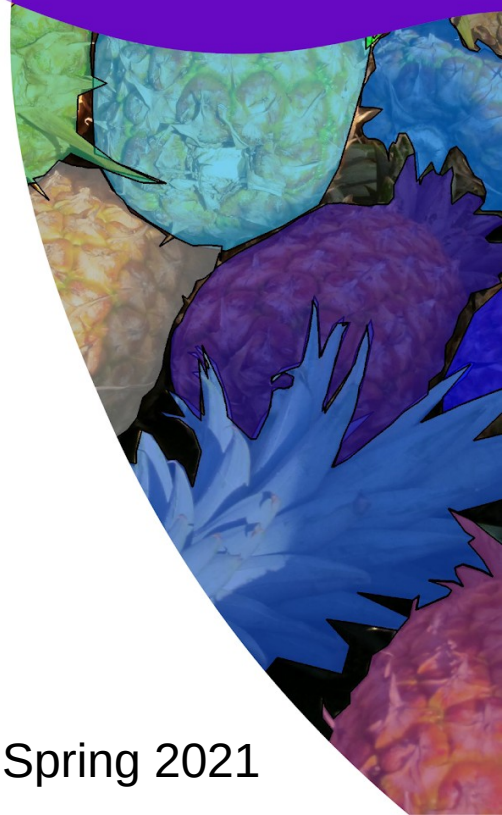
NEW YORK UNIVERSITY

Optimization for Deep Learning



Yann LeCun
NYU - Courant Institute & Center for Data Science
Facebook AI Research
With material from **Aaron Defazio** (FAIR)

The Convergence of Gradient Descent

parameter

training sample

$$f(w) = \frac{1}{P}\sum_{i=1}^{P} L(x_i, y_i, w)$$

objective

per-sample loss

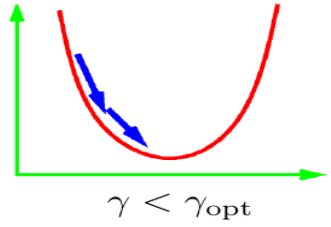
learning rate

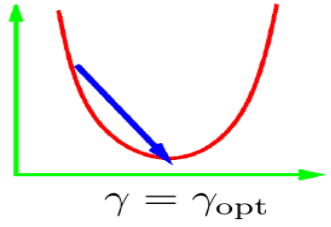
$$w_{k+1} \leftarrow w_k - \gamma_k \frac{\partial f(w_k)}{\partial w}^T$$

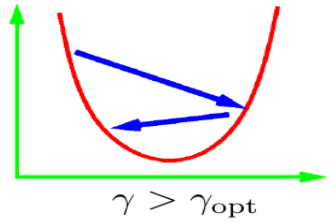
new parameter

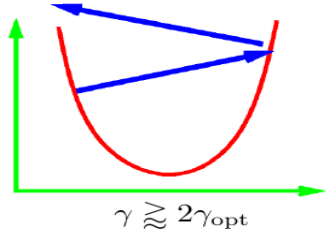
Gradient (transposed)

- **f(w): objective function**
  - average of many terms
- **Gradient descent**
  - uses local slope information of a function to move towards a minimum.
- **Requires a step size**
  - aka “learning rate”



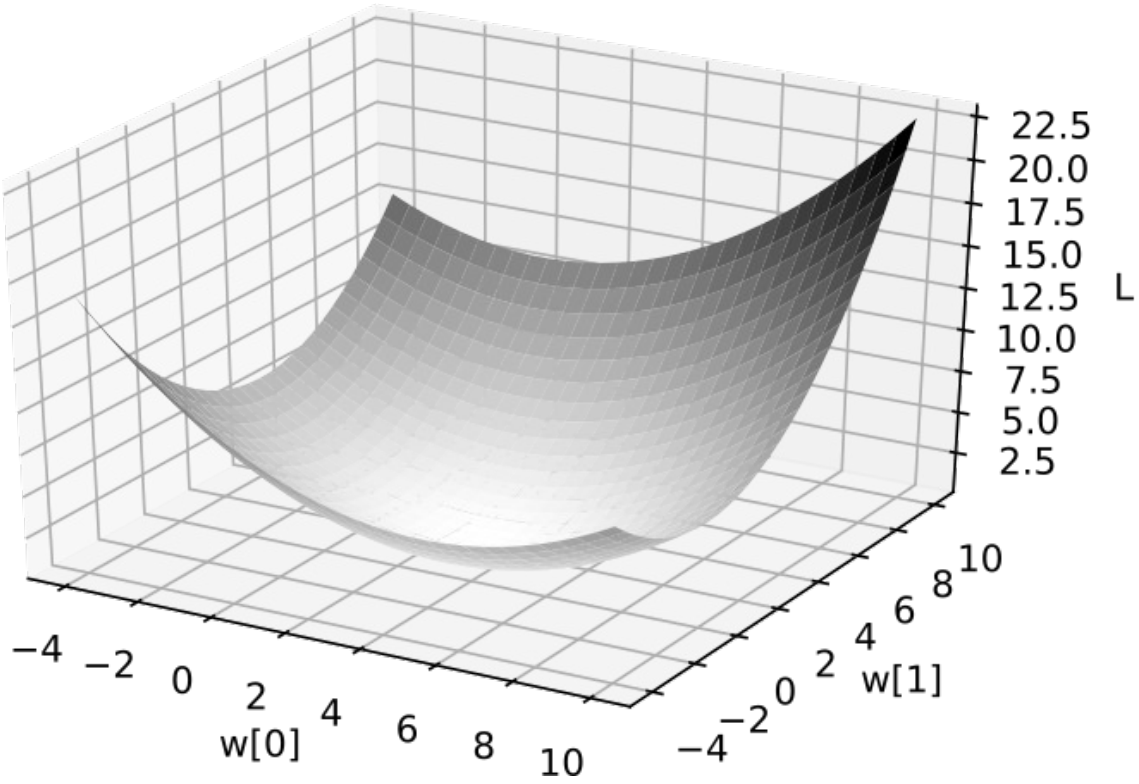


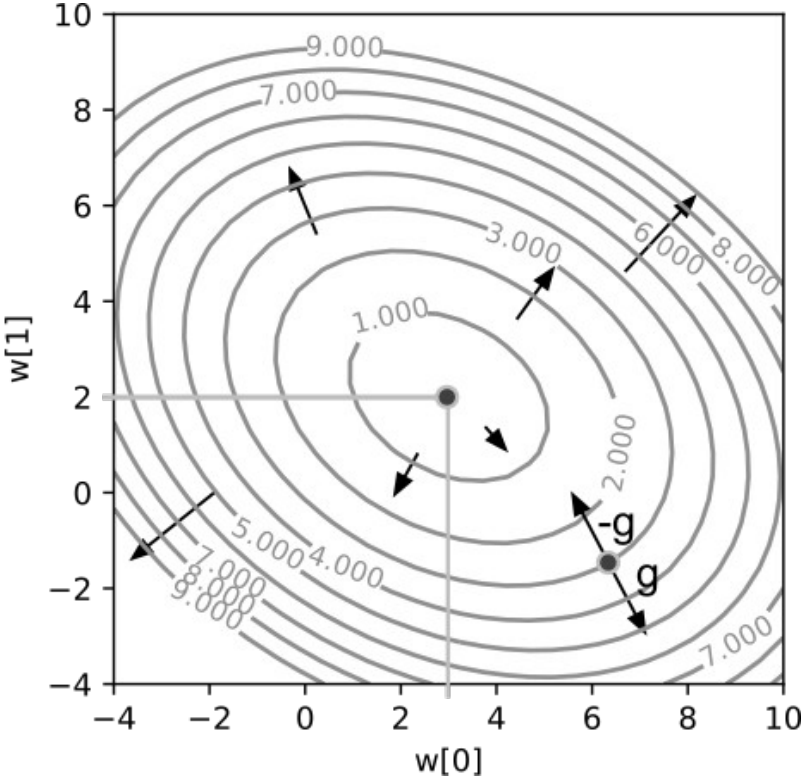




Gradient descent

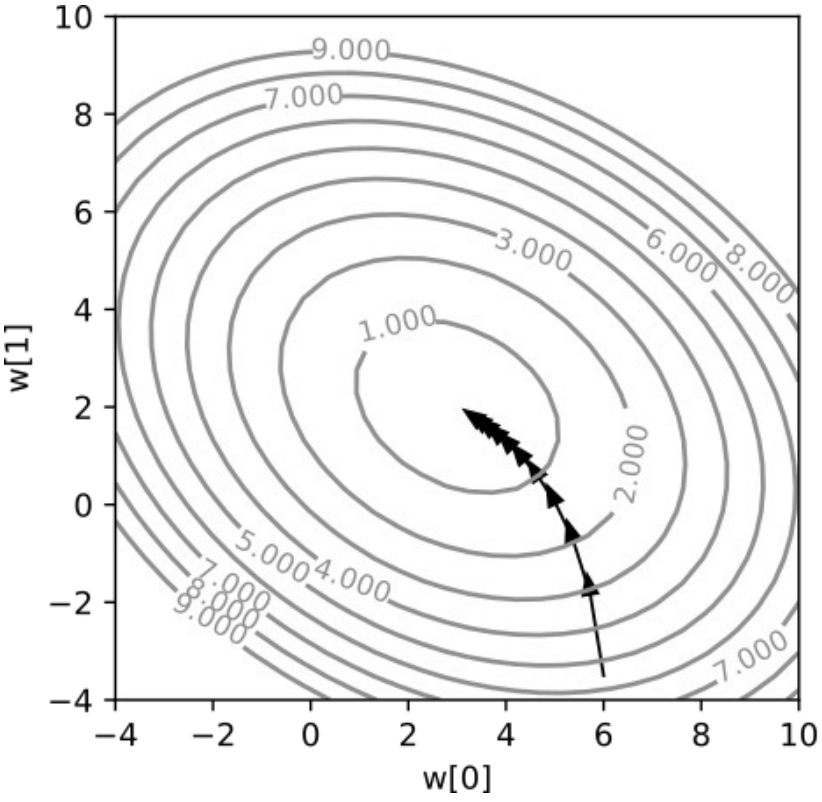
- **Gradient indicates the direction of steepest ascent.**
- **Convex, quadratic case.**

