CSC 561: Neural Networks and Deep Learning

Optimization (part 1)

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THINK BIG  WE DO℠

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

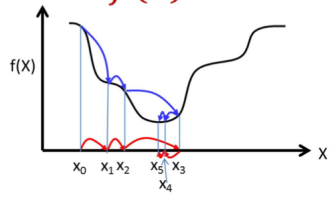
MLSP MachineLearning For SignalProcessing Group

Neural Networks: Optimization Part 1

Intro to Deep Learning, Spring 2025

Recap: Gradient Descent Algorithm

- In order to minimize any function $f(x)$ w.r.t. x
- Initialize:
  - x^0
  - $k = 0$



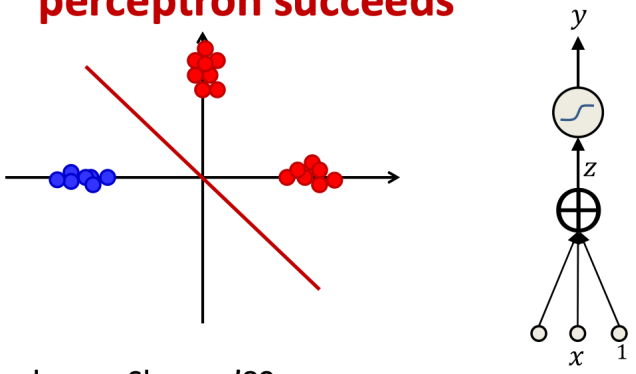
- Do
  - $k = k + 1$
  - $x^{k+1} = x^k - \eta \nabla_x f^T$
- while $\left| f\left(x^k\right) - f\left(x^{k-1}\right) \right| > \varepsilon$

Does backprop do the right thing?

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

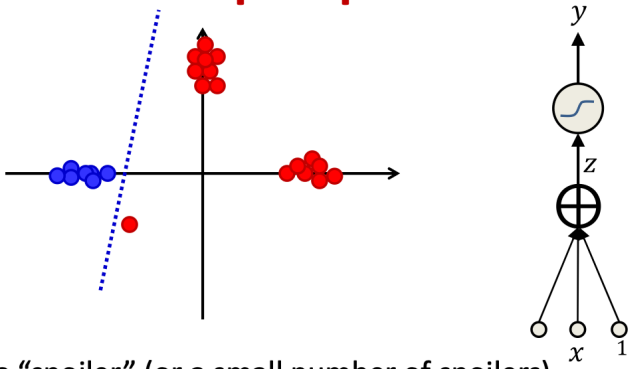
(Actual question: Does gradient descent find the right solution, even when it finds the actual minimum)

Backprop fails to separate where perceptron succeeds



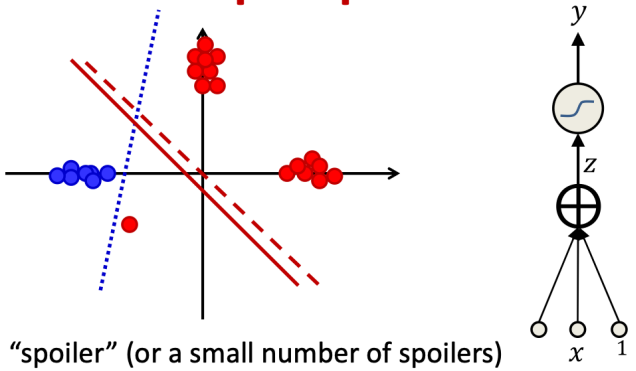
- Brady, Raghavan, Slawny, '89
- *Several* linearly separable training examples
- Simple setup: **both backprop and perceptron algorithms find solutions**

A more complex problem



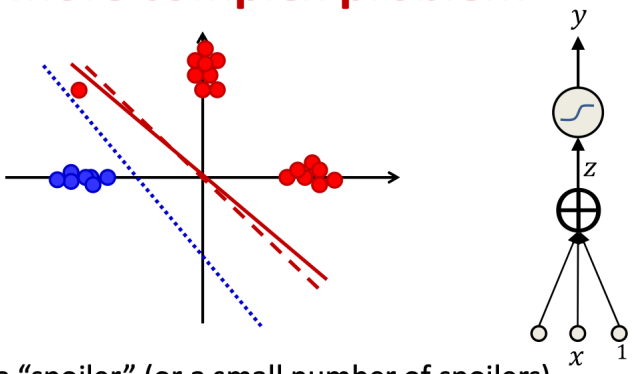
- Adding a "spoiler" (or a small number of spoilers)
  - Perceptron finds the linear separator,

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**

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
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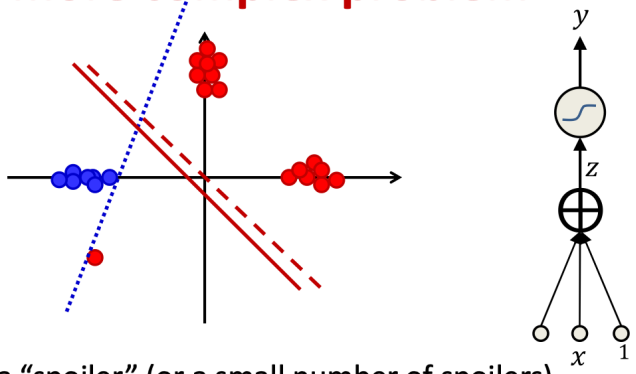
A more complex problem



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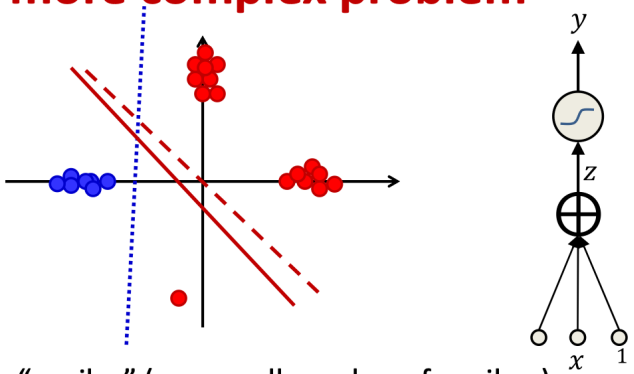

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So what is happening here?

