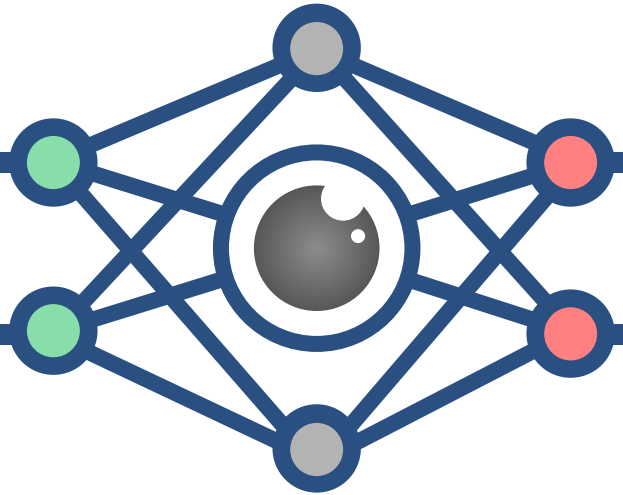
CS3485

# Deep Learning for Computer Vision



*Lec 4*: Optimization and Regularization

# Announcements

- Labs:
  - Lab1 is due today at 11:59pm.
  - Lab2 will be released this afternoon (report in latex).

# (Tentative) Lecture Roadmap

## Basics of Deep Learning

- Intro to Computer Vision
- Linear Classifiers and Perceptron
- Multilayer Perceptron and Intro to Deep Learning
- Optimization and Regularization
- Pytorch
- Convolutional Neural Networks
- Data Augmentation and Deep CNNs
- Transfer Learning and Residual Nets
- Inception Net and what CNNs learn
- Adversarial Examples and Self-supervision

## Computer Vision Tasks

- Intro to Object Detection
- Fast Object Detection
- Intro to Image Segmentation
- Applications of Detection and Segmentation
- Autoencoders
- Image Generation with GANs
- Advanced GANs
- Transformers and ChatGPT
- Image Generation by Prompt

# Finding the best weights

- Previously, we saw that we can learn the weights of a simple perceptron using the **Perceptron Algorithm**.
- We can extend that to multiclasses, by using multiple perceptron units and training each one separately.
- However, when we add the softmax layer, or add hidden layers, or changed the activation functions, the **perceptron algorithm is not helpful anymore**.
- Today we'll see how to find the weights of general neural networks using **optimization**!
- We'll also learn some techniques to avoid model overfitting using **regularization**.

# Loss minimization

- We saw that a Multilayer Perceptron classifies a data point $x$ into a class $y$ using:

$$\hat{y} = NN_\theta(x) = \text{softmax}(W_L a(W_{L-1} \cdots a(W_0 x) \cdots))$$

  where $NN_\theta$ is a shorthand notation for **the whole neural network** as **a function** and $\theta$ represents the weights $W_0$, $W_1$, ..., $W_L$ in it.
- Since we want to do **supervised learning**, we have a set of $n$ points $x^{(1)}$, ..., $x^{(n)}$ in $D$ dimensions, each with a class $y^{(1)}$, ..., $y^{(n)}$, of $K$ different classes.
- We can now assess $NN_\theta$ at classifying the points in our dataset via the average loss:

$$L(\theta) = \frac{1}{n} \sum_{i=1}^{n} l(\hat{y}^{(i)}, y^{(i)}) = \frac{1}{n} \sum_{i=1}^{n} l(NN_\theta(x^{(i)}), y^{(i)})$$

- Naturally, we'd like to find best $\theta$, i.e, those that **minimize** $L(\theta)$.
- Which means that learning in Deep Learning is "just" an **optimization problem.**

# Minimization Techniques

- To minimize a **differentiable** function* $f(x)$ one can use **Gradient Descent (GD)**, which starting from some $x_0$, it finds $x_1$ such that $f(x_1)$ is lower than $f(x_2)$, and then repeats.
- It uses the derivative of $f$, defined as $df/dx$, to check its slope at each point to know where to go next.
- GD works just like a climber who wants to quickly go down a mountain:
  - He first steps around where he “feels” the **slope** of his location,
  - Then decides to take the direction where the slope is the **steepest**,
  - After that he walks a **step** on that direction.
  - He then **repeats** the process until he is at the bottom of the mountain.

* We’ll work on the general case for now and get back to Neural Networks/Deep Learning later.

# Gradient Descent in 1D

- We use this intuition to mathematically formulate our **minimizer** for functions in 1D:

$$x_{t+1} = x_t - \eta \frac{df}{dx}(x_t)$$

where $\eta$ (called step size or **learning rate**) is a constant*. This equation simply says:

  - If you are at $x_t$, the next point you should go to is on the opposite direction of the slope of $f$ at $x_t$.
  - Then walk a step of size proportional to how steep that slope is in the direction.

- With this definition, the **gradient descent algorithm** in 1D is very simple:
  1. Pick a random starting point $x_0$,
  2. Repeat for $t = 0, 1, 2, \ldots$ until $|grad| < \epsilon$**
     a. Compute $grad = df(x_t)/dx$
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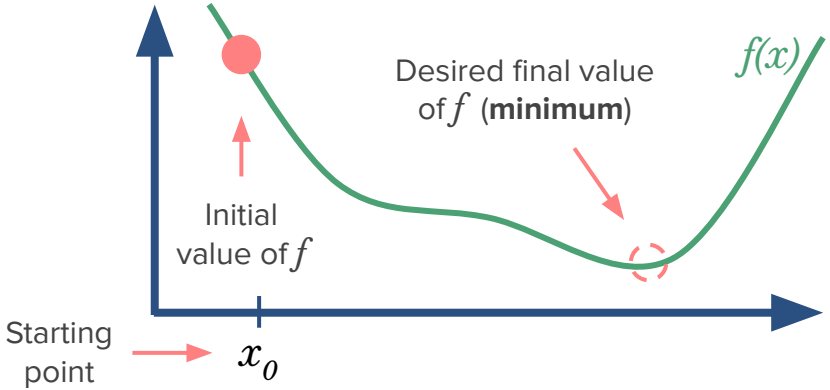


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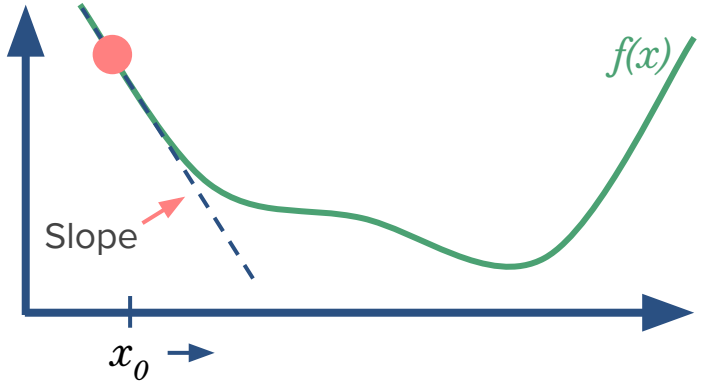


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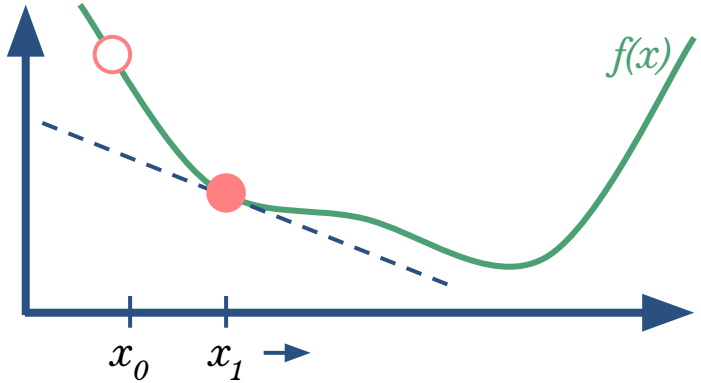


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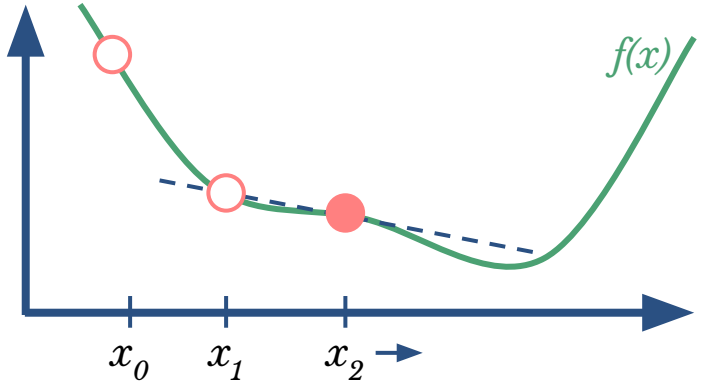


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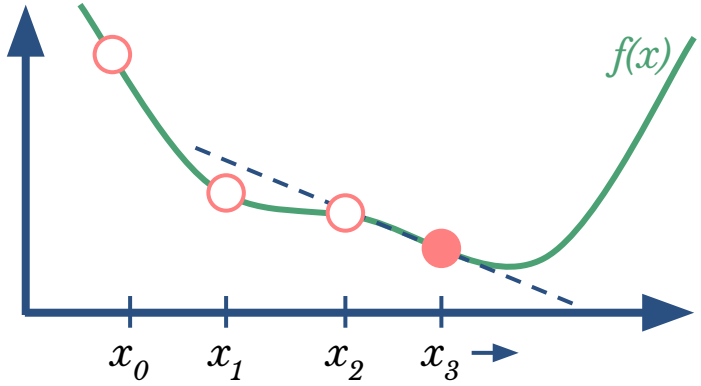


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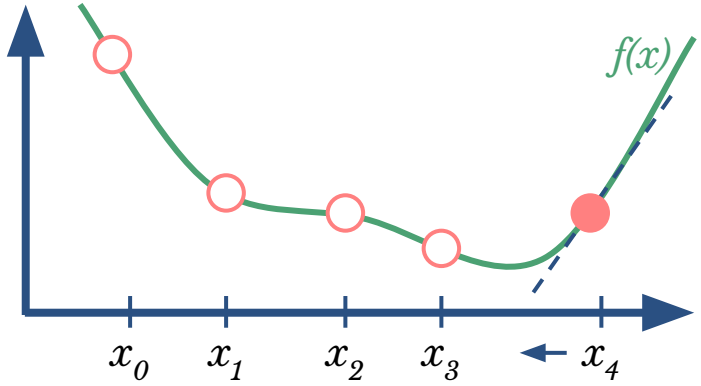


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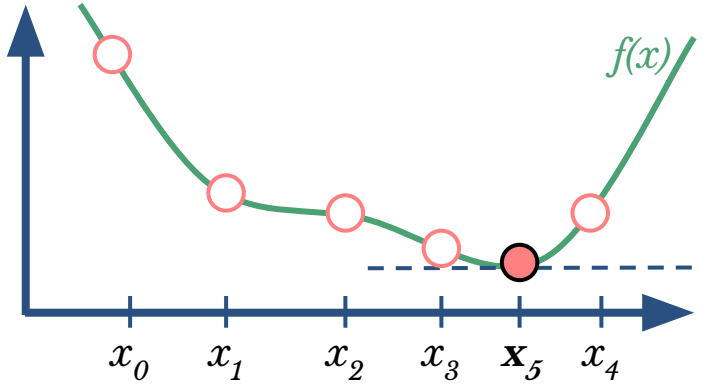


