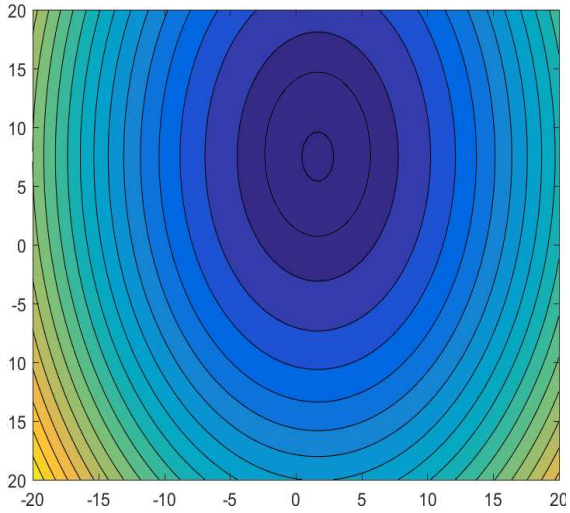
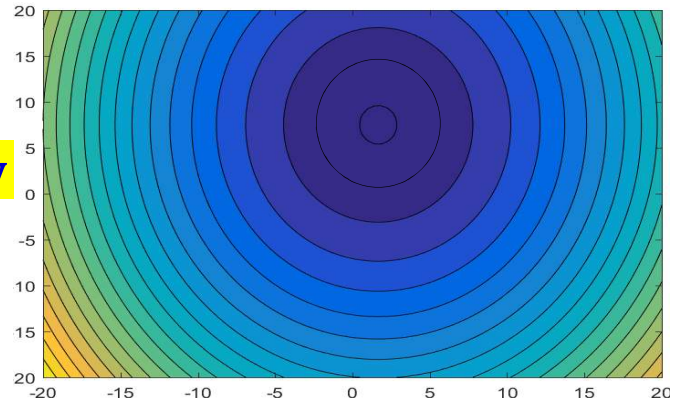
Modified update rule



$$\hat{\mathbf{w}} = \mathbf{A}^{0.5}\mathbf{w}$$



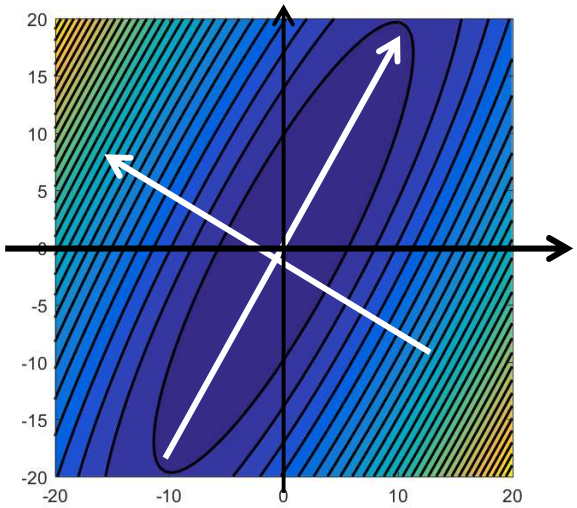
$$E = \frac{1}{2}\mathbf{w}^T\mathbf{A}\mathbf{w} + \mathbf{b}^T\mathbf{w} + c$$

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

- $\hat{\mathbf{w}}^{(k+1)} = \hat{\mathbf{w}}^{(k)} - \eta\nabla_{\hat{\mathbf{w}}}E\left(\hat{\mathbf{w}}^{(k)}\right)^T$
- Leads to the modified gradient descent rule

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

For non-axis-aligned quadratics..

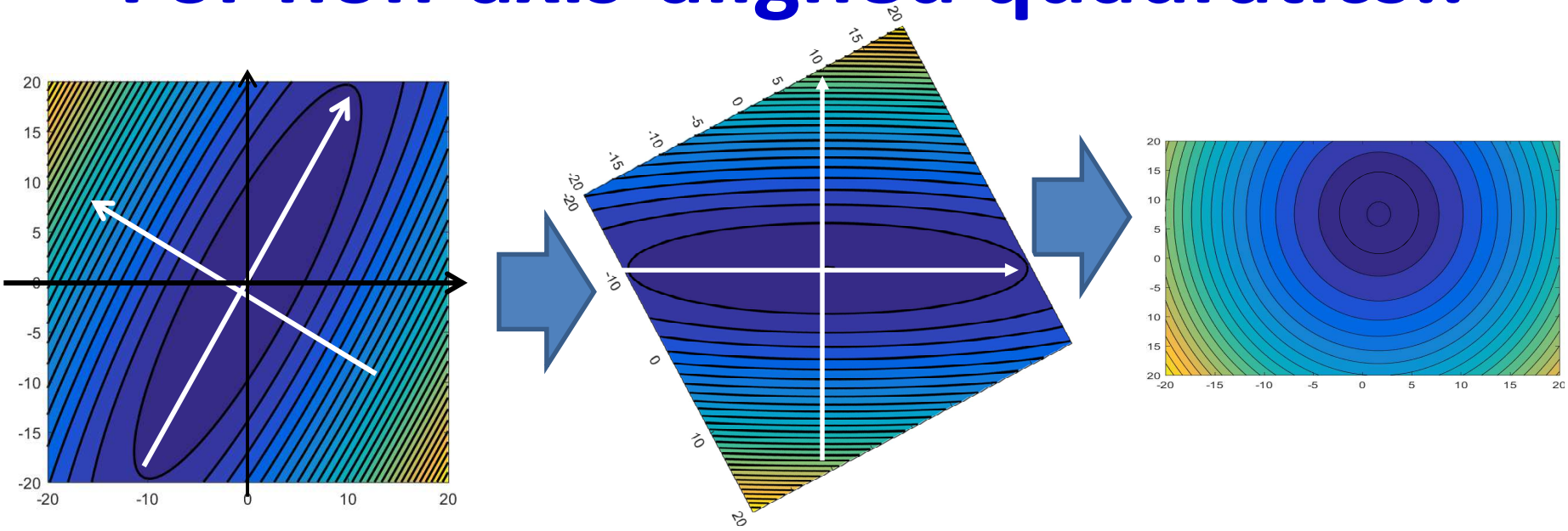


$$E = \frac{1}{2}\mathbf{w}^T\mathbf{A}\mathbf{w} + \mathbf{w}^T\mathbf{b} + c$$

$$E = \frac{1}{2}\sum_i a_{ii}w_i^2 + \sum_{i\neq j} a_{ij}w_i w_j + \sum_i b_i w_i + c$$

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

For non-axis-aligned quadratics..

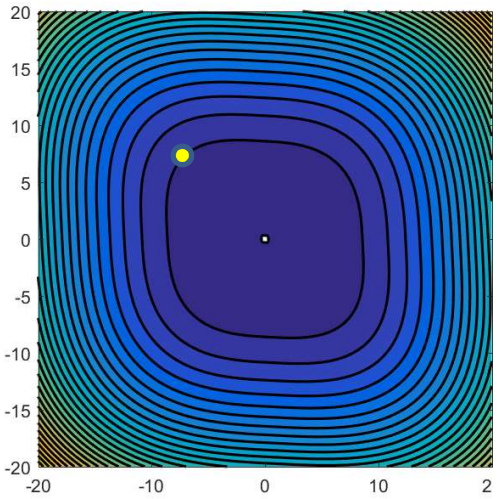


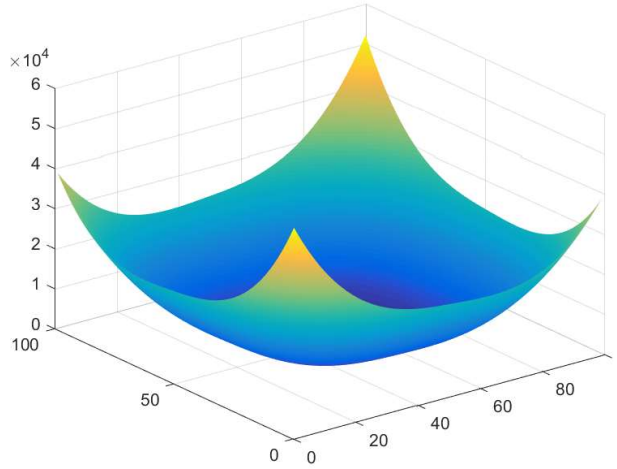
- The component-wise optimal learning rates along the major and minor axes of the contour ellipsoids will differ, causing problems
  - Inversely proportional to the *eigenvalues* of $\mathbf{A}$

- This can be fixed as before by rotating and resizing the different directions to obtain the same *normalized* update rule as before:

$$\mathbf{w}^{(k+1)} = \mathbf{w}^{(k)} - \eta \mathbf{A}^{-1}\mathbf{b}$$

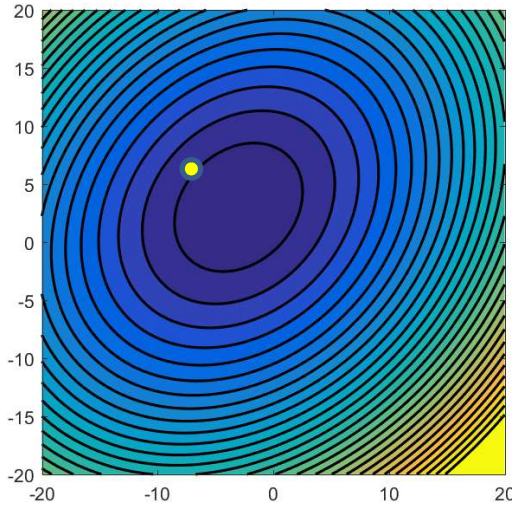
Generic differentiable *multivariate* convex functions

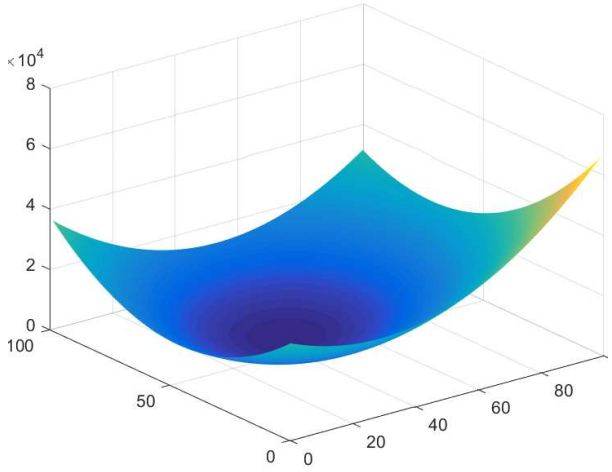




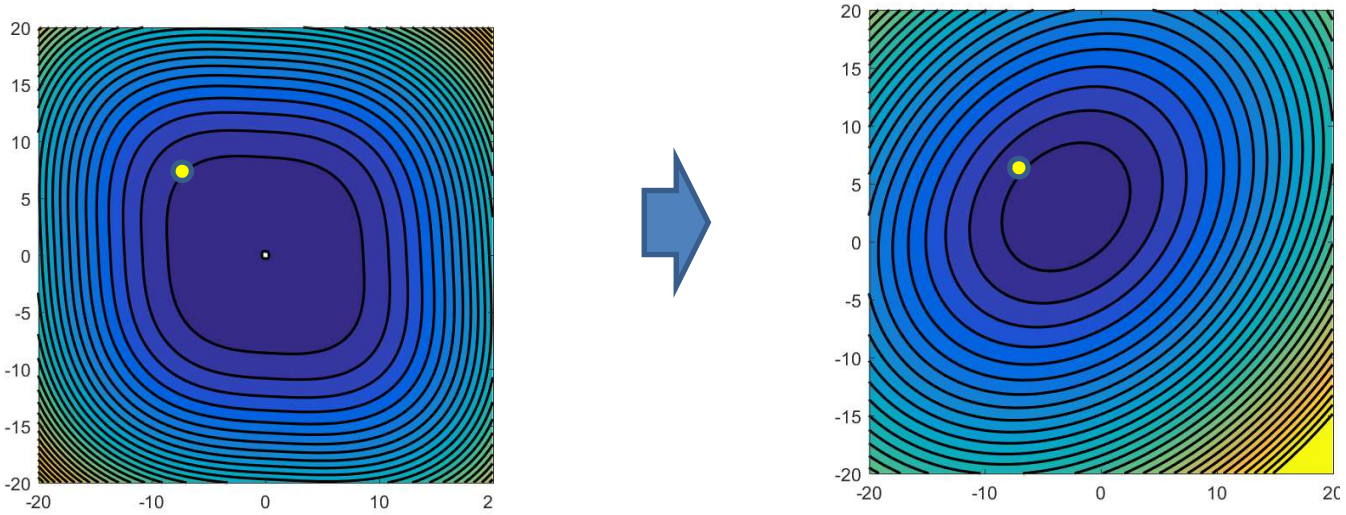
- Taylor expansion

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





Generic differentiable *multivariate* convex functions



- Taylor expansion

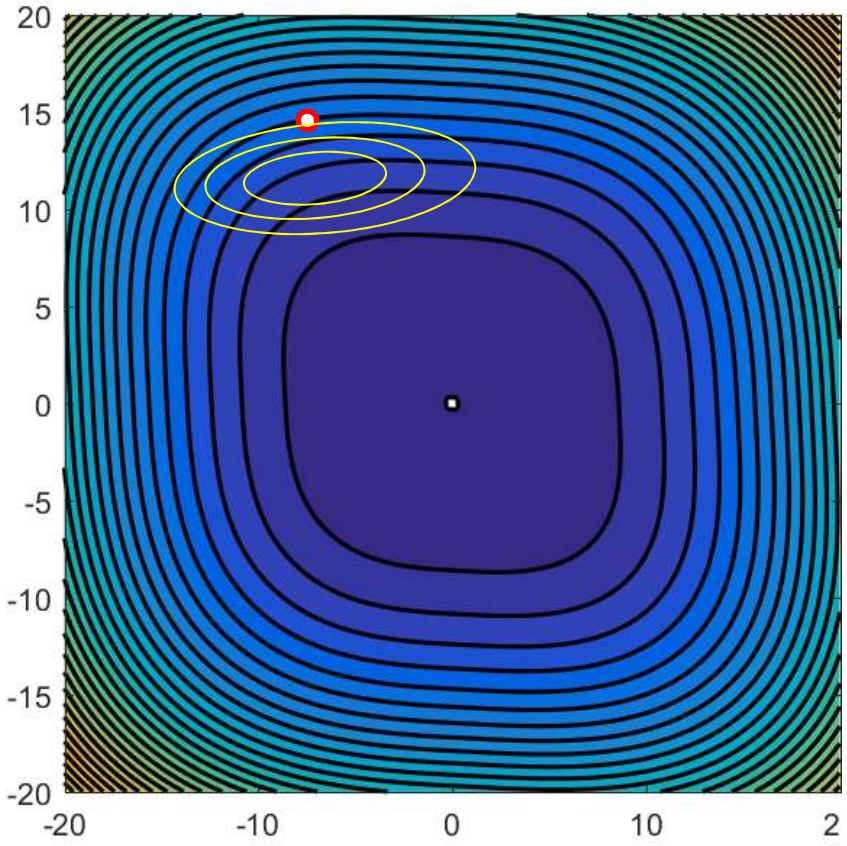
$$\boldsymbol{E}(\mathbf{w}) \approx \boldsymbol{E}\left(\mathbf{w}^{(k)}\right) + \boldsymbol{\nabla}_{\mathbf{w}}\boldsymbol{E}\left(\mathbf{w}^{(k)}\right)\left(\mathbf{w} - \boldsymbol{w}^{(k)}\right) + \frac{\mathbf{1}}{\mathbf{2}}\left(\mathbf{w} - \boldsymbol{w}^{(k)}\right)^{\boldsymbol{T}}\boldsymbol{H}_{\boldsymbol{E}}\left(\boldsymbol{w}^{(k)}\right)\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

