Optimization

Designing, Visualizing and Understanding Deep Neural Networks

CS W182/282A

Instructor: Sergey Levine
UC Berkeley

How does gradient descent work?

The loss “landscape”

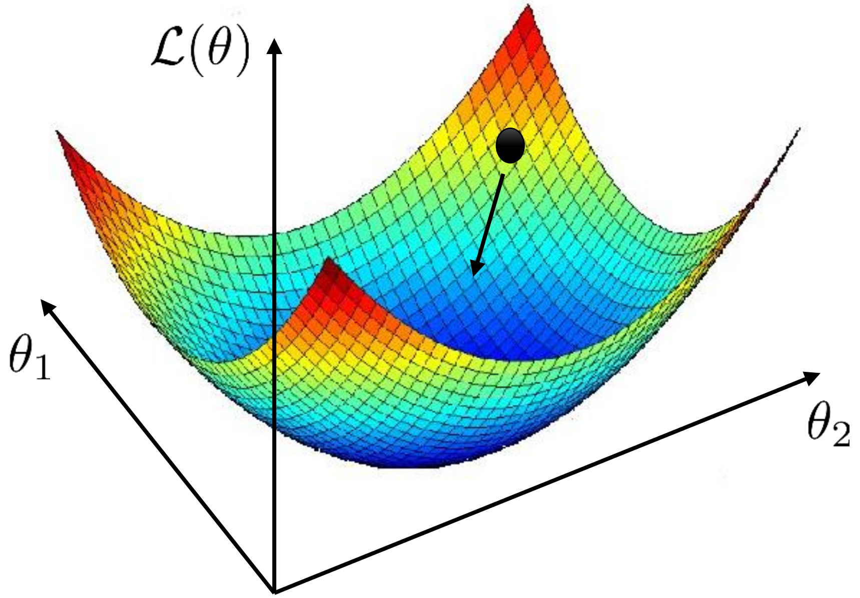
$$\theta^\star \leftarrow \arg\min_\theta \underbrace{- \sum_i \log p_\theta(y_i|x_i)}_{\mathcal{L}(\theta)}$$

let’s say θ is 2D

An algorithm:

1. Find a *direction* v where $\mathcal{L}(\theta)$ decreases
2. $\theta \leftarrow \theta + \alpha v$

some small constant called “learning rate” or “step size”



Gradient descent

An algorithm:

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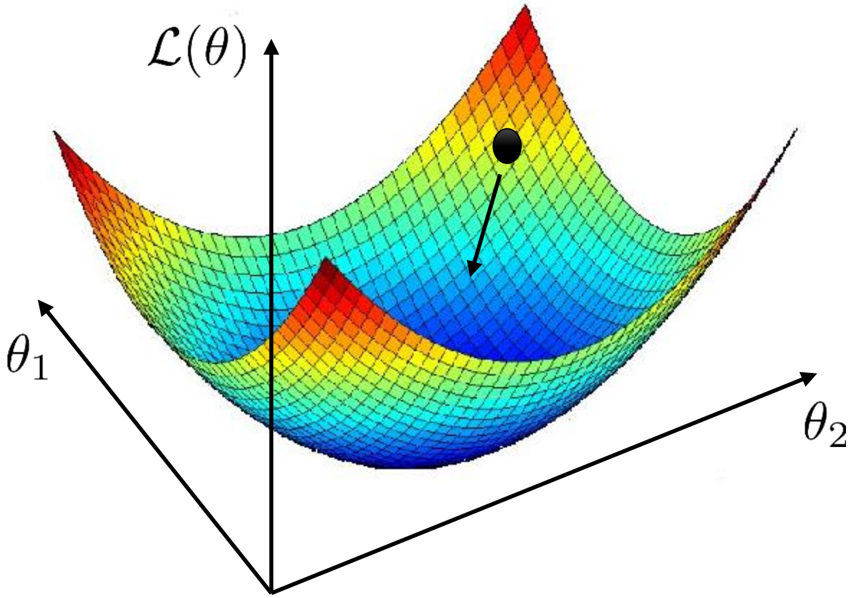
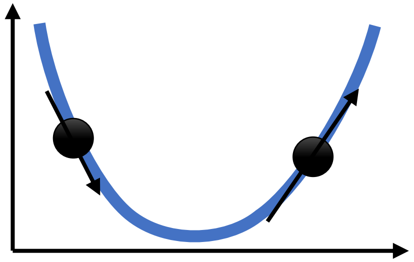


Which way does $\mathcal{L}(\theta)$ decrease?



negative slope = go to the right

positive slope = go to the left

in general:

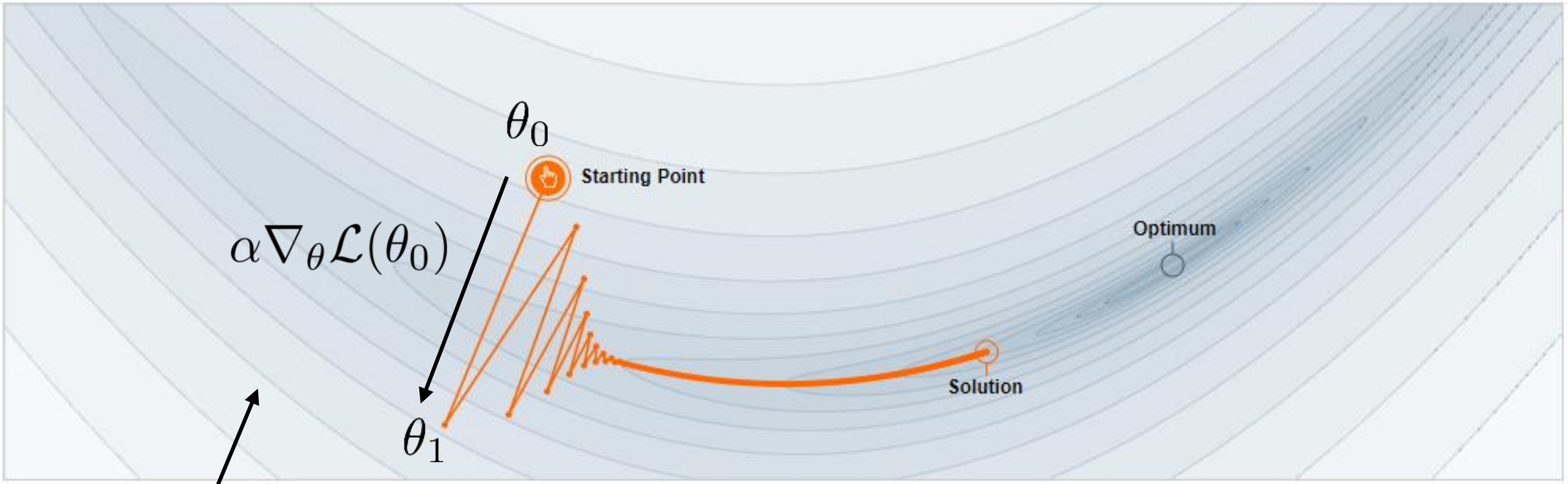
for each dimension, go in the direction opposite the slope **along that dimension**

$$v_1 = -\frac{d\mathcal{L}(\theta)}{d\theta_1} \quad v_2 = -\frac{d\mathcal{L}(\theta)}{d\theta_2} \quad \text{etc.}$$

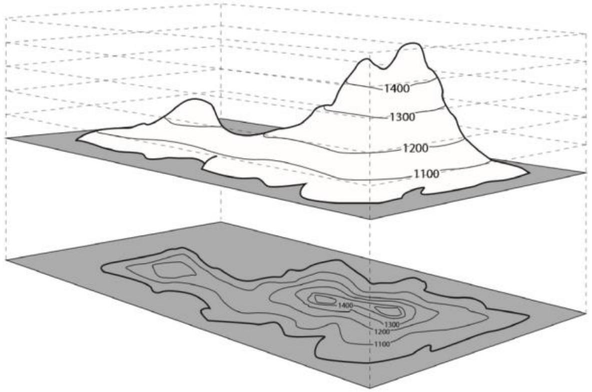
gradient:

$$\nabla_\theta \mathcal{L}(\theta) = \begin{pmatrix} \frac{d\mathcal{L}(\theta)}{d\theta_1} \\ \frac{d\mathcal{L}(\theta)}{d\theta_2} \\ \vdots \\ \frac{d\mathcal{L}(\theta)}{d\theta_n} \end{pmatrix}$$