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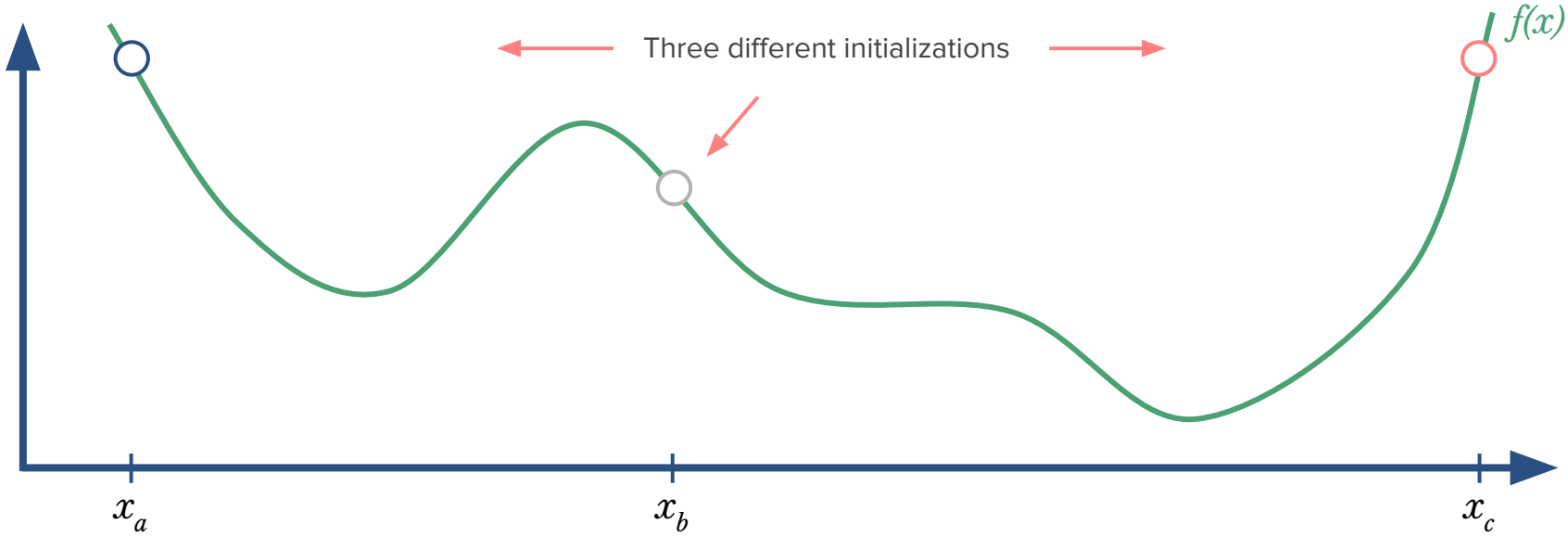
# When Gradient descent is suboptimal

- Unfortunately, GD **doesn't always** find the best $x$, the **global minimum**.
- Depending on where it is initialized, it output two possible **suboptimal solutions**: a **local minimum** or a **saddle point**.



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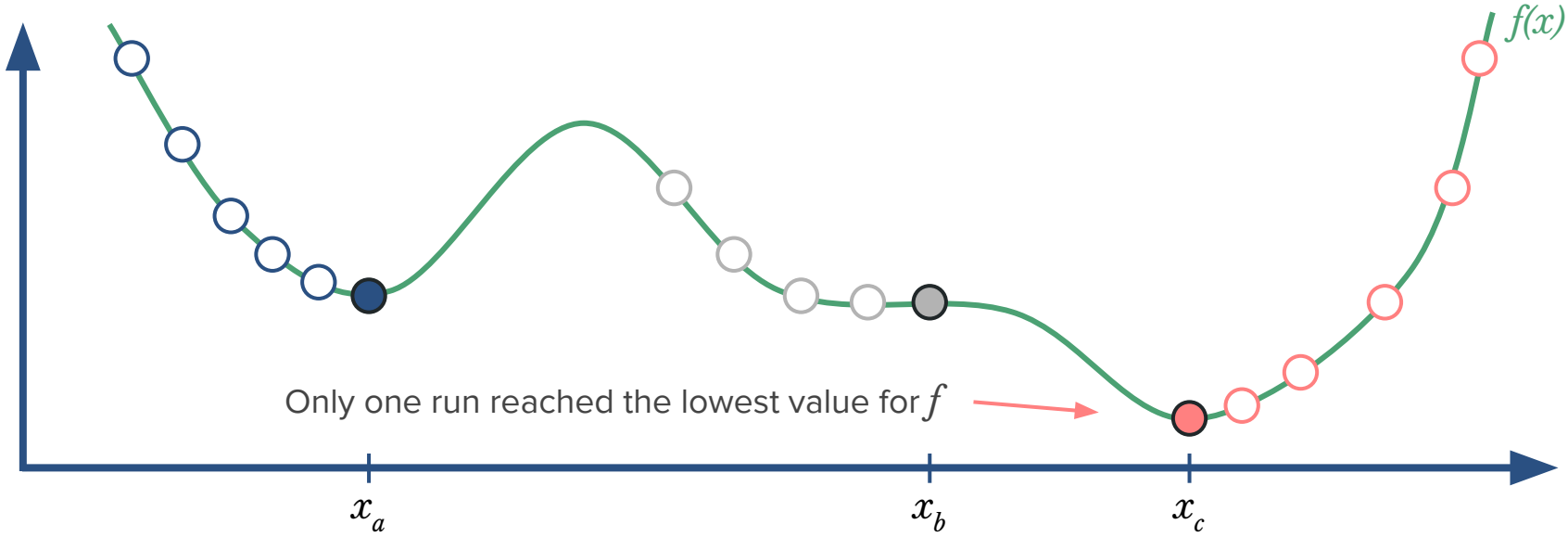

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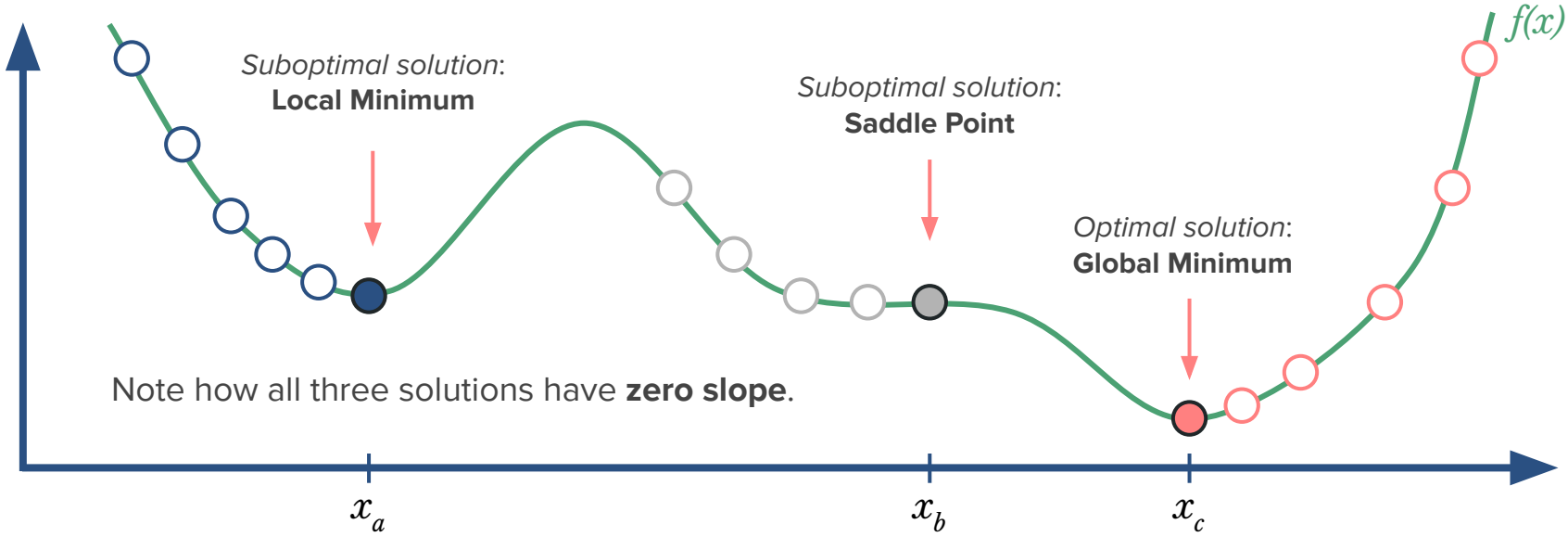

# How about more dimensions?

- What we did for 1D can be readily generalized to functions $f(x_1, \ldots, x_D)$ in $D$ dimensions.
- Call $x = [x_1, \ldots, x_D]^T$ the vector of variables. Then, the Gradient Descent formula is now:

$$x_{t+1} = x_t - \eta \nabla_x f(x_t)$$

where $\nabla_x f = [df/dx_1, \ldots, df/dx_D]^T$ is the gradient of $f$.

- The principle is the same as in 1D, but now we have a direction in $D$ dimensions to follow: **the negative of the function's gradient**, $-\nabla_x f(x)$.

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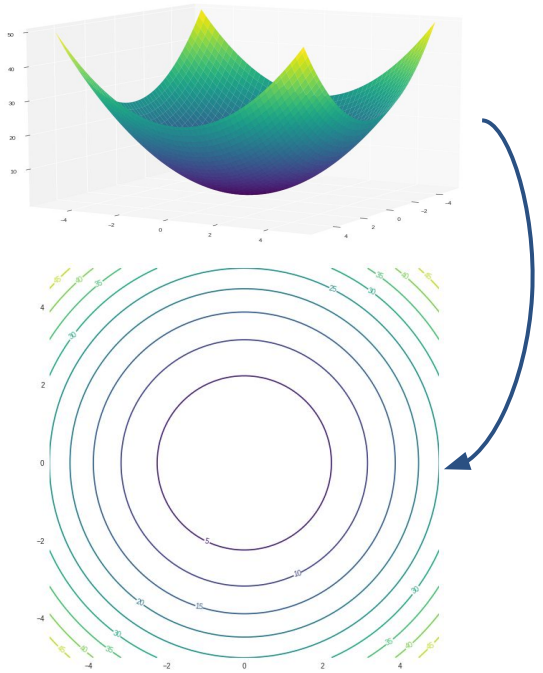