- Note that this has the form $\frac{1}{2}\mathbf{w}^T\mathbf{A}\mathbf{w} + \mathbf{w}^T\mathbf{b} + c$
- Using the same logic as before, we get the 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 a quadratic function, the optimal η is 1 (which is exactly Newton's method)**
  - **And should not be greater than 2!**

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



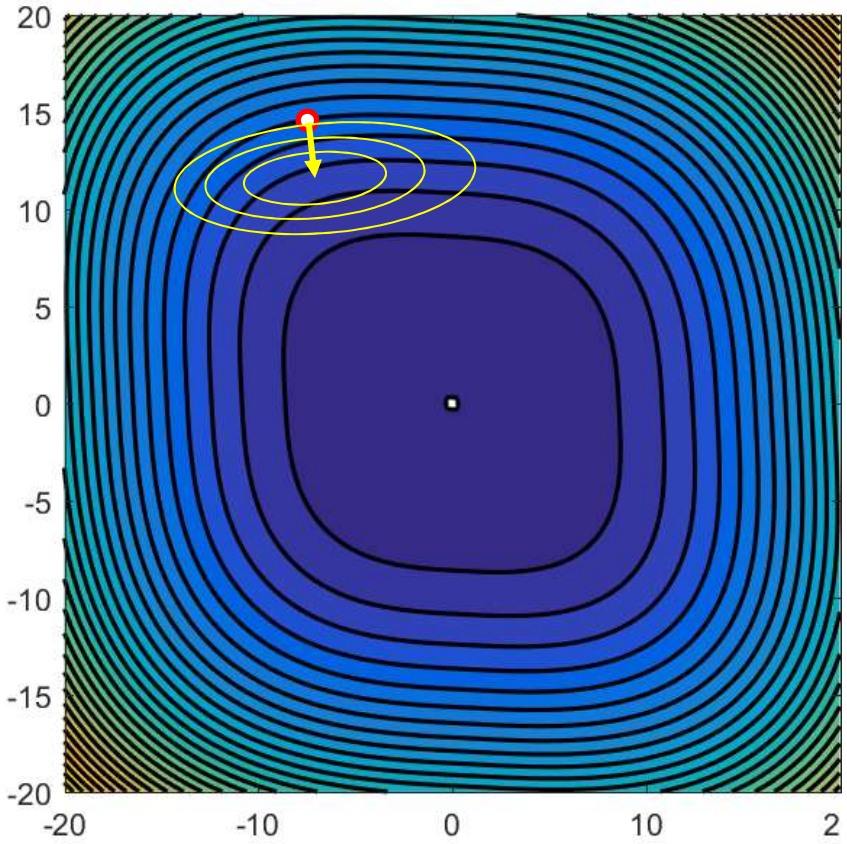
Fit a quadratic at each point and find the minimum of that quadratic

- Iterated localized optimization with quadratic approximations

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

$- \eta = 1$

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



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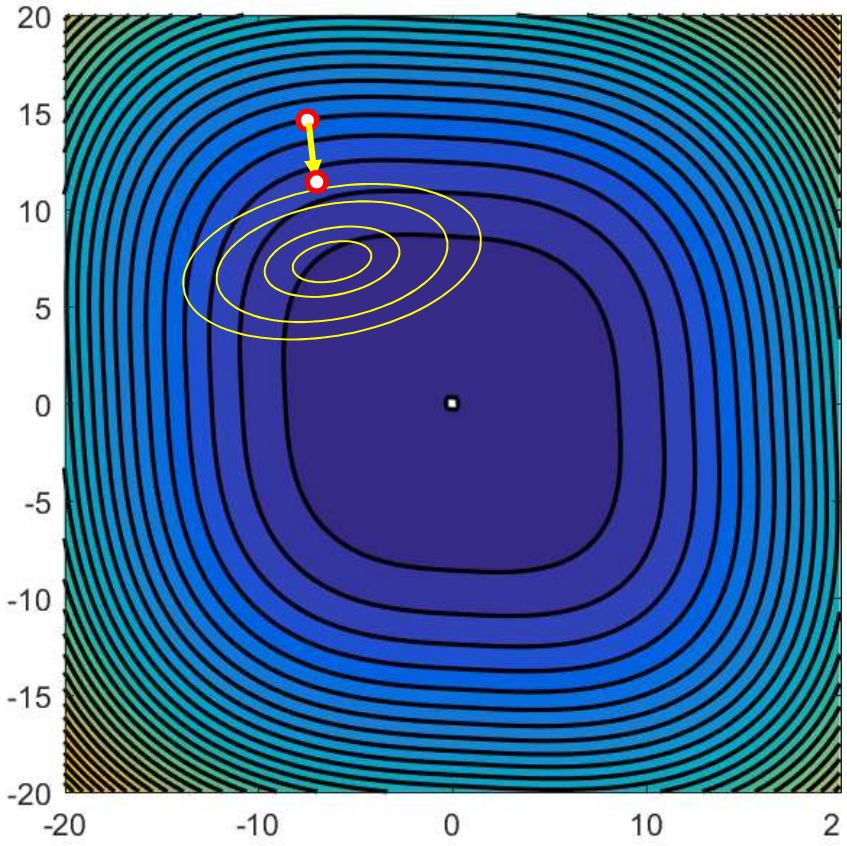

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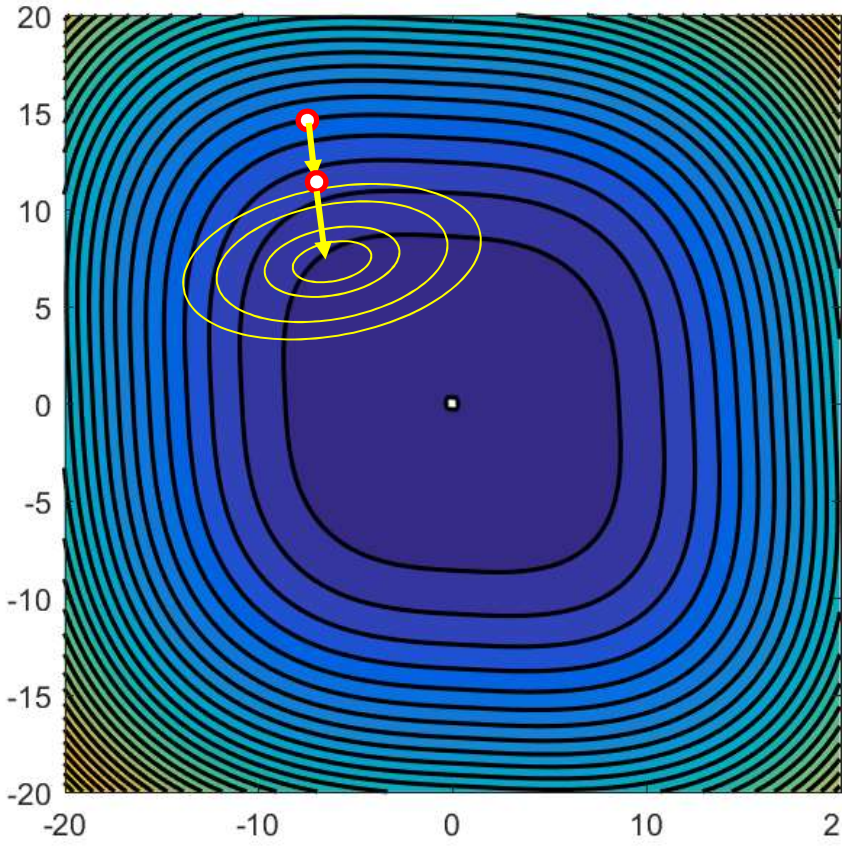

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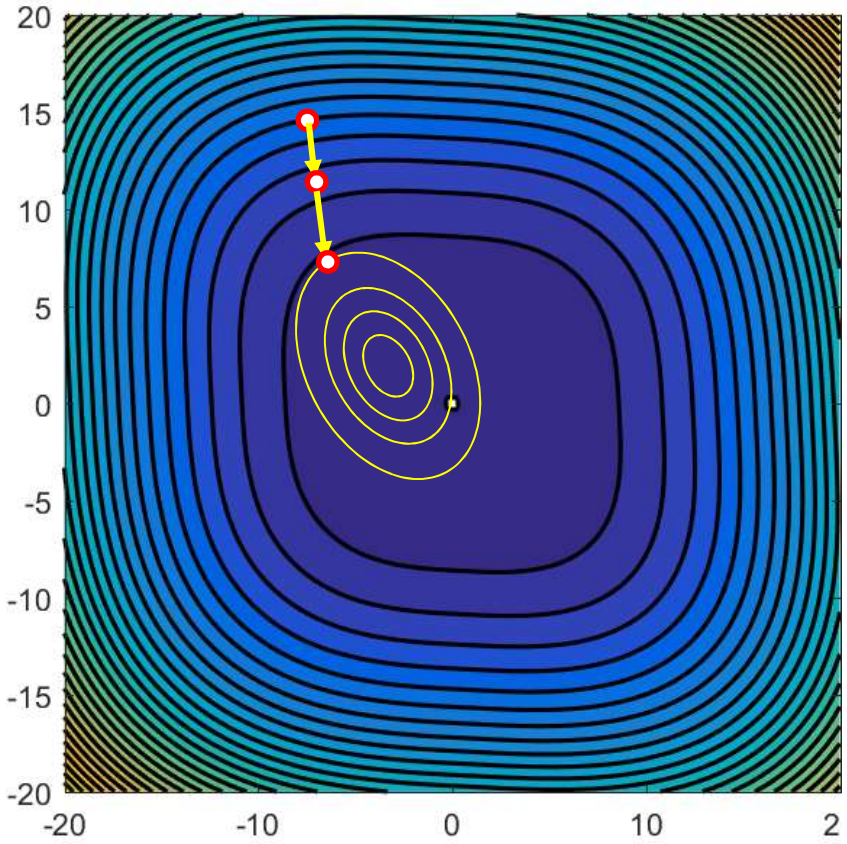

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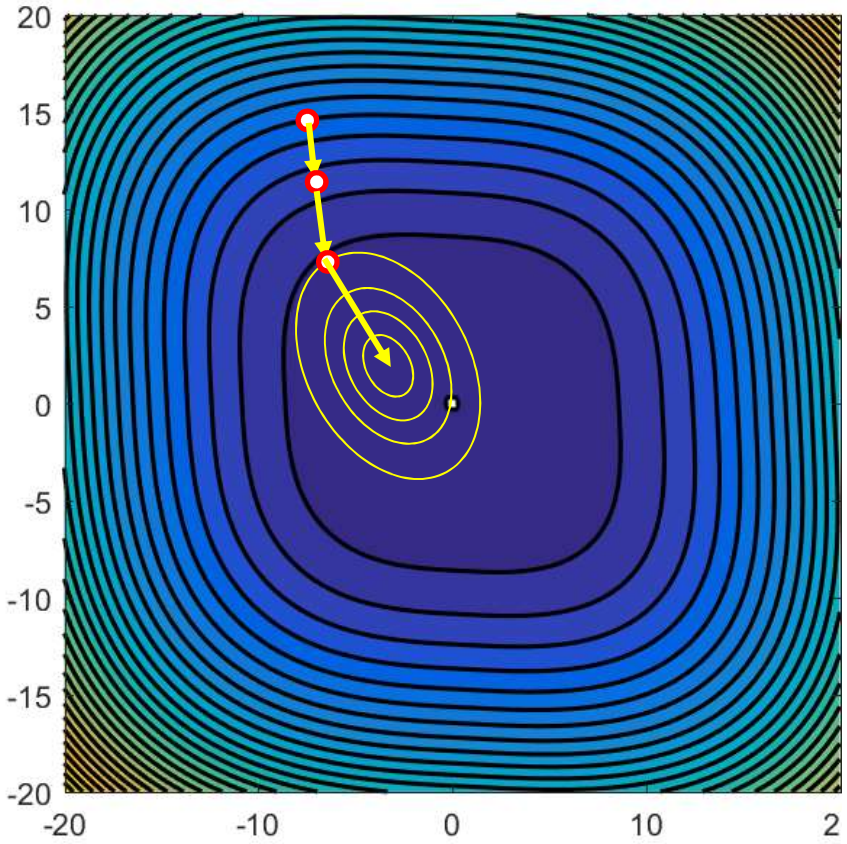

