Deep Learning 1

2025-2026 - Pascal Mettes

Lecture 3

Deep learning optimization I

Previous lecture

Lecture	Title
1	Intro and history of deep learning
3	Deep learning optimization I
5	Convolutional deep learning
7	Graph deep learning
9	Multi-modal deep learning
11	What doesn't work in deep learning
13	Q&A

Lecture	Title
2	AutoDiff
4	Deep learning optimization II
6	Attention-based deep learning
8	From supervised to unsupervised deep learning
10	Generative deep learning
12	Non-Euclidean deep learning
14	Deep learning for videos

This lecture

Stochastic gradient descent

Advanced optimizers


have model
• Architecture
• Weights initialisation
compute loss
• Gradient Descent, dataloader
• Augmentations
• Regularisation
compute gradient
• Loss functions
• Backprop
update weights
• Gradient Descent
• Advanced Optimizers

Optimization versus learning

Optimization

- given a parametric definition of model and a set of data, we want to discover the optimal parameter that minimize a certain objective function, given some data.
- E.g., find the optimal flight schedule given resources and population.

Learning

- We have observed and unobserved data.
- Reduce errors on the observed data (training data) to *generalize* to unseen data (test data).
- The goal is to reduce the generalization error.

Minimizing risk

We want to optimize on observed data.

Minimizing a cost function, with extra regularizations

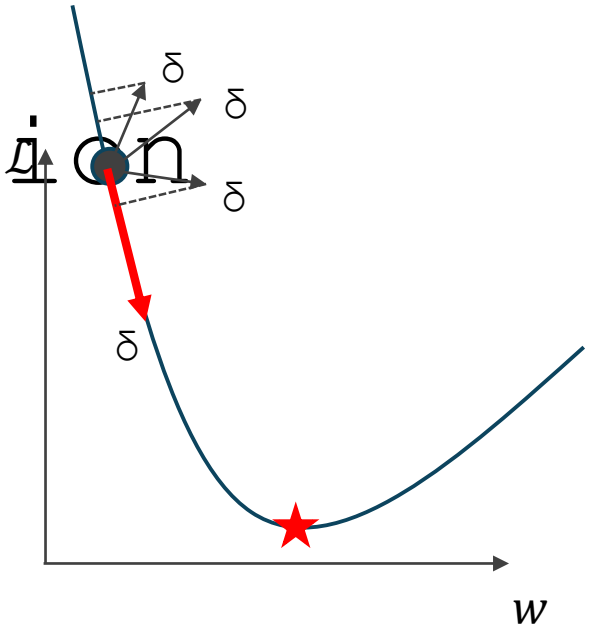
$$\min_{\mathbf{w}} \mathbb{E}_{\boldsymbol{x},\mathrm{y}\sim p_{data}}[\mathcal{L}(f(\boldsymbol{x},\boldsymbol{w}),y)] + \lambda\Omega(\boldsymbol{w})$$

where $\hat{y} = f(\boldsymbol{x},\boldsymbol{w}) = h_L \circ h_{L-1} \circ \cdots \circ h_1(\boldsymbol{x})$ is the prediction and each h_l comes with parameters $\boldsymbol{w}_l$.

In simple words: (1) predictions are not too wrong, while (2): not being "too geared" towards the observed data.

Problem: the true distribution p_{data} is not available.

Empirical risk minimization



In practice having p_{data} is not possible.

We only have a training set of data

$$\min_{\mathbf{w}} \mathbb{E}_{\boldsymbol{x},\mathbf{y}\sim\hat{p}_{data}}[\mathcal{L}(f(\boldsymbol{x},\boldsymbol{w}),y)] + \lambda\Omega(\boldsymbol{w})$$

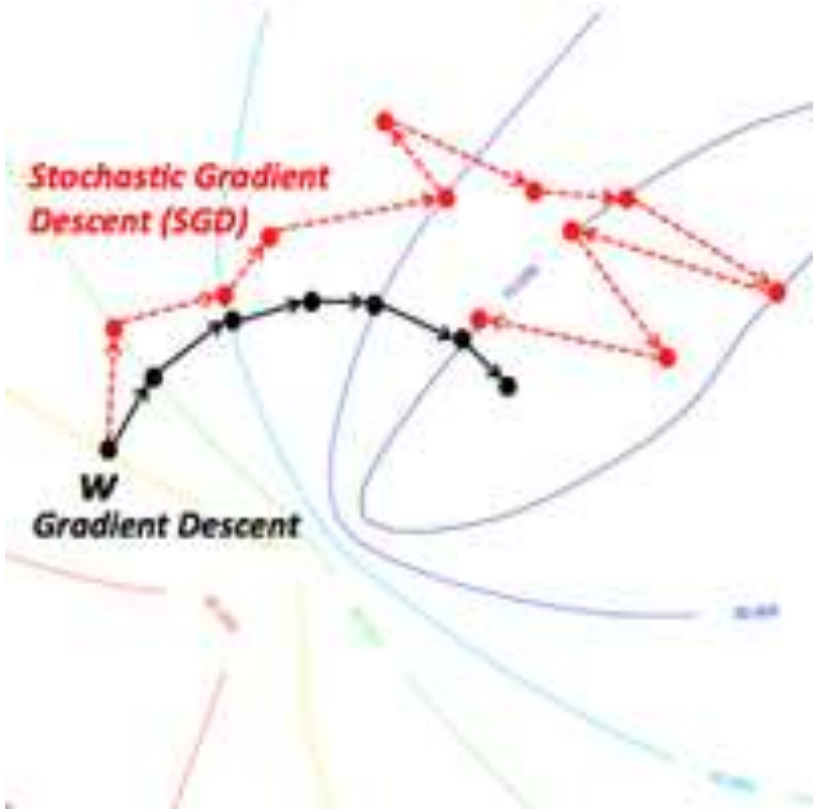
with $\hat{p}_{data}$ the empirical data distribution, defined by a set of training examples.

To minimize any function, we take a step δ. Our best bet: the (negative) gradient

$$-\sum\frac{d}{dw}\mathcal{L}(f(\boldsymbol{x},\boldsymbol{w}),y)$$

Gradient descent based on optimization.

Stochastic gradient descent



Instead of using the entire dataset to calculate gradients, perform parameter update for each mini-batch.

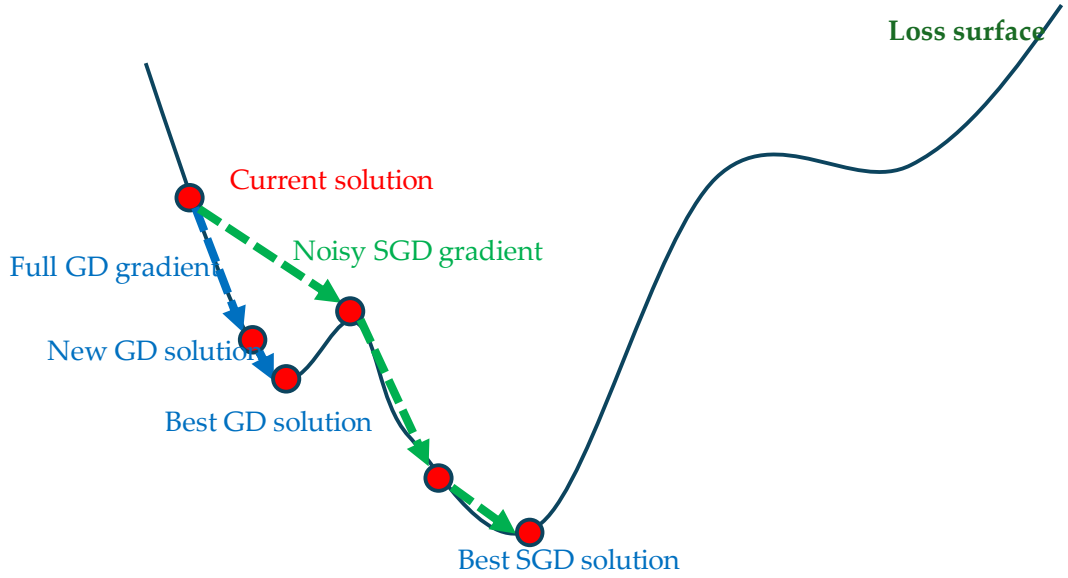
Properties of SGD

Randomness actually reduces overfitting.

Reshuffling is important!

One epoch = go through all mini-batches.

Be careful to balance class/data per batch.




```
trainset = torchvision.datasets.CIFAR10(root='./data', train=True,
                                        download=True, transform=transform)
trainloader = torch.utils.data.DataLoader(trainset, batch_size=batch_size,
                                          shuffle=True, num_workers=2)
```

On batch size

Large batch size: more accurate estimation of the gradient.

Very small batch size: underutilizes hardware, but can act as regularizer.

General rule: batch size and learning rate are coupled (double BS = double LR)

(*Accurate, Large Minibatch SGD: Training ImageNet in 1 Hour.* Goyal et al. 2017: Batchsize of 8K)

Guideline: use the largest batch size that fits on the GPU and is a power of 2.

Why does mini-batch SGD work?

Gradient descent is already an approximation; the true data distribution is unknown.

Reduced sample size does not imply reduced gradient quality.

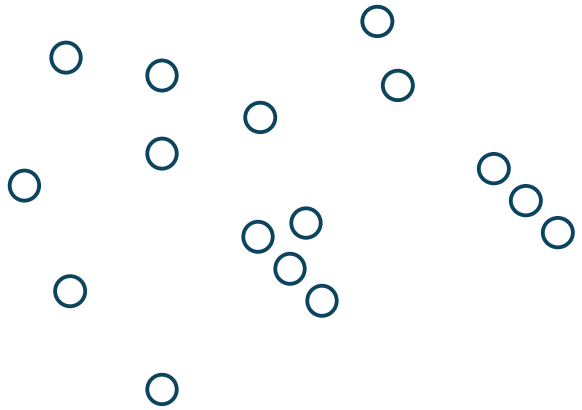
The training samples may have lots of noises or outliers or biases.

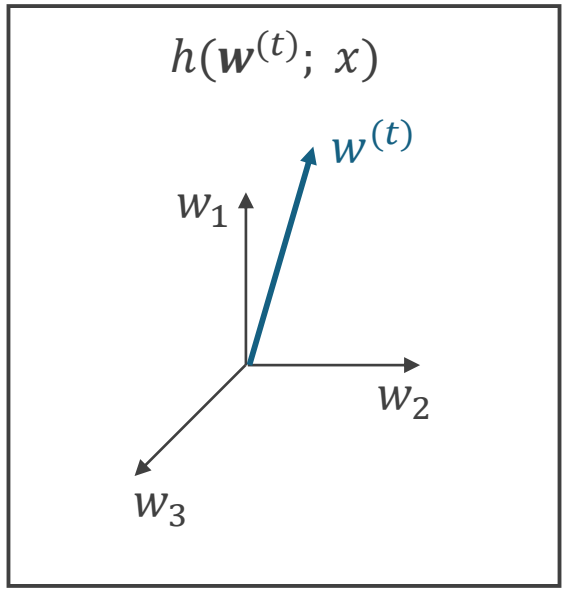
- A randomly sampled minibatch may reflect the true data generating distribution better (or worse).

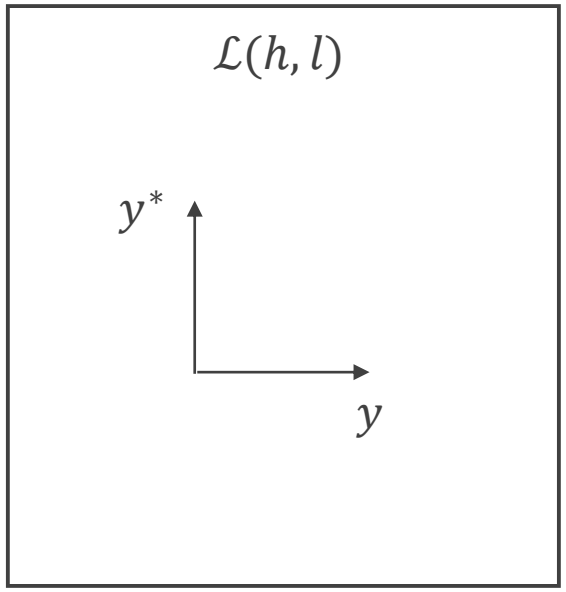
Real gradient might get stuck into a local minima.

