Neural Networks: Optimization Part 1

Intro to Deep Learning, Fall 2022
• Neural networks are universal approximators
  – Can model any odd thing
  – Provided they have the right architecture
• We must *train* them to approximate any function
  – Specify the architecture
  – Learn their weights and biases
• Networks are trained to minimize total “loss” on a training set
  – We do so through empirical risk minimization
• We use variants of gradient descent to do so
• The gradient of the error with respect to network parameters is computed through backpropagation
Recap: Gradient Descent Algorithm

• In order to minimize any function $f(x)$ w.r.t. $x$

• Initialize:
  – $x^0$
  – $k = 0$

• Do
  – $k = k + 1$
  – $x^{k+1} = x^k - \eta \nabla_x f^T$

• while $|f(x^k) - f(x^{k-1})| > \varepsilon$
Recap: Training Neural Nets by Gradient Descent

Total training error:

\[ \text{Loss} = \frac{1}{T} \sum_{t} \text{Div}(Y_t, d_t; W_1, W_2, ..., W_K) \]

• Gradient descent algorithm:
  • Initialize all weights \( W_1, W_2, ..., W_K \)
  • Do:
    - For every layer \( k \), compute:
      - \( \nabla_{W_k} \text{Loss} = \frac{1}{T} \sum_{t} \nabla_{W_k} \text{Div}(Y_t, d_t) \)
        - Computed using backprop
      - \( W_k = W_k - \eta \nabla_{W_k} \text{Loss}^T \)
  • Until \( \text{Loss} \) has converged
Neural network training algorithm

• Initialize all weights and biases \((W_1, b_1, W_2, b_2, \ldots, W_N, b_N)\)

• Do:

  – **Loss** = 0

  – For all \(k\), initialize \(\nabla_{W_k} Loss = 0, \nabla_{b_k} Loss = 0\)

  – For all \(t = 1:T\)  # Loop through training instances

    • Forward pass: Compute
      – Output \(Y(X_t)\),
      – Divergence \(Div(Y_t, d_t)\)

    • Backward pass: For all \(k\) compute:
      – \(\nabla_{W_k} Div(Y_t, d_t), \nabla_{b_k} Div(Y_t, d_t)\)
      – \(\nabla_{W_k} Loss += \nabla_{W_k} Div(Y_t, d_t); \ nabla_{b_k} Loss += \nabla_{b_k} Div(Y_t, d_t)\)

    – For all \(k\), update:

      \[
      W_k = W_k - \frac{\eta}{T} (\nabla_{W_k} Loss)^T; \quad b_k = b_k - \frac{\eta}{T} (\nabla_{W_k} Loss)^T
      \]

• Until **Loss** has converged
Issues

• Convergence: How well does it learn
  – And how can we improve it

• How well will it generalize (outside training data)

• What does the output really mean?

• Etc..
Backpropagating from the kth layer, which is the derivative for the weights $W_k$?

- $y_{k-1} \cdot \nabla_{z_k} Div$: The product of the output $y$ of the $k-1$th layer and the derivative for the affine value $z$ of the $k$th layer (in that order)

- $\nabla_{z_k} Div \ y_{k-1}$: The product of the derivative for the affine value $z$ at the $k$th layer and the output $y$ of the $k-1$th layer (in that order)

- $y^\top_{k-1} \cdot \nabla_{z_k} Div$: The product of the transpose of the output $y$ of the $k-1$th layer and the derivative for the affine value $z$ of the $k$th layer (in that order)

- $\nabla_{z_k} Div \ y^\top_{k-1}$: The product of the derivative for the affine value $z$ at the $k$th layer and the transpose output $y$ of the $k-1$th layer (in that order)
Backpropagating from the kth layer, which is the derivative for the weights $W_k$?

- $y_{k-1} \cdot \nabla_{z_k} Div$: The product of the output $y$ of the $k - 1$th layer and the derivative for the affine value $z$ of the $k$th layer (in that order)
- $\nabla_{z_k}Div y_{k-1}$: The product of the derivative for the affine value $z$ at the $k$th layer and the output $y$ of the $k - 1$th layer (in that order)
- $y_{k-1}^T \cdot \nabla_{z_k} Div$: The product of the transpose of the output $y$ of the $k - 1$th layer and the derivative for the affine value $z$ of the $k$th layer (in that order)
- $\nabla_{z_k} Div. y_{k-1}^T$: The product of the derivative for the affine value $z$ at the $k$th layer and the transpose output $y$ of the $k - 1$th layer (in that order)
Onward
Onward

• Does backprop always work?
• Convergence of gradient descent
  – Rates, restrictions,
  – Hessians
  – Acceleration and Nestorov
  – Alternate approaches
• Modifying the approach: Stochastic gradients
• Speedup extensions: RMSprop, Adagrad
Does backprop do the right thing?

- Is backprop always right?
  - Assuming it actually finds the minimum of the divergence function?

(Actual question: Does gradient descent find the right solution, even when it finds the actual minimum)
Recap: The differentiable activation

- Threshold activation: Equivalent to counting errors
  - Shifting the threshold from $T_1$ to $T_2$ does not change classification error
  - Does not indicate if moving the threshold left was good or not

- Differentiable activation: Computes “distance to answer”
  - “Distance” == divergence
  - Perturbing the function changes this quantity,
    - Even if the classification error itself doesn’t change
Does backprop do the right thing?

• **Is backprop always right?**
  – Assuming it actually finds the global minimum of the loss (average divergence)?

• In classification problems, the classification error is a non-differentiable function of weights

• The divergence function minimized is only a *proxy* for classification error

• Minimizing divergence may not minimize classification error
Backprop fails to separate where perceptron succeeds

- Brady, Raghavan, Slawny, ’89
- Simple problem, 3 training instances, single neuron
- Perceptron training rule trivially find a perfect solution
Backprop vs. Perceptron

- Back propagation using logistic function and $L_2$ divergence ($Div = (y - d)^2$)
- Unique minimum trivially proved to exist, backprop finds it
Unique solution exists

- Let $u = f^{-1}(1 - \varepsilon)$
  - E.g. $u = f^{-1}(0.99)$ representing a 99% confidence in the class
- From the three points we get three independent equations:

\[
\begin{align*}
wx\cdot 1 + wy\cdot 0 + b &= u \\
wx\cdot 0 + wy\cdot 1 + b &= u \\
wx\cdot -1 + wy\cdot 0 + b &= -u
\end{align*}
\]

- Unique solution ($wx = u, wx = u, b = 0$) exists
  - represents a unique line regardless of the value of $u$
• Now add a fourth point
• $t$ is very large (point near $-\infty$)
• Perceptron trivially finds a solution (may take $t^2$ iterations)
Consider backprop:

Contribution of fourth point to derivative of $L_2$ error:

\[
\begin{align*}
\text{div}_4 &= \left(1 - \varepsilon - \sigma(-w_y t + b)\right)^2 \\
\frac{d \text{div}_4}{dw_y} &= 2 \left(1 - \varepsilon - \sigma(-w_y t + b)\right) \sigma'(-w_y t + b) t \\
\frac{d \text{div}_4}{db} &= -2 \left(1 - \varepsilon - \sigma(-w_y t + b)\right) \sigma'(-w_y t + b)
\end{align*}
\]

Notation:

