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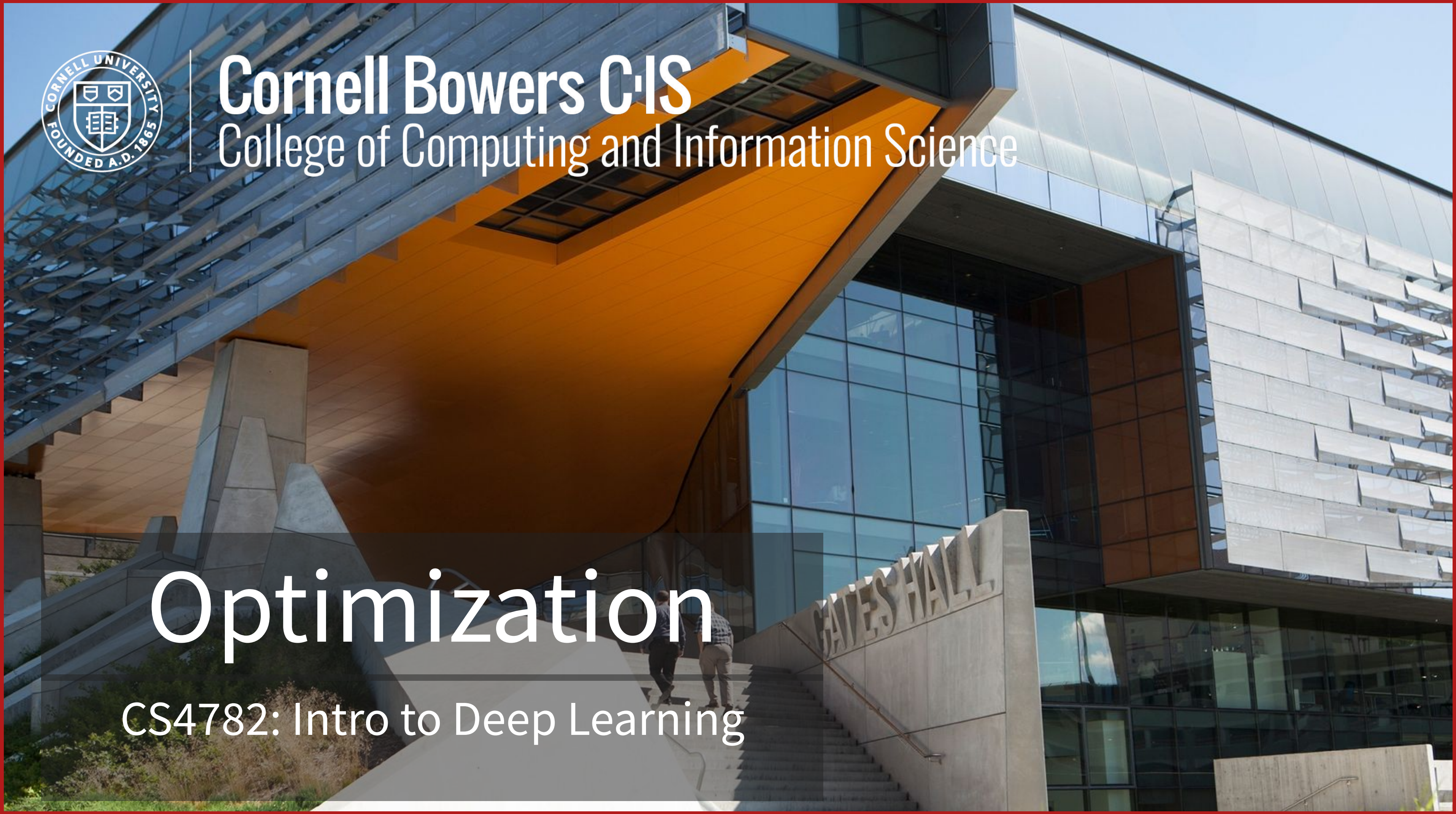
College of Computing and Information Science



Optimization

CS4782: Intro to Deep Learning

Quiz on Canvas!
(code-1234)

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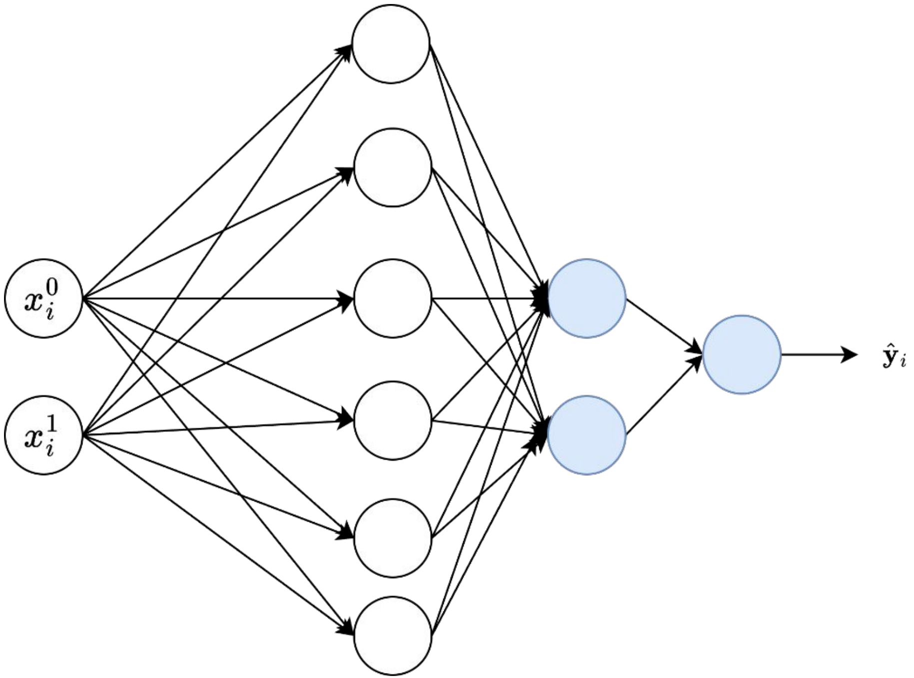
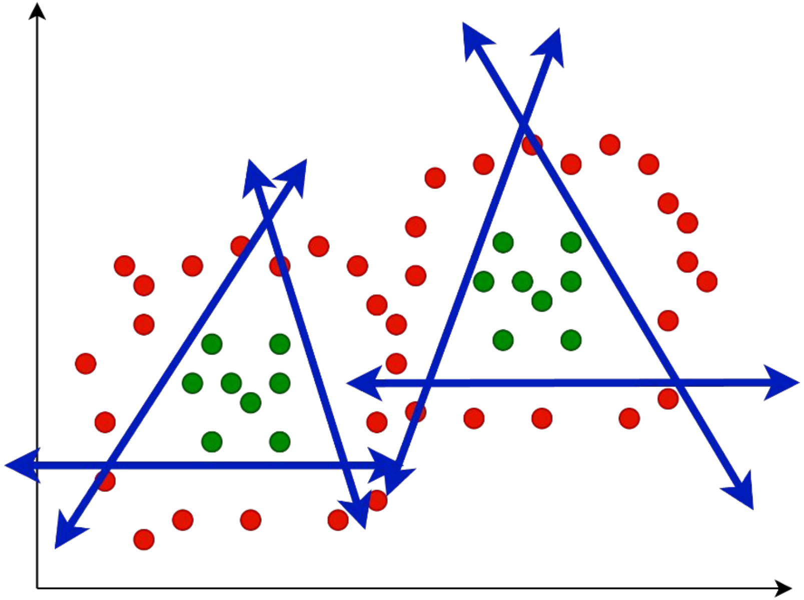
Agenda

- Backpropagation
- Optimizers
  - Gradient Descent
  - Stochastic Gradient Descent
  - SGD w. Momentum
  - AdaGrad
  - RMSProp
  - Adam
- Learning rate scheduling
- Hyperparameter Optimization