- While *more random gradient* computed with minibatch might not.

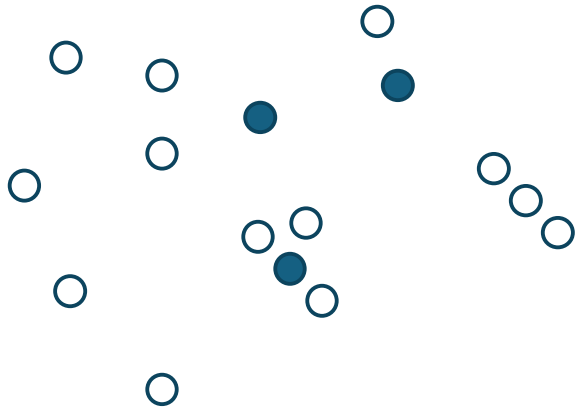
Stochastic gradient descent



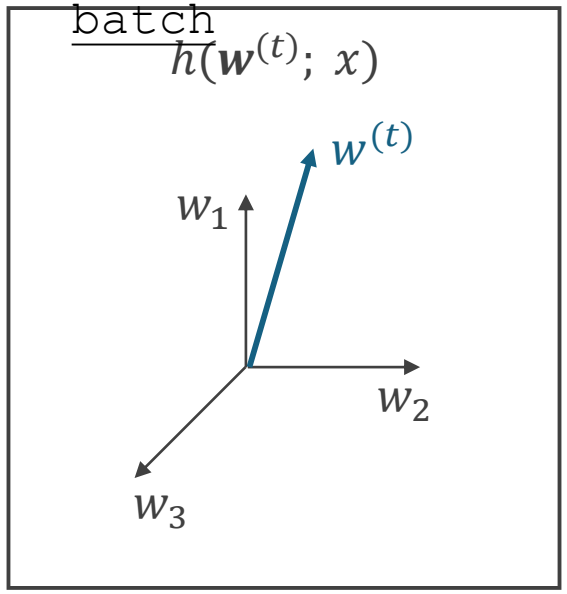


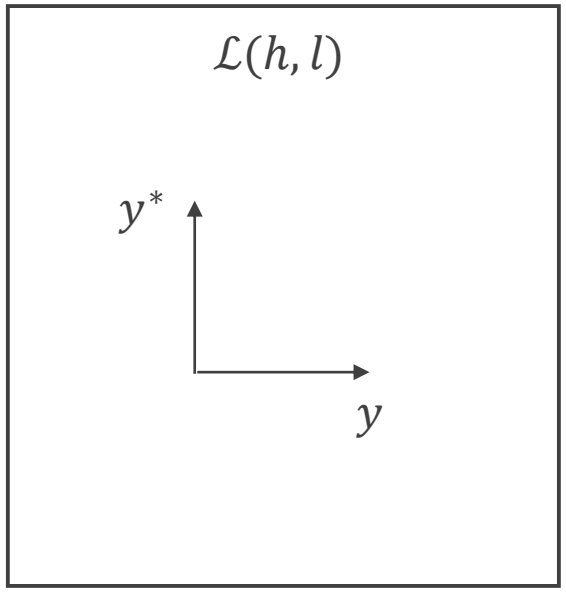


Stochastic gradient descent

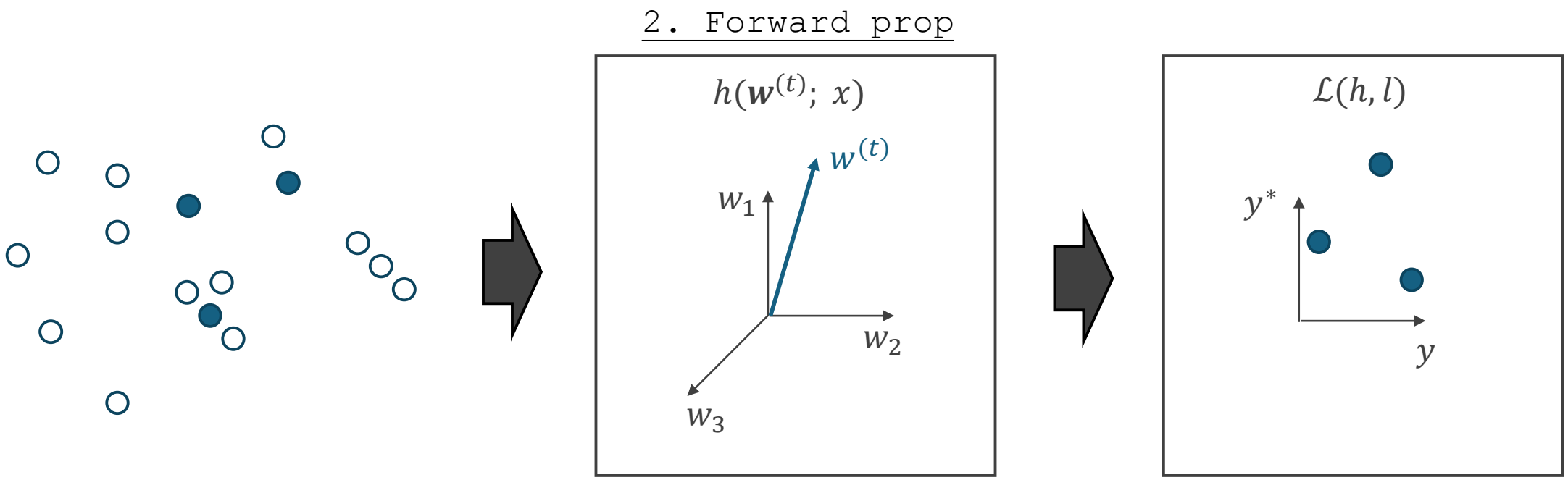


1. Sample mini-batch

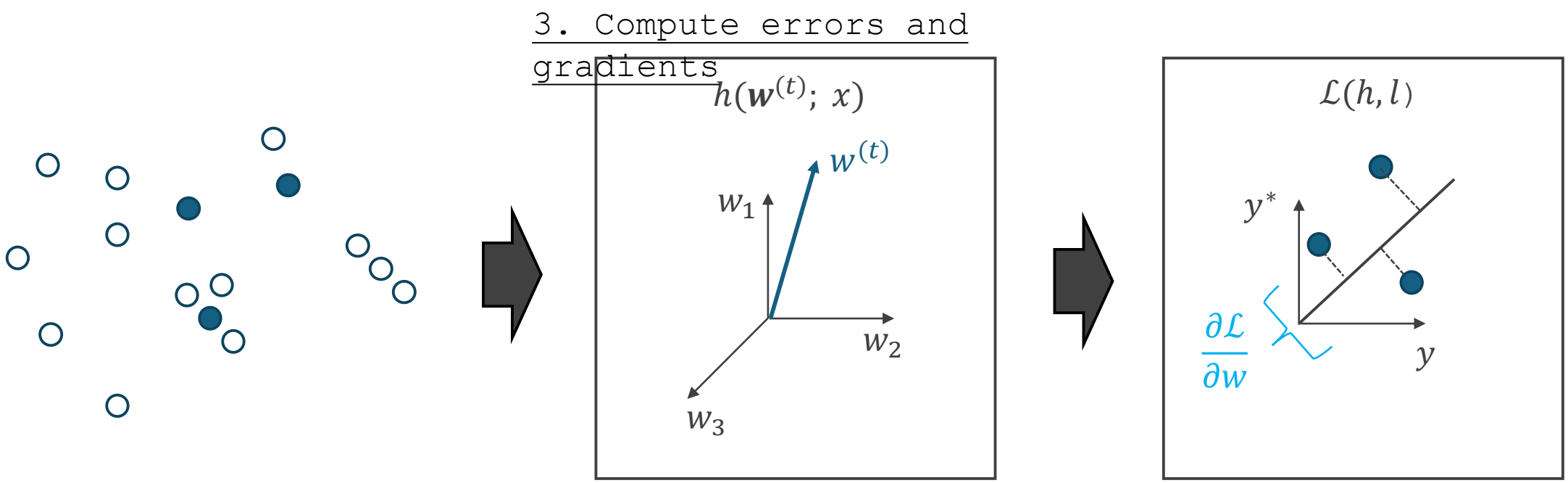




Stochastic gradient descent

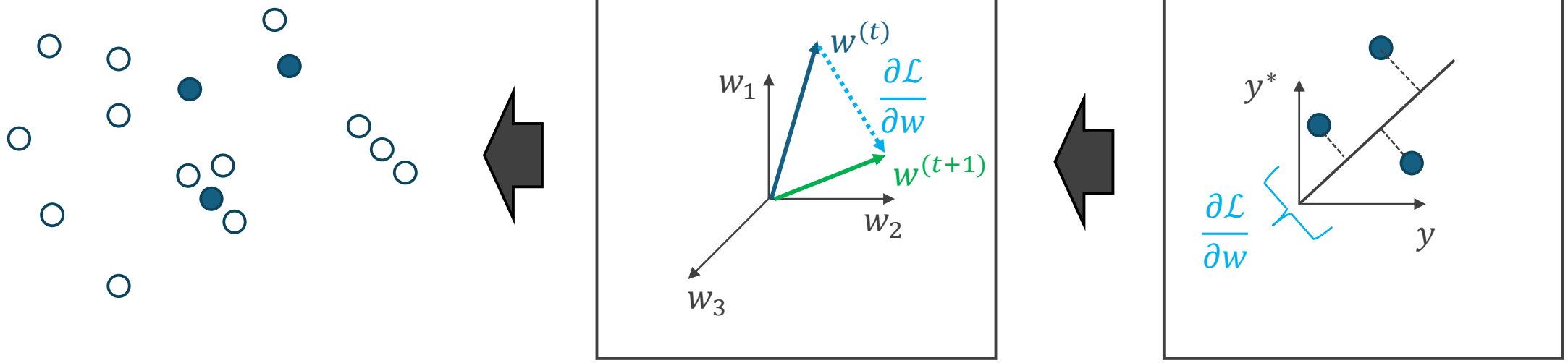


Stochastic gradient descent



Stochastic gradient descent

4. Update model parameters and repeat



In a nutshell

First, define your neural network

$$y = h_L \circ h_{L-1} \circ \cdots \circ h_1 (\boldsymbol{x})$$

where each module h_l comes with parameters $\boldsymbol{w}_l$

Finding an "optimal" neural network means minimizing a loss function

$$\boldsymbol{w}^* = \underset{\boldsymbol{w}}{\operatorname{argmin}} L(\boldsymbol{w}) = \sum_{(\boldsymbol{x},y)\in(X,Y)} \mathcal{L}(\, f(\boldsymbol{x},\boldsymbol{w}), y) + \lambda\Omega(\boldsymbol{w})$$

