Neural Networks: Optimization Part 1

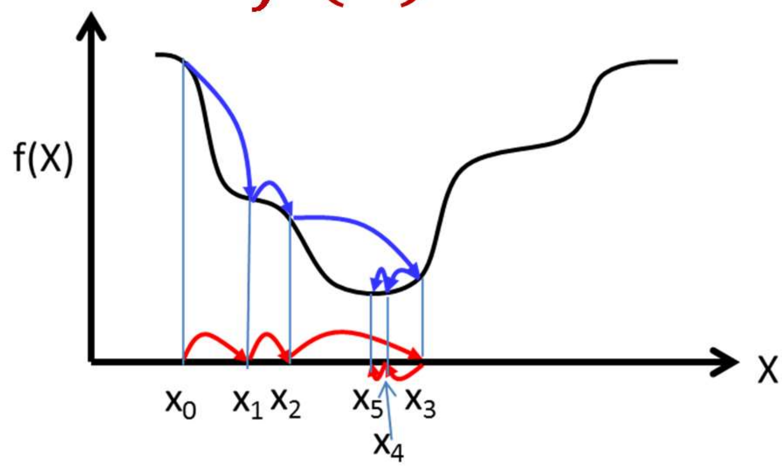
Intro to Deep Learning, Spring 2024

Story so far

- 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 $\left|f(x^k) - f(x^{k-1})\right| > \varepsilon$

Recap: Training Neural Nets by Gradient Descent

Total training error:

$$Loss = \frac{1}{T}\sum_t Div(\boldsymbol{Y}_t, \boldsymbol{d}_t; \mathbf{W}_1, \mathbf{W}_2, \ldots, \mathbf{W}_K)$$

- Gradient descent algorithm:
- Initialize all weights $\mathbf{W}_1, \mathbf{W}_2, \ldots, \mathbf{W}_K$
- Do:
  - For every layer k, compute:
    - $\nabla_{\mathbf{W}_k} Loss = \frac{1}{T}\sum_t \nabla_{\mathbf{W}_k} Div(\boldsymbol{Y}_t, \boldsymbol{d}_t)$
    - $\mathbf{W}_k = \mathbf{W}_k - \eta \nabla_{\mathbf{W}_k} Loss^T$
- Until $Loss$ has converged

Computed using backprop

Neural network training algorithm

- Initialize all weights and biases $(\mathbf{W}_1, \mathbf{b}_1, \mathbf{W}_2, \mathbf{b}_2, \dots, \mathbf{W}_N, \mathbf{b}_N)$
- Do:
  - $Loss = 0$
  - For all k, initialize $\nabla_{\mathbf{W}_k} Loss = 0$, $\nabla_{\mathbf{b}_k} Loss = 0$
  - For all $t = 1:T$ # Loop through training instances
    - Forward pass : Compute
      - Output $\boldsymbol{Y}(\boldsymbol{X}_t)$,
      - Divergence $\boldsymbol{Div}(\boldsymbol{Y}_t, \boldsymbol{d}_t)$
    - Backward pass: For all k compute:
      - $\nabla_{\mathbf{W}_k} \boldsymbol{Div}(\boldsymbol{Y}_t, \boldsymbol{d}_t)$, $\nabla_{\mathbf{b}_k} \boldsymbol{Div}(\boldsymbol{Y}_t, \boldsymbol{d}_t)$
      - $\nabla_{\mathbf{W}_k} Loss \mathrel{+}= \nabla_{\mathbf{W}_k} \boldsymbol{Div}(\boldsymbol{Y}_t, \boldsymbol{d}_t)$; $\nabla_{\mathbf{b}_k} Loss \mathrel{+}= \nabla_{\mathbf{b}_k} \boldsymbol{Div}(\boldsymbol{Y}_t, \boldsymbol{d}_t)$

    Computing gradient (uses backprop)
  - For all k, update:

$$\mathbf{W}_k = \mathbf{W}_k - \frac{\eta}{T}\left(\nabla_{\mathbf{W}_k} Loss\right)^T; \qquad \mathbf{b}_k = \mathbf{b}_k - \frac{\eta}{T}\left(\nabla_{\mathbf{W}_k} Loss\right)^T$$

Gradient descent

- 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.*.

Poll 0 (@380)

Backpropagating from the kth layer, which is the derivative for the weights W_k?

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

Poll 0

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Onward

Onward

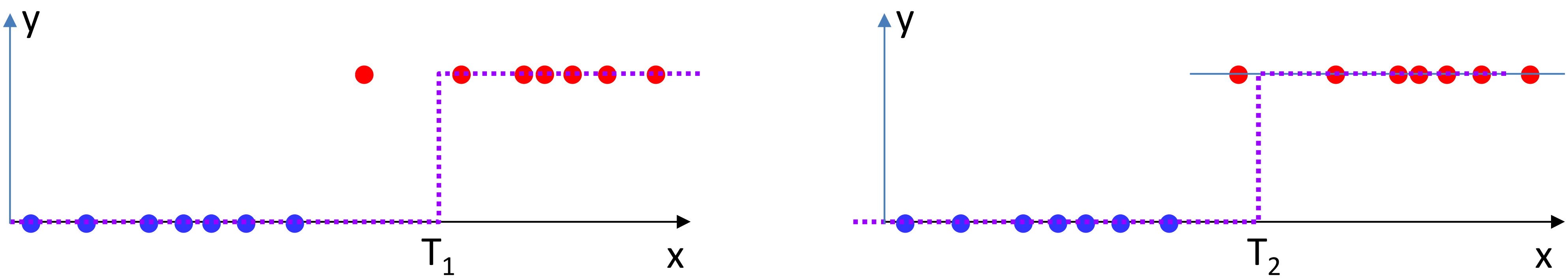
- Does backprop always work?
- Convergence of gradient descent
  - Rates, restrictions,
  - Hessians
  - Acceleration and Nestorov
  - Alternate approaches
- Modifying the approach: Stochastic gradients
- Speedup extensions: RMSprop, Adagrad

Does backprop do the right thing?

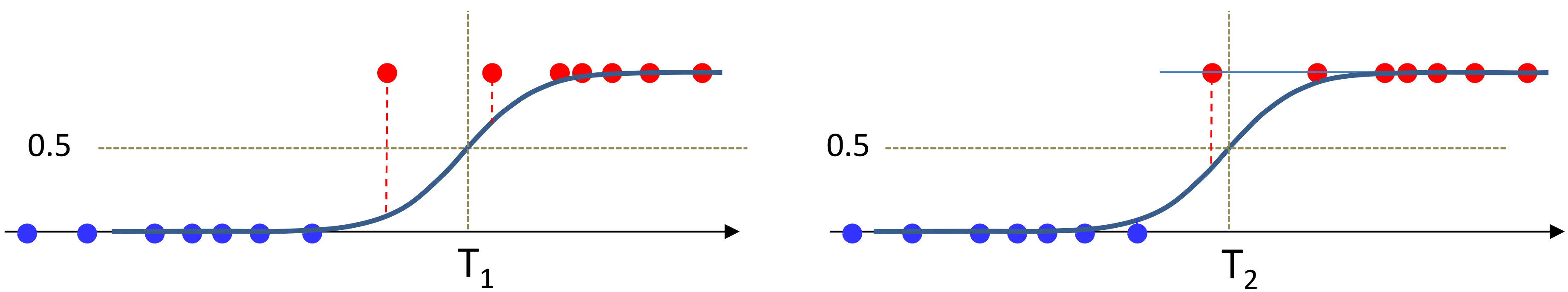
- **Is backprop always right?**
  - Assuming it actually finds the minimum of the divergence function?

(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



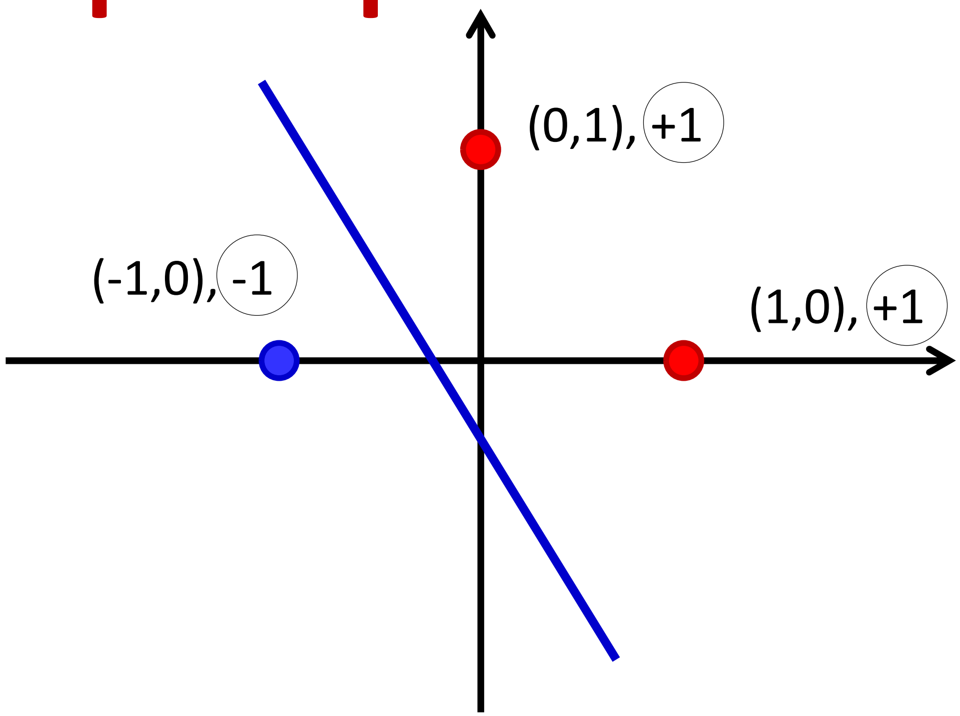
- Differentiable activation: Computes "distance to answer"
  - "Distance" == divergence
  - Perturbing the function changes this quantity,
    - Even if the classification error itself doesn't change

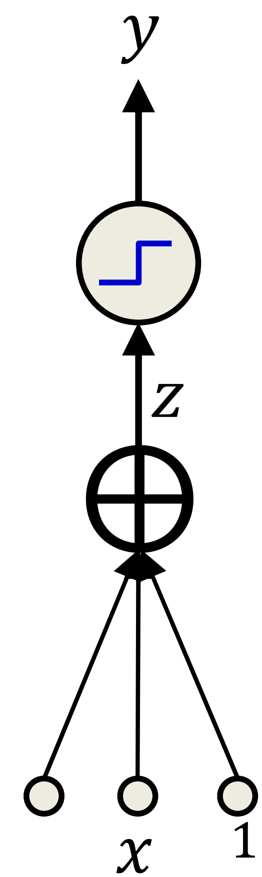
Does backprop do the right thing?

- **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

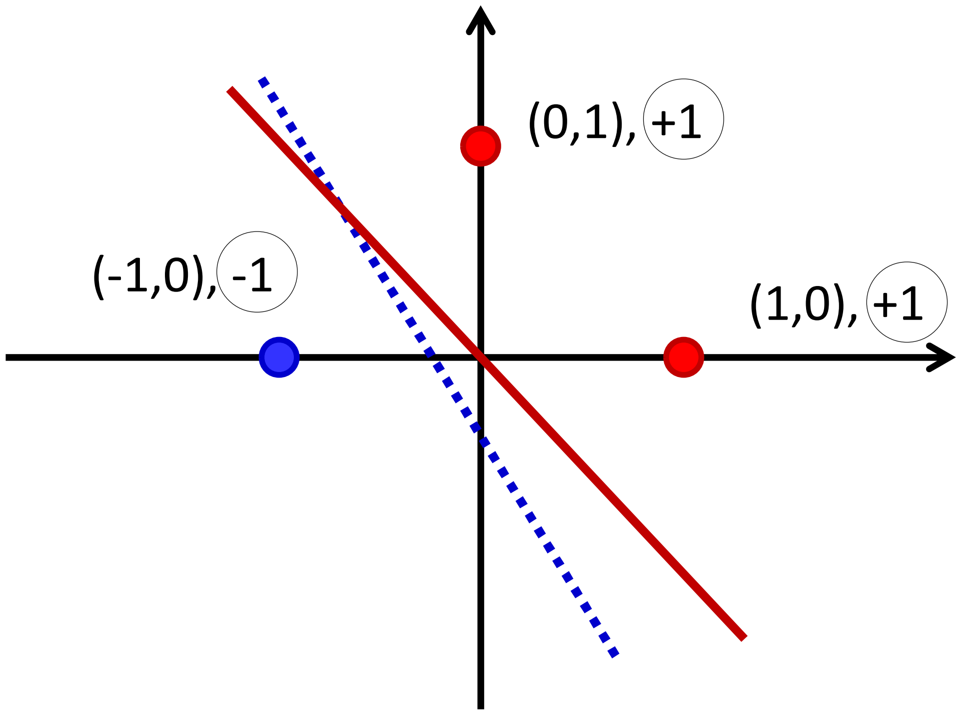
Backprop fails to separate where perceptron succeeds

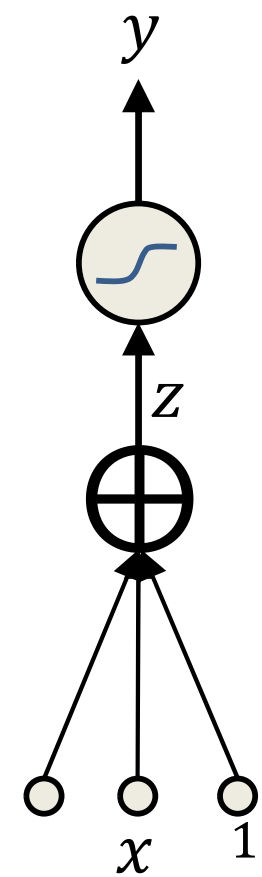




- Brady, Raghavan, Slawny, ’89
- Simple problem, 3 training instances, single neuron
- Perceptron training rule trivially find a perfect solution

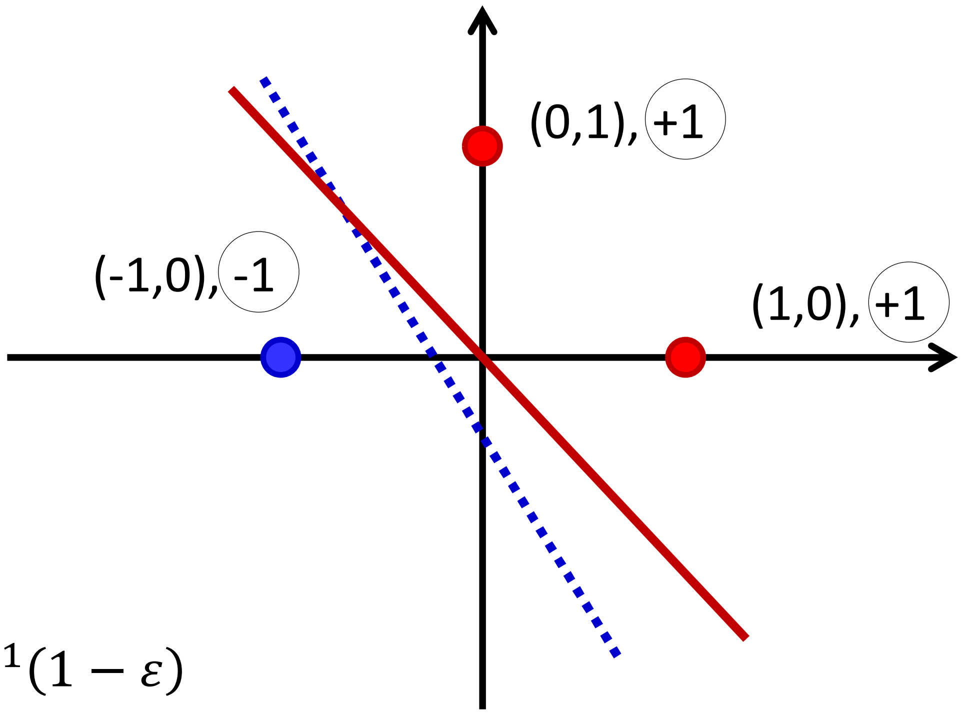
Backprop vs. Perceptron

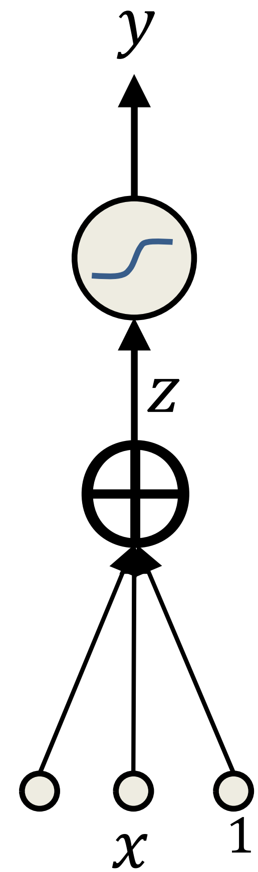




- Back propagation using logistic function and L_2 divergence $(Div = (y - d)^2)$
- Unique minimum trivially proved to exist, backprop finds it

Unique solution exists



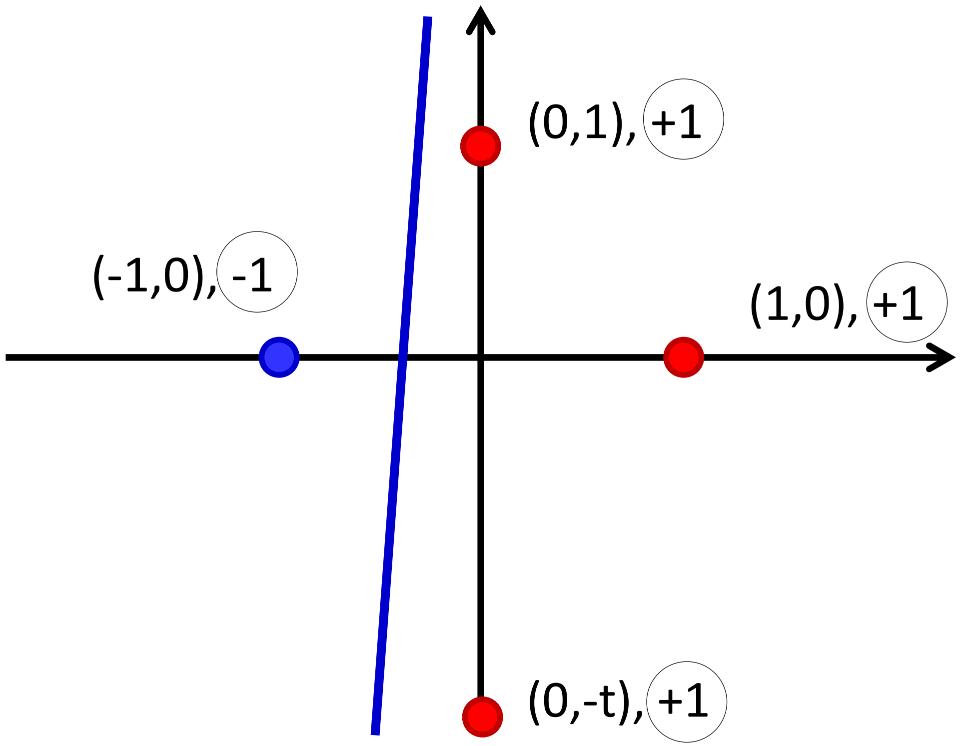


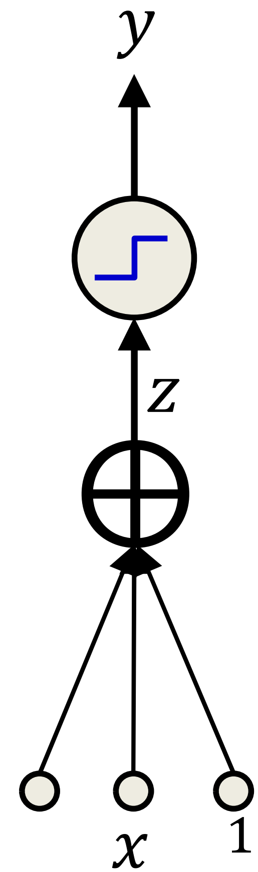
- Let $u = f^{-1}(1-\varepsilon)$
  - E.g. $u = f^{-1}(0.99)$ representing a 99% confidence in the class
- From the three points we get three independent equations:

$$w_x.1 + w_y.0 + b = u$$
$$w_x.0 + w_y.1 + b = u$$
$$w_x.-1 + w_y.0 + b = -u$$

- Unique solution $(w_x = u, w_x = u, b = 0)$ exists
  - represents a unique line regardless of the value of u

Backprop vs. Perceptron

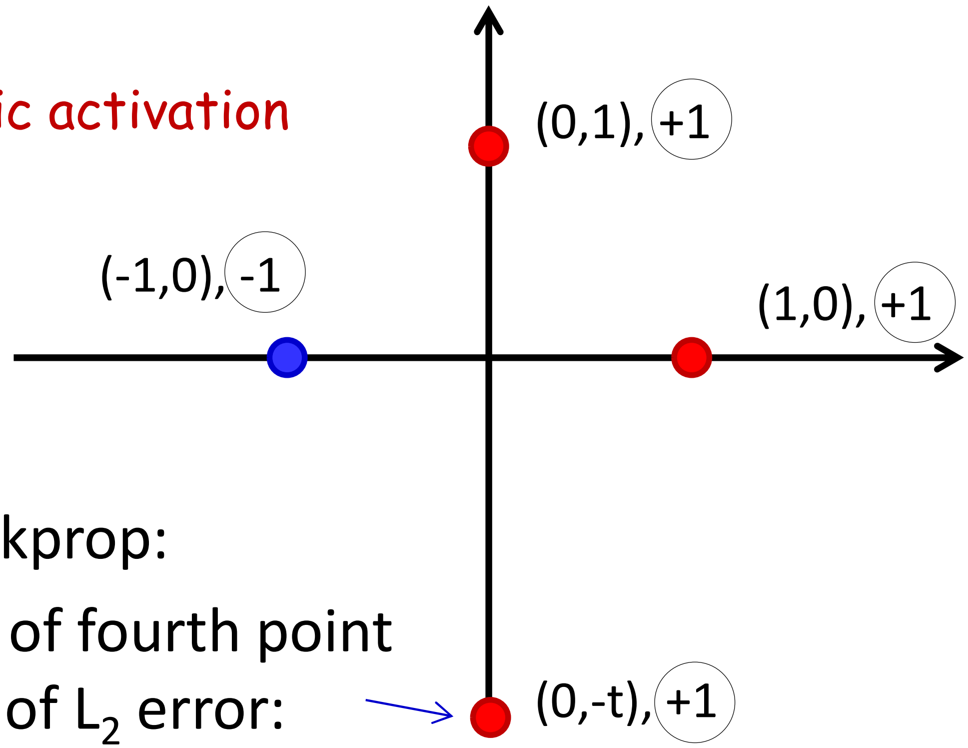


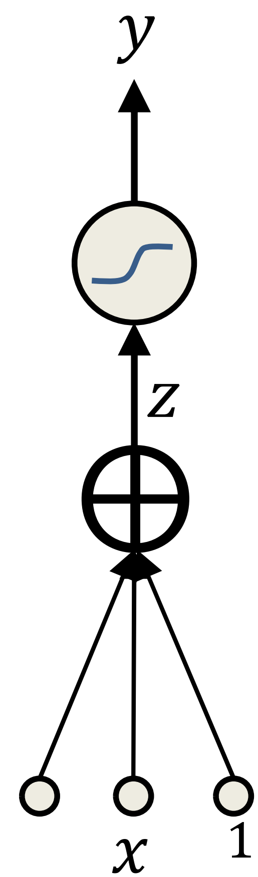


- Now add a fourth point
- t is very large (point near $-\infty$)
- Perceptron trivially finds a solution (may take t^2 iterations)

Backprop

Notation:
$y = \sigma(z)$ = logistic activation





- Consider backprop:
- Contribution of fourth point to derivative of L_2 error:

$$div_4 = \left(1 - \varepsilon - \sigma(-w_y t + b)\right)^2$$

$$\frac{d\ div_4}{dw_y} = 2\left(1 - \varepsilon - \sigma(-w_y t + b)\right)\sigma'(-w_y t + b)t$$

$$\frac{d\ div_4}{db} = -2\left(1 - \varepsilon - \sigma(-w_y t + b)\right)\sigma'(-w_y t + b)$$

1-ε is the actual *achievable value*

Backprop

Notation:
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$$div_4 = \left(1 - \varepsilon - \sigma(-w_y t + b)\right)^2$$

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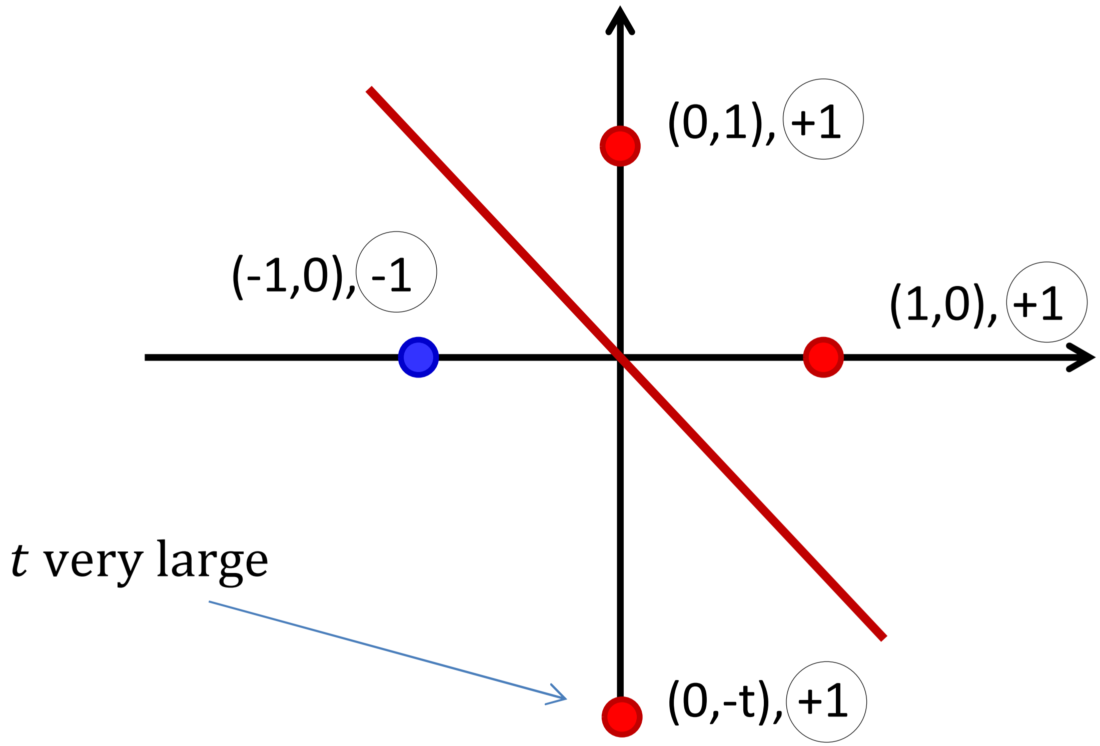
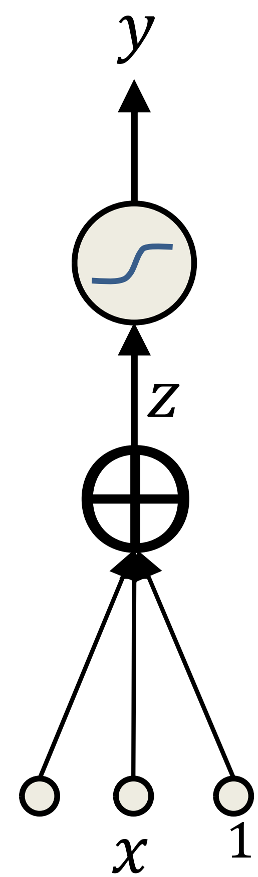
$$\frac{d\,div_4}{db} = 2\left(1 - \sigma(-w_y t + b)\right)\sigma'(-w_y t + b)t$$

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

$$\frac{d\,div_4}{dw_y} = \frac{d\,div_4}{db} = 0$$

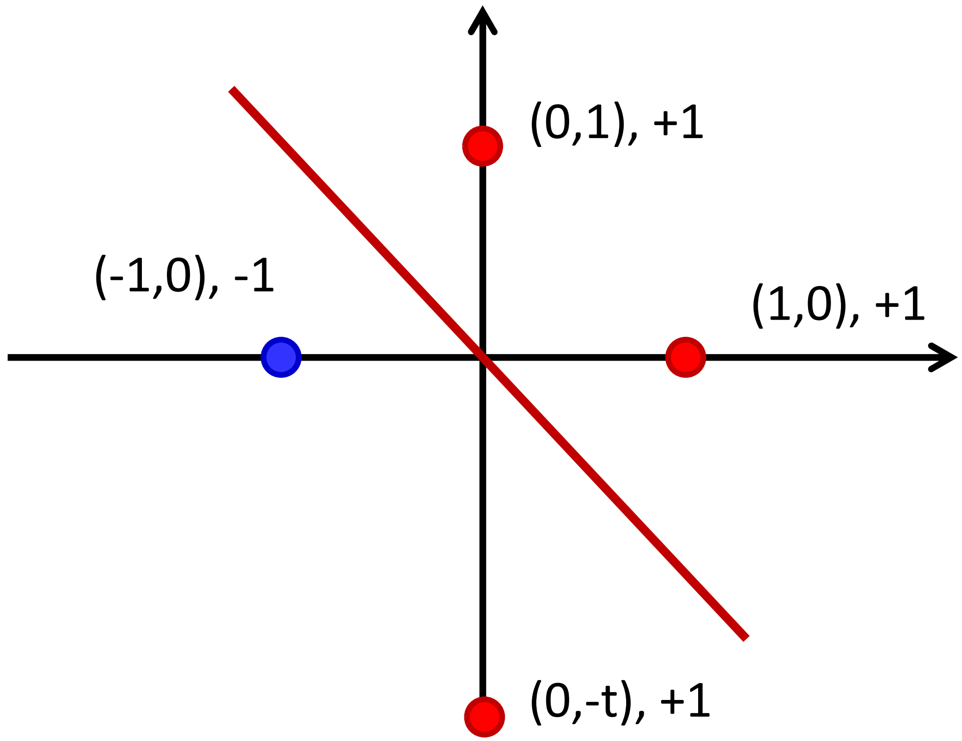
Backprop

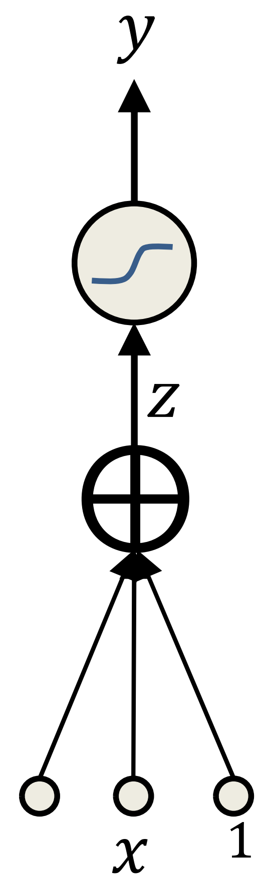




- The fourth point at $(0, -t)$ does not change the gradient of the L_2 divergence near the optimal solution for 3 points
- The optimum solution for 3 points is also a broad *local* minimum (0 gradient) for the 4-point problem!
  - Will be found by backprop nearly all the time
    - Although the global minimum with unbounded weights will separate the classes correctly

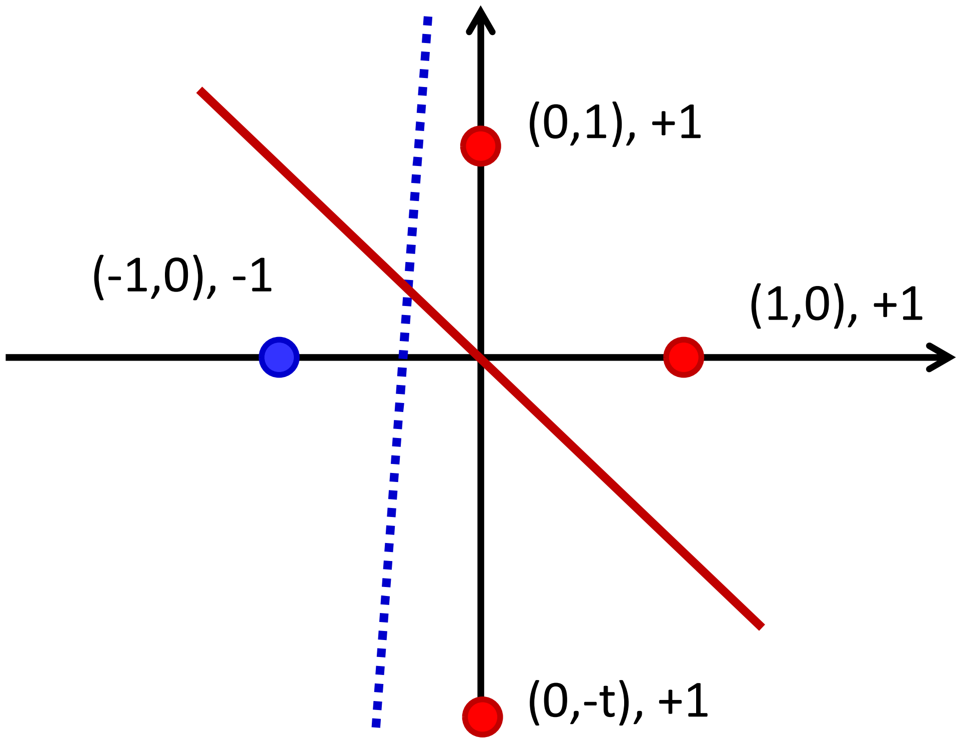
Backprop

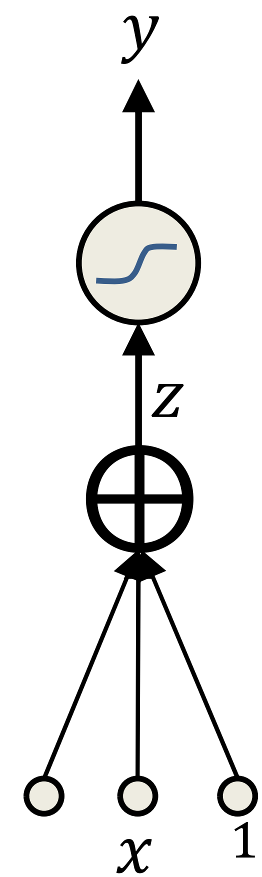




- Local optimum solution found by backprop
- Does not separate the points *even though the points are linearly separable!*