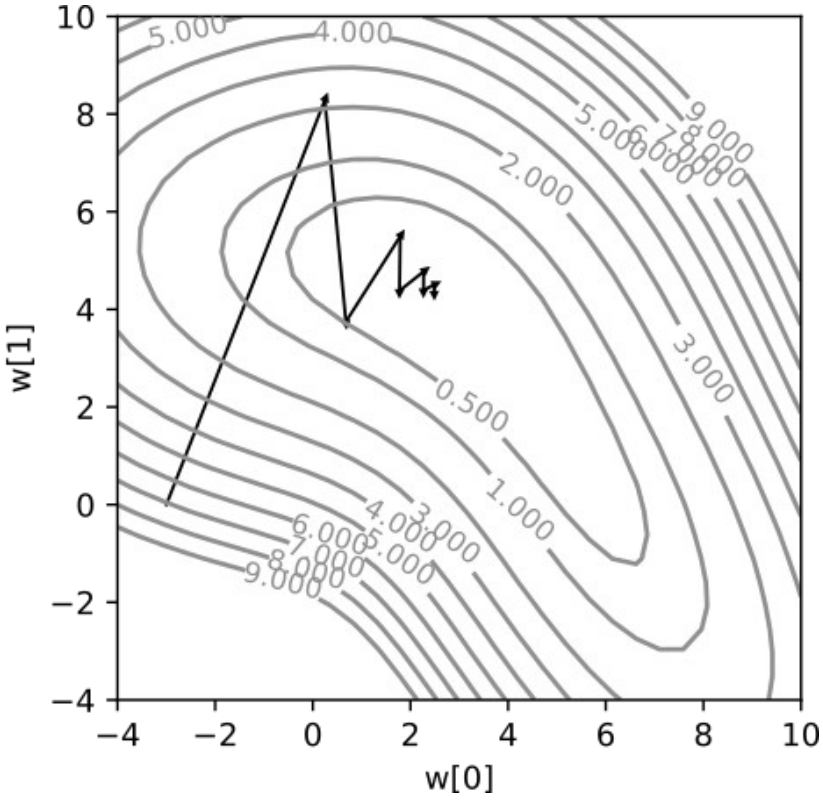




Gradient descent

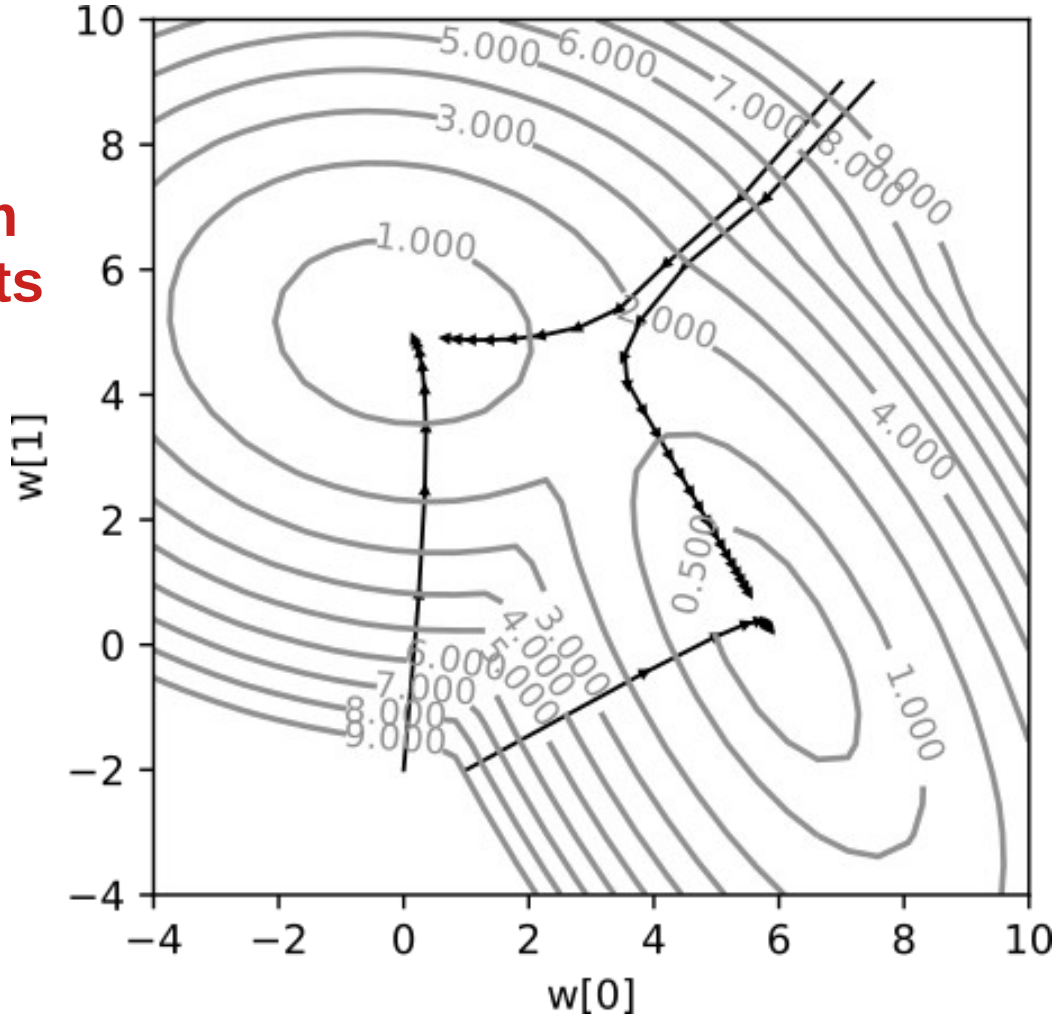
- **Small learning rate, Large learning rate**





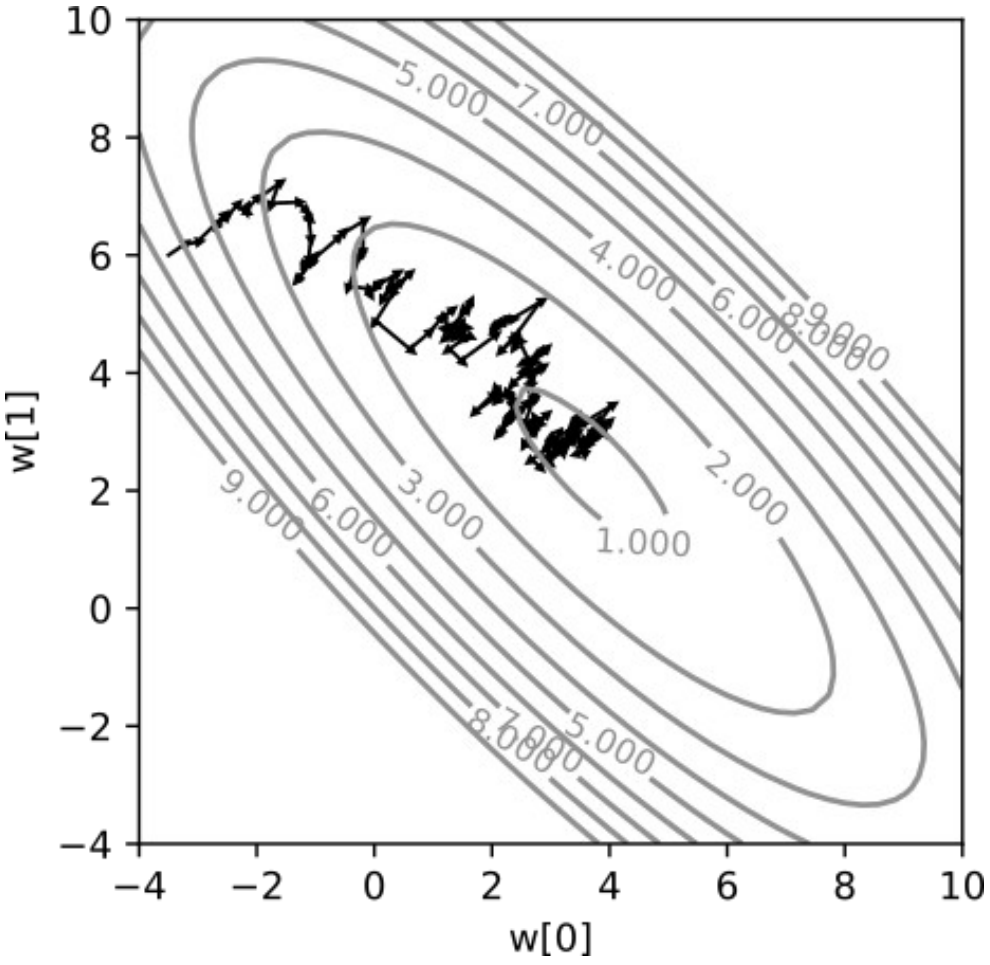
Gradient descent

- **Non convex objective**
- **This is not as much of a problem as you might think for neural nets**
  - Because of the high dimension
  - More on this later



Stochastic Gradient {Descent,Optimization}

- **For when the objective is an average of many similar terms**
- **Erratic but fast convergence**
- **Exploits the redundancy in the data**
- **Difficult to prove the convergence theoretically**
  - Bottou, L., Curtis, F. E., & Nocedal, J. (2018). Optimization methods for large-scale machine learning. Siam Review, 60(2), 223-311.



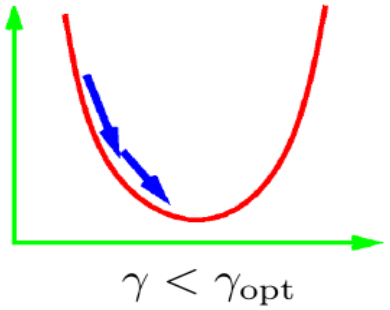
The Convergence of Gradient Descent

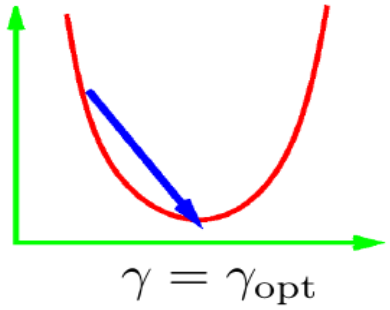
$$w_{k+1} \leftarrow w_k - \gamma_k \frac{\partial f(w_k)}{\partial w}$$

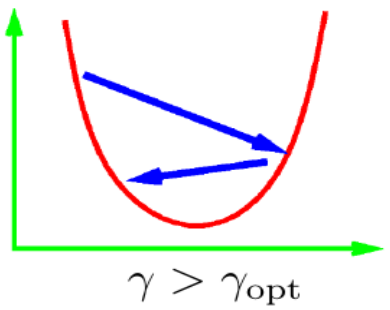
$$f(w) = \frac{1}{P} \sum_{i=1}^{P} L(x_i, y_i, w)$$

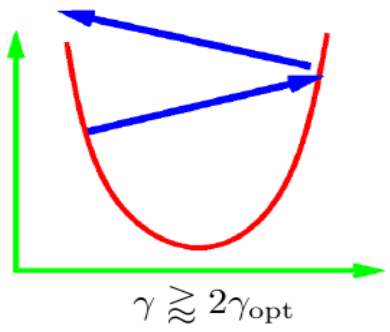
- **Batch Gradient**
- **There is an optimal learning rate**
- **Equal to inverse 2nd derivative**

$$\gamma_{opt} = \left(\frac{\partial^2 f(w)}{\partial w^2} \right)^{-1}$$









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- **Batch Gradient**
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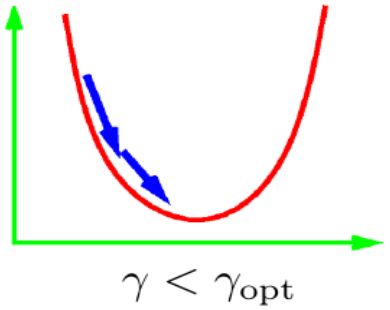
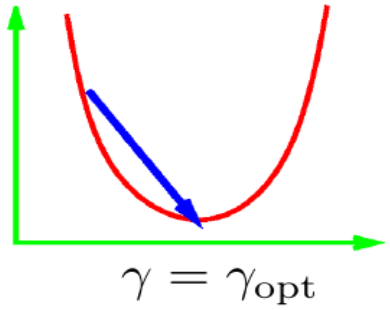
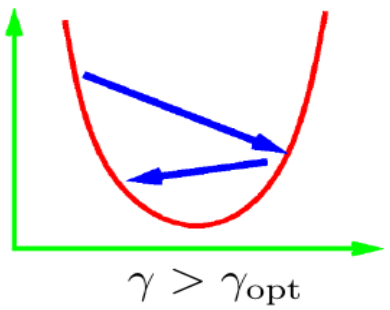
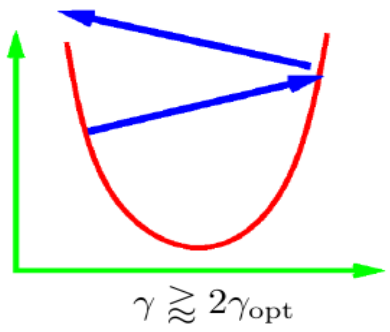