$y = \sigma(z) = \text{logistic activation}$

$1 - \varepsilon$ is the actual achievable value.
Backprop

Notation: 
\[ y = \sigma(z) = \text{logistic activation} \]

\[ \text{div}_4 = \left(1 - \varepsilon - \sigma(-w_y t + b)\right)^2 \]

\[
\frac{d \text{div}_4}{dw_y} = 2 \left(1 - \varepsilon - \sigma(-w_y t + b)\right) \sigma'(-w_y t + b)t \\
\frac{d \text{div}_4}{db} = 2 \left(1 - \sigma(-w_y t + b)\right) \sigma'(-w_y t + b)t
\]

- For very large positive \( t \), \( |w_y| > \varepsilon \) (where \( w = [w_x, w_y, b] \))
- \( \left(1 - \varepsilon - \sigma(-w_y t + b)\right) \to 1 \) as \( t \to \infty \)
- \( \sigma'(-w_y t + b) \to 0 \) exponentially as \( t \to \infty \)
- Therefore, for very large positive \( t \)

\[
\frac{d \text{div}_4}{dw_y} = \frac{d \text{div}_4}{db} = 0
\]
- The fourth point at \((0, -t)\) does not change the gradient of the \(L_2\) divergence near the optimal solution for 3 points.
- The optimum solution for 3 points is also a broad *local* minimum (0 gradient) for the 4-point problem!
  - Will be found by backprop nearly all the time.
- Although the global minimum with unbounded weights will separate the classes correctly.
• Local optimum solution found by backprop
• Does not separate the points *even though the points are linearly separable!*
• Solution found by backprop
• Does not separate the points *even though the points are linearly separable!*
• Compare to the perceptron: *Backpropagation fails to separate where the perceptron succeeds*
Backprop fails to separate where perceptron succeeds

- Brady, Raghavan, Slawny, ’89
- Several linearly separable training examples
- Simple setup: both backprop and perceptron algorithms find solutions
A more complex problem

- Adding a “spoiler” (or a small number of spoilers)
  - Perceptron finds the linear separator,
A more complex problem

- Adding a “spoiler” (or a small number of spoilers)
  - Perceptron finds the linear separator,
  - Backprop does not find a separator
    - A single additional input does not change the loss function significantly
      - Assuming weights are constrained to be bounded
• Adding a “spoiler” (or a small number of spoilers)
  – Perceptron finds the linear separator,
  – For bounded $w$, backprop does not find a separator
    • A single additional input does not change the loss function significantly
A more complex problem

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A more complex problem

- Adding a “spoiler” (or a small number of spoilers)
  - Perceptron finds the linear separator,
  - For bounded $w$, backprop does not find a separator
    - A single additional input does not change the loss function significantly
So what is happening here?

• The perceptron may change greatly upon adding just a single new training instance
  – But it fits the training data well
  – The perceptron rule has low bias
    • Makes no errors if possible
  – But high variance
    • Swings wildly in response to small changes to input

• Backprop is minimally changed by new training instances
  – Prefers consistency over perfection
  – It is a low-variance estimator, at the potential cost of bias
Backprop fails to separate even when possible

- This is not restricted to single perceptrons
- An MLP learns non-linear decision boundaries that are determined from the entirety of the training data
- Adding a few “spoilers” will not change their behavior
Backprop fails to separate even when possible

- This is not restricted to single perceptrons
- An MLP learns non-linear decision boundaries that are determined from the entirety of the training data
- Adding a few “spoilers” will not change their behavior
Backpropagation: Finding the separator

- Backpropagation will often not find a separating solution even though the solution is within the class of functions learnable by the network.

- This is because the separating solution is not a feasible optimum for the loss function.

- One resulting benefit is that a backprop-trained neural network classifier has lower variance than an optimal classifier for the training data.
Minimizing the (differentiable) loss function will also minimize classification error, true or false

- True
- False
Minimizing the (differentiable) loss function will also minimize classification error, true or false

- True
- False (true)
The Loss Surface

- The example (and statements) earlier assumed the loss objective had a single global optimum that could be found
  - Statement about variance is assuming global optimum

- What about local optima
The Loss Surface

- **Popular hypothesis:**
  - In large networks, saddle points are far more common than local minima
    - Frequency of occurrence exponential in network size
  - Most local minima are equivalent
    - And close to global minimum
  - This is not true for small networks

- **Saddle point:** A point where
  - The slope is zero
  - The surface increases in some directions, but decreases in others
    - Some of the Eigenvalues of the Hessian are positive; others are negative
  - Gradient descent algorithms often get “stuck” in saddle points
The Controversial Loss Surface

• *Baldi and Hornik (89),* “Neural Networks and Principal Component Analysis: Learning from Examples Without Local Minima” : An MLP with a single hidden layer has only saddle points and no local Minima

• *Dauphin et. al (2015),* “Identifying and attacking the saddle point problem in high-dimensional non-convex optimization” : An exponential number of saddle points in large networks

• *Chomoranksa et. al (2015),* “The loss surface of multilayer networks” : For large networks, most local minima lie in a band and are equivalent
  – Based on analysis of spin glass models

• *Swirszc et. al. (2016),* “Local minima in training of deep networks”, In networks of finite size, trained on finite data, you *can* have horrible local minima

• Watch this space...
Story so far

• Neural nets can be trained via gradient descent that minimizes a loss function

• Backpropagation can be used to derive the derivatives of the loss

• Backprop *is not guaranteed* to find a “true” solution, even if it exists, and lies within the capacity of the network to model
  – The optimum for the loss function may not be the “true” solution

• For large networks, the loss function may have a large number of unpleasant saddle points or local minima
  – Which backpropagation may find
Convergence

• In the discussion so far we have assumed the training arrives at a local minimum

• Does it always converge?
• How long does it take?

• Hard to analyze for an MLP, but we can look at the problem through the lens of convex optimization
A quick tour of (convex) optimization

The streetlight effect is a type of observational bias where people only look for whatever they are searching by looking where it is easiest.

“I’m searching for my keys.”
Convex Loss Functions

• A surface is “convex” if it is continuously curving upward
  – We can connect any two points on or above the surface without intersecting it
  – Many mathematical definitions that are equivalent

• Caveat: Neural network loss surface is generally not convex
  – Streetlight effect
Convergence of gradient descent

• An iterative algorithm is said to *converge* to a solution if the value updates arrive at a fixed point
  – Where the gradient is 0 and further updates do not change the estimate

• The algorithm may not actually converge
  – It may jitter around the local minimum
  – It may even diverge

• Conditions for convergence?
**Convergence and convergence rate**

- **Convergence rate:** How fast the iterations arrive at the solution

- Generally quantified as

  \[ R = \frac{|f(x^{(k+1)}) - f(x^*)|}{|f(x^{(k)}) - f(x^*)|} \]

  - \(x^{(k+1)}\) is the k-th iteration
  - \(x^*\) is the optimal value of \(x\)

- If \(R\) is a constant (or upper bounded), the convergence is *linear*
  - In reality, its arriving at the solution exponentially fast

  \[ |f(x^{(k)}) - f(x^*)| \leq R^k |f(x^{(0)}) - f(x^*)| \]
Convergence for quadratic surfaces