Visualizing gradient descent

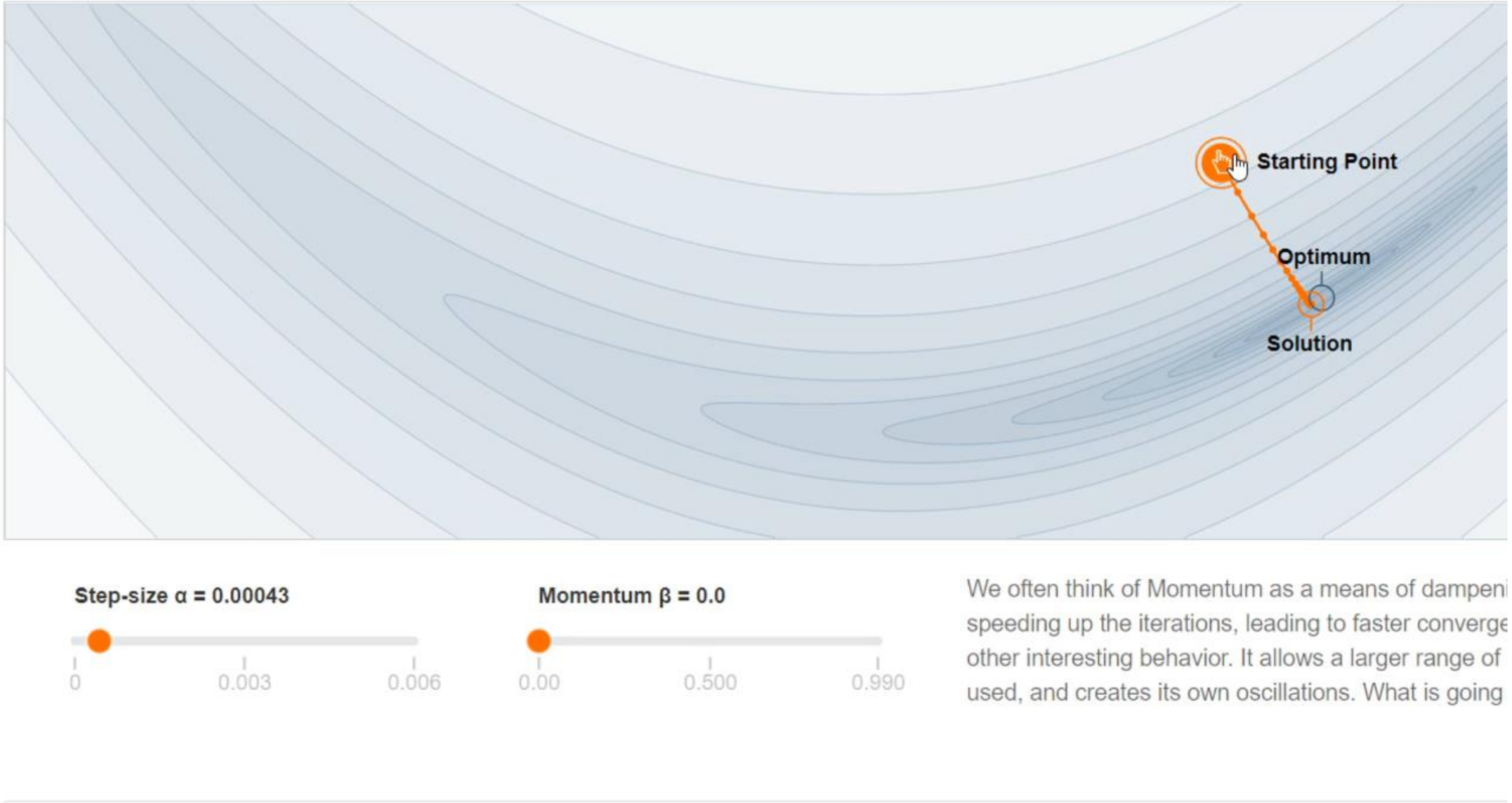


level set contours
for all θ values along a line
$\mathcal{L}(\theta)$ takes on the same value



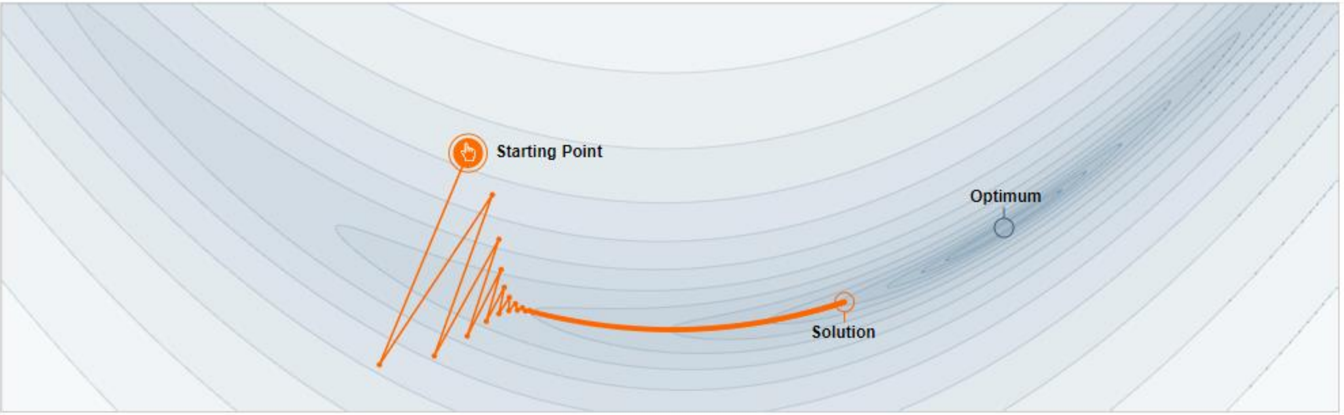
visualizations based on Gabriel Goh’s distill.pub article: https://distill.pub/2017/momentum/

Demo time!

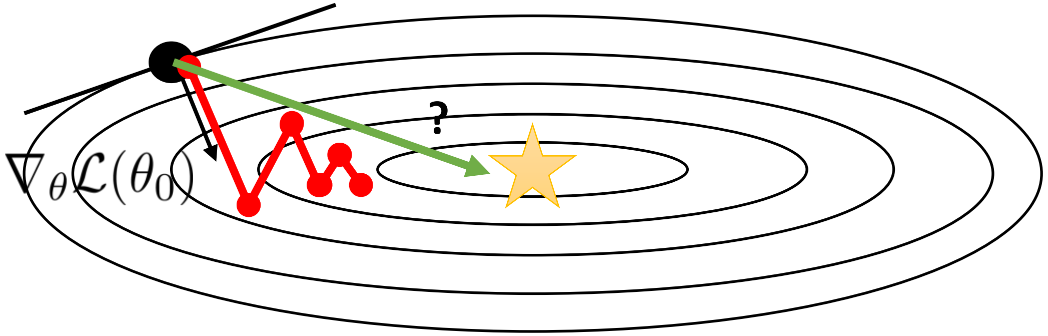


visualizations based on Gabriel Goh's distill.pub article: https://distill.pub/2017/momentum/

What's going on?



we don't always move toward the optimum!



the steepest direction is not always best!

more on this later…

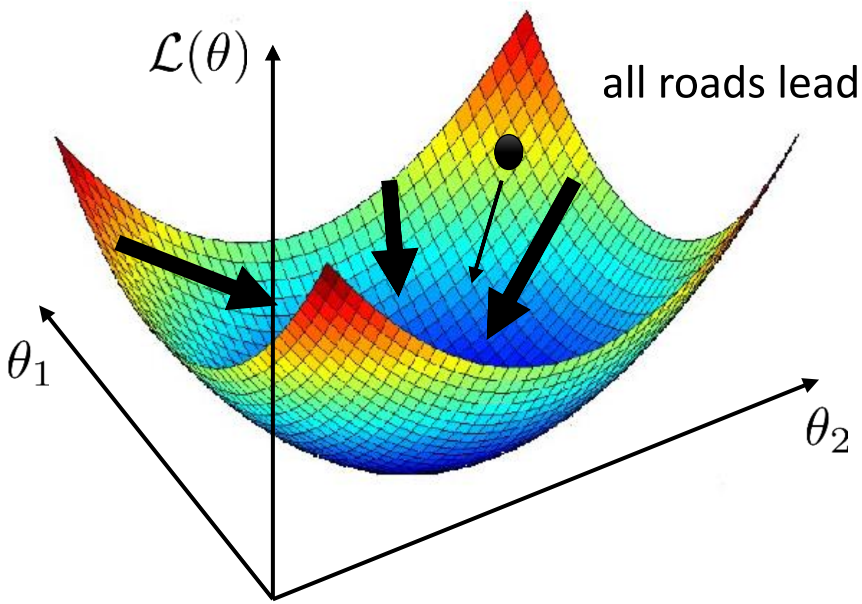
The loss surface

Logistic regression:

$$p_\theta(y = i|x) = \frac{\exp(x^T\theta_i)}{\sum_{j=1}^{m}\exp(x^T\theta_j)}$$

Negative likelihood loss for **logistic regression** is guaranteed to be **convex**

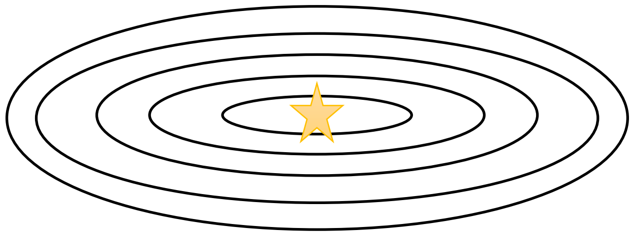
(this is **not** an obvious or trivial statement!)



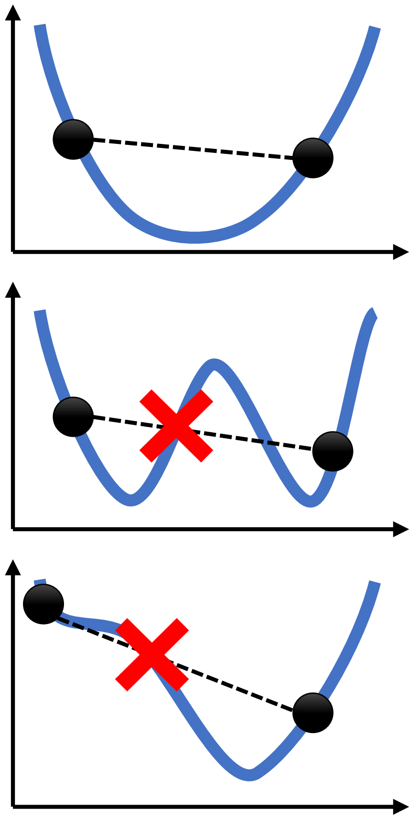
all roads lead to Rome

This is a *very* nice loss surface   Why?