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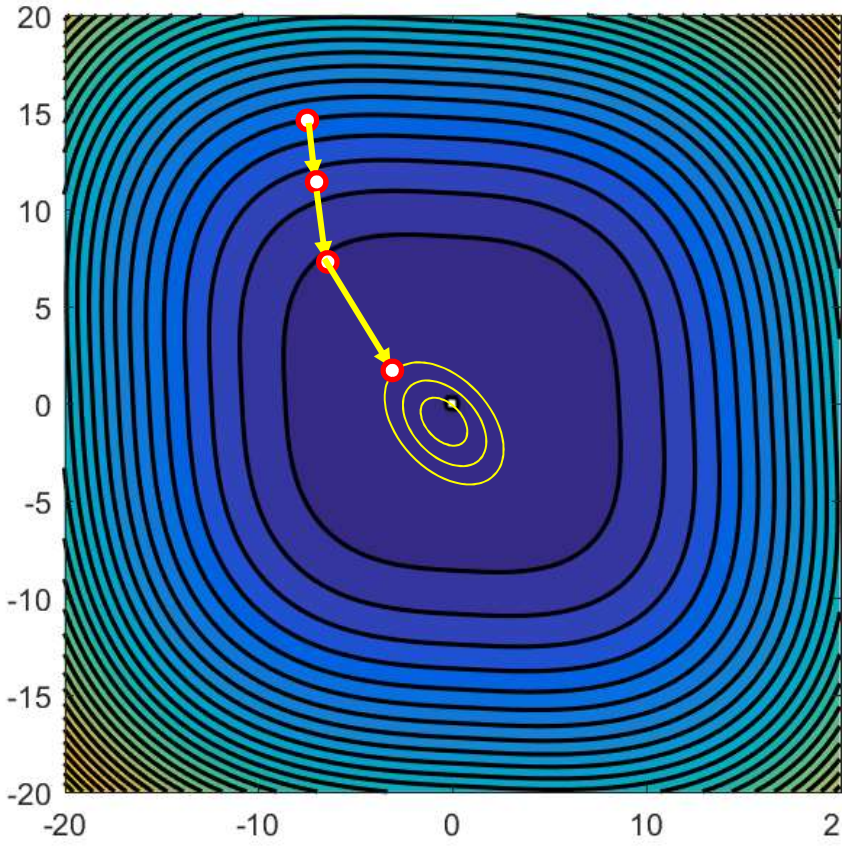

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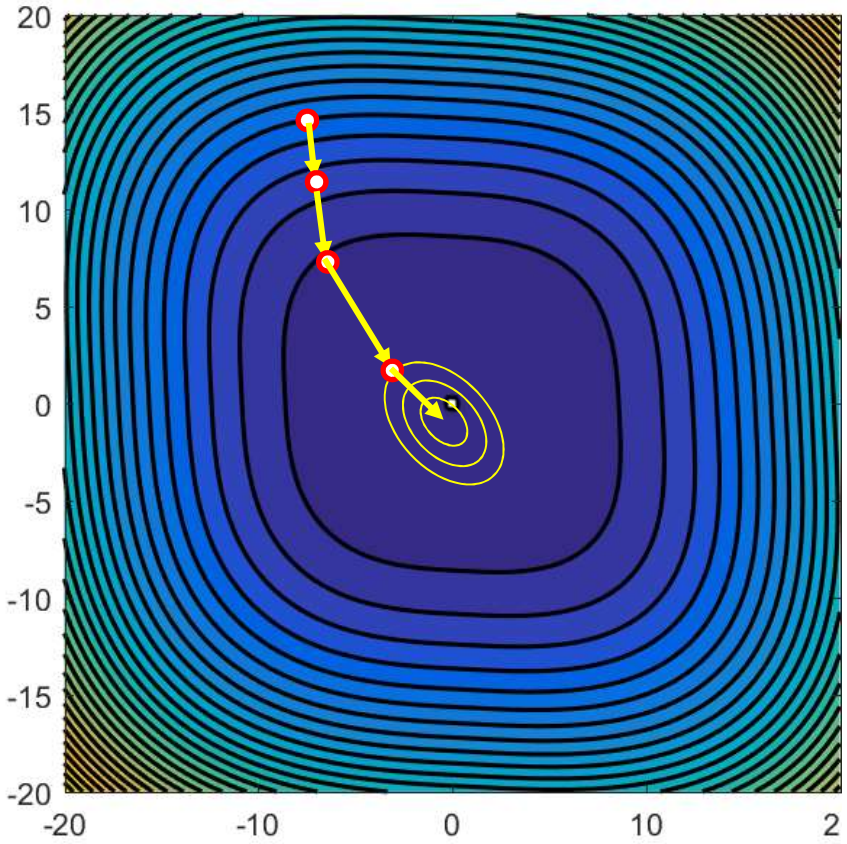

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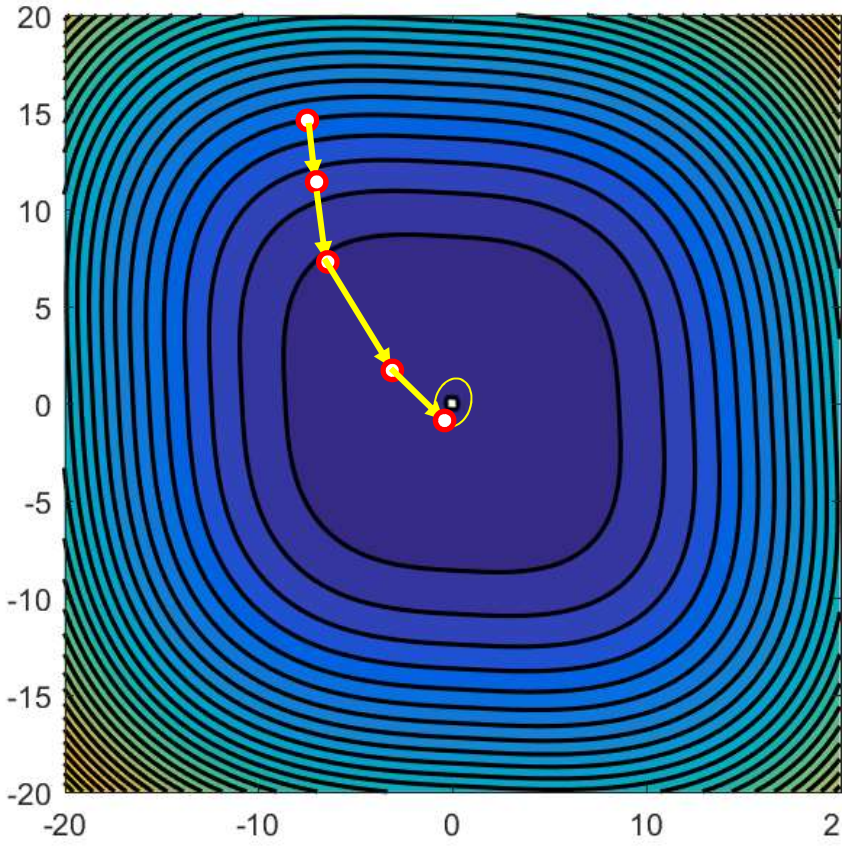

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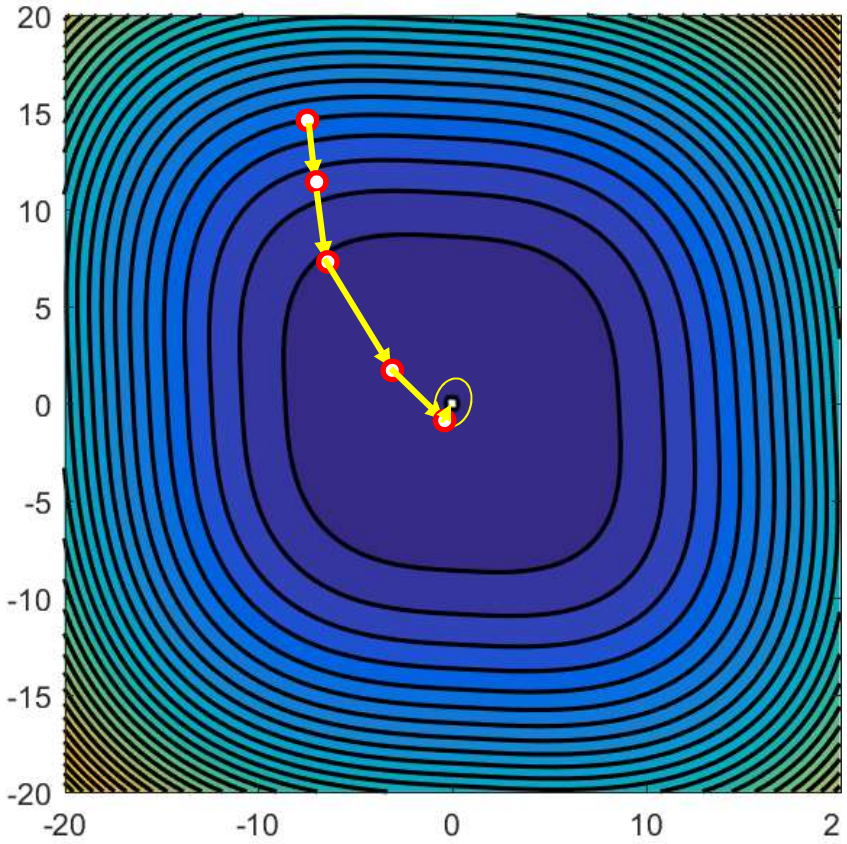
Minimization by Newton's method



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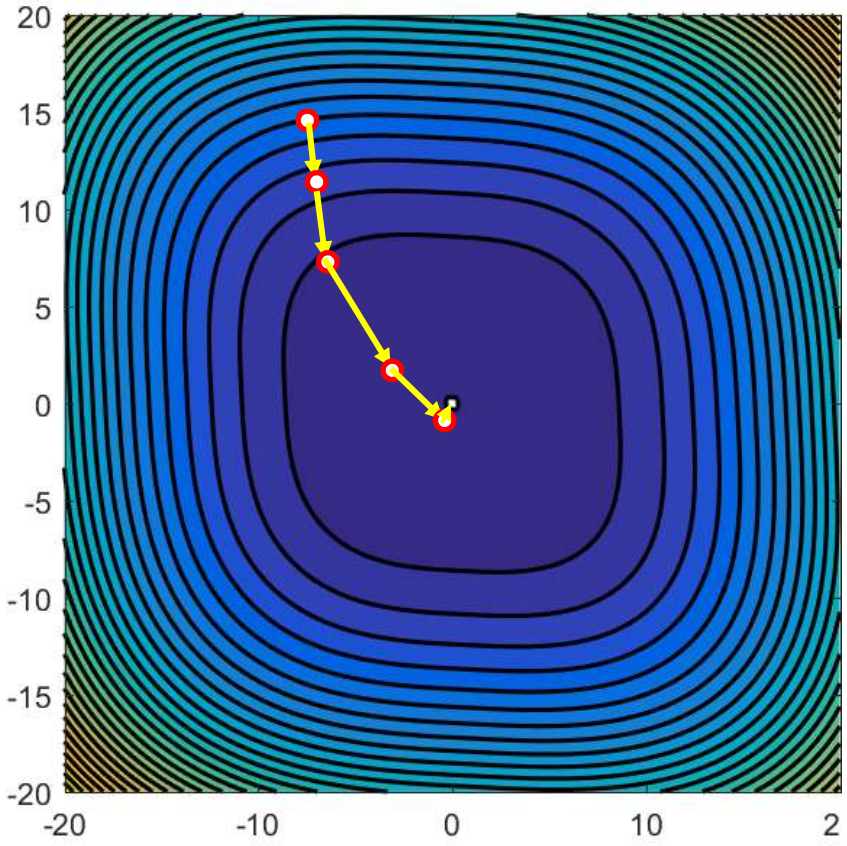