Rely on stochastic gradient descent methods to obtain desired parameters

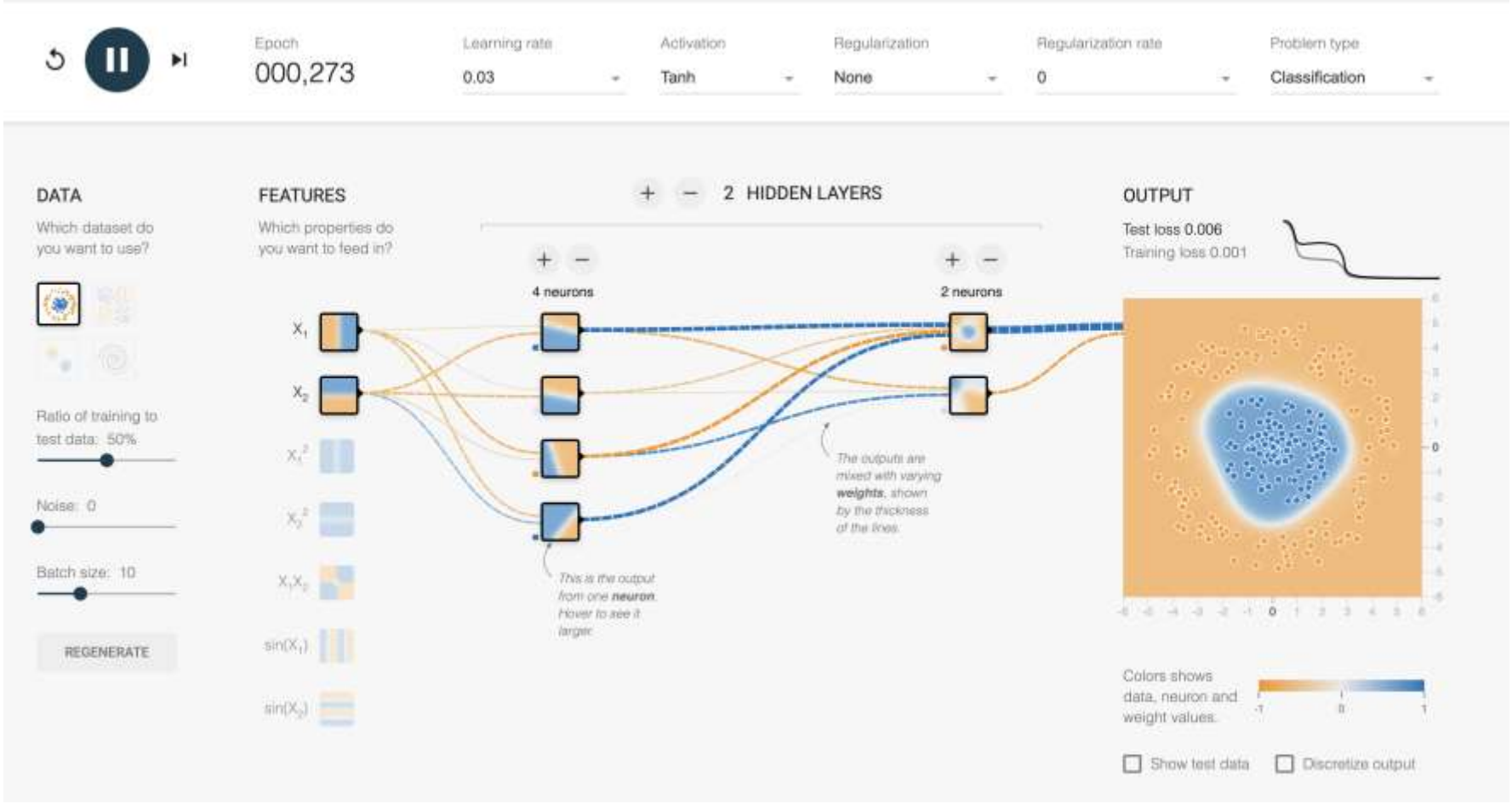
$$\boldsymbol{w}^{(t+1)} = \boldsymbol{w}^{(t)} - \eta \frac{dL}{d\boldsymbol{w}}$$

where η is the step size or learning rate.

Gradient vs Stochastic Gradient Descent

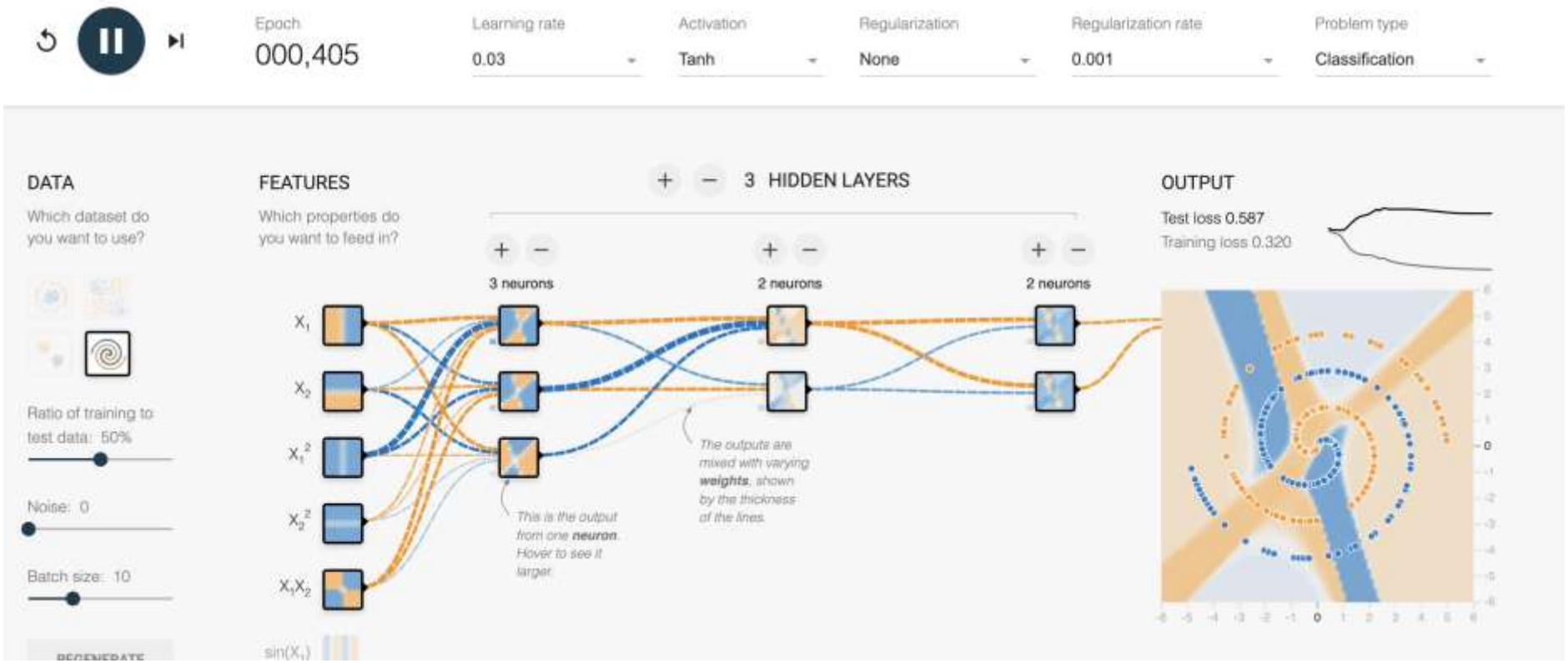
Gradient Descent	Stochastic Gradient Descent
Computes gradient using the whole training dataset	Computes gradient using a single training sample
Not suggested for huge training samples	Can be used for large training samples
Deterministic in nature	Stochastic in nature
No random shuffling of points required	Shuffling needed. More hyperparameters, e.g. batch size
Can’t escape shallow local minima easily	Can escape shallow local minima more easily
Convergence is slow	Reaches the convergence faster

Practical examples



https://playground.tensor

Practical examples



https://playground.tensor

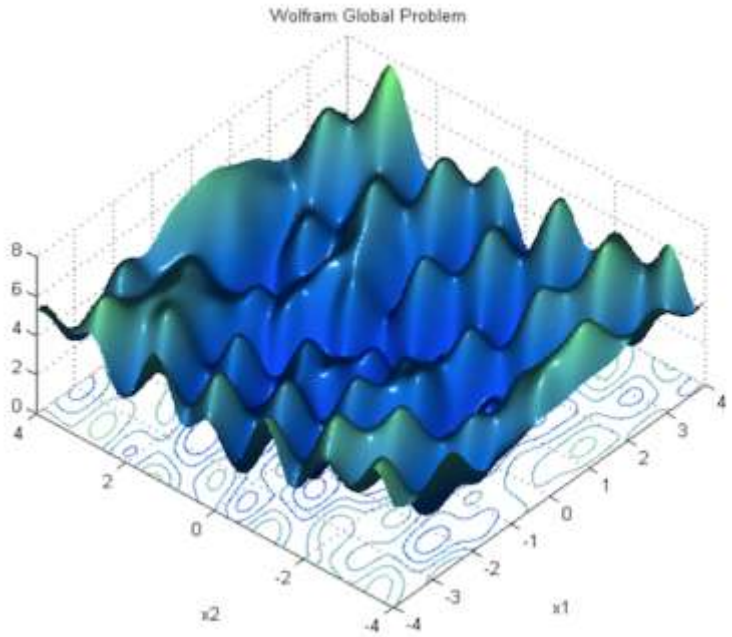
Challenges of optimizing deep networks

Neural network training is **non-convex** optimization.

- Involves a function which has multiple optima.
- Extremely difficult to locate the global optimum.

This raises many problems:

- How do we avoid getting stuck in loc
- What is a reasonable learning rate t
- What if the loss surface morphology
- …



Main challenges in optimization

1. Ill conditioning → a strong gradient might not even be good enough
2. Local optimization is susceptive to local minima
3. Ravines, plateaus, cliffs, and pathological curvatures
4. Vanishing and exploding gradients
5. Long-term dependencies

1. Ill conditioning

Hessian matrix *H*

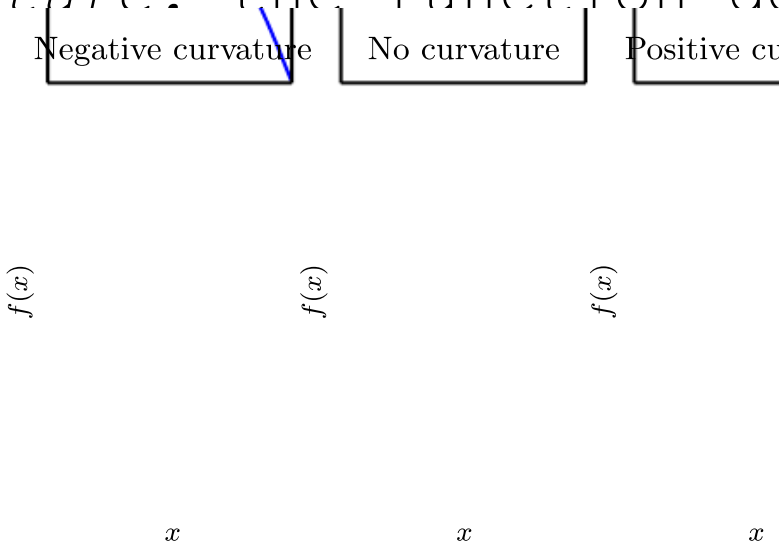
- Square matrix of second-order partial derivatives of *a scalar-valued function.*
- The *Hessian* describes the local *curvature* of a function of many variables.
- The Hessian mat[illegible]

$$\mathbf{H} = \begin{bmatrix} \frac{\partial^2 f}{\partial x_1^2} & \frac{\partial^2 f}{\partial x_1\,\partial x_2} & \cdots & \frac{\partial^2 f}{\partial x_1\,\partial x_n} \\ \frac{\partial^2 f}{\partial x_2\,\partial x_1} & \frac{\partial^2 f}{\partial x_2^2} & \cdots & \frac{\partial^2 f}{\partial x_2\,\partial x_n} \\ \vdots & \vdots & \ddots & \vdots \\ \frac{\partial^2 f}{\partial x_n\,\partial x_1} & \frac{\partial^2 f}{\partial x_n\,\partial x_2} & \cdots & \frac{\partial^2 f}{\partial x_n^2} \end{bmatrix}$$