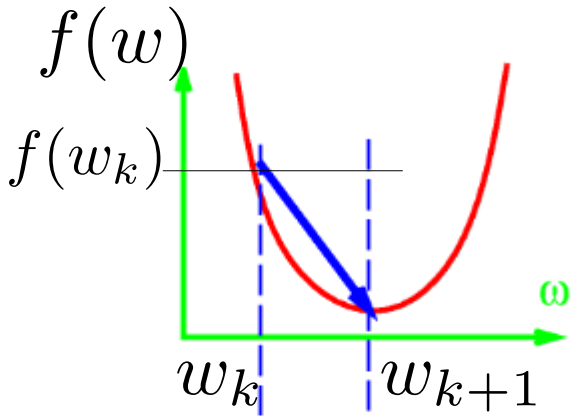


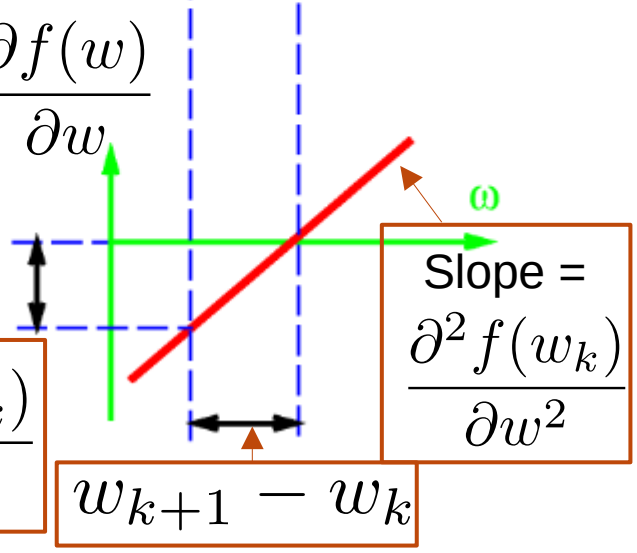


Optimal learning rate in 1D (with formulas for multidim)

- **Quadratic objective function: parabola**
- **Gradient (derivative): line**
- **Slope of gradient line: 2nd derivative**
- **For what value of w does the gradient line intersect the x axis (zero gradient)?**

$$(w_{k+1} - w_k)^T \frac{\partial^2 f(w_k)}{\partial w^2} = \frac{\partial f(w_{k+1})}{\partial w} - \frac{\partial f(w_k)}{\partial w}$$





Optimal learning rate in 1D (with formulas for multidim)

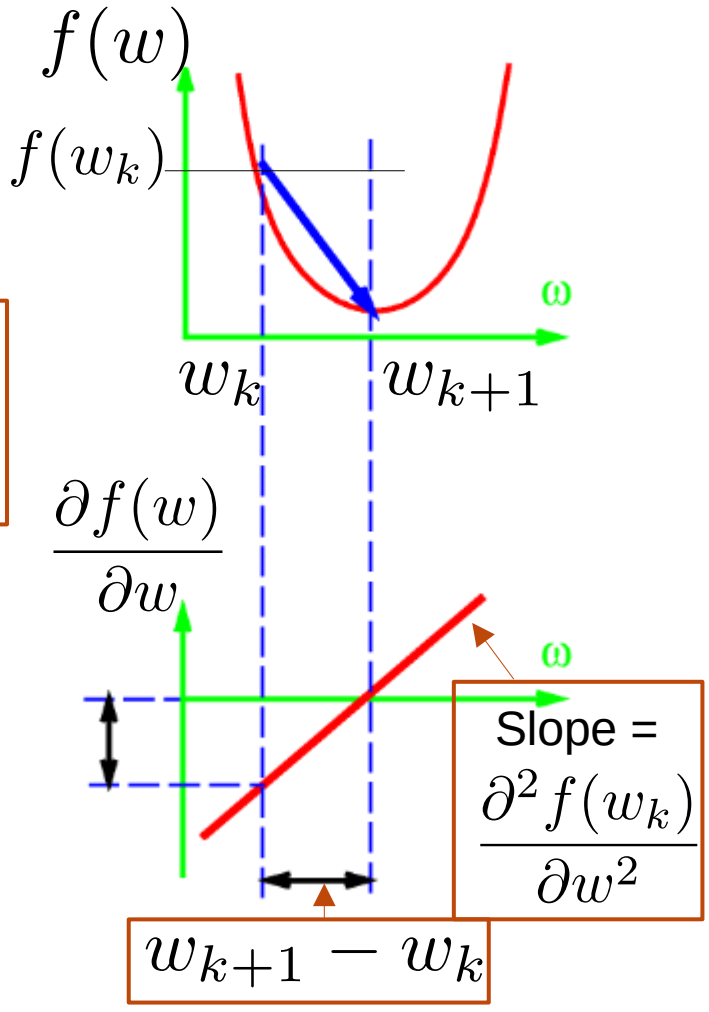
- **Solve for w with gradient at $w_{k+1} = 0$**

$$\frac{\partial^2 f(w_k)}{\partial w^2}^T (w_{k+1} - w_k) = \frac{\partial f(w_{k+1})}{\partial w}^T - \frac{\partial f(w_k)}{\partial w}^T$$

$$\frac{\partial f(\check{w})}{\partial w}^T = 0 \qquad \boxed{\frac{\partial^2 f(w_k)}{\partial w^2}(\check{w} - w_k) = -\frac{\partial f(w_k)}{\partial w}^T}$$

$$\check{w} = w_k - \frac{\partial^2 f(w_k)}{\partial w^2}^{-1} \frac{\partial f(w_k)}{\partial w}^T$$

$$\boxed{\gamma_{opt} = \left(\frac{\partial^2 f(w)}{\partial w^2}\right)^{-1}}$$



Theory for the quadratic case

Theory in the quadratic (positive definite) case

$$f(w) = \frac{1}{2} w^\top A w - b^\top w$$
$$\nabla f(w) = Aw - b$$
$$w_* = A^{-1} b$$

$$w_{k+1} = w_k - \gamma \nabla f(w_k)$$

$$\begin{aligned}
\|w_{k+1} - w_*\| &= \|w_k - \gamma(Aw_k - b) - w_*\| \\
&= \|w_k - \gamma A(w_k - A^{-1}b) - w_*\| \\
&= \|w_k - \gamma A(w_k - w_*) - w_*\| \\
&= \|(I - \gamma A)(w_k - w_*)\| \\
&\leq \|I - \gamma A\| \, \|w_k - w_*\|
\end{aligned}$$

Let μ be the minimum eigenvalue of A and L the max. Then the extremal eigenvalues of $I - \gamma A$ are $1 - \mu\gamma$ and $1 - L\gamma$, so:

$$\|I - \gamma A\| = \max\{|1 - \mu\gamma|, |1 - L\gamma|\}$$

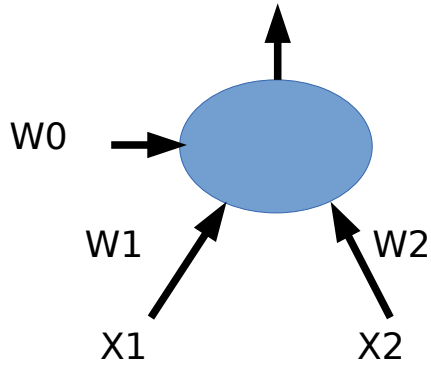
If we use two large a step size $1 - L\gamma$ becomes negative. A standard value is $\gamma = 1/L$ which gives:

$$\|w_{k+1} - w_*\| \leq \left(1 - \frac{\mu}{L}\right) \|w_k - w_*\|$$

[Defazio 2020]

Let's Look at a single linear unit

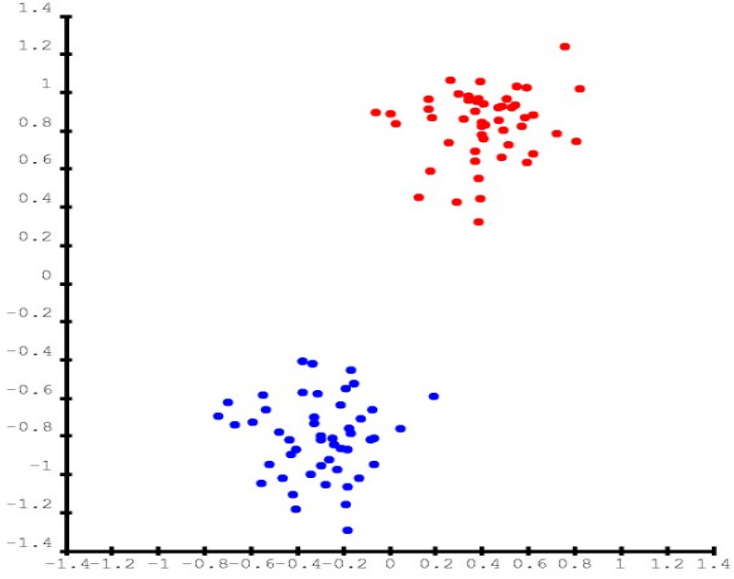
- **Single unit, 2 inputs**
- **Quadratic loss** $L(x, y, w) = (y - w^t x)^2$



- **Dataset: classification: y=-1 for blue, +1 for red.**
- **Second derivative matrix = Hessian**
- **is covariance matrix of input vectors**

$$H = \frac{\partial^2 f(w)}{\partial w} = \frac{1}{P} \sum_{i=1}^{p} x(i) x(i)^T$$

- **To avoid ill conditioning: normalize the in**
  - Zero mean
  - Unit variance for all variable