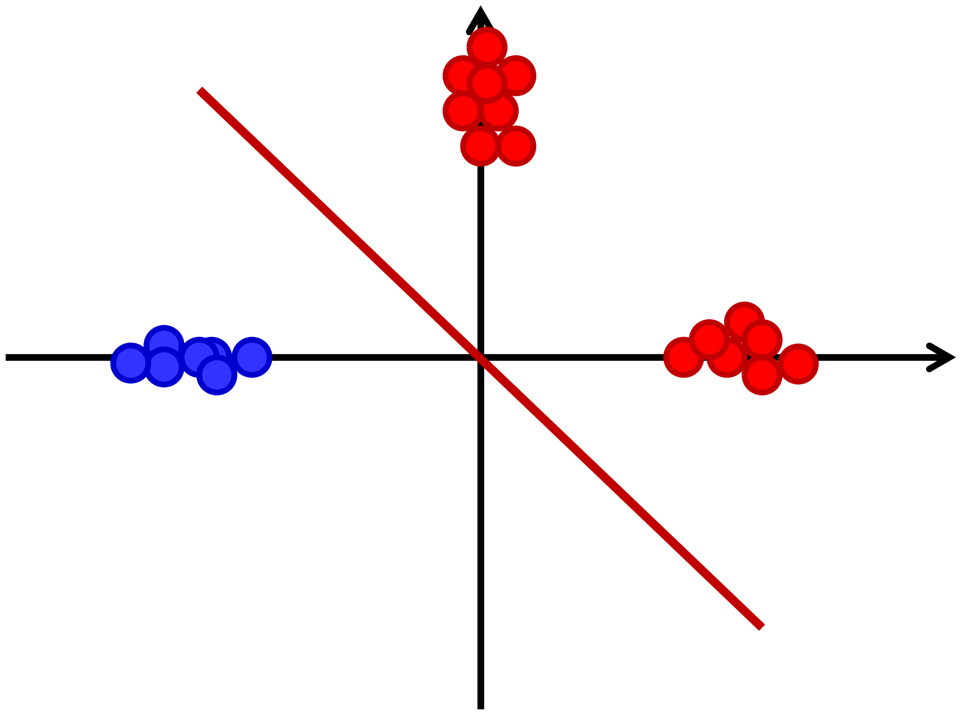
Backprop

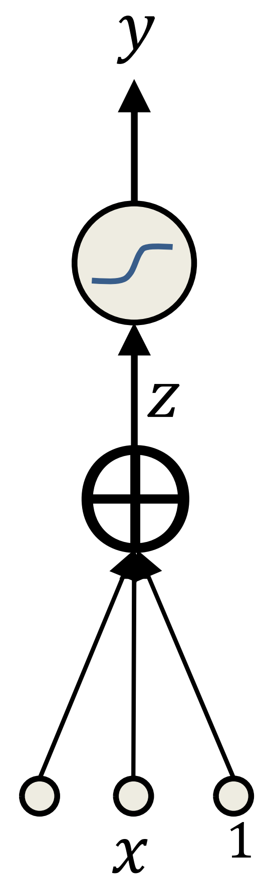




- Solution found by backprop
- Does not separate the points *even though the points are linearly separable!*
- Compare to the perceptron: *Backpropagation fails to separate where the perceptron succeeds*

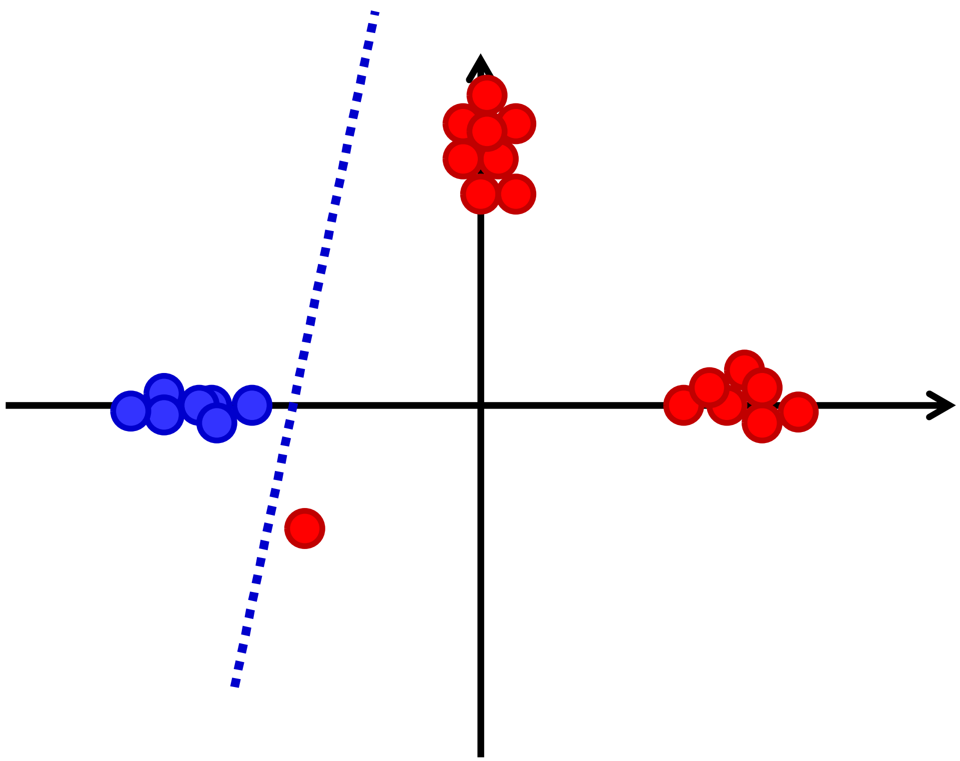
Backprop fails to separate where perceptron succeeds

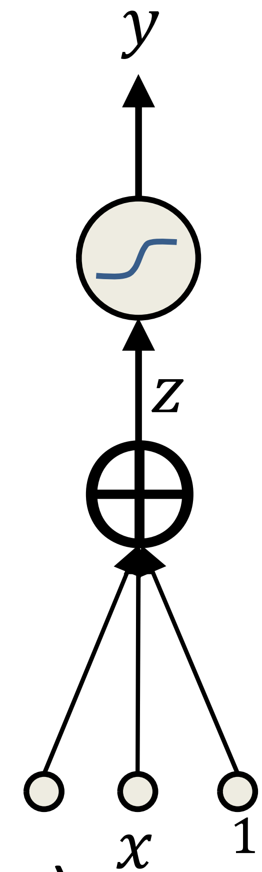




- Brady, Raghavan, Slawny, ’89
- *Several* linearly separable training examples
- Simple setup: **both backprop and perceptron algorithms find solutions**

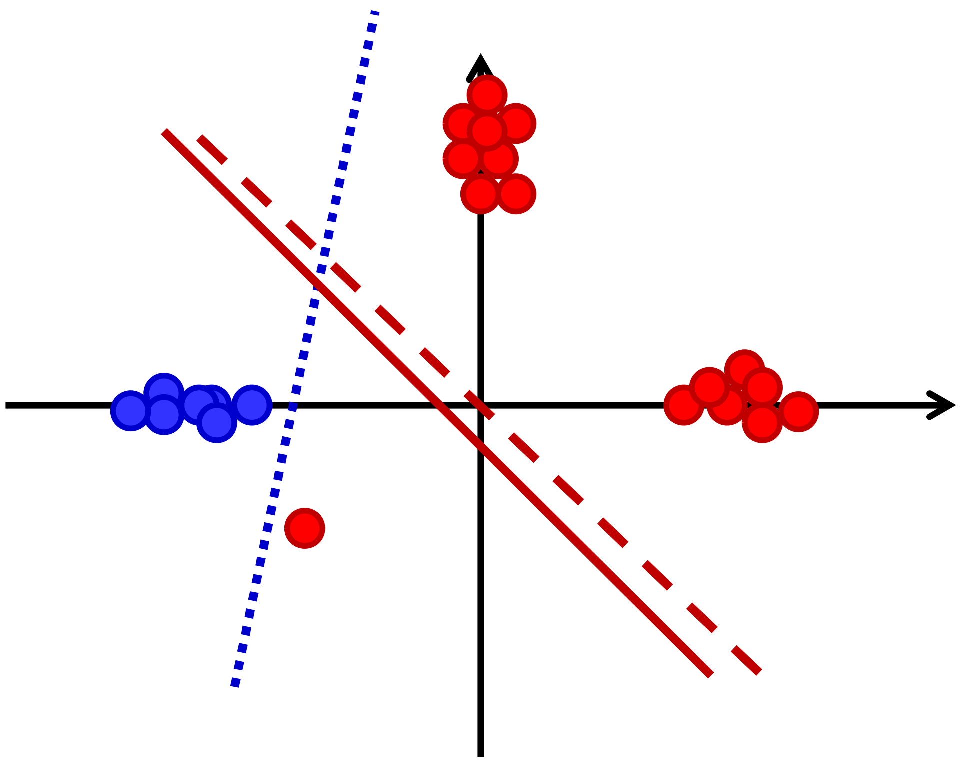
A more complex problem

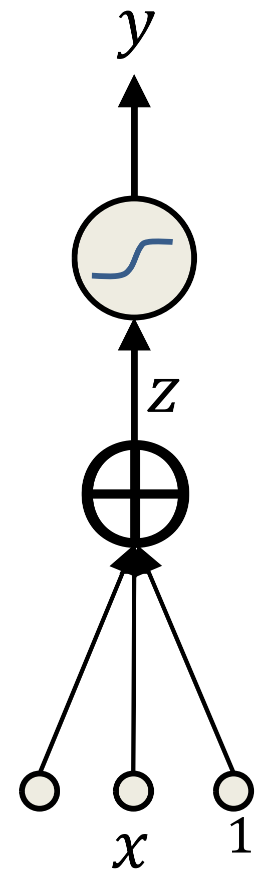




- Adding a "spoiler" (or a small number of spoilers)
  – Perceptron finds the linear separator,

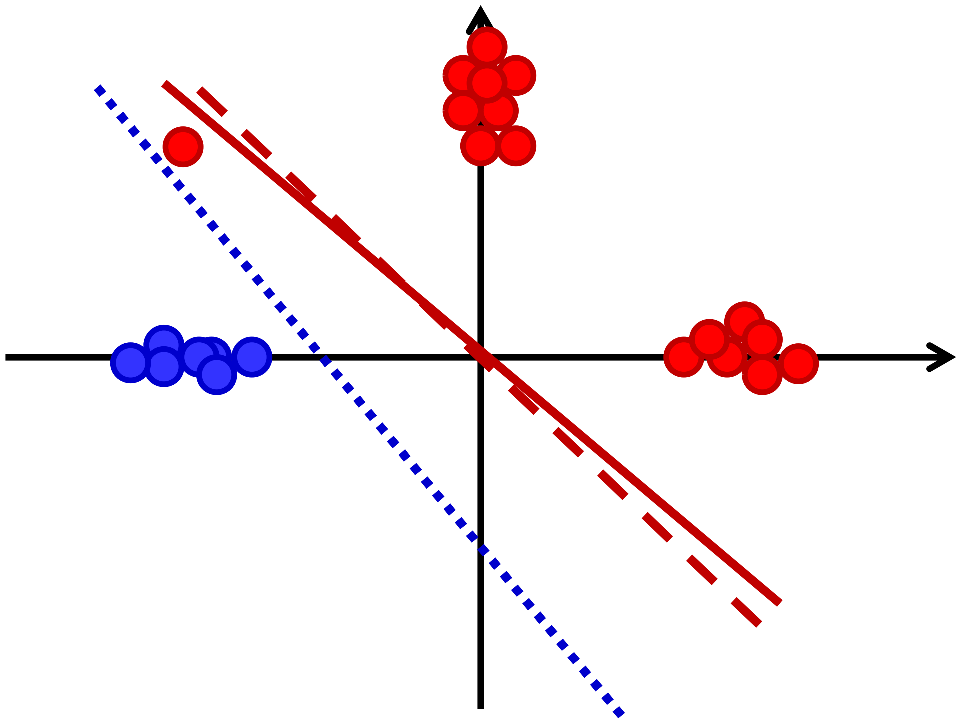
A more complex problem

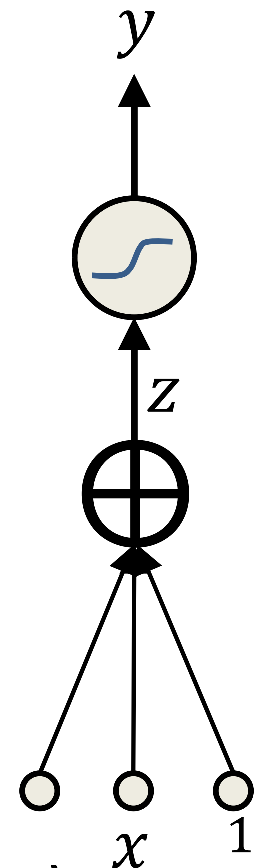




- Adding a "spoiler" (or a small number of spoilers)
  - Perceptron finds the linear separator,
  - Backprop does not find a separator
    - A single additional input does not change the loss function significantly
      - **Assuming weights are constrained to be bounded**

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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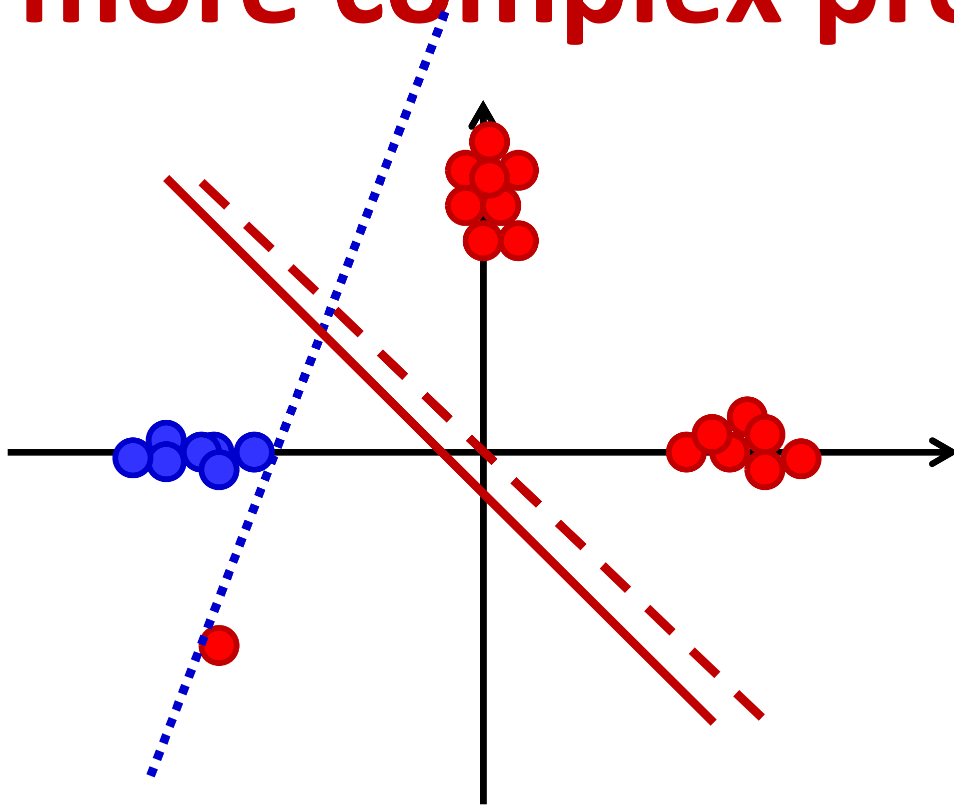
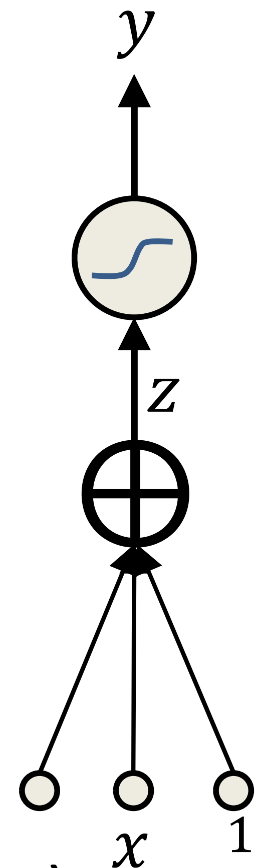
A more complex problem





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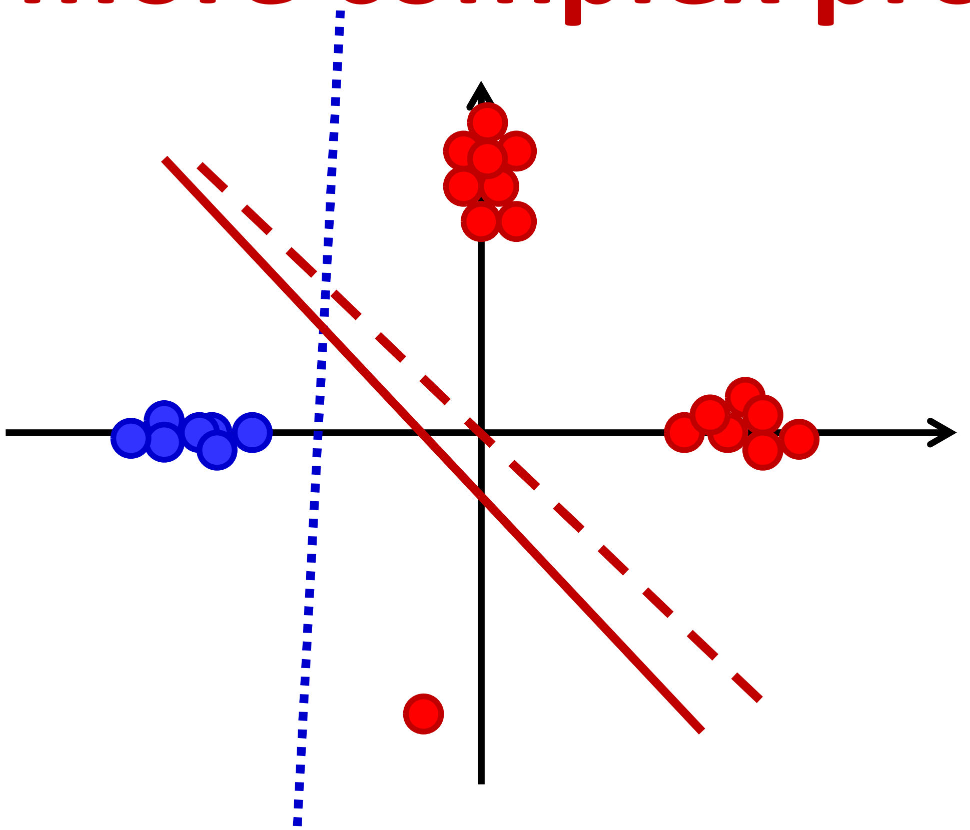

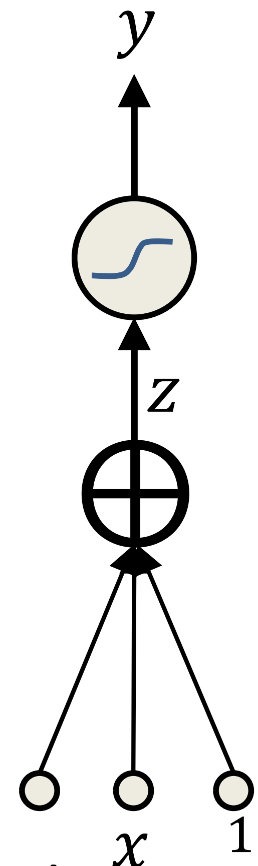

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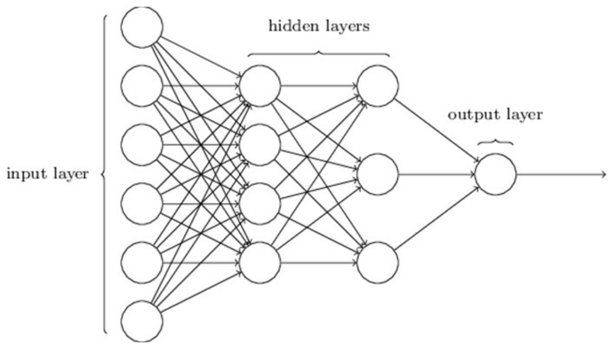
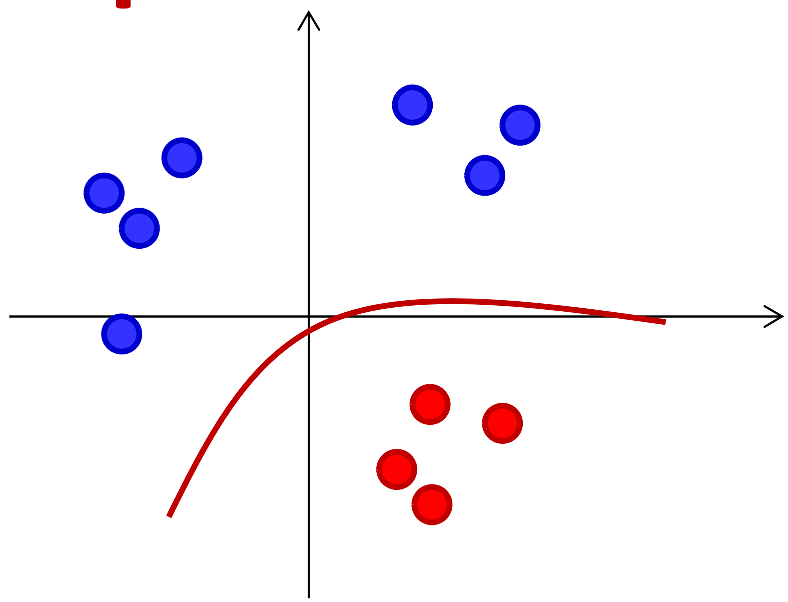
So what is happening here?

- 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

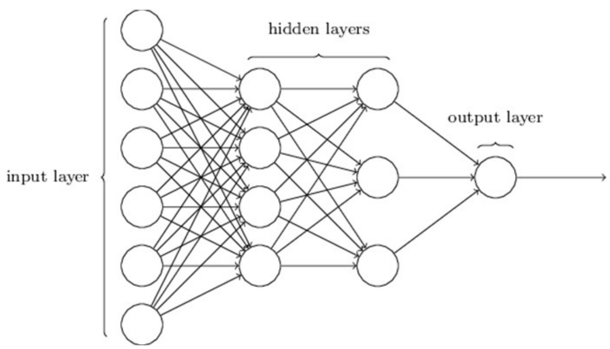
Backprop fails to separate even when possible

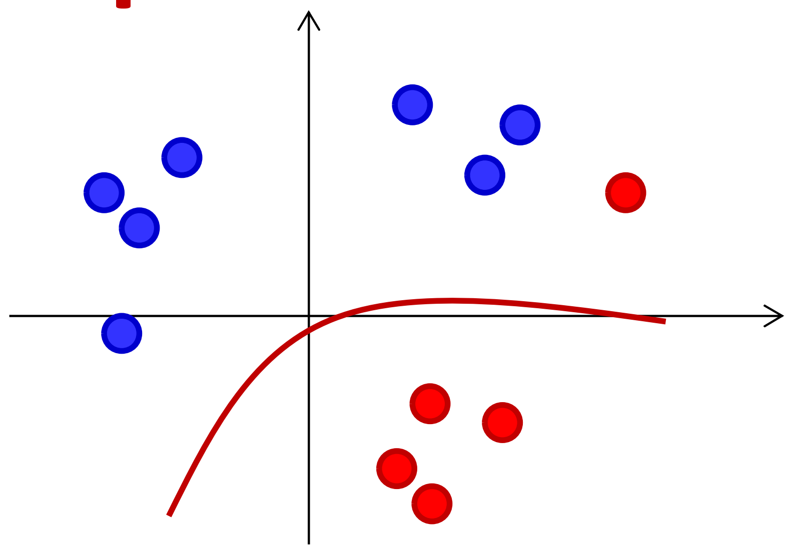




- This is not restricted to single perceptrons
- An MLP learns non-linear decision boundaries that are determined from the entirety of the training data
- Adding a few "spoilers" will not change their behavior

Backprop fails to separate even when possible





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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

Poll (@381)

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

- True
- False

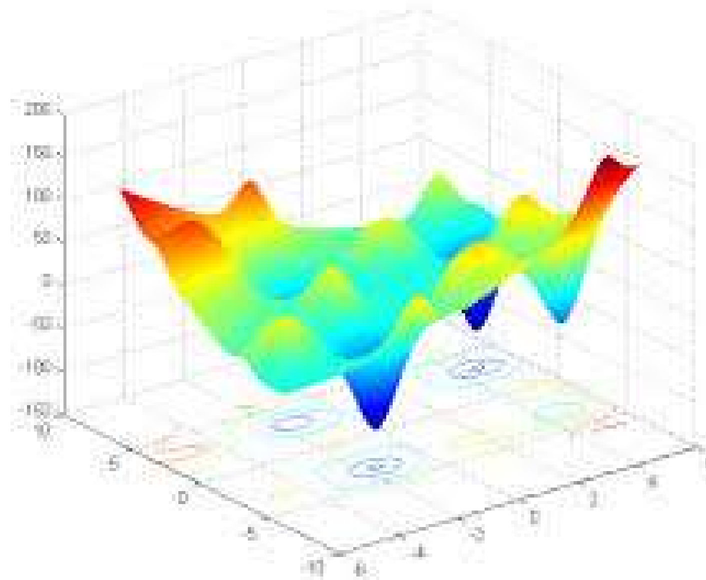
Poll 1

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

- True
- False **(true)**

The Loss Surface

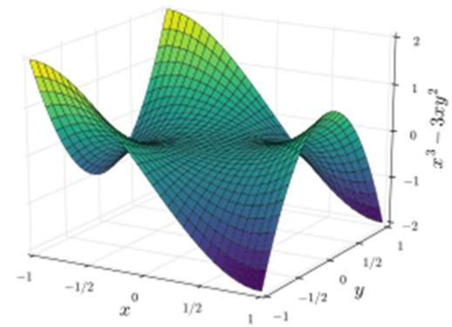
- The example (and statements) earlier assumed the loss objective had a single global optimum that could be found
  - Statement about variance is assuming global optimum

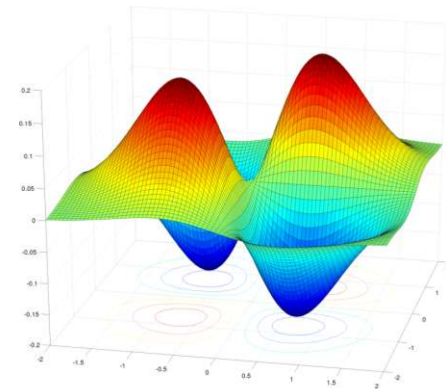


- What about local optima

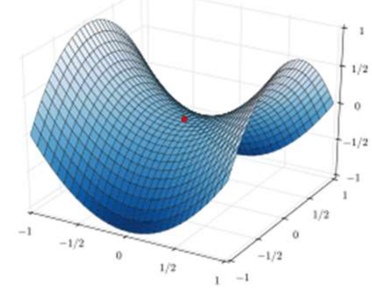
The Loss Surface

- **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

- **Swirscz 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

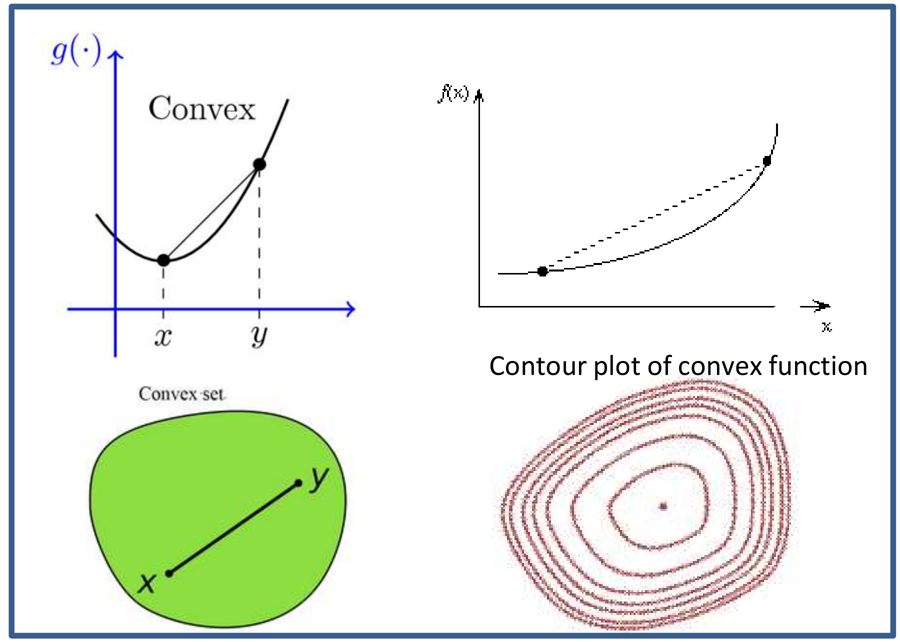
A quick tour of (convex) optimization

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

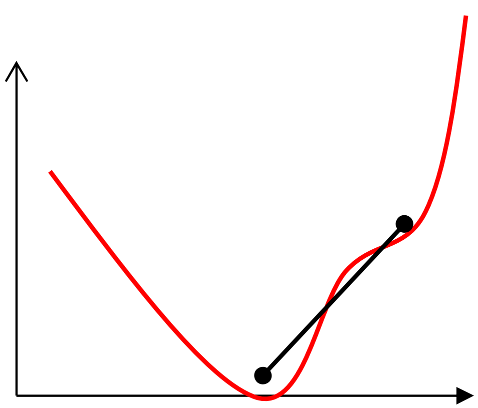
"I'm searching for my keys."

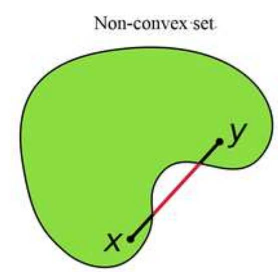
Convex Loss Functions

- 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



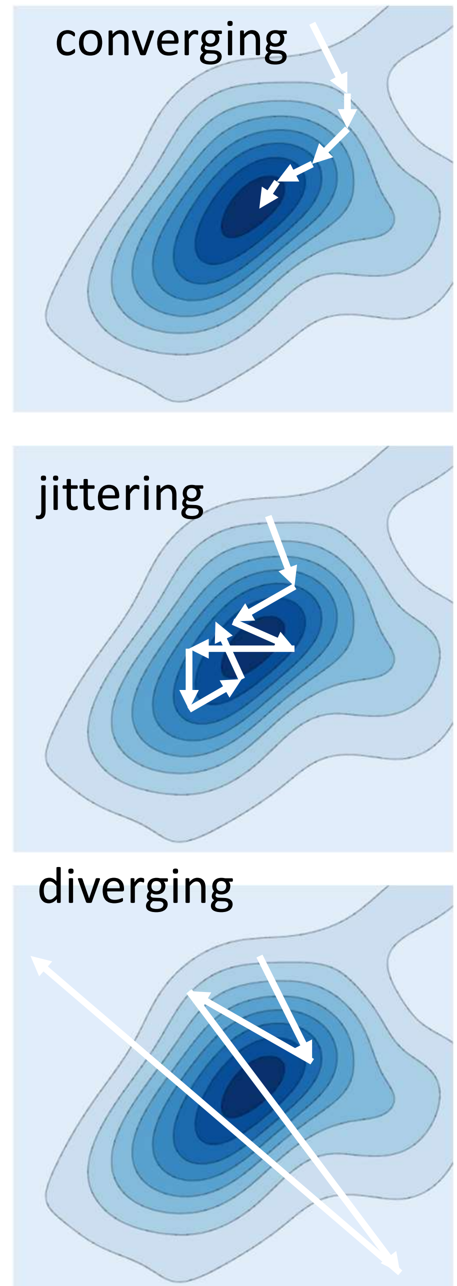


Convergence of gradient descent

- 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?