Is our loss actually this nice?



Convexity:



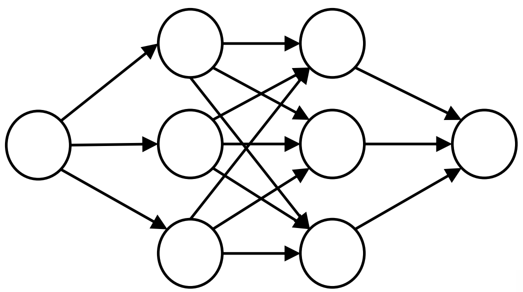
a function is convex if a line segment between any two points lies entirely "above" the graph

convex functions are "nice" in the sense that simple algorithms like gradient descent have strong guarantees

the **doesn't** mean that gradient descent works well for all convex functions!

The loss surface…

…of a neural network



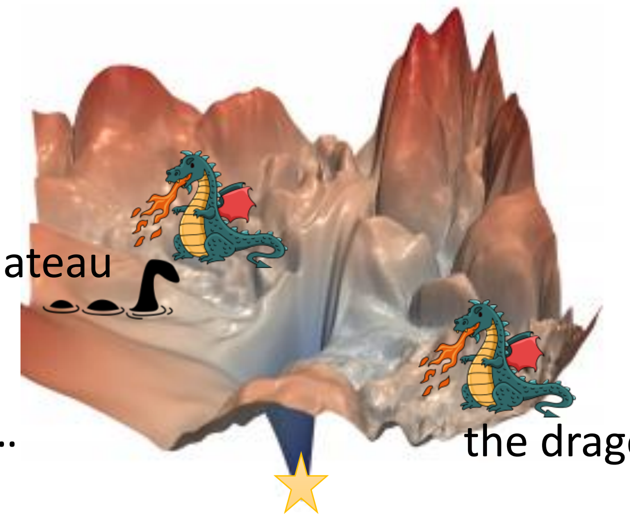
pretty hard to visualize, because neural networks have very large numbers of parameters

but let's give it a try!

Visualizing the Loss Landscape of Neural Nets

Hao Li[1], Zheng Xu[1], Gavin Taylor[2], Christoph Studer[3], Tom Goldstein[1]
[1]University of Maryland, College Park [2]United States Naval Academy [3]Cornell University
{haoli,xuzh,tomg}@cs.umd.edu, taylor@usna.edu, studer@cornell.edu

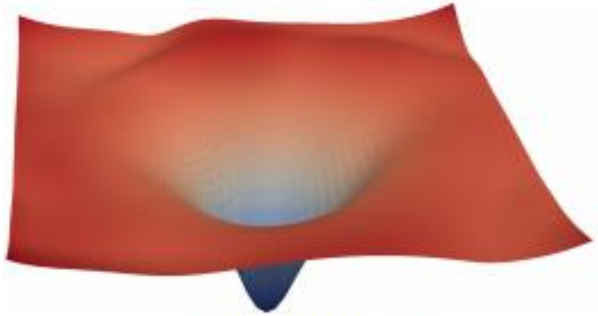
…though some networks are better!



the monster of the plateau

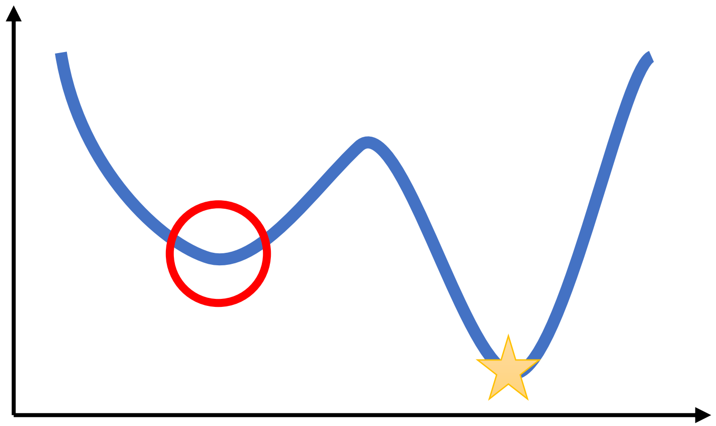
Oh no…

the dragon of local optima

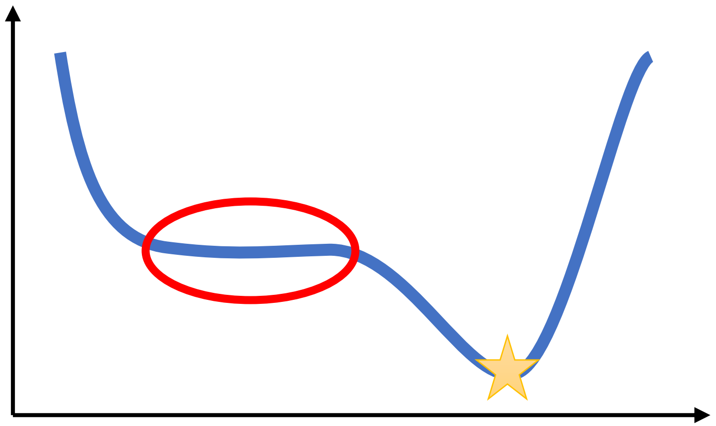


(b) with skip connections

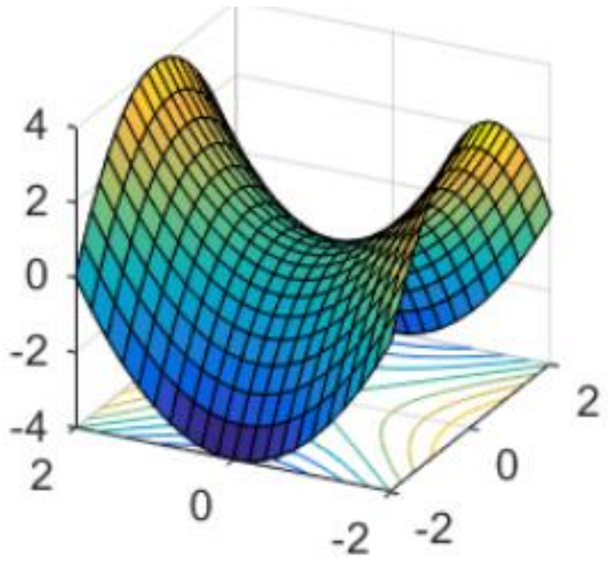
The geography of a loss landscape



the local optimum

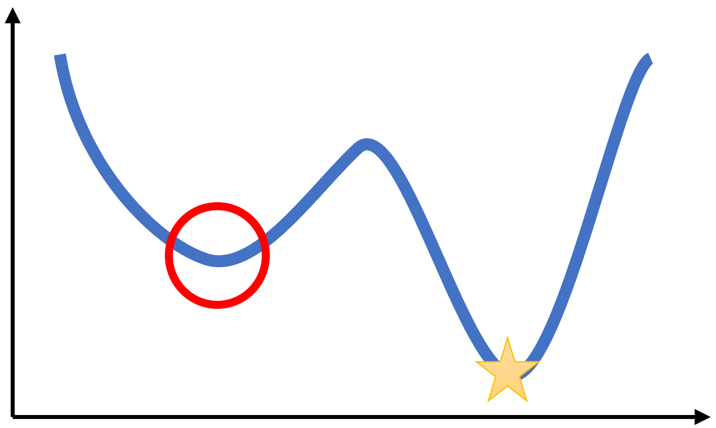


the plateau



the saddle point

Local optima



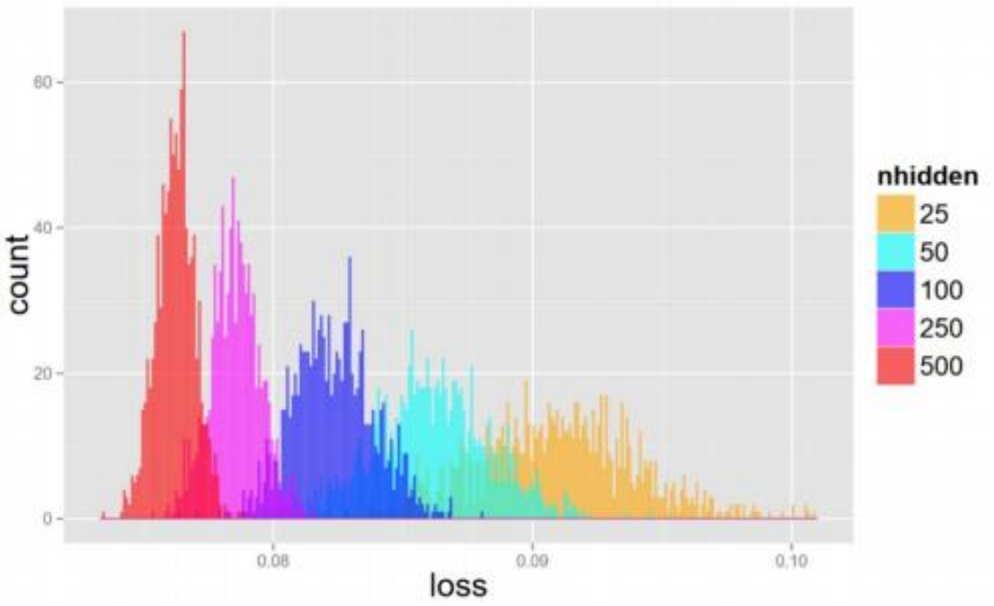
the most obvious issue with non-convex loss landscapes

one of the big reasons people used to worry about neural networks!

very scary in principle, since gradient descent could converge to a solution that is arbitrarily worse than the global optimum!