Recap

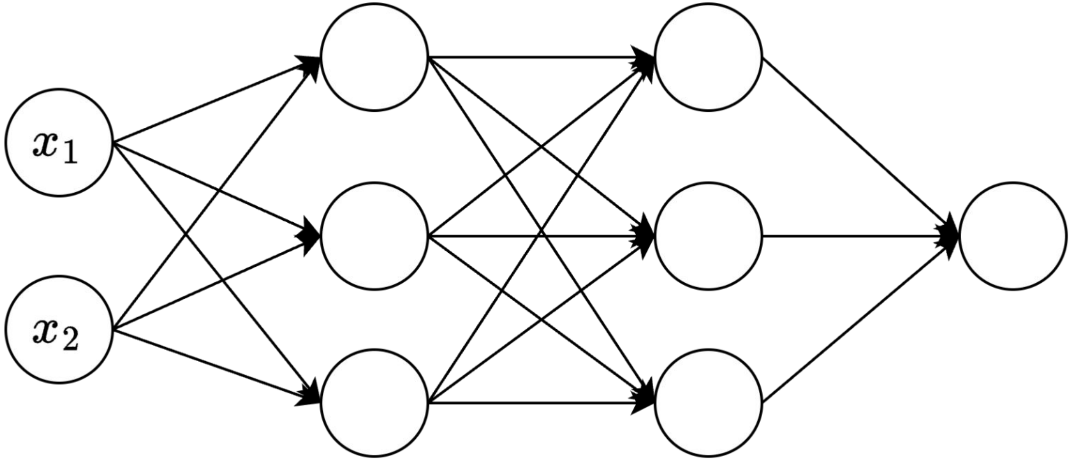
MLPs can learn complex decision boundaries!





Forward Pass - MLP

$$\mathbf{a}^{[1]} = \mathbf{W}^{[1]}\mathbf{z}^{[0]} + \mathbf{b}^{[1]}$$



$$\mathbf{z}^{[0]} = \mathbf{x}$$

Discuss

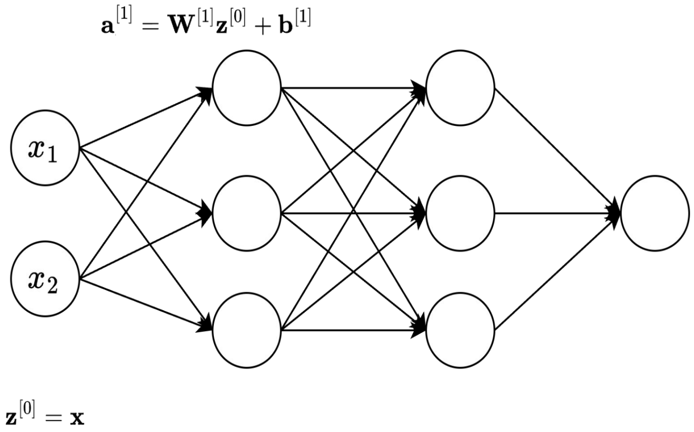
What are the dimensions of $W^{[1]}$ and $b^{[1]}$?

x: (2, 1)

$\mathbf{W}^{[1]}$:

$\mathbf{b}^{[1]}$:

$\mathbf{a}^{[1]}$:



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Discuss

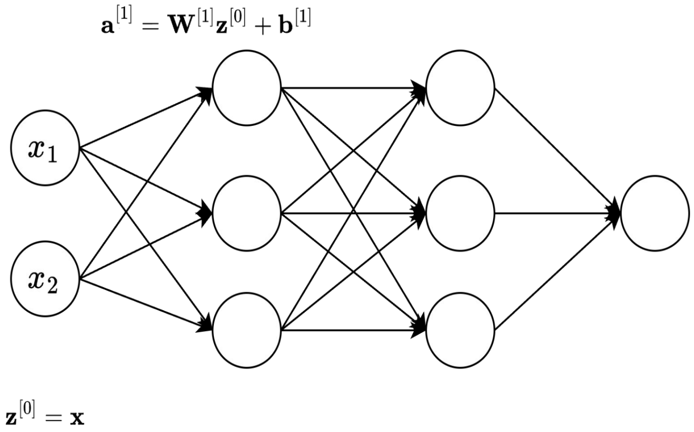
What are the dimensions of W[1] and b[1]?

x: (2, 1)

$\mathbf{W}^{[1]}$: (3, 2)

$\mathbf{b}^{[1]}$: (3, 1)

$\mathbf{a}^{[1]}$: (3, 1)



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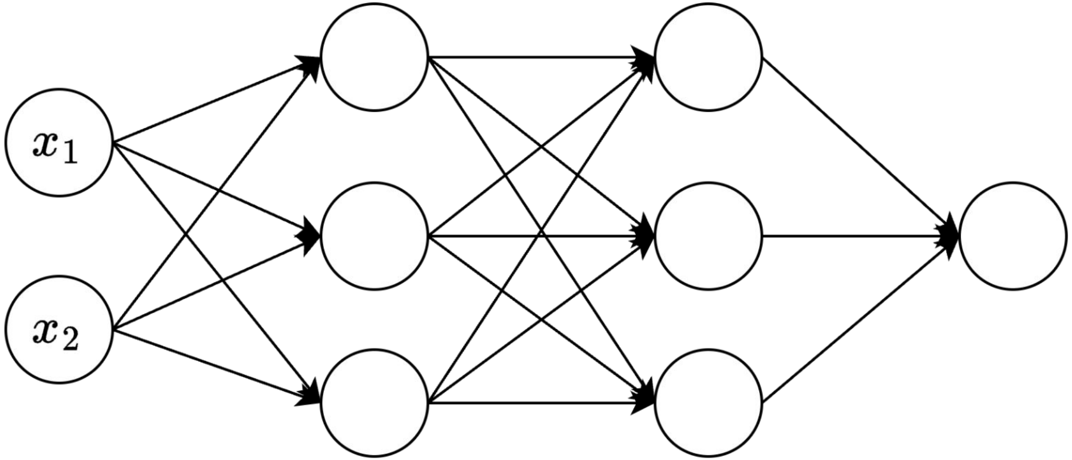
Forward Pass - MLP