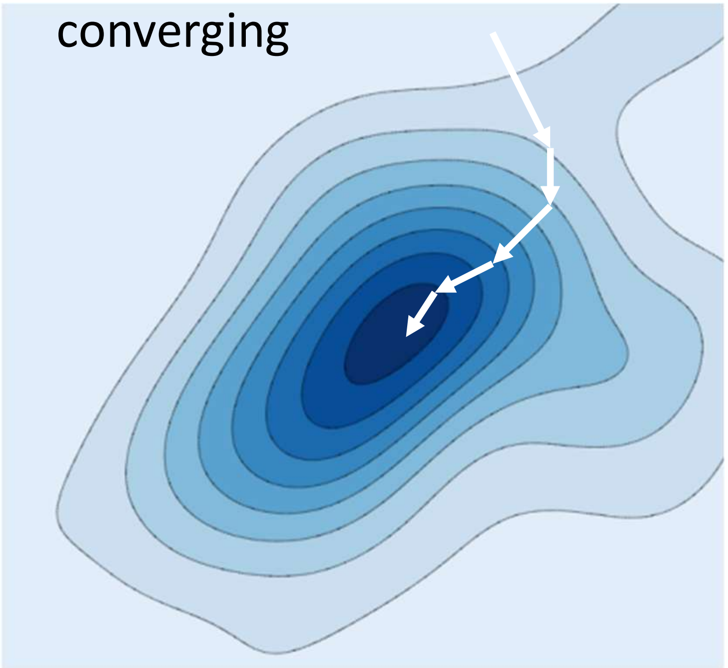


Convergence and convergence rate

- Convergence rate: How fast the iterations arrive at the solution
- Generally quantified as

$$R = \frac{\left|f\left(x^{(k+1)}\right) - f(x^*)\right|}{\left|f\left(x^{(k)}\right) - f(x^*)\right|}$$

  – $x^{(k+1)}$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

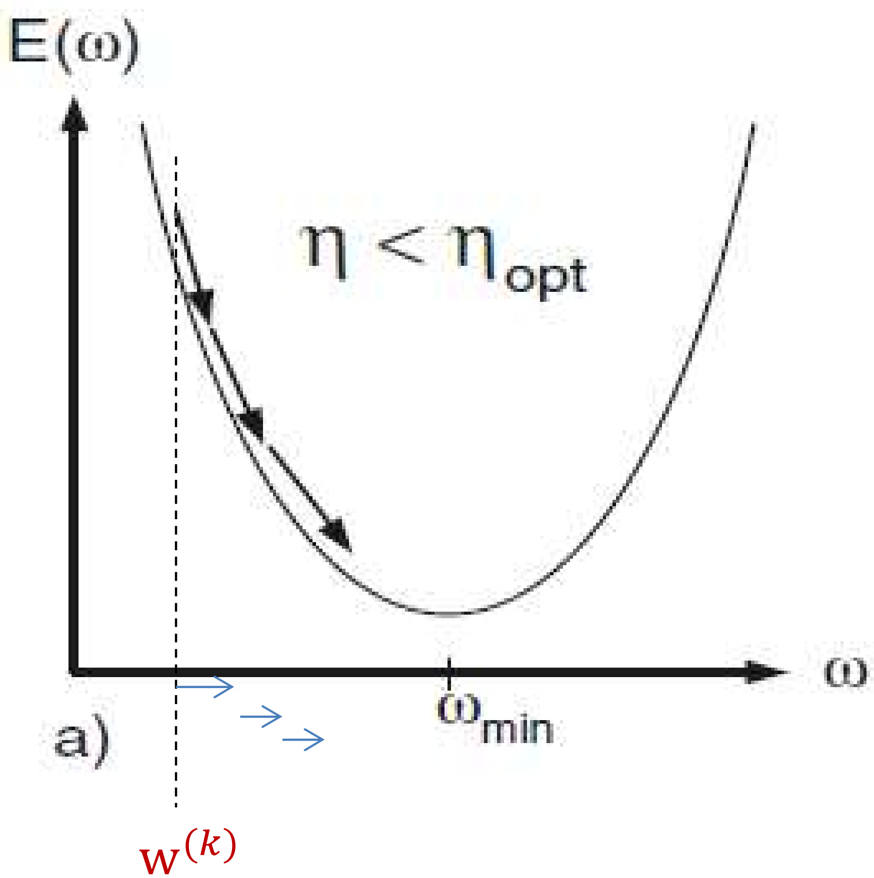
$$\left|f\left(x^{(k)}\right) - f(x^*)\right| \leq R^k \left|f\left(x^{(0)}\right) - f(x^*)\right|$$

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



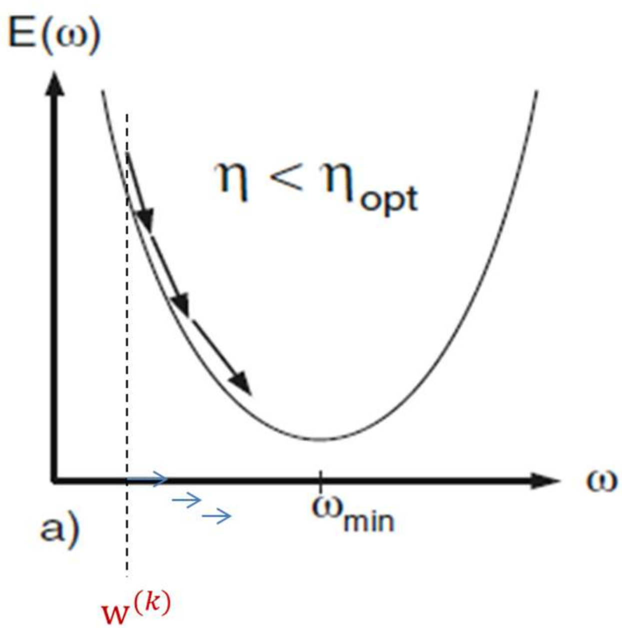
- Gradient descent to find the optimum of a quadratic, starting from $\mathrm{w}^{(k)}$

- Assuming fixed step size η
- What is the optimal step size η to get there fastest?

Convergence for quadratic surfaces

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

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



- Any quadratic objective can be written as

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

  – Taylor expansion

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

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

- Note:

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

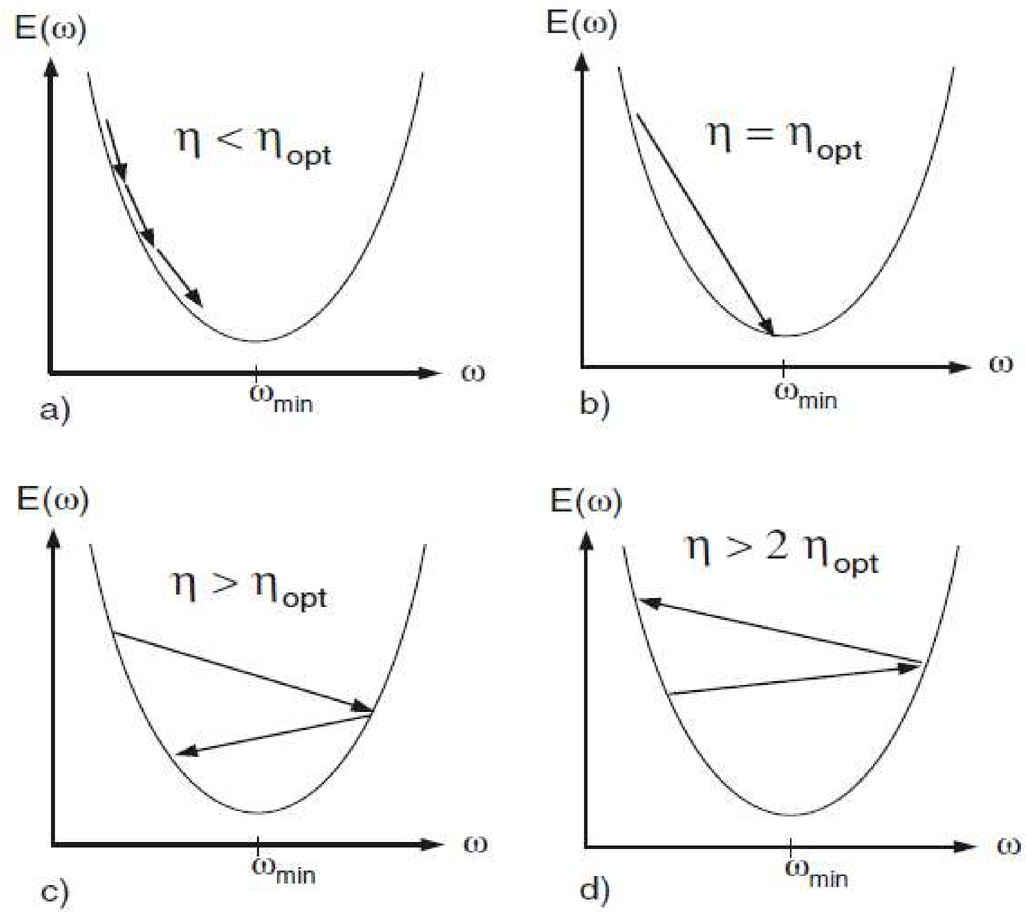
- Comparing to the gradient descent rule, we see that we can arrive at the optimum in a single step using the optimum step size

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

With non-optimal step size

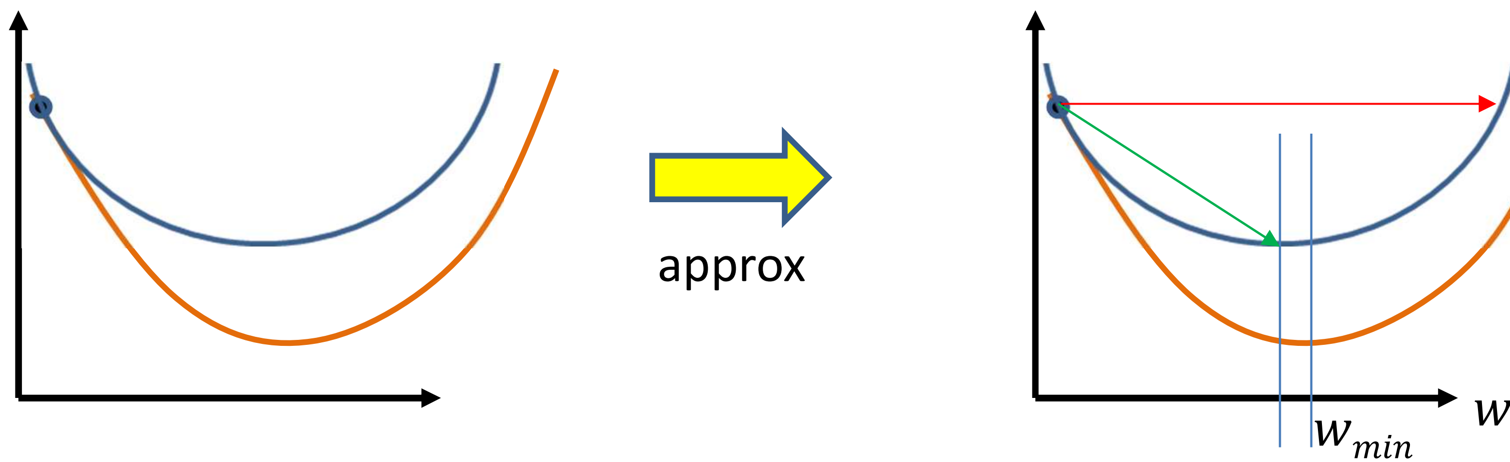
$$w^{(k+1)} = w^{(k)} - \eta \frac{dE\left(w^{(k)}\right)}{dw}$$

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

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

  - Taylor expansion

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

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

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

For functions of *multivariate* inputs

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

- Consider a simple quadratic convex (paraboloid) function

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

  – Since $E^T = E$ (E is scalar), $\mathbf{A}$ can always be made symmetric
    - For strictly **convex** E, $\mathbf{A}$ is always positive definite, and has positive eigenvalues

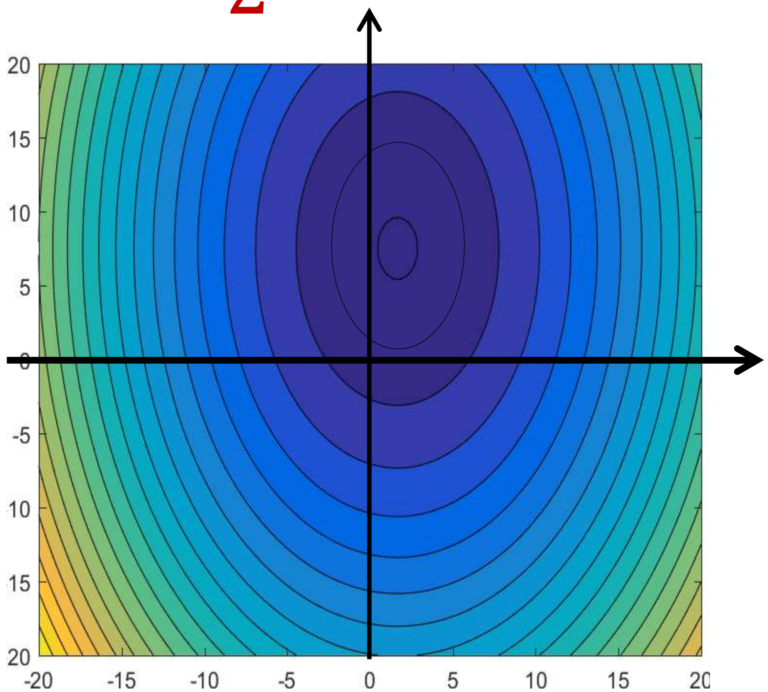
- When $\mathbf{A}$ is diagonal:

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

  – The w_is 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

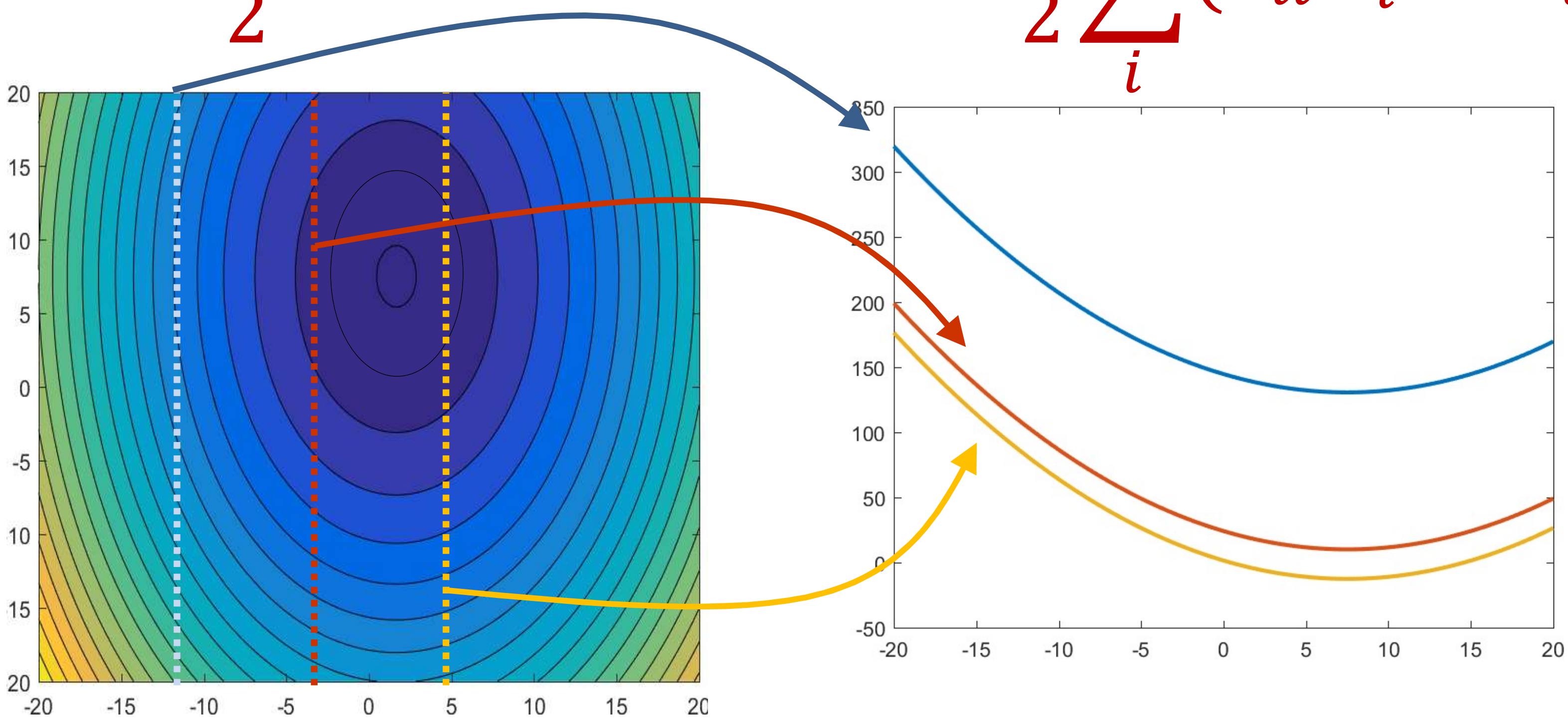
$$E = \frac{1}{2}\mathbf{w}^T\mathbf{A}\mathbf{w} + \mathbf{w}^T\mathbf{b} + c = \frac{1}{2}\sum_i \left(a_{ii}w_i^2 + b_i w_i\right) + c$$



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

Multivariate Quadratic with Diagonal A

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

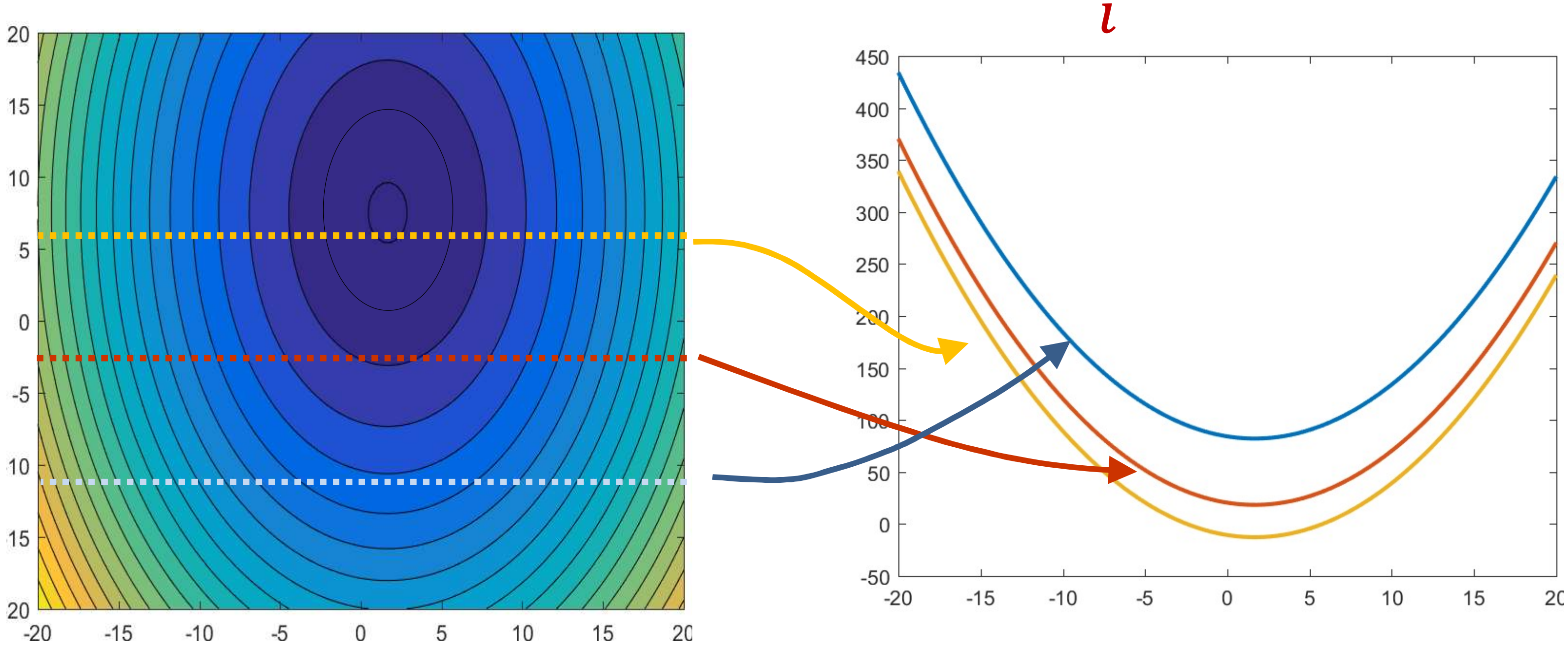


- Equal-value contours will be parallel to the axes
  - All “slices” parallel to an axis are shifted versions of one another

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

Multivariate Quadratic with Diagonal A

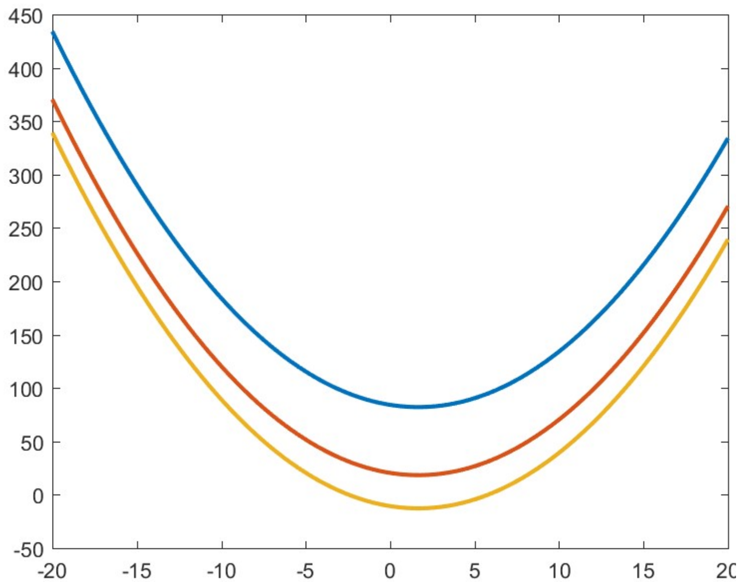
$$E = \frac{1}{2}\mathbf{w}^T\mathbf{A}\mathbf{w} + \mathbf{w}^T\mathbf{b} + c = \frac{1}{2}\sum_i \left(a_{ii}w_i^2 + b_i w_i\right) + c$$

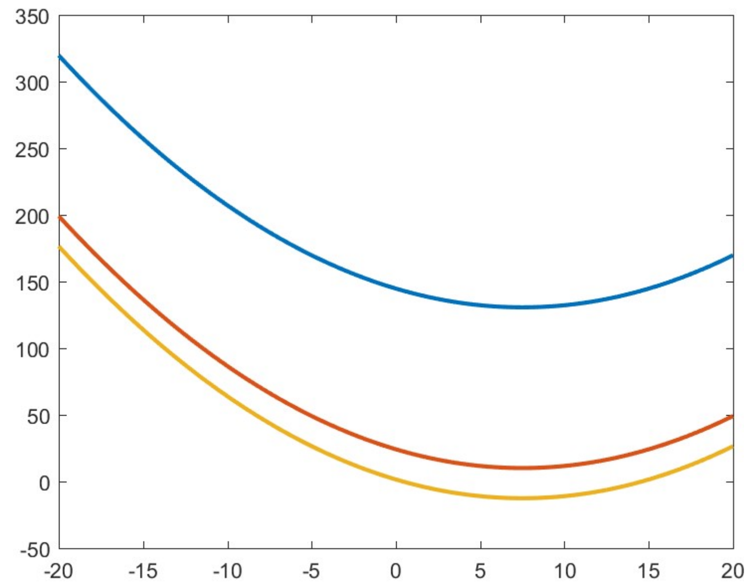


- Equal-value contours will be parallel to the axis
  - All “slices” parallel to an axis are shifted versions of one another

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

“Descents” are uncoupled



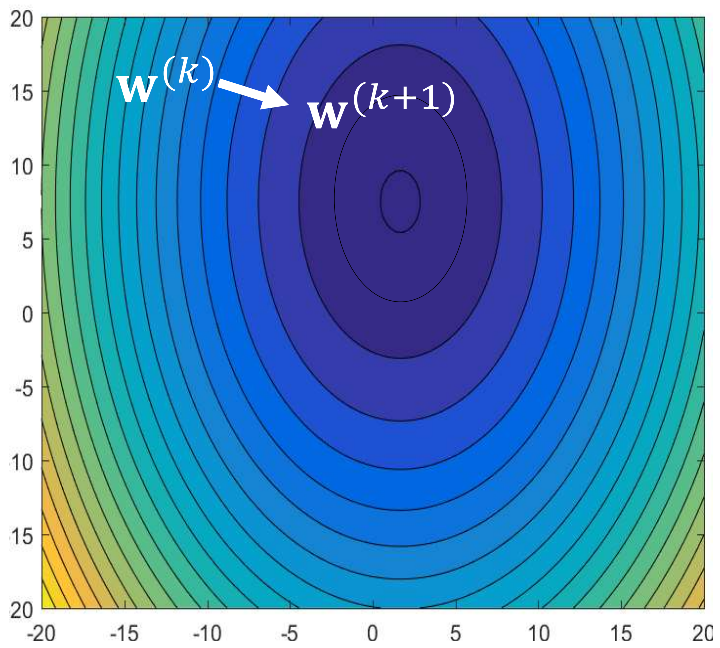


$$E = \frac{1}{2}a_{11}w_1^2 + b_1 w_1 + c + C(\neg w_1) \qquad E = \frac{1}{2}a_{22}w_2^2 + b_2 w_2 + c + C(\neg w_2)$$

$$\eta_{1,opt} = a_{11}^{-1} \qquad \eta_{2,opt} = a_{22}^{-1}$$

- 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



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

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

- 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

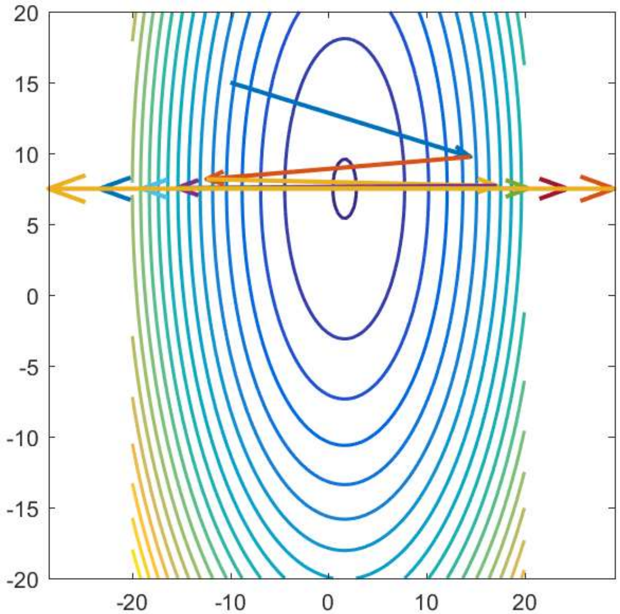
Problem with vector update rule

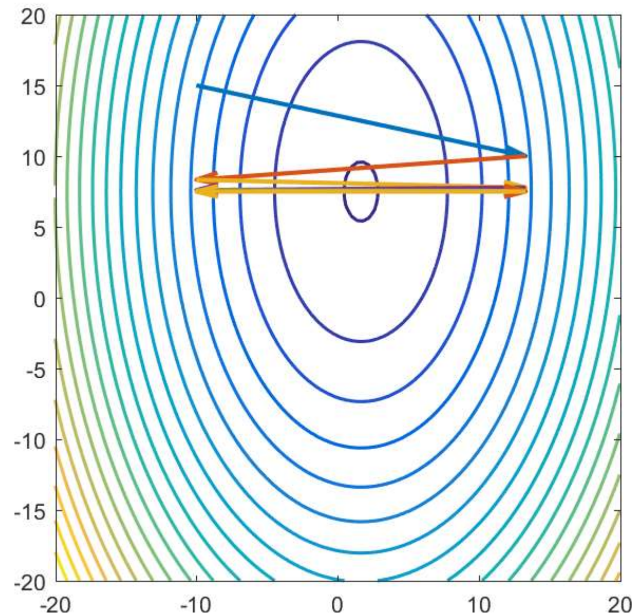
$$\mathbf{w}^{(k+1)} \leftarrow \mathbf{w}^{(k)} - \eta \nabla_{\mathbf{w}} E^T$$

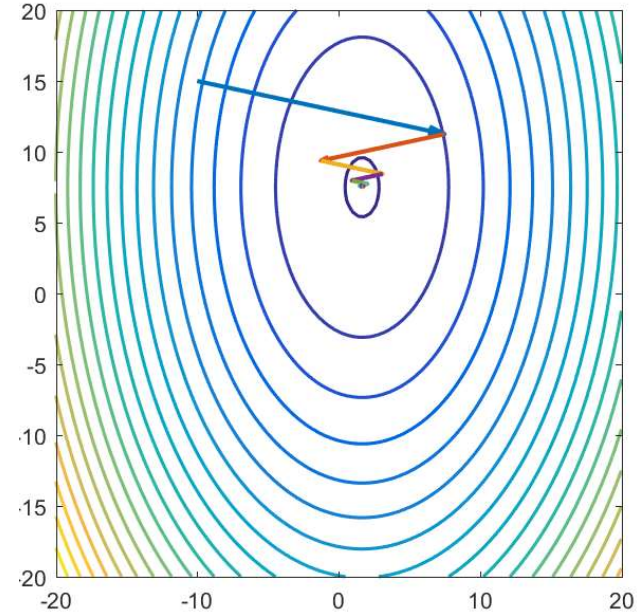
$$w_i^{(k+1)} = w_i^{(k)} - \eta \frac{\partial E\left(w_i^{(k)}\right)}{\partial \mathrm{w}}$$

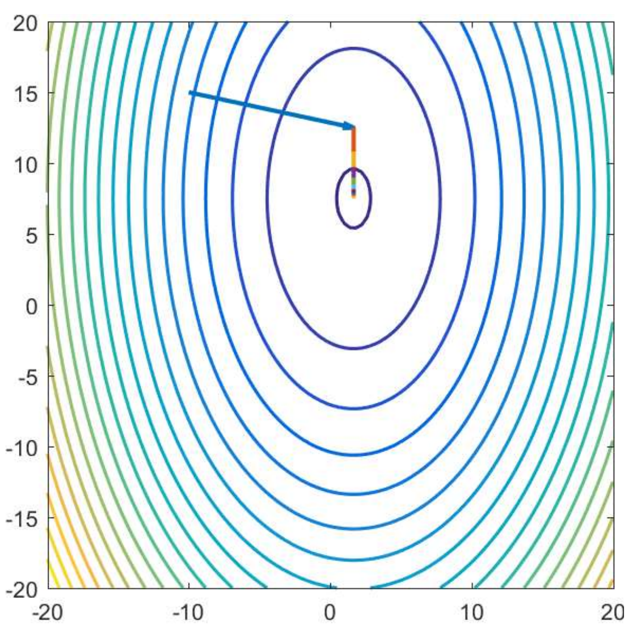
$$\eta_{i,opt} = \left(\frac{\partial^2 E\left(w_i^{(k)}\right)}{\partial w_i^2}\right)^{-1} = a_{ii}^{-1}$$