- Iterated localized optimization with quadratic approximations

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

$-\ \eta = 1$

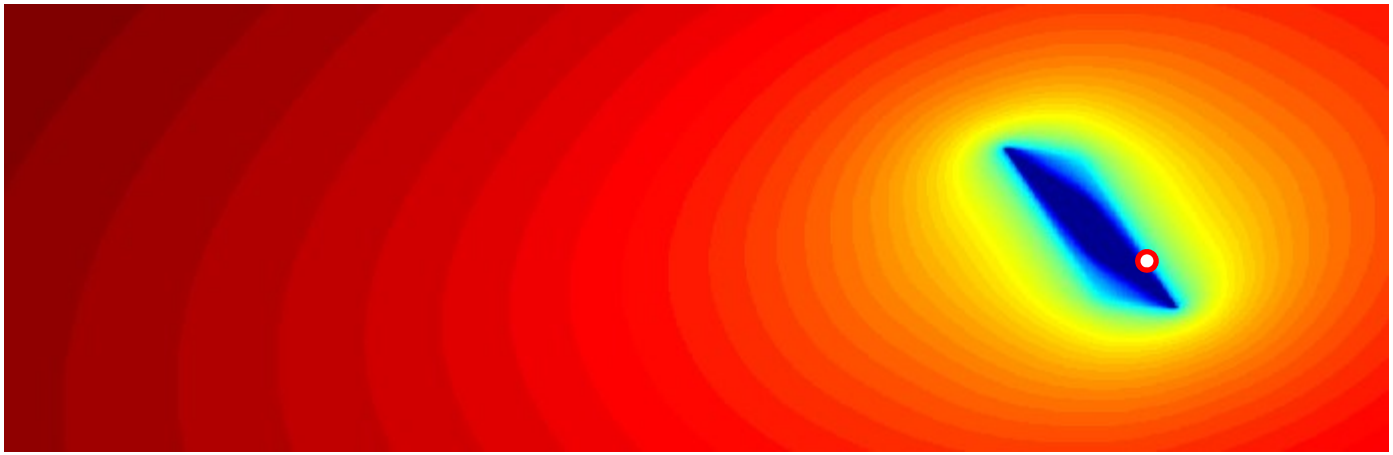
Issues: 1. The Hessian

- Normalized update rule

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

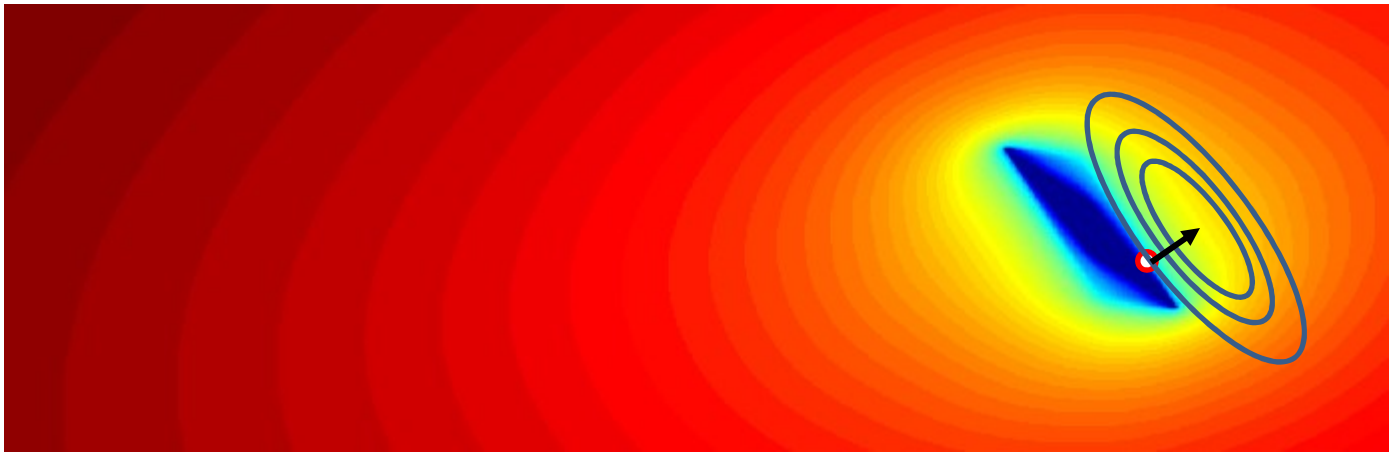
- For complex models such as neural networks, with a very large number of parameters, the Hessian $H_E\left(\boldsymbol{w}^{(k)}\right)$ is extremely difficult to compute
  - For a network with only 100,000 parameters, the Hessian will have 10^{10} cross-derivative terms
  - And its even harder to invert, 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

Issues: 1. The Hessian



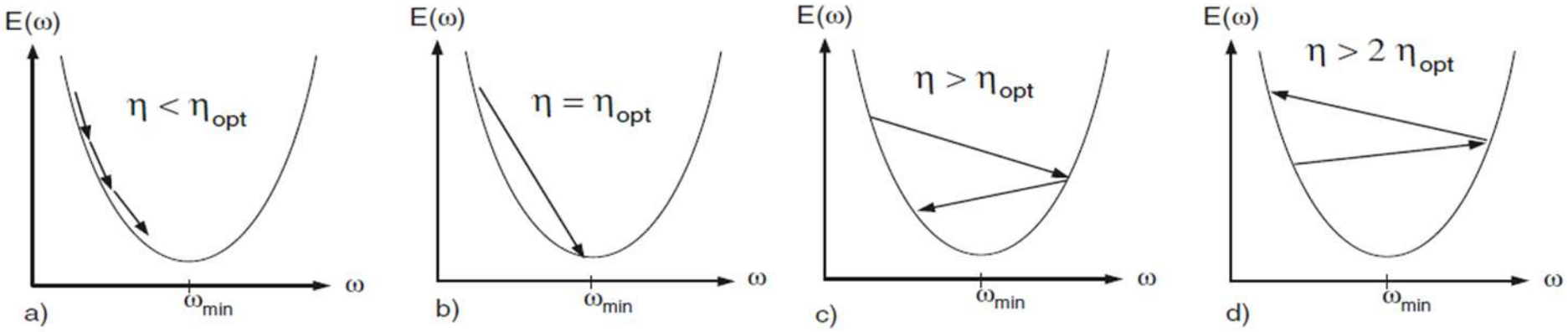
- For non-convex functions, the Hessian may not be positive semi-definite, in which case the algorithm can *diverge*
  - Goes away from, rather than towards the minimum
  - Now requires additional checks to avoid movement in directions corresponding to –ve Eigenvalues of the Hessian

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

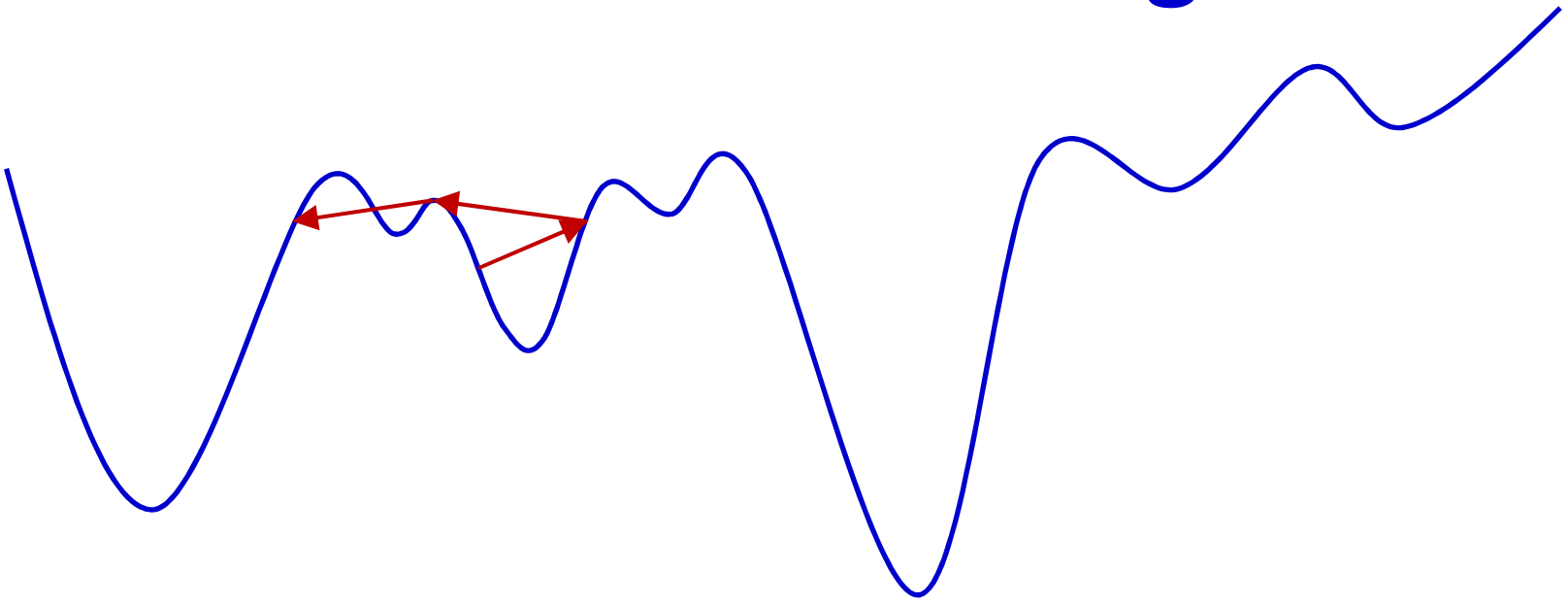
- Not particularly popular anymore for large neural networks..

Issues: 2. The learning rate



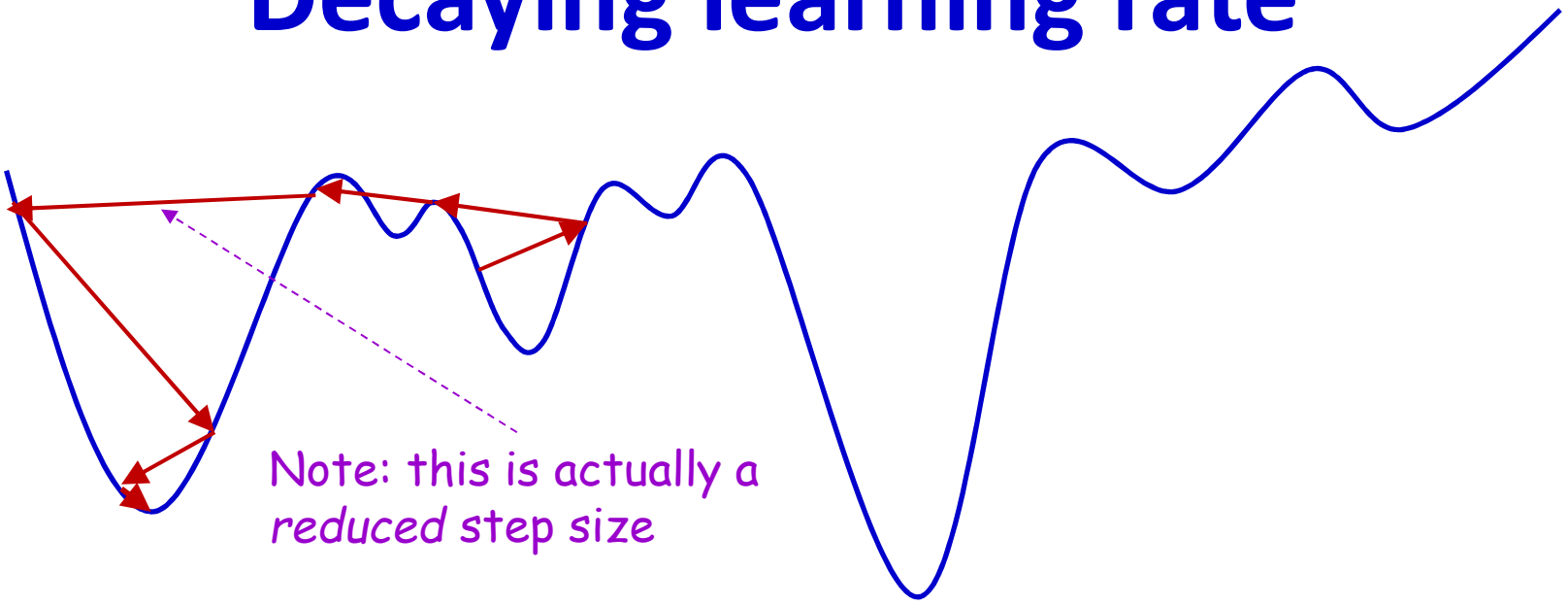
- Much of the analysis we just saw was based on trying to ensure that the step size was not so large as to cause divergence within a convex region
  - $\eta < 2\eta_{opt}$

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



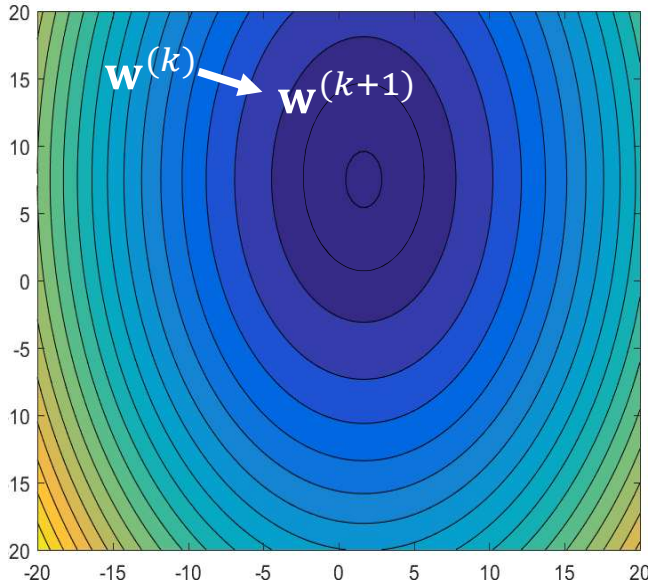
- Start with a large learning rate
  - Greater than 2 (assuming Hessian normalization)
  - Gradually reduce it with iterations

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

Lets take a step back



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

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

- Problems arise because of requiring a fixed step size across all dimensions
  - Because step are "tied" to the gradient
- Lets try releasing this requirement