Minimize \( E = \frac{1}{2} aw^2 + bw + c \)

\[
\begin{align*}
\mathbf{w}^{(k+1)} &= \mathbf{w}^{(k)} - \eta \frac{dE(\mathbf{w}^{(k)})}{d\mathbf{w}} \\
\end{align*}
\]

Gradient descent with fixed step size \( \eta \) to estimate scalar parameter \( \mathbf{w} \)

- Gradient descent to find the optimum of a quadratic, starting from \( \mathbf{w}^{(k)} \)
- Assuming fixed step size \( \eta \)
- What is the optimal step size \( \eta \) to get there fastest?
Convergence for quadratic surfaces

- Any quadratic objective can be written as
  \[ E(w) = E(w^{(k)}) + E'(w^{(k)})(w - w^{(k)}) + \frac{1}{2}E''(w^{(k)})(w - w^{(k)})^2 \]
  - Taylor expansion

- Minimizing w.r.t \( w \), we get (Newton’s method)
  \[ w_{min} = w^{(k)} - E''(w^{(k)})^{-1}E'(w^{(k)}) \]

- Note:
  \[ \frac{dE(w^{(k)})}{dw} = E'(w^{(k)}) \]

- Comparing to the gradient descent rule, we see that we can arrive at the optimum in a single step using the optimum step size
  \[ \eta_{opt} = E''(w^{(k)})^{-1} = \alpha^{-1} \]
With non-optimal step size

Gradient descent with fixed step size $\eta$ to estimate scalar parameter $w$

\[ w^{(k+1)} = w^{(k)} - \eta \frac{dE(w^{(k)})}{dw} \]

- For $\eta < \eta_{opt}$ the algorithm will converge monotonically.
- For $2\eta_{opt} > \eta > \eta_{opt}$ we have oscillating convergence.
- For $\eta > 2\eta_{opt}$ we get divergence.
For generic differentiable convex objectives

- Any differentiable convex objective $E(w)$ can be approximated as

$$E \approx E(w^{(k)}) + (w - w^{(k)}) \frac{dE(w^{(k)})}{dw} + \frac{1}{2} (w - w^{(k)})^2 \frac{d^2E(w^{(k)})}{dw^2} + \ldots$$

  - Taylor expansion

- Using the same logic as before, we get (Newton’s method)

$$\eta_{opt} = \left( \frac{d^2E(w^{(k)})}{dw^2} \right)^{-1}$$

- We can get divergence if $\eta \geq 2\eta_{opt}$
For functions of *multivariate* inputs

\[ E = g(w), \text{ } w \text{ is a vector } w = [w_1, w_2, \ldots, w_N] \]

- Consider a simple quadratic convex (paraboloid) function
  \[ E = \frac{1}{2} w^T A w + w^T b + c \]
  - Since \( E^T = E \) (\( E \) is scalar), \( A \) can always be made symmetric
    - For strictly convex \( E \), \( A \) is always positive definite, and has positive eigenvalues

- When \( A \) is diagonal:
  \[ E = \frac{1}{2} \sum_{i} (a_{ii}w_i^2 + b_i w_i) + c \]
  - The \( w_i \)s are uncoupled
  - For paraboloid (convex) \( E \), the \( a_{ii} \) values are all positive
  - Just a sum of \( N \) independent quadratic functions
Multivariate Quadratic with Diagonal $A$

$$E = \frac{1}{2} w^T A w + w^T b + c = \frac{1}{2} \sum_i (a_{ii} w_i^2 + b_i w_i) + c$$

- Equal-value contours will ellipses with principal axes parallel to the spatial axes
Multivariate Quadratic with Diagonal $A$

$$E = \frac{1}{2} w^T A w + w^T b + c = \frac{1}{2} \sum_i (a_{ii} w_i^2 + b_i w_i) + c$$

- Equal-value contours will be parallel to the axes
  - All “slices” parallel to an axis are shifted versions of one another

$$E = \frac{1}{2} a_{ii} w_i^2 + b_i w_i + c + C(-w_i)$$
Multivariate Quadratic with Diagonal $\mathbf{A}$

$$E = \frac{1}{2} \mathbf{w}^T \mathbf{A} \mathbf{w} + \mathbf{w}^T \mathbf{b} + c = \frac{1}{2} \sum_{i} (a_{ii} w_i^2 + b_i w_i) + c$$

- Equal-value contours will be parallel to the axis
  - All “slices” parallel to an axis are shifted versions of one another

$$E = \frac{1}{2} a_{ii} w_i^2 + b_i w_i + c + C(\neg w_i)$$
“Descents” are uncoupled

- The optimum of each coordinate is not affected by the other coordinates
  - I.e. we could optimize each coordinate independently
- Note: Optimal learning rate is different for the different coordinates

\[ E = \frac{1}{2} a_{11} w_1^2 + b_1 w_1 + c + C(\neg w_1) \]
\[ \eta_{1,\text{opt}} = a_{11}^{-1} \]

\[ E = \frac{1}{2} a_{22} w_2^2 + b_2 w_2 + c + C(\neg w_2) \]
\[ \eta_{2,\text{opt}} = a_{22}^{-1} \]
Conventional vector update rules for gradient descent:
update entire vector against direction of gradient

- Note: Gradient is perpendicular to equal value contour
- The same learning rate is applied to all components
Problem with vector update rule

\[ w^{(k+1)} \leftarrow w^{(k)} - \eta \nabla_w E^T \]

\[ w_i^{(k+1)} = w_i^{(k)} - \eta \frac{\partial E (w_i^{(k)})}{\partial w} \]

\[ \eta_{i,\text{opt}} = \left( \frac{\partial^2 E (w_i^{(k)})}{\partial w_i^2} \right)^{-1} = a_{ii}^{-1} \]
Dependence on learning rate

- $\eta_{1,\text{opt}} = 1; \eta_{2,\text{opt}} = 0.33$
- $\eta = 2.1\eta_{2,\text{opt}}$
- $\eta = 2\eta_{2,\text{opt}}$
- $\eta = 1.5\eta_{2,\text{opt}}$
- $\eta = \eta_{2,\text{opt}}$
- $\eta = 0.75\eta_{2,\text{opt}}$
**Problem with vector update rule**

\[
\begin{align*}
    w^{(k+1)} & \leftarrow w^{(k)} - \eta \nabla_w E^T \\
    w_i^{(k+1)} &= w_i^{(k)} - \eta \frac{\partial E (w_i^{(k)})}{\partial w} \\
    \eta_{i,\text{opt}} &= \left( \frac{\partial^2 E (w_i^{(k)})}{\partial w_i^2} \right)^{-1} = a_{ii}^{-1}
\end{align*}
\]

- The learning rate must be lower than twice the *smallest* optimal learning rate for any component
  \[
  \eta < 2 \min_i \eta_{i,\text{opt}}
  \]
  - Otherwise the learning will diverge
- This, however, makes the learning very slow
  - And will oscillate in all directions where \( \eta_{i,\text{opt}} \leq \eta < 2 \eta_{i,\text{opt}} \)
Dependence on learning rate

- $\eta_{1,\text{opt}} = 1$; $\eta_{2,\text{opt}} = 0.91$; $\eta = 1.9 \eta_{2,\text{opt}}$
Generic differentiable *multivariate* convex functions