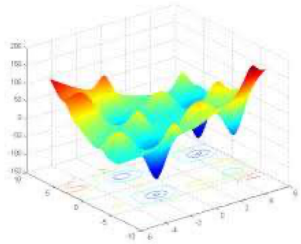
- The perceptron may change greatly upon adding just a single new training instance
  - But it fits the training data well
  - The perceptron rule has *low bias*
    - Makes no errors if possible
  - But high variance
    - Swings wildly in response to small changes to input
- Backprop is minimally changed by new training instances
  - Prefers consistency over perfection
  - It is a *low-variance* estimator, at the potential cost of bias

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

The Loss Surface

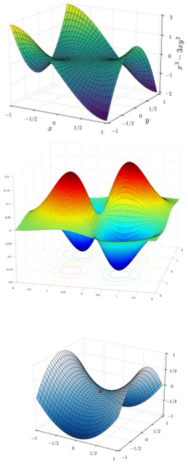
- The example (and statements) earlier assumed the loss objective had a single global optimum that could be found
  - Statement about variance is assuming global optimum



- 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

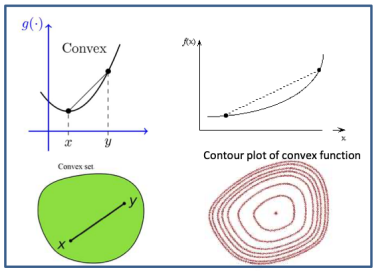


Convergence

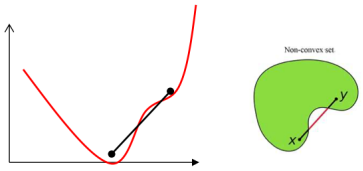
- In the discussion so far we have assumed the training arrives at a local minimum
- Does it always converge?
- How long does it take?
- Hard to analyze for an MLP, but we can look at the problem through the lens of convex optimization

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

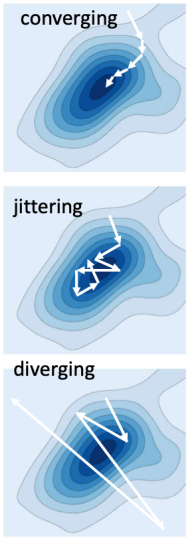


- Caveat: Neural network loss surface is generally not convex
  - Streetlight effect



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?

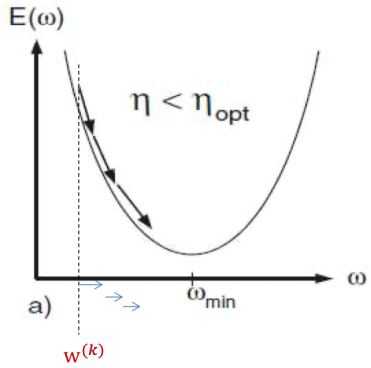


Convergence for quadratic surfaces

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

$$\mathrm{w}^{(k+1)} = \mathrm{w}^{(k)} - \eta \frac{dE\left(\mathrm{w}^{(k)}\right)}{d\mathrm{w}}$$

Gradient descent with fixed step size η to estimate *scalar* parameter w



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

Convergence for quadratic surfaces

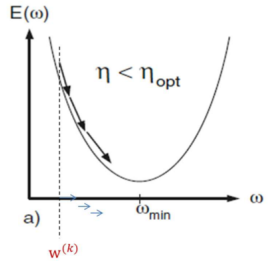
$$E = \frac{1}{2}aw^2 + bw + c$$

$$\mathrm{w}^{(k+1)} = \mathrm{w}^{(k)} - \eta \frac{dE\left(\mathrm{w}^{(k)}\right)}{d\mathrm{w}}$$

- Any quadratic objective can be written as

$$E(w) = E\left(\mathrm{w}^{(k)}\right) + E'\left(\mathrm{w}^{(k)}\right)\left(w - \mathrm{w}^{(k)}\right) + \frac{1}{2}E''\left(\mathrm{w}^{(k)}\right)\left(w - \mathrm{w}^{(k)}\right)^2$$

  - Taylor expansion



- Minimizing w.r.t w, we get (Newton's method)

$$w_{min} = \mathrm{w}^{(k)} - E''\left(\mathrm{w}^{(k)}\right)^{-1} E'\left(\mathrm{w}^{(k)}\right)$$

- Note:

$$\frac{dE\left(\mathrm{w}^{(k)}\right)}{d\mathrm{w}} = E'\left(\mathrm{w}^{(k)}\right)$$