Same function seen from above

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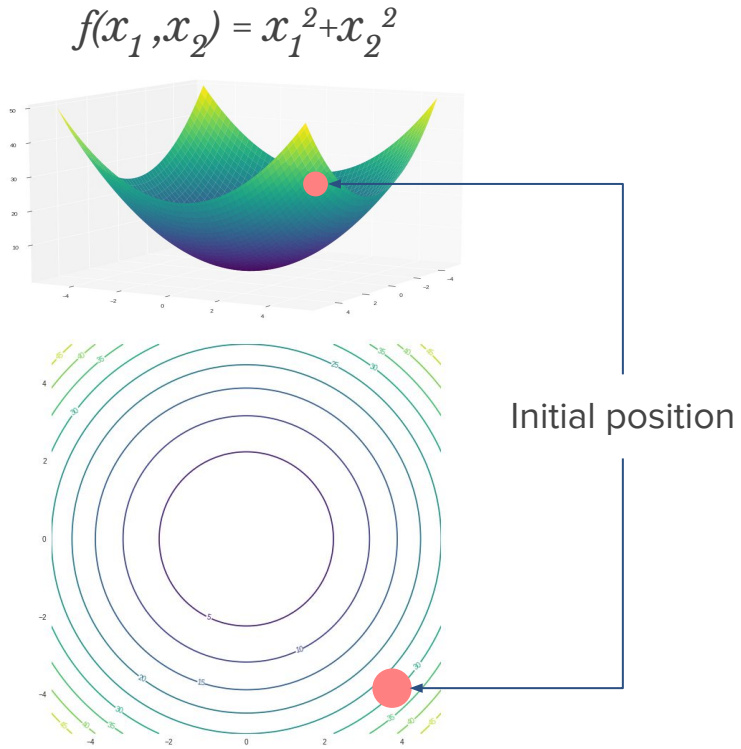

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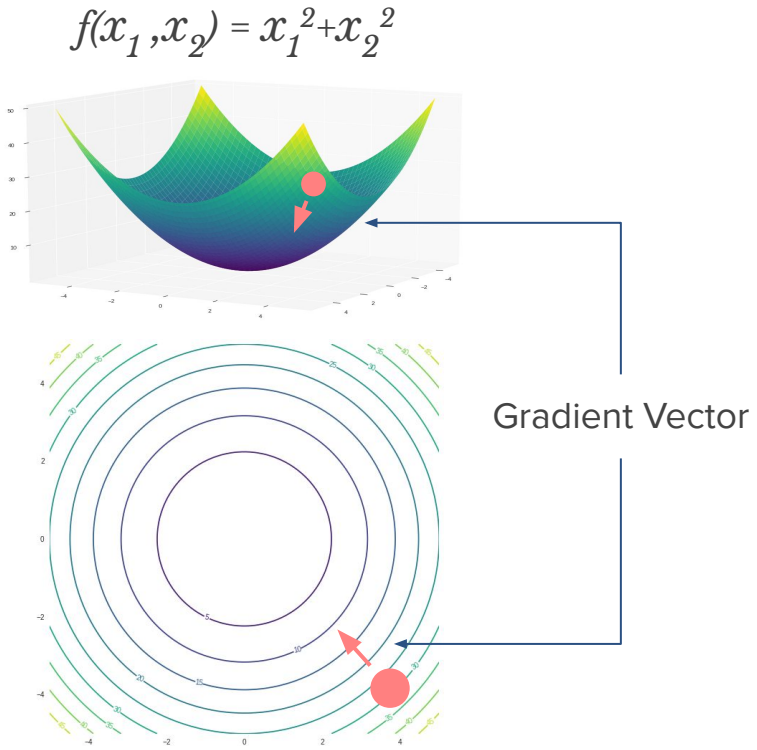

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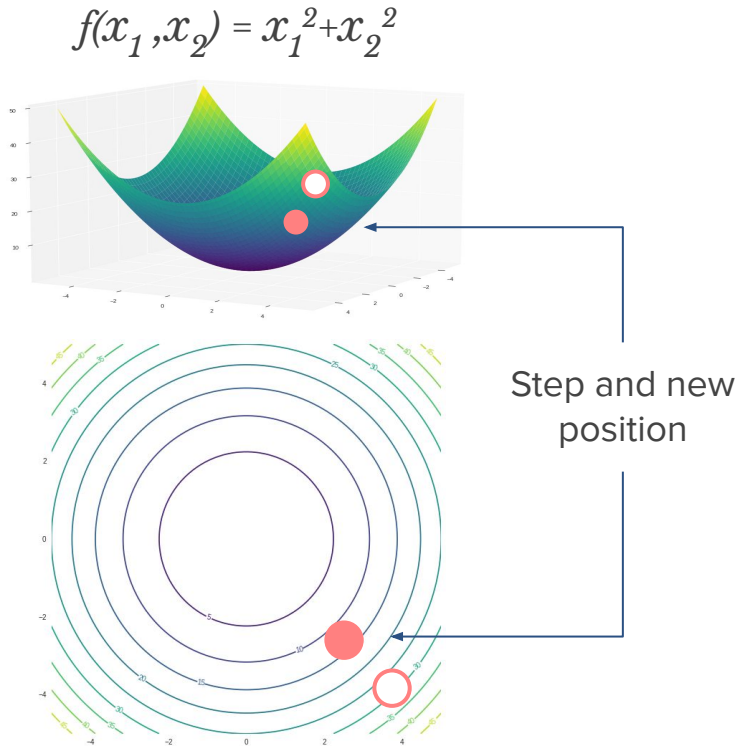

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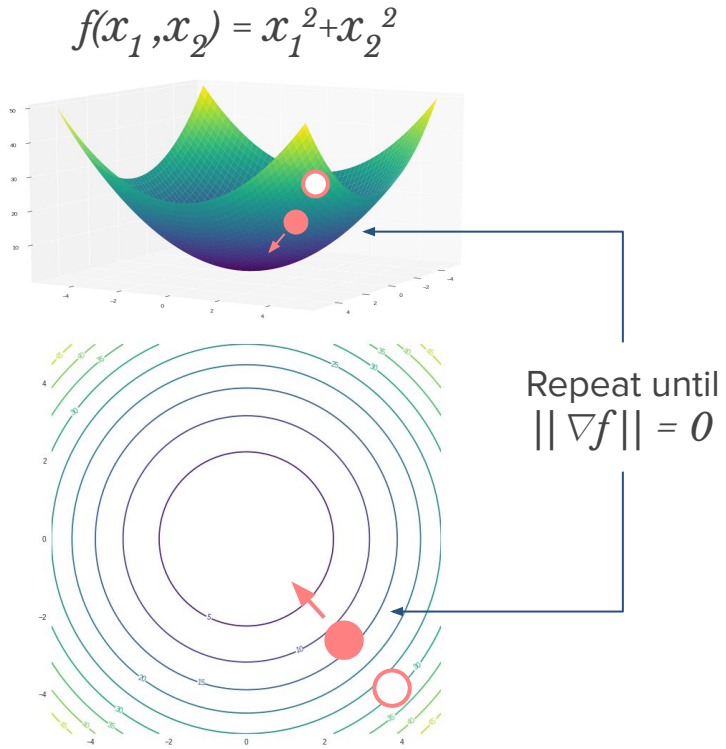

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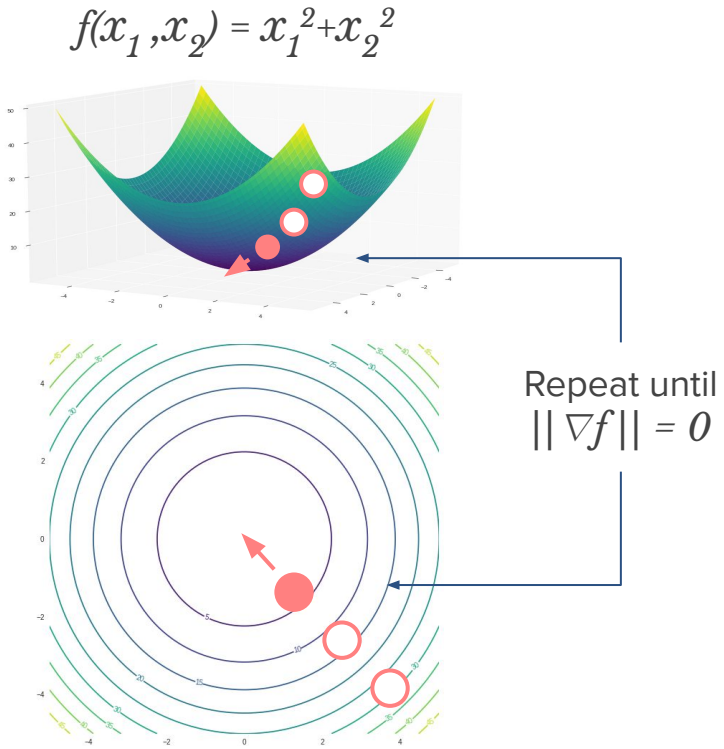

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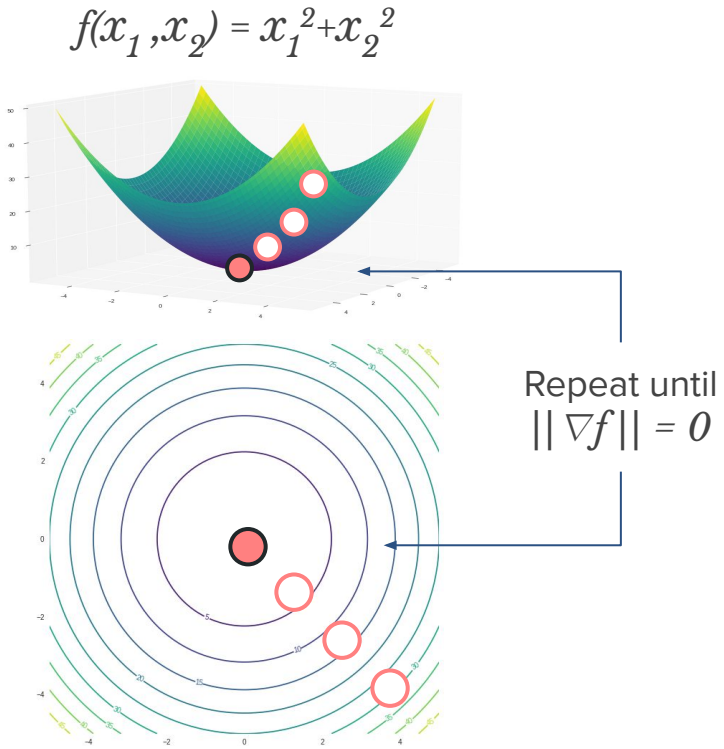

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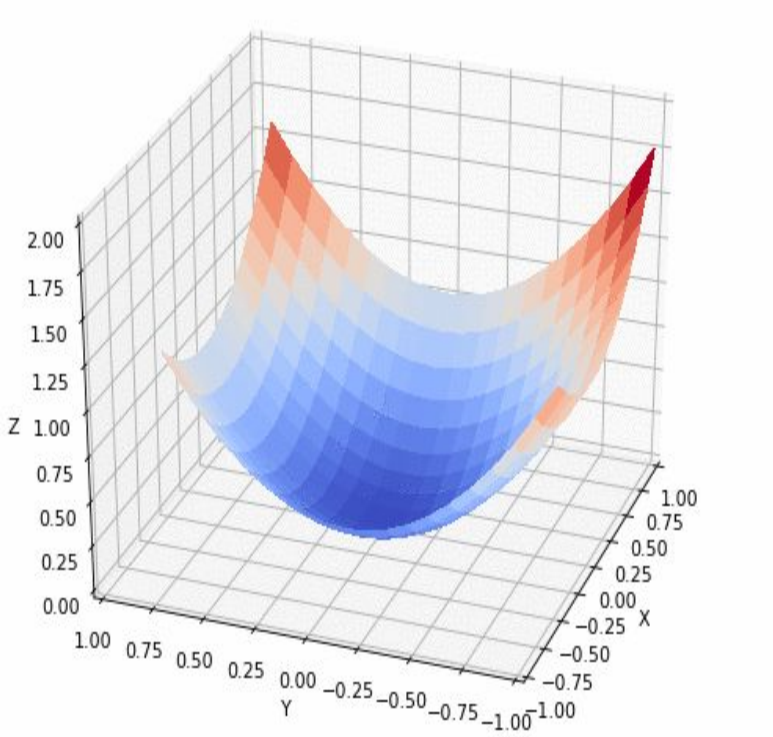