- For generic convex multivariate functions (not necessarily quadratic), we can employ quadratic Taylor series expansions and much of the analysis still applies
- Taylor expansion

\[ E(w) \approx E(w^{(k)}) + \nabla_w E(w^{(k)})(w - w^{(k)}) + \frac{1}{2} (w - w^{(k)})^T H_E(w^{(k)})(w - w^{(k)}) \]

- The optimal step size is inversely proportional to the Eigen values of the Hessian
  - The second derivative along the orthogonal coordinates
  - For the smoothest convergence, these must all be equal
Convergence

• Convergence behaviors become increasingly unpredictable as dimensions increase

• For the fastest convergence, ideally, the learning rate $\eta$ must be close to both, the largest $\eta_{i,\text{opt}}$ and the smallest $\eta_{i,\text{opt}}$
  – To ensure convergence in every direction
  – Generally infeasible

• Convergence is particularly slow if $\frac{\max_i \eta_{i,\text{opt}}}{\min_i \eta_{i,\text{opt}}}$ is large
  – The “condition” number
    • Must be close to 1.0 for fast convergence

• Following (hidden) slides discuss solutions that “normalize the space by stretching different directions differently to standardize optimal step size
  – A big topic for optimization
  – Unfortunately, infeasible for neural networks
Comments on the quadratic

• Why are we talking about quadratics?
  – Quadratic functions form some kind of benchmark
  – Convergence of gradient descent is linear
    • Meaning it converges to solution exponentially fast

• The convergence for other kinds of functions can be viewed against this benchmark

• Actual losses will not be quadratic, but may locally have other structure
  – Local between current location and nearest local minimum

• Some examples in the following slides..
  – Strong convexity
  – Lifschitz continuity
  – Lifschitz smoothness
  – ..and how they affect convergence of gradient descent
Quadratic convexity

- A quadratic function has the form $\frac{1}{2}w^T A w + w^T b + c$
  - Every “slice” is a quadratic bowl
- In some sense, the “standard” for gradient-descent based optimization
  - Others convex functions will be steeper in some regions, but flatter in others
- Gradient descent solution will have linear convergence
  - Take $O(\log 1/\epsilon)$ steps to get within $\epsilon$ of the optimal solution
• A strongly convex function is \textit{at least} quadratic in its convexity
  – Has a lower bound to its second derivative
• The function sits within a quadratic bowl
  – At any location, you can draw a quadratic bowl of fixed convexity (quadratic constant equal to lower bound of 2\textsuperscript{nd} derivative) touching the function at that point, which contains it
• Convergence of gradient descent algorithms at least as good as that of the enclosing quadratic
• A strongly convex function is *at least* quadratic in its convexity
  – Has a lower bound to its second derivative
• The function sits within a quadratic bowl
  – At any location, you can draw a quadratic bowl of fixed convexity (quadratic constant equal to lower bound of 2\textsuperscript{nd} derivative) touching the function at that point, which contains it
• Convergence of gradient descent algorithms at least as good as that of the enclosing quadratic

**Strong convexity**
Types of continuity

• Most functions are not strongly convex (if they are convex)
• Instead we will talk in terms of Lifschitz smoothness
• But first: a definition

• **Lifschitz continuous:** The function always lies outside a cone
  – The slope of the outer surface is the Lifschitz constant
  – \(|f(x) - f(y)| \leq L|x - y|\)
Lifschitz smoothness

- Lifschitz smooth: The function’s derivative is Lifschitz continuous
  - Need not be convex (or even differentiable)
  - Has an upper bound on second derivative (if it exists)
- Can always place a quadratic bowl of a fixed curvature within the function
  - Minimum curvature of quadratic must be $\geq$ upper bound of second derivative of function (if it exists)
• **Lifschitz smooth**: The function’s *derivative* is Lifschitz continuous
  – Need not be convex (or even differentiable)
  – Has an *upper bound* on second derivative (if it exists)

• **Can always place a quadratic bowl of a fixed curvature within the function**
  – Minimum curvature of quadratic must be $\geq$ upper bound of second derivative of function (if it exists)
Types of smoothness

- A function can be both strongly convex and Lipschitz smooth
  - Second derivative has upper and lower bounds
  - Convergence depends on curvature of strong convexity (at least linear)

- A function can be convex and Lipschitz smooth, but not strongly convex
  - Convex, but upper bound on second derivative
  - Weaker convergence guarantees, if any (at best linear)
  - This is often a reasonable assumption for the local structure of your loss function
Types of smoothness

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Convergence Problems

• For quadratic (strongly) convex functions, gradient descent is exponentially fast
  ‒ Linear convergence
    • Assuming learning rate is non-divergent

• For generic (Lifschitz Smooth) convex functions however, it is very slow
  \[ |f(w^{(k)}) - f(w^*)| \propto \frac{1}{k} |f(w^{(0)}) - f(w^*)| \]
  ‒ And inversely proportional to learning rate
  \[ |f(w^{(k)}) - f(w^*)| \leq \frac{1}{2\eta k} |w^{(0)} - w^*| \]
  ‒ Takes \( O(1/\epsilon) \) iterations to get to within \( \epsilon \) of the solution
  ‒ An inappropriate learning rate will destroy your happiness

• Second order methods will \textit{locally} convert the loss function to quadratic
  ‒ Convergence behavior will still depend on the nature of the original function

• \textit{Continuing with the quadratic-based explanation...}
Convergence

• Convergence behaviors become increasingly unpredictable as dimensions increase

• For the fastest convergence, ideally, the learning rate $\eta$ must be close to both, the largest $\eta_{i,\text{opt}}$ and the smallest $\eta_{i,\text{opt}}$
  – To ensure convergence in every direction
  – Generally infeasible

• Convergence is particularly slow if $\frac{\max_i \eta_{i,\text{opt}}}{\min_i \eta_{i,\text{opt}}}$ is large
  – The “condition” number is small
One reason for the problem

- The objective function has different eccentricities in different directions
  - Resulting in different optimal learning rates for different directions
  - The problem is more difficult when the ellipsoid is not axis aligned: the steps along the two directions are coupled! Moving in one direction changes the gradient along the other

- Solution: *Normalize* the objective to have identical eccentricity in all directions
  - Then all of them will have identical optimal learning rates
  - Easier to find a working learning rate
Solution: Scale the axes

- Scale (and rotate) the axes, such that all of them have identical (identity) “spread”
  - Equal-value contours are circular
  - Movement along the coordinate axes become independent
- **Note:** equation of a quadratic surface with circular equal-value contours can be written as

\[
E = \frac{1}{2} \hat{w}^T S \hat{w} + \hat{b}^T \hat{w} + c
\]
Scaling the axes

• Original equation:

\[ E = \frac{1}{2} w^T A w + b^T w + c \]

• We want to find a (diagonal) scaling matrix \( S \) such that

\[ S = \begin{bmatrix} s_1 & \cdots & 0 \\ \vdots & \ddots & \vdots \\ 0 & \cdots & s_N \end{bmatrix}, \quad \hat{w} = Sw \]

• And

\[ E = \frac{1}{2} \hat{w}^T \hat{w} + \hat{b}^T \hat{w} + c \]
Scaling the axes

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• We want to find a (diagonal) scaling matrix \( S \) such that

\[
S = \begin{bmatrix}
    s_1 & \cdots & 0 \\
    \vdots & \ddots & \vdots \\
    0 & \cdots & s_N \\
\end{bmatrix}, \quad \hat{w} = Sw
\]

