strongly convex functions
  - More generally, the learning rates are heuristically determined
- If the loss is convex, SGD converges to the optimal solution
- For non-convex losses SGD converges to a local minimum

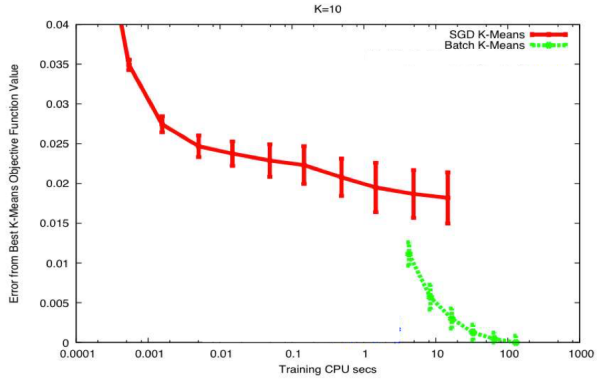
Batch gradient convergence

- In contrast, using the batch update method, for *strongly convex* functions,

$$\left|f\left(W^{(k)}\right) - f(W^*)\right| < c^k \left|f\left(W^{(0)}\right) - f(W^*)\right|$$

  - Giving us the iterations to ϵ convergence as $O\left(log\left(\frac{1}{\epsilon}\right)\right)$
- For generic convex functions, iterations to ϵ convergence is $O\left(\frac{1}{\epsilon}\right)$
- Batch gradients converge "faster"
  - But SGD performs T updates for every batch update

SGD example

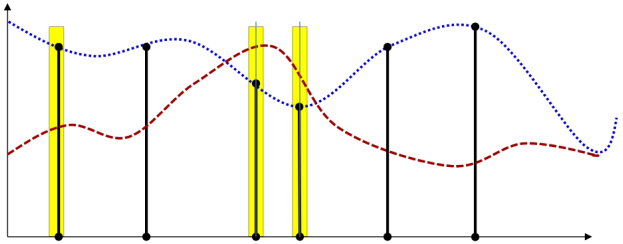


- A simpler problem: K-means
- Note: SGD converges faster
- But also has large variation between runs

SGD vs batch

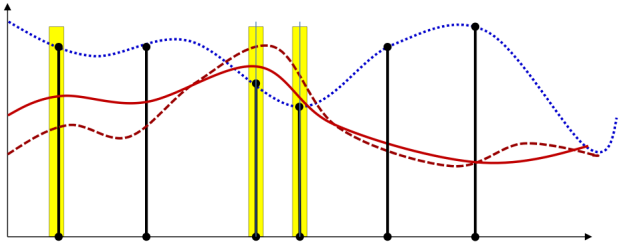
- SGD uses the gradient from only one sample at a time, and is consequently high variance
- But also provides significantly quicker updates than batch
- Is there a good medium?

Alternative: Mini-batch update



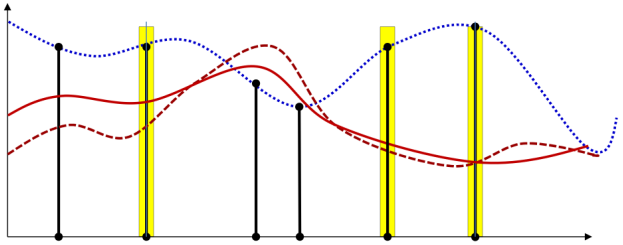
- Alternative: adjust the function at a small, randomly chosen subset of points
  - Keep adjustments small
  - If the subsets cover the training set, we will have adjusted the entire function
- As before, vary the subsets randomly in different passes through the training data

Alternative: Mini-batch update



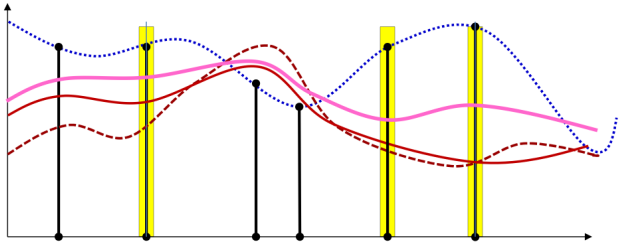
- Alternative: adjust the function at a small, randomly chosen subset of points
  - Keep adjustments small
  - If the subsets cover the training set, we will have adjusted the entire function
- As before, vary the subsets randomly in different passes through the training data