$$\mathbf{a}^{[1]} = \mathbf{W}^{[1]}\mathbf{z}^{[0]} + \mathbf{b}^{[1]}$$



$$\mathbf{z}^{[0]} = \mathbf{x}$$

$$\mathbf{z}^{[1]} = \sigma(\mathbf{a}^{[1]})$$

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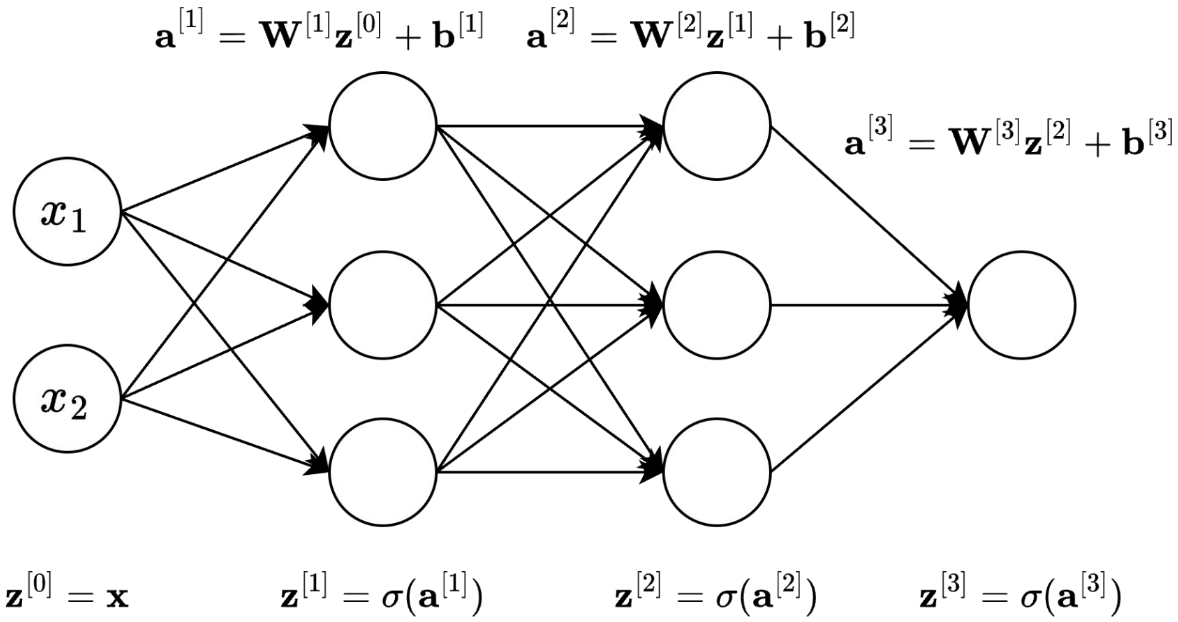
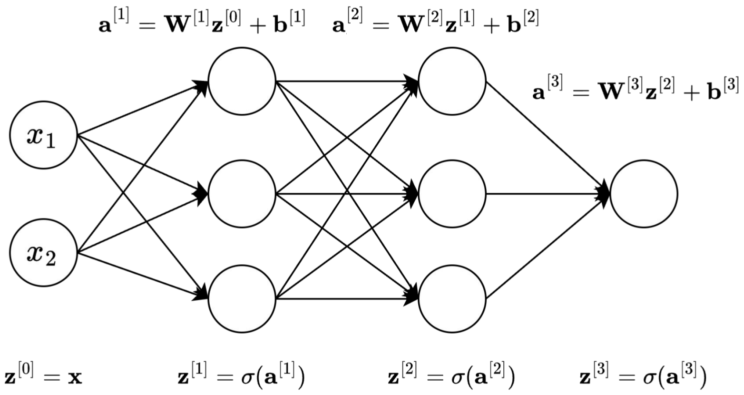
Forward Pass - MLP



Forward Pass - MLP

Algorithm Forward Pass through MLP

Input: input $\mathbf{x}$, weight matrices $\mathbf{W}^{[1]}, \ldots, \mathbf{W}^{[L]}$, bias vectors $\mathbf{b}^{[1]}, \ldots, \mathbf{b}^{[L]}$
$\mathbf{z}^{[0]} = \mathbf{x}$ ▷ Initialize input
for $l = 1$ **to** L **do**
    $\mathbf{a}^{[l]} = \mathbf{W}^{[l]}\mathbf{z}^{[l-1]} + \mathbf{b}^{[l]}$ ▷ Linear transformation
    $\mathbf{z}^{[l]} = \sigma^{[l]}(\mathbf{a}^{[l]})$ ▷ Nonlinear activation
end for
Output: $\mathbf{z}^{[L]}$



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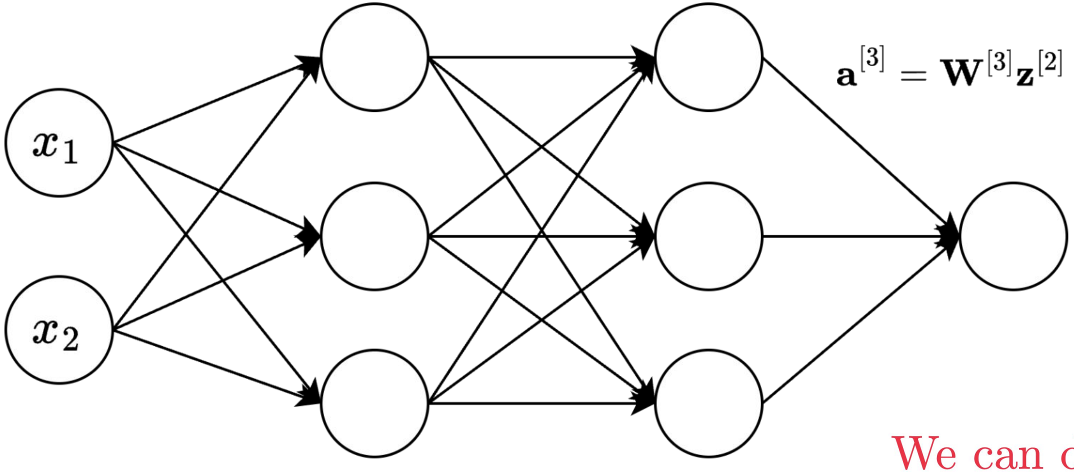
Backpropagation- MLPs

$\mathbf{a}^{[1]} = \mathbf{W}^{[1]}\mathbf{z}^{[0]} + \mathbf{b}^{[1]}$ $\quad$ $\mathbf{a}^{[2]} = \mathbf{W}^{[2]}\mathbf{z}^{[1]} + \mathbf{b}^{[2]}$

$\mathbf{a}^{[3]} = \mathbf{W}^{[3]}\mathbf{z}^{[2]} + \mathbf{b}^{[3]}$



$\text{Loss} = \mathcal{L}$

We can directly compute $\frac{\partial \mathcal{L}}{\partial \mathbf{z}^{[3]}}$!

$\mathbf{z}^{[0]} = \mathbf{x}$ $\quad$ $\mathbf{z}^{[1]} = \sigma(\mathbf{a}^{[1]})$ $\quad$ $\mathbf{z}^{[2]} = \sigma(\mathbf{a}^{[2]})$ $\quad$ $\mathbf{z}^{[3]} = \sigma(\mathbf{a}^{[3]})$

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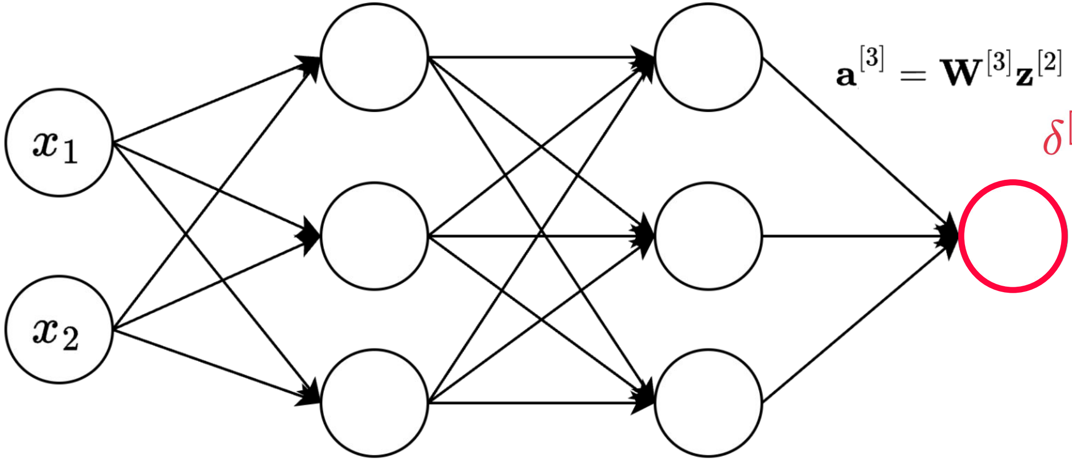
Backpropagation- MLPs

$$\mathbf{a}^{[1]} = \mathbf{W}^{[1]}\mathbf{z}^{[0]} + \mathbf{b}^{[1]} \qquad \mathbf{a}^{[2]} = \mathbf{W}^{[2]}\mathbf{z}^{[1]} + \mathbf{b}^{[2]}$$

$$\mathbf{a}^{[3]} = \mathbf{W}^{[3]}\mathbf{z}^{[2]} + \mathbf{b}^{[3]}$$

$$\delta^{[3]} = \frac{\partial \mathcal{L}}{\partial \mathbf{a}^{[3]}} = \frac{\partial \mathcal{L}}{\partial \mathbf{z}^{[3]}} \frac{\partial \mathbf{z}^{[3]}}{\partial \mathbf{a}^{[3]}}$$

$$= \frac{\partial \mathcal{L}}{\partial \mathbf{z}^{[3]}} \odot \sigma^{[3]\prime}$$



$$\mathbf{z}^{[0]} = \mathbf{x} \qquad \mathbf{z}^{[1]} = \sigma(\mathbf{a}^{[1]}) \qquad \mathbf{z}^{[2]} = \sigma(\mathbf{a}^{[2]}) \qquad \mathbf{z}^{[3]} = \sigma(\mathbf{a}^{[3]})$$