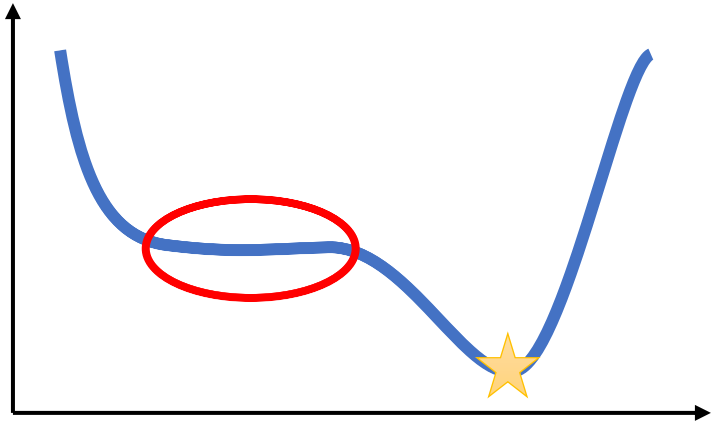
a bit surprisingly, this becomes less of an issue as the number of parameters increases!

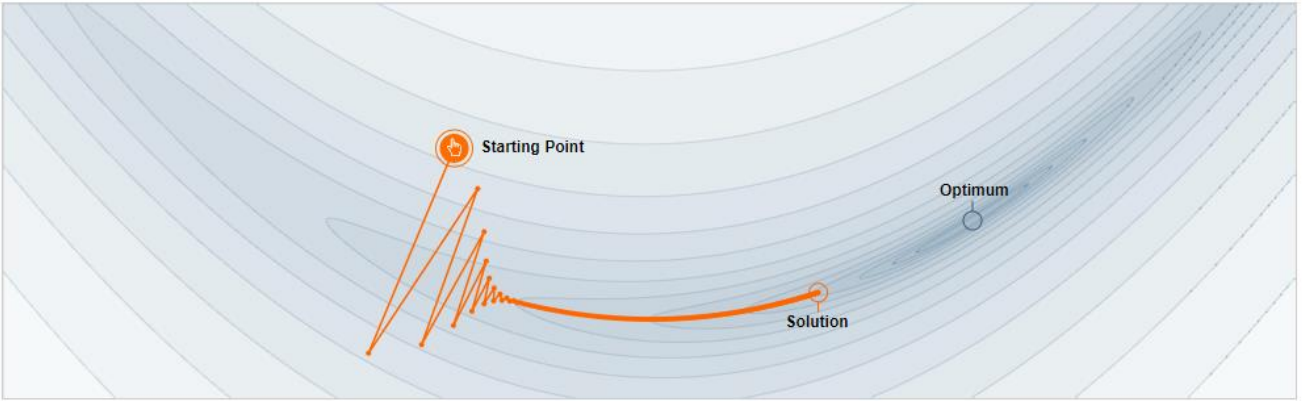
for big networks, local optima exist, but tend to be not much worse than global optima



Choromanska, Henaff, Mathieu, Ben Arous, LeCun.
The Loss Surface of Multilayer Networks.

Plateaus



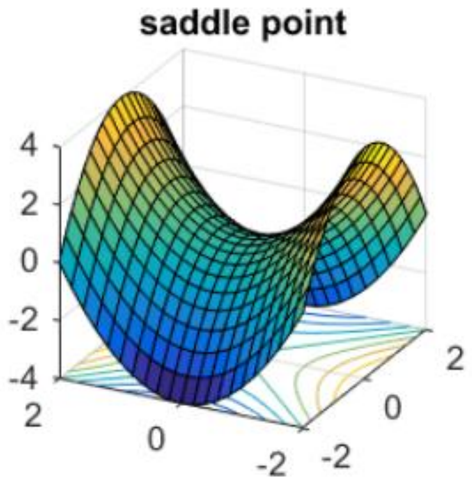


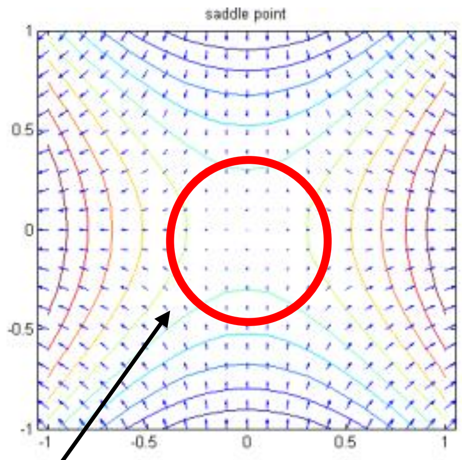
Can’t just choose tiny learning rates to prevent oscillation!

Need learning rates to be large enough not to get stuck in a plateau

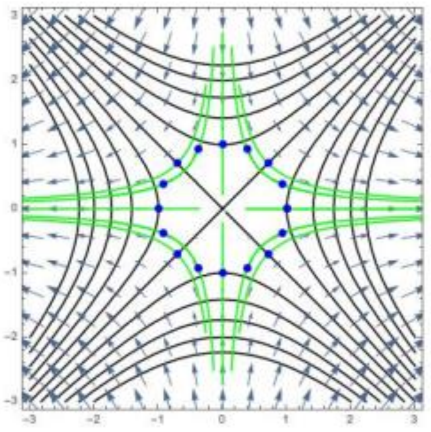
We’ll learn about **momentum**, which really helps with this

Saddle points





Gradient vectors



Gradient flows (green)

the gradient here is very small

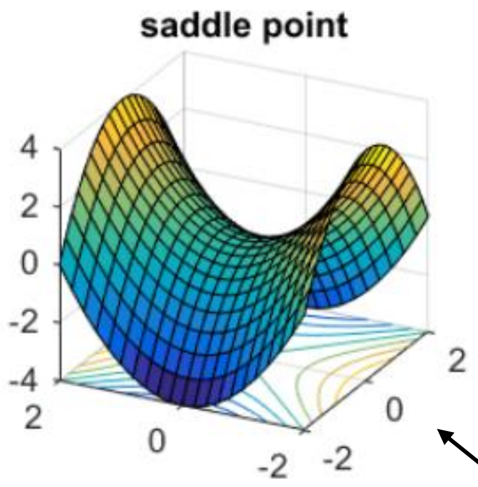
it takes a long time to get out of saddle points

this seems like a **very** special structure, does it really happen **that** often?

Yes! in fact, most critical points in neural net loss landscapes are saddle points

A saddle point is a critical point that is not a local extrema.
Or, a point where the slopes (or derivatives) in orthogonal directions are all zero. However, the point is not the highest or lowest point in its neighbourhood.

Saddle points



Critical points:

any point where $\nabla_\theta \mathcal{L}(\theta) = 0$

is it a **maximum**, **minimum**, or **saddle**?

In higher dimensions:

Hessian matrix:

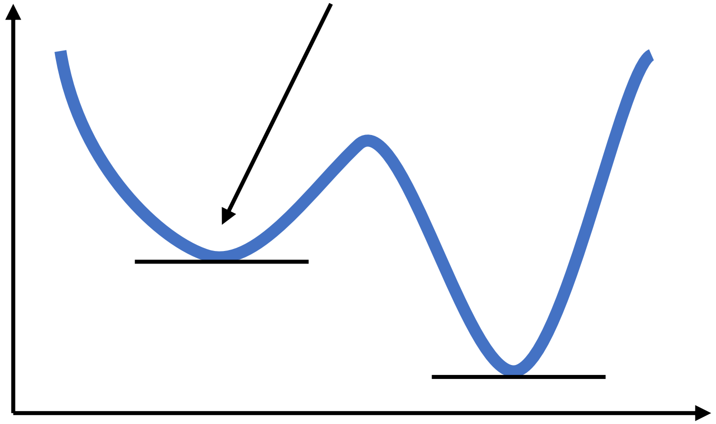
$$\begin{bmatrix} \frac{d^2\mathcal{L}}{d\theta_1 d\theta_1} & \frac{d^2\mathcal{L}}{d\theta_1 d\theta_2} & \frac{d^2\mathcal{L}}{d\theta_1 d\theta_3} \\ \frac{d^2\mathcal{L}}{d\theta_2 d\theta_1} & \frac{d^2\mathcal{L}}{d\theta_2 d\theta_2} & \frac{d^2\mathcal{L}}{d\theta_2 d\theta_3} \\ \frac{d^2\mathcal{L}}{d\theta_3 d\theta_1} & \frac{d^2\mathcal{L}}{d\theta_3 d\theta_2} & \frac{d^2\mathcal{L}}{d\theta_3 d\theta_3} \end{bmatrix}$$

$$\begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}$$

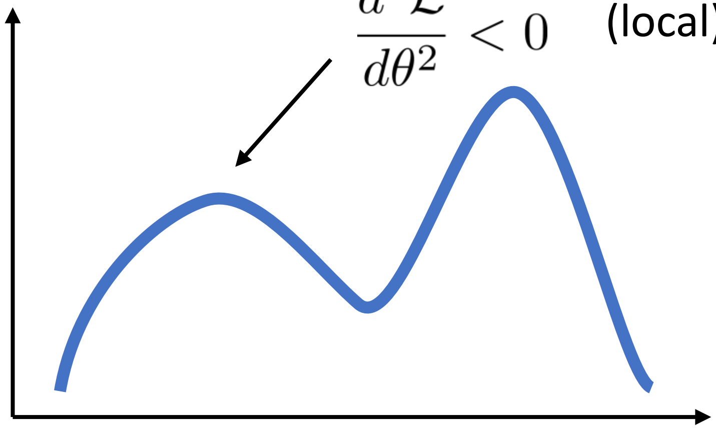
only maximum or minimum if all diagonal entries are positive or negative!

how often is that the case?