• And

\[ E = \frac{1}{2} \hat{w}^T \hat{w} + \hat{b}^T \hat{w} + c \]

By inspection:

\[ S = A^{0.5} \]
Scaling the axes

- We have

\[ E = \frac{1}{2} w^T A w + b^T w + c \]

\[ \hat{w} = S w \]

\[ E = \frac{1}{2} \hat{w}^T \hat{w} + \hat{b}^T \hat{w} + c \]

\[ = \frac{1}{2} w^T S^T S w + \hat{b}^T S w + c \]

- Equating linear and quadratic coefficients, we get

\[ S^T S = A, \quad \hat{b}^T S = b^T \]

- Solving:

\[ S = A^{0.5}, \quad \hat{b} = A^{-0.5} b \]
Scaling the axes

• We have

\[
E = \frac{1}{2} w^T A w + b^T w + c
\]

\[
\hat{w} = Sw
\]

\[
E = \frac{1}{2} \hat{w}^T \hat{w} + b^T \hat{w} + c
\]

• Solving for \( S \) we get

\[
\hat{w} = A^{0.5} w, \quad \hat{b} = A^{-0.5} b
\]
Scaling the axes

• We have

\[
E = \frac{1}{2} w^T A w + b^T w + c
\]

\[
\hat{w} = Sw
\]

\[
E = \frac{1}{2} \hat{w}^T \hat{w} + \hat{b}^T \hat{w} + c
\]

• Solving for \( S \) we get

\[
\hat{w} = A^{0.5} w, \quad \hat{b} = A^{-0.5} b
\]
The Inverse Square Root of A

• For any positive definite $A$, we can write
  $$A = E\Lambda E^T$$
  – Eigen decomposition
  – $E$ is an orthogonal matrix
  – $\Lambda$ is a diagonal matrix of non-zero diagonal entries

• Defining $A^{0.5} = E\Lambda^{0.5}E^T$
  – Check $(A^{0.5})^T A^{0.5} = E\Lambda E^T = A$

• Defining $A^{-0.5} = E\Lambda^{-0.5}E^T$
  – Check: $(A^{-0.5})^T A^{-0.5} = E\Lambda^{-1}E^T = A^{-1}$
Returning to our problem

\[ E = \frac{1}{2} \hat{\mathbf{w}}^T \hat{\mathbf{w}} + \hat{\mathbf{b}}^T \hat{\mathbf{w}} + c \]

- Computing the gradient, and noting that \( \mathbf{A}^{0.5} \) is symmetric, we can relate \( \nabla_{\hat{\mathbf{w}}} E \) and \( \nabla_{\mathbf{w}} E \):

  \[
  \nabla_{\hat{\mathbf{w}}} E = \hat{\mathbf{w}}^T + \hat{\mathbf{b}}^T \\
  = \mathbf{w}^T \mathbf{A}^{0.5} + \mathbf{b}^T \mathbf{A}^{-0.5} \\
  = (\mathbf{w}^T \mathbf{A} + \mathbf{b}^T) \mathbf{A}^{-0.5} \\
  = \nabla_{\mathbf{w}} E \cdot \mathbf{A}^{-0.5}
  \]
Returning to our problem

- Gradient descent rule:
  \[ E = \frac{1}{2} \hat{\mathbf{w}}^T \hat{\mathbf{w}} + \hat{\mathbf{b}}^T \hat{\mathbf{w}} + c \]

- Learning rate is now independent of direction

- Using \( \hat{\mathbf{w}} = \mathbf{A}^{0.5} \mathbf{w} \), and \( \nabla_{\hat{\mathbf{w}}} E(\hat{\mathbf{w}})^T = \mathbf{A}^{-0.5} \nabla_{\mathbf{w}} E(\mathbf{w})^T \)

\[ \mathbf{w}^{(k+1)} = \mathbf{w}^{(k)} - \eta \mathbf{A}^{-1} \nabla_{\mathbf{w}} E(\mathbf{w}^{(k)})^T \]
Modified update rule

\[ E = \frac{1}{2} \mathbf{w}^T A \mathbf{w} + \mathbf{b}^T \mathbf{w} + c \]

\[ \hat{\mathbf{w}} = A^{0.5} \mathbf{w} \]

\[ E = \frac{1}{2} \hat{\mathbf{w}}^T \hat{\mathbf{w}} + \hat{\mathbf{b}}^T \hat{\mathbf{w}} + c \]

- \( \hat{\mathbf{w}}^{(k+1)} = \hat{\mathbf{w}}^{(k)} - \eta \nabla_{\hat{\mathbf{w}}} E(\hat{\mathbf{w}}^{(k)})^T \)

- Leads to the modified gradient descent rule

\[ \mathbf{w}^{(k+1)} = \mathbf{w}^{(k)} - \eta A^{-1} \nabla_{\mathbf{w}} E(\mathbf{w}^{(k)})^T \]
For non-axis-aligned quadratics..

If $A$ is not diagonal, the contours are not axis-aligned
- Because of the cross-terms $a_{ij}w_iw_j$
- The major axes of the ellipsoids are the Eigenvectors of $A$, and their diameters are proportional to the Eigen values of $A$

But this does not affect the discussion
- This is merely a rotation of the space from the axis-aligned case
- The component-wise optimal learning rates along the major and minor axes of the equal-contour ellipsoids will be different, causing problems
  - The optimal rates along the axes are Inversely proportional to the eigenvalues of $A$
For non-axis-aligned quadratics..

- The component-wise optimal learning rates along the major and minor axes of the contour ellipsoids will differ, causing problems
  - Inversely proportional to the eigenvalues of $A$

- This can be fixed as before by rotating and resizing the different directions to obtain the same normalized update rule as before:
  $$w^{(k+1)} = w^{(k)} - \eta A^{-1}b$$
Generic differentiable \textit{multivariate} convex functions

- Taylor expansion

\[
E(w) \approx E(w^{(k)}) + \nabla_w E(w^{(k)})(w - w^{(k)}) + \frac{1}{2} (w - w^{(k)})^T H_E(w^{(k)})(w - w^{(k)}) + \ldots
\]
Generic differentiable *multivariate* convex functions

- Taylor expansion

\[ E(w) \approx E(w^{(k)}) + \nabla_w E(w^{(k)})(w - w^{(k)}) + \frac{1}{2} (w - w^{(k)})^T H_E(w^{(k)})(w - w^{(k)}) + \cdots \]

- Note that this has the form \( \frac{1}{2} w^T A w + w^T b + c \)
- Using the same logic as before, we get the normalized update rule

\[ w^{(k+1)} = w^{(k)} - \eta H_E(w^{(k)})^{-1} \nabla_w E(w^{(k)})^T \]
- For a quadratic function, the optimal \( \eta \) is 1 (which is exactly Newton’s method)
  - And should not be greater than 2!
Minimization by Newton’s method \((\eta = 1)\)

- Iterated localized optimization with quadratic approximations

\[
\mathbf{w}^{(k+1)} = \mathbf{w}^{(k)} - \eta H_E(\mathbf{w}^{(k)})^{-1} \nabla_w E(\mathbf{w}^{(k)})^T
\]

- \(\eta = 1\)
Minimization by Newton’s method \((\eta = 1)\)