Theory for the quadratic case

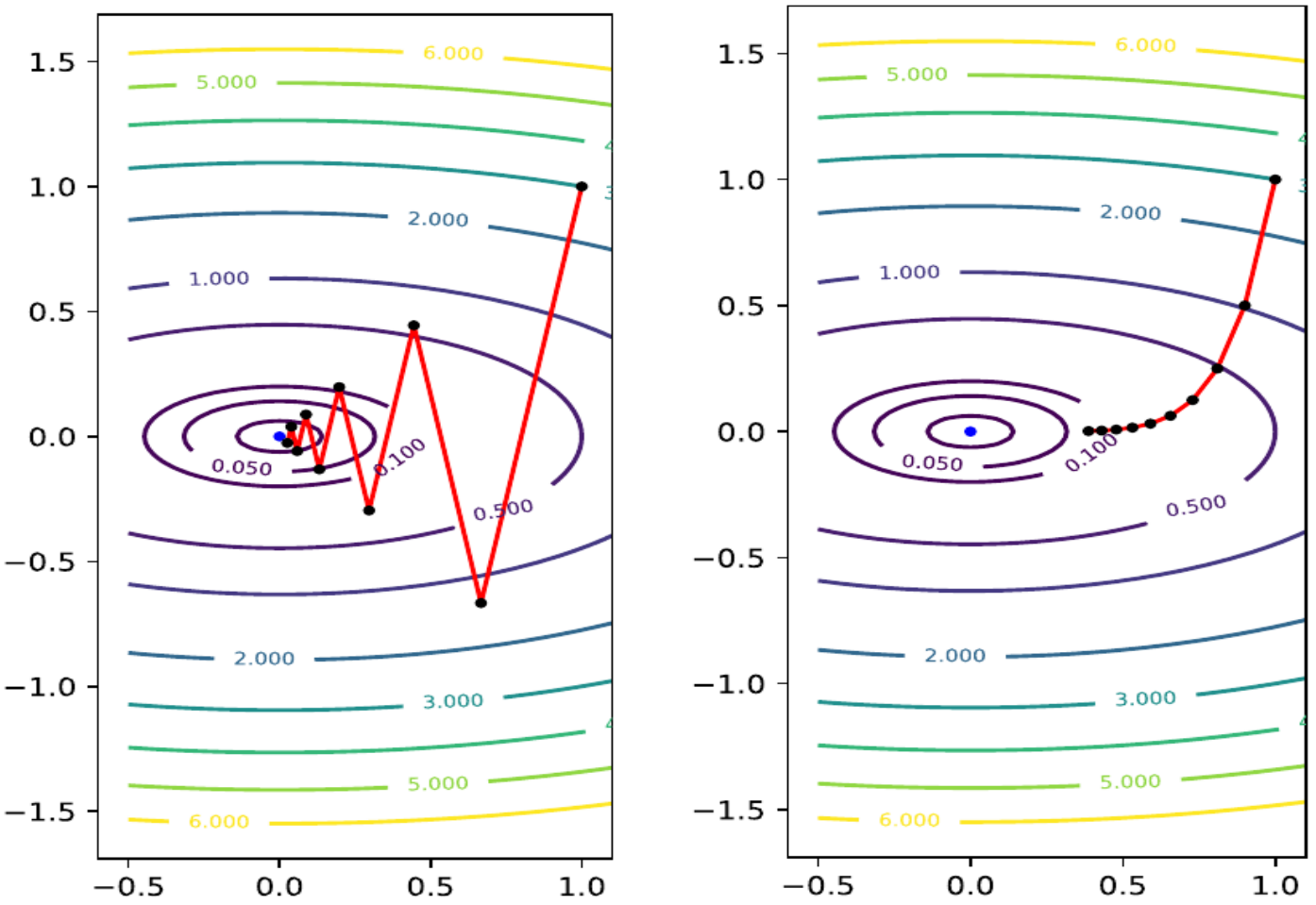
The convergence of optimization methods depends on the condition number of a problem

Inverse of the condition number

$$\|w_{k+1} - w_*\| \leq \left(1 - \frac{\mu}{L}\right) \|w_k - w_*\|$$

The condition number only formally makes sense on simple problems ("strongly convex")
But we often talk about "**poorly conditioned**" and "**well conditioned**" problems in machine learning informally

Step size should be as large as possible



Convergence is Slow When Hessian has Different Eigenvalues

Batch Gradient, small learning rate

Learning rate:

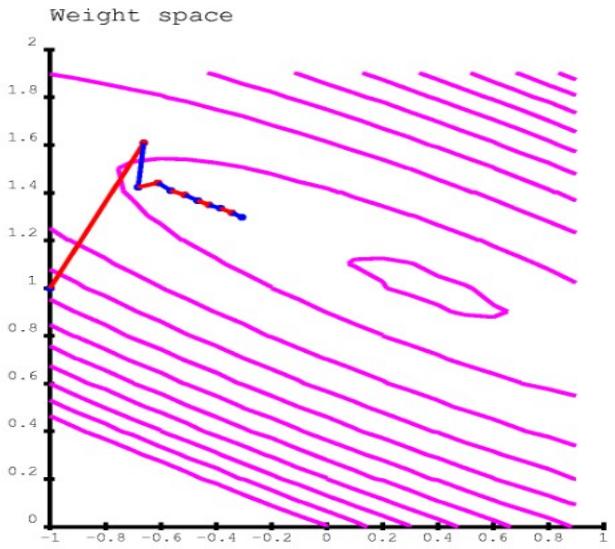
$\eta = 1.5$

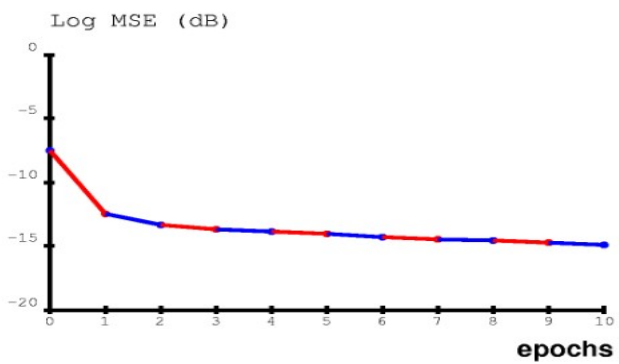
Hessian largest eigenvalue:

$\lambda_{max} = 0.84$

Maximum admissible Learning rate:

$\eta_{max} = 2.38$





Batch Gradient, large learning rate

Learning rate:

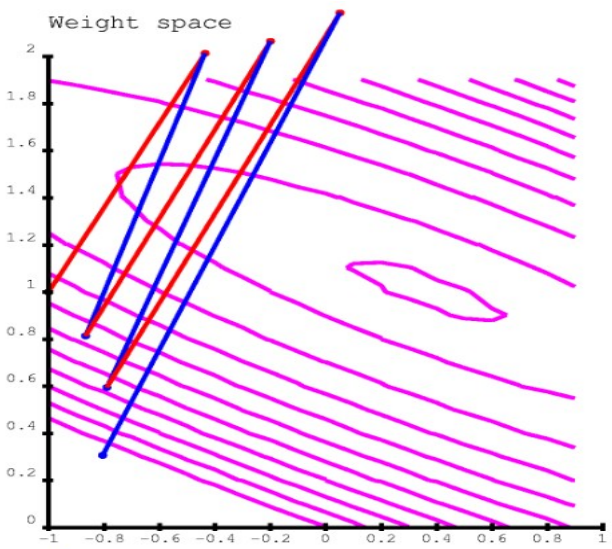
$\eta = 2.5$

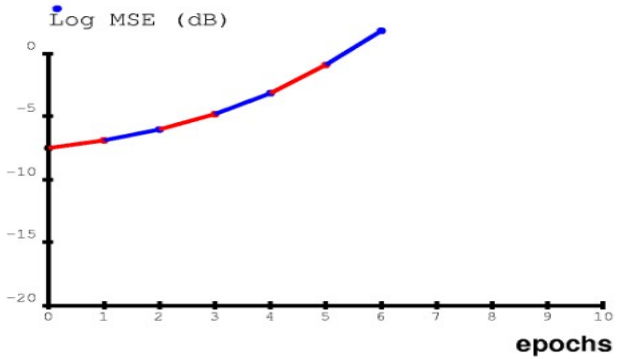
Hessian largest eigenvalue:

$\lambda_{max} = 0.84$

Maximum admissible Learning rate:

$\eta_{max} = 2.38$





Convergence is Slow When Hessian has Different Eigenvalues

- **Batch Gradient, small learning rate**

Learning rate:

$\eta = 1.5$

Hessian largest eigenvalue:

$\lambda_{max} = 0.84$

Maximum admissible Learning rate:

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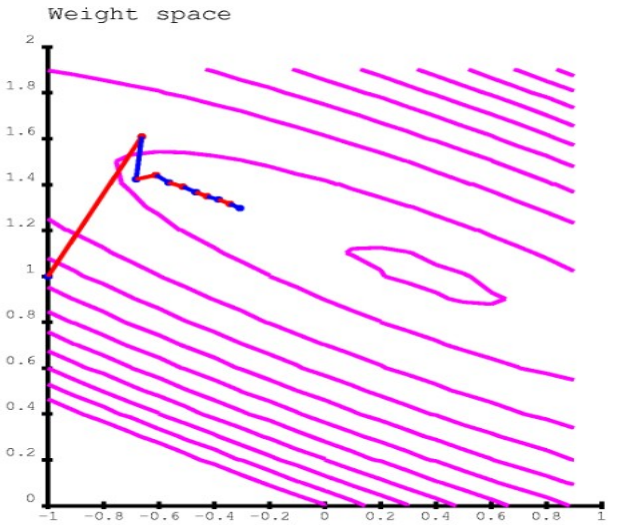
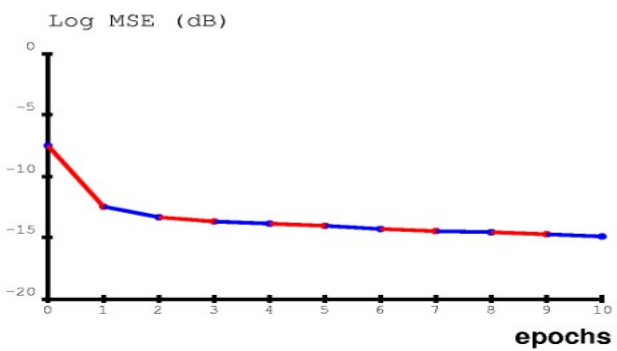




- **Stochastic Gradient: Much Faster**
- **But fluctuates near the minimum**

Learning rate:

$\eta = 0.2$

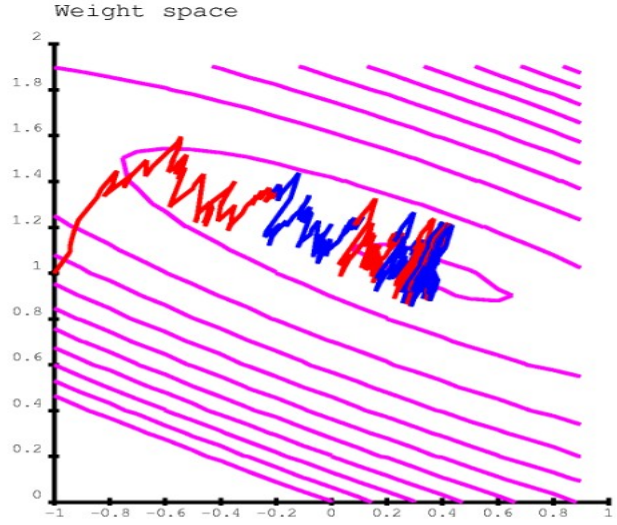
(equivalent to a batch learning rate of 20)