Derivative-*inspired* algorithms

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

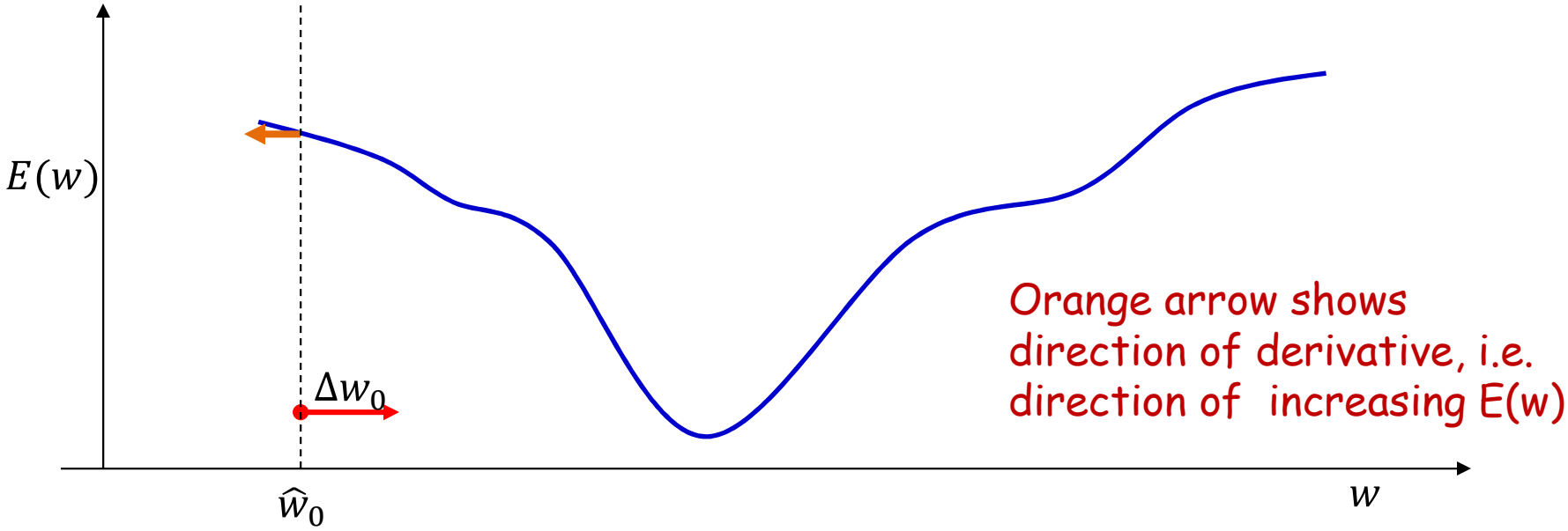
- Rprop
- Quick prop

RProp

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

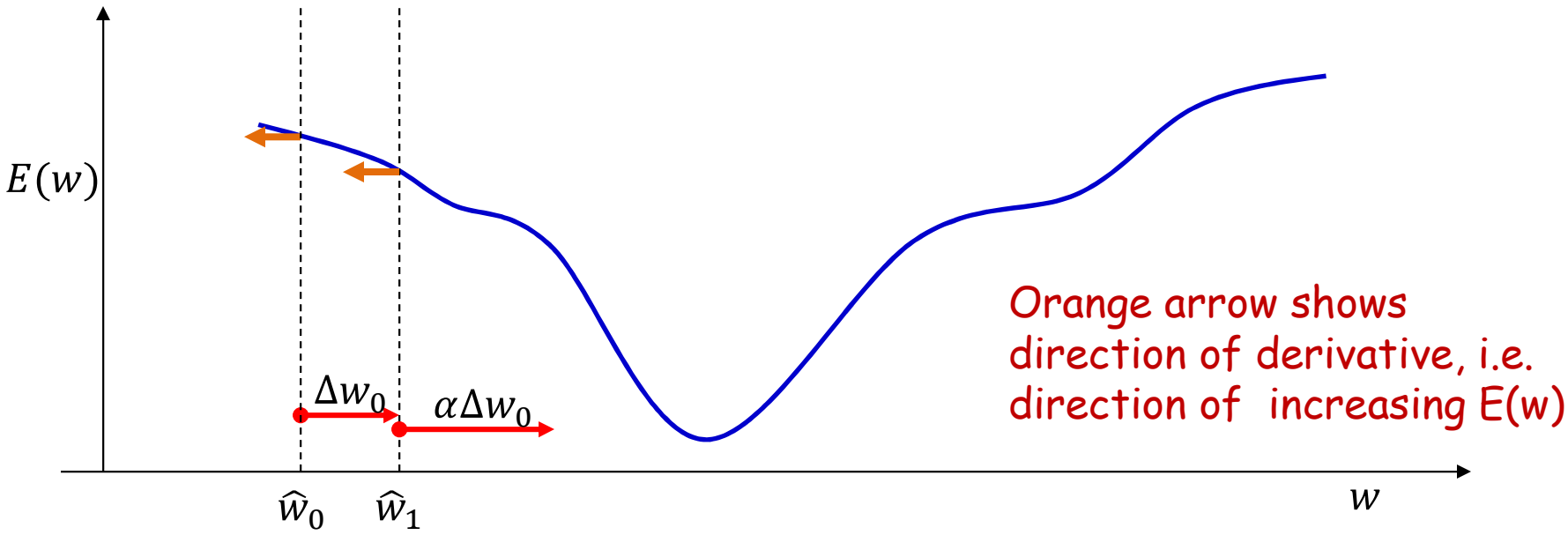
- At each time
  - If the derivative at the current location recommends continuing in the same direction as before (i.e. has not changed sign from earlier):
    - *increase* the step, and continue in the same direction
  - If the derivative has changed sign (i.e. we've overshot a minimum)
    - *reduce*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

Rprop



- Select an initial value $\widehat{w}$ and compute the derivative
  - Take an initial step Δw against the derivative
    - In the direction that reduces the function
      - $\Delta w = sign\left(\frac{dE(\widehat{w})}{dw}\right)\Delta w$
      - $\widehat{w} = \widehat{w} - \Delta w$

Rprop

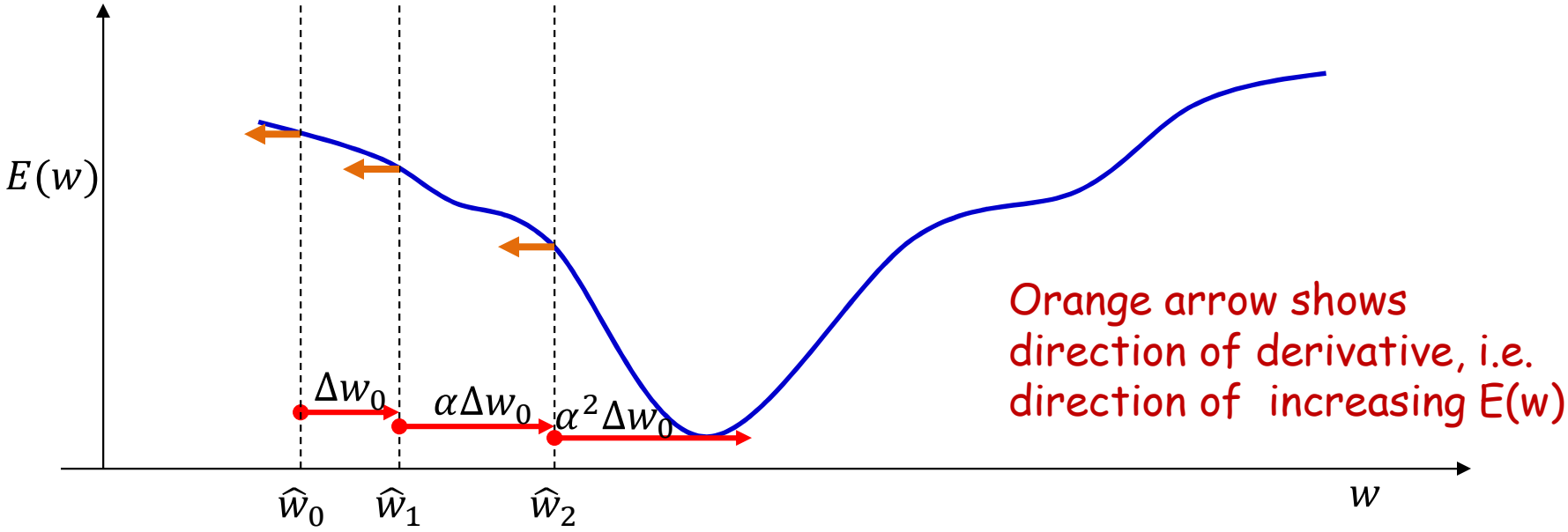


- Compute the derivative in the new location
  - If the derivative has not changed sign from the previous location, increase the step size and take a longer step

$\alpha > 1$

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

Rprop



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- $\Delta w = \alpha\Delta w$
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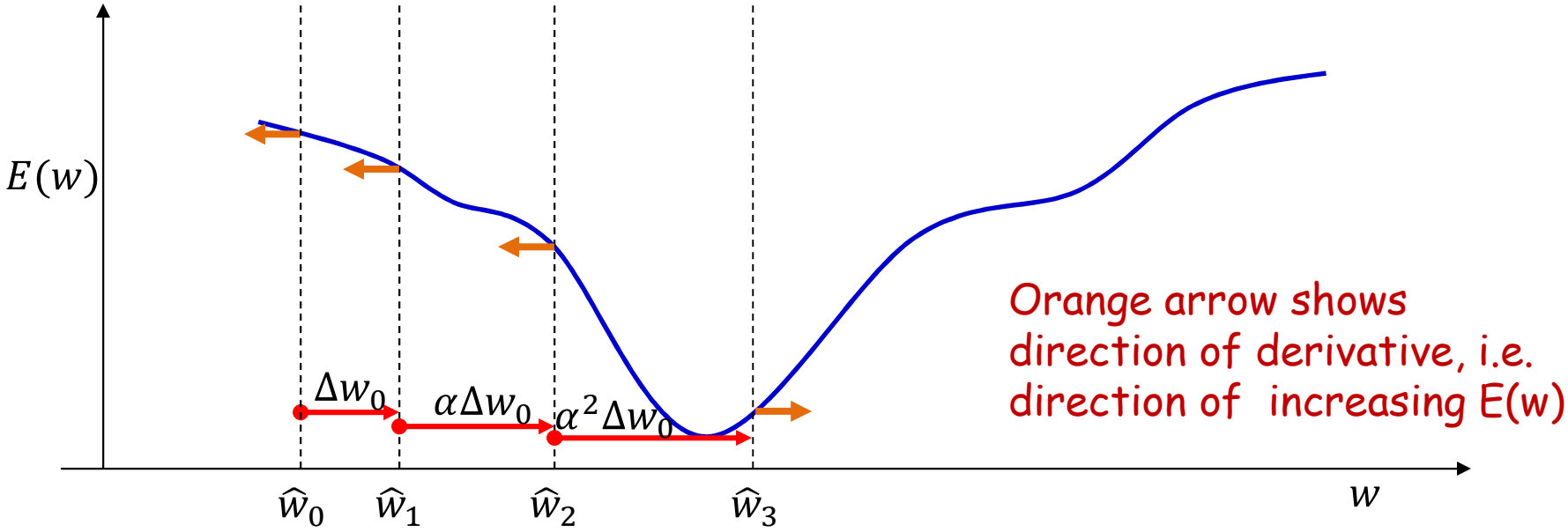
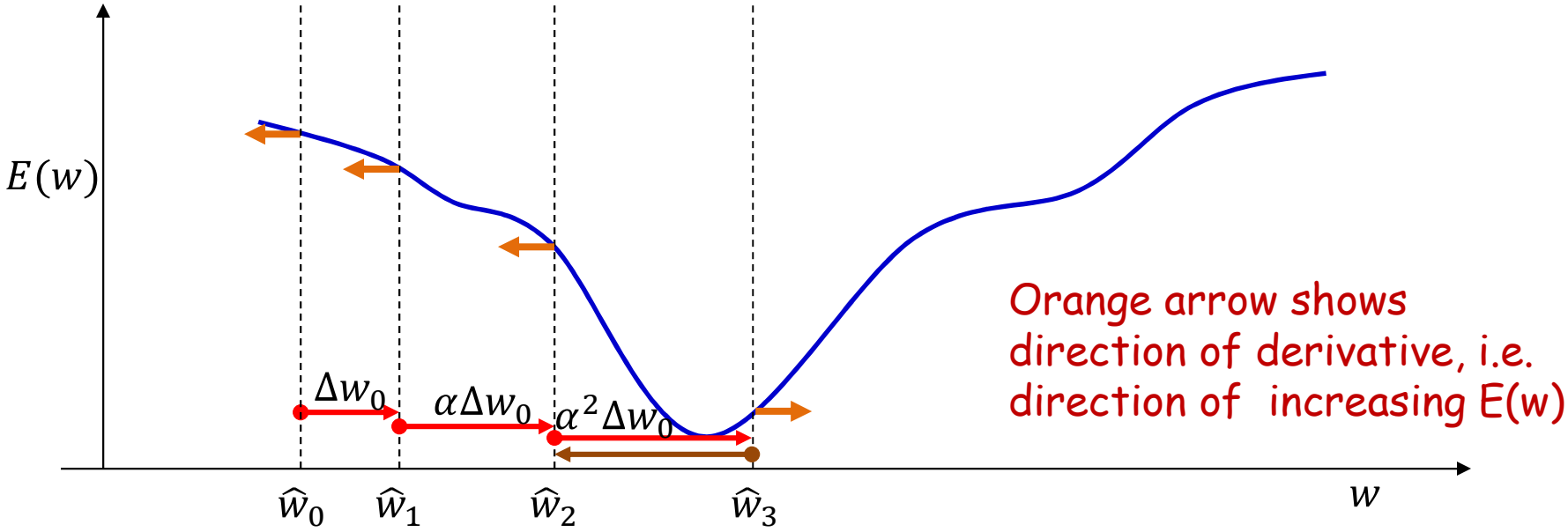
Rprop