1. Ill conditioning

Curvature is determined by the second derivative

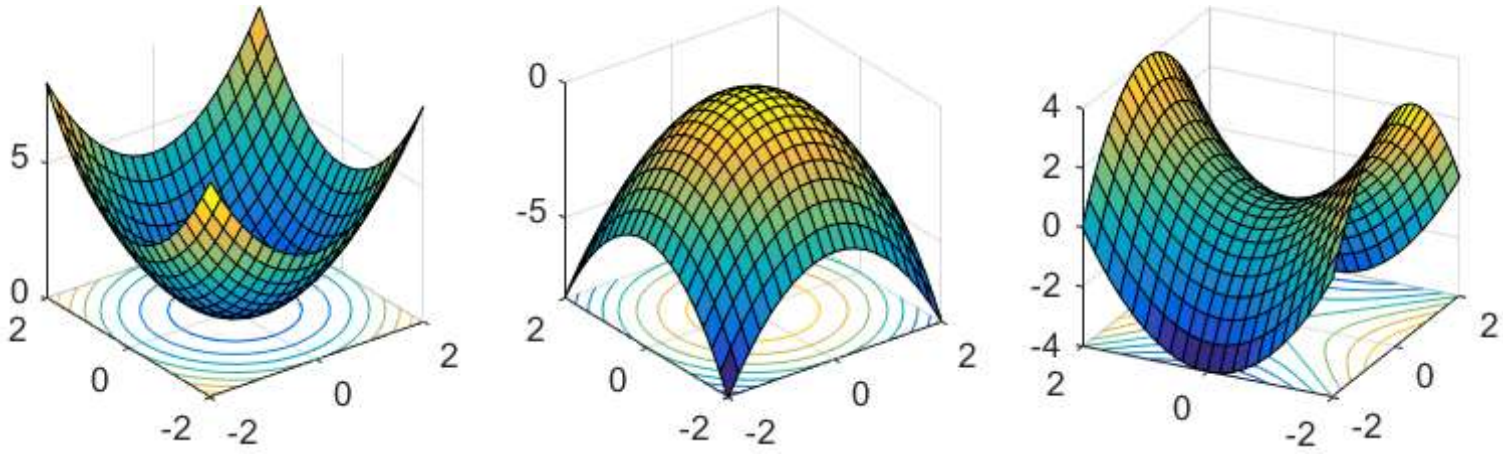
- *Negative curvature:* cost function decreases faster than the gradient predicts.
- *No curvature:* the gradient predicts the decrease correctly.
- *Positive curvature:* the function decreases slower than expected and e ease.



1. Ill conditioning

Critical points – Hessian matrix

- *A local minimum:* positive definite (all its eigenvalues are positive)
- *A local maximum:* negative definite (all its eigenvalues are negative)
- *A saddle point:* at least one eigenvalue is positive and a is this bad?



Prevalence of saddle points: https://ganguli-gang.stanford.edu/pdf/14.SaddlePoint.NIPS.pdf

1. Ill conditioning

Consider the Hessian matrix H has an eigenvalue decomposition.

Its condition numbe $\max_{i,j} \left| \frac{\lambda_i}{\lambda_j} \right|$

This is the ratio of the magnitude of the largest (i) and smallest eigenvalue (j).

Measures show much the second derivatives differ from each other.

With a poor (large) condition number, gradient descent performs poorly.

- In one direction derivative increases rapidly, in another it increases slowly.

2. Local minima

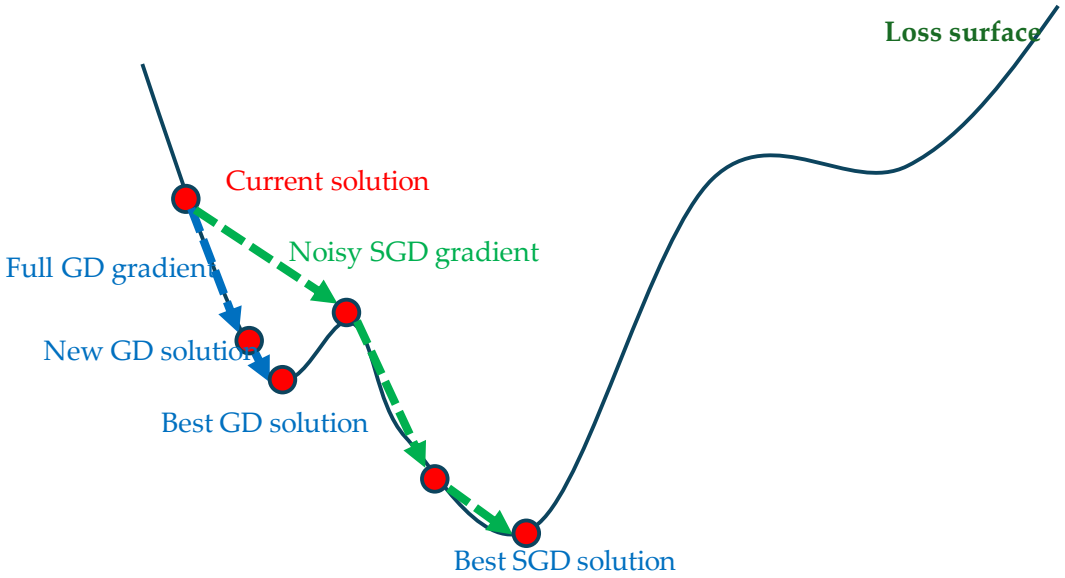
Model identifiability

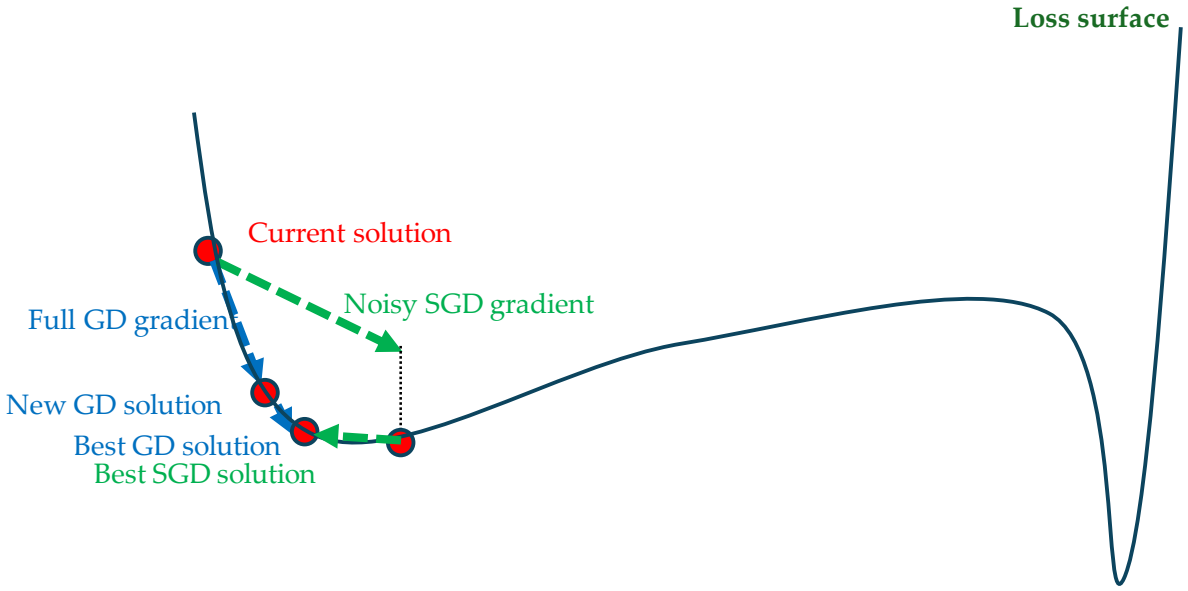
- A model is said to be identifiable if a sufficiently large training set can rule out all but one setting of the model's parameters.
- Models with latent variables are often not identifiable because we can obtain equivalent models by exchanging latent variables with each other.

Local minima can be extremely numerous

- However, all local minima from non-identifiability are equivalent in cost function value.
- *Those* local minima are not a problematic form of non-convexity.
- The other local minima (next slides) are.

Local minima

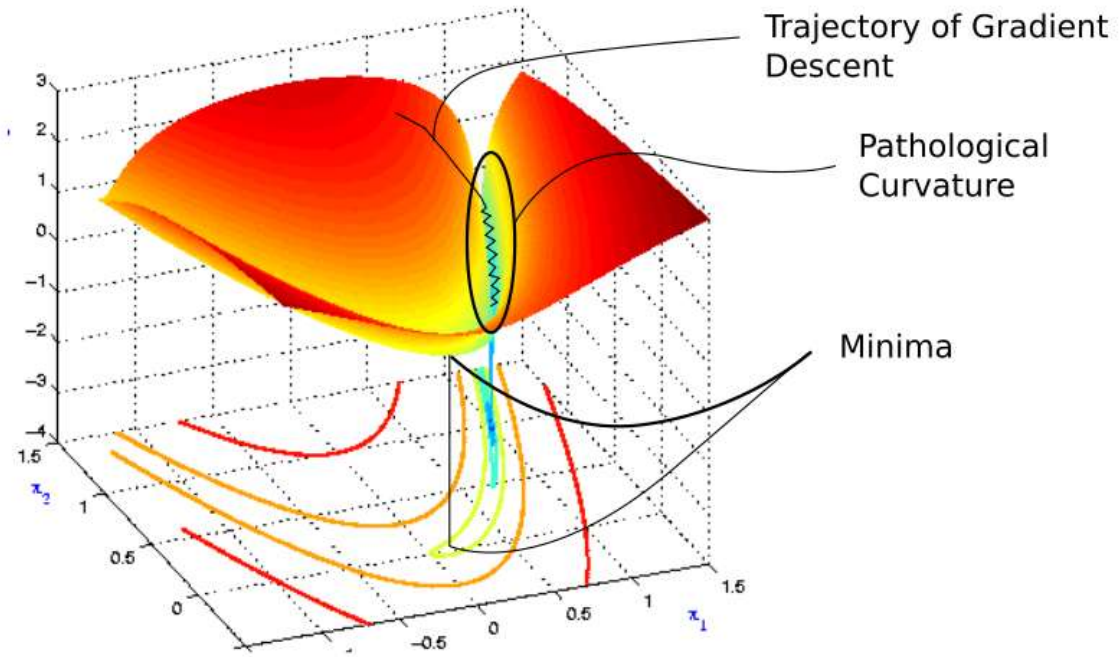


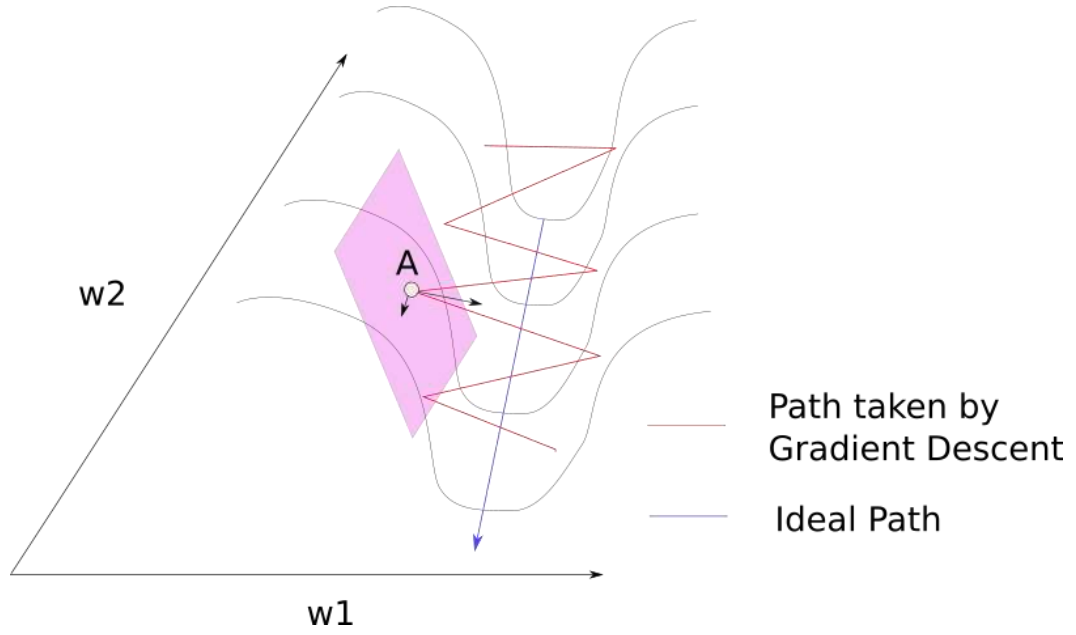


With gradient descent, we are blind to what the landscape looks like.