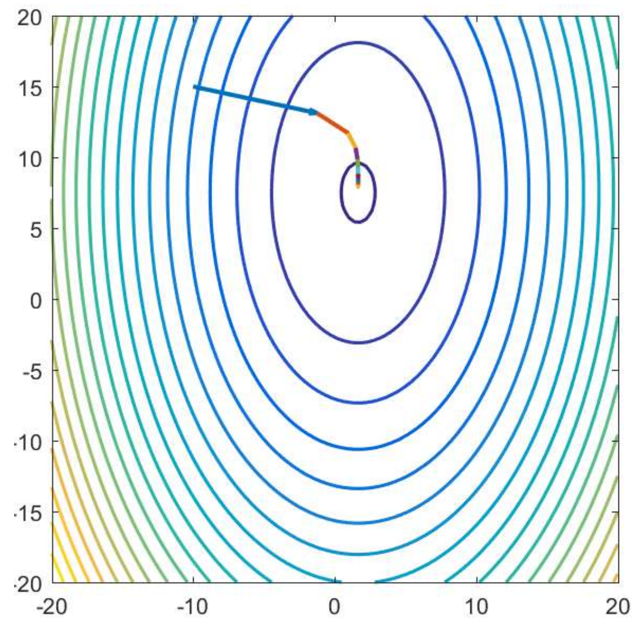
Dependence on learning rate











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

Problem with vector update rule

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

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

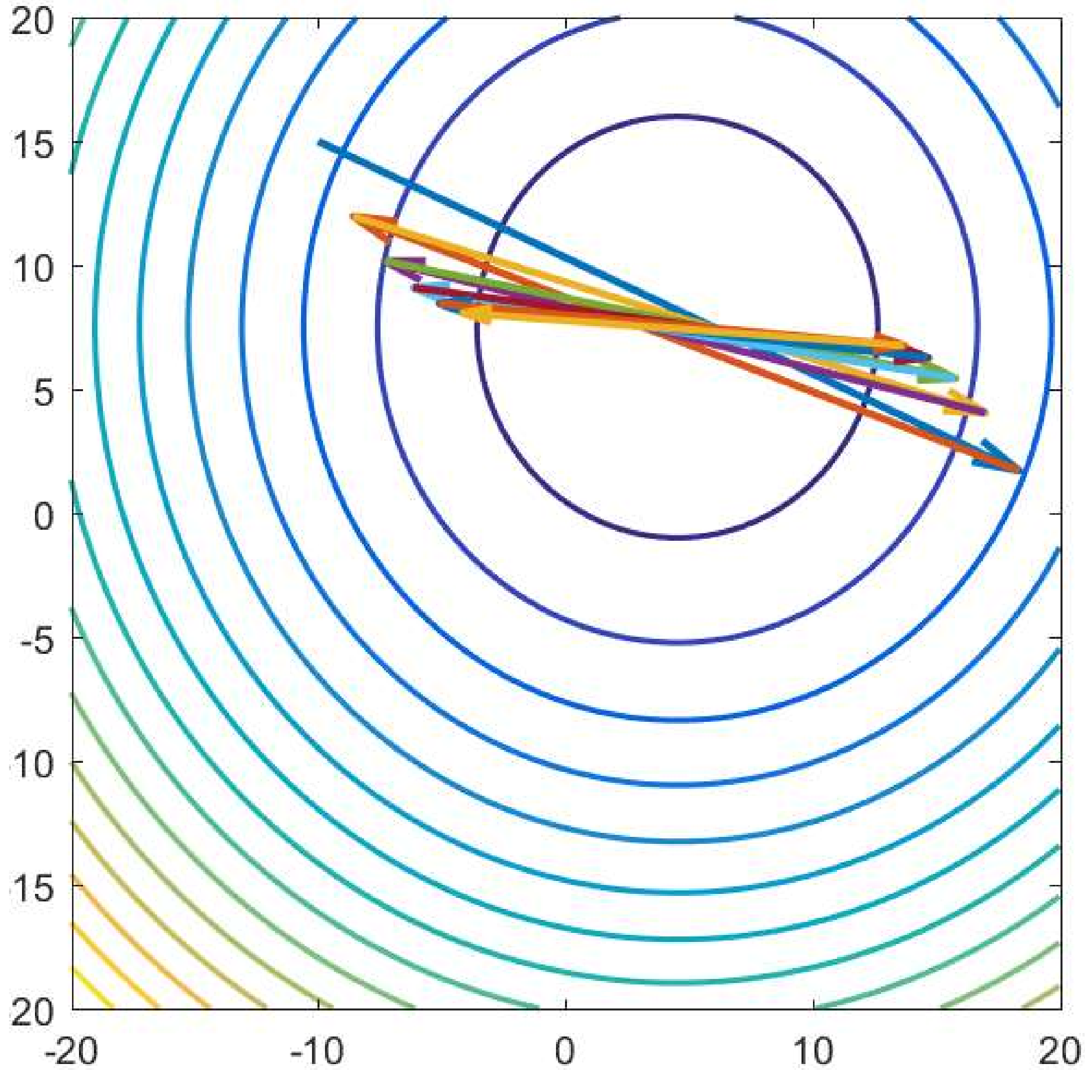
$$\eta_{i,opt} = \left(\frac{\partial^2 E\left(w_i^{(k)}\right)}{\partial w_i^2}\right)^{-1} = a_{ii}^{-1}$$

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

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

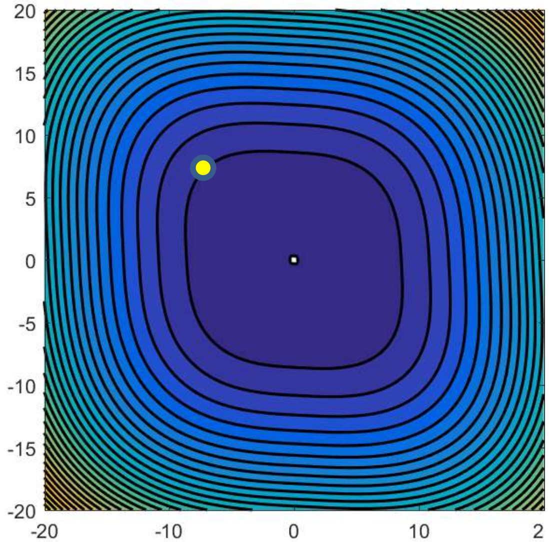
  – Otherwise the learning will diverge
- This, however, makes the learning very slow
  – And will oscillate in all directions where $\eta_{i,opt} \leq \eta < 2\eta_{i,opt}$

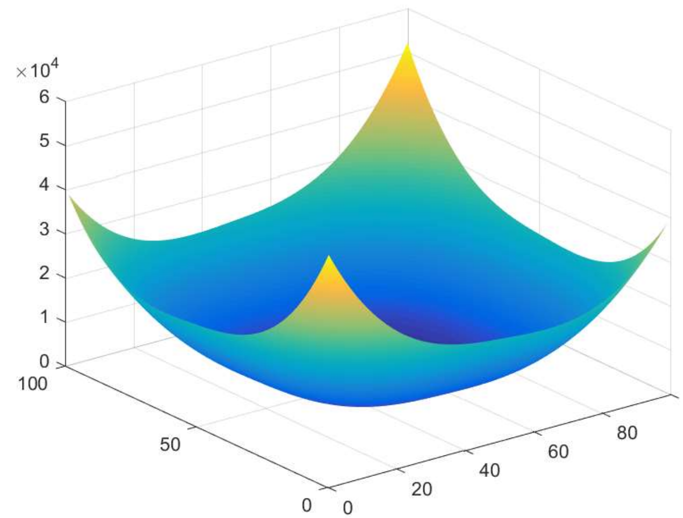
Dependence on learning rate



- $\eta_{1,opt} = 1;\ \eta_{2,opt} = 0.91;\qquad \eta = 1.9\,\eta_{2,opt}$

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

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

- 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 η must be close to both, the largest $\eta_{i,opt}$ and the smallest $\eta_{i,opt}$
  - To ensure convergence in every direction
  - Generally infeasible

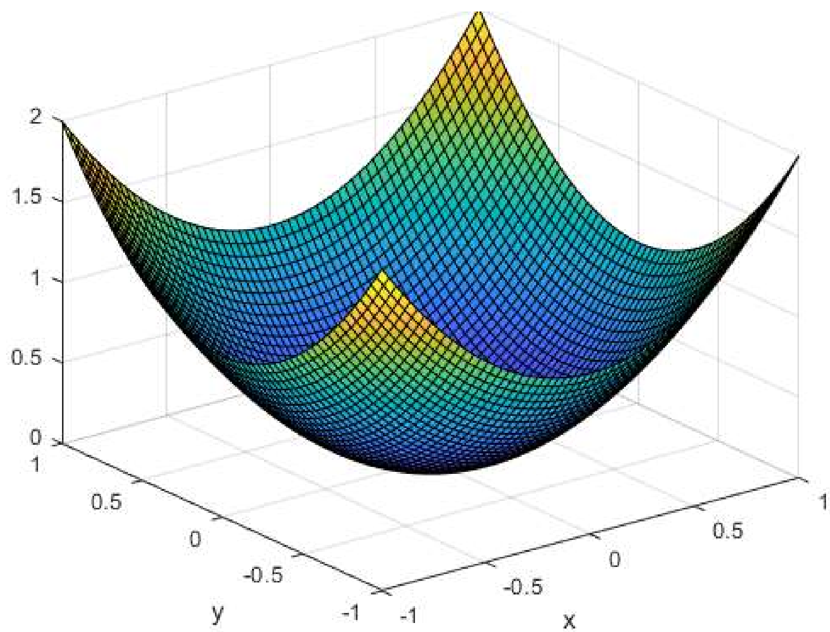
- Convergence is particularly slow if $\frac{\max_i \eta_{i,opt}}{\min_i \eta_{i,opt}}$ is large
  - The "condition" number
    - Must be close to 1.0 for fast convergence

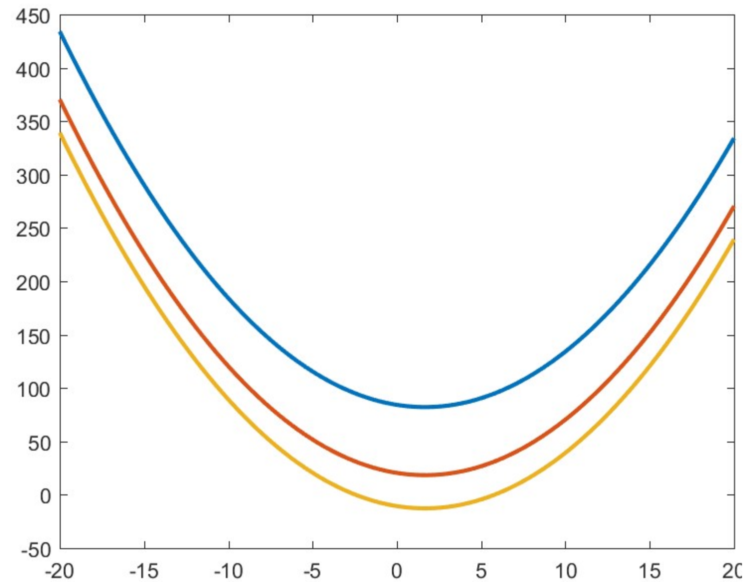
- Following (hidden) slides discuss solutions that "normalize the space by stretching different directions differently to standardize optimal step size
  - A big topic for optimization
  - Unfortunately, infeasible for neural networks

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

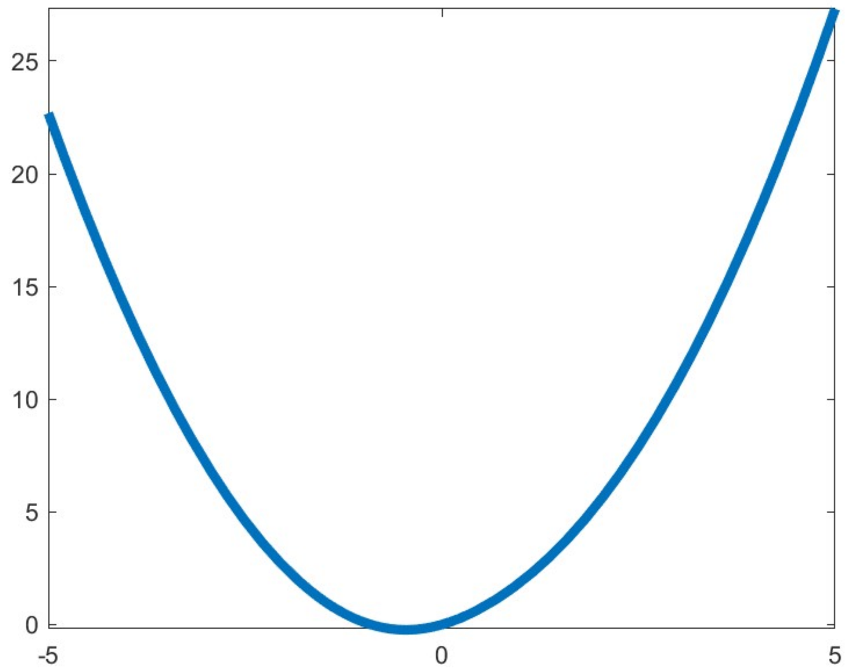
Quadratic convexity

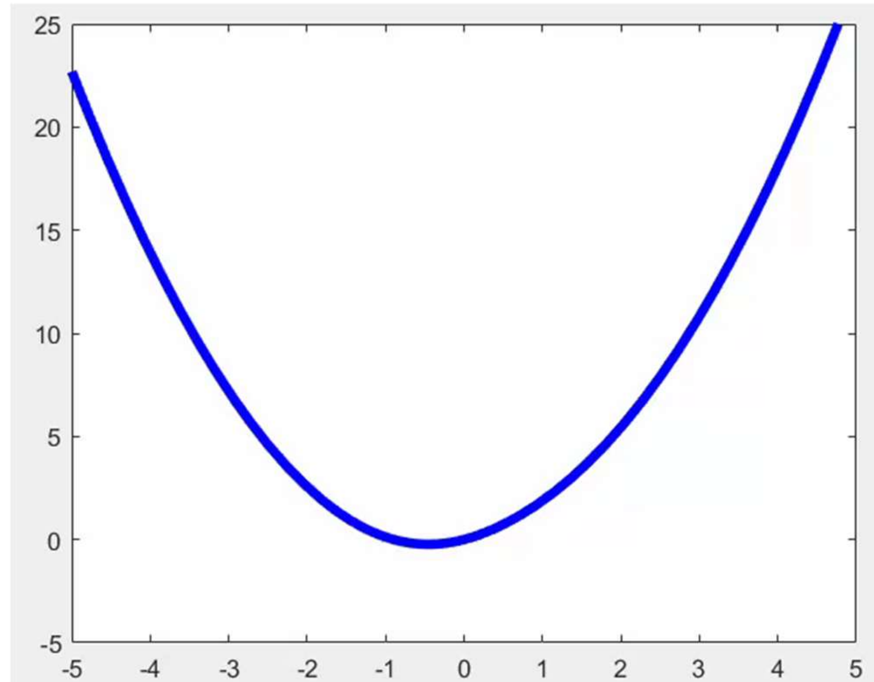




- A quadratic function has the form $\frac{1}{2}\mathbf{w}^T\mathbf{A}\mathbf{w} + \mathbf{w}^T\mathbf{b} + c$
  - Every “slice” is a quadratic bowl
- In some sense, the “standard” for gradient-descent based optimization
  - Others convex functions will be steeper in some regions, but flatter in others
- Gradient descent solution will have linear convergence
  - Take $O(\log 1/\varepsilon)$ steps to get within ε of the optimal solution

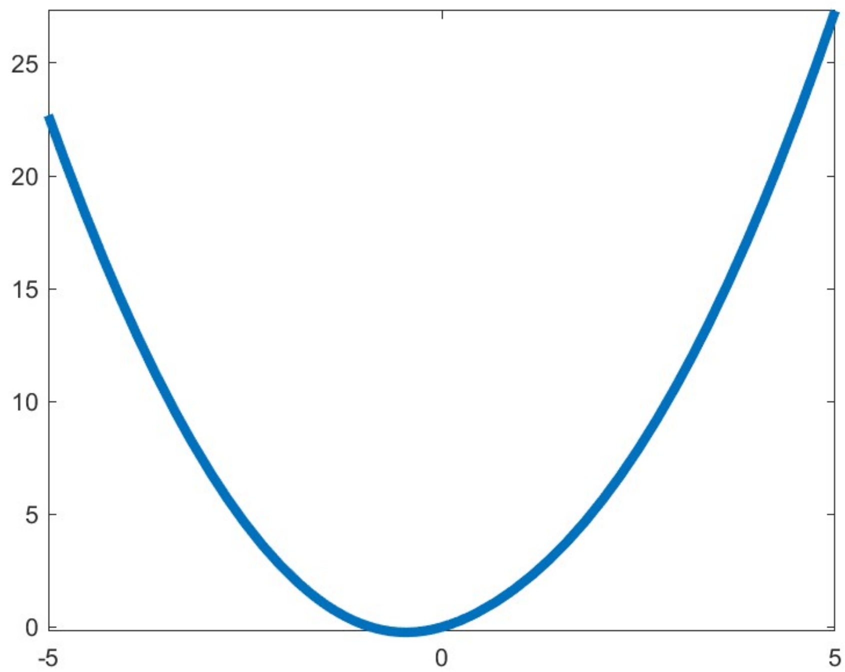
Strong convexity

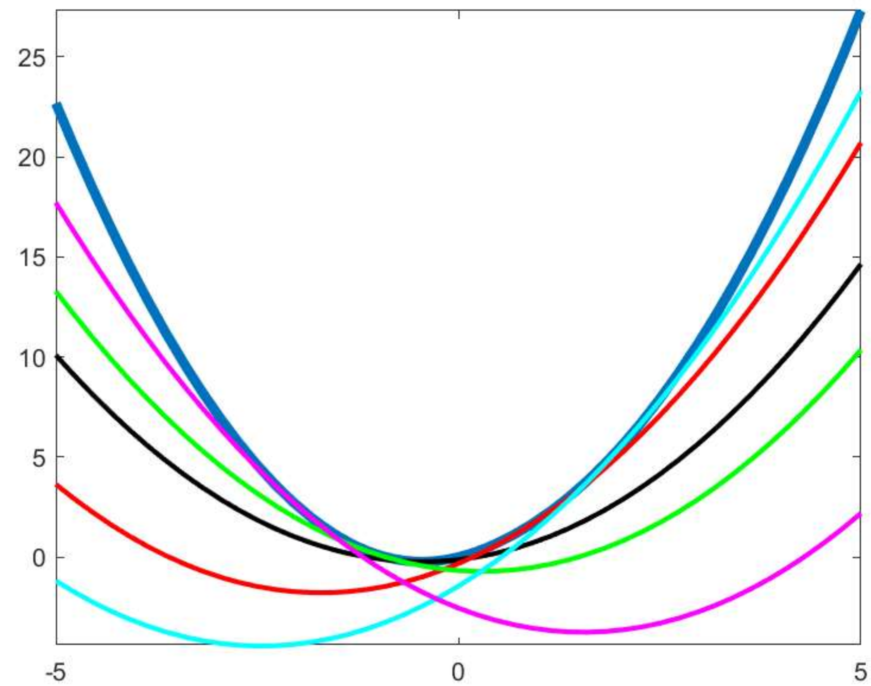




- A strongly convex function is *at least* quadratic in its convexity
  - Has a lower bound to its second derivative
- The function sits within a quadratic bowl
  - At any location, you can draw a quadratic bowl of fixed convexity (quadratic constant equal to lower bound of 2nd derivative) touching the function at that point, which contains it
- Convergence of gradient descent algorithms at least as good as that of the enclosing quadratic

Strong convexity





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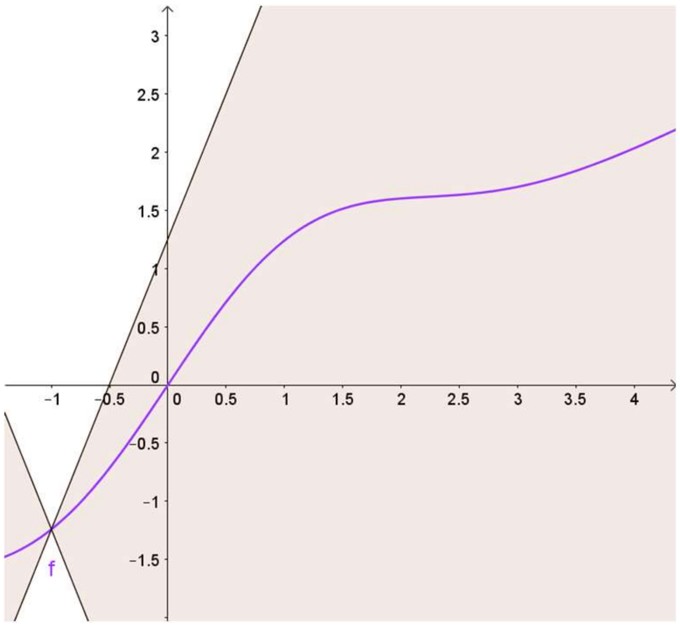
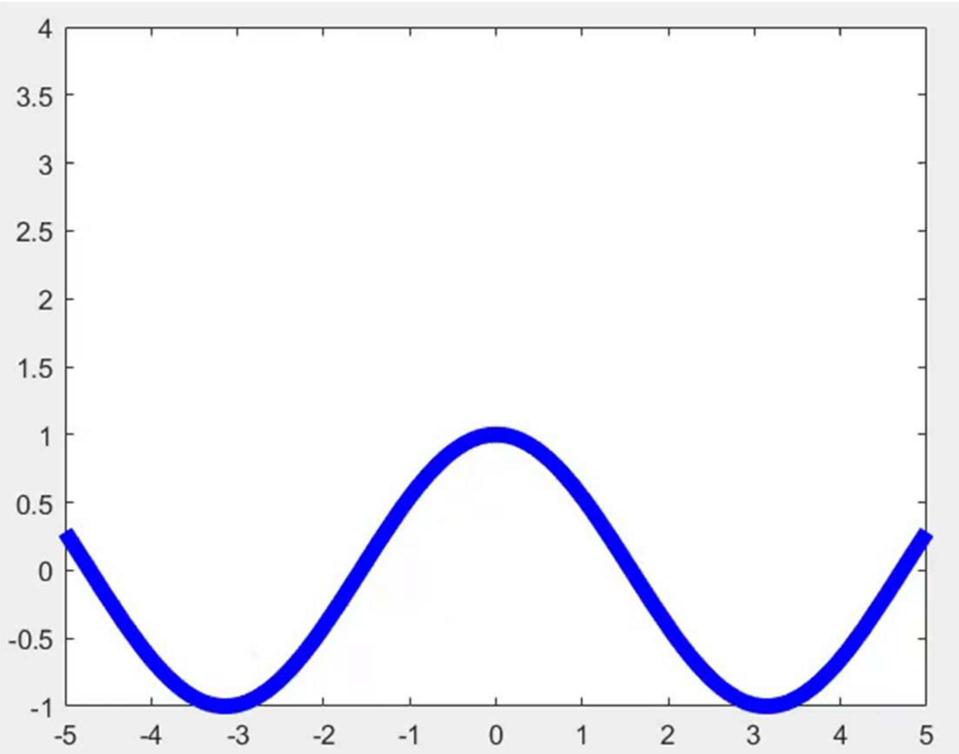
Types of continuity

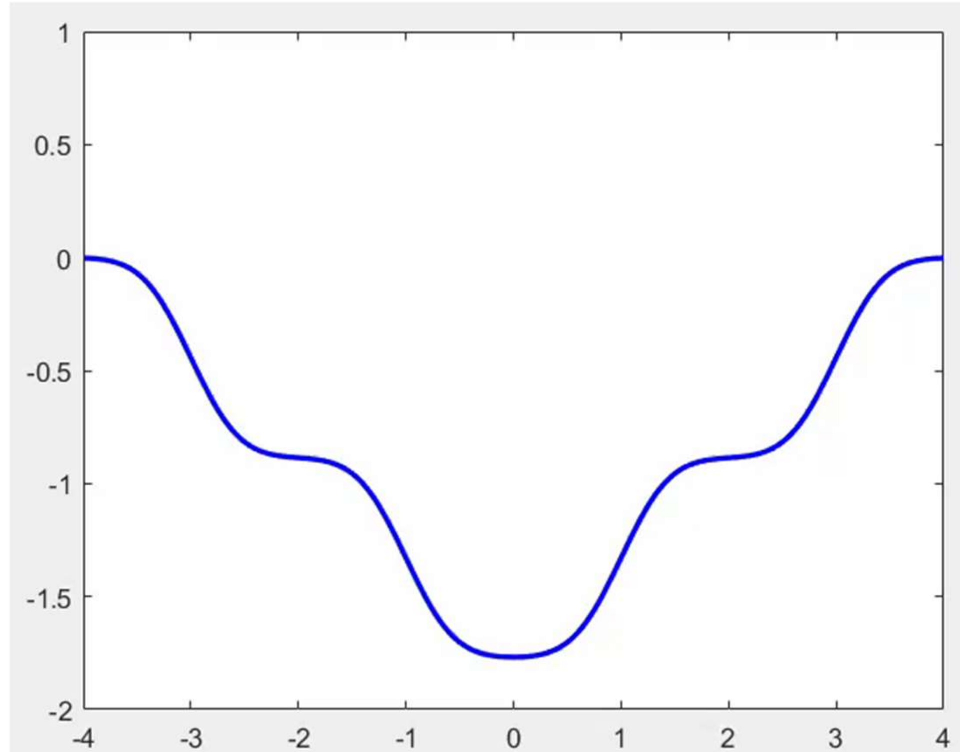


From wikipedia

- 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
  - $|f(x) - f(y)| \leq L|x - y|$

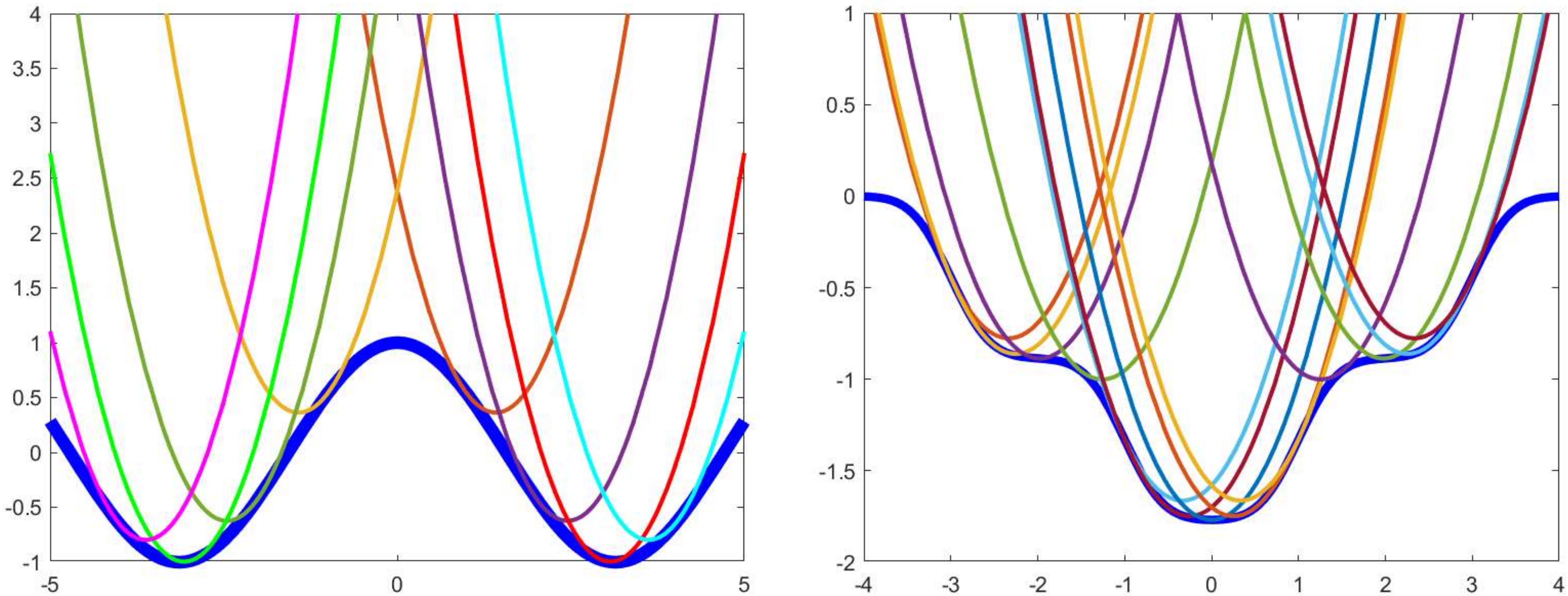
Lifschitz *smoothness*





- 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 >= upper bound of second derivative of function (if it exists)

Lifschitz *smoothness*



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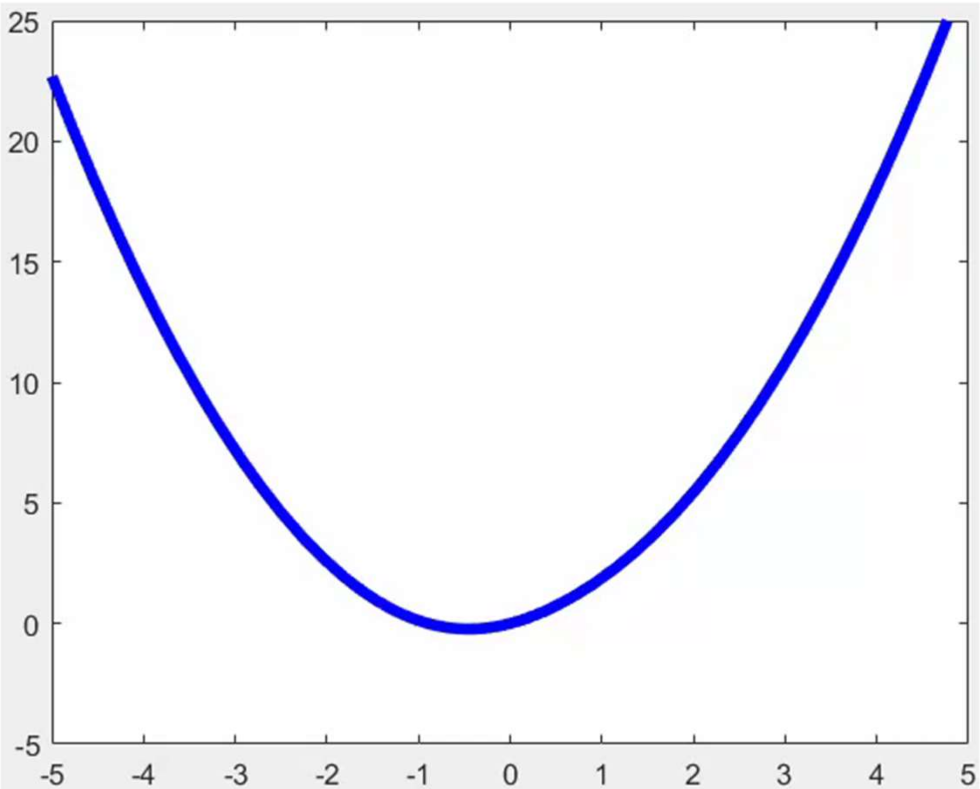
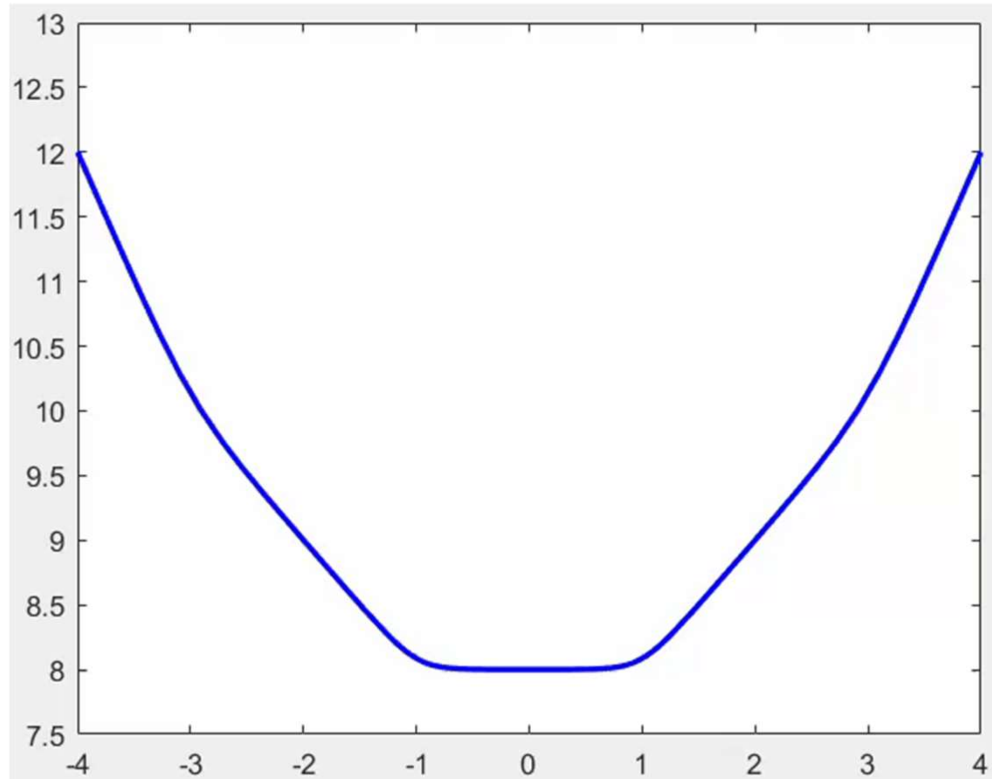
Types of smoothness