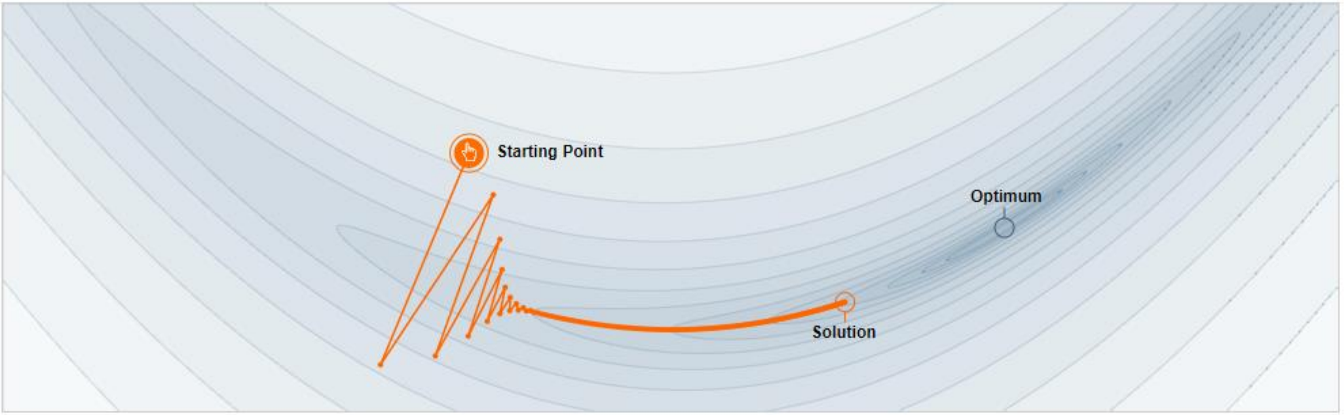
$\frac{d^2\mathcal{L}}{d\theta^2} > 0$ (local) minimum



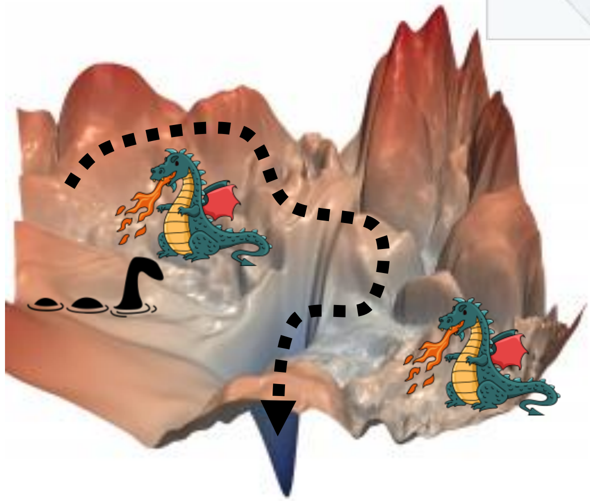
$\frac{d^2\mathcal{L}}{d\theta^2} < 0$ (local) maximum

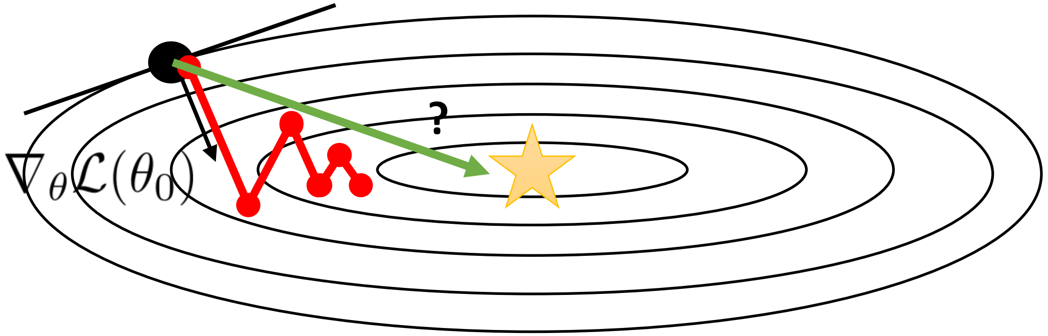


Which way do we go?



we don't always move toward the optimum!



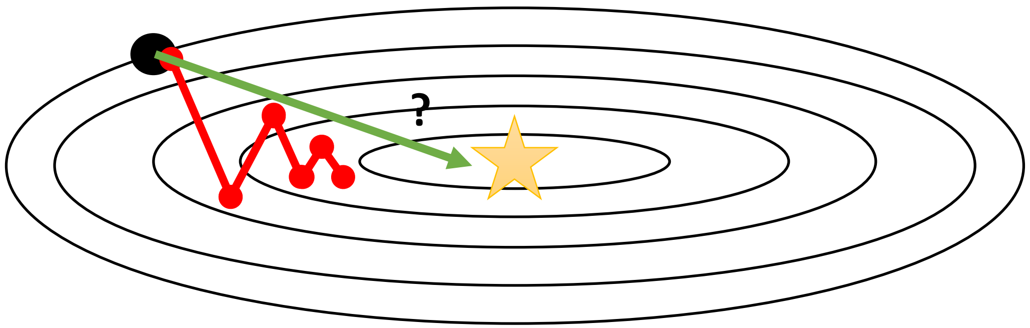


the steepest direction is not always best!

more on this later…

Improvement directions

A better direction...



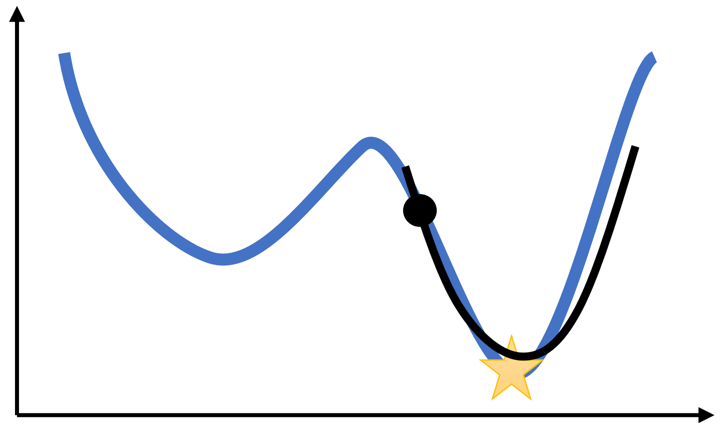
can we find this direction?

yes, with Newton's method!

we won't use Newton's method (can't afford it)

but it's an "ideal" to aspire to

Newton's method

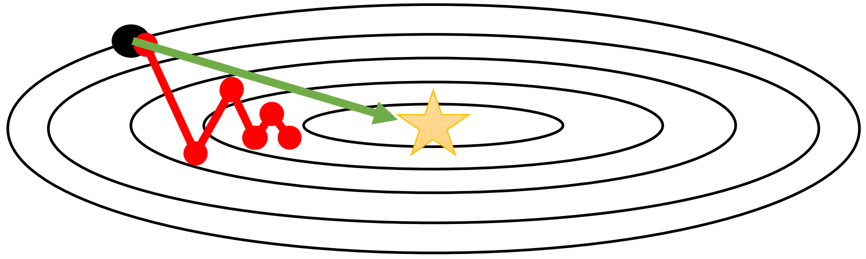


Taylor expansion:

$$f(x) \approx f(x_0) + f'(x_0)(x - x_0) + \frac{1}{2} f''(x_0)(x - x_0)^2$$

multivariate case:

$$\mathcal{L}(\theta) \approx \mathcal{L}(\theta_0) + \underbrace{\nabla_\theta \mathcal{L}(\theta_0)}_{\text{gradient}}(\theta - \theta_0) + \frac{1}{2}(\theta - \theta_0)^T \underbrace{\nabla_\theta^2 \mathcal{L}(\theta_0)}_{\text{Hessian}}(\theta - \theta_0)$$



$$\begin{bmatrix} \frac{d^2\mathcal{L}}{d\theta_1 d\theta_1} & \frac{d^2\mathcal{L}}{d\theta_1 d\theta_2} & \frac{d^2\mathcal{L}}{d\theta_1 d\theta_3} \\ \frac{d^2\mathcal{L}}{d\theta_2 d\theta_1} & \frac{d^2\mathcal{L}}{d\theta_2 d\theta_2} & \frac{d^2\mathcal{L}}{d\theta_2 d\theta_3} \\ \frac{d^2\mathcal{L}}{d\theta_3 d\theta_1} & \frac{d^2\mathcal{L}}{d\theta_3 d\theta_2} & \frac{d^2\mathcal{L}}{d\theta_3 d\theta_3} \end{bmatrix}$$

can optimize this analytically!