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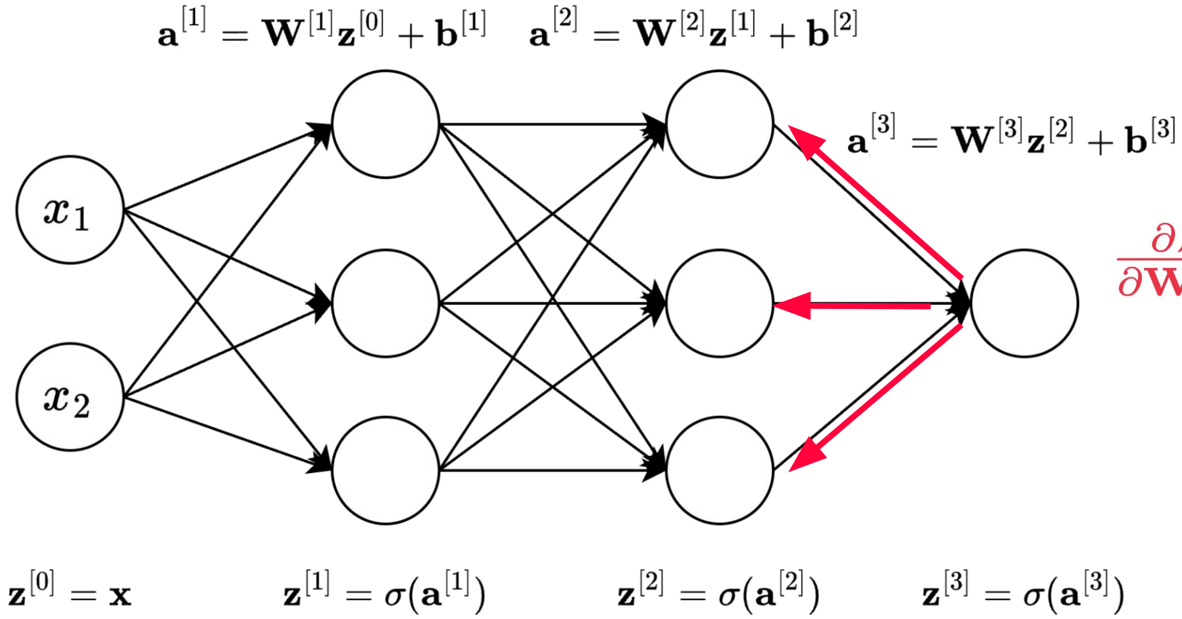
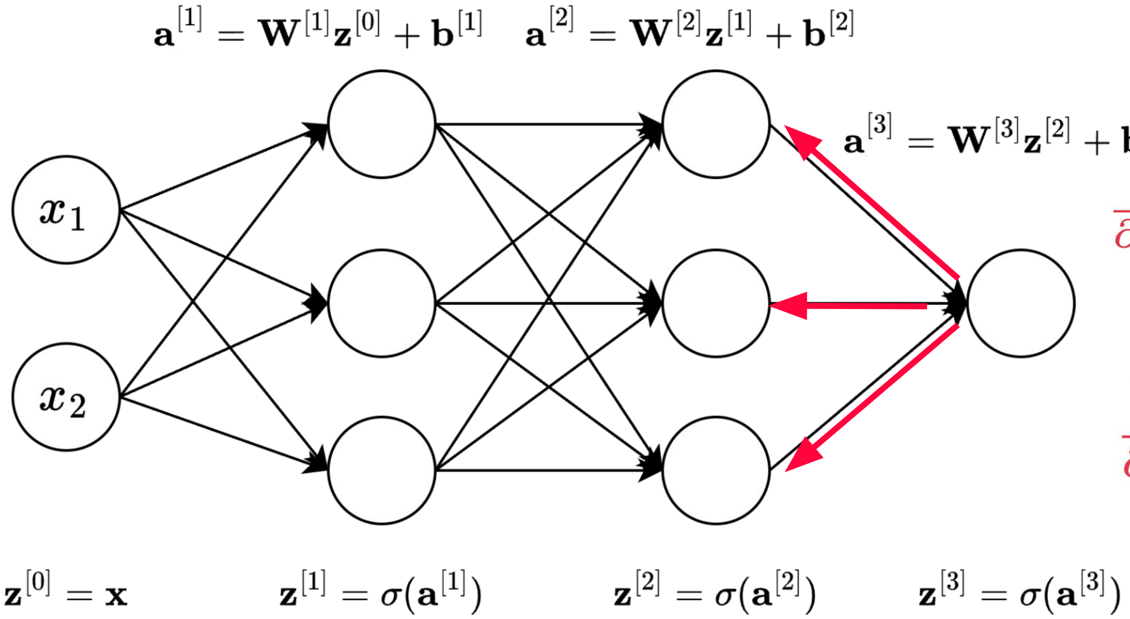
Backpropagation- MLPs



$$\frac{\partial \mathcal{L}}{\partial \mathbf{W}^{[3]}} = \frac{\partial \mathcal{L}}{\partial \mathbf{a}^{[3]}} \frac{\partial \mathbf{a}^{[3]}}{\partial \mathbf{W}^{[3]}}$$

Simplify further!

Backpropagation- MLPs



$$\frac{\partial \mathcal{L}}{\partial \mathbf{W}^{[3]}} = \frac{\partial \mathcal{L}}{\partial \mathbf{a}^{[3]}} \frac{\partial \mathbf{a}^{[3]}}{\partial \mathbf{W}^{[3]}}$$

$$= \delta^{[3]} (\mathbf{z}^{[2]})^T$$

$$\frac{\partial \mathcal{L}}{\partial \mathbf{b}^{[3]}} = \frac{\partial \mathcal{L}}{\partial \mathbf{a}^{[3]}} \frac{\partial \mathbf{a}^{[3]}}{\partial \mathbf{b}^{[3]}}$$

$$= \delta^{[3]}$$

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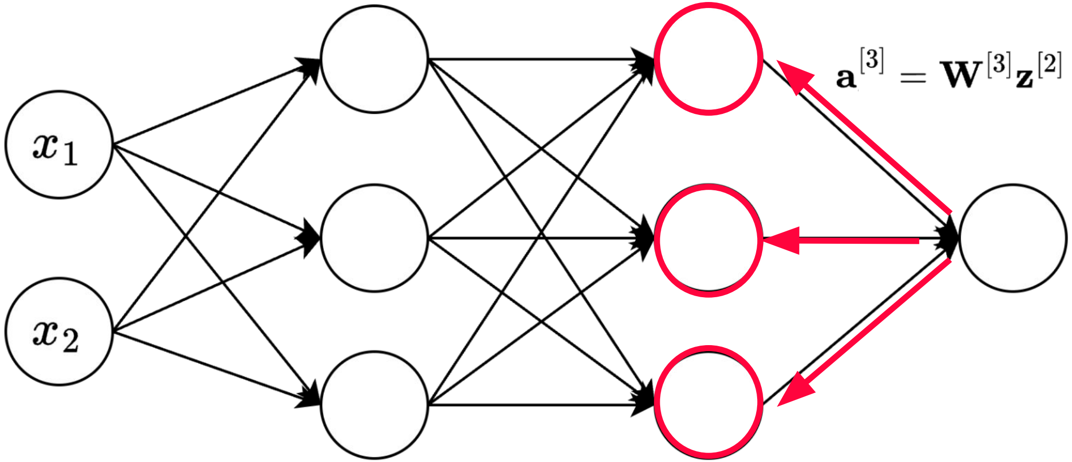
Backpropagation- MLPs