Alternative: Mini-batch update



- Alternative: adjust the function at a small, randomly chosen subset of points
  - Keep adjustments small
  - If the subsets cover the training set, we will have adjusted the entire function
- As before, vary the subsets randomly in different passes through the training data

Alternative: Mini-batch update



- Alternative: adjust the function at a small, randomly chosen subset of points
  - Keep adjustments small
  - If the subsets cover the training set, we will have adjusted the entire function
- As before, vary the subsets randomly in different passes through the training data

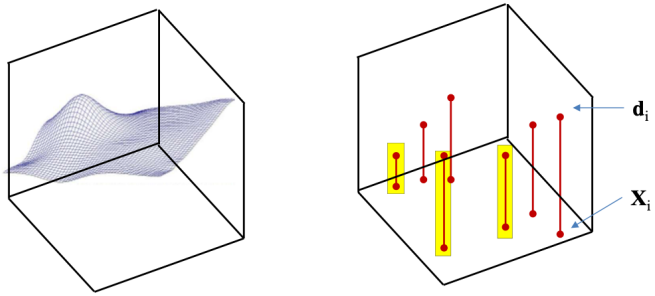
Incremental Update: Mini-batch update

- Given (X_1, d_1), (X_2, d_2),…, (X_T, d_T)
- Initialize all weights $W_1, W_2, \ldots, W_K$; $j = 0$
- Do:
  - Randomly permute (X_1, d_1), (X_2, d_2),…, (X_T, d_T)
  - For $t = 1 : b : T$
    - $j = j + 1$
    - For every layer k:
      - $\Delta W_k = 0$
    - For t' = t : t+b-1
      - For every layer k:
        - Compute $\nabla_{W_k} Div(Y_t, d_t)$
        - $\Delta W_k = \Delta W_k + \frac{1}{b} \nabla_{W_k} Div(Y_t, d_t)^T$
    - Update
      - For every layer k:
        - $W_k = W_k - \eta_j \Delta W_k$
- Until Err has converged

Mini-batch size

Shrinking step size

Mini Batches



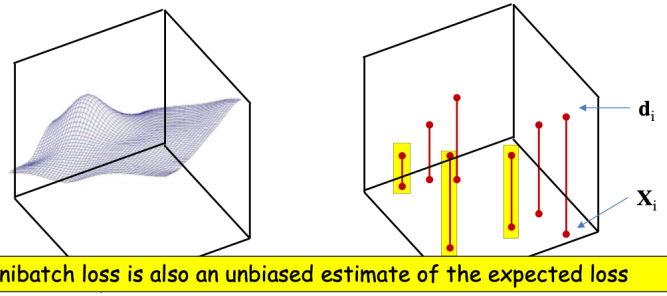
- Mini-batch updates compute and minimize a *batch loss*

$$MiniBatchLoss(W) = \frac{1}{b}\sum_{i=1}^{b} div(f(X_i; W), d_i)$$

- The *expected value* of the *batch loss* is also the *expected divergence*

$$E[MiniBatchLoss(W)] = E\left[div(f(X; W), g(X))\right]$$

Mini Batches



The minibatch loss is also an unbiased estimate of the expected loss

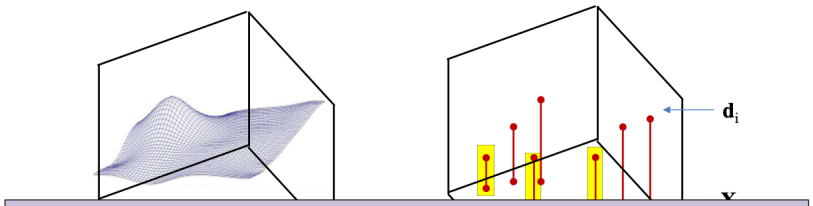
- Mini-batch updates compute and minimize a *batch loss*

$$MiniBatchLoss(W) = \frac{1}{b}\sum_{i=1}^{b} div(f(X_i; W), d_i)$$

- The *expected value* of the *batch loss* is also the *expected divergence*

$$E[MiniBatchLoss(W)] = E\left[div(f(X; W), g(X))\right]$$

Mini Batches



The variance of the minibatch loss: var(BatchLoss) = 1/b var(div)
This will be much smaller than the variance of the sample error in SGD