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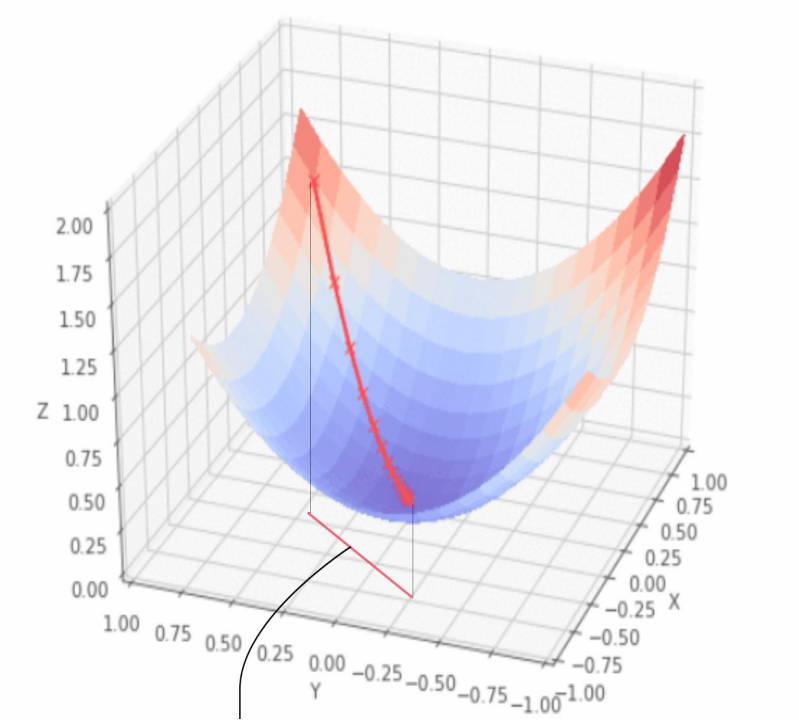
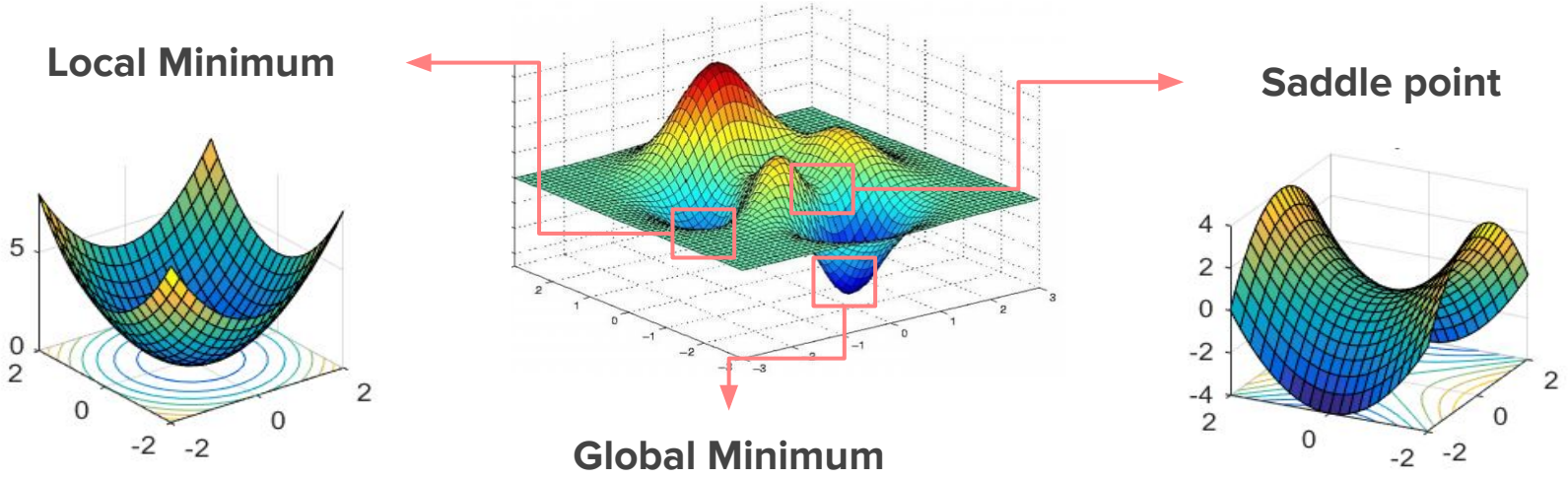



Trajectory of $x$

# When Gradient Descent is suboptimal

- Also, just like in 1D, gradient descent can get stuck in multidimensional suboptimal solutions and miss the global minimum:




- In fact, one can show that these points are prevalent in **Deep Learning loss surfaces**.
- How can we address this issue?

# Exercise (*In pairs*)

- Implement gradient descent for a function that you know the derivative of and its global minimum (like $f(x) = x^2$). Set $\eta$ to $0.1$ and make sure to print the value of the function as you do your GD interactions. *Hint*: create two Python functions `f(x)` and `df(x)`.
- Now try $\eta$ equal to $0.01, 1, 100, 1000$. What do you observe? What does this tell you about weakness of gradient descent?
- Now change that implementation for a function of 2 variables (like, $f(x, y) = x^2 + y^2$). How does your code change?

# Going back to Neural Networks

- As a recap, in Neural Networks our goal is to find a set of weights $\theta^*$ defined by:

$$\theta^* = \arg\min_{\theta} L(\theta)$$

  which reads as "$\theta^*$ *is the value for* $\theta$ *that minimizes* $L(\theta)$ *over all possible* $\theta$" and where:

$$L(\theta) = \frac{1}{n}\sum_{i=1}^{n} l(NN_\theta(x^{(i)}), y^{(i)})$$

- In GD, we need to compute the gradient of $L(\theta)$, which is:

$$\nabla_\theta L(\theta) = \frac{1}{n}\sum_{i=1}^{n} \nabla_\theta l(NN_\theta(x^{(i)}), y^{(i)})$$

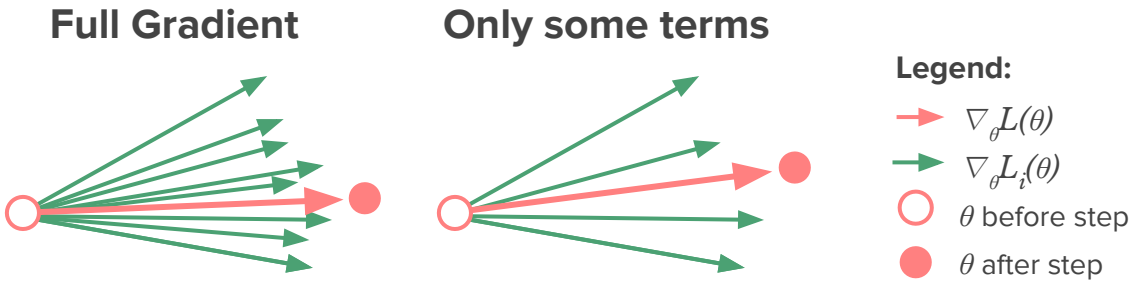
- That is, as we search for $\theta^*$, we have to compute evaluate $n$ gradients at each GD step.
- *One problem*: In modern datasets, $n > 100000$!

# Going back to Neural Networks

- Ok, let's summarize our problems with GD so far:
  1. GD is prone to local minima and saddle points,
  2. It is very computationally expensive to compute a step of GD in modern Neural Networks.
- We'll try to solve both problems with the same solution: **randomness**!
- First, to make things easier, let's use the following shorthand notation:

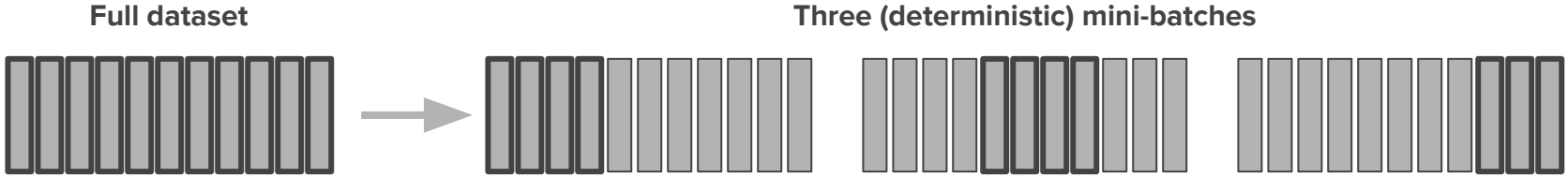
$$L_i(\theta) = l(NN_\theta(x^{(i)}), y^{(i)})$$

- That is, the gradient vector $\nabla_\theta L(\theta)$ is just an average sum of many vectors $\nabla_\theta L_i(\theta)$!
- *In other words*: we can compute the average of a few $\nabla_\theta L_i(\theta)$ and **the result won't be too far off** from the full gradient $\nabla_\theta L(\theta)$.



# Stochastic Gradient Descent

- If we **randomly** choose the datapoints to compute these few $\nabla_\theta L_i(\theta)$ vectors, we are now dealing with **Stochastic* Gradient Descent (SGD)**.
- Since we won't be using the whole dataset to compute one step of SGD anymore, we need to introduce a bit more of deep learning linguo:
  - The set of chosen datapoints used to compute one step of SD is called **mini-batch** (or just batch**). The batches don't need to be exactly of the same size.




  - SGD will go over each batch and then restart. An **epoch** is over when it has finished going over all batches (and therefore all data points) once.

* In most contexts, "stochastic" simply means "random". ** "*Batch Gradient Descent*" is sometimes used to refer to GD using all datapoints.