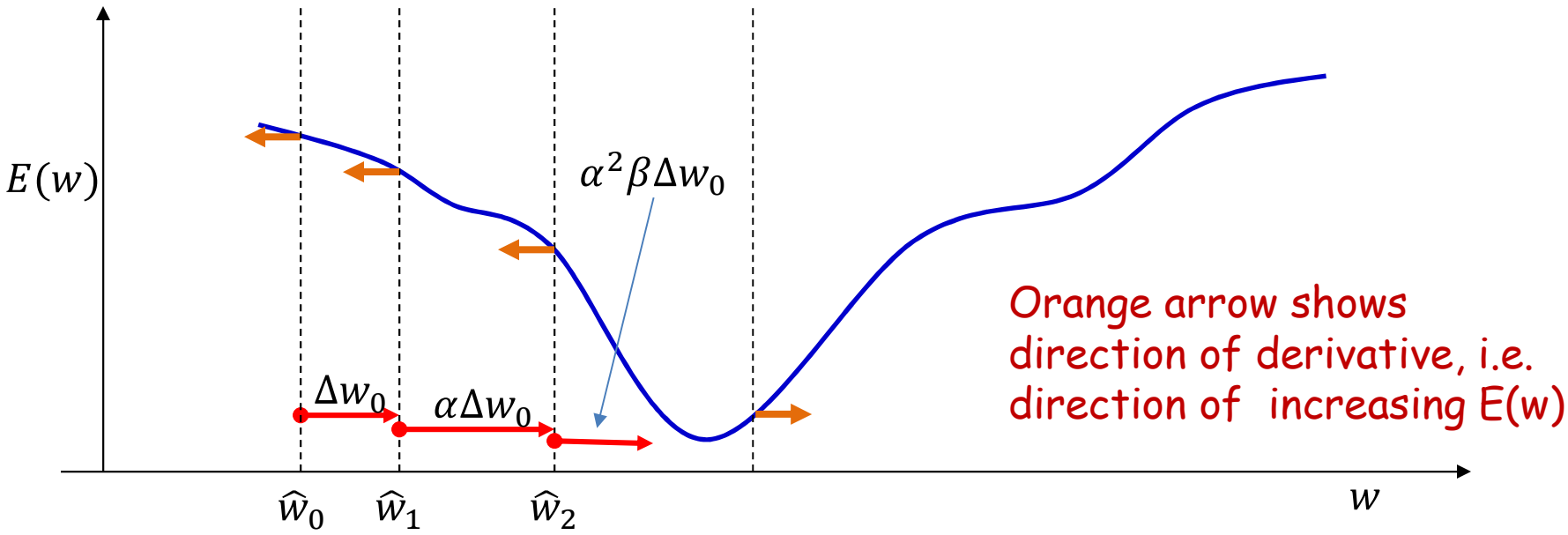
- Compute the derivative in the new location
  - If the derivative has changed sign

Rprop



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

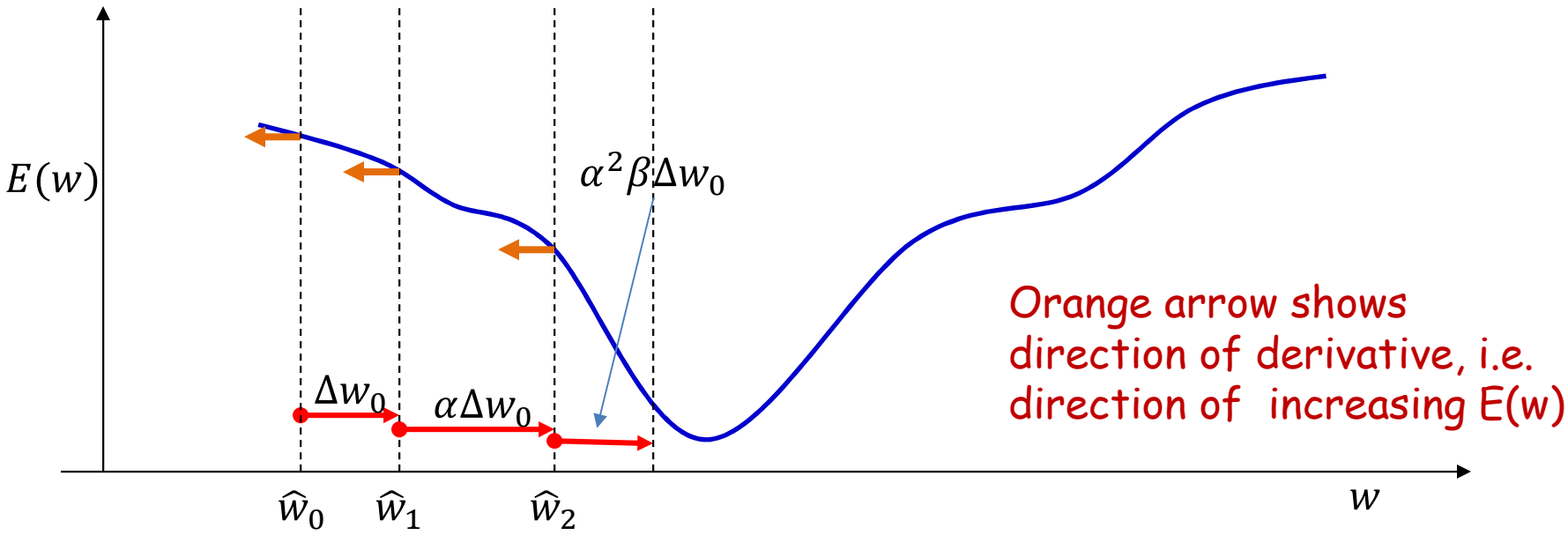
Rprop



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

$\beta < 1$

Rprop (simplified)

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

Ceiling and floor on step

Rprop (simplified)

- Set $\alpha = 1.2, \beta = 0.5$
- For each layer l, for each i, j:
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  - $\Delta w_{l,i,j} = \text{sign}\big(prevD(l,i,j)\big)\Delta w_{l,i,j}$
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    - $w_{l,i,j} = w_{l,i,j} - \Delta w_{l,i,j}$
    - $D(l,i,j) = \frac{dErr(w_{l,i,j})}{dw_{l,i,j}}$
    - If $\text{sign}\big(prevD(l,i,j)\big) == \text{sign}\big(D(l,i,j)\big)$:
      - $\Delta w_{l,i,j} = \alpha \Delta w_{l,i,j}$
      - $prevD(l,i,j) = D(l,i,j)$
    - else:
      - $w_{l,i,j} = w_{l,i,j} + \Delta w_{l,i,j}$
      - $\Delta w_{l,i,j} = \beta \Delta w_{l,i,j}$

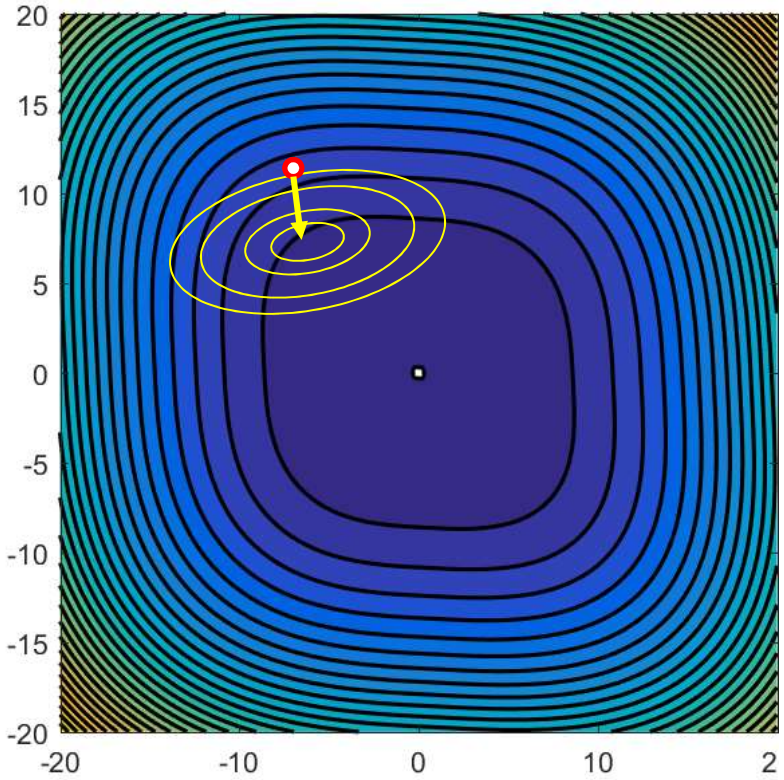
Obtained via backprop

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

QuickProp

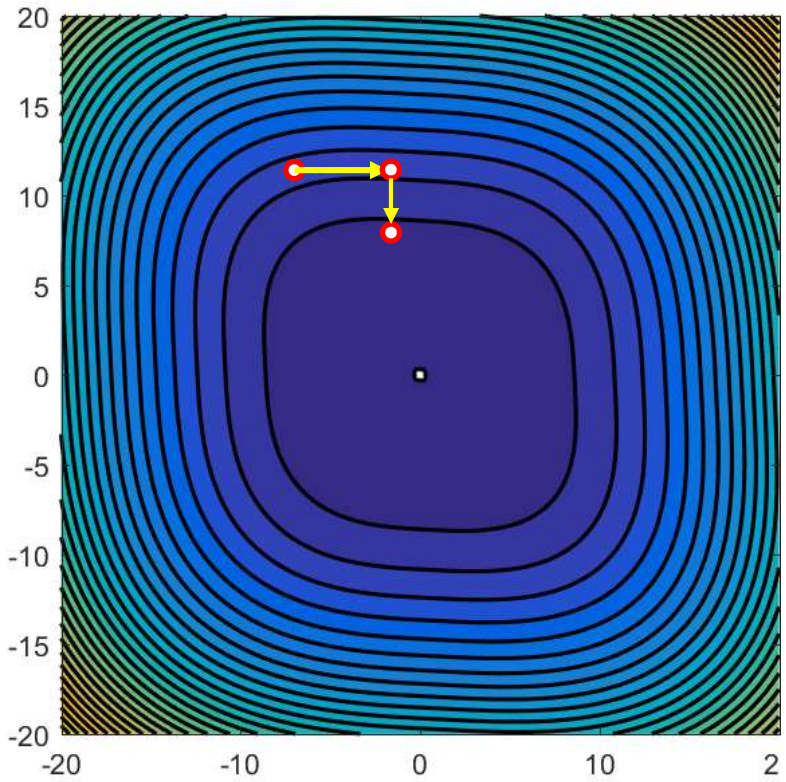


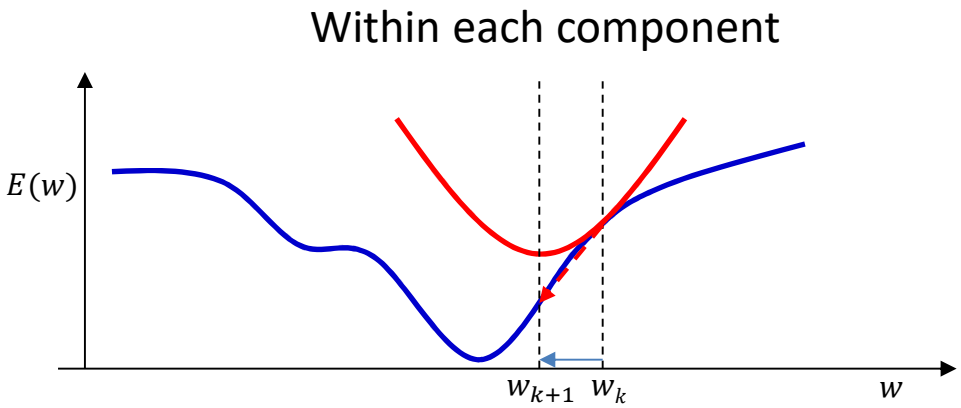
- Quickprop employs the Newton updates with two modifications

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

- But with two modifications

QuickProp: Modification 1



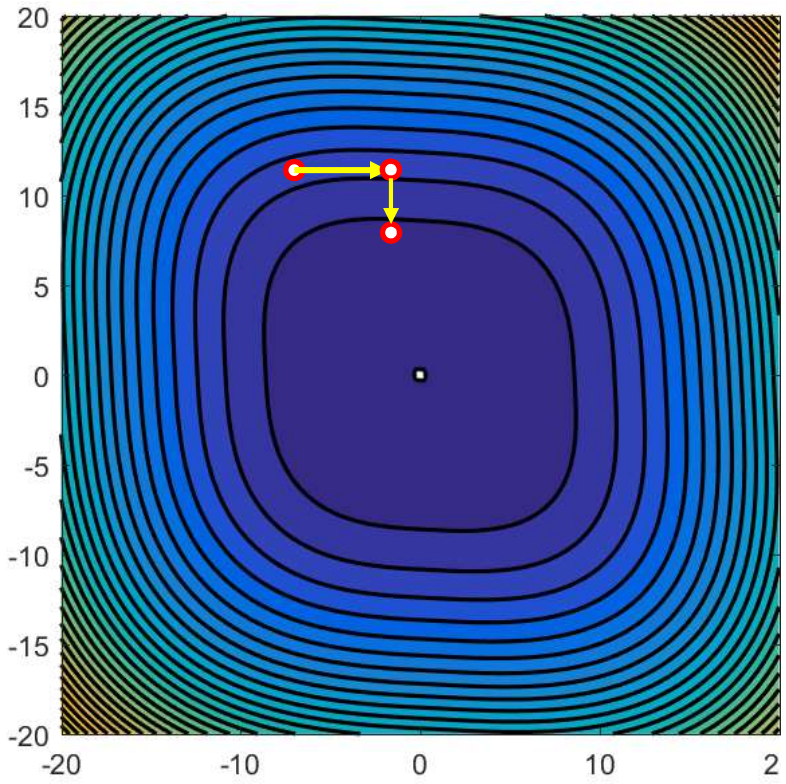


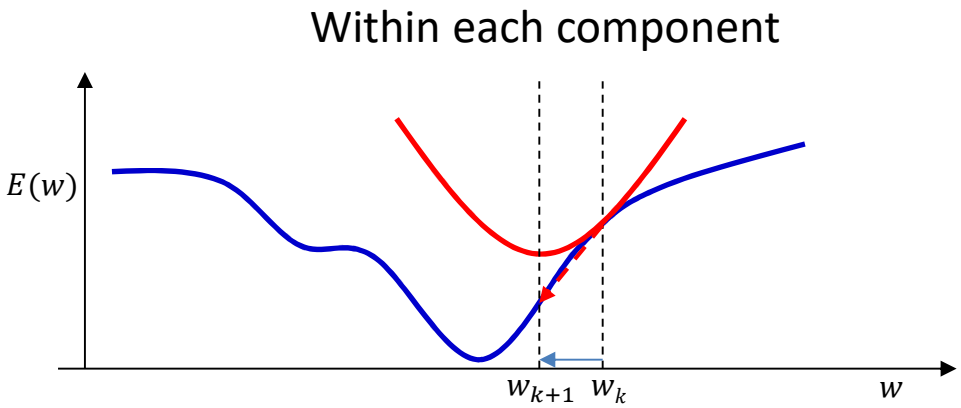
- It treats each dimension independently
- For $i = 1{:}N$

$$w_i^{k+1} = w_i^k - E''\left(w_i^k | w_j^k, j \neq i\right)^{-1} E'\left(w_i^k | w_j^k, j \neq i\right)$$