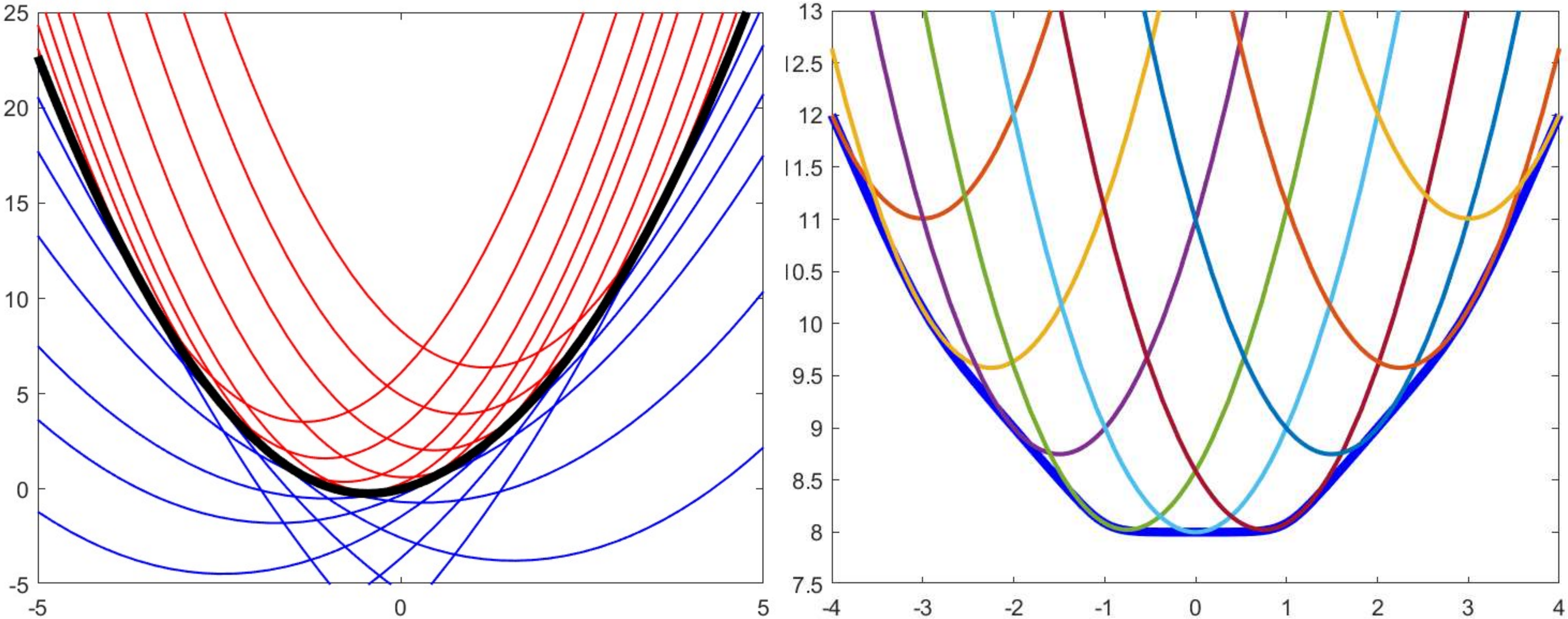




- A function can be both strongly convex and Lipschitz smooth
  - Second derivative has upper *and* lower bounds
  - Convergence depends on curvature of strong convexity (at least linear)

- A function can be convex and Lifschitz 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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  - This is often a reasonable assumption for the local structure of your loss function

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

$$\left|f\left(w^{(k)}\right) - f(w^*)\right| \propto \frac{1}{k}\left|f\left(w^{(0)}\right) - f(w^*)\right|$$

  - And inversely proportional to learning rate

$$\left|f\left(w^{(k)}\right) - f(w^*)\right| \leq \frac{1}{2\eta k}\left|w^{(0)} - w^*\right|$$

  - Takes $O(1/\epsilon)$ iterations to get to within ϵ of the solution

  - An inappropriate learning rate will destroy your happiness

- Second order methods will *locally* convert the loss function to quadratic
  - Convergence behavior will still depend on the nature of the original function

- ***Continuing with the quadratic-based explanation…***

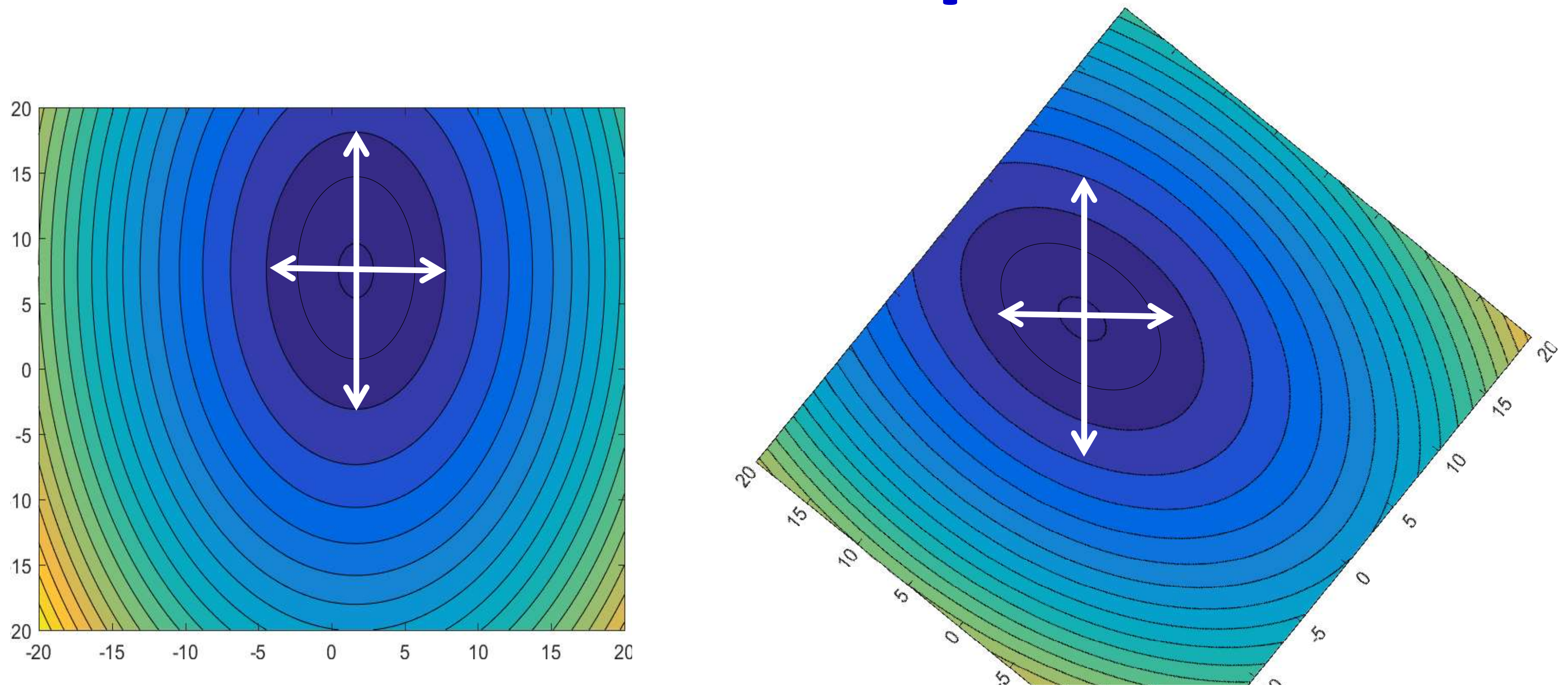
Convergence

- Convergence behaviors become increasingly unpredictable as dimensions increase

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

- Convergence is particularly slow if $\frac{\max_i \eta_{i,opt}}{\min_i \eta_{i,opt}}$ is large
  - The "condition" number is small

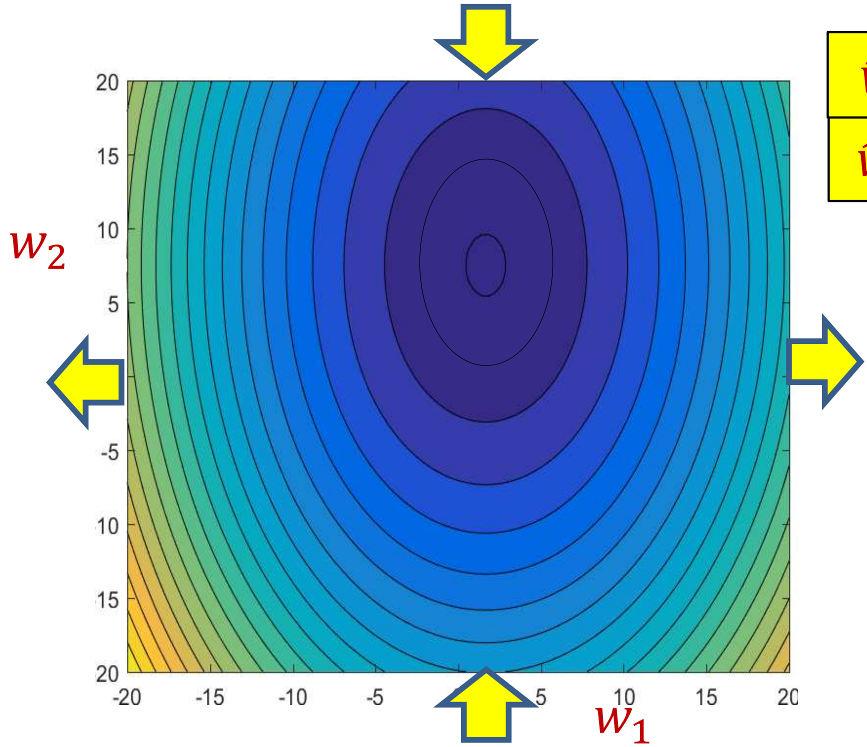
One reason for the problem



- 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

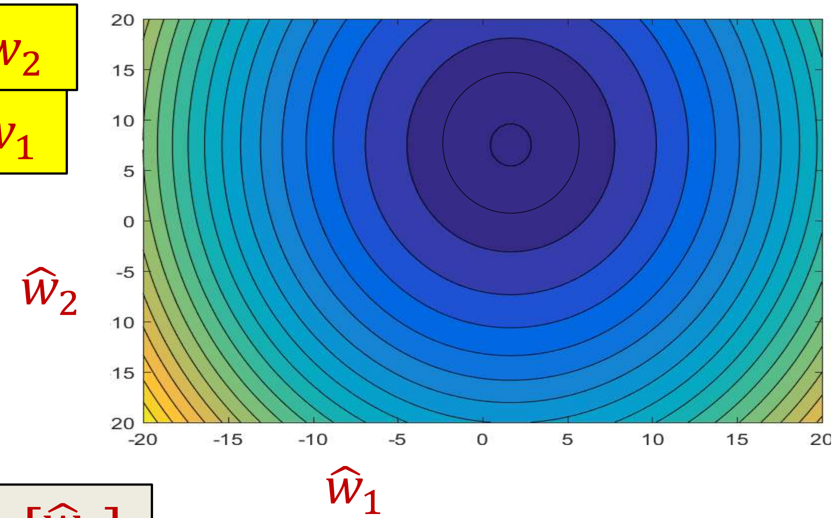
- Solution: *Normalize* the objective to have identical eccentricity in all directions
  - Then all of them will have identical optimal learning rates
  - Easier to find a working learning rate

Solution: Scale the axes



$\widehat{w}_2 = s_2 w_2$

$\widehat{w}_1 = s_1 w_1$



$\widehat{\mathbf{w}} = \begin{bmatrix} \widehat{w}_1 \\ \widehat{w}_2 \end{bmatrix}$

$\mathbf{w} = \begin{bmatrix} w_1 \\ w_2 \end{bmatrix}$

$S = \begin{bmatrix} s_1 & 0 \\ 0 & s_2 \end{bmatrix}$

$\widehat{\mathbf{w}} = S\mathbf{w}$

- 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

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

Scaling the axes

- Original equation:

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

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

$$\mathrm{S} = \begin{bmatrix} s_1 & \cdots & 0 \\ \vdots & \ddots & \vdots \\ 0 & \cdots & s_N \end{bmatrix}, \qquad \widehat{\mathbf{w}} = \mathrm{S}\mathbf{w}$$

- And

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

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- And

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

By inspection:
$\mathrm{S} = \mathbf{A}^{0.5}$

Scaling the axes

- We have

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

$$\widehat{\mathbf{w}} = S\mathbf{w}$$

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

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

- Equating linear and quadratic coefficients, we get

$$S^T S = \mathbf{A}, \qquad \hat{\mathbf{b}}^T S = \mathbf{b}^T$$

- Solving: $S = \mathbf{A}^{0.5}, \qquad \hat{\mathbf{b}} = \mathbf{A}^{-0.5}\mathbf{b}$

Scaling the axes

- We have

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

$$\widehat{\mathbf{w}} = S\mathbf{w}$$

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

- Solving for S we get

$$\widehat{\mathbf{w}} = \mathbf{A}^{0.5}\mathbf{w}, \qquad \hat{\mathbf{b}} = \mathbf{A}^{-0.5}\mathbf{b}$$

Scaling the axes

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

- Solving for S we get

$$\widehat{\mathbf{w}} = \mathbf{A}^{0.5}\mathbf{w}, \qquad \hat{\mathbf{b}} = \mathbf{A}^{-0.5}\mathbf{b}$$

The Inverse Square Root of A

- For *any* positive definite $\mathbf{A}$, we can write

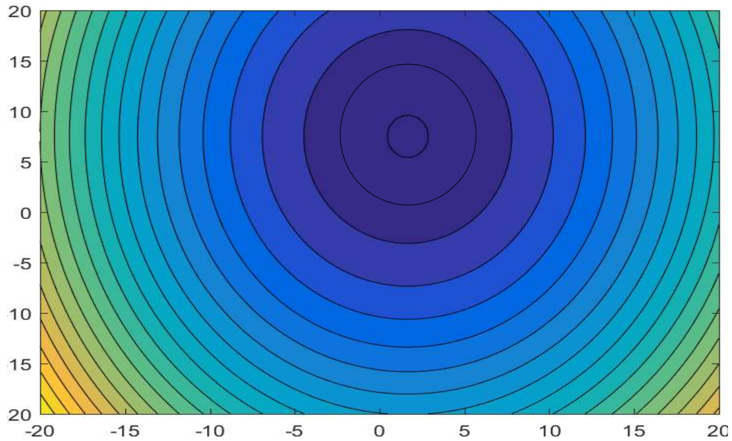
$$\mathbf{A} = \mathbf{E}\boldsymbol{\Lambda}\mathbf{E}^{\mathrm{T}}$$

  - Eigen decomposition
  - $\mathbf{E}$ is an orthogonal matrix
  - $\boldsymbol{\Lambda}$ is a diagonal matrix of non-zero diagonal entries

- Defining $\mathbf{A}^{0.5} = \mathbf{E}\boldsymbol{\Lambda}^{0.5}\mathbf{E}^{\mathrm{T}}$
  - Check $(\mathbf{A}^{0.5})^{\mathrm{T}}\mathbf{A}^{0.5} = \mathbf{E}\boldsymbol{\Lambda}\mathbf{E}^{\mathrm{T}} = \mathbf{A}$

- Defining $\mathbf{A}^{-0.5} = \mathbf{E}\boldsymbol{\Lambda}^{-0.5}\mathbf{E}^{\mathrm{T}}$
  - Check: $(\mathbf{A}^{-0.5})^{\mathrm{T}}\mathbf{A}^{-0.5} = \mathbf{E}\boldsymbol{\Lambda}^{-1}\mathbf{E}^{\mathrm{T}} = \mathbf{A}^{-1}$

Returning to our problem

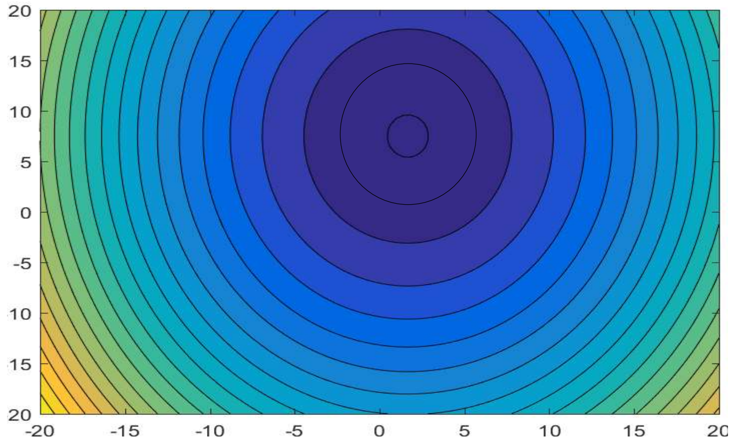


$$E = \frac{1}{2}\hat{\mathbf{w}}^T\hat{\mathbf{w}} + \hat{\mathbf{b}}^T\hat{\mathbf{w}} + c$$

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

$$\nabla_{\hat{\mathbf{w}}}E = \hat{\mathbf{w}}^T + \hat{\mathbf{b}}^T$$
$$= \mathbf{w}^T\mathbf{A}^{0.5} + \mathbf{b}^T\mathbf{A}^{-0.5}$$
$$= (\mathbf{w}^T\mathbf{A} + \mathbf{b}^T)\mathbf{A}^{-0.5}$$
$$= \nabla_{\mathbf{w}}E.\mathbf{A}^{-0.5}$$

Returning to our problem

- 

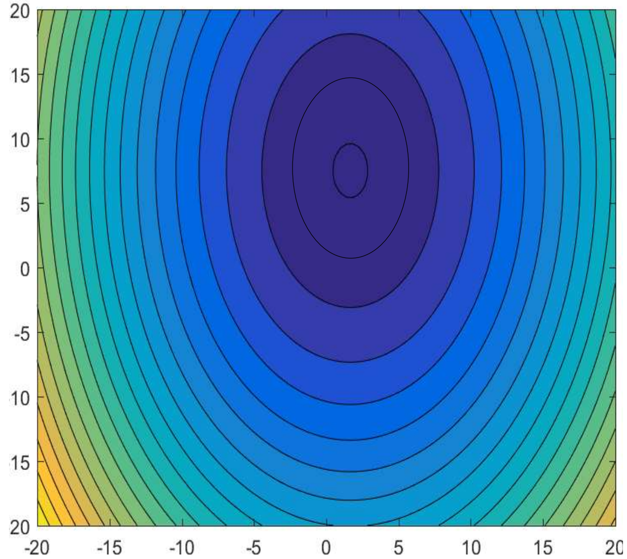
$$E = \frac{1}{2}\widehat{\mathbf{w}}^T\widehat{\mathbf{w}} + \hat{\mathbf{b}}^T\widehat{\mathbf{w}} + c$$

- Gradient descent rule:
  - $\widehat{\mathbf{w}}^{(k+1)} = \widehat{\mathbf{w}}^{(k)} - \eta \nabla_{\widehat{\mathbf{w}}} E\left(\widehat{\mathbf{w}}^{(k)}\right)^T$
  - Learning rate is now independent of direction

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

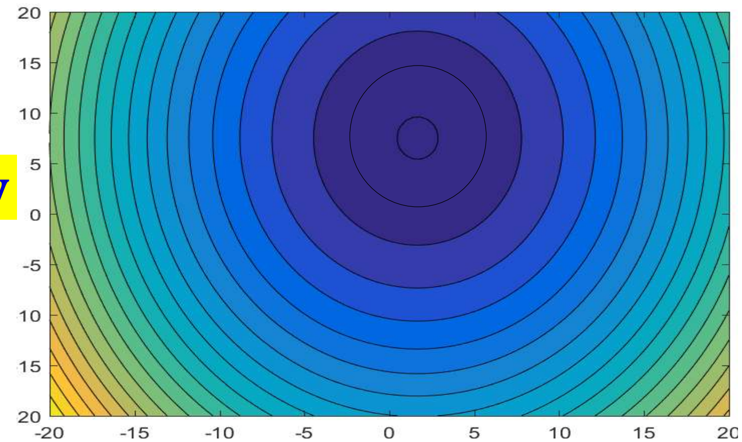
$$\mathbf{w}^{(k+1)} = \mathbf{w}^{(k)} - \eta\mathbf{A}^{-1}\nabla_{\mathbf{w}} E\left(\mathbf{w}^{(k)}\right)^T$$

Modified update rule



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

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

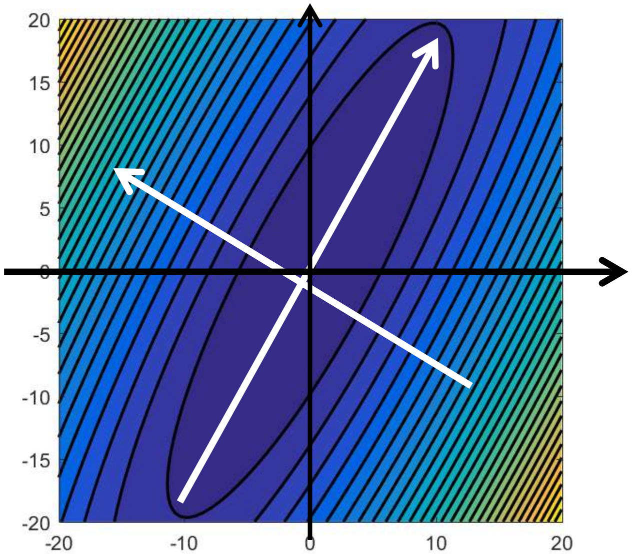


$$E = \frac{1}{2}\hat{\mathbf{w}}^T\hat{\mathbf{w}} + \hat{\mathbf{b}}^T\hat{\mathbf{w}} + c$$

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



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

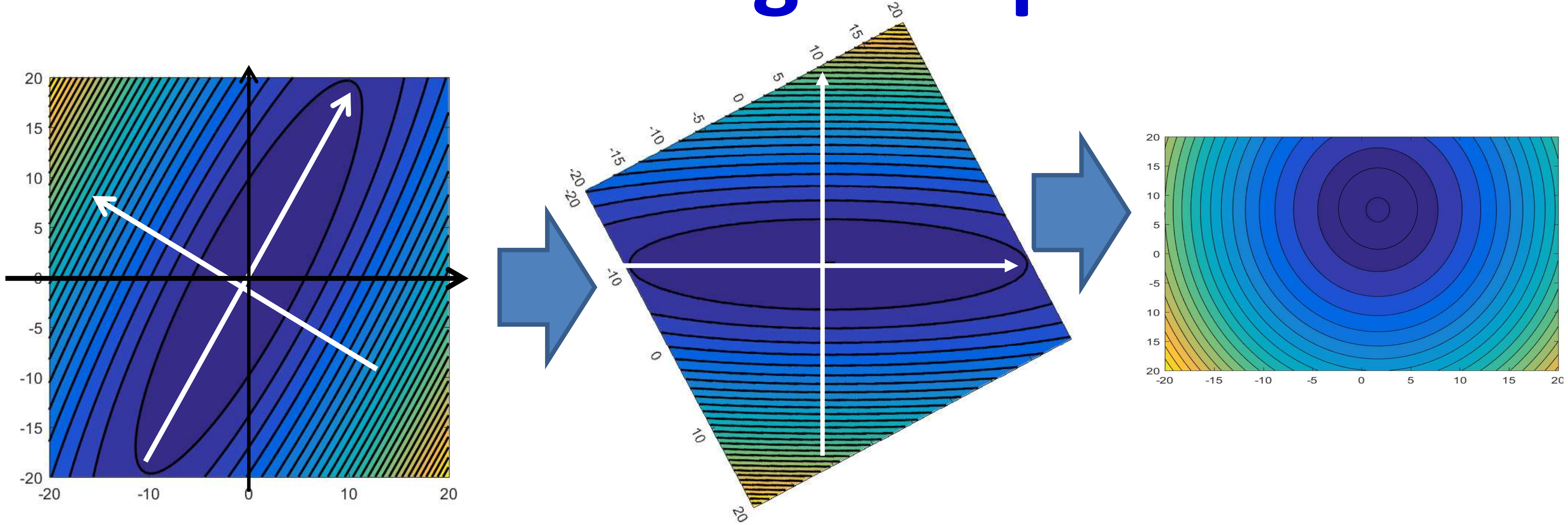
$$E = \frac{1}{2}\sum_i a_{ii}w_i^2 + \sum_{i \neq j} a_{ij}w_iw_j$$

$$+ \sum_i b_iw_i + c$$

- If $\mathbf{A}$ 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 $\mathbf{A}$, 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..

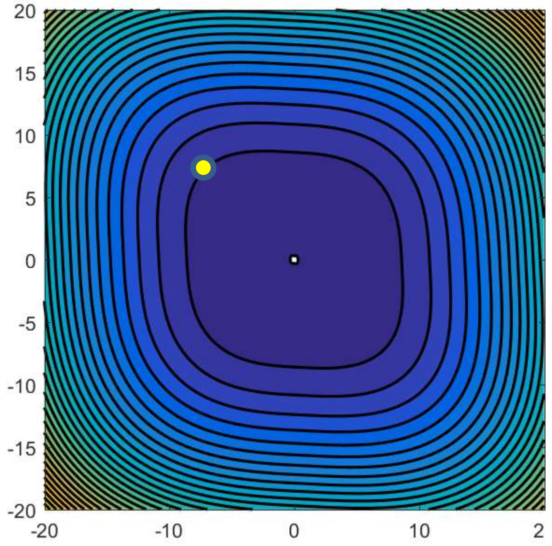


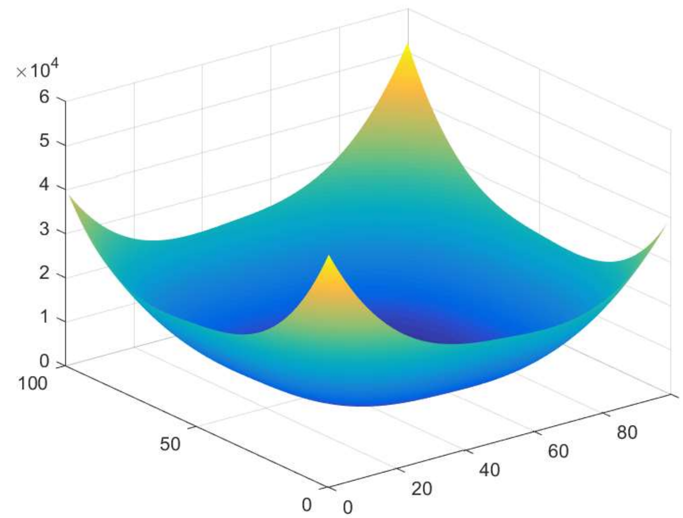
- The component-wise optimal learning rates along the major and minor axes of the contour ellipsoids will differ, causing problems
  - Inversely proportional to the *eigenvalues* of $\mathbf{A}$

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

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

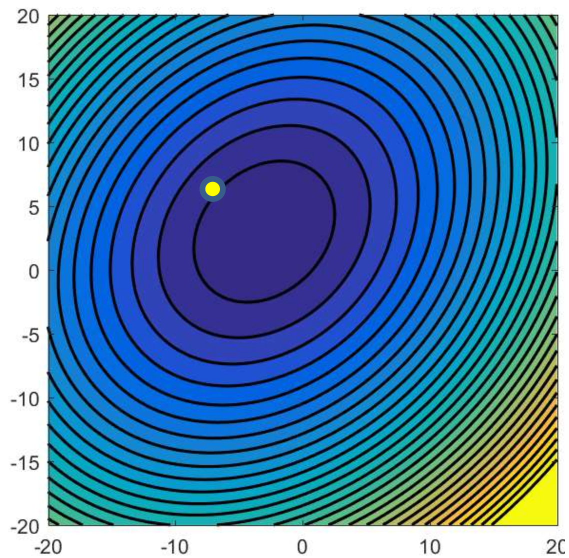
Generic differentiable *multivariate* convex functions

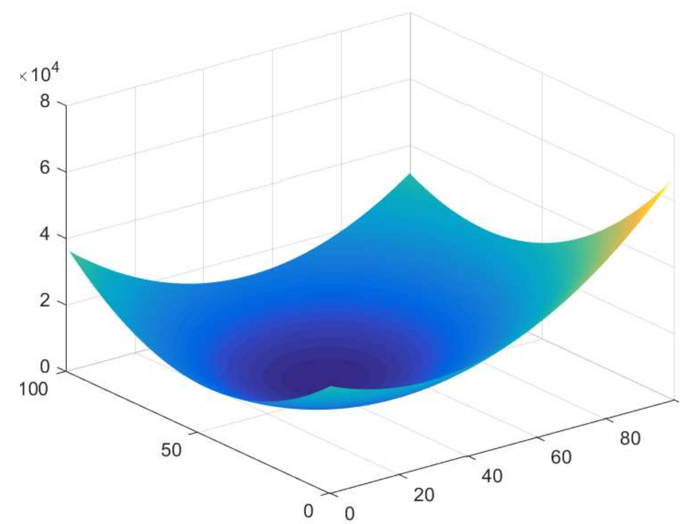




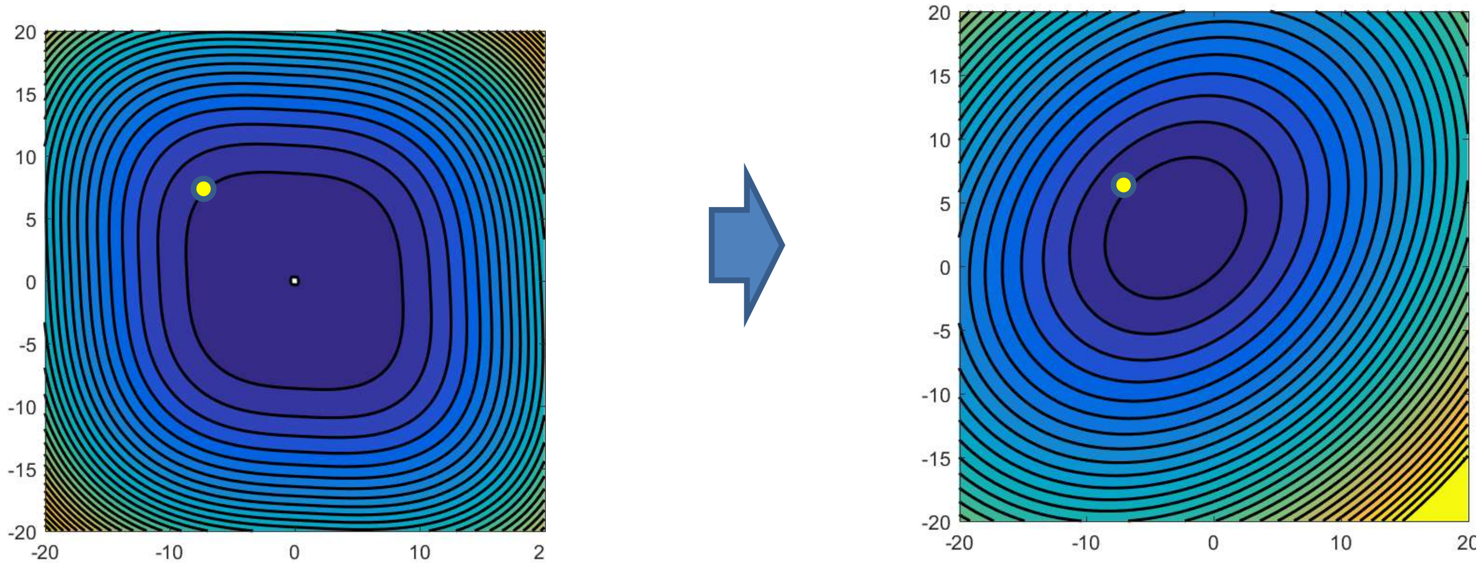
- Taylor expansion

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





Generic differentiable *multivariate* convex functions



- Taylor expansion

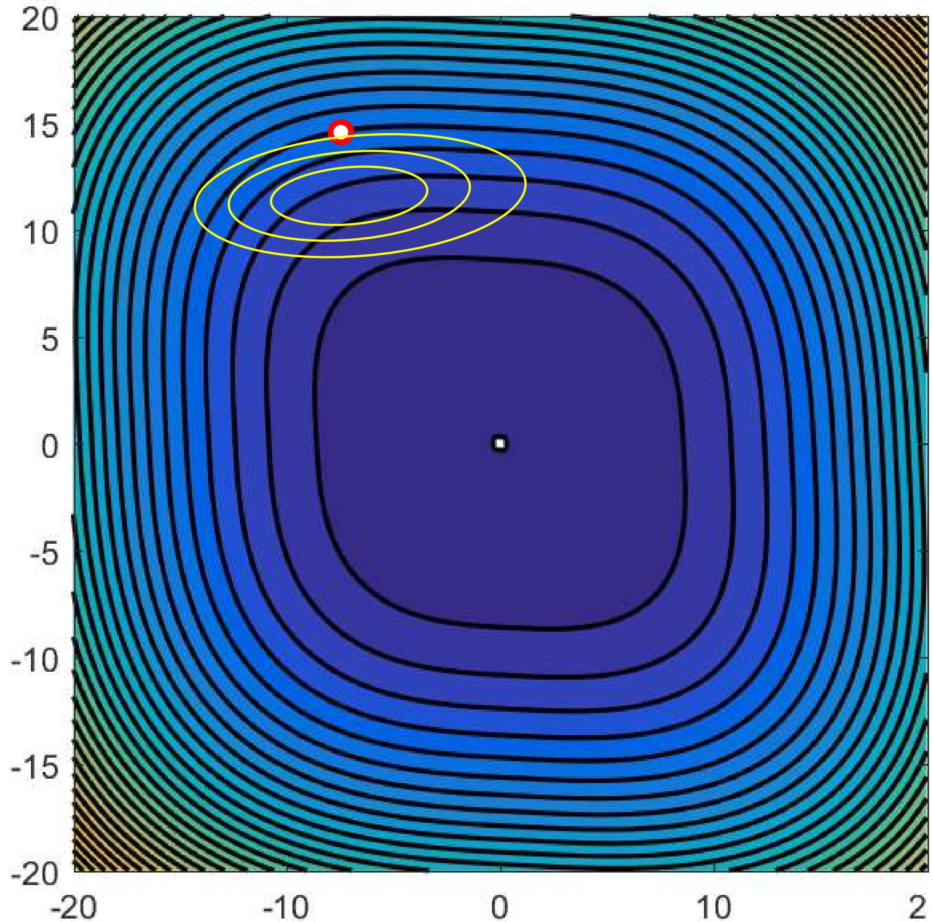
$$\boldsymbol{E(\mathbf{w}) \approx E\left(\mathbf{w}^{(k)}\right) + \nabla_{\mathbf{w}} E\left(\mathbf{w}^{(k)}\right)\left(\mathbf{w} - \mathbf{w}^{(k)}\right) + \frac{1}{2}\left(\mathbf{w} - \mathbf{w}^{(k)}\right)^T H_E\left(\mathbf{w}^{(k)}\right)\left(\mathbf{w} - \mathbf{w}^{(k)}\right) + \cdots}$$