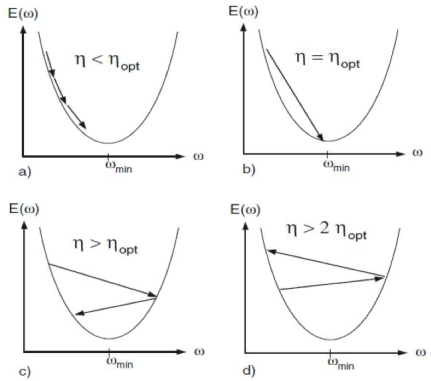
- Comparing to the gradient descent rule, we see that we can arrive at the optimum in a single step using the optimum step size

$$\eta_{opt} = E''\left(\mathrm{w}^{(k)}\right)^{-1} = \boldsymbol{a^{-1}}$$

With non-optimal step size

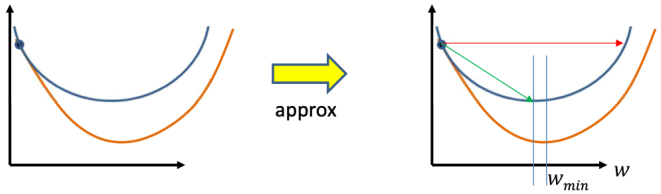
$$w^{(k+1)} = w^{(k)} - \eta \frac{dE\left(w^{(k)}\right)}{dw}$$

Gradient descent with fixed step size η to estimate scalar parameter w



- 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

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

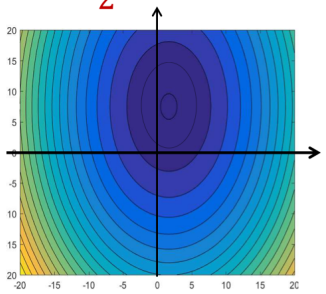
  - Taylor expansion
- Using the same logic as before, we get (Newton's method)

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

- We can get divergence if $\eta \geq 2\eta_{opt}$

Multivariate Quadratic with Diagonal A

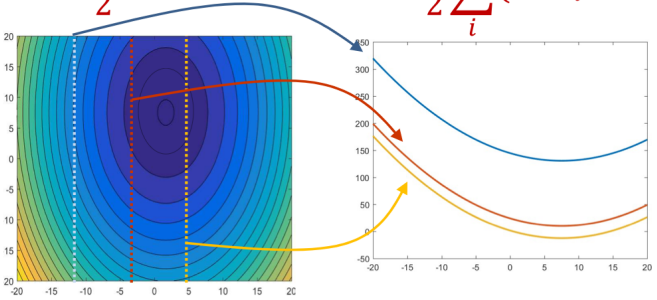
$$E = \frac{1}{2}\mathbf{w}^T\mathbf{A}\mathbf{w} + \mathbf{w}^T\mathbf{b} + c = \frac{1}{2}\sum_i \left(a_{ii}w_i^2 + b_i w_i\right) + c$$



- Equal-value contours will ellipses with principal axes parallel to the spatial axes

Multivariate Quadratic with Diagonal A

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



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

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

Multivariate Quadratic with Diagonal A

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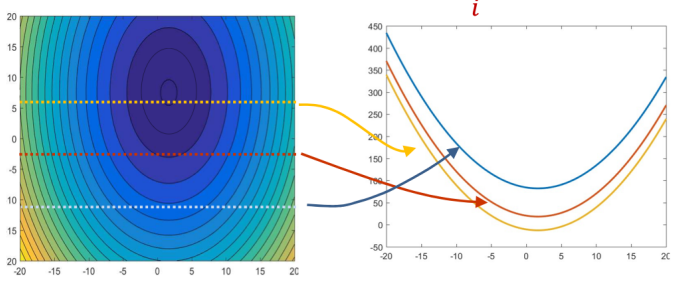

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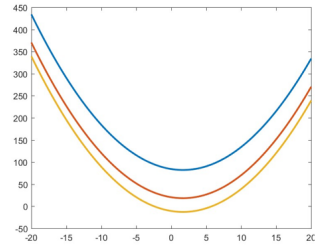
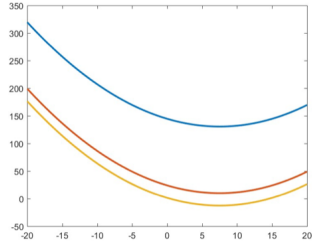
$$E = \frac{1}{2}a_{ii}w_i^2 + b_i w_i + c + C(\neg w_i)$$