- Iterated localized optimization with quadratic approximations

\[
\mathbf{w}^{(k+1)} = \mathbf{w}^{(k)} - \eta H_E(\mathbf{w}^{(k)})^{-1} \nabla_{\mathbf{w}} E(\mathbf{w}^{(k)})^T
\]
Minimization by Newton’s method \((\eta = 1)\)

• Iterated localized optimization with quadratic approximations

\[
\mathbf{w}^{(k+1)} = \mathbf{w}^{(k)} - \eta H_E(\mathbf{w}^{(k)})^{-1} \nabla_w E(\mathbf{w}^{(k)})^T
\]

\(- \eta = 1\)
Minimization by Newton’s method ($\eta = 1$)

- Iterated localized optimization with quadratic approximations

$$\mathbf{w}^{(k+1)} = \mathbf{w}^{(k)} - \eta H_E(\mathbf{w}^{(k)})^{-1} \nabla_w E(\mathbf{w}^{(k)})^T$$

$- \eta = 1$
Minimization by Newton’s method

- Iterated localized optimization with quadratic approximations

\[ w^{(k+1)} = w^{(k)} - \eta H_E(w^{(k)})^{-1} \nabla_w E(w^{(k)})^T - \eta = 1 \]
Minimization by Newton’s method

- Iterated localized optimization with quadratic approximations

\[ \mathbf{w}^{(k+1)} = \mathbf{w}^{(k)} - \eta H_E(\mathbf{w}^{(k)})^{-1} \nabla_w E(\mathbf{w}^{(k)})^T \]

\[- \eta = 1 \]
Minimization by Newton’s method

- Iterated localized optimization with quadratic approximations

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\mathbf{w}^{(k+1)} = \mathbf{w}^{(k)} - \eta H_E(\mathbf{w}^{(k)})^{-1} \nabla_w E(\mathbf{w}^{(k)})^T - \eta = 1
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\[ - \eta = 1 \]
Minimization by Newton’s method

- Iterated localized optimization with quadratic approximations

\[ \mathbf{w}^{(k+1)} = \mathbf{w}^{(k)} - \eta \nabla_{\mathbf{w}} E(\mathbf{w}^{(k)})^{-1} \nabla_{\mathbf{w}} E(\mathbf{w}^{(k)})^T \]

- \( \eta = 1 \)
Minimization by Newton’s method

- Iterated localized optimization with quadratic approximations

\[ \mathbf{w}^{(k+1)} = \mathbf{w}^{(k)} - \eta H_E(\mathbf{w}^{(k)})^{-1} \nabla_w E(\mathbf{w}^{(k)})^T \]

- \( \eta = 1 \)
Issues: 1. The Hessian

• Normalized update rule

\[ w^{(k+1)} = w^{(k)} - \eta H_E(w^{(k)})^{-1} \nabla_w E(w^{(k)})^T \]

• For complex models such as neural networks, with a very large number of parameters, the Hessian \( H_E(w^{(k)}) \) is extremely difficult to compute
  – For a network with only 100,000 parameters, the Hessian will have \( 10^{10} \) cross-derivative terms
  – And its even harder to invert, since it will be enormous
Issues: 1. The Hessian

- For non-convex functions, the Hessian may not be positive semi-definite, in which case the algorithm can *diverge*
  - Goes away from, rather than towards the minimum
Issues: 1. The Hessian

- For non-convex functions, the Hessian may not be positive semi-definite, in which case the algorithm can **diverge**
  - Goes away from, rather than towards the minimum
  - Now requires additional checks to avoid movement in directions corresponding to –ve Eigenvalues of the Hessian
A great many approaches have been proposed in the literature to approximate the Hessian in a number of ways and improve its positive definiteness

- Boyden-Fletcher-Goldfarb-Shanno (BFGS)
  - And “low-memory” BFGS (L-BFGS)
  - Estimate Hessian from finite differences
- Levenberg-Marquardt
  - Estimate Hessian from Jacobians
  - Diagonal load it to ensure positive definiteness
- Other “Quasi-newton” methods

Hessian estimates may even be local to a set of variables

Not particularly popular anymore for large neural networks..
Issues: 2. The learning rate

- Much of the analysis we just saw was based on trying to ensure that the step size was not so large as to cause divergence within a convex region
  - $\eta < 2\eta_{opt}$
Issues: 2. The learning rate

• For complex models such as neural networks the loss function is often not convex
  – Having $\eta > 2\eta_{opt}$ can actually help escape local optima
• However always having $\eta > 2\eta_{opt}$ will ensure that you never ever actually find a solution
• Start with a large learning rate
  – Greater than 2 (assuming Hessian normalization)
  – Gradually reduce it with iterations

Note: this is actually a reduced step size
Decaying learning rate

• Typical decay schedules

   - Linear decay: $\eta_k = \frac{\eta_0}{k+1}$
   - Quadratic decay: $\eta_k = \frac{\eta_0}{(k+1)^2}$
   - Exponential decay: $\eta_k = \eta_0 e^{-\beta k}$, where $\beta > 0$

• A common approach (for nnets):

  1. Train with a fixed learning rate $\eta$ until loss (or performance on a held-out data set) stagnates
  2. $\eta \leftarrow \alpha \eta$, where $\alpha < 1$ (typically 0.1)
  3. Return to step 1 and continue training from where we left off
Story so far: Convergence

• Gradient descent can miss obvious answers
  – And this may be a good thing

• Convergence issues abound
  – The loss surface has many saddle points
    • Although, perhaps, not so many bad local minima
    • Gradient descent can stagnate on saddle points
  – Vanilla gradient descent may not converge, or may converge toooooo slowly
    • The optimal learning rate for one component may be too high or too low for others
Mark all true statements

- Step sizes that are greater than twice the inverse of the second derivative can cause gradient descent to diverge
- This is always a bad thing
- Gradient descent will not converge without decaying learning rates
Mark all true statements

- Step sizes that are greater than twice the inverse of the second derivative can cause gradient descent to diverge **(true)**
- This is always a bad thing
- Gradient descent will not converge without decaying learning rates
Story so far: Second-order methods

Second-order methods “normalize” the variation along the components to mitigate the problem of different optimal learning rates for different components.

- But this requires computation of inverses of second-order derivative matrices.
- Computationally infeasible.
- Not stable in non-convex regions of the loss surface.
- Approximate methods address these issues, but simpler solutions may be better.
• Divergence-causing learning rates may not be a bad thing
  – Particularly for ugly loss functions

• *Decaying* learning rates provide good compromise between escaping poor local minima and convergence

• *Many of the convergence issues arise because we force the same learning rate on all parameters*
• Problems arise because of requiring a fixed step size across all dimensions
  – Because step are “tied” to the gradient
• Let’s try releasing this requirement
Derivative-inspired algorithms

- Algorithms that use derivative information for trends, but do not follow them absolutely
  - Rprop
  - Quick prop
RProp

- Resilient propagation
- Simple algorithm, to be followed independently for each component
  - I.e. steps in different directions are not coupled

- At each time
  - If the derivative at the current location recommends continuing in the same direction as before (i.e. has not changed sign from earlier):
    - increase the step, and continue in the same direction
  - If the derivative has changed sign (i.e. we’ve overshot a minimum)
    - reduce the step and reverse direction
Rprop