- 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

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

- **For a quadratic function, the optimal $\boldsymbol{\eta}$ is 1 (which is exactly Newton's method)**
  - **And should not be greater than 2!**

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



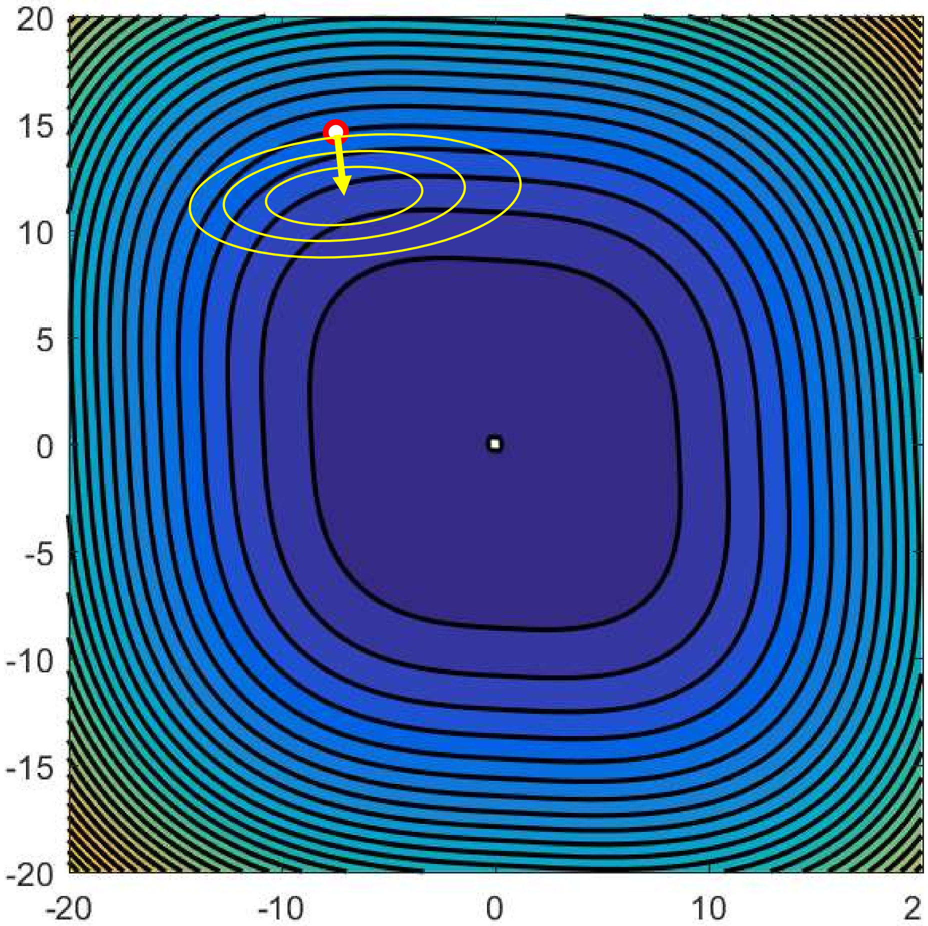
Fit a quadratic at each point and find the minimum of that quadratic

- Iterated localized optimization with quadratic approximations

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

– $\eta = 1$

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



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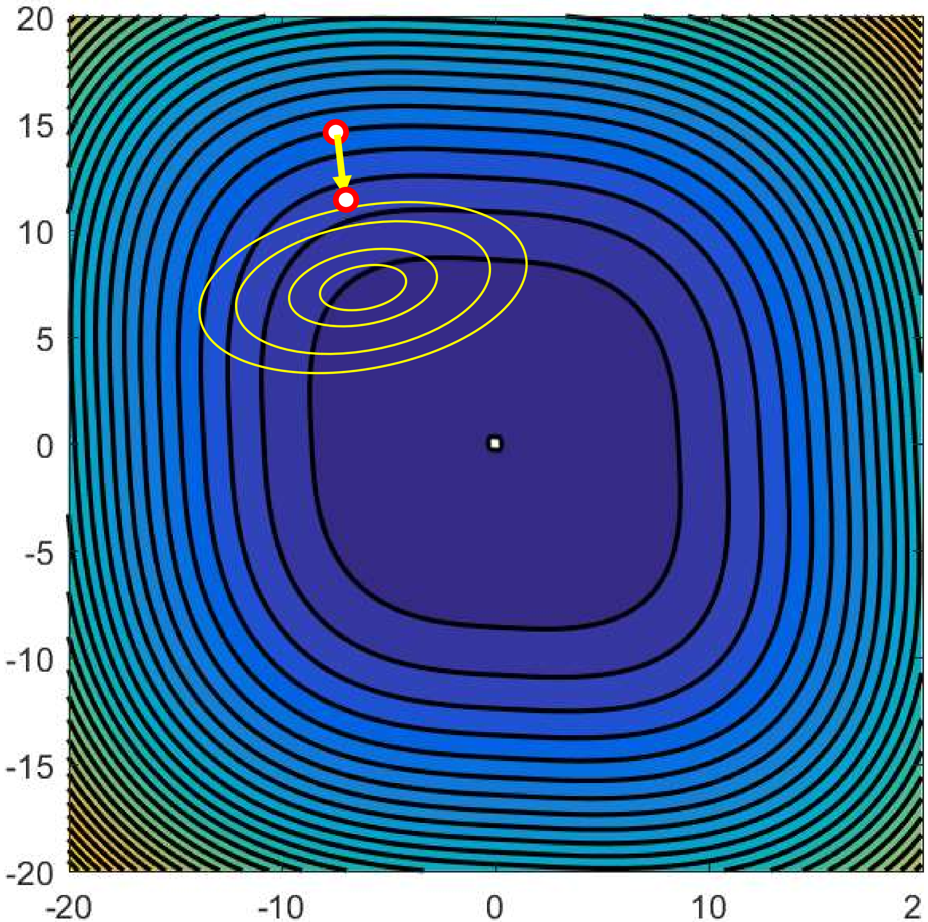

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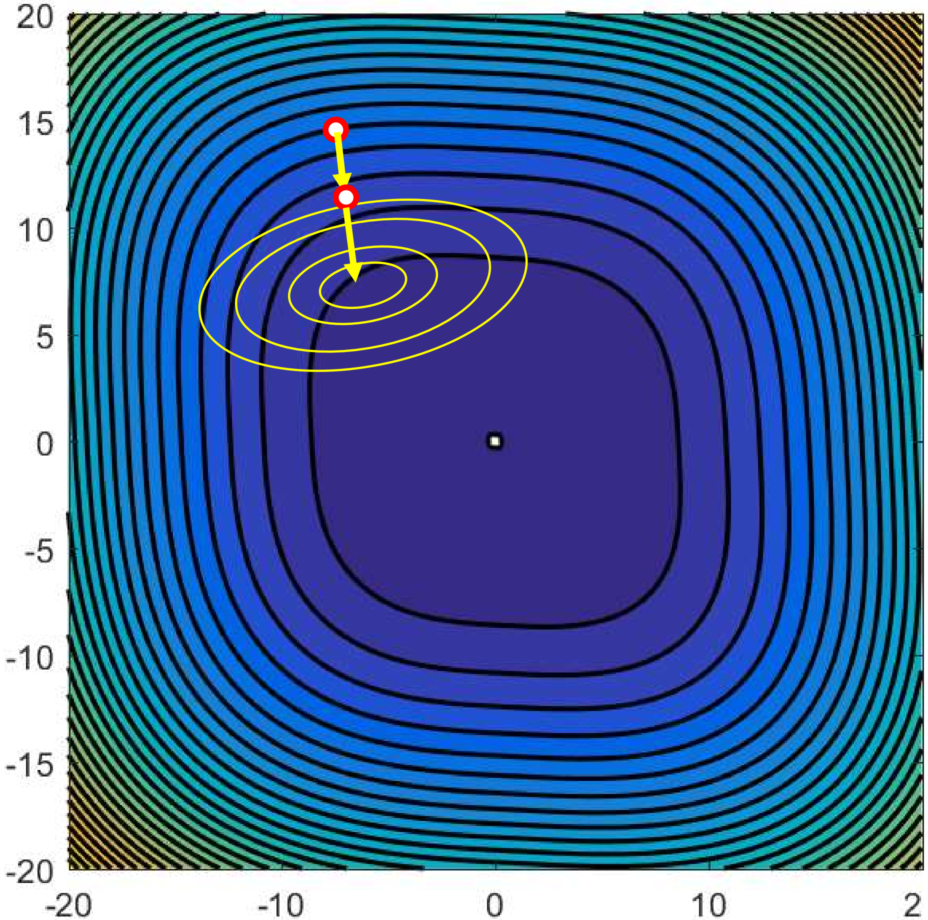

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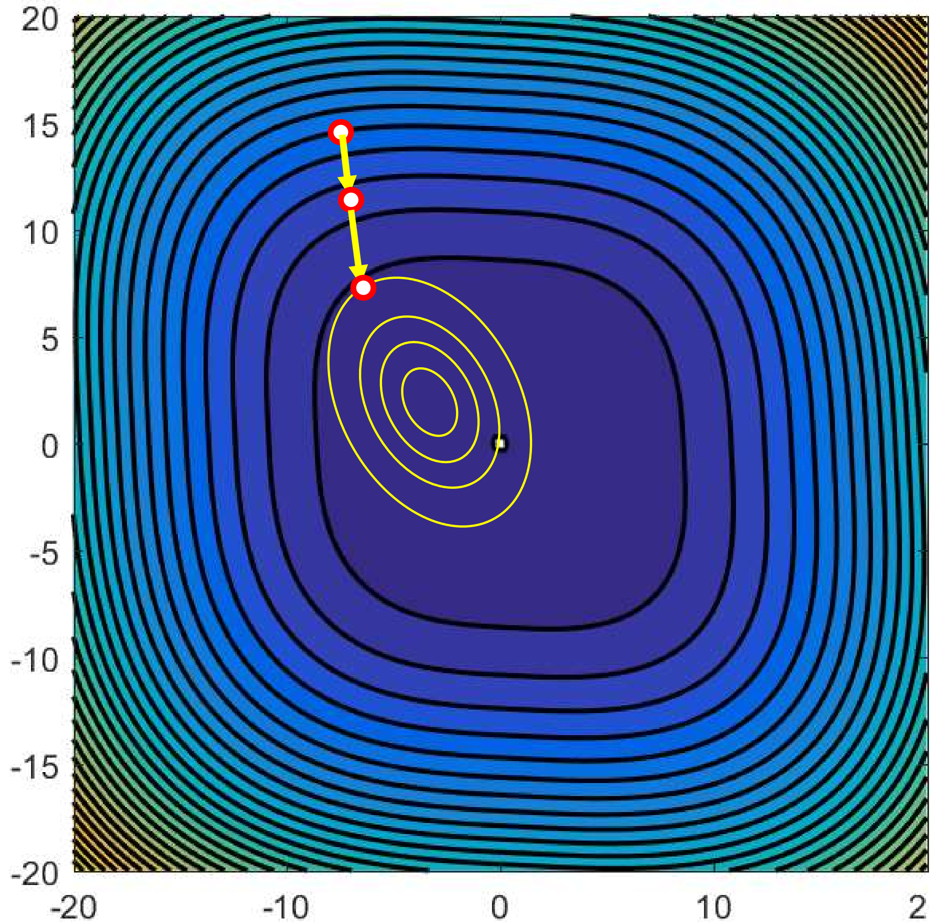

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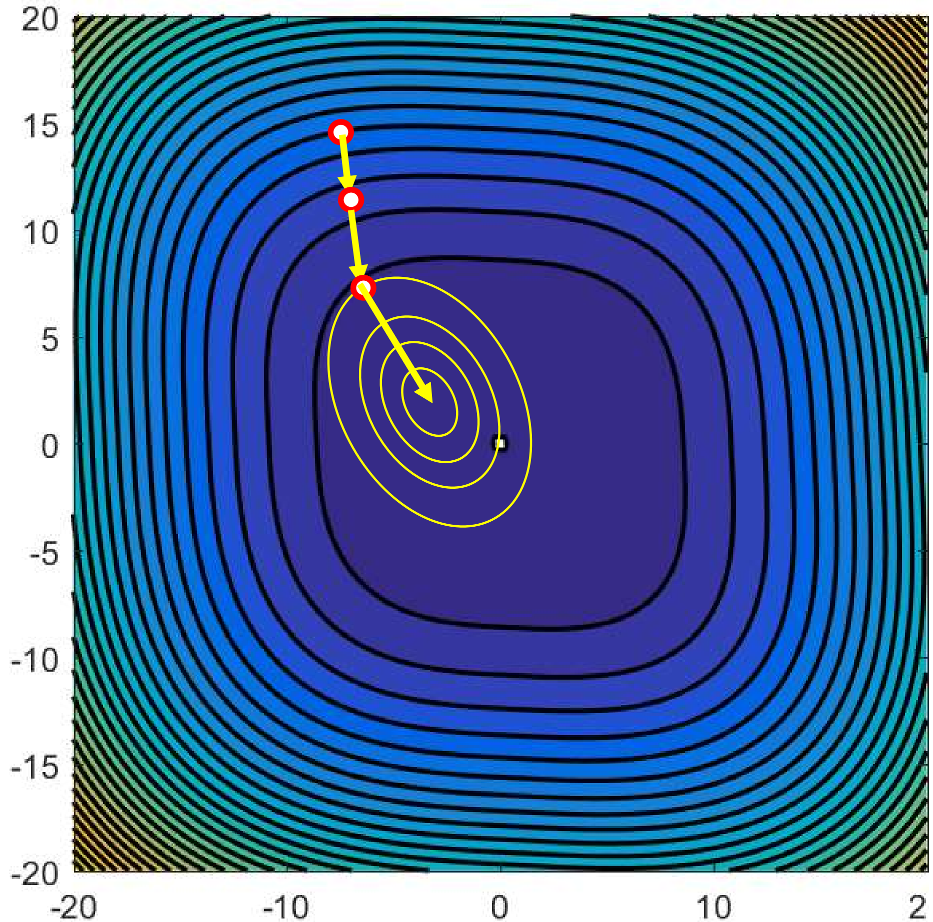
Minimization by Newton's method



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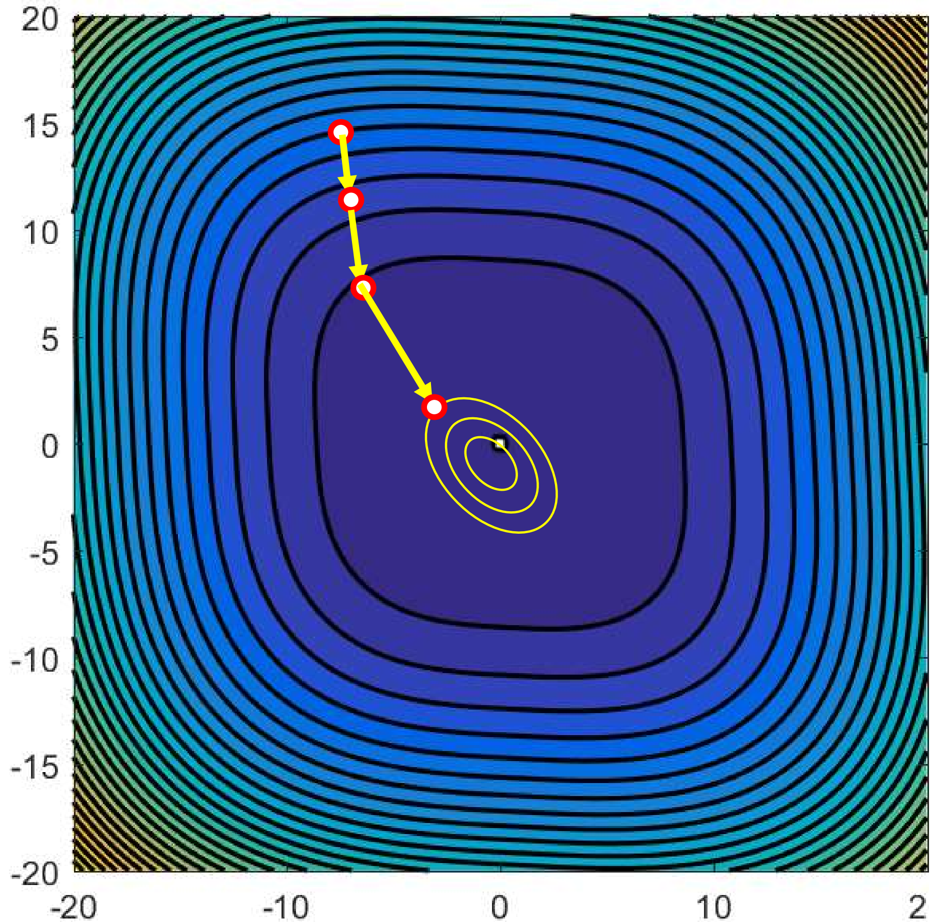
Minimization by Newton's method



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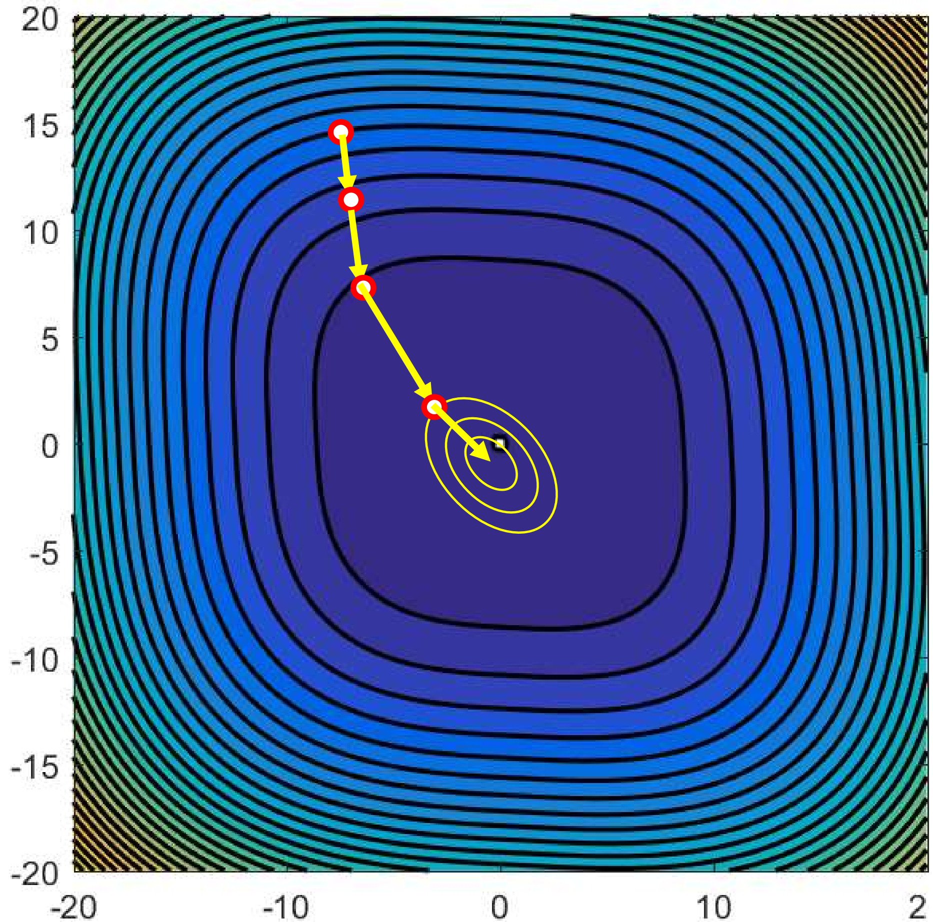
Minimization by Newton's method



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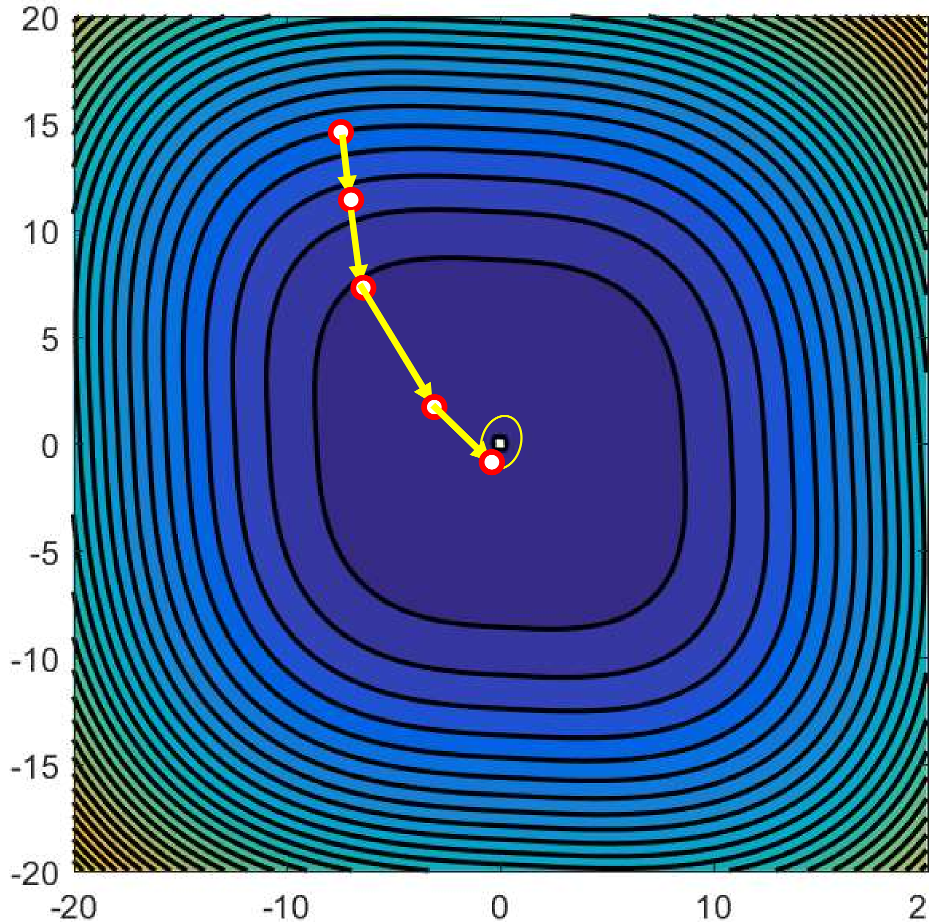
Minimization by Newton's method



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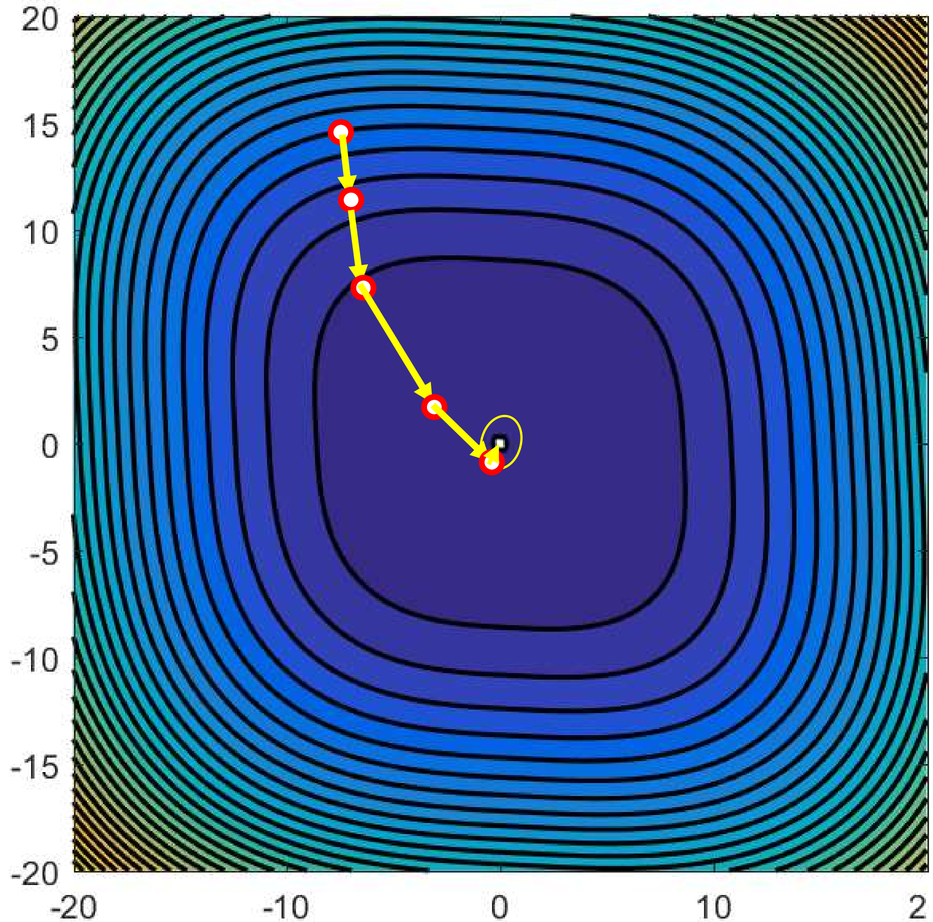
Minimization by Newton's method



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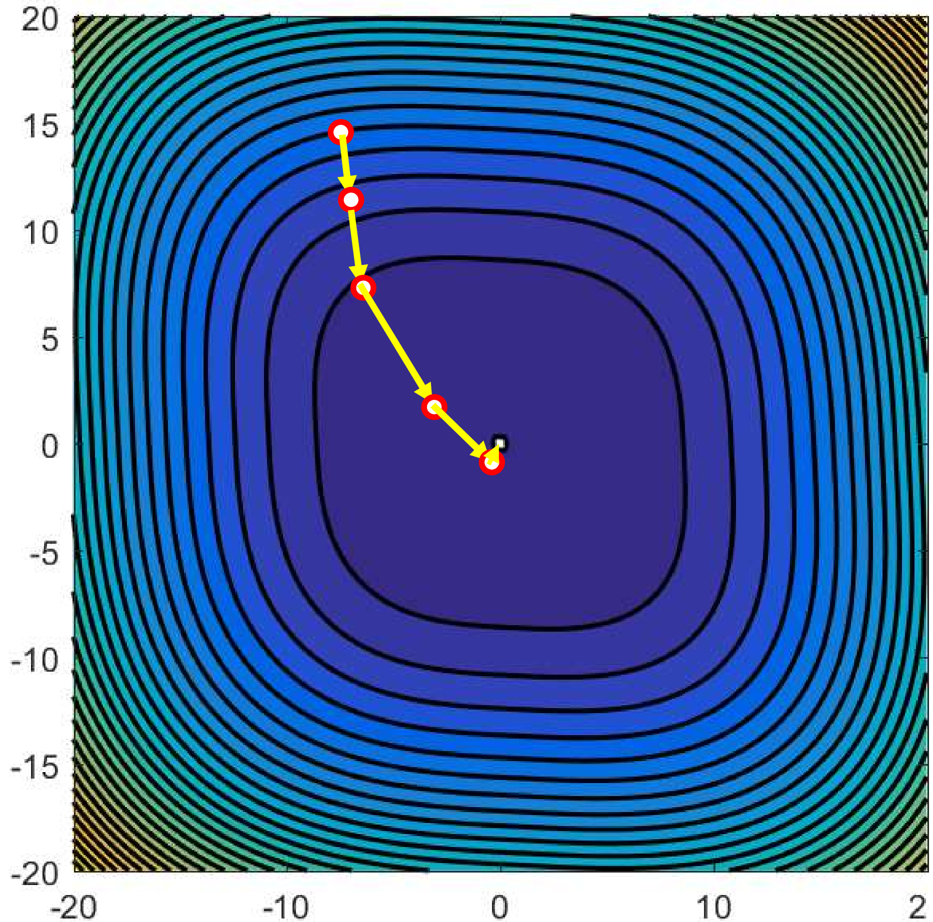
Minimization by Newton's method



- Iterated localized optimization with quadratic approximations

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

– $\eta = 1$

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

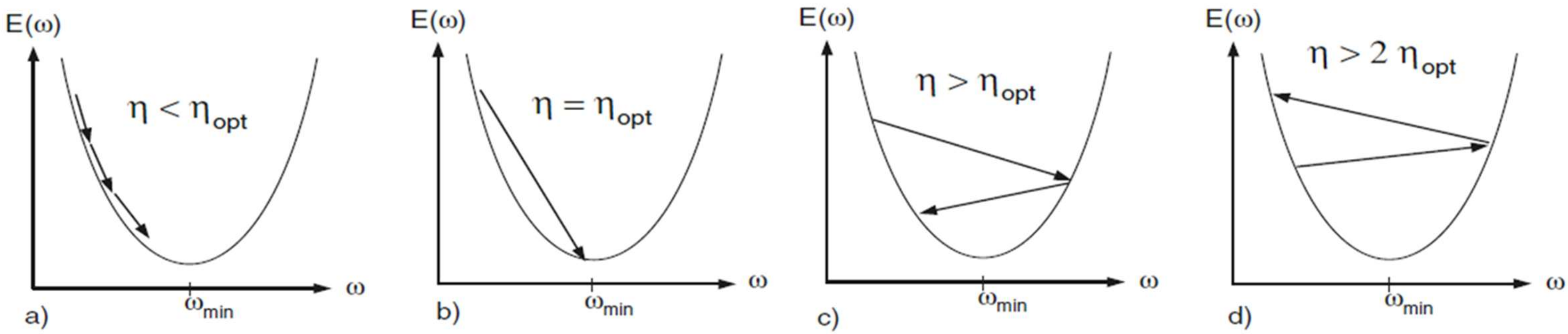
- For non-convex functions, the Hessian may not be positive semi-definite, in which case the algorithm can *diverge*
  - Goes away from, rather than towards the minimum
  - Now requires additional checks to avoid movement in directions corresponding to –ve Eigenvalues of the Hessian

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

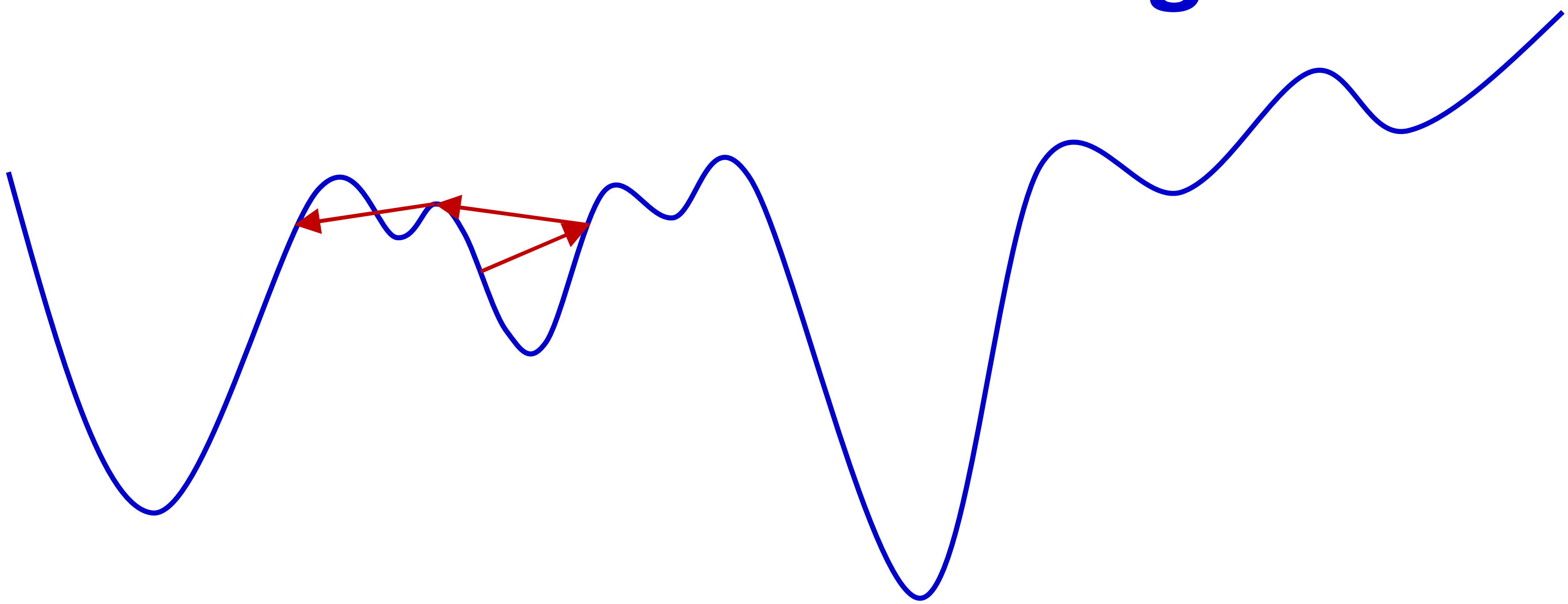
- Not particularly popular anymore for large neural networks..