"Descents" are uncoupled



$$E = \frac{1}{2}a_{11}w_1^2 + b_1 w_1 + c + C(\neg w_1)$$

$$\eta_{1,opt} = a_{11}^{-1}$$

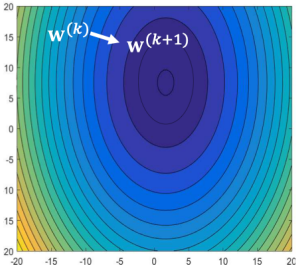


$$E = \frac{1}{2}a_{22}w_2^2 + b_2 w_2 + c + C(\neg w_2)$$

$$\eta_{2,opt} = a_{22}^{-1}$$

- 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**

Vector update rule

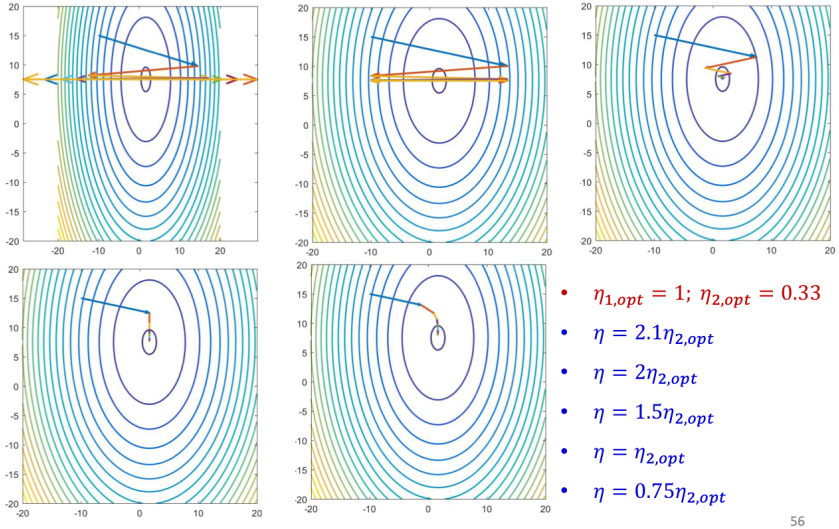


$$\mathbf{w}^{(k+1)} \leftarrow \mathbf{w}^{(k)} - \eta\nabla_w E^\top$$

$$w_i^{(k+1)} = w_i^{(k)} - \eta\frac{\partial E\left(w_i^{(k)}\right)}{d\partial \mathrm{w}}$$

- 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

Dependence on learning rate



- $\eta_{1,opt} = 1;\ \eta_{2,opt} = 0.33$
- $\eta = 2.1\eta_{2,opt}$
- $\eta = 2\eta_{2,opt}$
- $\eta = 1.5\eta_{2,opt}$
- $\eta = \eta_{2,opt}$
- $\eta = 0.75\eta_{2,opt}$

Problem with vector update rule

$$\mathbf{w}^{(k+1)} \leftarrow \mathbf{w}^{(k)} - \eta \nabla_{\mathbf{w}} E^T \qquad w_i^{(k+1)} = w_i^{(k)} - \eta \frac{\partial E\left(w_i^{(k)}\right)}{\partial \mathrm{w}}$$

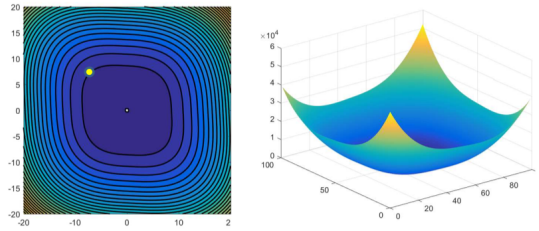
$$\eta_{i,opt} = \left(\frac{\partial^2 E\left(w_i^{(k)}\right)}{\partial w_i^2}\right)^{-1} = a_{ii}^{-1}$$

- The learning rate must be lower than twice the *smallest* optimal learning rate for any component

$$\eta < 2 \min_i \eta_{i,opt}$$

  - Otherwise the learning will diverge
- This, however, makes the learning very slow
  - And will oscillate in all directions where $\eta_{i,opt} \leq \eta < 2\eta_{i,opt}$

Generic differentiable *multivariate* convex functions

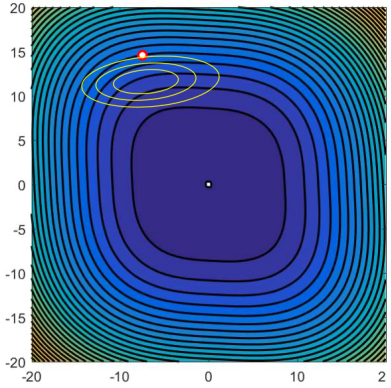


- For generic convex multivariate functions (not necessarily quadratic), we can employ quadratic Taylor series expansions and much of the analysis still applies
- Taylor expansion

$$E(\mathbf{w}) \approx E\left(\mathbf{w}^{(k)}\right) + \nabla_{\mathbf{w}} E\left(\mathbf{w}^{(k)}\right)\left(\mathbf{w} - \mathbf{w}^{(k)}\right) + \frac{1}{2}\left(\mathbf{w} - \mathbf{w}^{(k)}\right)^T \boldsymbol{H}_E\left(\mathbf{w}^{(k)}\right)\left(\mathbf{w} - \mathbf{w}^{(k)}\right)$$

- 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

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



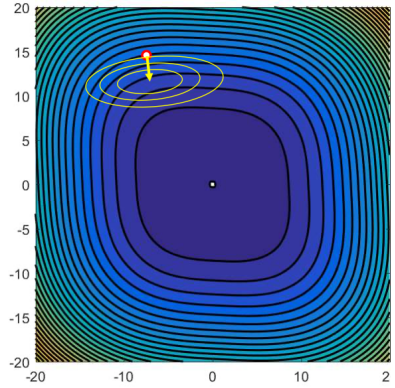
Fit a quadratic at each point and find the minimum of that quadratic

- Iterated localized optimization with quadratic approximations

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

  - $\eta = 1$

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



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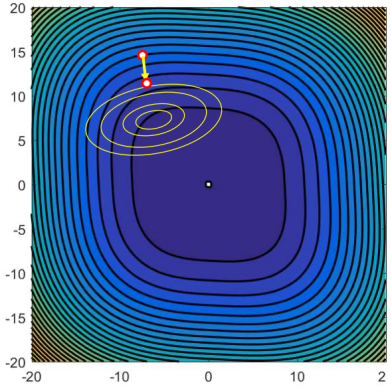
Minimization by Newton's method ($\eta = 1$)



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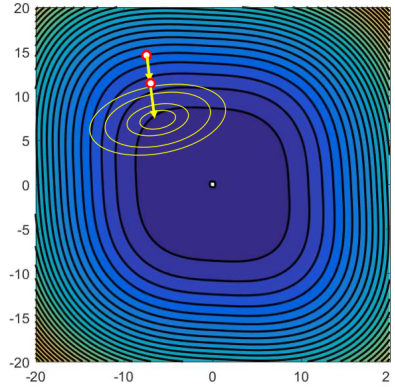
– $\eta = 1$