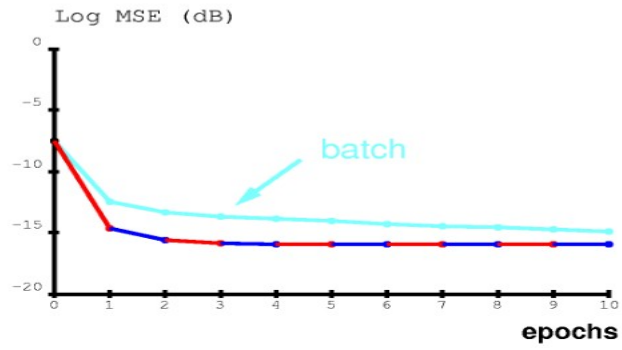
Hessian largest eigenvalue:

$\lambda_{max} = 0.84$

Maximum admissible Learning rate (for batch):

$\eta_{max} = 2.38$



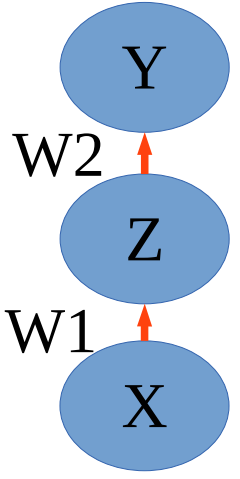


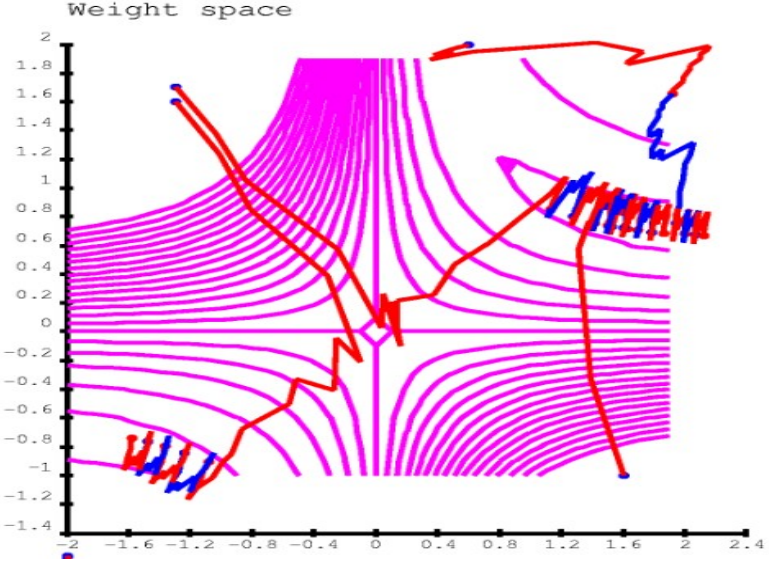
Convergence of GD

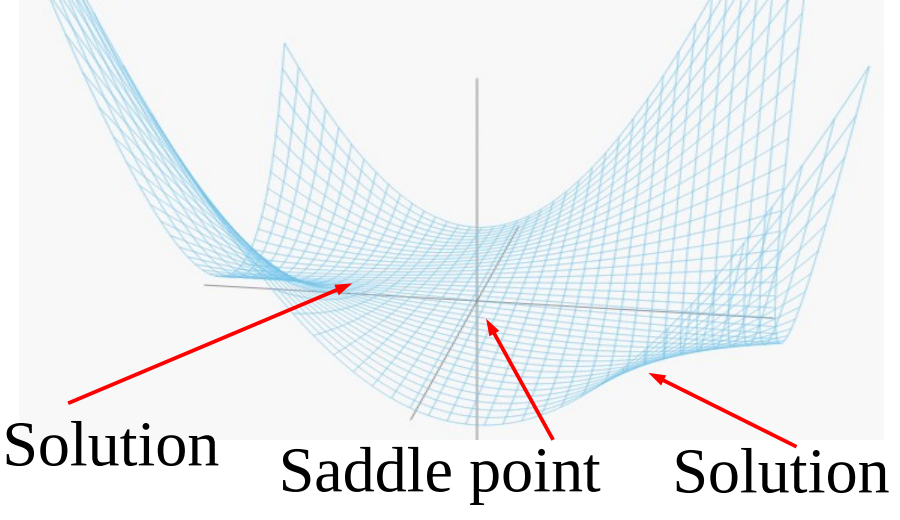
- **Convergence speed depends on conditioning**
- **Conditioning: ratio of largest to smallest non-zero eigenvalue of the Hessian**
- **How to condition?**
  - Center all the variables that enter a weight
  - Normalize the variance of all variables that enter a weight

Multilayer Nets Have Non-Convex Objective Functions

- **1-1-1 network**
  - Y = W1*W2*X
- **trained to compute the identity function with quadratic loss**
  - Single sample X=1, Y=1 L(W) = (1-W1*W2)^2
- **Solution: W2 = 1/W2 hyperbola.**







Stochastic Optimization

Stochastic optimization $\underset{w}{\text{minimize}}\ f(w) = \frac{1}{n}\sum_{i}^{n} f_i(w)$

Typically each f_i is the loss of the neural network on a single instance

$$f_i(w) = \ell(x_i, y_i, w)$$

Note: the optimization community uses f by convention, so I follow that notation here

$$w_{k+1} = w_k - \gamma_k \nabla f(w_k)$$ GD: *The WORST method in virtually all situations*

$$w_{k+1} = w_k - \gamma_k \nabla f_i(w_k)$$ SGD: *Often the BEST method available!*

(i chosen uniformly at random)

WHY?

SGD is GD in expectation...

Since:

$$\mathbb{E}[\nabla f_i(w_k)] = \nabla f(w_k)$$

The SGD step's expectation is just the gradient step:

$$\mathbb{E}\left[w_{k+1}\right] = w_k - \gamma_k \nabla f(w_k)$$

It's useful to think of SGD as GD with **noise**.

SGD exploits the redundancy in the samples

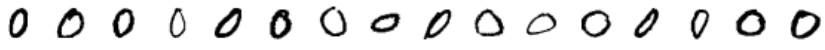
Advantages of SGD

$$w_{k+1} = w_k - \gamma_k \nabla f_i(w_k)$$

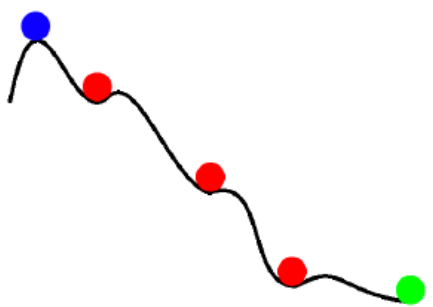
$$\underset{w}{\text{minimize}}\ f(w) = \frac{1}{n}\sum_{i}^{n} f_i(w)$$

$$f_i(w) = \ell(x_i, y_i, w)$$

- There is redundant information across instances (i.e. MNIST has thousands of near identical digits) the noise is lower when there is higher redundancy.



- At the early stages of optimization, the noise is small compared to the information in the gradient, so a SGD step is virtually as good as a GD step.
- The noise can prevent the optimizing converging to bad local minima, a phenomena called annealing
- Stochastic gradients are drastically cheaper to compute (proportional to your dataset size), so you can often take thousands of SGD steps for the cost of one GD step.



Minibatching: a necessary evil due to our hardware

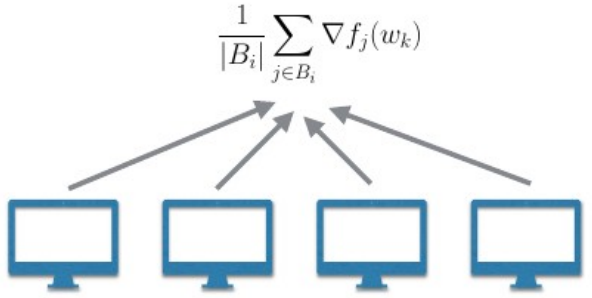
Mini-batching

$$w_{k+1} = w_k - \gamma_k \frac{1}{|B_i|} \sum_{j \in B_i} \nabla f_j(w_k)$$

Often we are able to make better use of our hardware by using mini batches instead of single instances

For instance, modern graphics cards are poorly utilized if we try and calculate single instance batches.

The most common distributing training technique on a cluster involves splitting a large mini batch between the machines and aggregating the resulting gradient.



All methods we discuss for stochastic optimization work with mini batches without issue

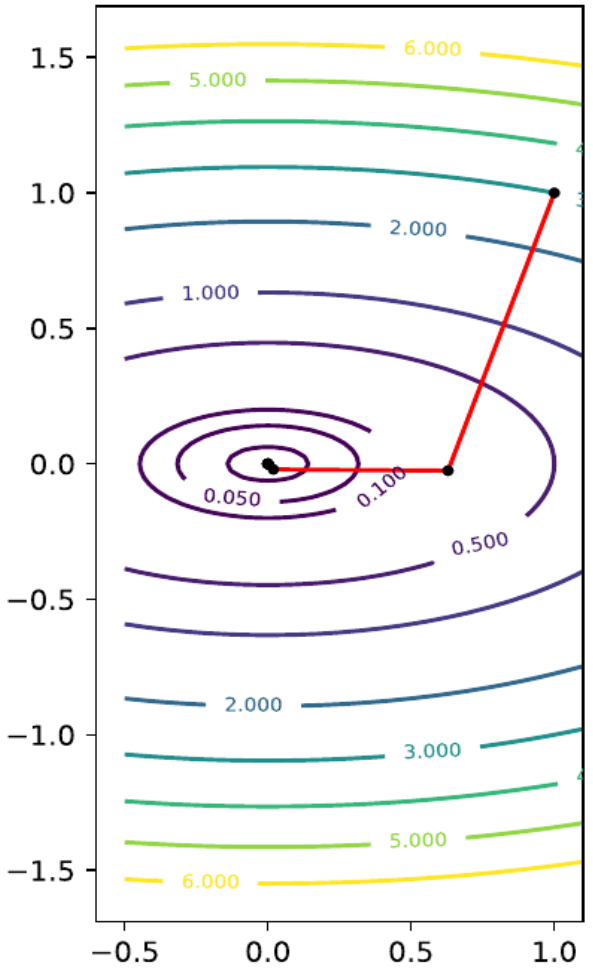
Don’t use full batch, but if you must...

If you must use a full-batch method ...

For batch optimization, **LBFGS** & Conjugate-Gradients are far better than vanilla gradient descent

`torch.optim.LBFGS` **scipy.optimize.fmin_l_bfgs_b**

BUT we don’t know how to best combine these techniques with stochasticity!
Plain SGD (with momentum) is still the best method for training many state-of-the-art neural networks such as ResNet models.



Liu, D. C.; Nocedal, J. (1989). "On the Limited Memory Method for Large Scale Optimization"

Momentum acceleration methods

The most misunderstood idea in optimization?

$$p_{k+1} = \hat{\beta}_k p_k + \nabla f_i(w_k)$$
$$w_{k+1} = w_k - \gamma_k p_{k+1}$$

Extra term on top of SGD

SGD + Momentum = Stochastic **heavy ball** method

$$w_{k+1} = w_k - \gamma_k \nabla f_i(w_k) + \beta_k (w_k - w_{k-1}) \qquad 0 \leq \beta < 1$$

This is mathematically equivalent to the previous form for a particular value of beta.