$$\mathbf{a}^{[1]} = \mathbf{W}^{[1]}\mathbf{z}^{[0]} + \mathbf{b}^{[1]} \qquad \mathbf{a}^{[2]} = \mathbf{W}^{[2]}\mathbf{z}^{[1]} + \mathbf{b}^{[2]}$$

$$\mathbf{a}^{[3]} = \mathbf{W}^{[3]}\mathbf{z}^{[2]} + \mathbf{b}^{[3]}$$



$$\mathbf{z}^{[0]} = \mathbf{x} \qquad \mathbf{z}^{[1]} = \sigma(\mathbf{a}^{[1]}) \qquad \mathbf{z}^{[2]} = \sigma(\mathbf{a}^{[2]}) \qquad \mathbf{z}^{[3]} = \sigma(\mathbf{a}^{[3]})$$

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Backpropagation- MLPs

Algorithm Backward Pass through MLP (Detailed)

1: **Input:** $\{\mathbf{z}^{[1]}, \ldots, \mathbf{z}^{[L]}\}$, $\{\mathbf{a}^{[1]}, \ldots, \mathbf{a}^{[L]}\}$, loss gradient $\frac{\partial \mathcal{L}}{\partial \mathbf{z}^{[L]}}$

2: $\delta^{[L]} = \frac{\partial \mathcal{L}}{\partial \mathbf{a}^{[L]}} = \frac{\partial \mathcal{L}}{\partial \mathbf{z}^{[L]}} \frac{\partial \mathbf{z}^{[L]}}{\partial \mathbf{a}^{[L]}} = \frac{\partial \mathcal{L}}{\partial \mathbf{z}^{[L]}} \odot \sigma^{[L]\prime}(\mathbf{a}^{[L]})$ ▷ Error term

3: **for** $l = L$ **to** 1 **do**

4: $\quad \frac{\partial \mathcal{L}}{\partial \mathbf{W}^{[l]}} = \frac{\partial \mathcal{L}}{\partial \mathbf{a}^{[l]}} \frac{\partial \mathbf{a}^{[l]}}{\partial \mathbf{W}^{[l]}} = \delta^{[l]} (\mathbf{z}^{[l-1]})^T$ ▷ Gradient of weights

5: $\quad \frac{\partial \mathcal{L}}{\partial \mathbf{b}^{[l]}} = \frac{\partial \mathcal{L}}{\partial \mathbf{a}^{[l]}} \frac{\partial \mathbf{a}^{[l]}}{\partial \mathbf{b}^{[l]}} = \delta^{[l]}$ ▷ Gradient of biases

6: $\quad \frac{\partial \mathcal{L}}{\partial \mathbf{z}^{[l-1]}} = \frac{\partial \mathcal{L}}{\partial \mathbf{a}^{[l]}} \frac{\partial \mathbf{a}^{[l]}}{\partial \mathbf{z}^{[l-1]}} = (\mathbf{W}^{[l]})^T \delta^{[l]}$

7: $\quad \delta^{[l-1]} = \frac{\partial \mathcal{L}}{\partial \mathbf{a}^{[l-1]}} = \frac{\partial \mathcal{L}}{\partial \mathbf{z}^{[l-1]}} \frac{\partial \mathbf{z}^{[l-1]}}{\partial \mathbf{a}^{[l-1]}} = ((\mathbf{W}^{[l]})^T \delta^{[l]}) \odot \sigma^{[l-1]\prime}(\mathbf{a}^{[l-1]})$

8: **end for**

9: **Output:** $\frac{\partial \mathcal{L}}{\partial \mathbf{W}^{[1:L]}}, \frac{\partial \mathcal{L}}{\partial \mathbf{b}^{[1:L]}}$

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Backpropagation- MLPs

Algorithm Backward Pass through MLP

1: **Input:** $\{\mathbf{z}^{[1]}, \ldots, \mathbf{z}^{[L]}\}$, $\{\mathbf{a}^{[1]}, \ldots, \mathbf{a}^{[L]}\}$, loss gradient $\frac{\partial \mathcal{L}}{\partial \mathbf{z}^{[L]}}$

2: $\delta^{[L]} = \frac{\partial \mathcal{L}}{\partial \mathbf{z}^{[L]}} \odot \sigma^{[L]'}(\mathbf{a}^{[L]})$ ▷ Error term

3: **for** $l = L$ **to** 1 **do**

4: $\quad \frac{\partial \mathcal{L}}{\partial \mathbf{W}^{[l]}} = \delta^{[l]}(\mathbf{z}^{[l-1]})^T$ ▷ Gradient of weights

5: $\quad \frac{\partial \mathcal{L}}{\partial \mathbf{b}^{[l]}} = \delta^{[l]}$ ▷ Gradient of biases

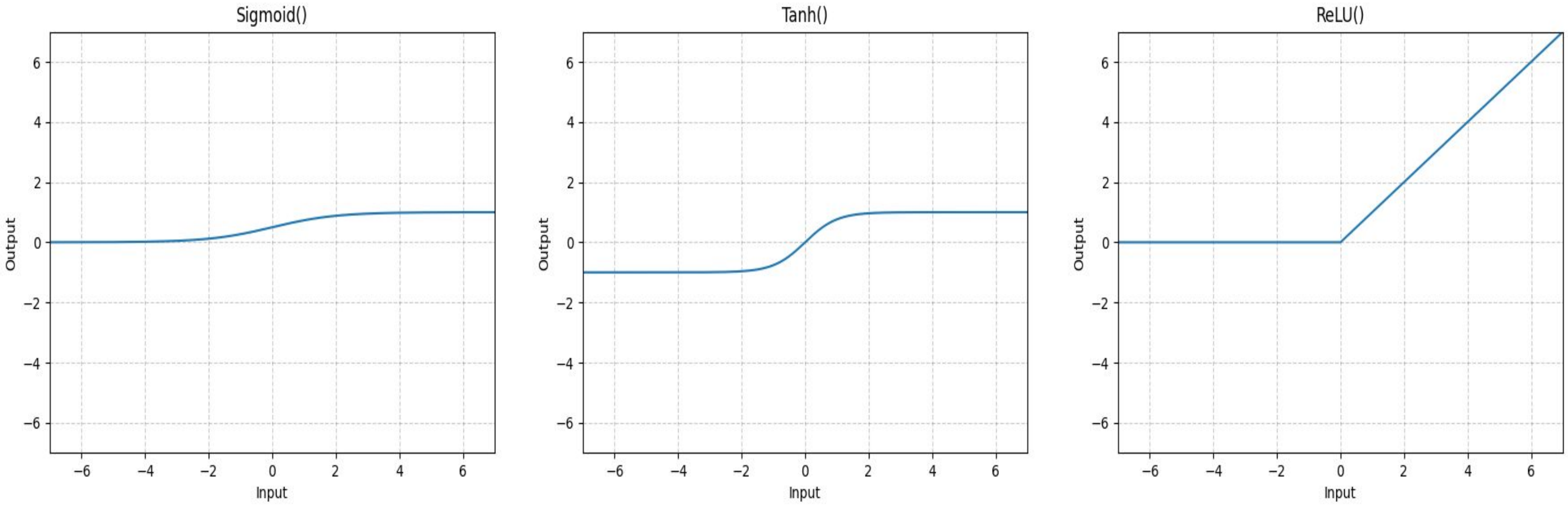
6: $\quad \delta^{[l-1]} = ((\mathbf{W}^{[l]})^T \delta^{[l]}) \odot \sigma^{[l-1]'}(\mathbf{a}^{[l-1]})$

7: **end for**

8: **Output:** $\frac{\partial \mathcal{L}}{\partial \mathbf{W}^{[1:L]}}, \frac{\partial \mathcal{L}}{\partial \mathbf{b}^{[1:L]}}$

Discuss: Activation functions

- How do different activation functions behave during backprop?
    - Visualize their derivatives!