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



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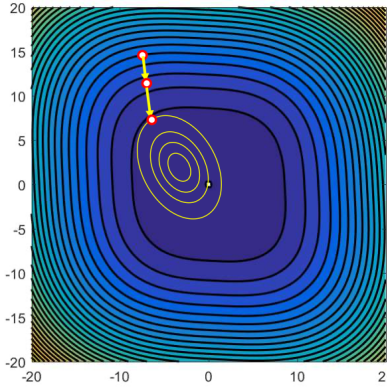
– $\eta = 1$

Minimization by Newton's method

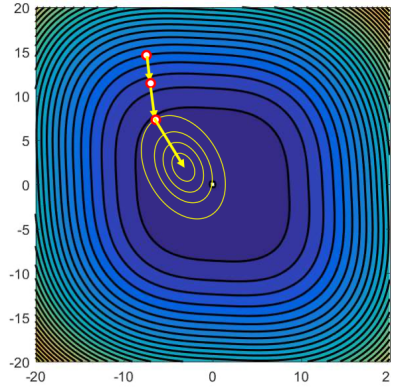


- Iterated localized optimization with quadratic approximations

$$\mathbf{w}^{(k+1)} = \mathbf{w}^{(k)} - \eta H_E\left(\boldsymbol{w}^{(k)}\right)^{-1} \nabla_{\mathbf{w}} E\left(\mathbf{w}^{(k)}\right)^T$$

– $\eta = 1$

Minimization by Newton's method

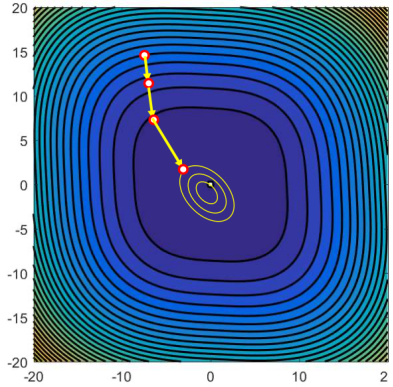


- Iterated localized optimization with quadratic approximations

$$\mathbf{w}^{(k+1)} = \mathbf{w}^{(k)} - \eta H_E\left(\boldsymbol{w}^{(k)}\right)^{-1} \nabla_{\mathbf{w}} E\left(\mathbf{w}^{(k)}\right)^T$$

– $\eta = 1$

Minimization by Newton's method



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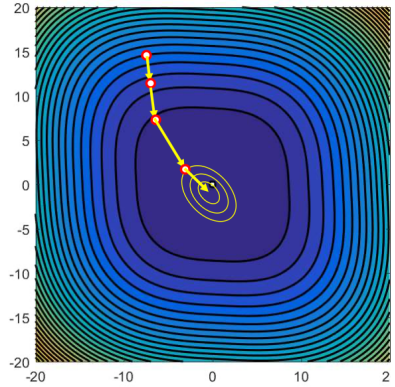
Minimization by Newton's method



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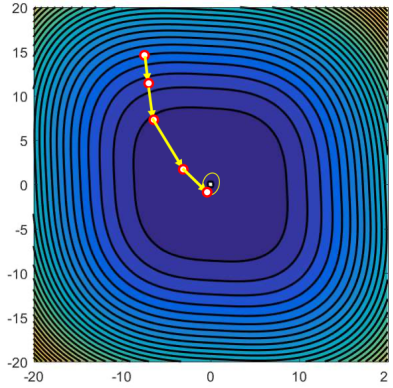
Minimization by Newton's method



- Iterated localized optimization with quadratic approximations

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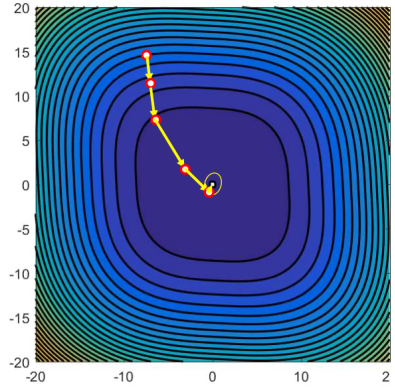
– $\eta = 1$

Minimization by Newton's method

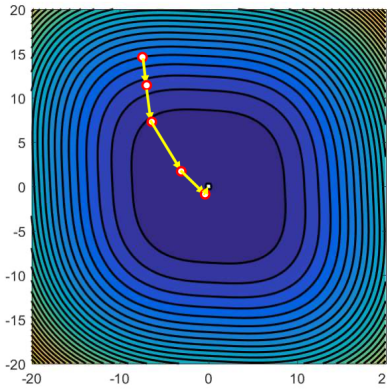


- Iterated localized optimization with quadratic approximations

$$\mathbf{w}^{(k+1)} = \mathbf{w}^{(k)} - \eta H_E\left(\boldsymbol{w}^{(k)}\right)^{-1} \nabla_{\mathbf{w}} E\left(\mathbf{w}^{(k)}\right)^T$$

– $\eta = 1$

Minimization by Newton's method



- Iterated localized optimization with quadratic approximations

$$\mathbf{w}^{(k+1)} = \mathbf{w}^{(k)} - \eta H_E\left(\boldsymbol{w}^{(k)}\right)^{-1} \nabla_{\mathbf{w}} E\left(\mathbf{w}^{(k)}\right)^T$$