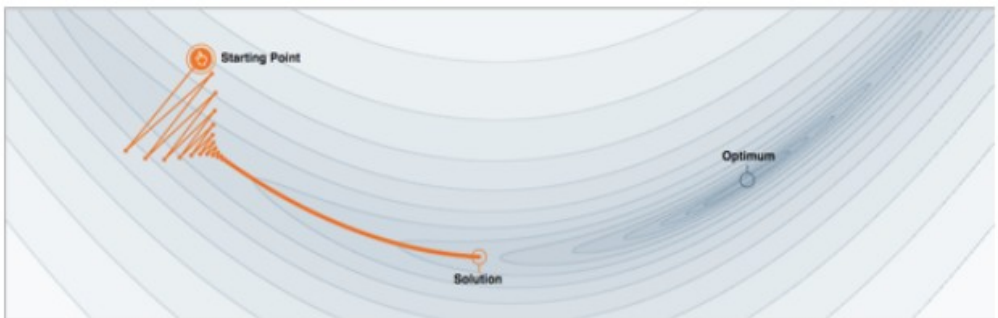
Key idea: The next step becomes a combination of the previous step's direction and the new negative gradient

Momentum acceleration methods

$$p_{k+1} = \hat{\beta}_k p_k + \nabla f_i(w_k)$$
$$w_{k+1} = w_k - \gamma_k p_{k+1}$$

The optimization process resembles a heavy ball rolling down a hill. The ball has momentum, so it doesn't change direction immediately when it encounters changes to the landscape!

Without momentum



With momentum

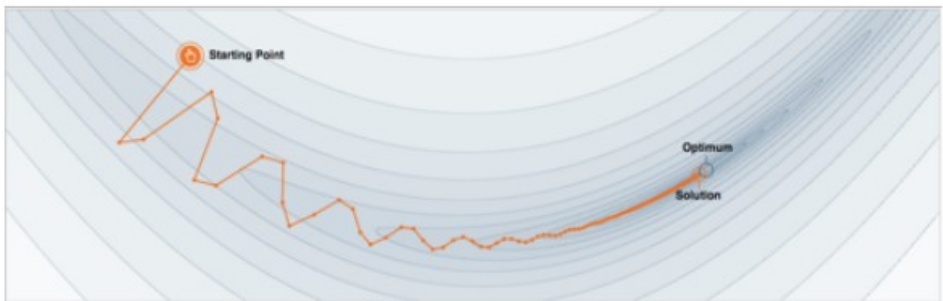
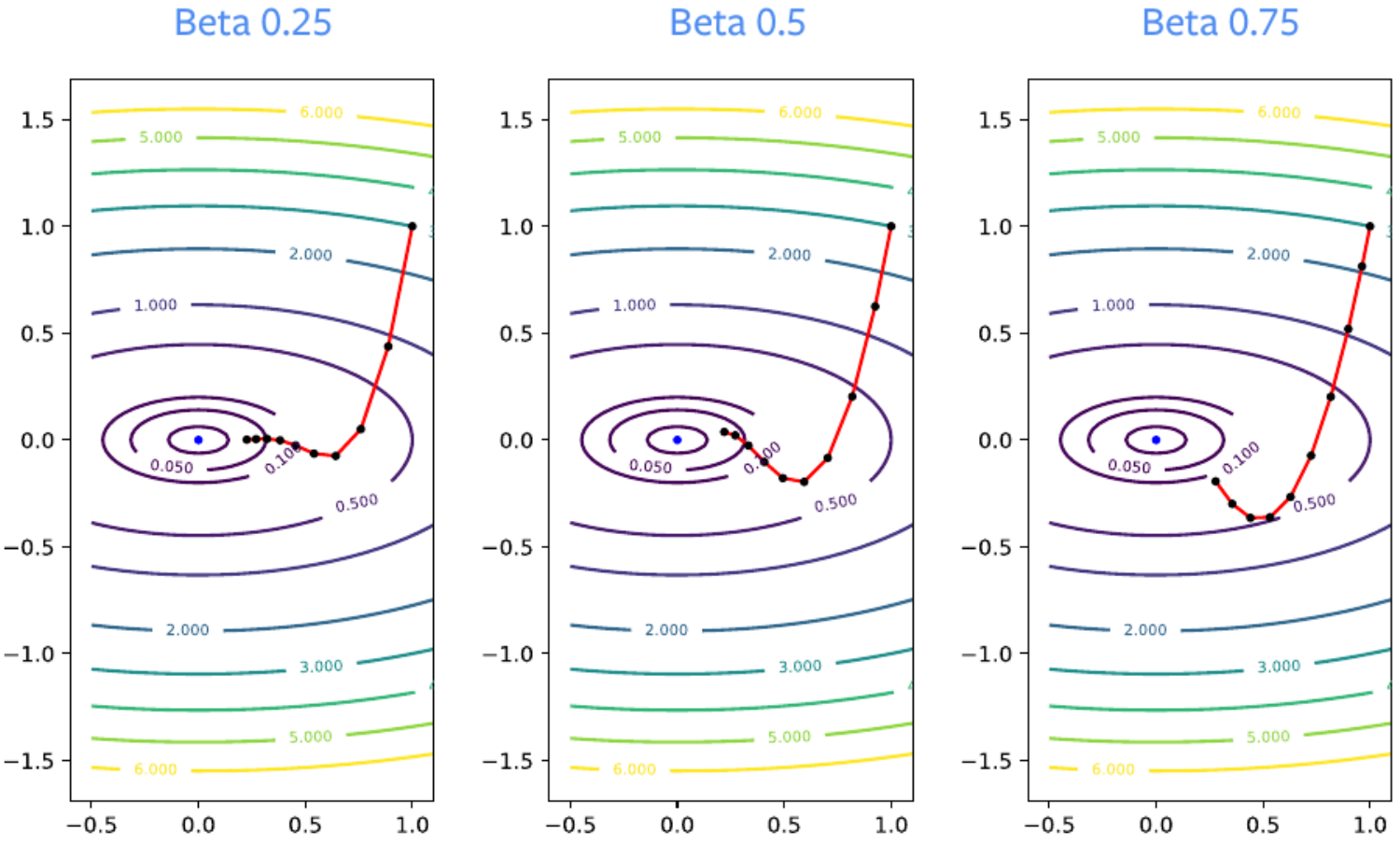


Image Source: https://distill.pub/2017/momentum/

Larger momentum → slower reactions to changes in landscape



Momentum in practice

Practical Aspects of momentum

$$p_{k+1} = \hat{\beta}_k p_k + \nabla f_i(w_k)$$
$$w_{k+1} = w_k - \gamma_k p_{k+1}$$

It's basically "free lunch", in almost all situations, SGD + momentum is better than SGD, and very rarely worse!

Recommended Parameters:

Beta = **0.9** or **0.99** almost always works well. Sometimes slight gains can be had by tuning it.

The step size parameter usually needs to be decreased when the momentum parameter is increased to maintain convergence.

Momentum accelerates

Explanation one: **Acceleration**

The momentum method is often conflated with Nesterov's momentum

Regular momentum

$$p_{k+1} = \hat{\beta}_k p_k + \nabla f_i(w_k)$$
$$w_{k+1} = w_k - \gamma_k p_{k+1}$$

Nesterov's momentum

$$p_{k+1} = \hat{\beta}_k p_k + \nabla f_i(w_k)$$
$$w_{k+1} = w_k - \gamma_k \left(\nabla f_i(w_k) + \hat{\beta}_k p_{k+1} \right)$$

`torch.optim.SGD(…, nesterov=True)`

Nesterov's momentum, when using **VERY** carefully chosen constants, provably "**accelerates**" convergence on problems with simple structure (convex)

Regular momentum is also accelerated: but only on **quadratics**!

There is no theory to suggest this acceleration occurs when training neural networks, although a practical speedup is often observed.

Surprisingly, Nesterov's momentum usually performs the same as regular momentum when training neural networks.

Acceleration alone does not explain momentum!

But momentum also smoothes the gradient noise

In optimization, we usually take the last w as our estimate of the best parameters at the end.

When using **SGD**, this is suboptimal! We should actually take an **average** over past time steps (with weights ideally depending on the problem structure)

$$\bar{w}_K = \frac{1}{K} \sum_{k=1}^{K} w_k$$

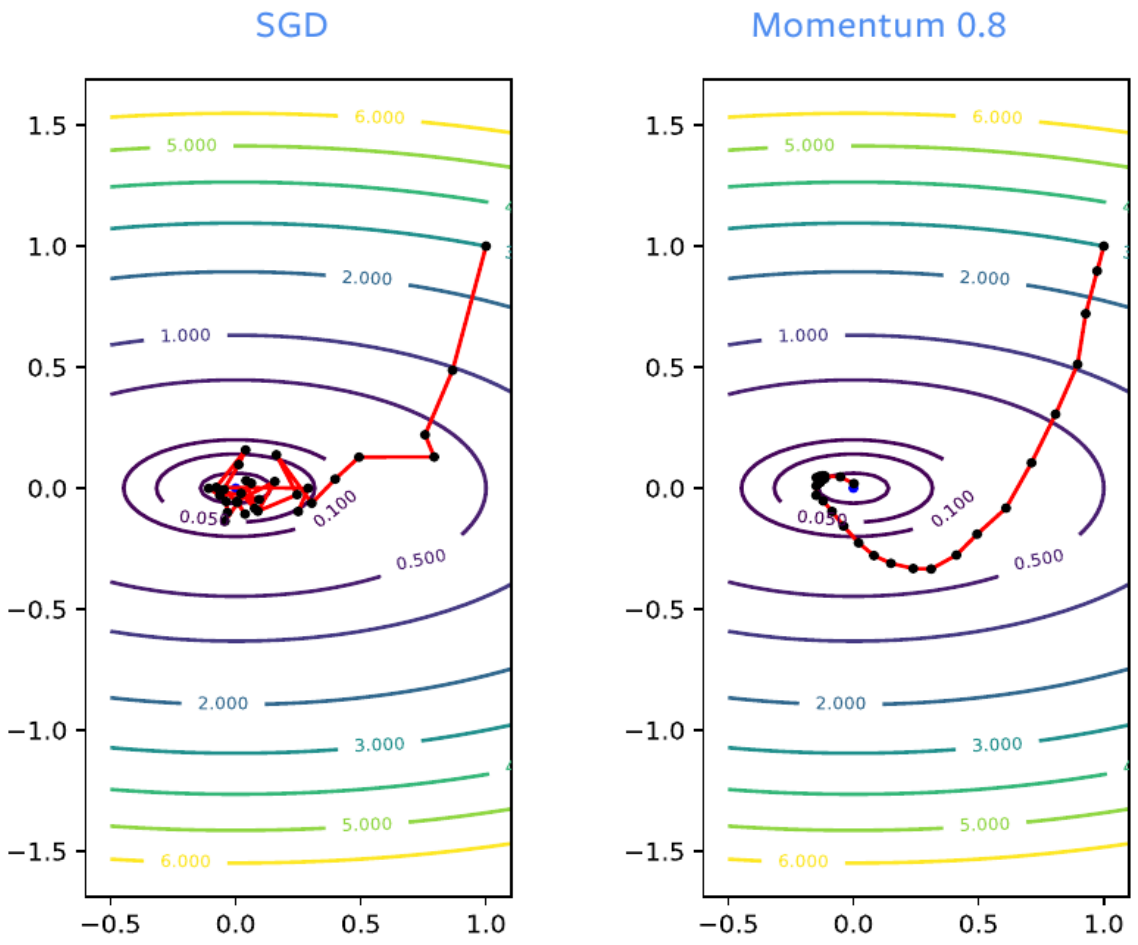
In contrast, theory suggests that SGD + Momentum requires **no averaging**, the **last value** may directly be returned!