set derivative to zero and solve:

$$\theta^\star \leftarrow \theta_0 - (\nabla_\theta^2 \mathcal{L}(\theta_0))^{-1} \nabla_\theta \mathcal{L}(\theta_0)$$

Tractable acceleration

Why is Newton's method not a viable way to improve neural network optimization?

$$\nabla_\theta \mathcal{L}(\theta) = \begin{pmatrix} \frac{d\mathcal{L}(\theta)}{d\theta_1} \\ \frac{d\mathcal{L}(\theta)}{d\theta_2} \\ \vdots \\ \frac{d\mathcal{L}(\theta)}{d\theta_n} \end{pmatrix} \; n$$

gradient descent: $\theta_{k+1} \leftarrow \theta_k - \alpha \nabla_\theta \mathcal{L}(\theta_k)$ runtime? $\mathcal{O}(n)$

Hessian

$$\underbrace{\begin{bmatrix} \frac{d^2\mathcal{L}}{d\theta_1 d\theta_1} & \frac{d^2\mathcal{L}}{d\theta_1 d\theta_2} & \frac{d^2\mathcal{L}}{d\theta_1 d\theta_3} \\ \frac{d^2\mathcal{L}}{d\theta_2 d\theta_1} & \frac{d^2\mathcal{L}}{d\theta_2 d\theta_2} & \frac{d^2\mathcal{L}}{d\theta_2 d\theta_3} \\ \frac{d^2\mathcal{L}}{d\theta_3 d\theta_1} & \frac{d^2\mathcal{L}}{d\theta_3 d\theta_2} & \frac{d^2\mathcal{L}}{d\theta_3 d\theta_3} \end{bmatrix}}_{n} \; n$$

$$\theta^\star \leftarrow \theta_0 - (\nabla_\theta^2 \mathcal{L}(\theta_0))^{-1} \nabla_\theta \mathcal{L}(\theta_0)$$

runtime?

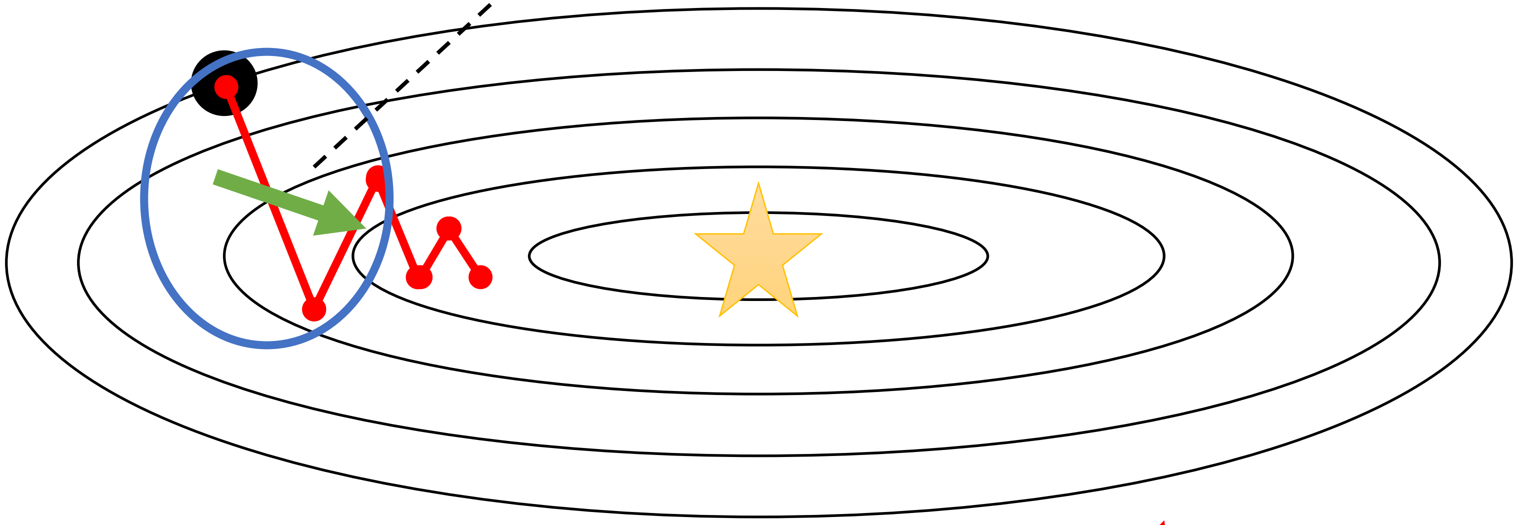
$\mathcal{O}(n^3)$

if using naïve approach, though fancy methods can be much faster if they avoid forming the Hessian explicitly

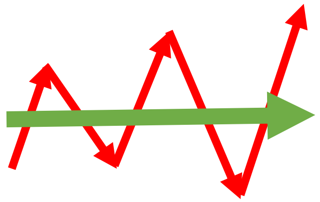
because of this, we would really prefer methods that don't require second derivatives, but somehow "accelerate" gradient descent instead

Momentum

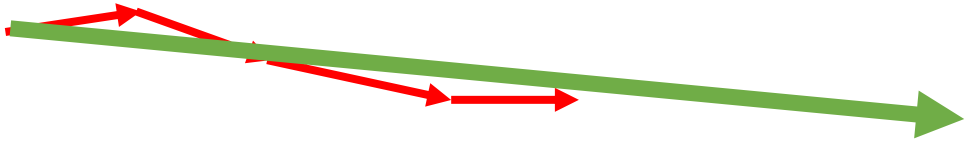
averaging together successive gradients
seems to yield a much better direction!



Intuition: if successive gradient steps point in **different** directions, we should **cancel off** the directions that disagree



if successive gradient steps point in **similar** directions, we should **go faster** in that direction



Momentum

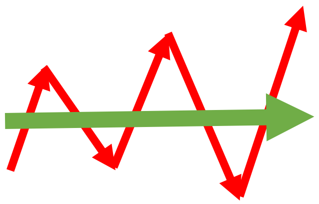
update rule:

$$\theta_{k+1} = \theta_k - \alpha g_k$$

before: $g_k = \nabla_\theta \mathcal{L}(\theta_k)$

now: $g_k = \nabla_\theta \mathcal{L}(\theta_k) + \underbrace{\mu g_{k-1}}$

"blend in" previous direction



this is a **very** simple update rule

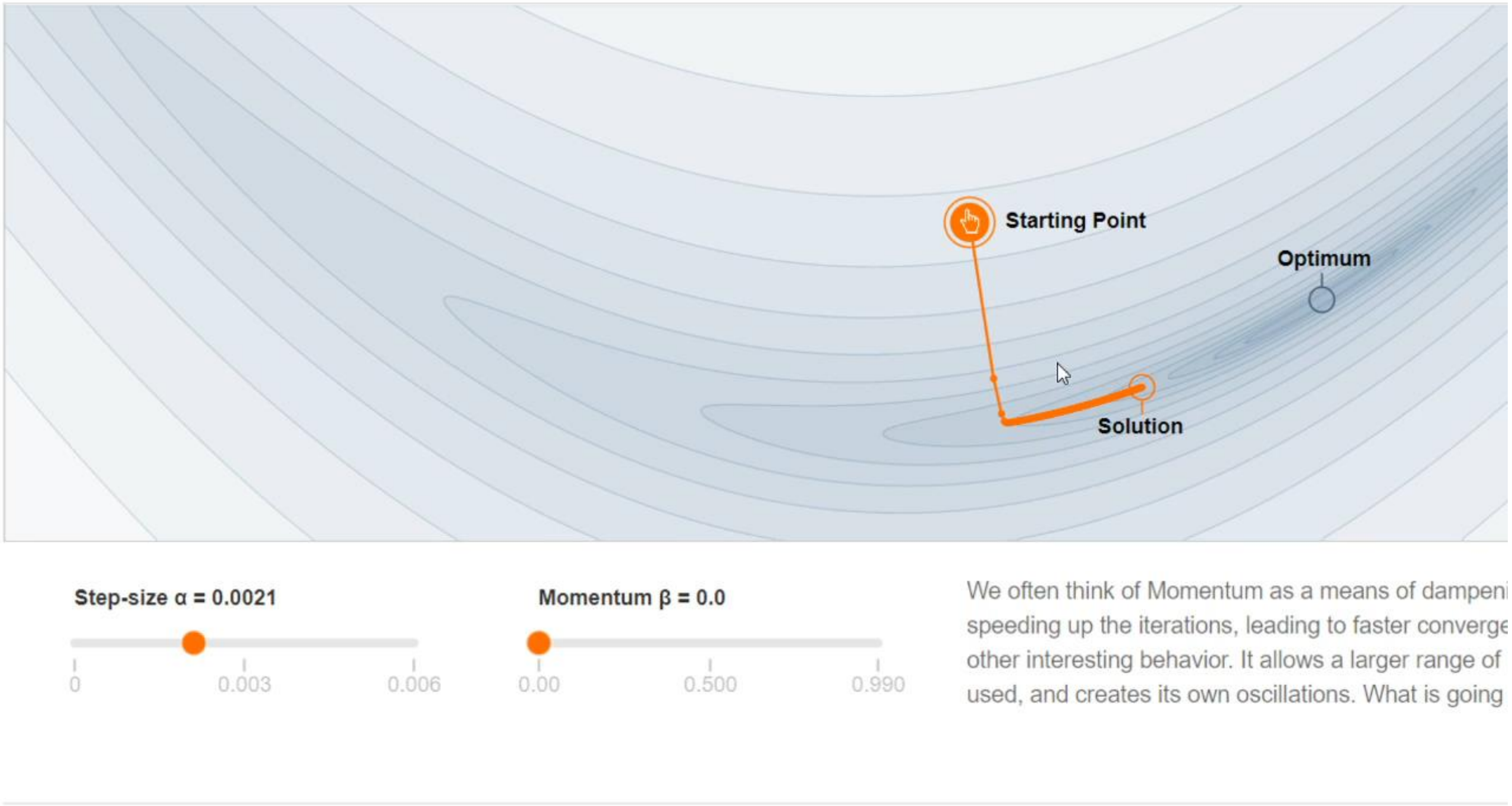
adding weight for previous direction also