  - $\eta = 1$

Issues: 1. The Hessian

- Normalized update rule

$$\mathbf{w}^{(k+1)} = \mathbf{w}^{(k)} - \eta H_E\left(\boldsymbol{w}^{(k)}\right)^{-1} \nabla_{\mathbf{w}} E\left(\mathbf{w}^{(k)}\right)^T$$

- For complex models such as neural networks, with a very large number of parameters, the Hessian $H_E\left(\boldsymbol{w}^{(k)}\right)$ 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

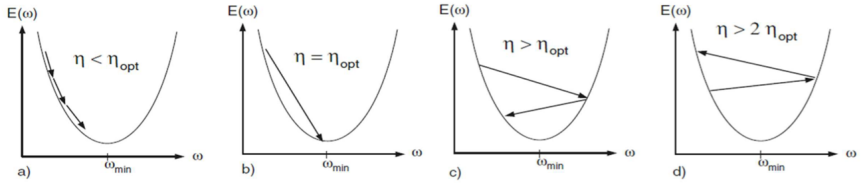
Issues: 1. The Hessian

- 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
  - Now requires additional checks to avoid movement in directions corresponding to –ve Eigenvalues of the Hessian

Issues: 1 – contd.

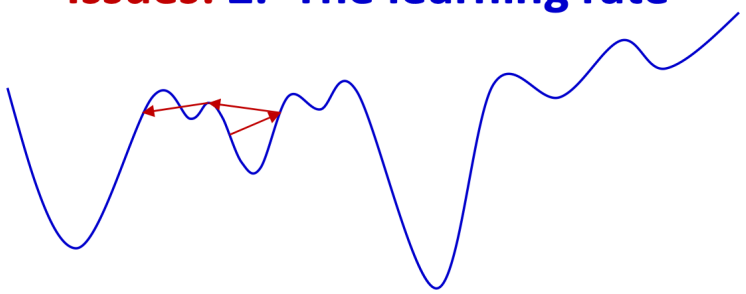
- A great many approaches have been proposed in the literature to *approximate* the Hessian in a number of ways and improve its positive definiteness
  - Boyden-Fletcher-Goldfarb-Shanno (BFGS)
    - And "low-memory" BFGS (L-BFGS)
    - Estimate Hessian from finite differences
  - Levenberg-Marquardt
    - 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



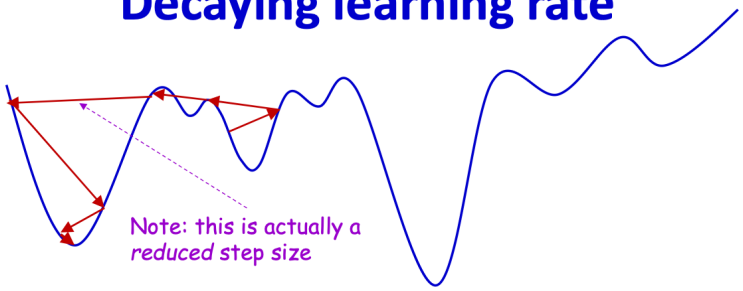
- Much of the analysis we just saw was based on trying to ensure that the step size was not so large as to cause divergence within a convex region
  - $\eta < 2\eta_{opt}$

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

Decaying learning rate



- Start with a large learning rate
  - Greater than 2 (assuming Hessian normalization)
  - Gradually reduce it with iterations

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 η 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

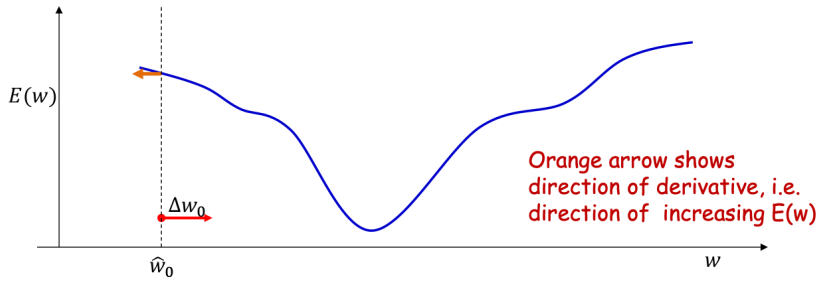
Derivative-*inspired* algorithms

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

RProp

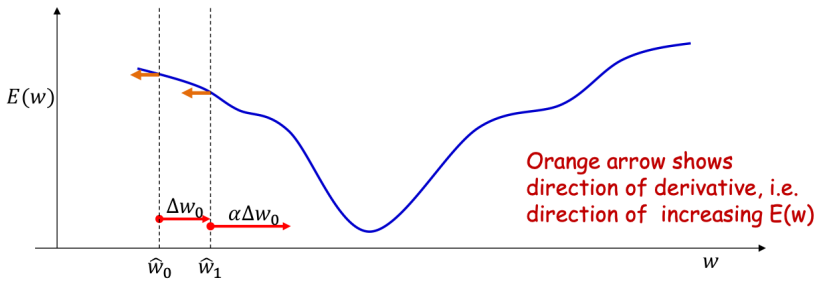
- *Resilient* propagation
- Simple algorithm, to be followed *independently* for each component
  - I.e. steps in different directions are not coupled
- At each time
  - If the derivative at the current location recommends continuing in the same direction as before (i.e. has not changed sign from earlier):
    - *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 $\hat{w}$ and compute the derivative
  - Take an initial step Δw against the derivative
    - In the direction that reduces the function
      - $\Delta w = sign\left(\frac{dE(\hat{w})}{dw}\right)\Delta w$
      - $\hat{w} = \hat{w} - \Delta w$