Momentum **smooths** the noise from the stochastic gradients

Both noise smoothing and acceleration contribute to the high performance of momentum

Is reducing the noise good or bad?

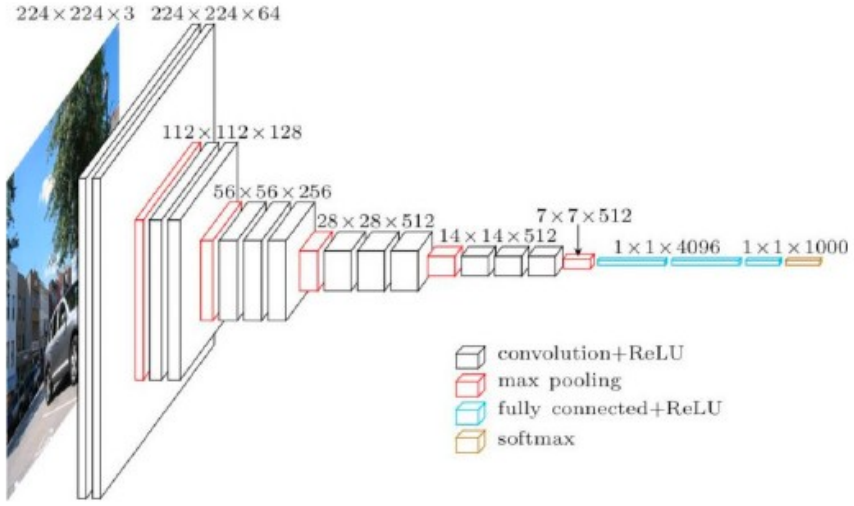
Quadratic with STD 1.0 noise injected into b



- **Noise can accelerate learning**
- **Noise can improve generalization**
- **Noise can drive the parameter to “flat” regions of the loss**

Automatic learning rate adjustment

The magnitude of the gradients often varies highly between layers due to, so a global learning rate may not work well.



General **IDEA**: Instead of using the same learning rate for every weight in our network, **maintain an estimate of a better rate separately for each weight**.

The exact way of adapting to the learning rates varies between algorithms,
But most methods either **adapt** to the **variance** of the weights, or to the l**ocal curvature** of the problem.

RMSprop

Key **IDEA**: normalize by the **root-mean-square** of the gradient

Exponential moving average

2nd moment estimate

Notation for element-wise squaring. i.e. square each element separately

$$v_{t+1} = \alpha v_t + (1-\alpha)\,\nabla f_i(w_t)^2$$

$$w_{t+1} = w_t - \gamma \frac{\nabla f_i(w_t)}{\sqrt{v_{t+1}} + \epsilon}$$

Global LR

RMS estimate + epsilon (epsilon avoids divide-by-zero)

Most adaptive methods use a moving average, it's a simple way to estimate a noisy quantity that changes over time.

If the expected value of gradient is small, this is similar to dividing by the standard deviation (i.e. whitening)

Adam

Adam: RMSprop with a kind of momentum

"Adaptive Moment Estimation"

Presented here without **bias-correction** (i.e. steady state Adam)

RMSProp

$$v_{t+1} = \alpha v_t + (1-\alpha)\,\nabla f_i(w_t)^2$$
$$w_{t+1} = w_t - \gamma \frac{\nabla f_i(w_t)}{\sqrt{v_{t+1}} + \epsilon}$$

Momentum (Exponential moving average)

2nd moment estimate (same as RMSProp)

$$m_{t+1} = \beta v_t + (1-\beta)\nabla f_i(w_t)$$
$$v_{t+1} = \alpha v_t + (1-\alpha)\,\nabla f_i(w_t)^2$$
$$w_{t+1} = w_t - \gamma \frac{m_t}{\sqrt{v_{t+1}} + \epsilon}$$

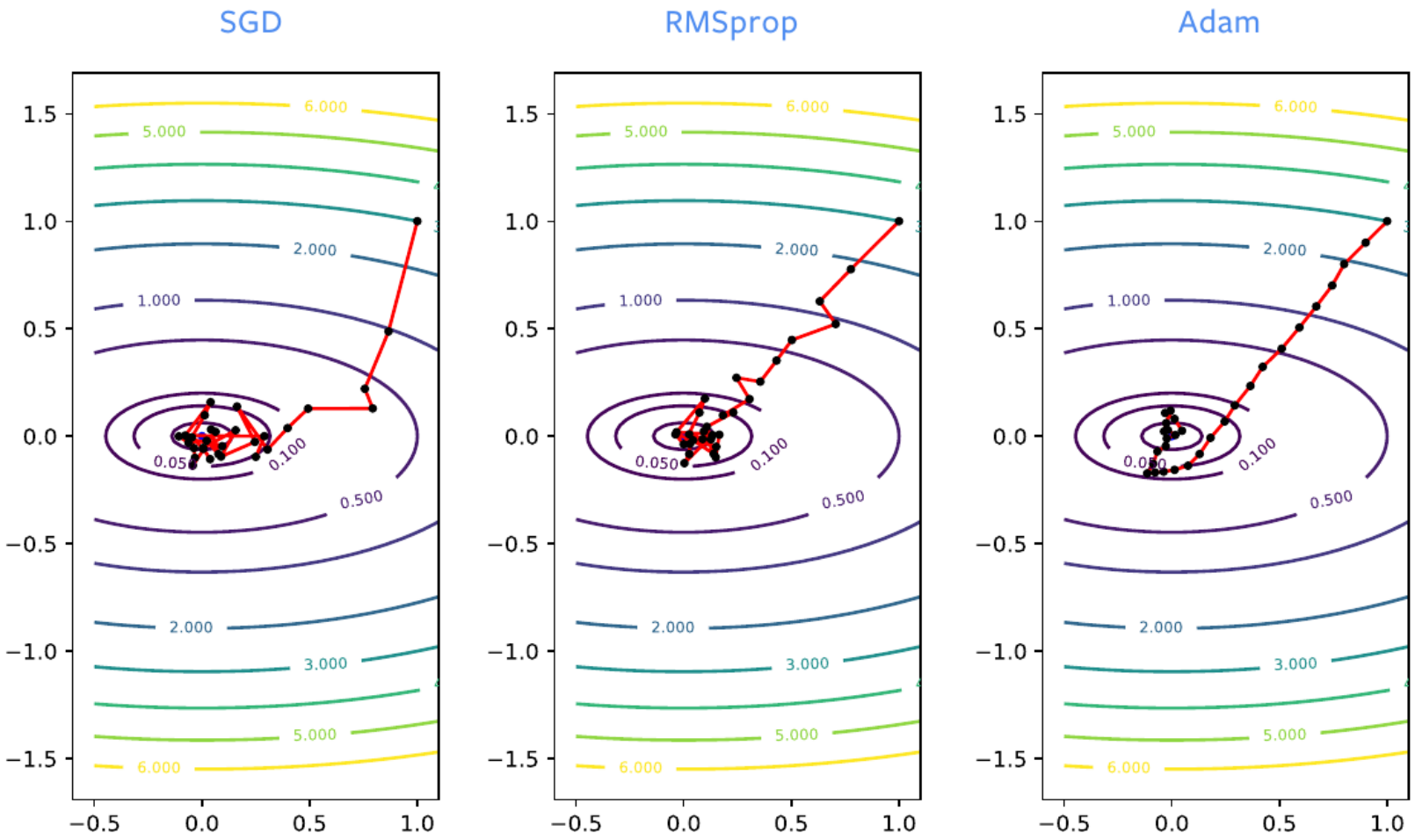
Use m instead of the gradient

Just as momentum improves SGD, it improves RMSProp as well.
The exponential-moving-average method of updating momentum is equivalent to the standard form under rescaling. Nothing mysterious.

The full version of Adam has **bias-correction** as well, which just keeps the moving averages **unbiased** during early iterations. The algorithm quickly approaches the above steady state form.

Diederik, Kingma; Ba, Jimmy (2014). "Adam: A method for stochastic optimization"

Pure SGD vs RMSprop vs Adam



Practical considerations

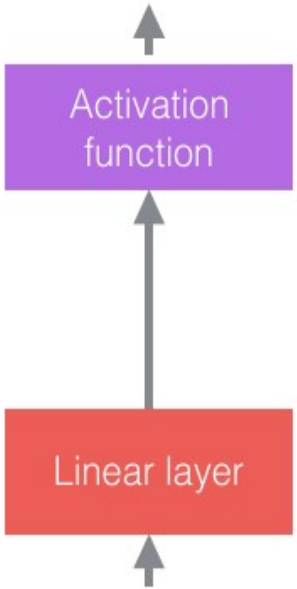
For poorly conditioned problems, Adam is often **much** better than SGD.
I recommend using Adam over RMSprop due to the clear advantages of momentum

BUT, Adam is poorly understood theoretically, and has known disadvantages:

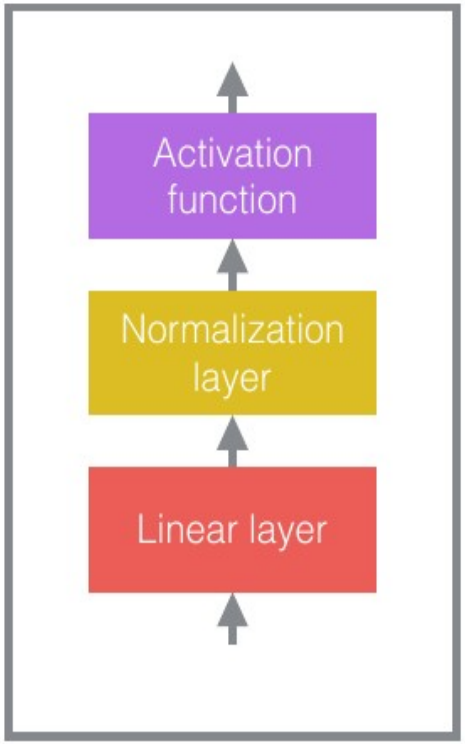
- Does not converge at all on some simple example problems!
- Gives worse generalization error on many computer vision problems (i.e. ImageNet)
- Requires more memory than SGD
- Has 2 momentum parameters, so some tuning may be needed

It's a good idea to try both SGD + momentum and Adam with a sweep of different learning rates, and use whichever works better on held out data