The minibatch loss is also an unbiased estimate of the expected error

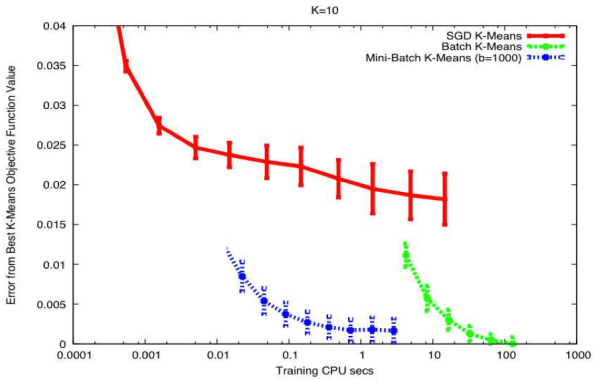
- Mini-batch updates compute and minimize a *batch loss*

$$MiniBatchLoss(W) = \frac{1}{b}\sum_{i=1}^{b} div(f(X_i;W), d_i)$$

- The *expected value* of the *batch loss* is also the *expected divergence*

$$E[MiniBatchLoss(W)] = E\left[div(f(X;W), g(X))\right]$$

SGD example



- Mini-batch performs comparably to batch training on this simple problem
  - But converges orders of magnitude faster

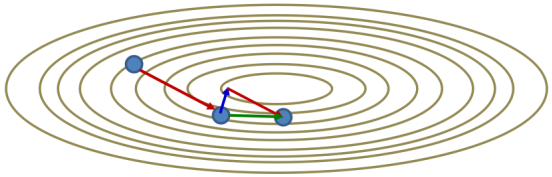
Training and minibatches

- In practice, training is usually performed using mini-batches
  - The mini-batch size is generally set to the largest that your hardware will support (in memory) without compromising overall compute time
    - Larger minibatches = less variance
    - Larger minibatches = few updates per epoch
- Convergence depends on learning rate
  - Simple technique: fix learning rate until the error plateaus, then reduce learning rate by a fixed factor (e.g. 10)
  - ***Advanced methods***: Adaptive updates, where the learning rate is itself determined as part of the estimation

Training and minibatches

- Convergence depends on learning rate
  - Simple technique: fix learning rate until the error plateaus, then reduce learning rate by a fixed factor (e.g. 10)
  - ***Advanced methods***: Adaptive updates, where the learning rate is itself determined as part of the estimation

Recall: Momentum Update

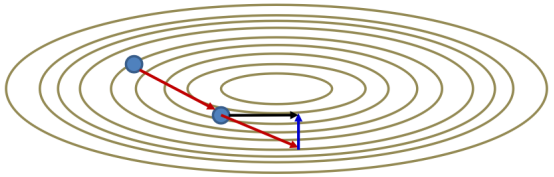


- The momentum method

$$\Delta W^{(k)} = \beta \Delta W^{(k-1)} - \eta \nabla_W Loss\left(W^{(k-1)}\right)^T$$

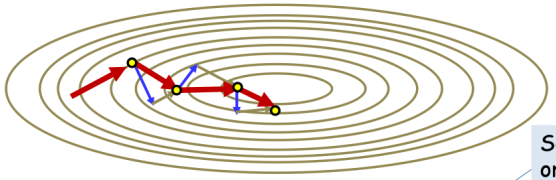
- At any iteration, to compute the current step:
  - First compute the gradient step at the current location
  - Then add in the scaled *previous* step
    - Which is actually a running average
  - To get the final step

Nestorov's Accelerated Gradient



- Change the order of operations
- At any iteration, to compute the current step:
  - First extend the previous step
  - Then compute the gradient step at the resultant position
  - Add the two to obtain the final step

Momentum and incremental updates



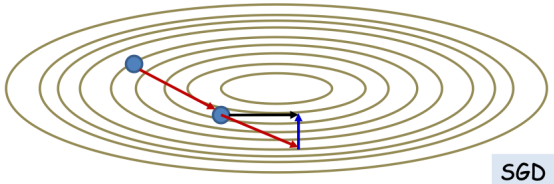
SGD instance or minibatch loss

- The momentum method

$$\Delta W^{(k)} = \beta \Delta W^{(k-1)} - \eta \nabla_W Loss\left(W^{(k-1)}\right)^T$$

- Incremental SGD and mini-batch gradients tend to have high variance
- Momentum smooths out the variations
  - Smoother and faster convergence