Rprop

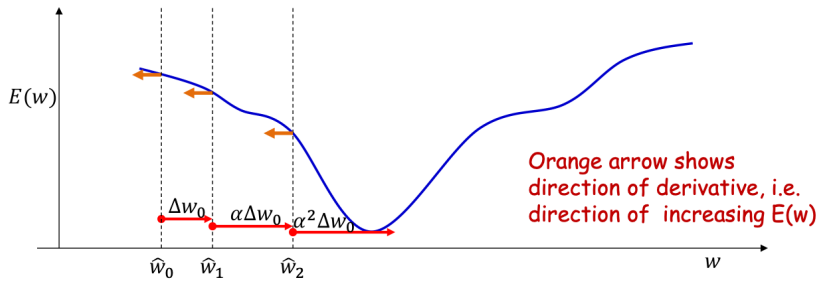


- Compute the derivative in the new location
  - If the derivative has not changed sign from the previous location, increase the step size and take a longer step

$\alpha > 1$

- $\Delta w = \alpha \Delta w$
- $\hat{w} = \hat{w} - \Delta w$

Rprop



- Compute the derivative in the new location
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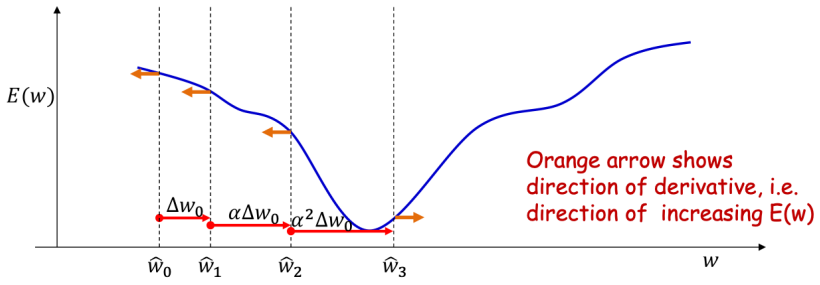
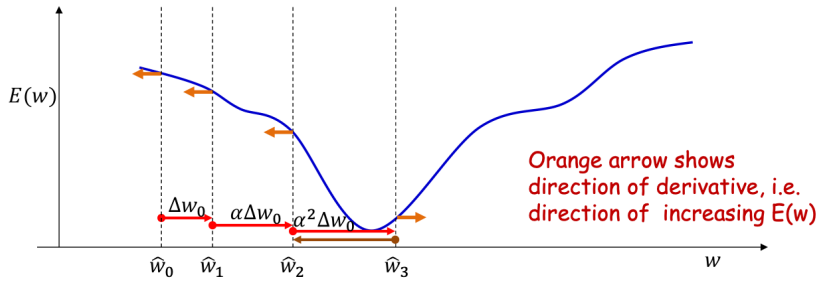
Rprop



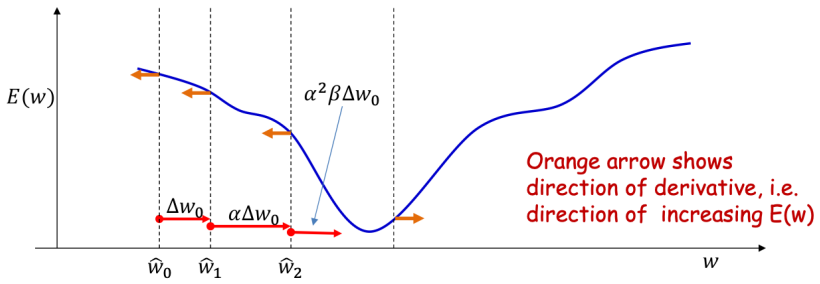
- Compute the derivative in the new location
  - If the derivative has changed sign

Rprop



- Compute the derivative in the new location
  - If the derivative has changed sign
  - Return to the previous location
    - $\hat{w} = \hat{w} + \Delta w$

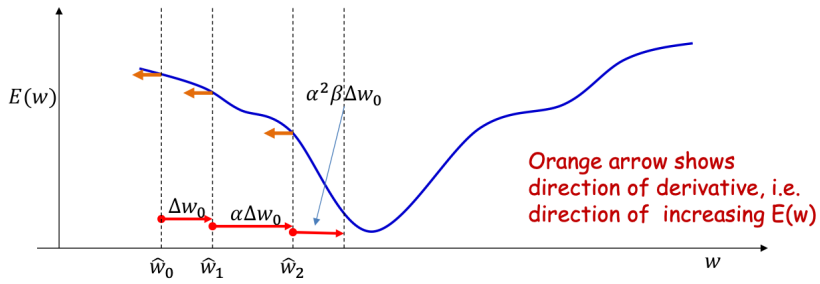
Rprop



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

$\beta < 1$

Rprop



- Compute the derivative in the new location
  - If the derivative has changed sign
  - Return to the previous location
    - $\hat{w} = \hat{w} + \Delta w$
  - Shrink the step
    - $\Delta w = \beta \Delta w$
  - Take the smaller step forward
    - $\hat{w} = \hat{w} - \Delta w$

$\beta < 1$

Rprop (simplified)

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

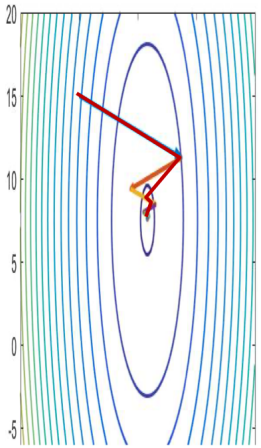
Note: Different parameters updated independently