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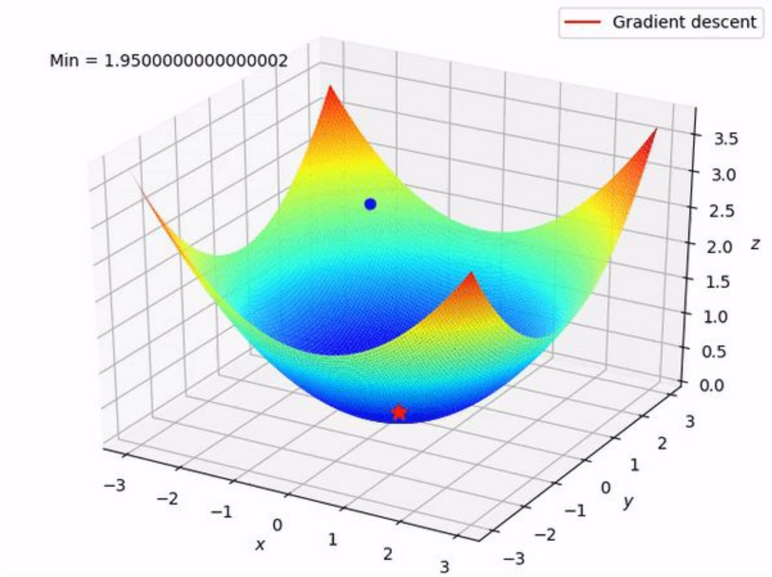
What is Optimization?



In deep learning, optimization methods attempt to find model weights that **minimize the loss function**.

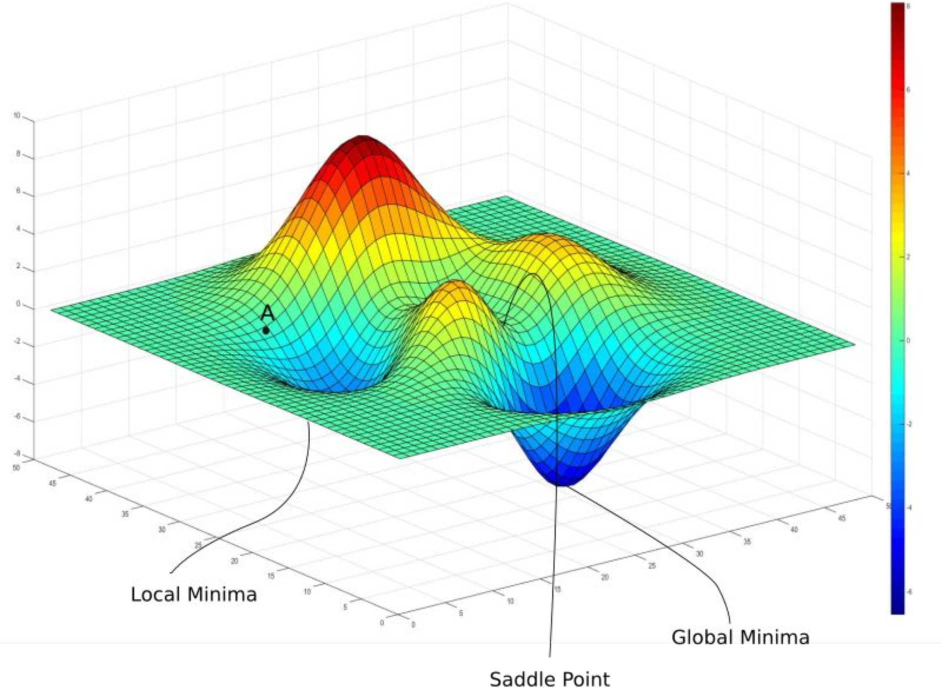
Loss function

Empirical Risk:

$$\mathcal{L}(\mathbf{w}_t) = \frac{1}{n} \sum_{i=1,\ldots,n} \ell(\mathbf{w}_t, \mathbf{x}_i)$$

t : at time step t
$\mathbf{w}_t$: Model weights (parameters) at time t
$\mathbf{x}_i$: The i-th input training data

$\mathcal{L}$: the Loss function (optimization target)
ℓ : per-sample loss



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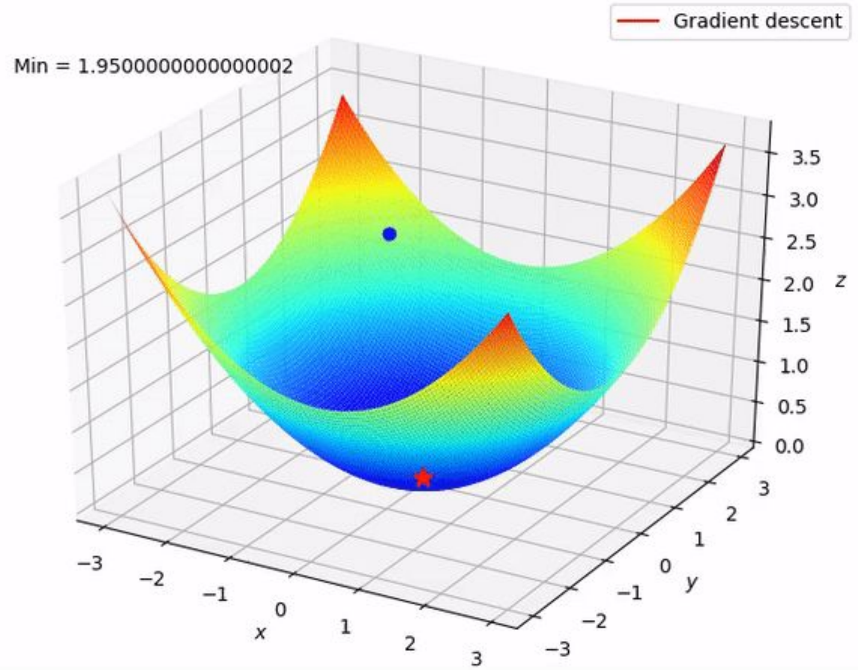
Gradient Descent (GD)

$$\mathbf{w}_{t+1} = \mathbf{w}_t - \alpha \nabla \mathcal{L}(\mathbf{w}_t)$$

α: the learning rate

$\nabla \mathcal{L}(\mathbf{w}_t)$: the gradient of Loss w.r.t. $\mathbf{w}_t$



What are some potential problems with gradient descent?