Picture credit: Team Pa

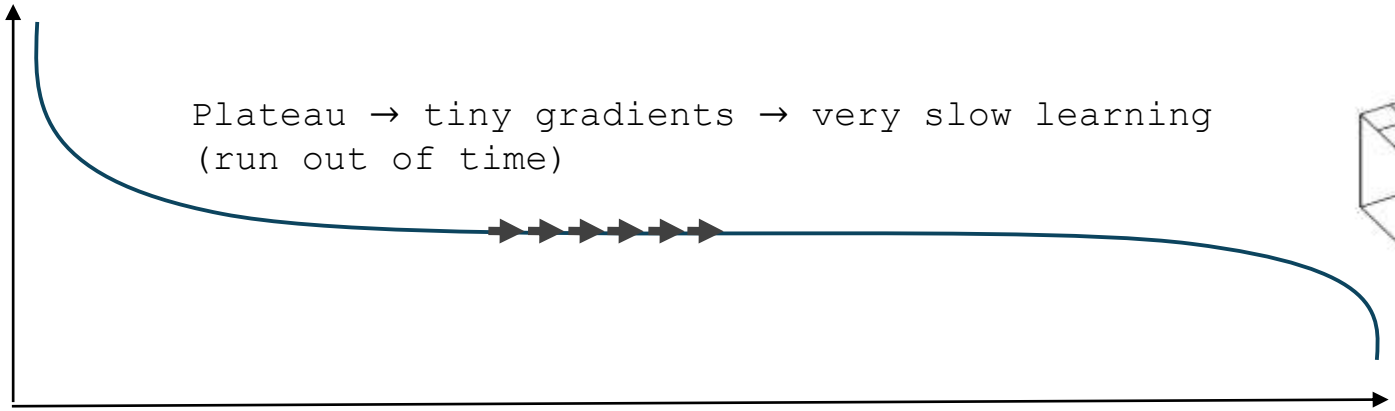
3. Ravines





Areas where the gradient is large in one direction and small in others.

3. Plateaus and flat areas



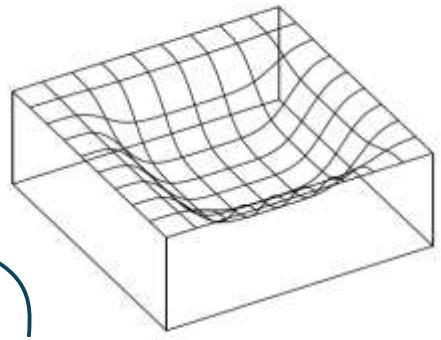


Figure 1: *Example of a "flat" minimum.*

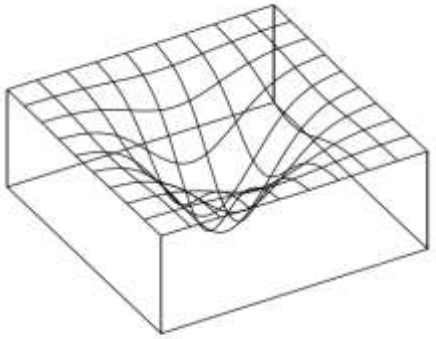


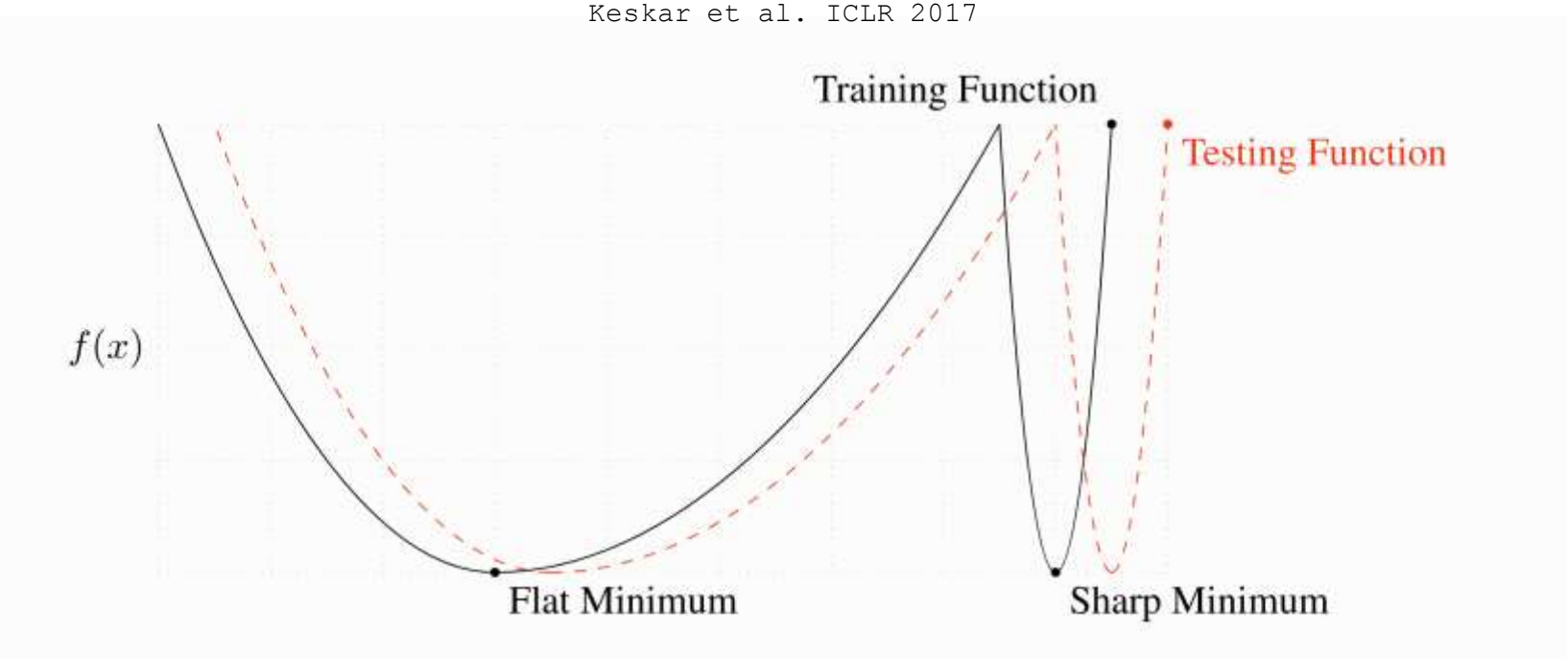
Figure 2: *Example of a "sharp" minimum.*

Link

Near zero gradients in flat areas, hence no learning.

Too step minima also a problem…

On Large-Batch Training for Deep Learning: Generalization Gap and Sharp Minima.
Keskar et al. ICLR 2017



Even if you miss the minimum of the test distribution slightly, still good results.

4. Cliffs and exploding gradients

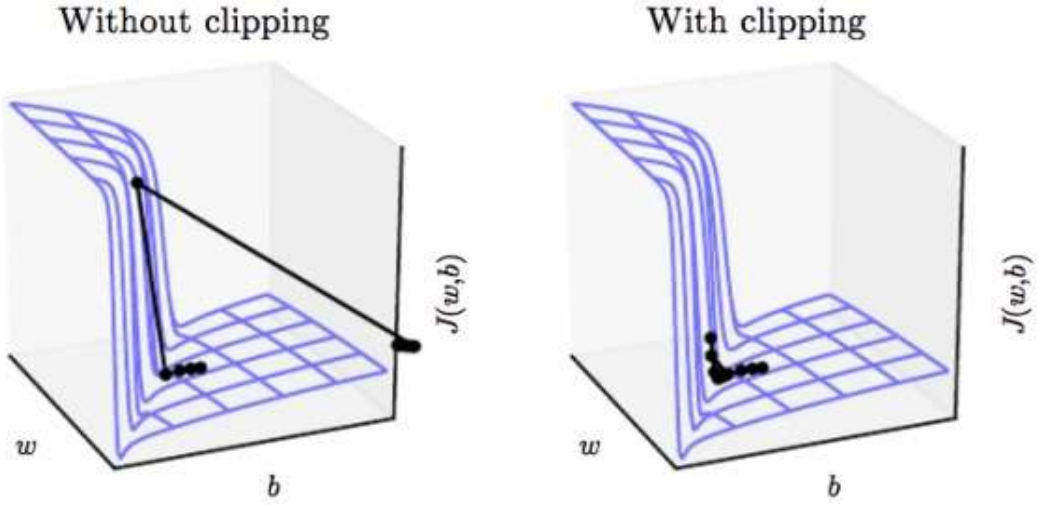
Neural networks with many layers often have steep regions resembling cliffs.

These result from the multiplication of several large weights together.

A simple trick: gradient clipp

if $\|\mathbf{g}\| > \eta$:

$$\mathbf{g} \leftarrow \frac{\eta \mathbf{g}}{\|\mathbf{g}\|}$$

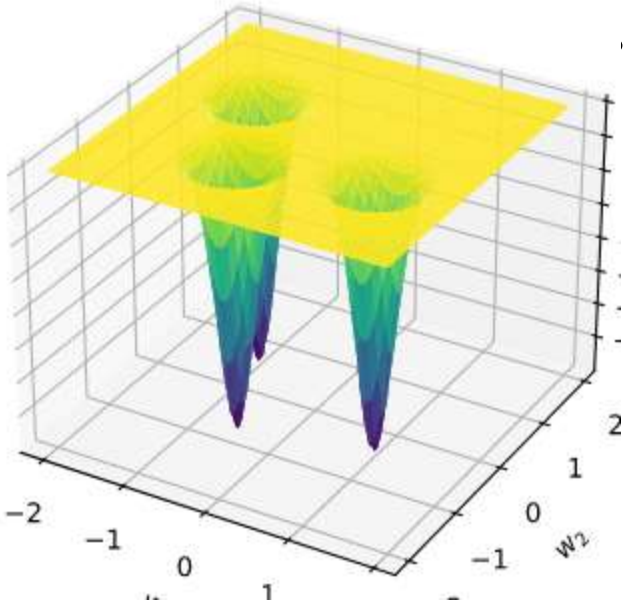


4. Flat areas and steep minima

When combining flat areas with very steep minima → very challenging

How do we even get to the area where the steep minima starts?

E.g.: temperate-sca s-entropy: p(y|x) = softmax(logits/0.00



5. Long-term dependencies

Especially for networks with many layers or recurrent neural networks.