- Select an initial value \( \hat{\omega} \) and compute the derivative
  - Take an initial step \( \Delta \omega \) against the derivative
    - In the direction that reduces the function
      \[
      \Delta \omega = \text{sign} \left( \frac{dE(\hat{\omega})}{d\omega} \right) \Delta \omega
      \]
      \[
      \hat{\omega} = \hat{\omega} - \Delta \omega
      \]
• Compute the derivative in the new location
  – If the derivative has not changed sign from the previous location, increase the step size and take a longer step

\[ \alpha > 1 \]

• \( \Delta w = \alpha \Delta w \)

• \( \hat{w} = \hat{w} - \Delta w \)
Rprop

- Compute the derivative in the new location
  - If the derivative has not changed sign from the previous location, increase the step size and take a step

\[ \alpha > 1 \]

- \[ \Delta w = \alpha \Delta w \]
- \[ \hat{w} = \hat{w} - \Delta w \]
Rprop

- Compute the derivative in the new location
  - If the derivative has changed sign

Orange arrow shows direction of derivative, i.e. direction of increasing $E(w)$
Rprop

- Compute the derivative in the new location
  - If the derivative has changed sign
  - Return to the previous location
- \( \hat{w} = \hat{w} + \Delta w \)
• Compute the derivative in the new location
  – If the derivative has changed sign
  – Return to the previous location
    • $\hat{w} = \hat{w} + \Delta w$
  – Shrink the step
    • $\Delta w = \beta \Delta w$

$\beta < 1$
• Compute the derivative in the new location
  – If the derivative has changed sign
  – Return to the previous location
    • \( \hat{\omega} = \hat{\omega} + \Delta \omega \)
  – Shrink the step
    • \( \Delta \omega = \beta \Delta \omega \)
  – Take the smaller step forward
    • \( \hat{\omega} = \hat{\omega} - \Delta \omega \)
Rprop (simplified)

- Set $\alpha = 1.2$, $\beta = 0.5$
- For each layer $l$, for each $i, j$:
  - Initialize $w_{l,i,j}, \Delta w_{l,i,j} > 0,$
  - $\text{prev}D(l, i, j) = \frac{dLoss(w_{l,i,j})}{dw_{l,i,j}}$
  - $\Delta w_{l,i,j} = \text{sign}(\text{prev}D(l, i, j)) \Delta w_{l,i,j}$
  - While not converged:
    - $w_{l,i,j} = w_{l,i,j} - \Delta w_{l,i,j}$
    - $D(l, i, j) = \frac{dLoss(w_{l,i,j})}{dw_{l,i,j}}$
    - If $\text{sign}(\text{prev}D(l, i, j)) == \text{sign}(D(l, i, j))$:
      - $\Delta w_{l,i,j} = \min(\alpha \Delta w_{l,i,j}, \Delta_{\text{max}})$
      - $\text{prev}D(l, i, j) = D(l, i, j)$
    - else:
      - $w_{l,i,j} = w_{l,i,j} + \Delta w_{l,i,j}$
      - $\Delta w_{l,i,j} = \max(\beta \Delta w_{l,i,j}, \Delta_{\text{min}})$

Ceiling and floor on step
Rprop (simplified)

- Set $\alpha = 1.2$, $\beta = 0.5$
- For each layer $l$, for each $i, j$:
  - Initialize $w_{l,i,j}$, $\Delta w_{l,i,j} > 0$,
  - $\text{prevD}(l, i, j) = \frac{d\text{Loss}(w_{l,i,j})}{dw_{l,i,j}}$
  - $\Delta w_{l,i,j} = \text{sign}(\text{prevD}(l, i, j))\Delta w_{l,i,j}$
  - While not converged:
    - $w_{l,i,j} = w_{l,i,j} - \Delta w_{l,i,j}$
    - $D(l, i, j) = \frac{d\text{Loss}(w_{l,i,j})}{dw_{l,i,j}}$
    - If $\text{sign}(\text{prevD}(l, i, j)) = \text{sign}(D(l, i, j))$:
      - $\Delta w_{l,i,j} = \alpha \Delta w_{l,i,j}$
      - $\text{prevD}(l, i, j) = D(l, i, j)$
    - else:
      - $w_{l,i,j} = w_{l,i,j} + \Delta w_{l,i,j}$
      - $\Delta w_{l,i,j} = \beta \Delta w_{l,i,j}$

Obtained via backprop

Note: Different parameters updated independently
RProp

• A remarkably simple first-order algorithm, that is frequently much more efficient than gradient descent.
  – And can even be competitive against some of the more advanced second-order methods

• Only makes minimal assumptions about the loss function
  – No convexity assumption
The derivative of the loss w.r.t a parameter \( w \), computed at the current estimate is positive. After taking a step (updating the parameter by a increment \( dw \)) the sign of the derivative becomes negative. Mark all true statements

- Rprop will revert to the earlier estimate and take a smaller step
- Rprop will change direction and begin taking steps in the opposite direction
The derivative of the loss w.r.t a parameter $w$, computed at the current estimate is positive. After taking a step (updating the parameter by a increment $dw$) the sign of the derivative becomes negative. Mark all true statements

- Rprop will revert to the earlier estimate and take a smaller step (true)
- Rprop will change direction and begin taking steps in the opposite direction
Quickprop employs the Newton updates with two modifications

$$w^{(k+1)} = w^{(k)} - \eta H_E(w^{(k)})^{-1} \nabla_w E(w^{(k)})^T$$

But with two modifications
QuickProp: Modification 1

- It treats each dimension independently
- For $i = 1: N$
  
  \[ w_i^{k+1} = w_i^k - E''(w_i^k | w_j^k, j \neq i)^{-1} E'(w_i^k | w_j^k, j \neq i) \]

- This eliminates the need to compute and invert expensive Hessians
QuickProp: Modification 2

- It approximates the second derivative through finite differences
- For $i = 1:N$
  \[
  w_i^{k+1} = w_i^k - D(w_i^k, w_i^{k-1})^{-1} E'(w_i^k | w_j^k, j \neq i)
  \]
- This eliminates the need to compute expensive double derivatives
QuickProp

\[ w^{(k+1)} = w^{(k)} - \left( \frac{E'(w^{(k)}) - E'(w^{(k-1)})}{\Delta w^{(k-1)}} \right)^{-1} E'(w^{(k)}) \]

Finite-difference approximation to double derivative obtained assuming a quadratic \( E() \)

- Updates are independent for every parameter
- For every layer \( l \), for every connection from node \( i \) in the \((l - 1)^{th}\) layer to node \( j \) in the \( l^{th}\) layer:

\[ \Delta w^{(k)}_{l,ij} = \frac{\Delta w^{(k-1)}_{l,ij}}{Err'(w^{(k)}_{l,ij}) - Err'(w^{(k-1)}_{l,ij})} Err'(w^{(k)}_{l,ij}) \]

\[ w^{(k+1)}_{l,ij} = w^{(k)}_{l,ij} - \Delta w^{(k)}_{l,ij} \]
QuickProp

\[ w^{(k+1)} = w^{(k)} - \left( \frac{E'(w^{(k)}) - E'(w^{(k-1)})}{\Delta w^{(k-1)}} \right)^{-1} E'(w^{(k)}) \]

Finite-difference approximation to double derivative obtained assuming a quadratic \( E() \)