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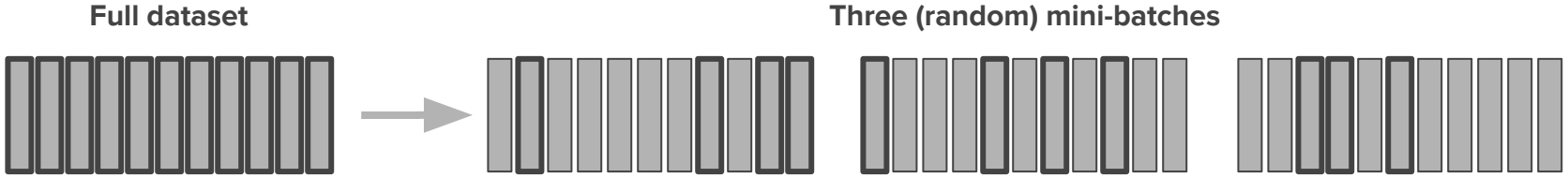


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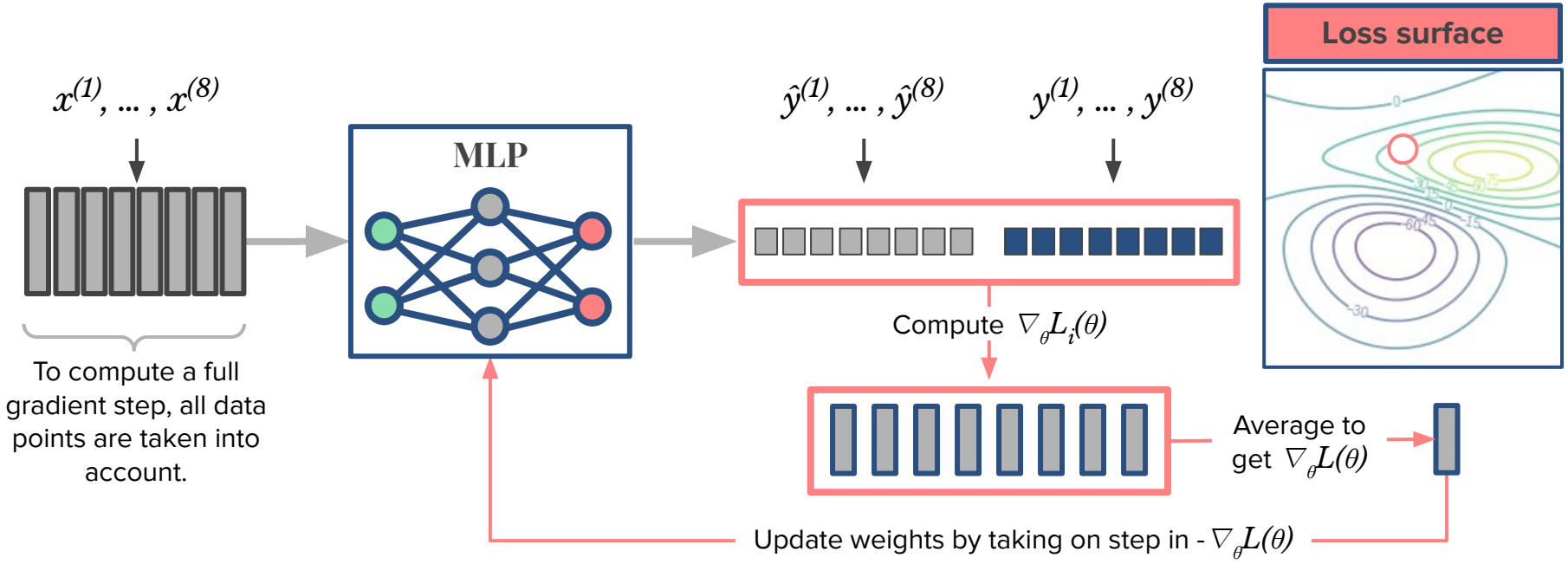
# GD vs SGD

- In normal gradient descent, we need to compute all datapoints gradients (eight in the example below) to make one step.



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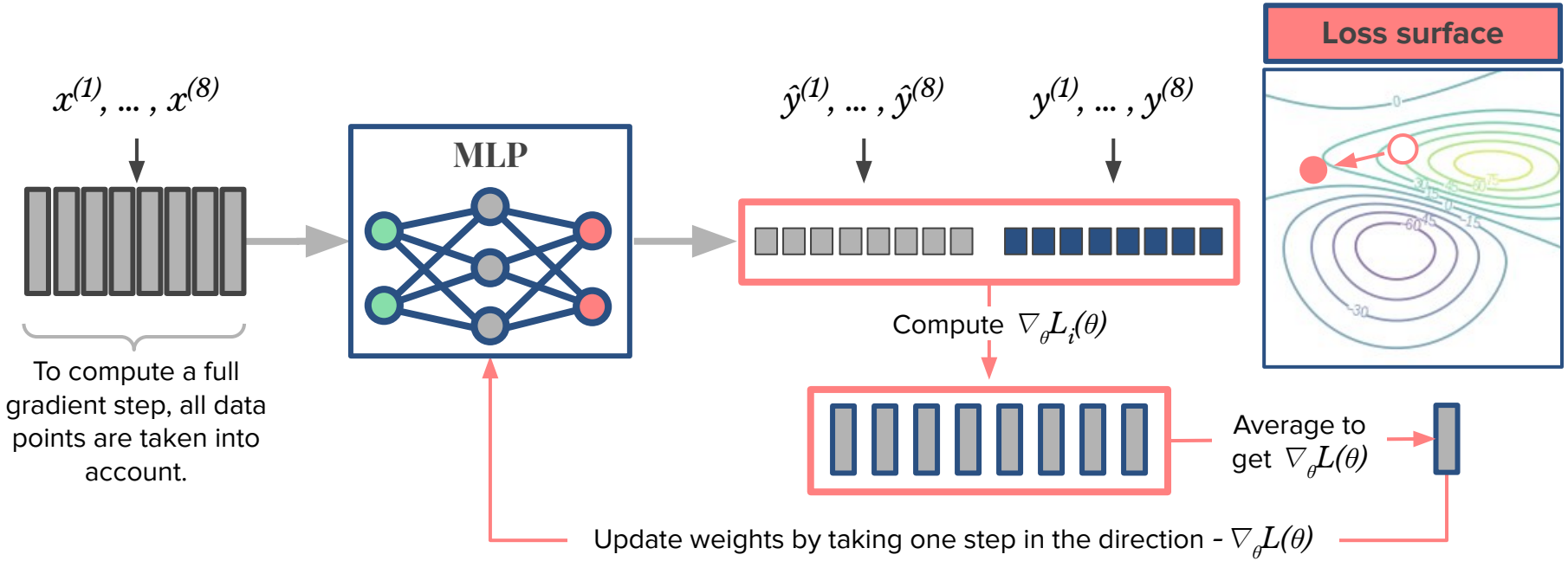
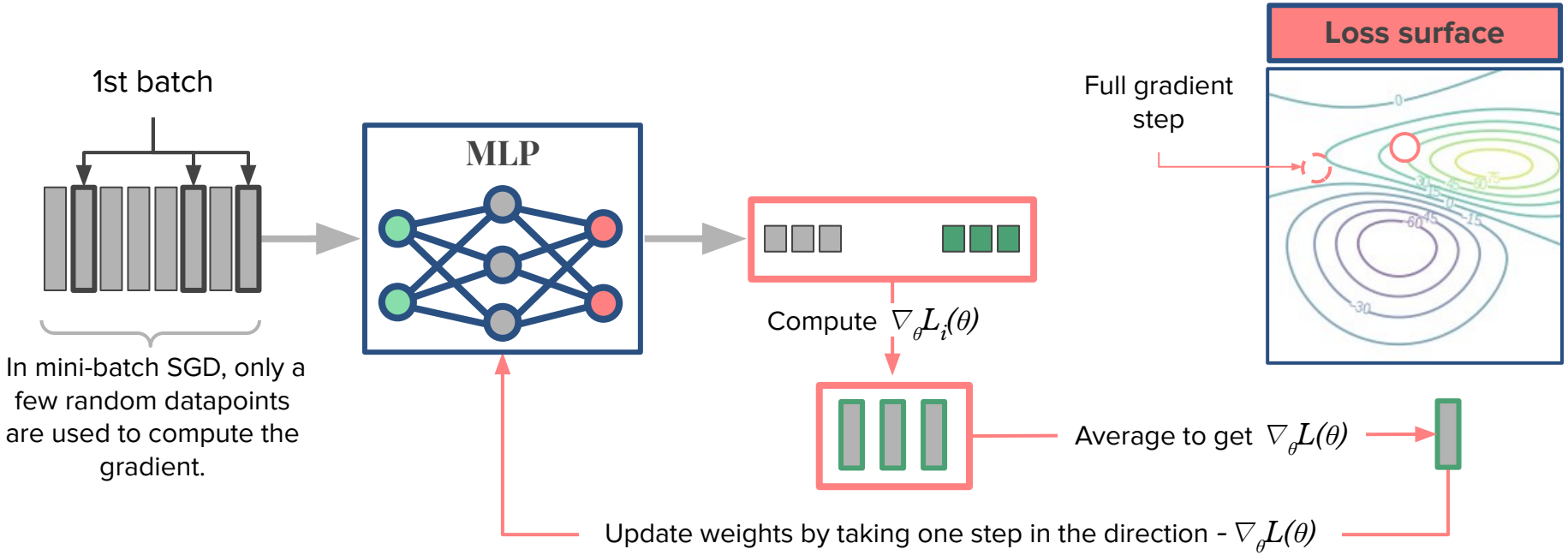


# GD vs SGD

- In stochastic gradient descent, we only compute the gradients respective to the mini-batches' points to make a step.