The vanishing and exploding gradient problem

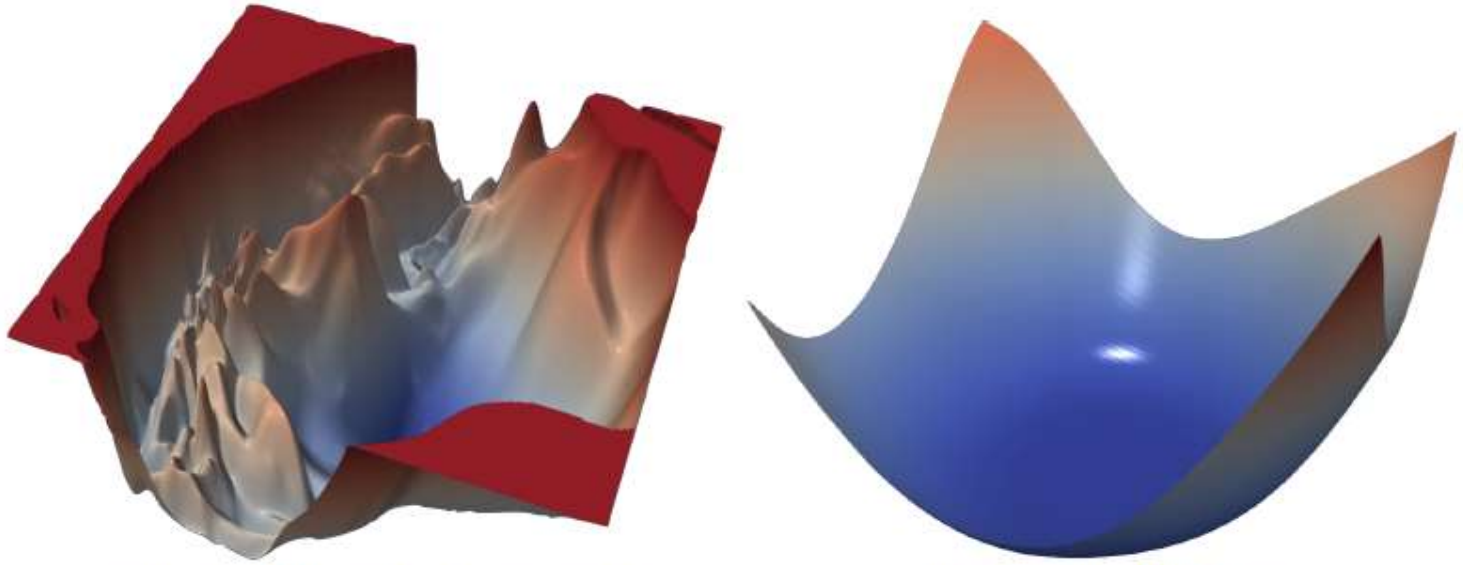
- Certain functions lead to a scaling of the gradient (potentially often).
- Vanishing gradients -> no direction to move
- Exploding gradients -> learning unstable.

For training-trajectory dependency: hard to recover from a bad start!

Is gradient descent even a good idea?

Global minima and local minima are nearby – Choromanska et al. (2015).

Architecture design and tricks have huge impact on loss landscapes



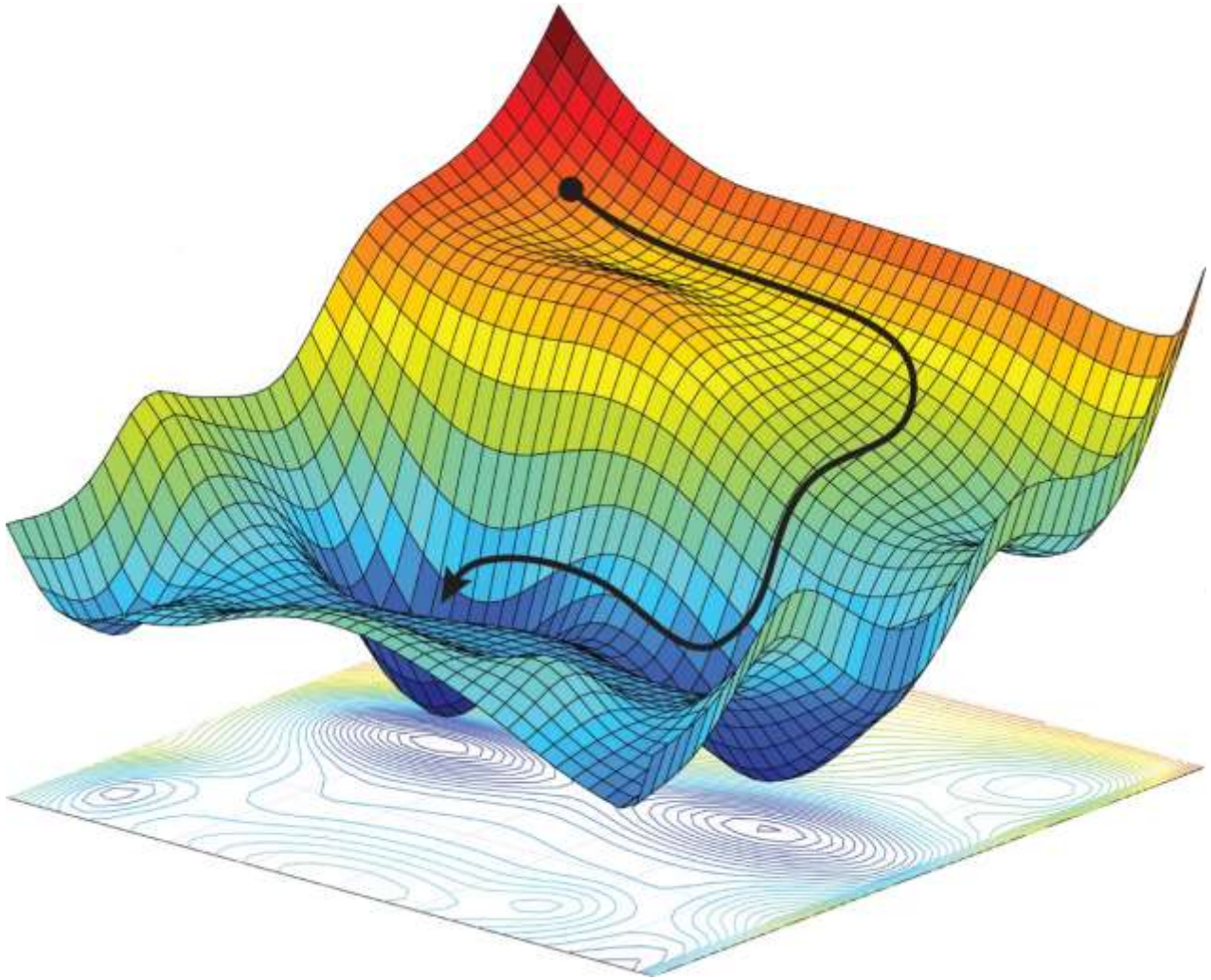
(a) ResNet-110, no skip connections

(b) DenseNet, 121 layers

Li et al. NeurIPS 2018

Break

Advanced optimizers



Gradient descent itself can be enhanced

$$\boldsymbol{w}^{(t+1)} = \boldsymbol{w}^{(t)} - \eta \frac{d\mathcal{L}(\boldsymbol{w})}{d\boldsymbol{w}}$$

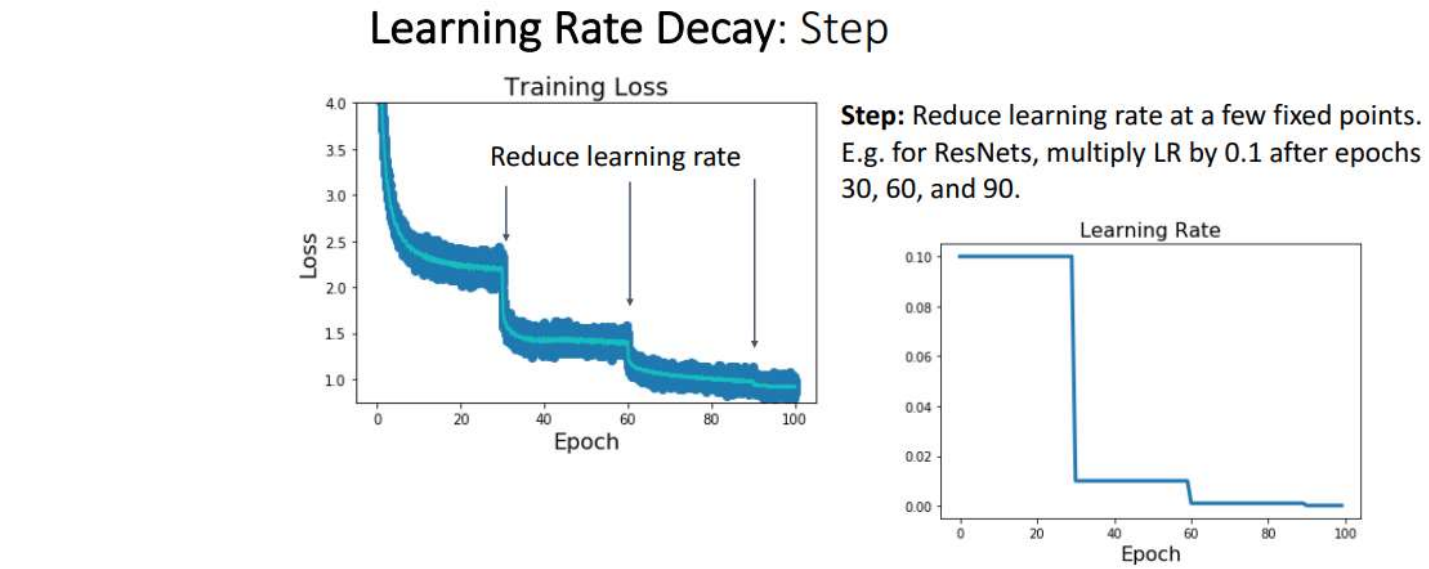
Can we improve the learning rate setting?

Can we get a better or more useful gradient?

Setting the learning rate

Truly an empirical endeavour, unique to each problem and dataset.

Big trick: learning rate schedulers.



Improving gradient descent

Stochastic Gradient Descent with momentum.

Nesterov momentum.

Stochastic Gradient Descent with adaptive learning rates.
E.g., AdaGrad, RMSProp, Adam

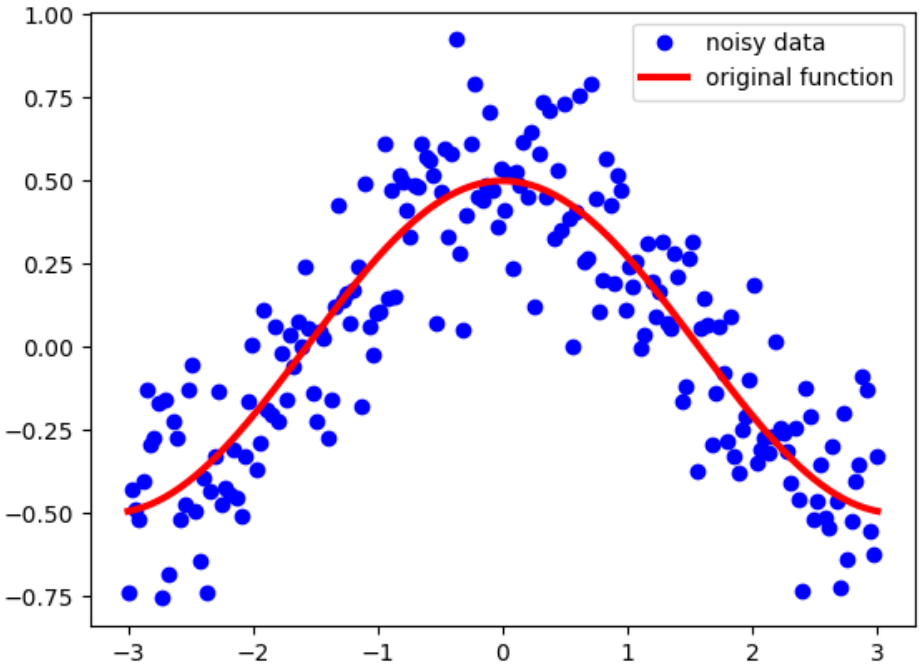
Second-order approximation, such as Newton's methods.

Momentum

Designed to accelerate learning, especially when loss is of high curvature.

We can understand momentum via exponentially weighted moving averages.