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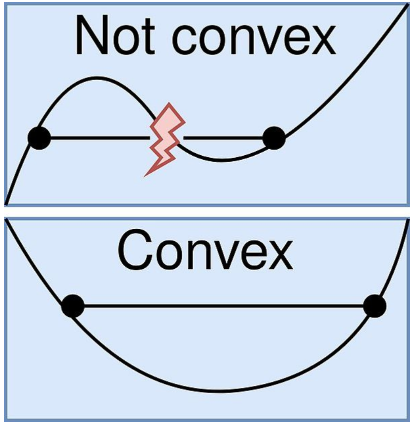
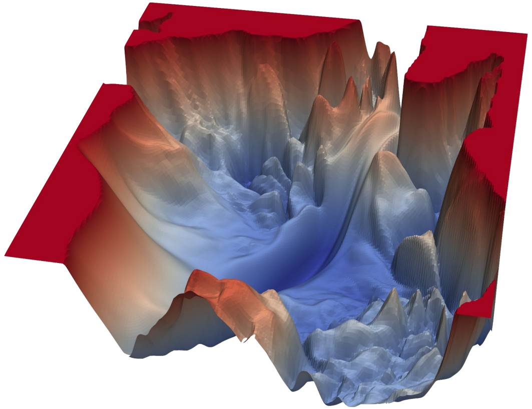
Convexity

- A function on a graph is **convex** if a line segment drawn through any two points on the line of the function, then it never lies below the curved line segment
- Convexity implies that every local minimum is **global minimum**.
- Neural networks are **not** convex!





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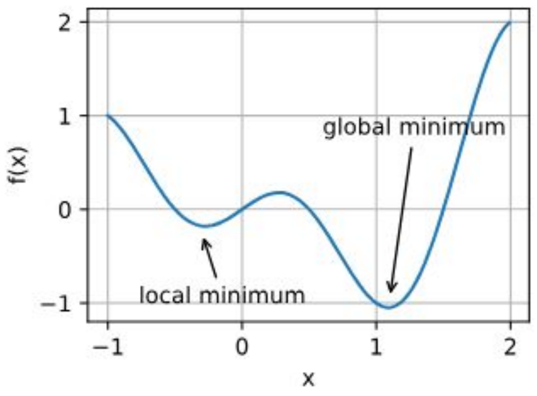
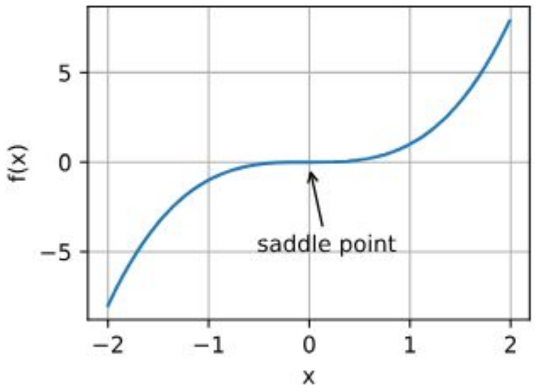
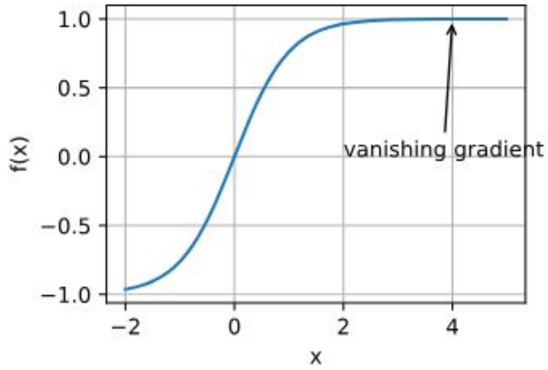
Challenges in Non-Convex Optimization



Local Minima vs. Global Minima



Saddle Points



Vanishing gradient

Gradient Descent (GD)

$$\mathcal{L}(\mathbf{w}_t) = \boxed{\frac{1}{n}\sum_{i=1}^{n}} \ell(\mathbf{w}_t, \mathbf{x}_i)$$

$$\nabla\mathcal{L}(\mathbf{w}_t) = \boxed{\frac{1}{n}\sum_{i=1}^{n}} \nabla\ell(\mathbf{w}_t, \mathbf{x}_i)$$

$$\mathbf{w}_{t+1} = \mathbf{w}_t - \alpha\nabla\mathcal{L}(\mathbf{w}_t)$$

Full gradient: $\mathcal{O}(n)$ time => ***Too expensive!***

- *Statistically, why don't we use 1 or a few samples from the training dataset to approximate the full gradient?*

Gradient Descent (GD)

$$\mathbf{w}_{t+1} = \mathbf{w}_t - \alpha \nabla \mathcal{L}(\mathbf{w}_t)$$

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Gradient Descent (GD)

$$\mathbf{w}_{t+1} = \mathbf{w}_t - \alpha \nabla \mathcal{L}(\mathbf{w}_t)$$

Select **1** example randomly each time

Gradient Descent (GD)

$$\mathbf{w}_{t+1} = \mathbf{w}_t - \alpha \nabla \mathcal{L}(\mathbf{w}_t)$$

$\downarrow$ Select **1** example randomly each time

Per-sample gradient is equivalent to full gradient in expectation!

$$\mathbb{E}[\nabla \ell(\mathbf{w}_t, \mathbf{x}_i)] = \frac{1}{n}\sum_{i=1}^{n} \nabla \ell(\mathbf{w}_t, \mathbf{x}_i) = \nabla \mathcal{L}(\mathbf{w}_t)$$

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Stochastic Gradient Descent (SGD)

$$\mathbf{w}_{t+1} = \mathbf{w}_t - \alpha \nabla \mathcal{L}(\mathbf{w}_t)$$

Select **1** example randomly each time

$$\mathbf{w}_{t+1} = \mathbf{w}_t - \alpha \nabla \ell(\mathbf{w}_t, \mathbf{x}_i)$$

Per-sample gradient is equivalent to full gradient in expectation!

$$\mathbb{E}[\nabla \ell(\mathbf{w}_t, \mathbf{x}_i)] = \frac{1}{n} \sum_{i=1}^{n} \nabla \ell(\mathbf{w}_t, \mathbf{x}_i) = \nabla \mathcal{L}(\mathbf{w}_t)$$

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Stochastic Gradient Descent (SGD)

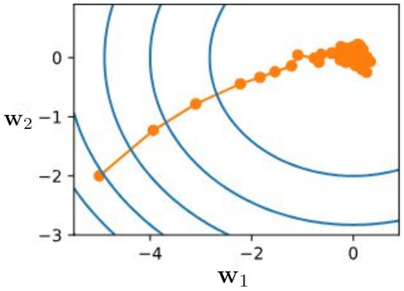
$$\mathbf{w}_{t+1} = \mathbf{w}_t - \alpha \nabla \mathcal{L}(\mathbf{w}_t)$$

Select **1** example randomly each time

$$\mathbf{w}_{t+1} = \mathbf{w}_t - \alpha \nabla \ell(\mathbf{w}_t, \mathbf{x}_i)$$

Trade off convergence*!*

Per-sample gradients not necessarily points to the local minimum, introducing a ***noise ball****...*



Stochastic Gradient Descent (SGD)

$$\mathbf{w}_{t+1} = \mathbf{w}_t - \alpha \nabla \mathcal{L}(\mathbf{w}_t)$$

Select **1** example randomly each time

$$\mathbf{w}_{t+1} = \mathbf{w}_t - \alpha \nabla \ell(\mathbf{w}_t, \mathbf{x}_i)$$

Select a batch $\mathcal{B}_t$ of examples randomly each time, with *batch size* b

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Minibatch SGD

$$\mathbf{w}_{t+1} = \mathbf{w}_t - \alpha \nabla \mathcal{L}(\mathbf{w}_t)$$

Select **1** example randomly each time

$$\mathbf{w}_{t+1} = \mathbf{w}_t - \alpha \nabla \ell(\mathbf{w}_t, \mathbf{x}_i)$$

Select a batch $\mathcal{B}_t$ of examples randomly each time, with *batch size* b

$$\mathbf{w}_{t+1} = \mathbf{w}_t - \alpha \cdot \frac{1}{b} \sum_{i \in \mathcal{B}_t} \nabla \ell(\mathbf{w}_t, \mathbf{x}_i)$$