Nestorov's Accelerated Gradient



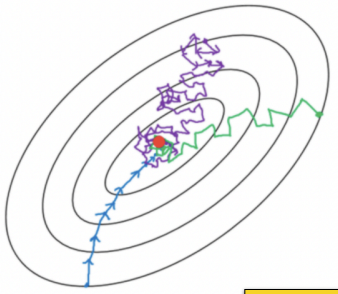
SGD instance or minibatch loss

- Nestorov's method

$$\Delta W^{(k)} = \beta \Delta W^{(k-1)} - \eta \nabla_W Loss(W^{(k-1)} + \beta \Delta W^{(k-1)})^T$$

$$W^{(k)} = W^{(k-1)} + \Delta W^{(k)}$$

Momentum update



momentum provides faster convergence with sgd and mini-bath gradient descent

The other term in the update

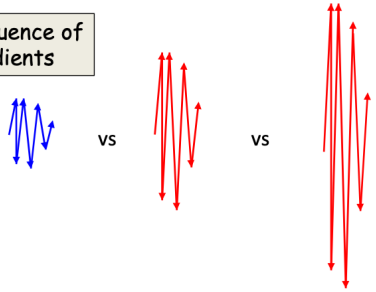
- Standard gradient descent rule

$$W \leftarrow W - \eta \nabla_W L(W)$$

- Gradient descent invokes two terms for updates
  - The derivative
  - and the learning rate
- Momentum methods fix this term to reduce unstable oscillation
- What about this term?

Adjusting the learning rate

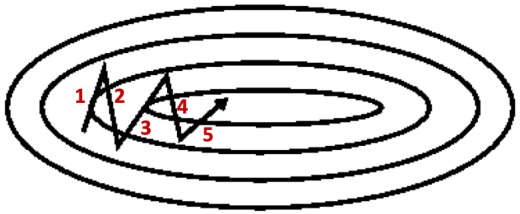
Sequence of gradients



With separate learning rates in each direction, which should have the lowest learning rate in the vertical direction?

- Have separate learning rates for each component
- Directions in which the derivatives swing more should likely have lower learning rates
  - Is likely indicative of more wildly swinging behavior
- Directions of greater swing are indicated by total movement
  - Direction of greater movement should have lower learning rate

Smoothing the trajectory

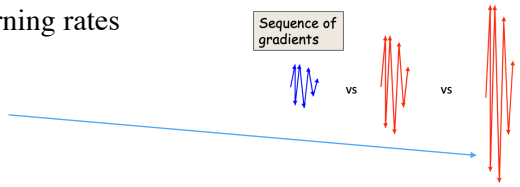


Step	X component	Y component
1	1	+2.5
2	1	-3
3	2	+2.5
4	1	-2
5	1.5	1.5

- Observation: Steps in "oscillatory" directions show large total movement
  - In the example, total motion in the vertical direction is much greater than in the horizontal direction
- Solution: Lower learning rate in the vertical direction than in the horizontal direction
  - Based on total motion
  - As quantified by RMS value

Adagrad

- Idea: per-parameter learning rates
  - steep directions
    - large "total movement"
    - want lower learning rates
  - flat directions
    - want larger learning rates
  - keep a historical sum of squares in each dimension
  - squares capture total motion on both sides of oscillation




```
dw_squared = 0
for i in range(n_iter):
    dw = gradient(w)
    dw_squared += dw * dw
    w = w - lr * dw / sqrt(dw_squared + eps)
```

step size decays to zero over time (denominator grows)

RMS Prop

- Notation:
  - Formulae are ***by parameter***
  - Derivative of loss w.r.t any individual parameter w is shown as $\partial_w D$
    - Batch or minibatch loss, or individual divergence for batch/minibatch/SGD
  - The ***squared*** derivative is $\partial_w^2 D = (\partial_w D)^2$
    - Short-hand notation represents the squared derivative, not the second derivative
  - The ***mean squared*** derivative is a running estimate of the average squared derivative. We will show this as $E[\partial_w^2 D]$
- Modified update rule: We want to
  - scale down learning rates for terms with large mean squared derivatives
  - scale up learning rates for terms with small mean squared derivatives