Suppose we have a sequence S which



Momentum

Exponentially weighted averages:

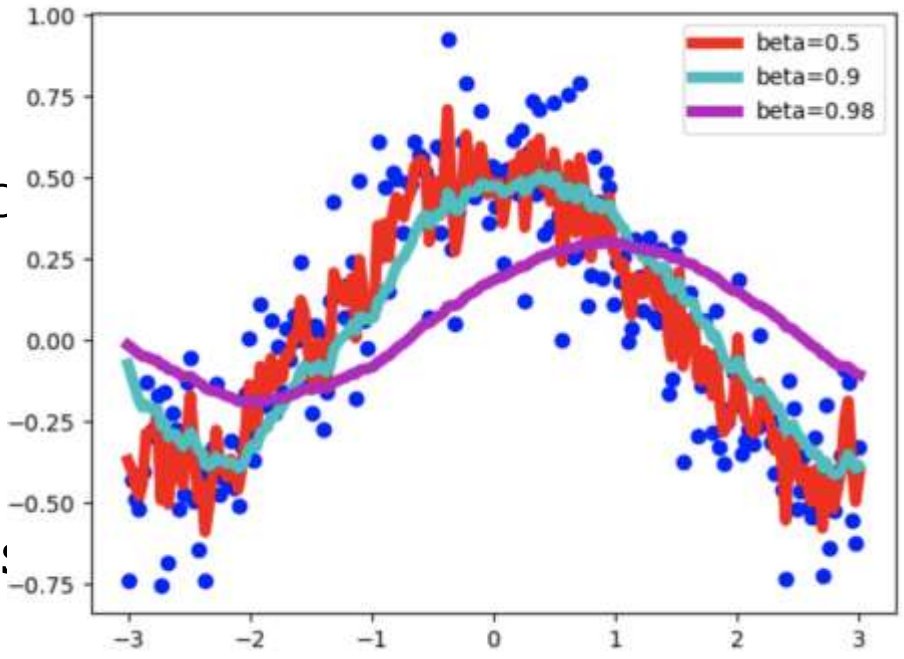
$$V_t = \beta V_{t-1} + (1-\beta) S_t,\ \beta \in [0\ 1],\ V_0 = 0$$

Small β leads to more fluctuatic

- β=0.9 provides a good balance

Bias correction.

- E.g., $V_1 = \beta V_0 + (1-\beta) S_1$: biased toward
- $V_t = \frac{V_t}{1-\beta^t}$



Stochastic gradient descent with momentum

Don't switch update direction all the time.

Maintain "*momentum*" from previous updates → dampens oscillations.

$$v_{t+1} = \gamma v_t + \eta_t g_t,$$

η_t = learning rate

$$w_{t+1} = w_t - v_{t+1}$$

Exponential averaging keeps steady direction.

Example: $\gamma = 0.9$ and $v_0 = 0$

- $v_1 \propto -g_1$
- $v_2 \propto -0.9g_1 - g_2$
- $v_3 \propto -0.81g_1 - 0.9g_2 - g_3$

Adding momentum is easy

SGD

$$w_{t+1} = w_t - \alpha \nabla f(w_t)$$

```
for t in range(num_steps):
  dw = compute_gradient(w)
  w -= learning_rate * dw
```

SGD+Momentum

$$v_{t+1} = \rho v_t + \nabla f(w_t)$$

$$w_{t+1} = w_t - \alpha v_{t+1}$$

```
v = 0
for t in range(num_steps):
  dw = compute_gradient(w)
  v = rho * v + dw
  w -= learning_rate * v
```

- Build up “velocity” as a running mean of gradients
- Rho gives “friction”; typically rho=0.9 or 0.99

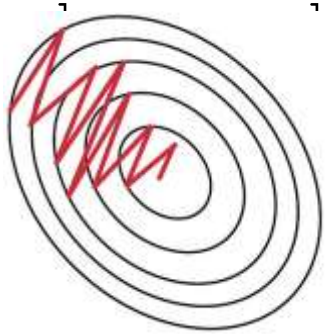
Sutskever et al, “On the importance of initialization and momentum in deep learning”, ICML 2013

Physical interpretation of momentum

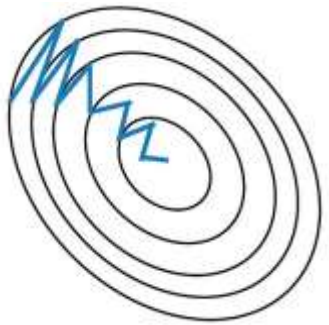
See gradient descent as rolling a ball down a hill.

The ball accumulates momentum, gaining speed down a straight path.

Momentum term increases for dimensions whose graidnets point in the same direction and reduces for dimesnions whose gradients

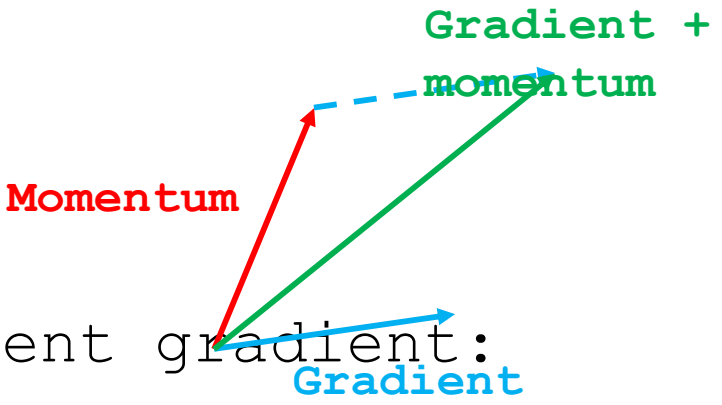


without momentum



with momentum

Nesterov momentum

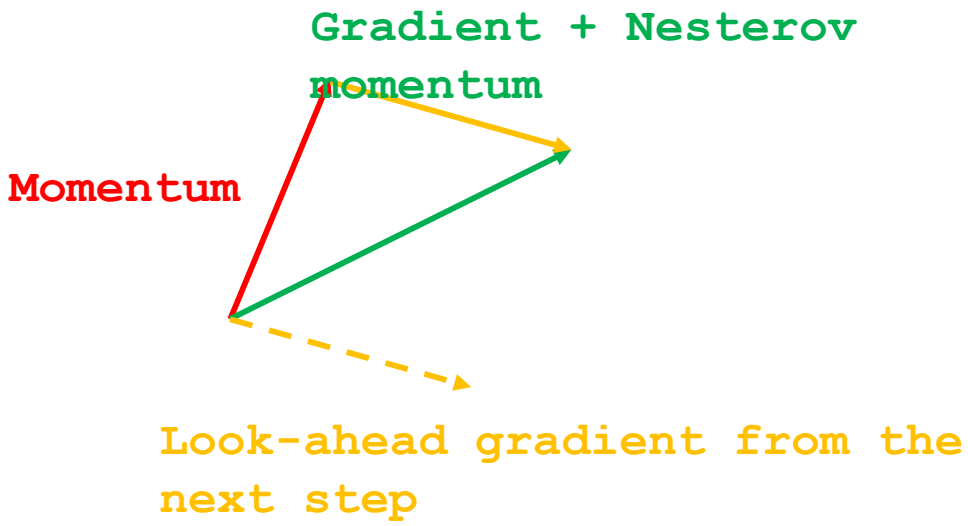


Use future gradient instead of current gradient:

$$v_{t+1} = \gamma v_t + \eta_t \nabla_w \mathcal{L}(w_t - \gamma v_t)$$
$$w_{t+1} = w_t - v_{t+1}$$

Prevents us from going too fast.

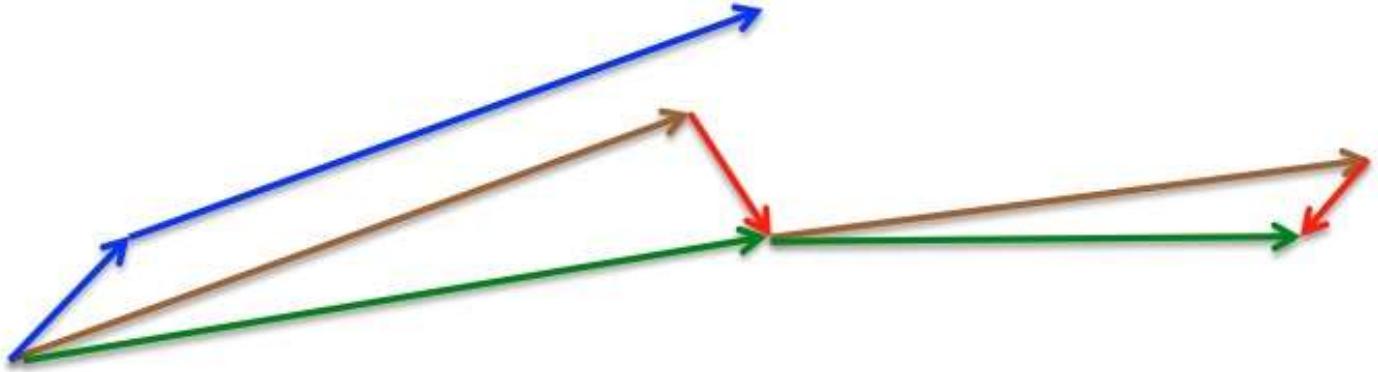
Also increases reponsiveness.



Nesterov momentum

First make a big jump in the direction of the previous accumulated gradient.

Then measure the gradient where you end up and make a correction



brown vector = jump;
red vector = correction;
green vector = accumulated gradient;
blue vectors = standard

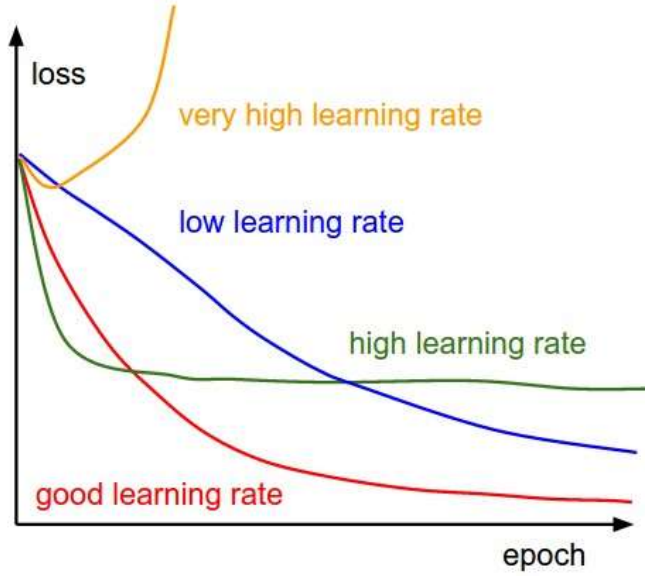
Picture from Hinton

Adaptive step sizes

A fixed learning rate is difficult to set.

Also has significant impact on performance and sensitive.

Is it possible to have a separate ac
learning rate for each parameter?



AdaGrad

Adaptive Gradient Algorithm – Adagrad:

- The learning rate is adapted **component-wise** to the parameters by incorporating knowledge of past observations.
- Rapid decrease in learning rates for parameters with large partial derivatives.
- Smaller decrease in learning rates for parameters with small partial derivatives.

Schedule

- $w_{t+1} = w_t - \frac{\eta}{\sqrt{r}+\varepsilon} \odot g_t$,
- where $r = \sum_t (\nabla_w \mathcal{L})^2$

learning rate

gradient

epsilon (avoid division by zero)

accumulation of squared gradients

RMSprop

Decay hyper-parameter
(usually 0.9)

Schedule

- $r_t = \alpha r_{t-1} + (1-\alpha) g_t^2$
- $v_t = \frac{\eta}{\sqrt{r_t}+\varepsilon} \odot g_t$
- $w_{t+1} = w_t - v_t$

Large gradients, e.g., too "noisy" loss surface

- Updates are tamed

Small gradients, e.g., stuck in plateau of loss surface

- Updates become more aggressive

Adam

One of the most popular algorithms.

Combines RMSprop and momentum.

- Computes adaptive learning rate for each parameter.
- Keeps an exponentially decaying average of past gradients (momentum).
- Introduces bias corrections to the estimates of moments.

Can be seen as a heavy ball with friction, hence a preference for flat minima.