RProp

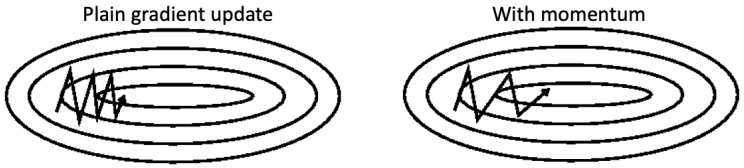
- A remarkably simple first-order algorithm, that is frequently much more efficient than gradient descent.
  - And can even be competitive against some of the more advanced second-order methods
- Only makes minimal assumptions about the loss function
  - No convexity assumption

The 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



Momentum Update



- The momentum method maintains a running average of all gradients until the *current* step

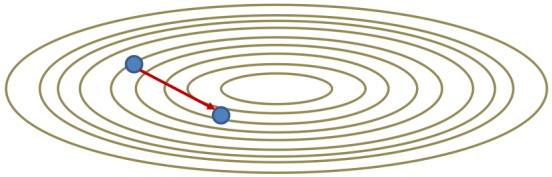
$$gradientstep = -\eta \nabla_W Loss\left(W^{(k-1)}\right)^T$$

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

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

  - Typical β 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

Momentum Update

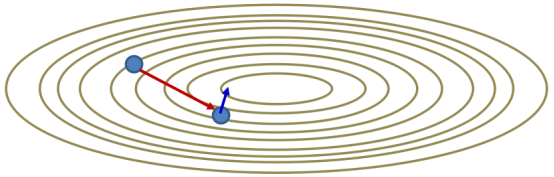


- The momentum method

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

- At any iteration, to compute the current step:

Momentum Update

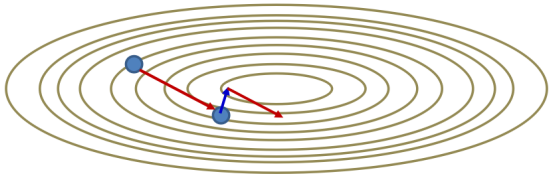


- The momentum method

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

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

Momentum Update

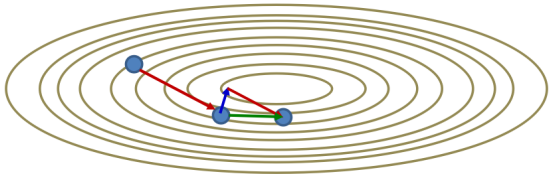


- The momentum method

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

- 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

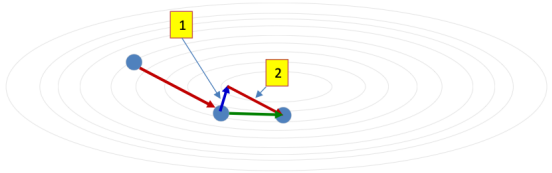


- The momentum method

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

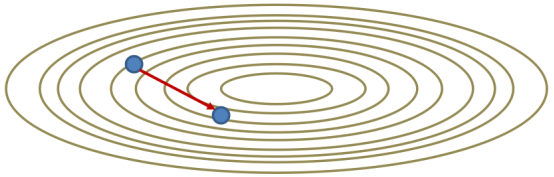
- At any iteration, to compute the current step:
  - First computes the gradient step at the current location
  - Then adds in the scaled *previous* step
    - Which is actually a running average
  - To get the final step

Momentum update



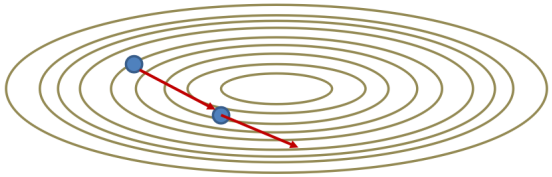
- Momentum update steps are actually computed in two stages
  - First: We take a step against the gradient at the current location
  - Second: Then we add a scaled version of the previous step
- The procedure can be made more optimal by reversing the order of operations..

Nestorov's Accelerated Gradient



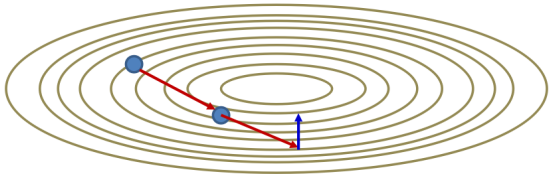
- Change the order of operations
- At any iteration, to compute the current step:

Nestorov's Accelerated Gradient



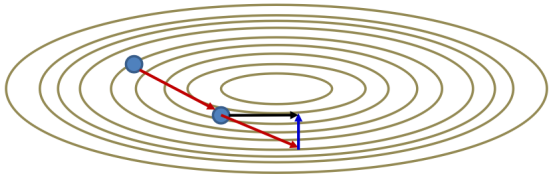
- Change the order of operations
- At any iteration, to compute the current step:
  - First extend the previous step

Nestorov's Accelerated Gradient



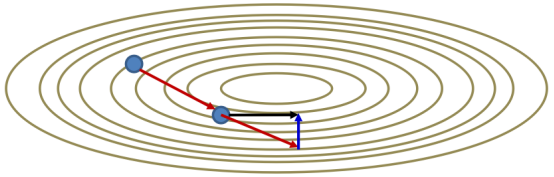
- Change the order of operations
- At any iteration, to compute the current step:
  - First extend the previous step
  - Then compute the gradient step at the resultant position

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



- Nestorov's method

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

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

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