in practice, it brings some of the benefits of Newton's method, at virtually no cost

this kind of momentum method has few guarantees

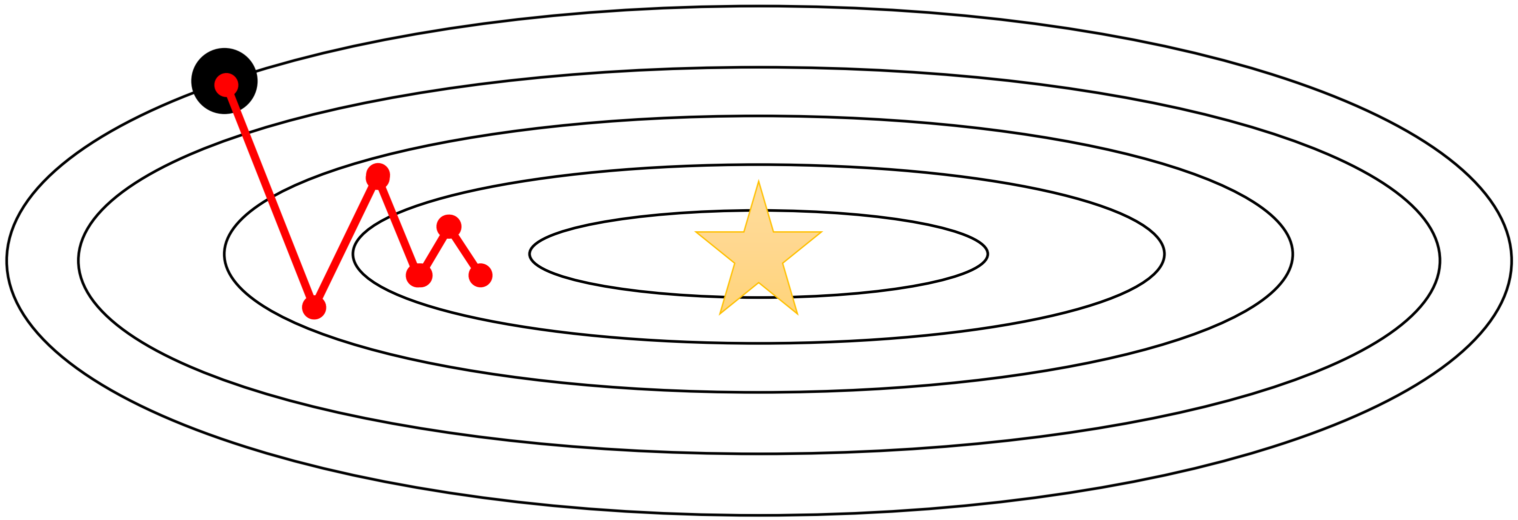
a closely related idea is "Nesterov accelerated gradient," which **does** carry very appealing guarantees (in practice we usually just momentum)

Momentum Demo



visualizations based on Gabriel Goh’s distill.pub article: https://distill.pub/2017/momentum/

Gradient scale



$$\nabla_\theta \mathcal{L}(\theta) = \begin{pmatrix} \frac{d\mathcal{L}(\theta)}{d\theta_1} \\ \frac{d\mathcal{L}(\theta)}{d\theta_2} \\ \vdots \\ \frac{d\mathcal{L}(\theta)}{d\theta_n} \end{pmatrix}$$

$$\mathcal{L}(\theta) = ||f_\theta(x) - y||^2$$

$$\nabla_\theta \mathcal{L}(\theta) = \underbrace{(f_\theta(x) - y)^T}_{\text{huge when far from optimum}} \frac{df}{d\theta}$$

Intuition: the **sign** of the gradient tells us which way to go along each dimension, but the magnitude is not so great

Even worse: overall magnitude of the gradient can change drastically over the course of optimization, making learning rates hard to tune

Idea: “normalize” out the magnitude of the gradient **along each dimension**

Algorithm: RMSProp

Estimate per-dimension magnitude (running average):

$s_k \leftarrow \beta s_{k-1} + (1-\beta)(\nabla_\theta \mathcal{L}(\theta_k))^2$ this is *roughly* the squared length of each dimension

$\theta_{k+1} = \theta_k - \alpha \frac{\nabla_\theta \mathcal{L}(\theta_k)}{\sqrt{s_k}}$ each dimension is divided by its magnitude

Algorithm: AdaGrad

Estimate per-dimension cumulative magnitude:

$$s_k \leftarrow s_{k-1} + (\nabla_\theta \mathcal{L}(\theta_k))^2$$

$$\theta_{k+1} = \theta_k - \alpha \frac{\nabla_\theta \mathcal{L}(\theta_k)}{\sqrt{s_k}}$$

RMSProp:

$$s_k \leftarrow \beta s_{k-1} + (1-\beta)(\nabla_\theta \mathcal{L}(\theta_k))^2$$

How does AdaGrad and RMSProp compare?

- AdaGrad has some appealing guarantees for **convex** problems
  - Learning rate effectively "decreases" over time, which is good for convex problems
  - But this only works if we find the optimum quickly before the rate decays too much

- RMSProp tends to be much better for deep learning (and most non-convex problems)

Algorithm: Adam

Basic idea: combine **momentum** and **RMSProp**

$$m_k = (1-\beta_1)\nabla_\theta \mathcal{L}(\theta_k) + \beta_1 m_{k-1}$$

first moment estimate ("momentum-like")

$$v_k = (1-\beta_2)(\nabla_\theta \mathcal{L}(\theta_k))^2 + \beta_2 v_{k-1}$$

second moment estimate

$$\hat{m}_k = \frac{m_k}{1-\beta_1^k}$$

why? $m_0 = 0$ $v_0 = 0$

so early on these values will be small, and this correction "blows them up" a bit for small *k*

$$\hat{v}_k = \frac{v_k}{1-\beta_2^k}$$

good default settings:

$\alpha = 0.001$

$\beta_1 = 0.9$

$\beta_2 = 0.999$

$$\theta_{k+1} = \theta_k - \alpha \frac{\hat{m}_k}{\sqrt{\hat{v}_k} + \epsilon}$$

small number to prevent division by zero

$\epsilon = 10^{-8}$

Stochastic optimization

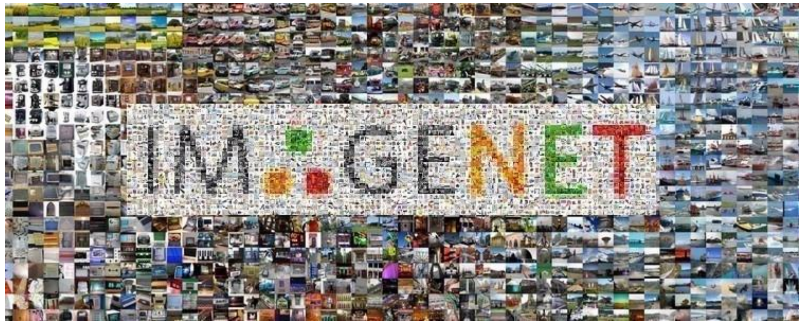
Why is gradient descent expensive?

$$\mathcal{L}(\theta) = -\underbrace{\frac{1}{N}\sum_{i=1}^{N} \log p_\theta(y_i|x_i)} \approx -E_{p_{\text{data}}(x,y)}[\log p_\theta(y_i|x_i)] \approx -\frac{1}{B}\sum_{j=1}^{B} \log p_\theta(y_{i_j}|x_{i_j})$$

requires summing over **all** datapoints in the dataset

could simply use **fewer** samples, and still have a correct (unbiased) estimator

$$B << N$$



ILSVRC (ImageNet), 2009: 1.5 **million** images

Stochastic gradient descent

with minibatches

1. Sample $\mathcal{B} \subset \mathcal{D}$
2. Estimate $g_k \leftarrow -\nabla_\theta \frac{1}{B} \sum_{i=1}^{B} \log p(y_i|x_i, \theta) \approx \nabla_\theta \mathcal{L}(\theta)$
3. $\theta_{k+1} \leftarrow \theta_k - \alpha g_k$

draw **B** datapoints at random from dataset of size **N**

(where sum is over elements in $\mathcal{B}$)

can also use momentum, ADAM, etc.