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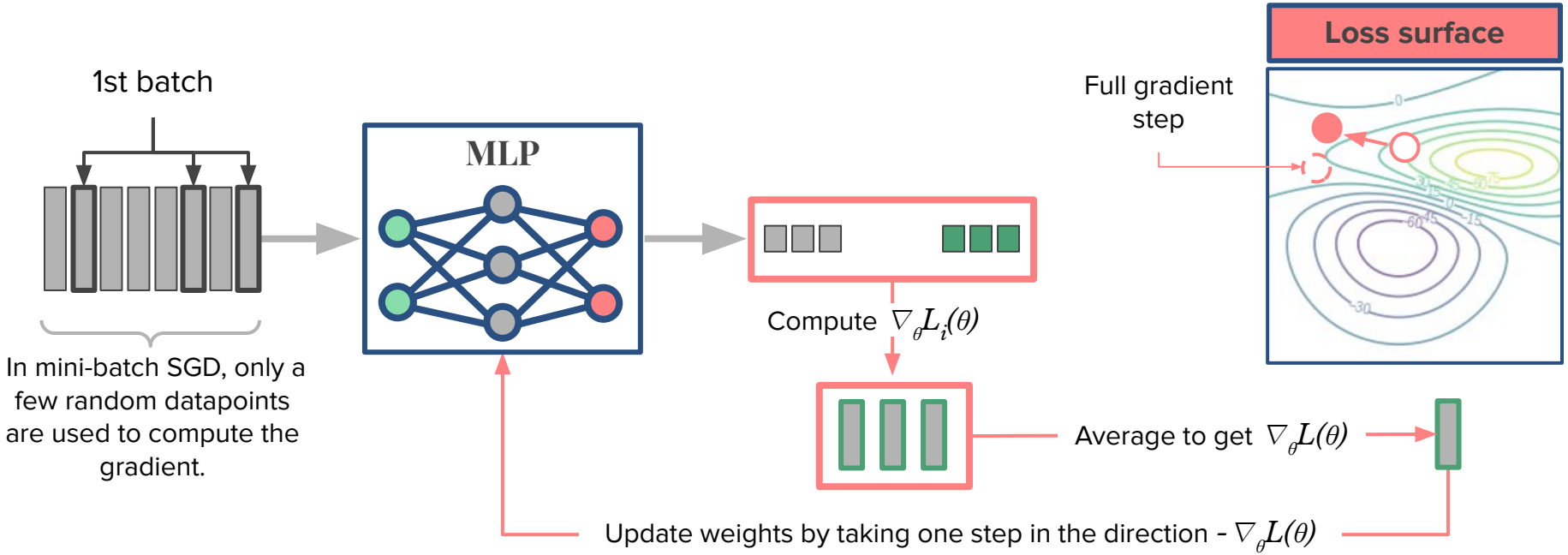
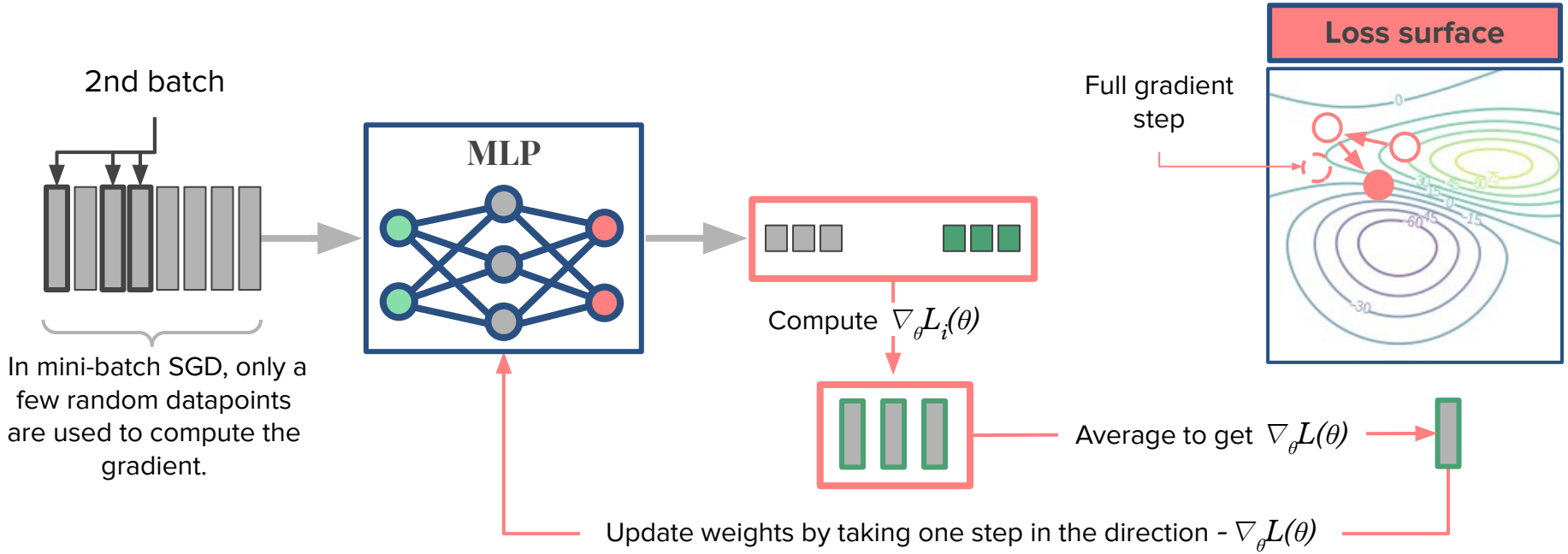


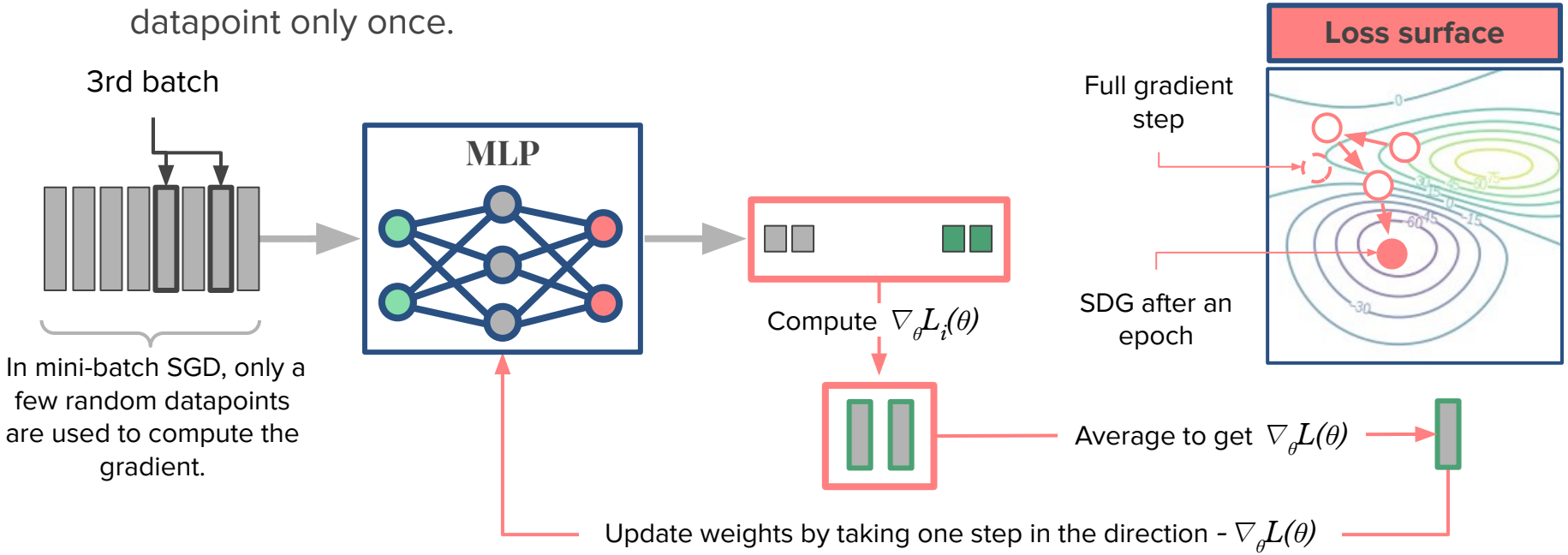
# GD vs SGD

- The next mini-batch's step will start from the location found by the previous step.



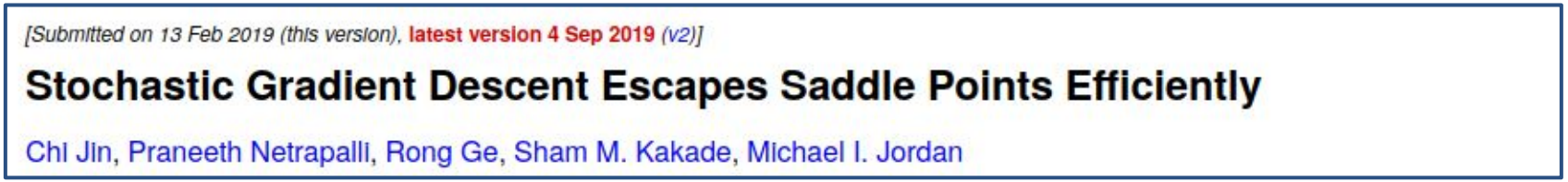
# GD vs SGD

- And we repeat that for the next batch and so on until we're done with one epoch. Note that **SGD made more progress than GD** using each datapoint only once.



# Analysing SGD

- SGD definitely makes the gradient computation quicker, but how about the local minima and saddle points?
- Well, the following recent paper seems convenient to answer this question:

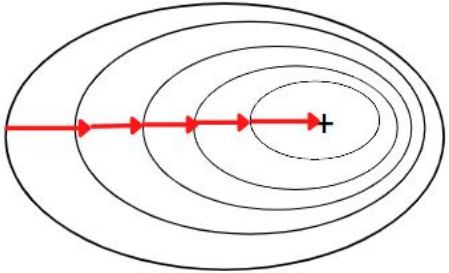



- Why does this happen? In simple english, it happened because SGD can be seen as **adding noise** to every step a full gradient would take.
- That means that it tries out directions that GD would not take, allowing it to **explore the loss surface better** and to hopefully “fall into” the global minimum region.
- This also means that SGD also makes more steps per datapoint than GD, due to this exploration feature.

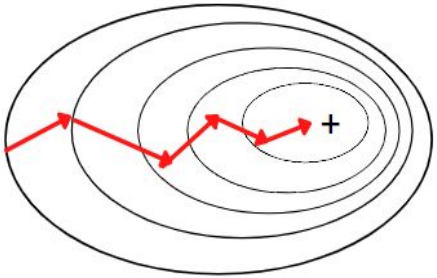
# Analysing SGD

- This behaviour is even more explicit when we change the batch size:
  - With a large batch size, SGD makes fewer steps per epoch and each step is more expensive. On the other hand, the full path is more stable.
  - With a smaller batch size, SGD explore the loss surface better and each step becomes cheaper. On the other hand, the path may be too erratic and SGD may take long to converge.

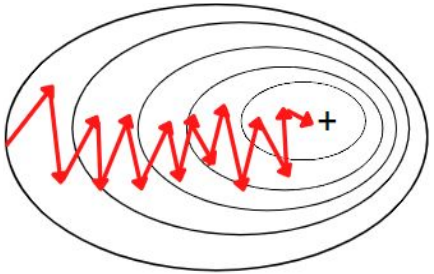
**GD**



**SGD with large batch size**



**SGD with small batch size**



- One solution to this issue is to use **smaller step sizes** (which may make the convergence even slower), other is to add **momentum**.

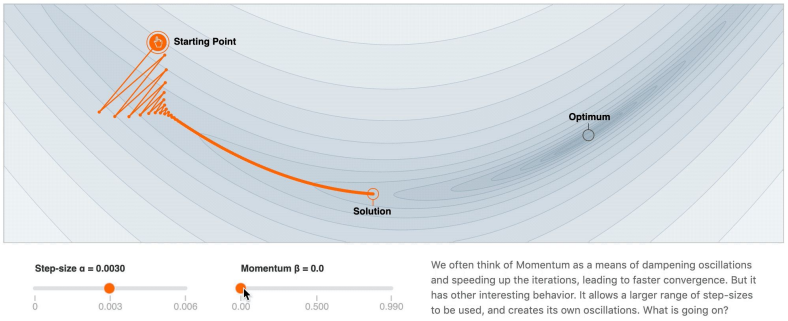
# Adding Momentum

- Adding momentum means **using previous steps (gradient directions)** to compute the current direction to go.
- Intuitively, it **hinders the walk from making very sharp turns** from one step to the next.
- Mathematically, we compute a step of SGD with momentum as follows:

$$g_t = \beta g_{t-1} + \nabla_x f(x_t) \qquad x_{t+1} = x_t - \eta g_t$$

where $\beta$ is called the **momentum parameter** (or simply momentum).

- In practice, adding some momentum makes SGD's path more stable/smooth*, leading to quicker convergences.
- However, adding too much momentum can also hurt convergence*.




* Check out this website and try adding momentum to GD yourself.