Issues: 2. The learning rate



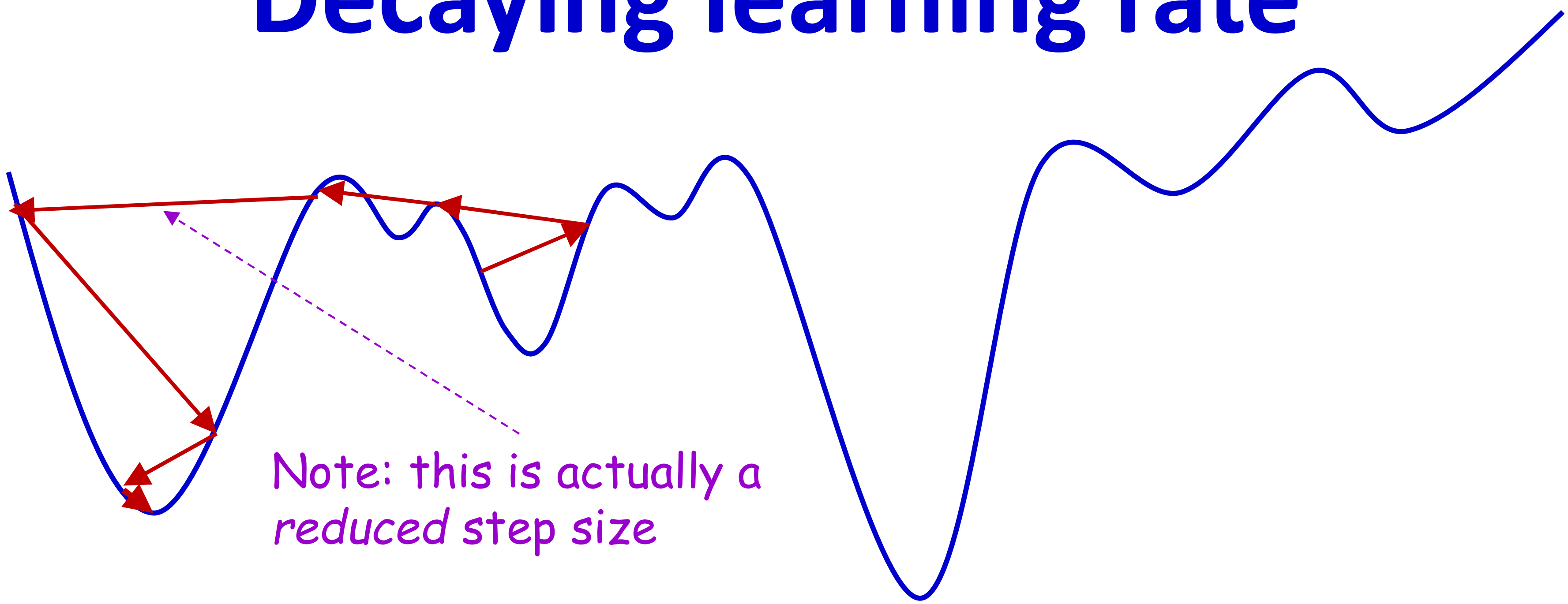
- Much of the analysis we just saw was based on trying to ensure that the step size was not so large as to cause divergence within a convex region
  - $\eta < 2\eta_{opt}$

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

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

Poll 2 (@382)

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

Poll 2

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

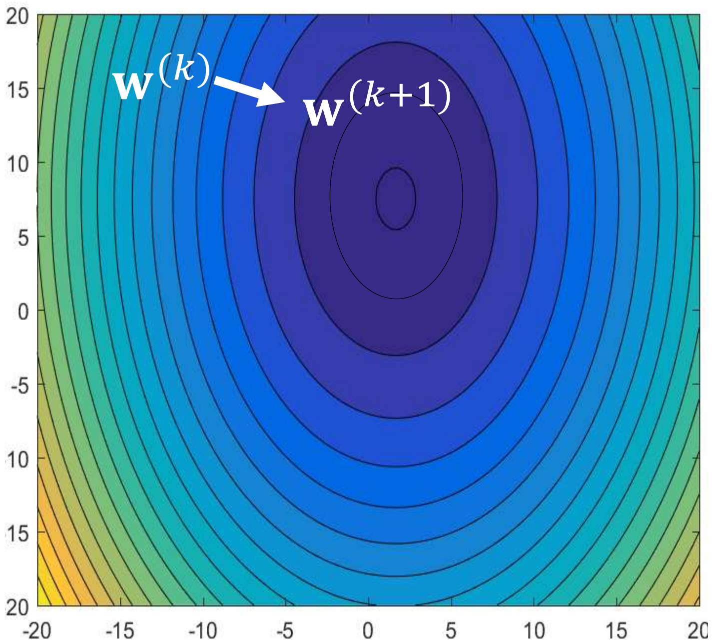
- Second-order methods “normalize” the variation along the components to mitigate the problem of different optimal learning rates for different components
  - But this requires computation of inverses of second-order derivative matrices
  - Computationally infeasible
  - Not stable in non-convex regions of the loss surface
  - Approximate methods address these issues, but simpler solutions may be better

Story so far : Learning rate

- 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*

Lets take a step back



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

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

- Problems arise because of requiring a fixed step size across all dimensions
  - Because steps 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

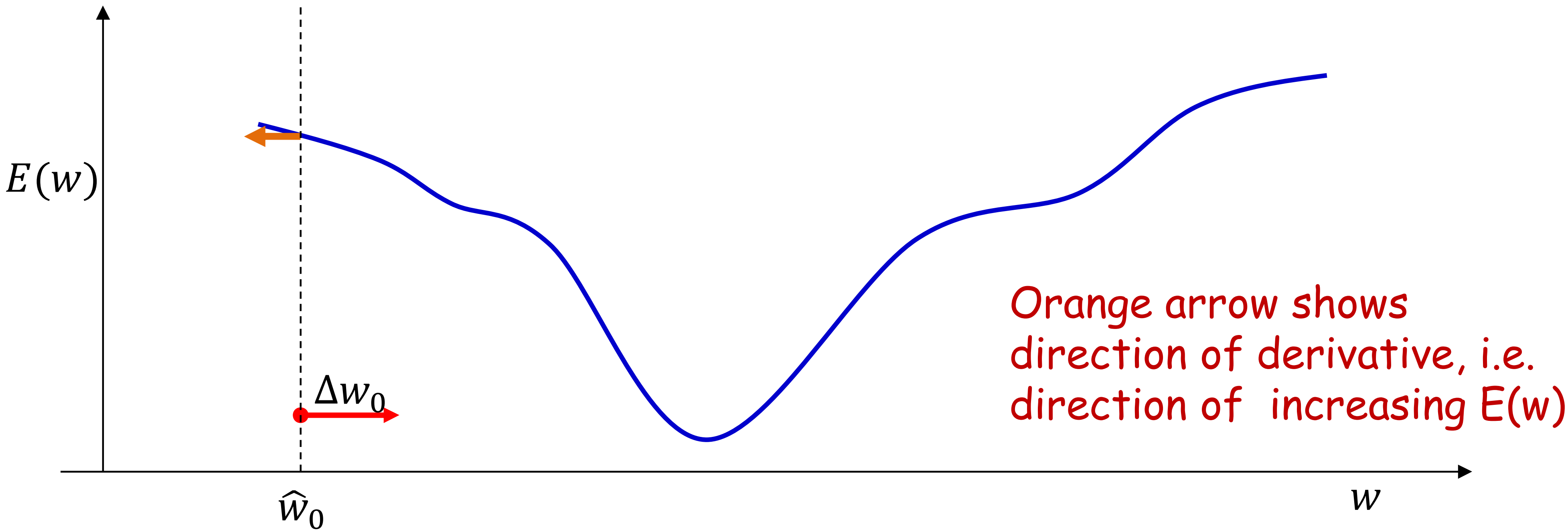
- Rprop
- Quick prop

RProp

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

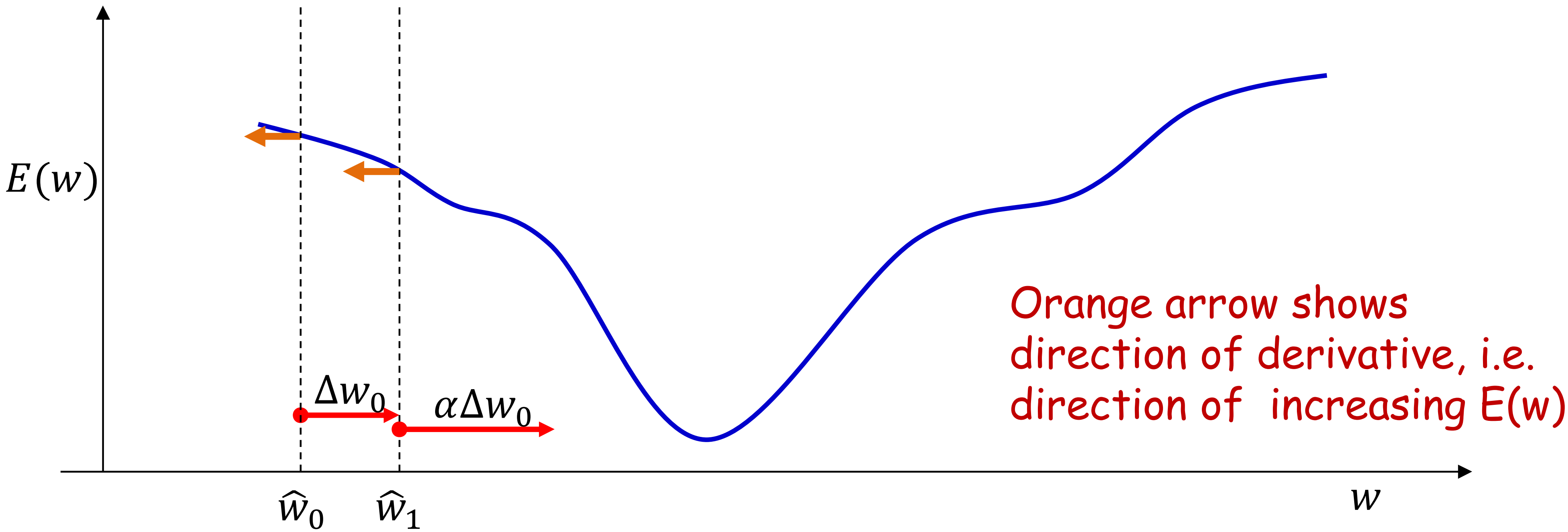
- At each time
  - If the derivative at the current location recommends continuing in the same direction as before (i.e. has not changed sign from earlier):
    - *increase* the step, and continue in the same direction
  - If the derivative has changed sign (i.e. we've overshot a minimum)
    - *reduce*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

Rprop



- Select an initial value $\hat{w}$ 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

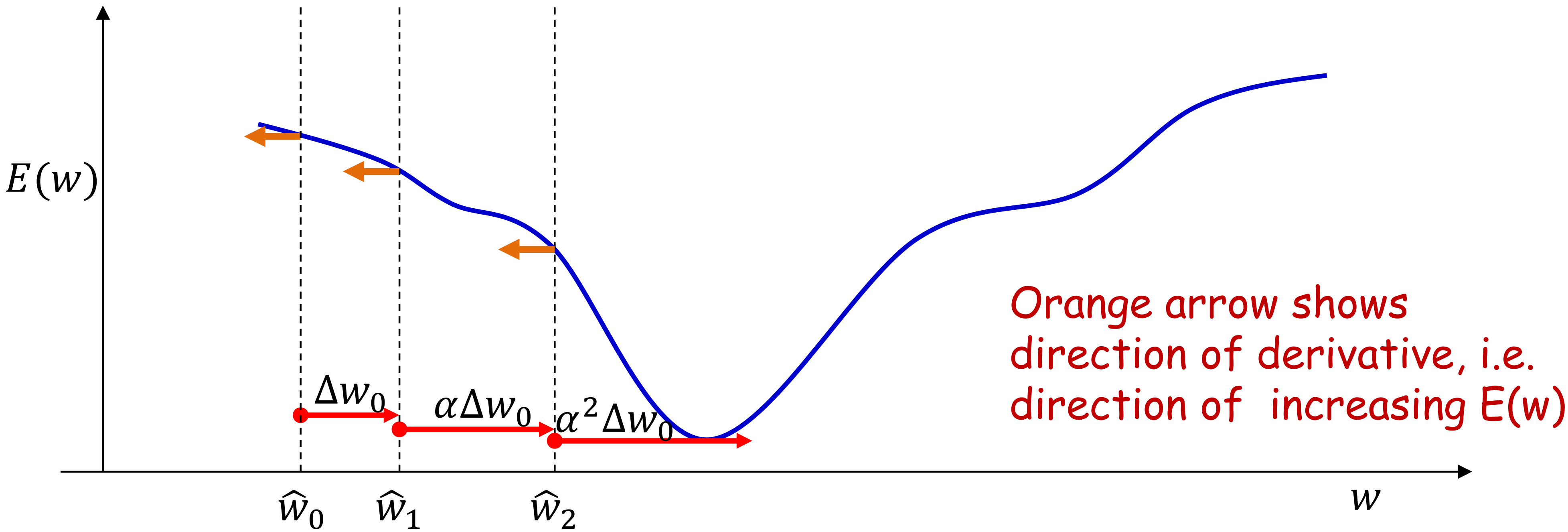


- Compute the derivative in the new location
  - If the derivative has not changed sign from the previous location, increase the step size and take a longer step

$\alpha > 1$

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

Rprop

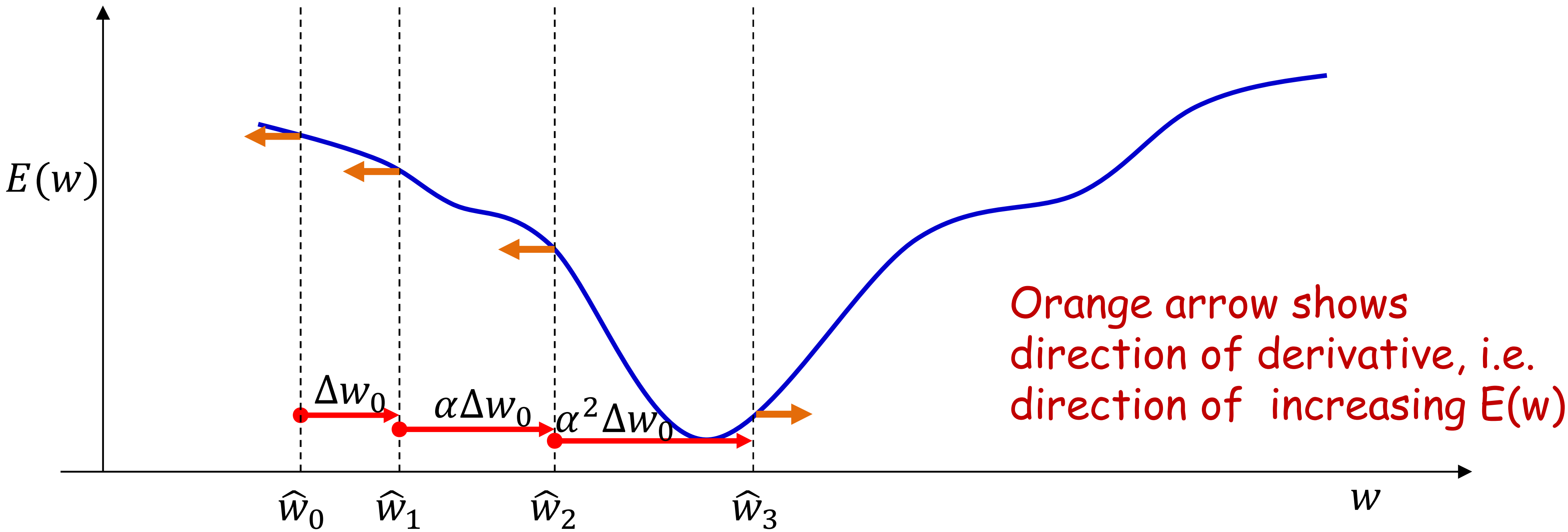


- Compute the derivative in the new location
  - If the derivative has not changed sign from the previous location, increase the step size and take a step

$\alpha > 1$

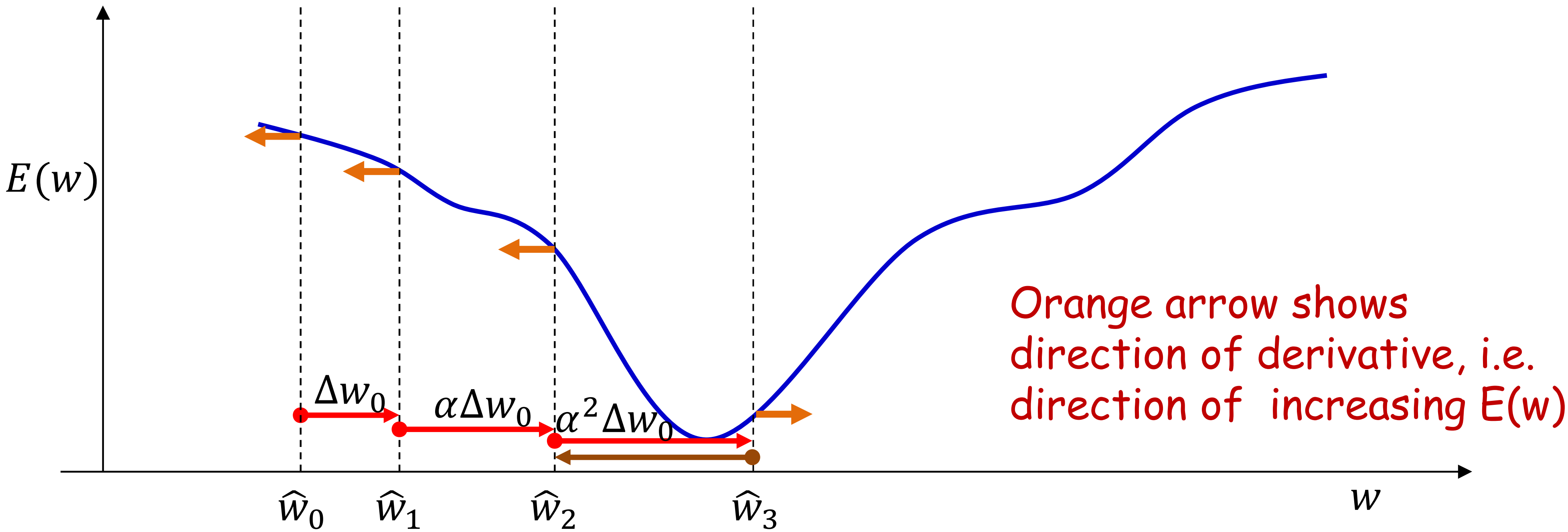
- $\Delta w = \alpha \Delta w$
- $\hat{w} = \hat{w} - \Delta w$

Rprop



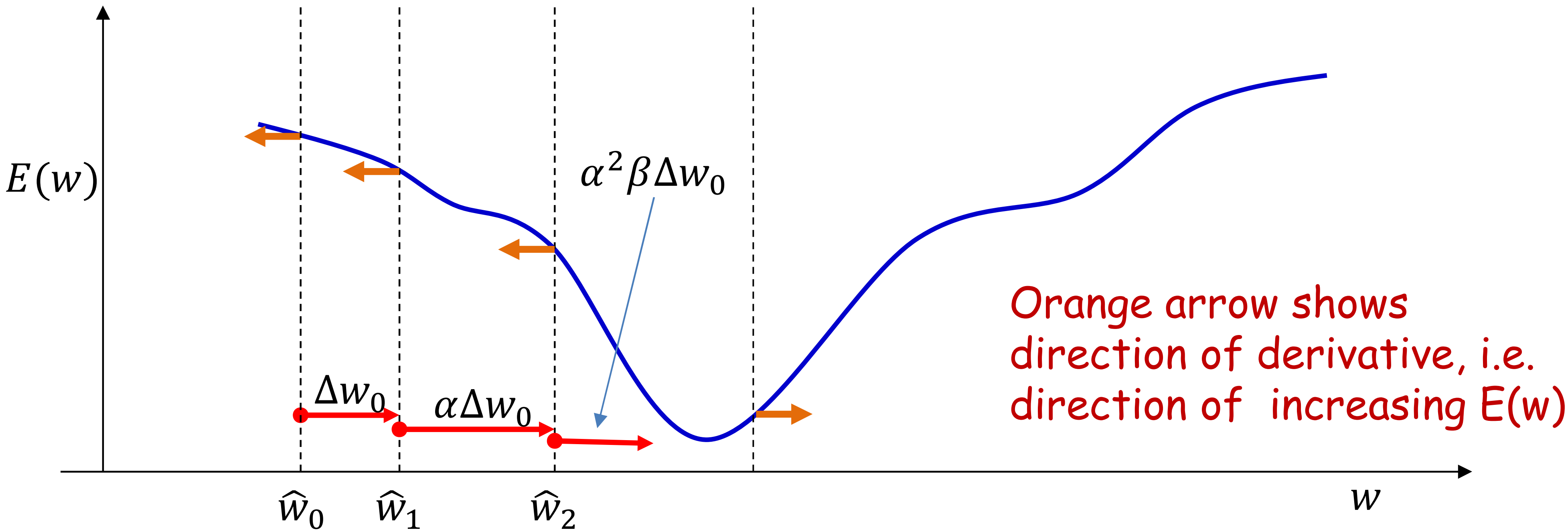
- Compute the derivative in the new location
  - If the derivative has changed sign

Rprop



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

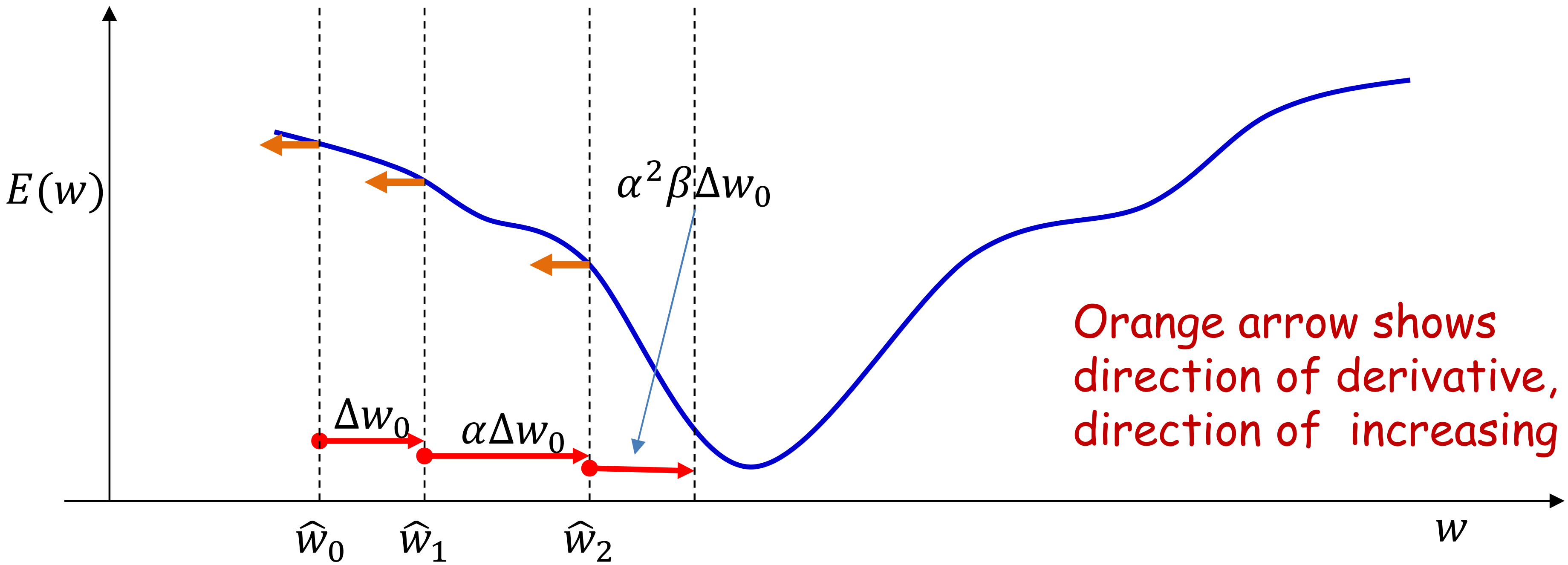
Rprop



- 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



Orange arrow shows direction of derivative, i.e. direction of increasing E(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
    - $\Delta w = \beta\Delta w$
  - 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 $w_{l,i,j}, \Delta w_{l,i,j} > 0,$
  - $prevD(l,i,j) = \frac{dLoss(w_{l,i,j})}{dw_{l,i,j}}$
  - $\Delta w_{l,i,j} = \text{sign}\big(prevD(l,i,j)\big)\Delta w_{l,i,j}$
  - While not converged:
    - $w_{l,i,j} = w_{l,i,j} - \Delta w_{l,i,j}$
    - $D(l,i,j) = \frac{dLos\ \ (w_{l,i,j})}{dw_{l,i,j}}$
    - 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:
  - Initialize $w_{l,i,j}, \Delta w_{l,i,j} > 0,$
  - $prevD(l,i,j) = \frac{dLoss(w_{l,i,j})}{dw_{l,i,j}}$
  - $\Delta w_{l,i,j} = \text{sign}\big(prevD(l,i,j)\big)\Delta w_{l,i,j}$
  - While not converged:
    - $w_{l,i,j} = w_{l,i,j} - \Delta w_{l,i,j}$
    - $D(l,i,j) = \frac{dLos\ (w_{l,i,j})}{dw_{l,i,j}}$
    - 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

Poll 3 (@384)

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

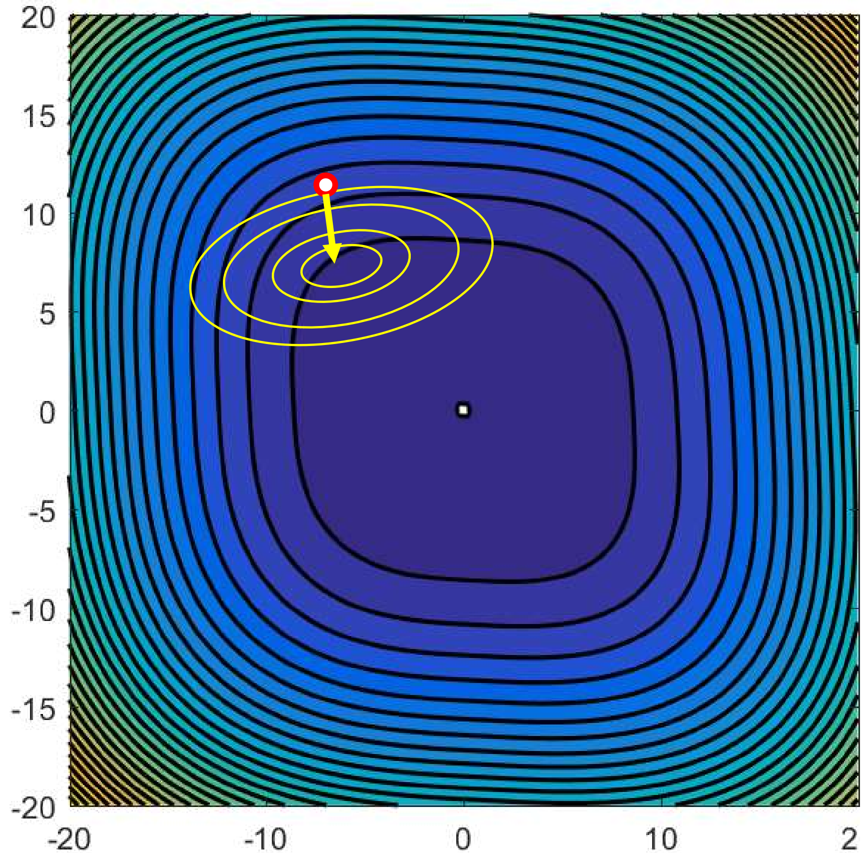
- Rprop will revert to the earlier estimate and take a smaller step
- Rprop will change direction and begin taking steps in the opposite direction

Poll 3

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

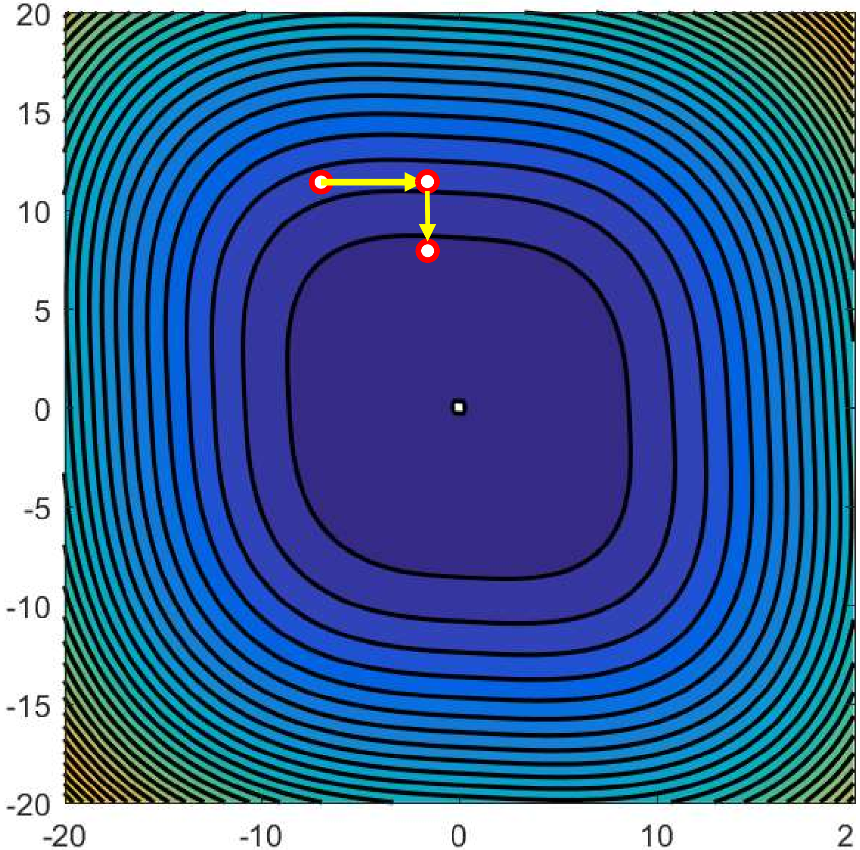


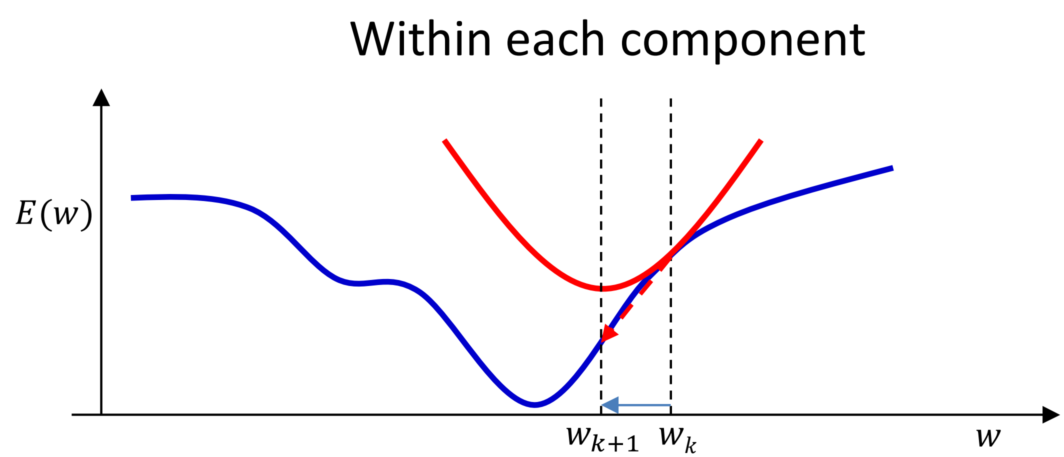
- Quickprop employs the Newton updates with two modifications