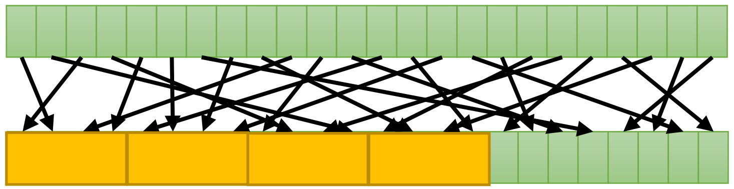
each iteration samples a different **minibatch**

Stochastic gradient descent **in practice:**

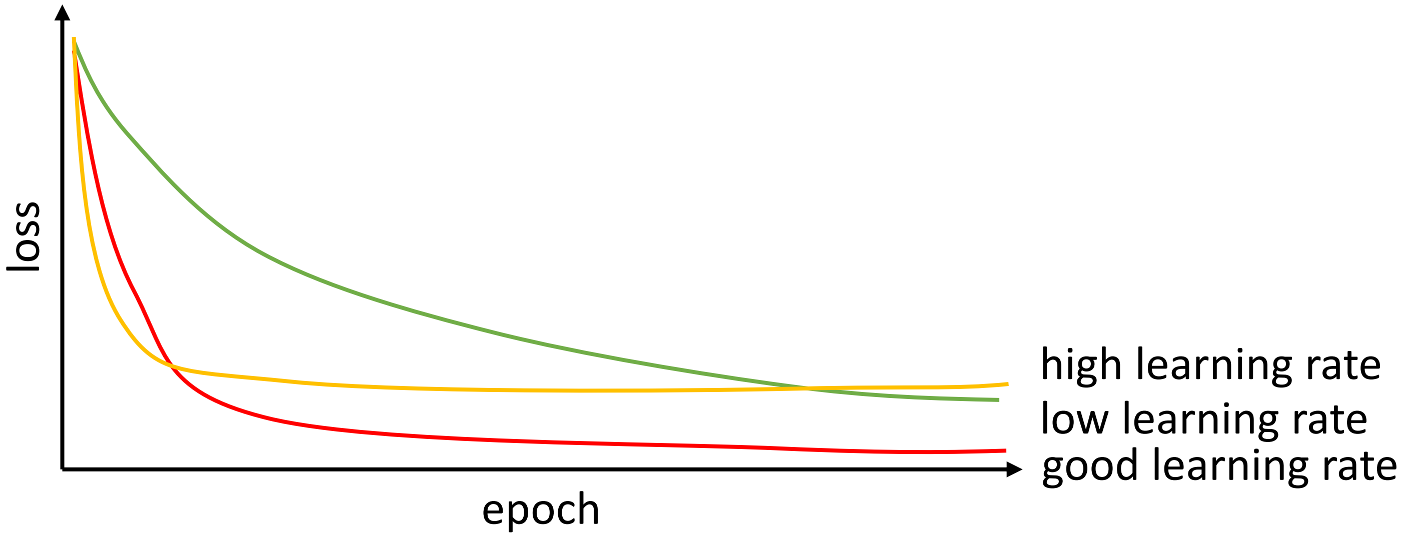
sampling randomly is slow due to random memory access

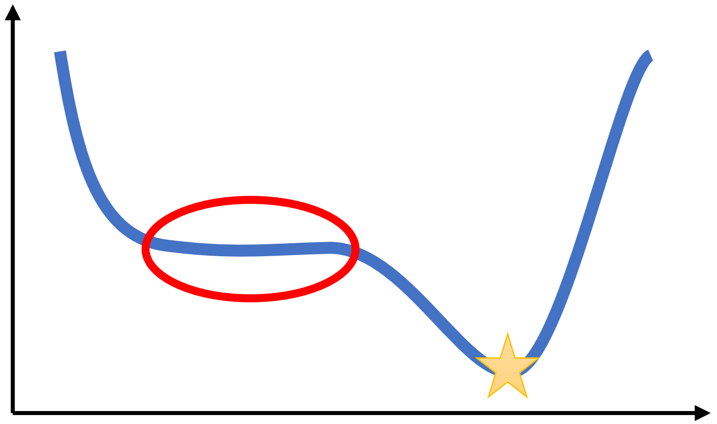
instead, shuffle the dataset (like a deck of cards…) once, in advance

then just construct batches out of consecutive groups of **B** datapoints

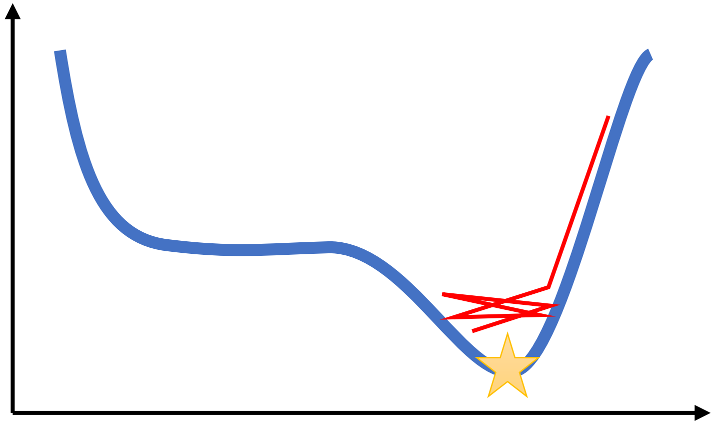


Learning rates



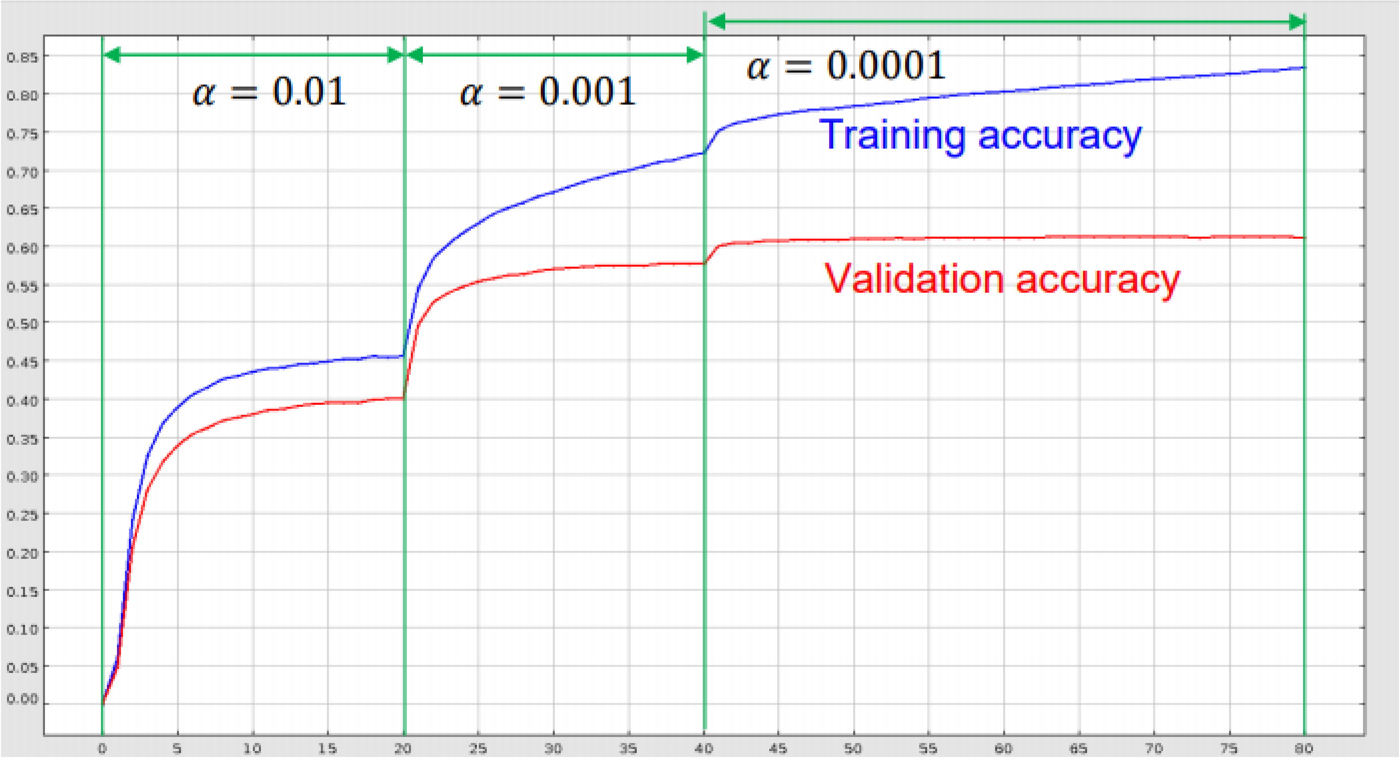


Low learning rates **can** result in convergence to worse values!
This is a bit counter-intuitive



Decaying learning rates

AlexNet trained on ImageNet



Learning rate decay schedules usually needed for best performance with SGD (+momentum)

Often not needed with ADAM

Opinions differ, some people think SGD + momentum is better than ADAM if you want the very best performance (but ADAM is easier to tune)

Tuning (stochastic) gradient descent

Hyperparameters:

batch size: B — larger batches = less noisy gradients, usually “safer” but more expensive

learning rate: α — best to use the biggest rate that still works, decay over time

momentum: μ — 0.99 is good

Adam parameters: β_1, β_2 — keep the defaults (usually)

Hyperparameters in Machine learning are those parameters that are explicitly defined by the user to control the learning process. These hyperparameters are used to improve the learning of the model, and their values are set before starting the learning process of the model.

What to tune hyperparameters on?

Technically we want to tune this on the **training** loss, since it is a parameter of the optimization

Often tuned on **validation** loss

Relationship between stochastic gradient and regularization is complex – some people consider it to be a good regularizer!
(this suggests we should use validation loss)

training loss is used to optimize the model's parameters during training, validation loss helps monitor the model's performance during training and detect overfitting