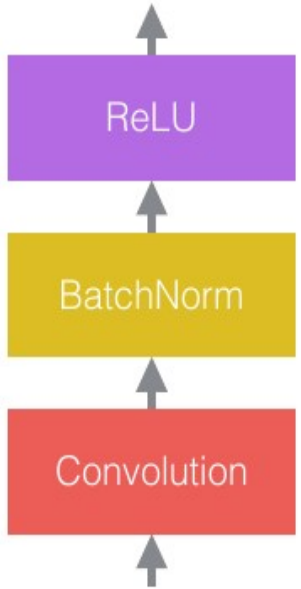
Normalization layers



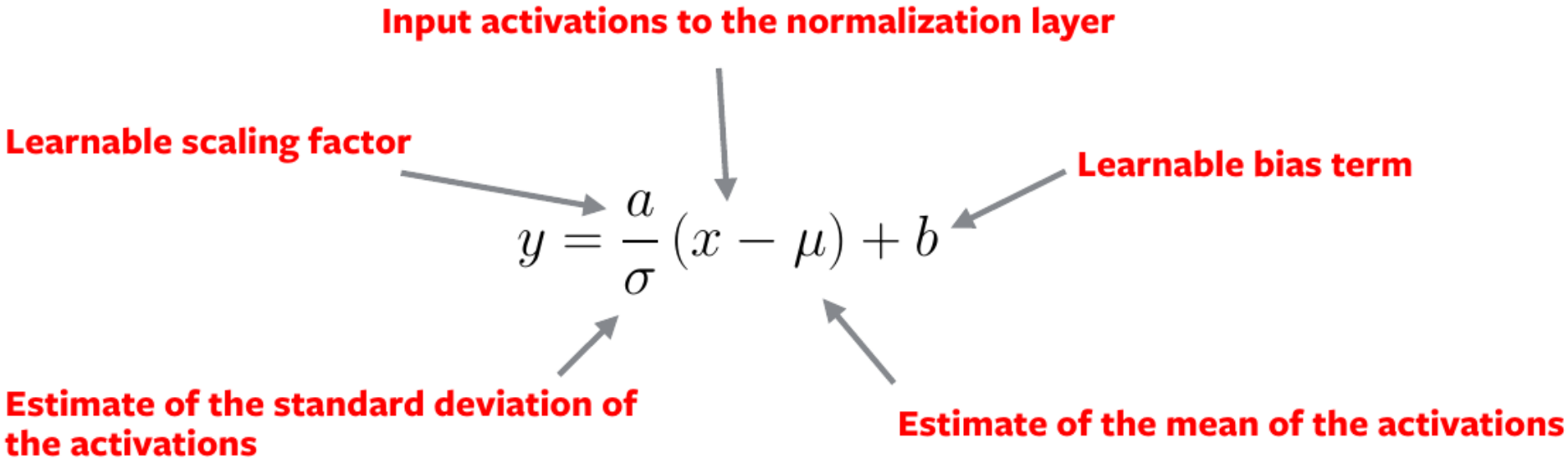
They are added in-between existing layers of a neural network



Typical image classification structure



Normalization layers whiten the activations



The extra a & b parameters keep the representation power of the network the same

But how do we estimate the mean and standard deviation? Does it differ across channels, spatial location, instances?

Normalization tricks

- **N=batch, C=channels, H,W space**
- **Batch norm: N,H,W**
- **Layer norm: C,H,W**
- **Instance norm: H,W**
- **Group norm: N, C subset**

- **Before non-linearity**
  - Needs scale and shift
- **After non-linearity**
  - Scale and shift may hurt

Input: Values of x over a mini-batch: $\mathcal{B} = \{x_{1...m}\}$;
Parameters to be learned: γ, β

Output: $\{y_i = \mathrm{BN}_{\gamma,\beta}(x_i)\}$

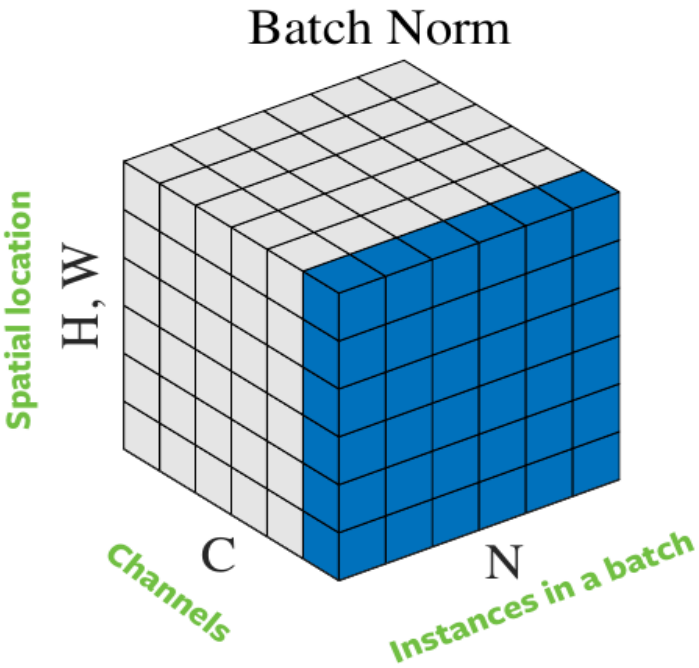
$$\mu_{\mathcal{B}} \leftarrow \frac{1}{m}\sum_{i=1}^{m} x_i \qquad \text{// mini-batch mean}$$

$$\sigma^2_{\mathcal{B}} \leftarrow \frac{1}{m}\sum_{i=1}^{m}(x_i - \mu_{\mathcal{B}})^2 \qquad \text{// mini-batch variance}$$

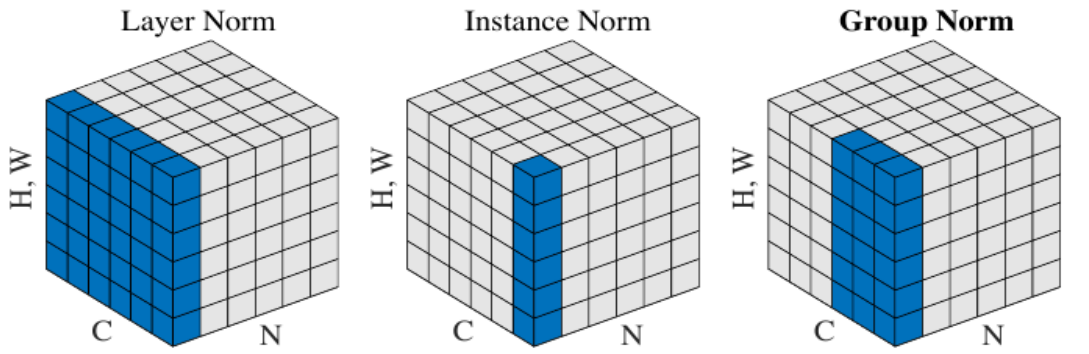
$$\widehat{x}_i \leftarrow \frac{x_i - \mu_{\mathcal{B}}}{\sqrt{\sigma^2_{\mathcal{B}} + \epsilon}} \qquad \text{// normalize}$$

$$y_i \leftarrow \gamma\widehat{x}_i + \beta \equiv \mathrm{BN}_{\gamma,\beta}(x_i) \qquad \text{// scale and shift}$$

Types of normalizations



Normalize across H,W,N
i.e. across the **batch**, and
Within each separate image channel

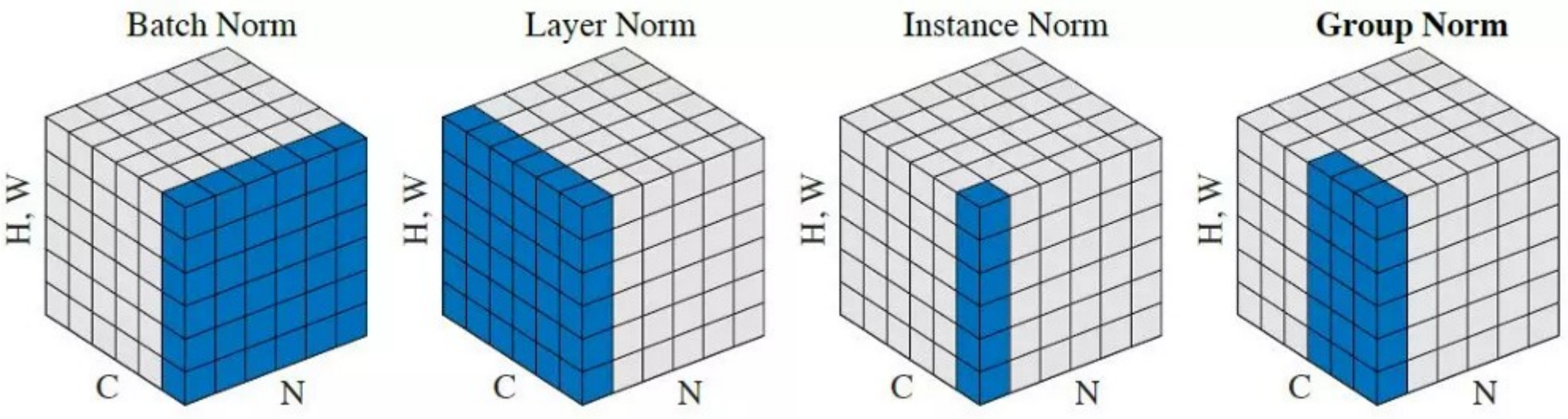


Normalize within
H,W and a **group** of
channels

In practice group/batch norm work well for computer vision problems, and instance/layer norm are heavily used for language problems.

IMG SOURCE: https://arxiv.org/pdf/1803.08494.pdf

Normalization tricks



- N=batch, C=channels, H,W space
- Batch norm: N,H,W
- Layer norm: C,H,W
- Instance norm: H,W
- Group norm: N, C subset

Why does normalization help?

This is still disputed

The original paper said that it "reduces internal covariate shift" whatever that means

As usual, we are using something we don't fully understand.

But, it's clearly a combination of a number of factors:

- Networks with normalization layers are easier to optimize, allowing for the use of larger learning rates. (Normalization has a **optimization** effect)
- The mean/std estimates are noisy, this extra "noise" results in better generalization in some cases (Normalization has an **regularization** effect)
- Normalization reduces sensitivity to weight initialization

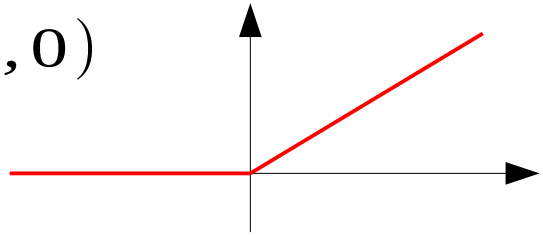
Normalization lets you be more "careless", you can combine almost any neural network building blocks together and have a good chance of training it without having to consider how poorly conditioned it might be.

For more info: https://myrtle.ai/how-to-train-your-resnet-7-batch-norm

Deep Nets with ReLUs and Max Pooling

- **Stack of linear transforms interspersed with Max operators**
- **Point-wise ReLUs:**

$$ReLU(x) = max(x, 0)$$



- **Max Pooling**
  - "switches" from one layer to the next
- **Input-output function**
  - Sum over active paths
  - Product of all weights along the path
  - Solutions are hyperbolas
- **Objective function is full of saddle points**