Adam

$$m_t = \beta_1 m_{t-1} + (1-\beta_1) g_t$$
$$v_t = \beta_2 v_{t-1} + (1-\beta_2) g_t^2$$

$$\hat{m}_t = \frac{m_t}{1-\beta_1^t}, \hat{v}_t = \frac{v_t}{1-\beta_2^t}$$

Bias corrections

$$u_t = \frac{\eta}{\sqrt{\hat{v}_t} + \varepsilon} \hat{m}_t$$
$$w_{t+1} = w_t - u_t$$

Recommended values: $\beta_1 = 0.9,\ \beta_2 = 0.999, \varepsilon = 10^{-8}$

Adaptive learning rate as RMSprop, but with momentum & bias correction

Adam is hyperparameter-free?

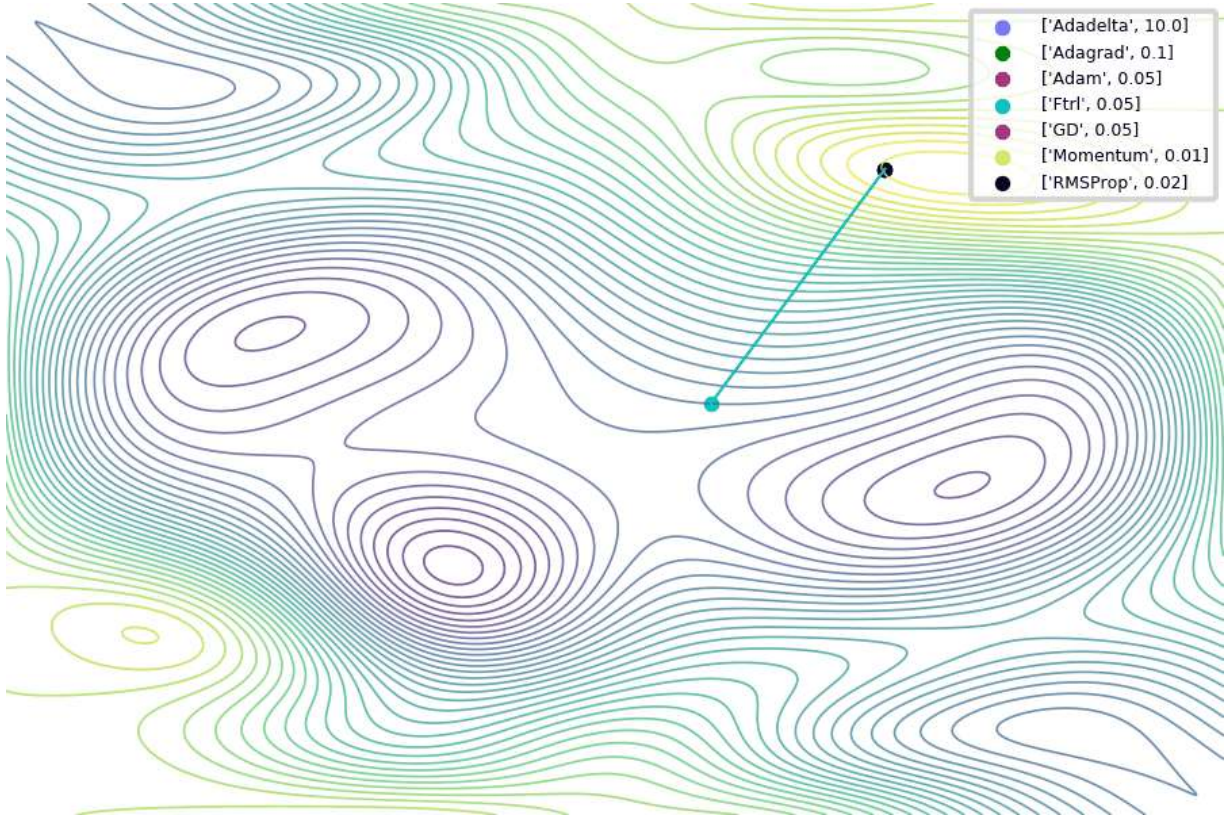
$$m_t = \beta_1 m_{t-1} + (1-\beta_1) g_t$$
$$v_t = \beta_2 v_{t-1} + (1-\beta_2) g_t^2$$

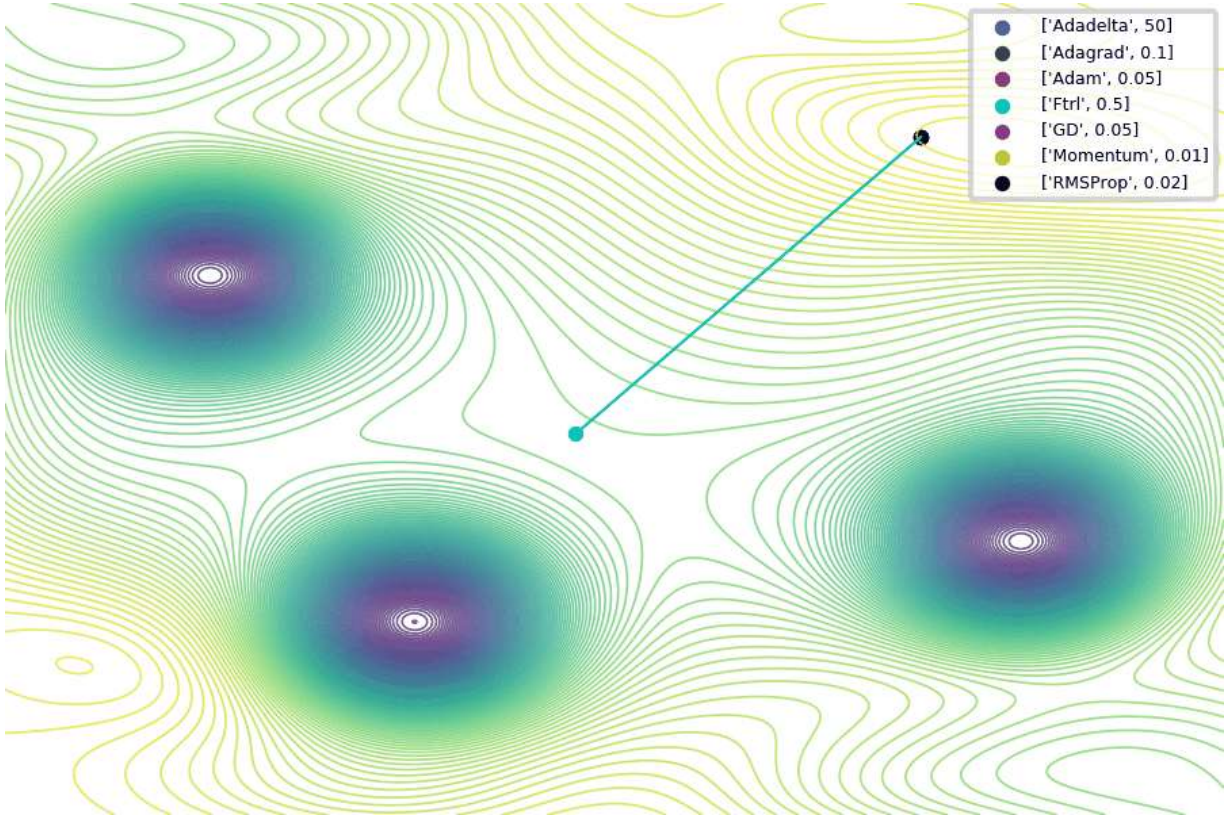
$$\hat{m}_t = \frac{m_t}{1-\beta_1^t}, \hat{v}_t = \frac{v_t}{1-\beta_2^t}$$

$$u_t = \frac{\eta}{\sqrt{\hat{v}_t} + \varepsilon} \hat{m}_t$$
$$w_{t+1} = w_t - u_t$$

More robust to different settings, but many values to set.

Visual overview





Picture credit:
Jaewan Yun

Which optimizer to use?

My go-to: SGD with momentum and learning rate decay.

For more complex models, Adam is often the preferred choice.

Adam with weight-decay (AdamW) is the standard for optimizing transformer architectures.

Oddity: even in “learning rate adjusting” optimizers like Adam, we add learning rate decays.

Interactive visualization

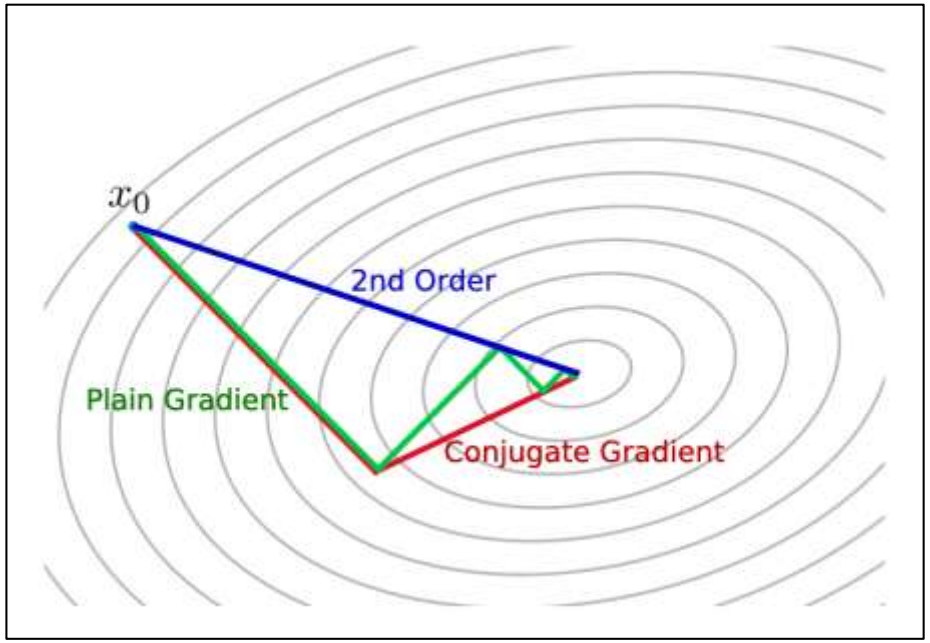
https://emiliendupont.github.io/2018/01/24/optimization-visualization/

Approximate second-order methods

SGD, Adam, etc are first-order: curvature information is ignored.

Benefits of second-order optimizati

- Better direction.
- Better step-size.
- Full step jumps directly to th
- of the local squared approx.
- Additional step size reducatio
- Dampening becomes easy.



Newton's method

A second-order Taylor series expansion to approximate $J(\theta)$ near some point θ_0, ignoring derivatives of higher order:

$$J(\boldsymbol{\theta}) \approx J(\boldsymbol{\theta}_0) + (\boldsymbol{\theta} - \boldsymbol{\theta}_0)^\top \nabla_{\boldsymbol{\theta}} J(\boldsymbol{\theta}_0) + \frac{1}{2}(\boldsymbol{\theta} - \boldsymbol{\theta}_0)^\top \boldsymbol{H}(\boldsymbol{\theta} - \boldsymbol{\theta}_0)$$

If we then solve for *the critical point* of this function, we obtain the Newton parameter update rule:

$$\boldsymbol{\theta}^* = \boldsymbol{\theta}_0 - \boldsymbol{H}^{-1} \nabla_{\boldsymbol{\theta}} J(\boldsymbol{\theta}_0)$$

For a locally quadratic function, Newton's method jumps directly to the minimum.

If convex but not quadratic (there are higher-order terms), *update can be iterated.*

Why we use first order optimization

Disadvantages:

- Super slow: need to compute inverse of Hessian matrix each time.
- More restrictive: 2nd order derivative needs to be possible to compute.
- Limited impact: no major improvement found in practice.

Learning and reflection

Understanding Deep Learning: Chapter 6

Understanding Deep Learning: Chapter 7

Next lecture

Lecture	Title
1	Intro and history of deep learning
3	Deep learning optimization I
5	Convolutional deep learning
7	Graph deep learning
9	Multi-modal deep learning
11	What doesn't work in deep learning
13	Q&A

Lecture	Title
2	AutoDiff
4	Deep learning optimization II
6	Attention-based deep learning
8	From supervised to unsupervised deep learning
10	Generative deep learning
12	Non-Euclidean deep learning
14	Deep learning for videos

Thank you!