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

- But with two modifications

QuickProp: Modification 1



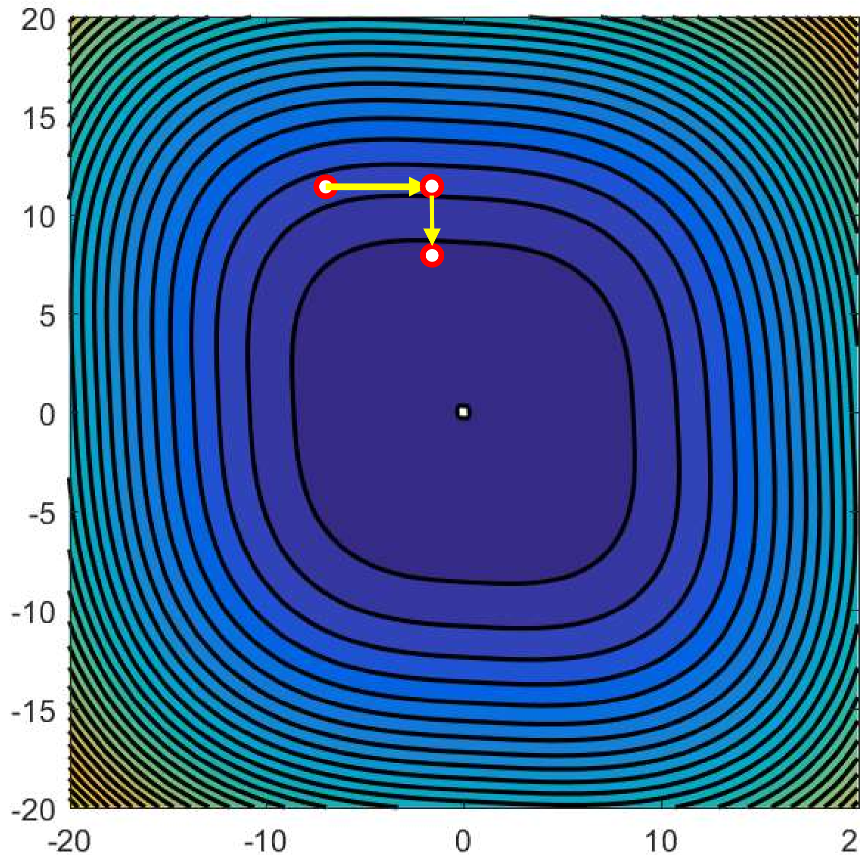


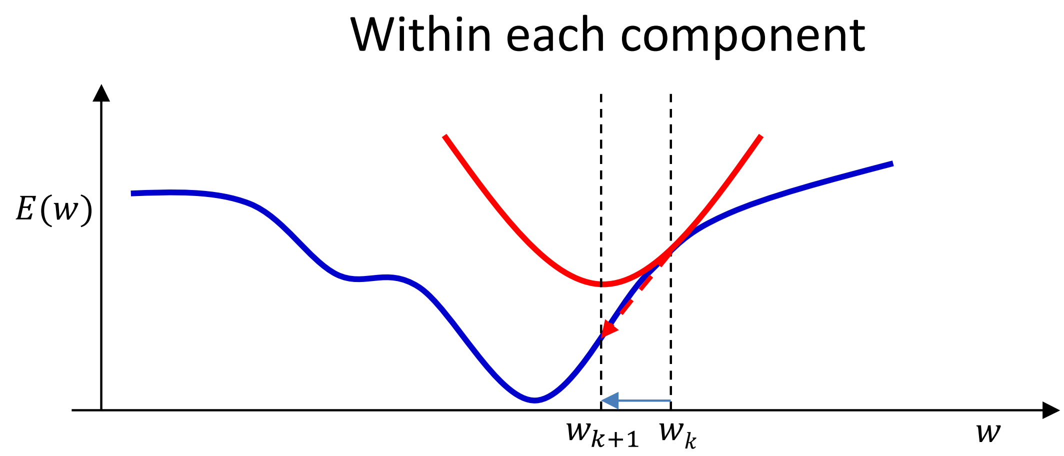
- It treats each dimension independently
- For $i = 1:N$

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

- 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

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

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

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

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:

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

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

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

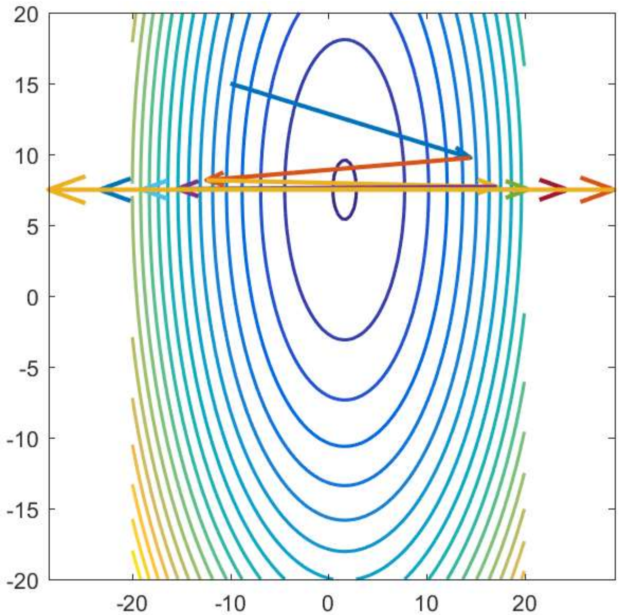
- Vanilla gradient descent may be too slow or unstable due to the differences between the dimensions

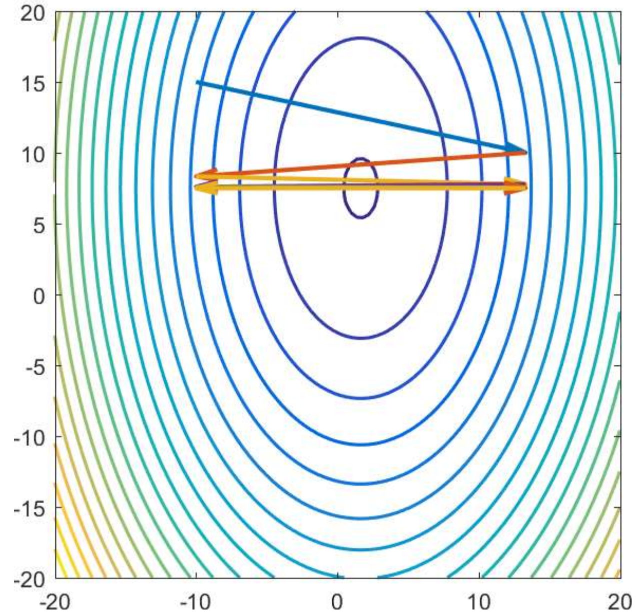
- Second order methods can normalize the variation across dimensions, but are complex

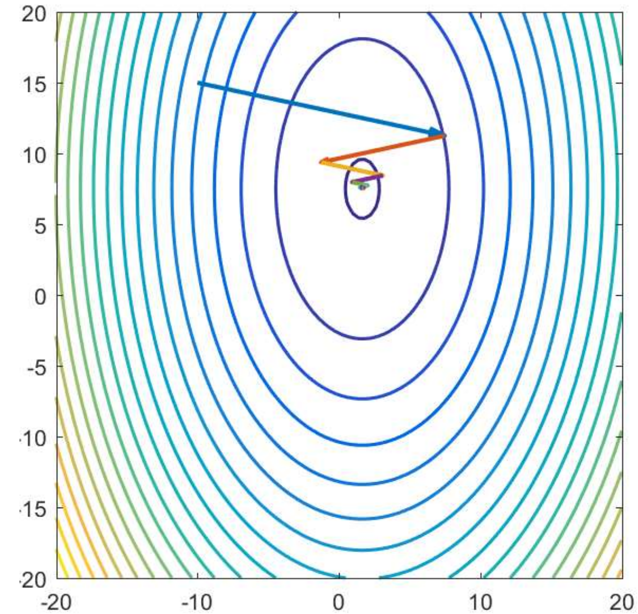
- Adaptive or decaying learning rates can improve convergence

- Methods that decouple the dimensions can improve convergence

A closer look at the convergence problem

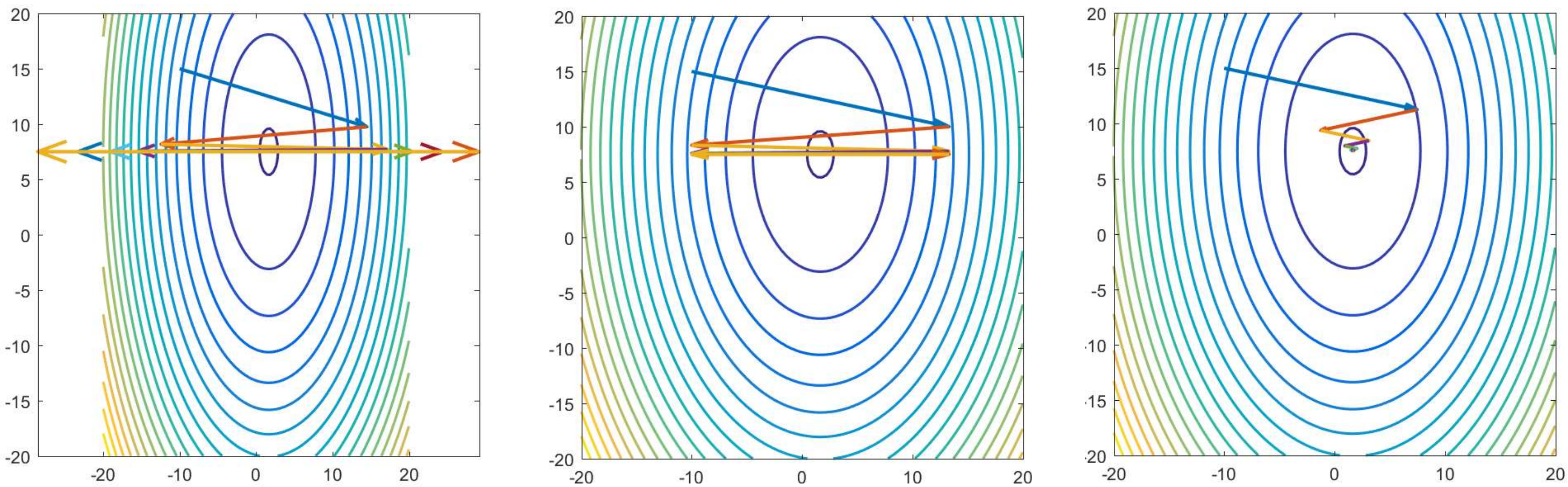






- With dimension-independent learning rates, the solution will converge smoothly in some directions, but oscillate or diverge in others

A closer look at the convergence problem

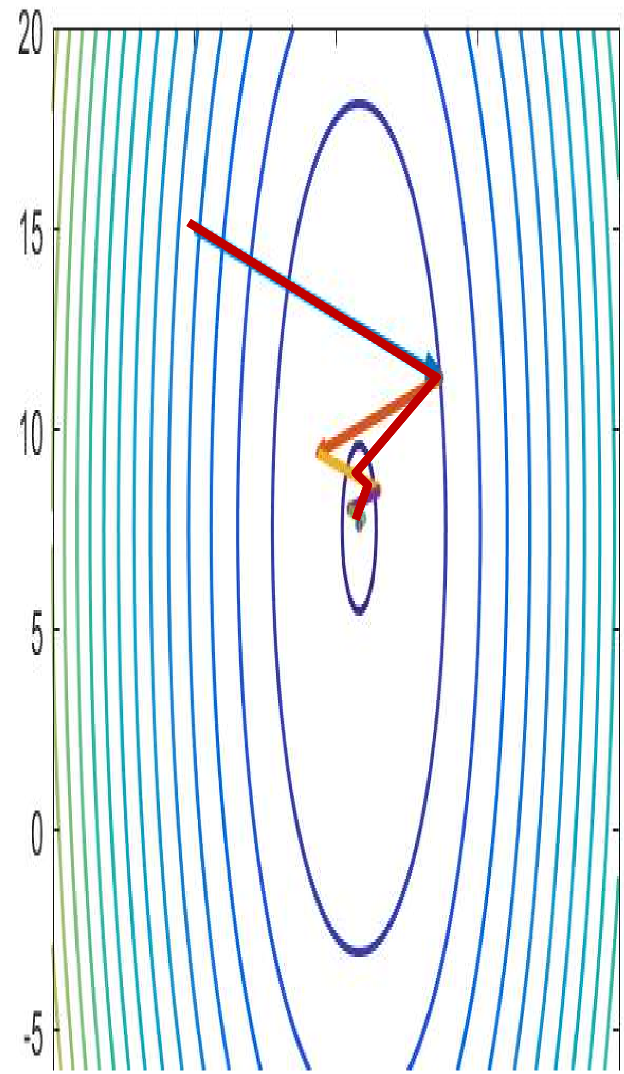


- With dimension-independent learning rates, the solution will converge smoothly in some directions, but oscillate or diverge in others

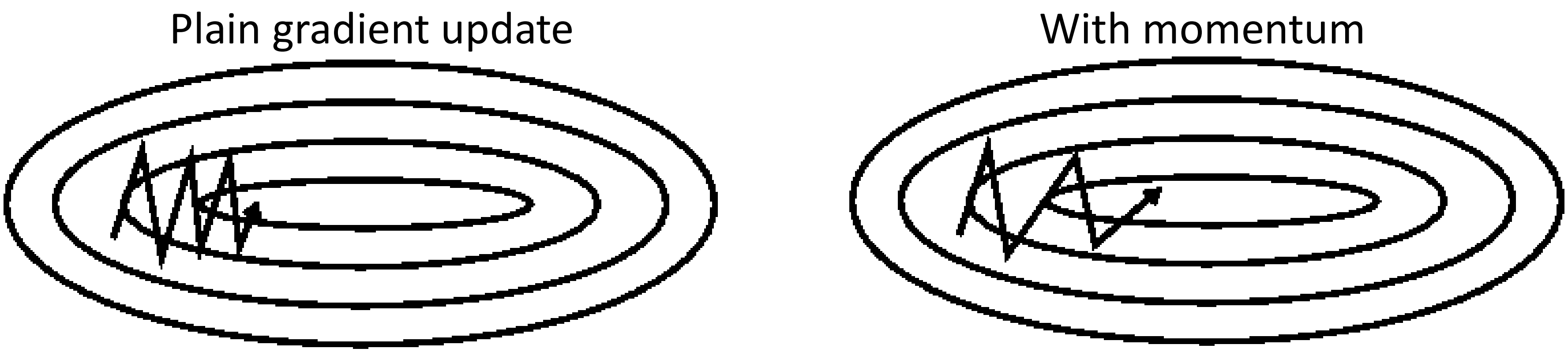
- **Proposal:**
  - Keep track of oscillations
  - Emphasize steps in directions that converge smoothly
  - Shrink steps in directions that bounce around..

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



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

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

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

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

Training by gradient descent

- Initialize all weights $\mathbf{W}_1, \mathbf{W}_2, \dots, \mathbf{W}_K$
- 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

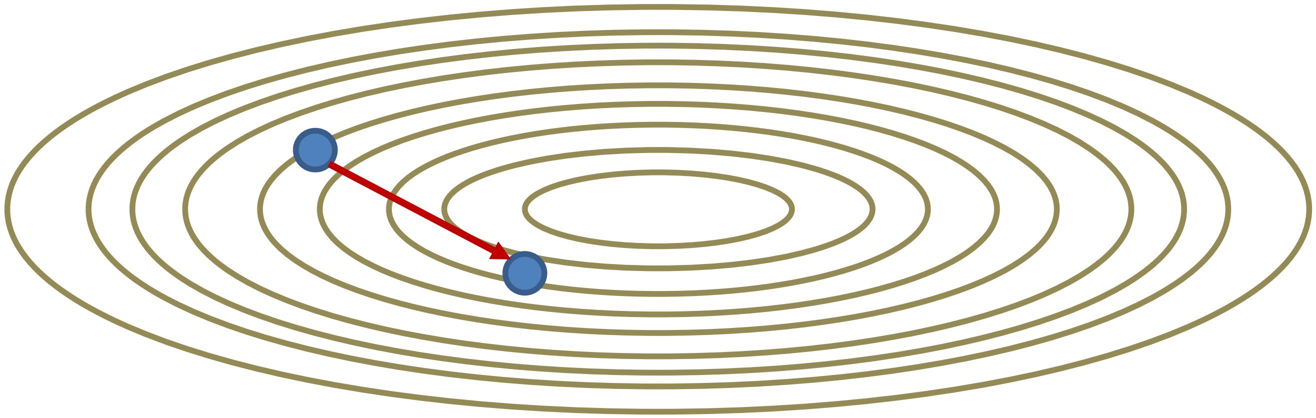
Training with momentum

- Initialize all weights $\mathbf{W}_1, \mathbf{W}_2, \dots, \mathbf{W}_K$
- 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

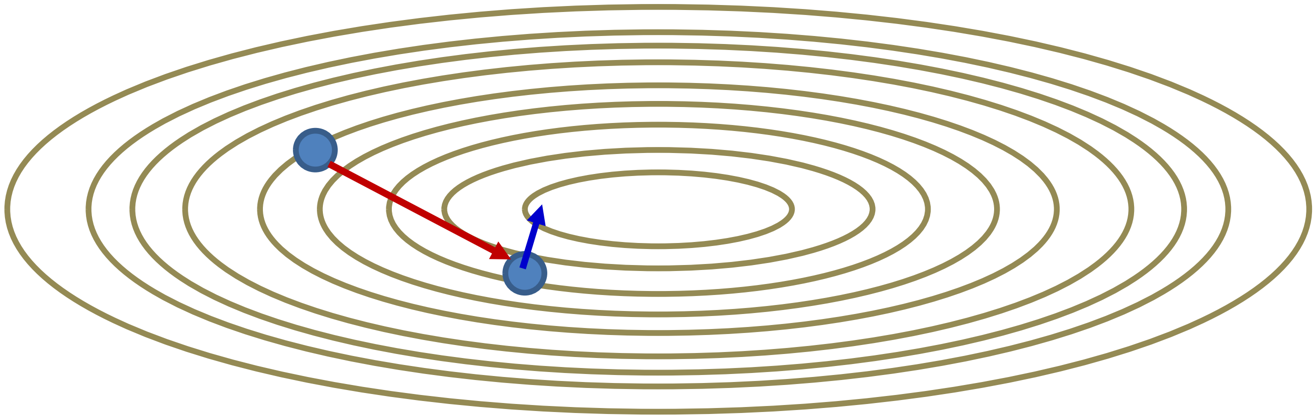


- The momentum method

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

- At any iteration, to compute the current step:

Momentum Update

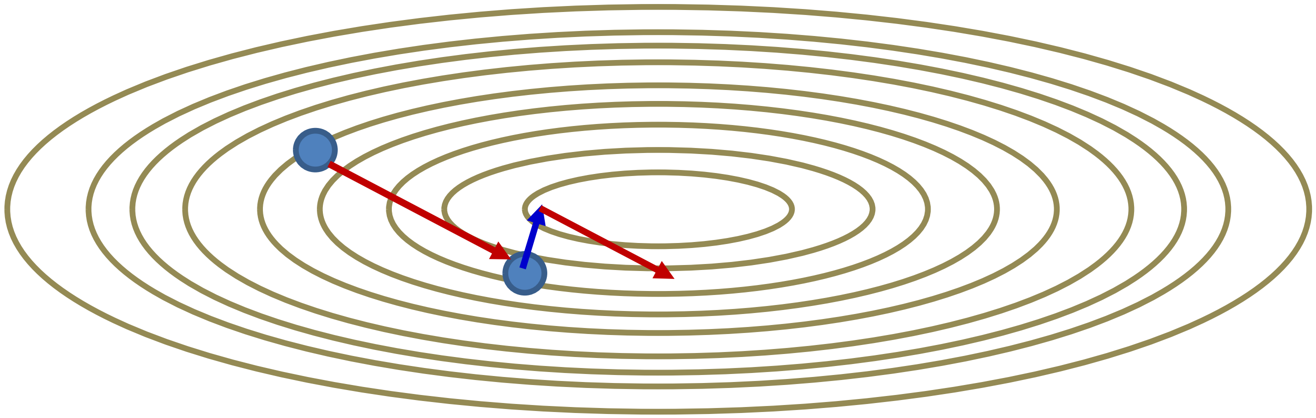


- The momentum method

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

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

Momentum Update

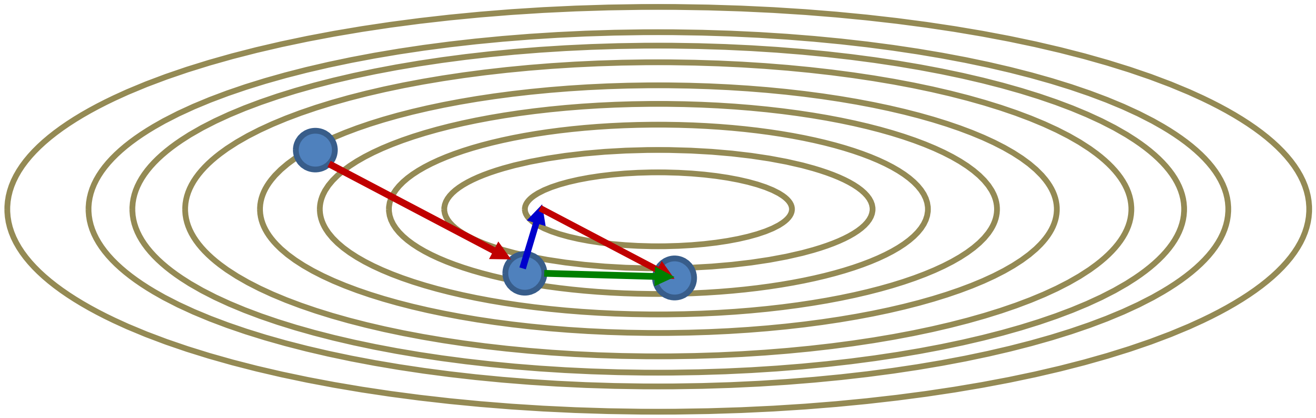


- The momentum method

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

- 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

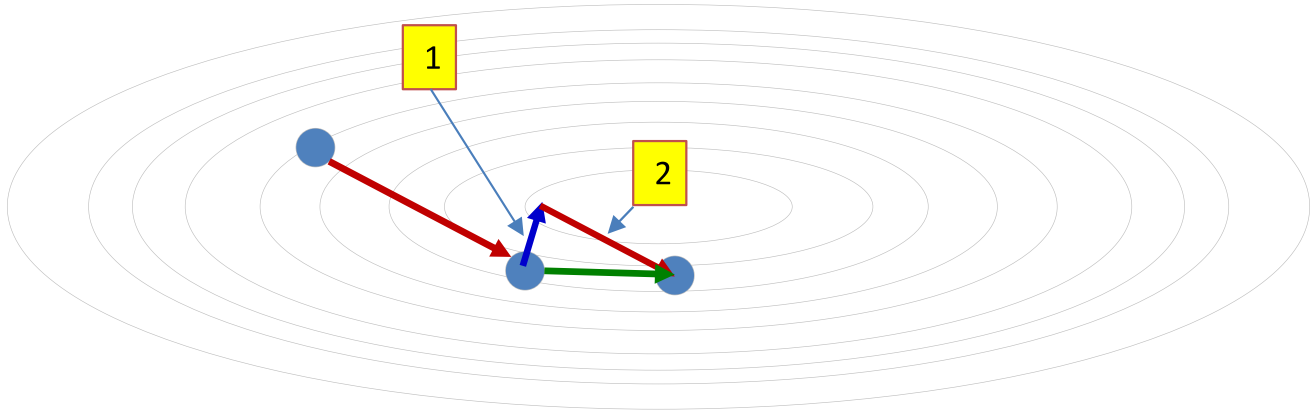


- The momentum method

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

- 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

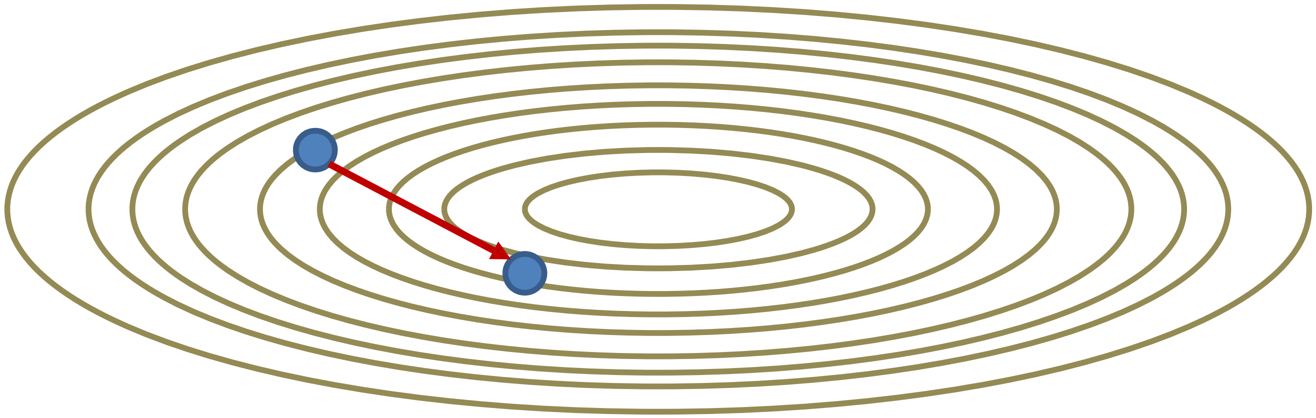
Momentum update



- 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

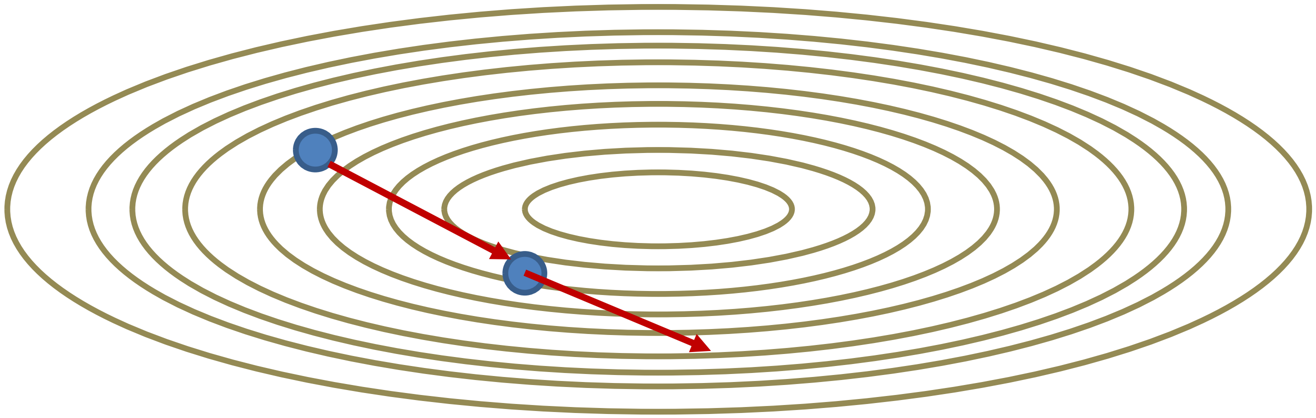
- The procedure can be made more optimal by reversing the order of operations..

Nestorov's Accelerated Gradient



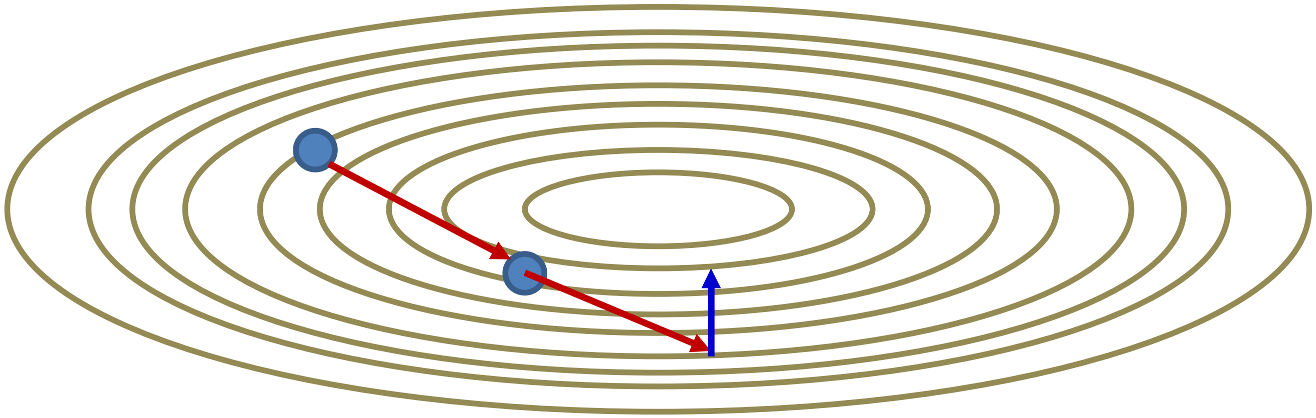
- Change the order of operations
- At any iteration, to compute the current step:

Nestorov's Accelerated Gradient



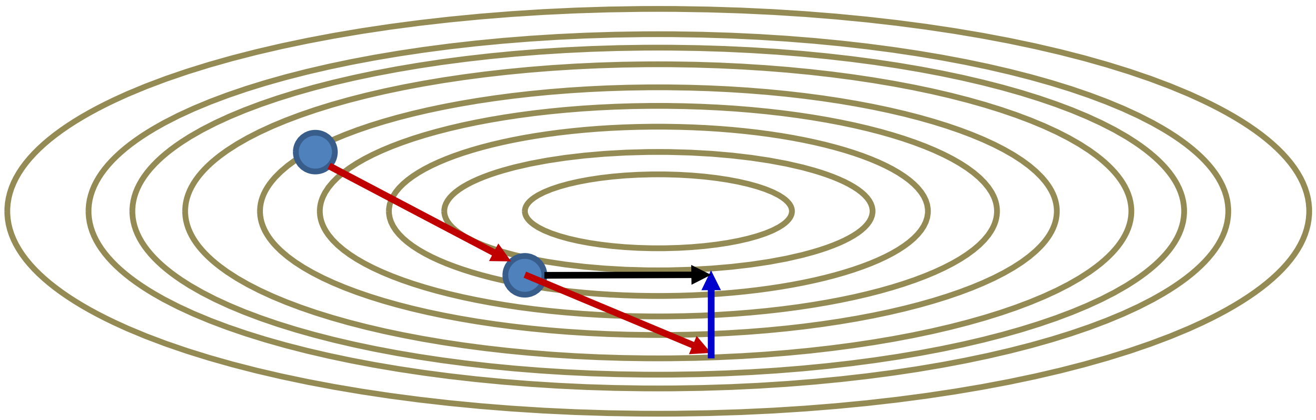
- Change the order of operations
- At any iteration, to compute the current step:
  - First extend the previous step

Nestorov's Accelerated Gradient



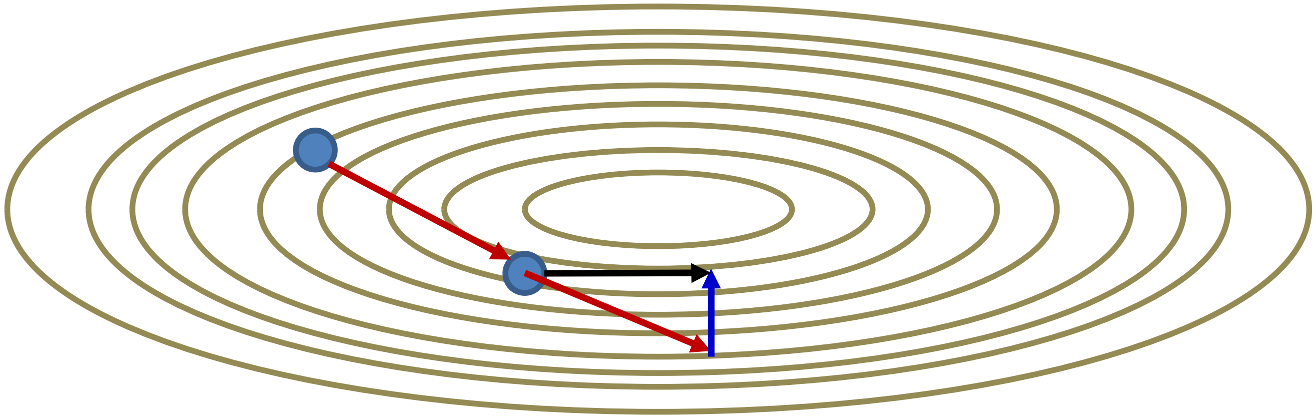
- Change the order of operations
- At any iteration, to compute the current step:
  - First extend the previous step
  - Then compute the gradient step at the resultant position

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

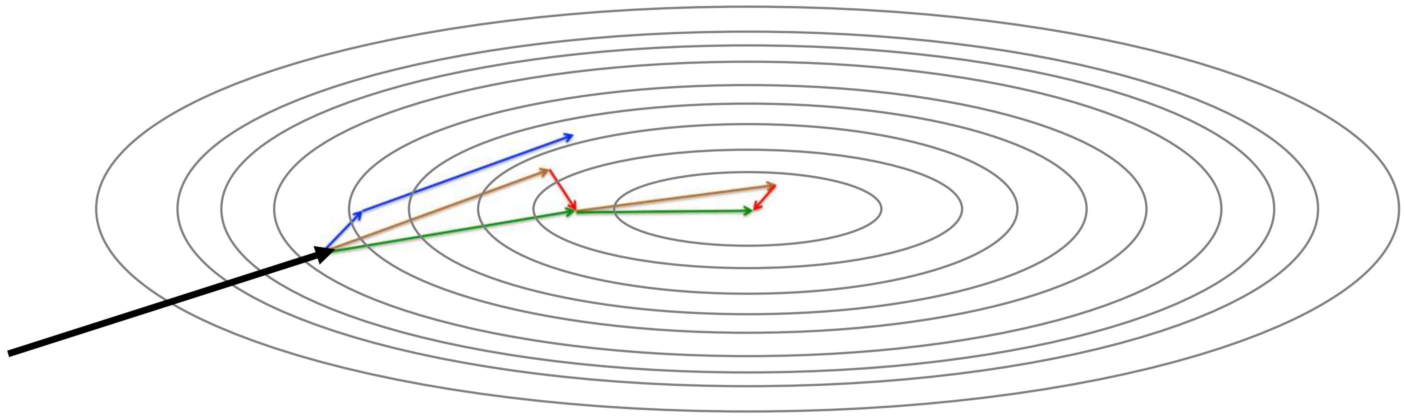


- Nestorov's method

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

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

Nestorov's Accelerated Gradient



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

Training with Nestorov

- Initialize all weights $\mathbf{W}_1, \mathbf{W}_2, \dots, \mathbf{W}_K$
- 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..

Poll 4 (@385)

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