- This eliminates the need to compute and invert expensive Hessians

QuickProp: Modification 2





- **It approximates the second derivative through finite differences**
- For $i = 1{:}N$

$$w_i^{k+1} = w_i^k - D\left(w_i^k, w_i^{k-1}\right)^{-1} E'\left(w_i^k | w_j^k, j \neq i\right)$$

- This eliminates the need to compute expensive double derivatives

QuickProp

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

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 $(l-1)^{\text{th}}$ layer to node j in the l^{th} layer:

$$\Delta w_{l,ij}^{(k)} = \frac{\Delta w_{l,ij}^{(k-1)}}{Err'\left(w_{l,ij}^{(k)}\right) - Err'\left(w_{l,ij}^{(k-1)}\right)} Err'\left(w_{l,ij}^{(k)}\right)$$

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

QuickProp

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

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

Computed using backprop

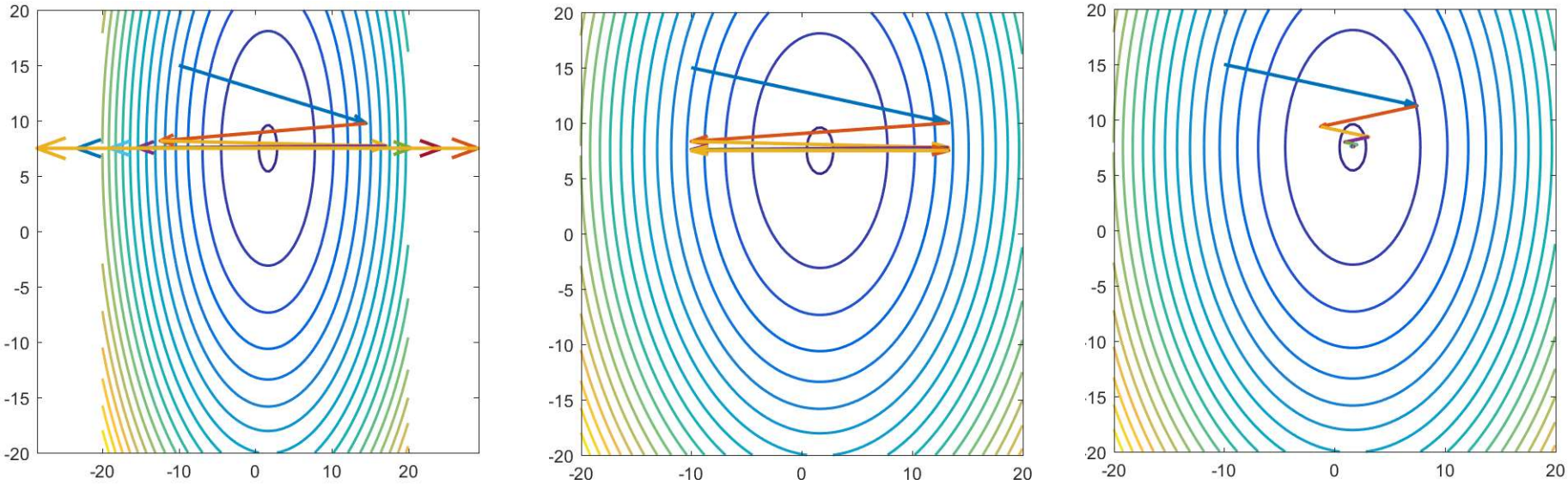
Quickprop

- 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

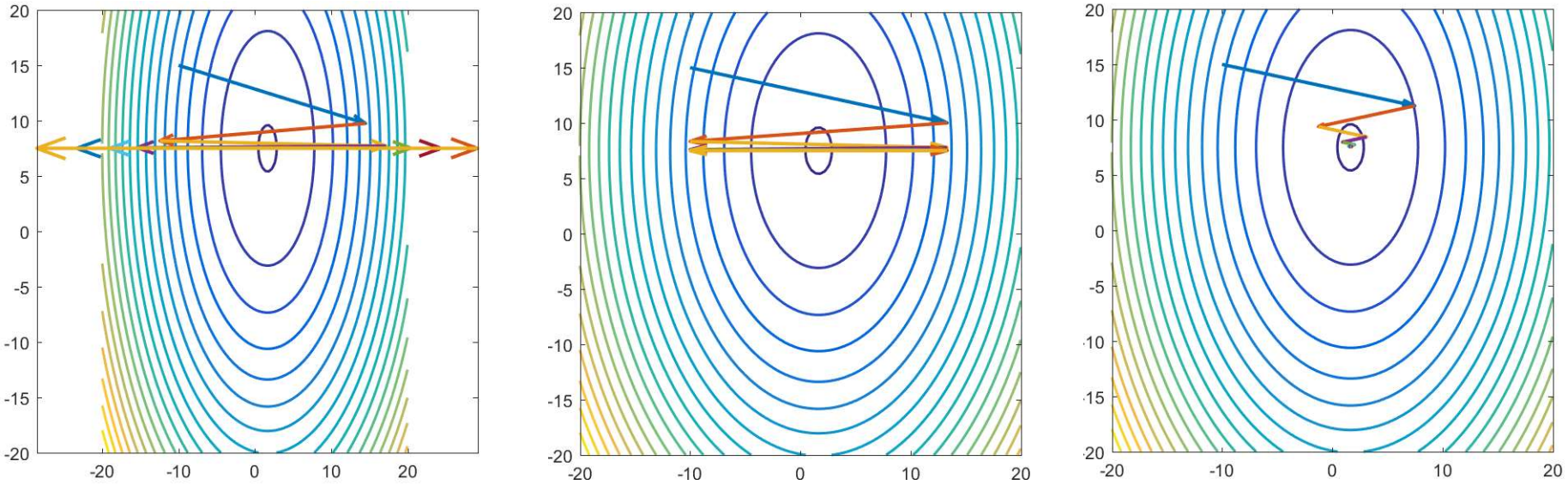
- Gradient descent can miss obvious answers
  - And this may be a *good* thing
- Vanilla gradient descent may be too slow or unstable due to the differences between the dimensions
- Second order methods can normalize the variation across dimensions, but are complex
- Adaptive or decaying learning rates 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

A closer look at the convergence problem

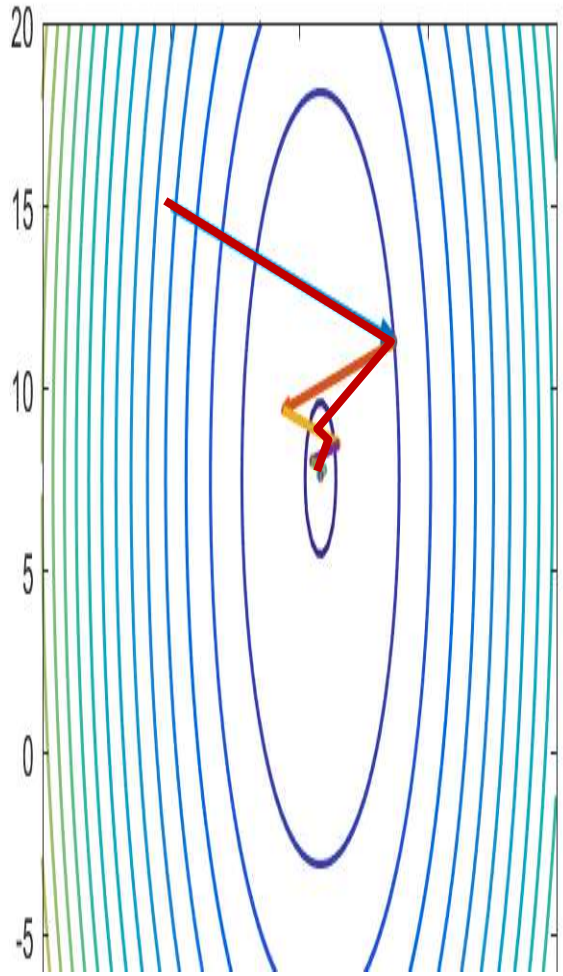


- With dimension-independent learning rates, the solution will converge smoothly in some directions, but oscillate or diverge in others

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

The momentum methods

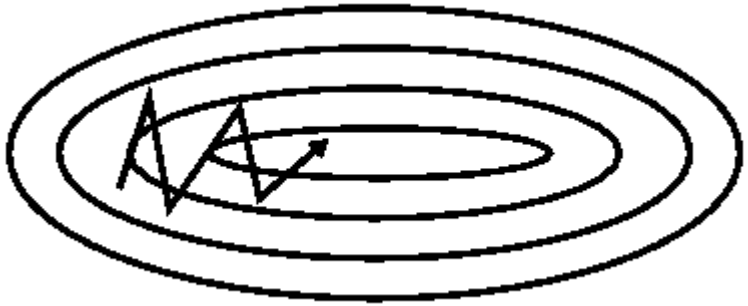
- Maintain a running average of all past steps
  - In directions in which the convergence is smooth, the average will have a large value
  - In directions in which the estimate swings, the positive and negative swings will cancel out in the average
- Update with the running average, rather than the current gradient



Momentum Update

Plain gradient update

With momentum



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

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

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

  - Typical β value is 0.9
- The running average steps
  - Get longer in directions where gradient stays in the same sign
  - Become shorter in directions where the sign keeps flipping

Training by gradient descent

- Initialize all weights $\mathbf{W}_1, \mathbf{W}_2, \ldots, \mathbf{W}_K$
- Do:
  - For all $i, j, k,$ initialize $\nabla_{W_k} Loss = 0$
  - For all $t = 1:T$
    - For every layer k:
      - Compute $\nabla_{W_k} \boldsymbol{Div}(Y_t, d_t)$
      - Compute $\nabla_{W_k} Loss \mathrel{+}= \frac{1}{T} \nabla_{W_k} \boldsymbol{Div}(Y_t, d_t)$
  - For every layer k:

$$W_k = W_k - \eta (\nabla_{W_k} Loss)^T$$

- Until $Loss$ has converged

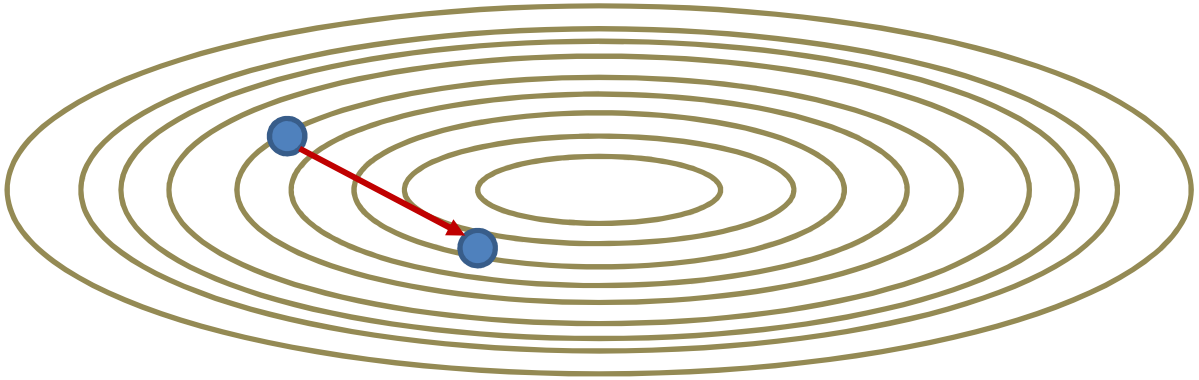
Training with momentum

- Initialize all weights $\mathbf{W}_1, \mathbf{W}_2, \ldots, \mathbf{W}_K$
- 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 $\nabla_{W_k} \boldsymbol{Div}(Y_t, d_t)$
      - $\nabla_{W_k} Loss \mathrel{+}= \frac{1}{T} \nabla_{W_k} \boldsymbol{Div}(Y_t, d_t)$
  - For every layer k

$$\Delta W_k = \beta \Delta W_k - \eta \left(\nabla_{W_k} Loss\right)^T$$
$$W_k = W_k + \Delta W_k$$

- Until $Loss$ has converged

Momentum Update

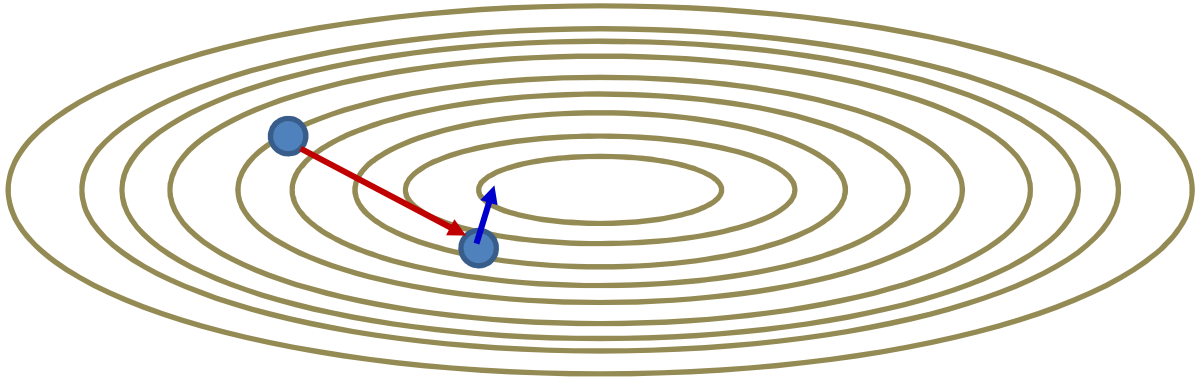


- The momentum method

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

- At any iteration, to compute the current step:

Momentum Update

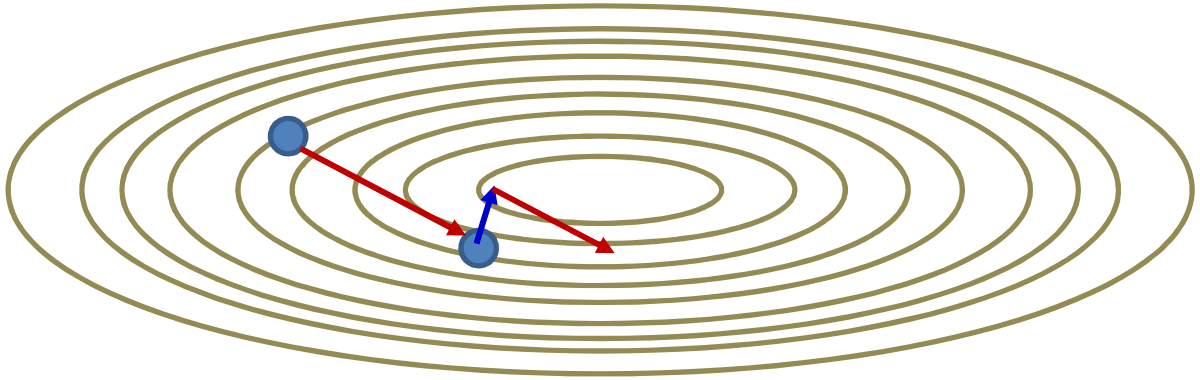


- The momentum method

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

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

Momentum Update

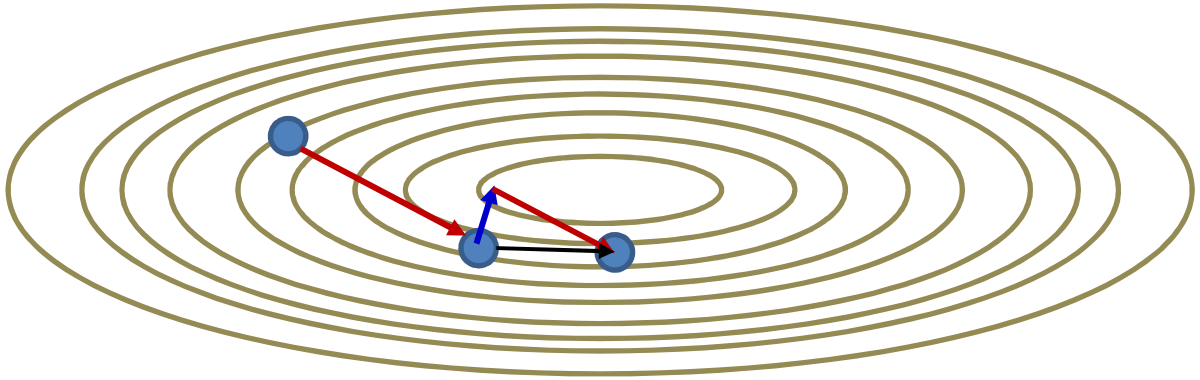


- The momentum method

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

- 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

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

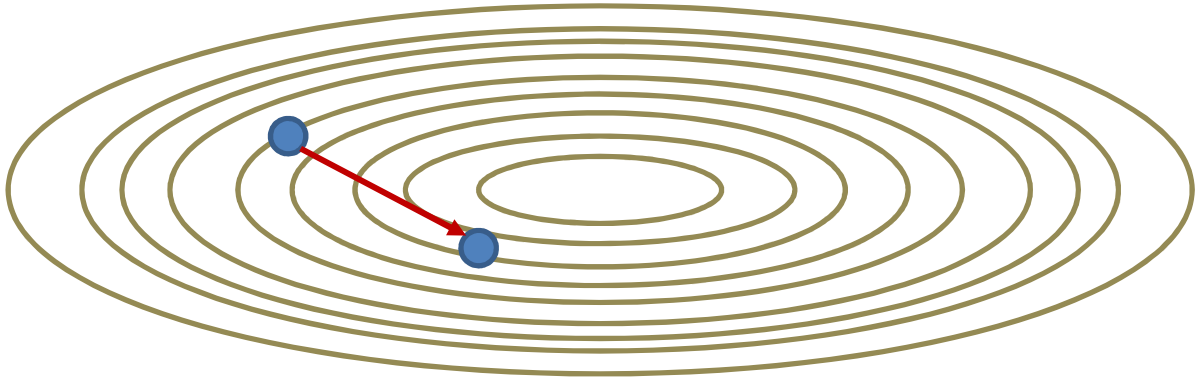
- At any iteration, to compute the current step:
  - First computes the gradient step at the current location
  - Then adds in the scaled *previous* step
    - Which is actually a running average
  - To get the final step

Momentum update

- Takes a step along the past running average *after* walking along the gradient

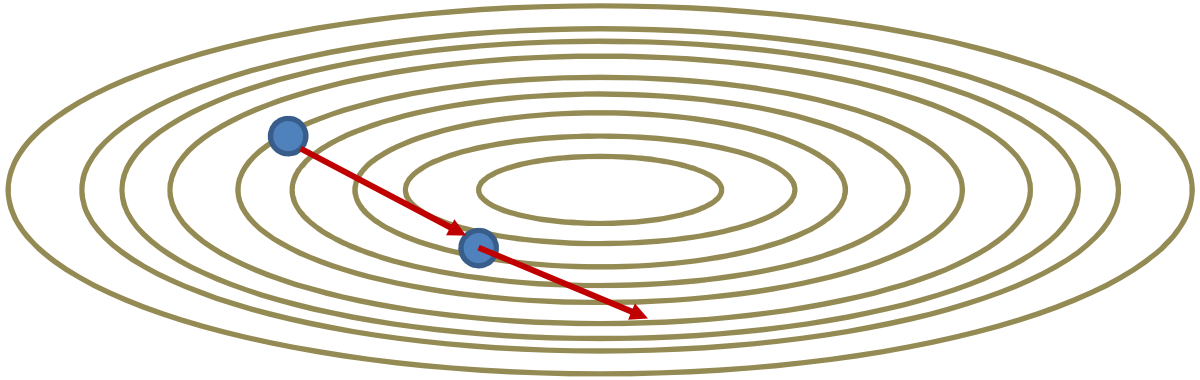
- The procedure can be made more optimal by reversing the order of operations..

Nestorov's Accelerated Gradient



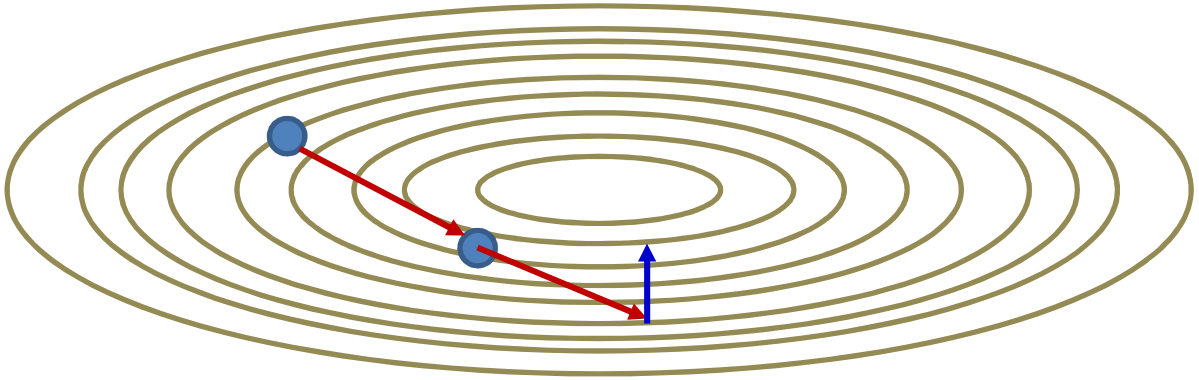
- Change the order of operations
- At any iteration, to compute the current step:

Nestorov's Accelerated Gradient



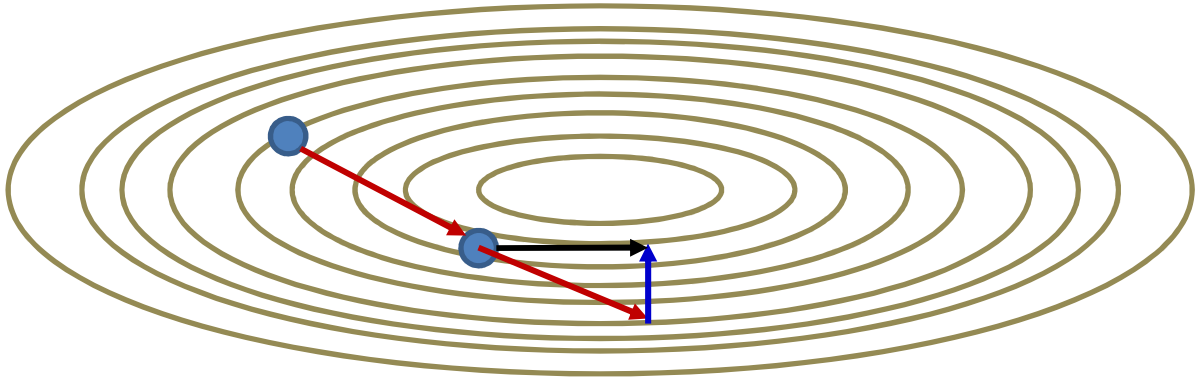
- Change the order of operations
- At any iteration, to compute the current step:
  - First extend the previous step

Nestorov's Accelerated Gradient



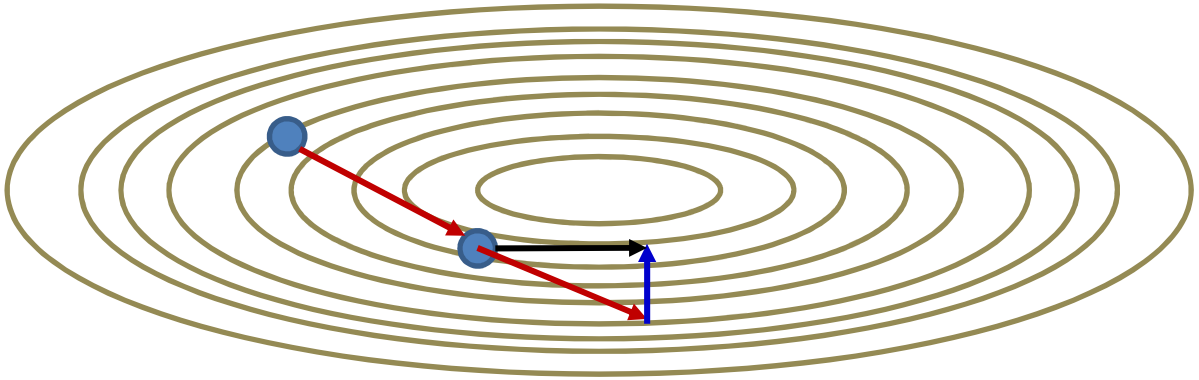
- Change the order of operations
- At any iteration, to compute the current step:
  - First extend the previous step
  - Then compute the gradient step at the resultant position

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

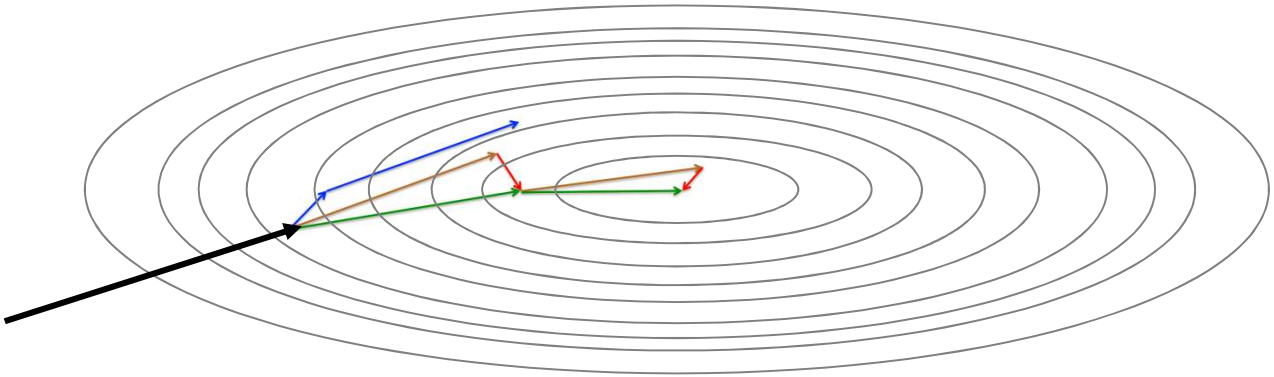


- Nestorov's method

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

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

Nestorov's Accelerated Gradient



- Comparison with momentum (example from Hinton)
- Converges much faster

Training with Nestorov

- Initialize all weights $\mathbf{W}_1, \mathbf{W}_2, \ldots, \mathbf{W}_K$
- Do:
  - For all layers k, initialize $\nabla_{W_k} Loss = 0$, $\Delta W_k = 0$
  - For every layer k

$$W_k = W_k + \beta \Delta W_k$$

  - For all $t = 1{:}T$
    - For every layer k:
      - Compute gradient $\nabla_{W_k} \boldsymbol{Div}(Y_t, d_t)$
      - $\nabla_{W_k} Loss \mathrel{+}= \frac{1}{T} \nabla_{W_k} \boldsymbol{Div}(Y_t, d_t)$
  - For every layer k

$$W_k = W_k - \eta (\nabla_{W_k} Loss)^T$$
$$\Delta W_k = \beta \Delta W_k - \eta (\nabla_{W_k} Loss)^T$$

- Until $Loss$ has converged

Momentum and trend-based methods..

- We will return to this topic again, very soon..

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
- 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