RMS Prop

- This is a variant on the *basic* mini-batch SGD algorithm
- **Procedure:**
  - Maintain a running estimate of the mean squared value of derivatives for each parameter
  - Scale learning rate of the parameter by the *inverse* of the *root mean squared* derivative

$$E[\partial_w^2 D]_k = \gamma E[\partial_w^2 D]_{k-1} + (1-\gamma)(\partial_w^2 D)_k$$

$$w_{k+1} = w_k - \frac{\eta}{\sqrt{E[\partial_w^2 D]_k + \epsilon}} \partial_w D$$

From Adagrad to RMSProp

Adagrad

```
dw_squared = 0
for i in range(n_iter):
    dw = gradient(w)
    dw_squared += dw * dw
    w = w - lr * dw / sqrt(dw_squared + eps)
```

step size decays to zero over time

RMSProp

```
dw_squared = 0
for i in range(n_iter):
    dw = gradient(w)
    dw_squared = dr * dw_squared + (1-dr) * dw * dw
    w = w - lr * dw / sqrt(dw_squared + eps)
```

decay rate

All the terms in gradient descent

- Standard gradient descent rule

$$W \leftarrow W - \eta \nabla_W L(W)$$

- RMSprop only adapts the learning rate
  - by total movement
- Momentum only smooths the gradient
- How about combining both?

Adam

- Previous methods
  - RMSProp adapts the learning rate per-parameter
  - Momentum smooths the gradient
- Adam (adaptive moments) combines both
  - moving averages for both the gradients (momentum) and the squared gradients (RMSProp)

```
first_moment = 0
second_moment = 0
for i in range(n_iter):
    dw = gradient(w)
    first_moment = beta1 * first_moment + (1-beta1) * dw
    second_moment = beta2 * second_moment + (1-beta2) * dw * dw
    w = w - lr * first_moment / (sqrt(second_moment) + eps)
```

Adam

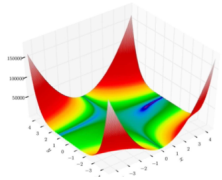
- Removing bias
  - as moments are initialized to zero, first update may be very large (small second_moment)

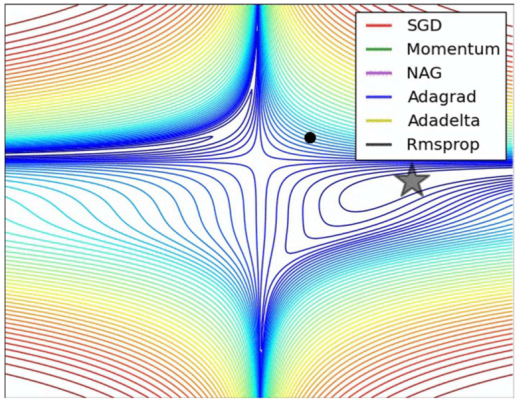
good starting points $\beta_1 = 0.9, \beta_2 = 0.999$

```
first_moment = 0
second_moment = 0
for i in range(n_iter):
    dw = gradient(w)
    first_moment = beta1 * first_moment + (1-beta1) * dw
    second_moment = beta2 * second_moment + (1-beta2) * dw * dw

    first = first_moment / (1 - beta1**(i+1))
    second = second_moment / (1 - beta2**(i+1))

    w = w - lr * first / (sqrt(second) + eps)
```

denominators approach 1 as i grows

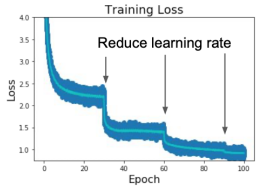
Visualizing the optimizers: Beale's Function



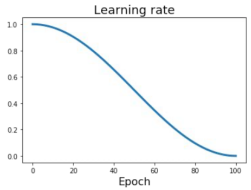


- http://www.denizyuret.com/2015/03/alec-radfords-animations-for.html

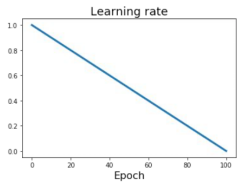
LR schedules (decaying over time)



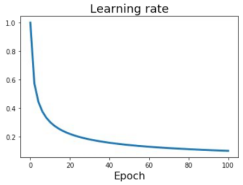
reduce LR at fixed intervals



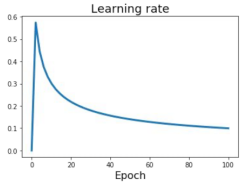
use cosine annealing



use linear decay



use inverse square root decay



use linear warmup