- Updates are independent for every parameter
- For every layer \( l \), for every connection from node \( i \) in the \((l - 1)^{th}\) layer to node \( j \) in the \( l^{th}\) layer:

\[ \Delta w_{l,ij}^{(k)} = \frac{\Delta w_{l,ij}^{(k-1)}}{E_{r}' (w_{l,ij}^{(k)}) - E_{r}' (w_{l,ij}^{(k-1)})} E_{r}' (w_{l,ij}^{(k)}) \]

\[ w_{l,ij}^{(k+1)} = w_{l,ij}^{(k)} - \Delta w_{l,ij}^{(k)} \]

Computed using backprop
Quickprop

• Employs Newton updates with empirically derived derivatives

• Prone to some instability for non-convex objective functions

• But is still one of the fastest training algorithms for many problems
Story so far : Convergence

• Gradient descent can miss obvious answers
  – And this may be a *good* thing

• Vanilla gradient descent may be too slow or unstable due to the differences between the dimensions

• Second order methods can normalize the variation across dimensions, but are complex

• Adaptive or decaying learning rates can improve convergence

• Methods that decouple the dimensions can improve convergence
A closer look at the convergence problem

- With dimension-independent learning rates, the solution will converge smoothly in some directions, but oscillate or diverge in others.

Proposal:
- Keep track of oscillations
- Emphasize steps in directions that converge smoothly
- Shrink steps in directions that bounce around.
A closer look at the convergence problem

- With dimension-independent learning rates, the solution will converge smoothly in some directions, but oscillate or diverge in others

- **Proposal:**
  - Keep track of oscillations
  - Emphasize steps in directions that converge smoothly
  - Shrink steps in directions that bounce around..
The momentum methods

• Maintain a running average of all past steps
  – In directions in which the convergence is smooth, the average will have a large value
  – In directions in which the estimate swings, the positive and negative swings will cancel out in the average

• Update with the running average, rather than the current gradient
The momentum method maintains a running average of all gradients until the current step. The plain gradient update is replaced by:

\[ \Delta W^{(k)} = \beta \Delta W^{(k-1)} - \eta \nabla_W \text{Loss}(W^{(k-1)})^T \]

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

- Typical \( \beta \) value is 0.9
- The running average steps:
  - Get longer in directions where gradient retains the same sign
  - Become shorter in directions where the sign keeps flipping
Training by gradient descent

- Initialize all weights $W_1, W_2, \ldots, W_K$

- Do:
  - For all $i, j, k$, initialize $\nabla_{W_k} Loss = 0$
  - For all $t = 1: T$
    - For every layer $k$:
      - Compute $\nabla_{W_k} Div(Y_t, d_t)$
      - Compute $\nabla_{W_k} Loss \leftarrow \frac{1}{T} \nabla_{W_k} Div(Y_t, d_t)$
    - For every layer $k$:
      $W_k = W_k - \eta (\nabla_{W_k} Loss)^T$

- Until $Loss$ has converged
Training with momentum

• Initialize all weights $W_1, W_2, ..., W_K$

• Do:
  – For all layers $k$, initialize $\nabla_{W_k} Loss = 0, \Delta W_k = 0$
  – For all $t = 1: T$
    • For every layer $k$:
      – Compute gradient $\nabla_{W_k} \text{Div}(Y_t, d_t)$
      – $\nabla_{W_k} Loss += \frac{1}{T} \nabla_{W_k} \text{Div}(Y_t, d_t)$
    – For every layer $k$
      \[
      \Delta W_k = \beta \Delta W_k - \eta (\nabla_{W_k} Loss)^T
      \]
      \[
      W_k = W_k + \Delta W_k
      \]
  – Until $Loss$ has converged
Momentum Update

- The momentum method

\[ \Delta W^{(k)} = \beta \Delta W^{(k-1)} - \eta \nabla_W \text{Loss}(W^{(k-1)})^T \]

- At any iteration, to compute the current step:
Momentum Update

• The momentum method

\[ \Delta W^{(k)} = \beta \Delta W^{(k-1)} - \eta \nabla_W \text{Loss}(W^{(k-1)})^T \]

• At any iteration, to compute the current step:
  - First computes the gradient step at the current location
Momentum Update

• The momentum method

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

• At any iteration, to compute the current step:
  – First computes the gradient step at the current location
  – Then adds in the scaled previous step
    • Which is actually a running average
Momentum Update

- The momentum method
  \[ \Delta W^{(k)} = \beta \Delta W^{(k-1)} - \eta \nabla_W \text{Loss}(W^{(k-1)})^T \]
- At any iteration, to compute the current step:
  - First computes the gradient step at the current location
  - Then adds in the scaled *previous* step
    - Which is actually a running average
  - To get the final step
Momentum update steps are actually computed in two stages
- First: We take a step against the gradient at the current location
- Second: Then we add a scaled version of the previous step

The procedure can be made more optimal by reversing the order of operations.
Nestorov’s Accelerated Gradient

- Change the order of operations
- At any iteration, to compute the current step:
Nestorov’s Accelerated Gradient

• Change the order of operations
• At any iteration, to compute the current step:
  – First extend the previous 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
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
Nestorov’s Accelerated Gradient

\[ \Delta W^{(k)} = \beta \Delta W^{(k-1)} - \eta \nabla_w \text{Loss}(W^{(k-1)} + \beta \Delta W^{(k-1)})^T \]

\[ W^{(k)} = W^{(k-1)} + \Delta W^{(k)} \]
Nestorov’s Accelerated Gradient

• Comparison with momentum (example from Hinton)
• Converges much faster
Training with Nestorov

- Initialize all weights $W_1, W_2, \ldots, W_K$
- Do:
  - For all layers $k$, initialize $\nabla_{W_k} \text{Loss} = 0$, $\Delta W_k = 0$
  - For every layer $k$
    - $W_k = W_k + \beta \Delta W_k$
  - For all $t = 1:T$
    - For every layer $k$:
      - Compute gradient $\nabla_{W_k} \text{Div}(Y_t, d_t)$
      - $\nabla_{W_k} \text{Loss} += \frac{1}{T} \nabla_{W_k} \text{Div}(Y_t, d_t)$
    - For every layer $k$
      - $W_k = W_k - \eta (\nabla_{W_k} \text{Loss})^T$
      - $\Delta W_k = \beta \Delta W_k - \eta (\nabla_{W_k} \text{Loss})^T$
- Until $\text{Loss}$ has converged
Momentum and trend-based methods..

• We will return to this topic again, very soon..
On a flat surface of constant slope momentum methods will converge faster than vanilla gradient descent, true or false

- True
- False
Poll 4

On a flat surface of constant slope momentum methods will converge faster than vanilla gradient descent, true or false

- True
- False (correct) – momentum only changes step size
Story so far

- Gradient descent can miss obvious answers
  - And this may be a *good* thing

- Vanilla gradient descent may be too slow or unstable due to the differences between the dimensions

- Second order methods can normalize the variation across dimensions, but are complex

- Adaptive or decaying learning rates can improve convergence

- Methods that decouple the dimensions can improve convergence

- Momentum methods which emphasize directions of steady improvement are demonstrably superior to other methods
Coming up

• Incremental updates
• Revisiting “trend” algorithms
• Generalization
• Tricks of the trade
  – Divergences..
  – Activations
  – Normalizations