# Adding adaptive learning rates

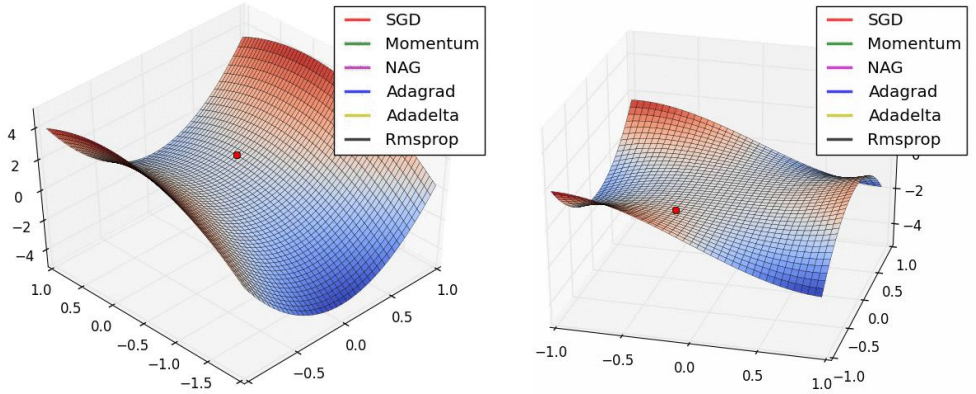
- The final trick to improve SGD is to use **adaptive learning rates (ALR)**, i.e. change the learning rates according to the “intensity” of previous steps.
- Mathematically, the new gradient descent formula would look like the following:

$$x_{t+1} = x_t - \frac{\eta}{\sqrt{\epsilon + \sum_{j=1}^{t} \|\nabla_x f(x_j)\|^2}} \nabla_x f(x_t)$$

  where $\epsilon$ is just a small number added to the numerator to avoid division by zero.
- Since the notation $||\nabla f(x)||^2$ in the numerator represents a gradient magnitude, the intuition behind the whole formula above is: **the larger the previous gradients/steps were, the smaller the next steps will be**.
- Most practical modern implementations of SGD for deep learning nowadays use ALR with slight changes, but keeping the same intuition.

# Modern Optimizers

- The literature offers many possible **optimizers** to find best the neural network weights.
- All of them employ one or more of the three main techniques: **Stochasticity**, **Momentum** and **Adaptive Learning Rates**.
- Below, we see how some of these optimizers* are able to escape saddle points.




- In practice, Deep Learning practitioners tend to use an optimizer called **ADAM (Adaptive Moment Estimation)**, since it uses the three techniques above in its algorithm**.

* NAG (Nestorov Accelerated Grad.) is a variation of momentum and Adagrad, Adadelta and RMSprop are different implementations of ALR.

** Here's two websites where you can compare ADAM's performance to SGD's, Momentum's and RMSprop's.

# Chain rule and Backpropagation

- After seeing all this theory of optimization, we only miss one thing: **how can we apply it to the neural networks we saw before???**
- Well, the first step is to write out the function we need to minimize.
- If we are using cross-entropy loss, this is the average loss function for our network:

$$L(\theta) = \frac{1}{n}\sum_{i=1}^{n} l(NN_\theta(x^{(i)}), y^{(i)}) = -\frac{1}{n}\sum_{i=1}^{n} [y^{(i)}]^\top \log(\text{softmax}(W_L a(W_{L-1} \cdots a(W_0 x^{(i)})...)))$$

- Now we "just" need to compute the gradient of $L(\theta)$ with respect to $\theta$! Although not straightforward, one just has to use the **Chain Rule** from calculus.
- Say that you have two **differentiable** functions $f$ and $g$. Let $y = f(g(x))$ and $u = g(x)$ for a value $x$. Then we have that:

$$\frac{dy}{dx} = \frac{dy}{du}\frac{du}{dx}$$

# Chain rule and Backpropagation

- *Example*: if $f(x) = x^2$ and $g(x) = 3x^3 + 2$, then the derivative of $y = f(g(x))$ (call $u = g(x)$):

$$\frac{dy}{dx} = \frac{dy}{du}\frac{du}{dx} = (2u)(9x^2) = (2(3x^3+2))(9x^2) = 54x^5+36x^2$$

- Using a similar approach one can consider $y = f_1(f_2(f_3...f_n(x)...))$. Let $u_1 = f_2(f_3...f_n(x)...)$, $u_2 = (f_3...f_n(x)...)$ and so on. Then we have that:

$$\frac{dy}{dx} = \frac{dy}{du_1}\frac{du_1}{du_2}\frac{du_2}{du_3}\cdots\frac{du_n}{dx}$$

- For (simple) neural networks, one only has to apply the chain rule to get the weight updates*.
- In that case the first step it to “see” our loss definition as a series of composed function such as $y = f_1(f_2(f_3...f_n(x)...))$.

* Mathematically speaking, the ReLU activation is not differentiable, which should complicate things. In practice, however, the deep learning community simply simply **disregards** this issue. This paper goes in detail about this issue.

# Chain rule and Backpropagation

- To make things simple, let's consider a network of just one hidden layer, the loss on only one datapoint (called $x$ with true label $y$) and that we just want to optimize $W_0$. Then:

$$u_0(W_0) = l(NN_\theta(x), y) = -y^\top \log(\text{softmax}(W_1 a(W_0 x)))$$

- Let $u_1(z) = -y^\top z$, $u_2(z) = log(z)$, $u_3(z) = \text{softmax}(z)$, $u_4(z) = W_1 z$, $u_5(z) = a(z)$, $u_6(z) = z^\top x$, where $z$ is a **vector** or a **matrix.** Then have that $u_0 = u_1(u_2(u_3(u_4(u_5(u_6(W_0))))))$ and that

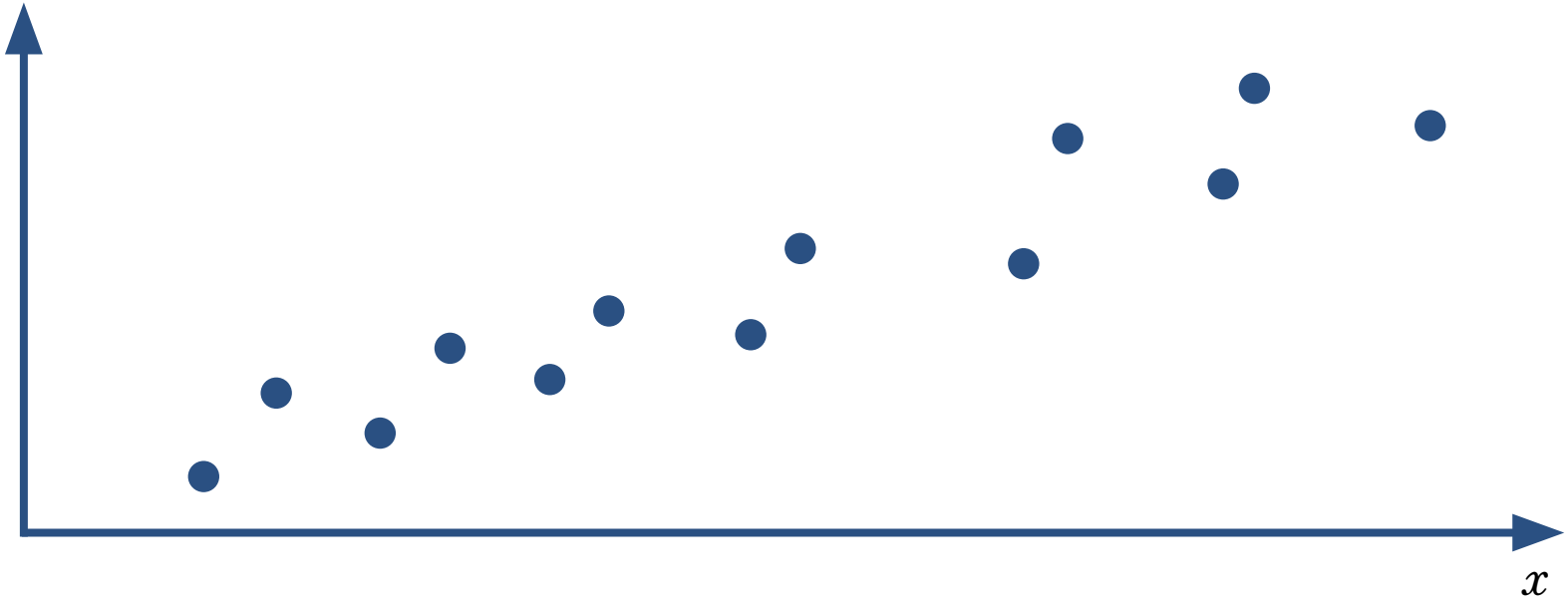
$$\frac{du_0}{dW_0} = \frac{du_0}{du_1}\frac{du_1}{du_2}\frac{du_2}{du_3}\frac{du_3}{du_4}\frac{du_4}{du_5}\frac{du_5}{du_6}\frac{du_6}{dW_0}$$

- Now things are much easier: for example, using matrix calculus*, we have $du_1/dz = -y$, $du_4(z)/dz = W_1$ and so on. Remember that one has to compute Jacobians sometimes here.
- Note that you'd need to do something similar to $W_1$ to optimize it too.

* Here, you can find more refreshing information on derivatives with respect to vectors and matrices

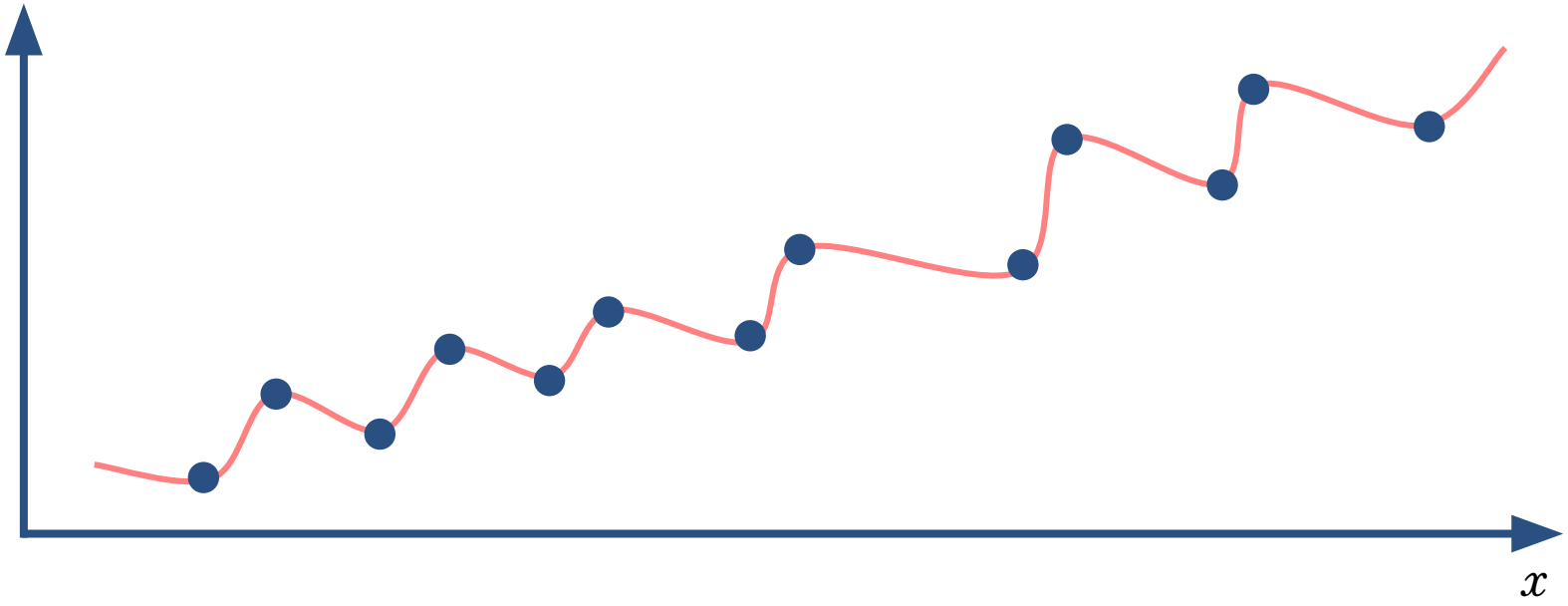
# Regularization in Deep Learning

- The final topic for today is **Regularization**. But, first one question: if you were to draw the function that generated the points below, how would it look like?



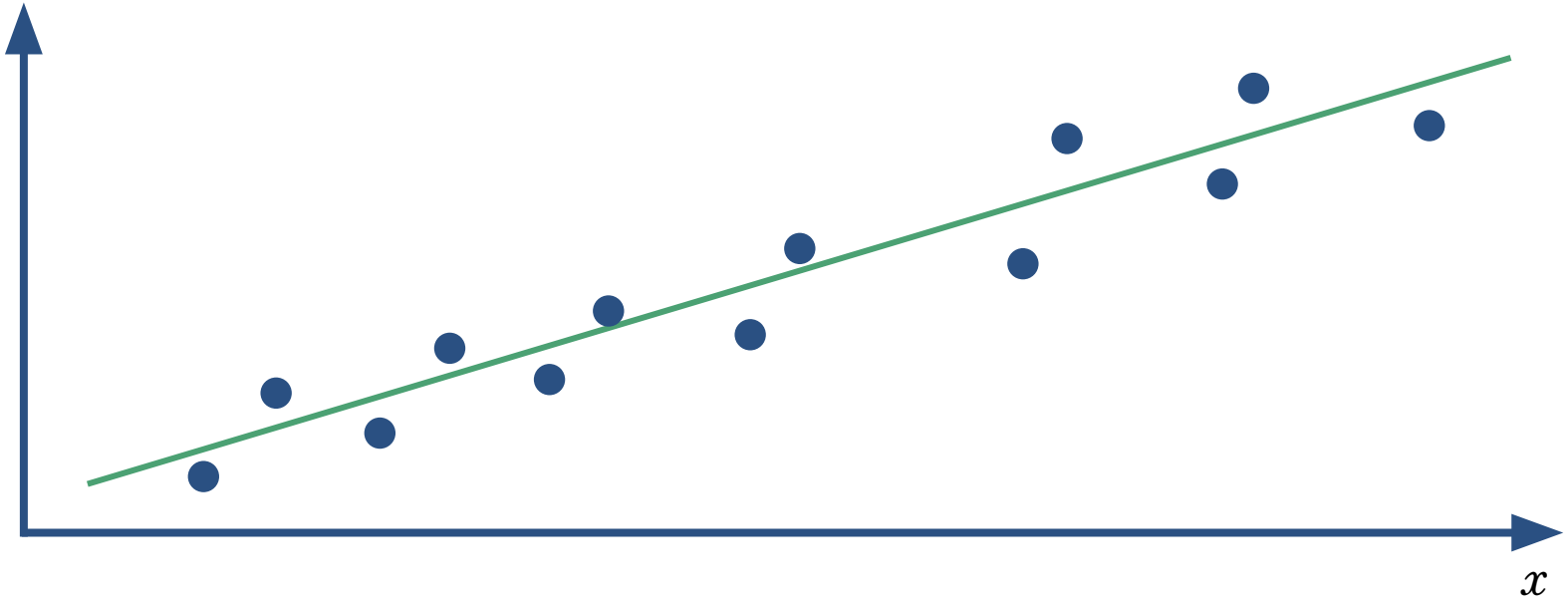
# Regularization in Deep Learning

- A possible solution is the following, where we made sure that the function went through all points:



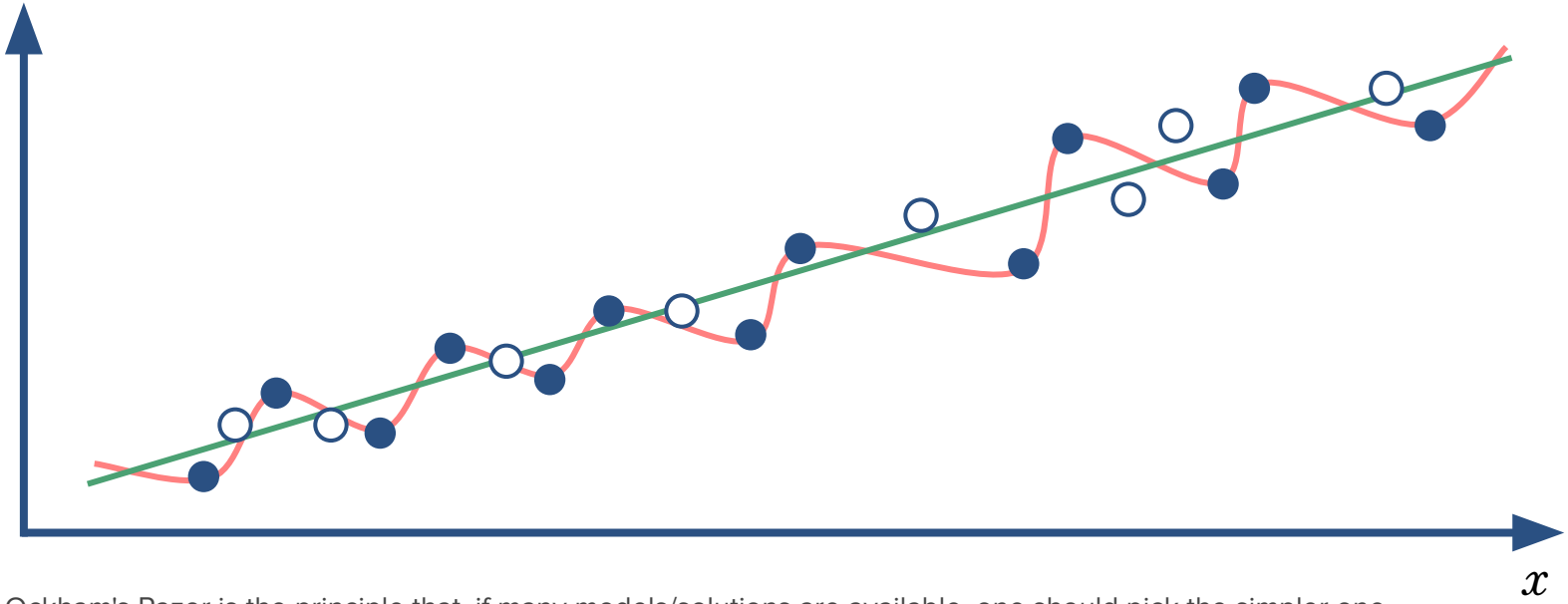
# Regularization in Deep Learning

- Another one, simpler, is a line, when we realize that these points are probably noisy samples from **regressor** function.



# Regularization in Deep Learning

- In general the second, simpler, option is preferred (using Ockham's Razor principle*), especially because it avoids fitting the intrinsic noise in the data (**overfitting**).




* Ockham's Razor is the principle that, if many models/solutions are available, one should pick the simpler one.

# Regularization in Deep Learning

- Despite the previous example of a regression problem, an analogous example can be traced to classification tasks.
- To add regularization to Deep Learning, the usual practice is to add a **regularizer** $R(\theta)$ to its average loss function:

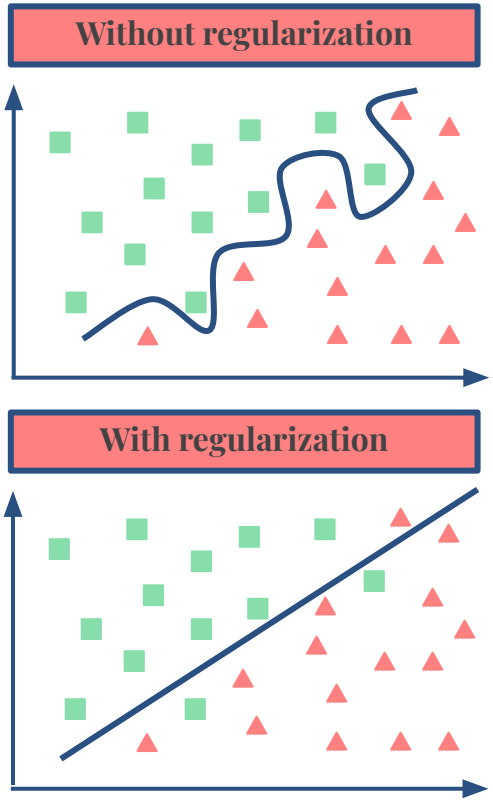
Encourages predictions to match training data

$$L(\theta) = \frac{1}{n}\sum_{i=1}^{n} l(NN_\theta(x^{(i)}), y^{(i)}) + \lambda R(\theta)$$

Prevents the model from doing too well on training data

where λ ("lambda") is a positive constant.

- In other words, $R(\theta)$ should ensure that the the network weights $W_0, W_1, ..., W_L$ are "well-behaved".



# Regularization in Deep Learning

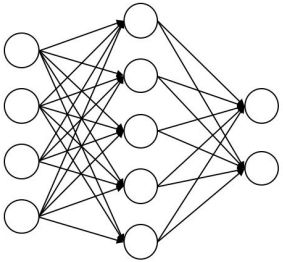
- Typical regularizers are the $L_1$ and $L_2$ norms, that consider that the network weights **shouldn't achieve very high values**.
- Another, quite unexpectedly, regularizer is **Dropout**, which consists in randomly ignoring certain nodes in a layer during training:

**Dropout: A Simple Way to Prevent Neural Networks from Overfitting**

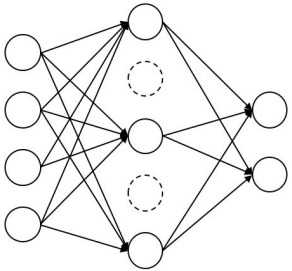
*Nitish Srivastava, Geoffrey Hinton, Alex Krizhevsky, Ilya Sutskever, Ruslan Salakhutdinov*, 15(56):1929–1958, 2014.

- In practice, when using dropout, we set a variable $p \in (0, 1)$ that indicates the percentage of units in a given layer will be "turn off" during training.
- At the beginning of each SGD epoch, another sampling of units to turn off is randomly chosen with probability $p$.

**Standart Network**



**Network With Dropout**



# *Video*: Go AlphaGo!