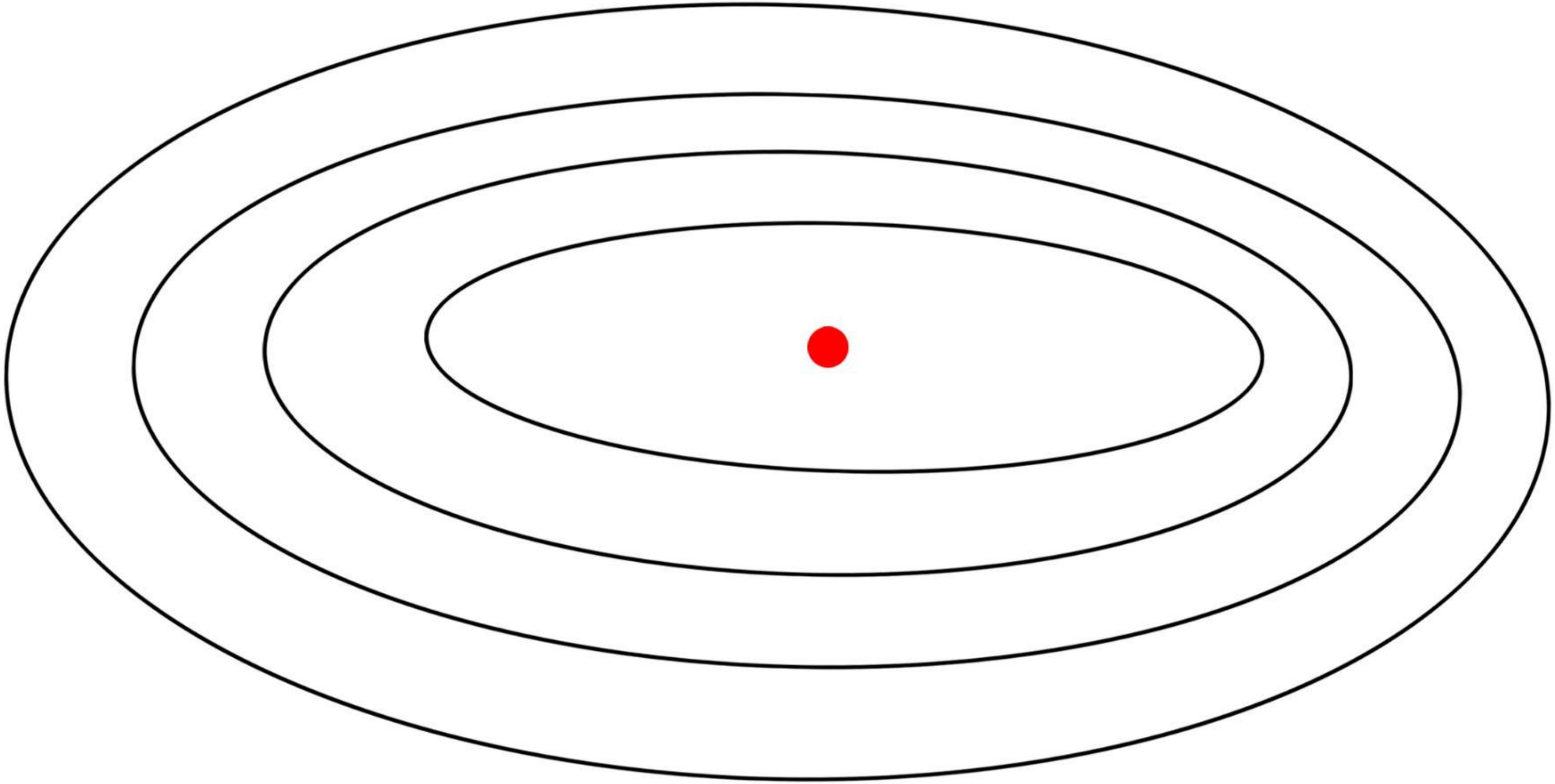
Minibatch SGD

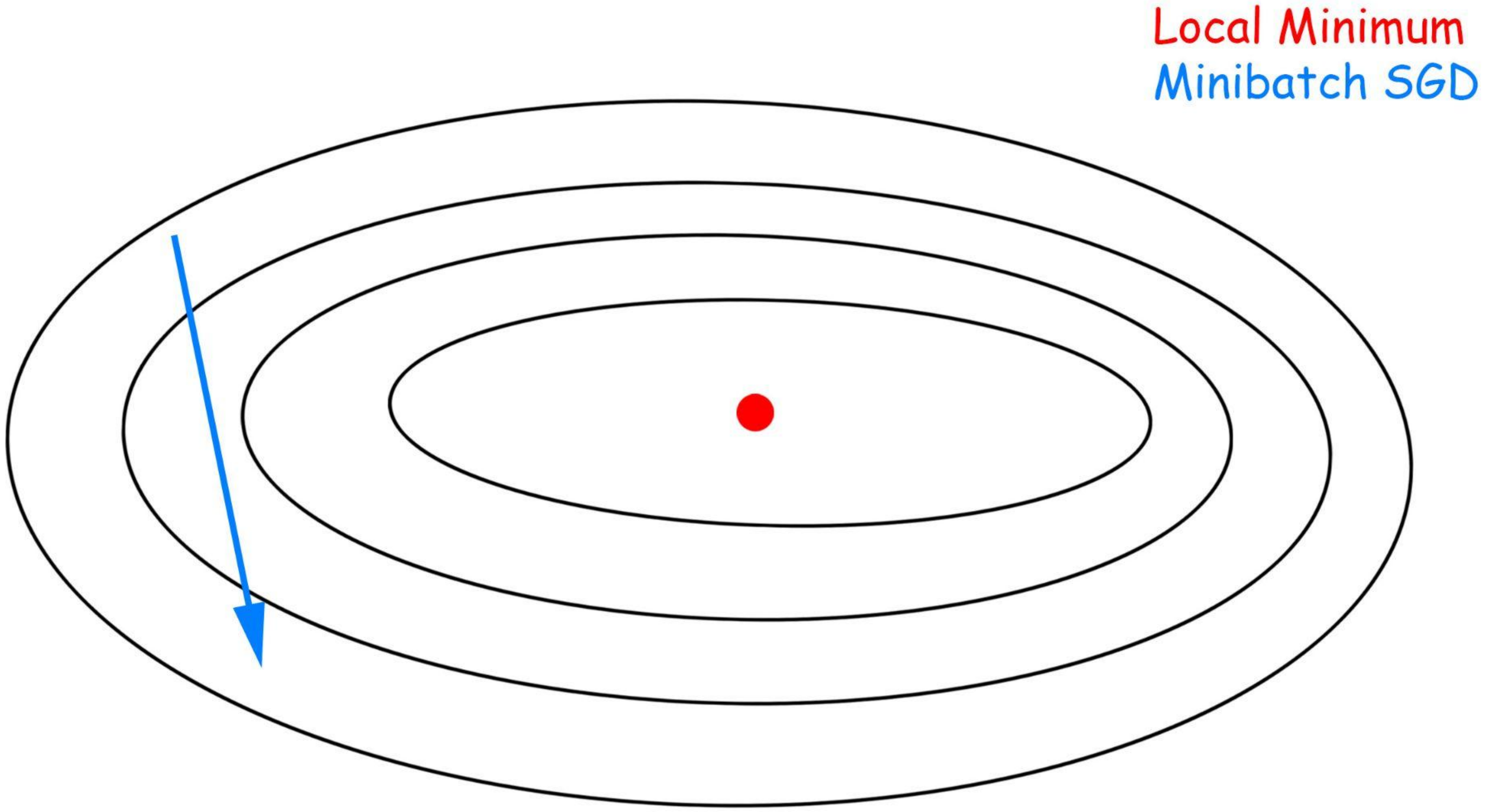
Best of both worlds: Computational and Statistical!

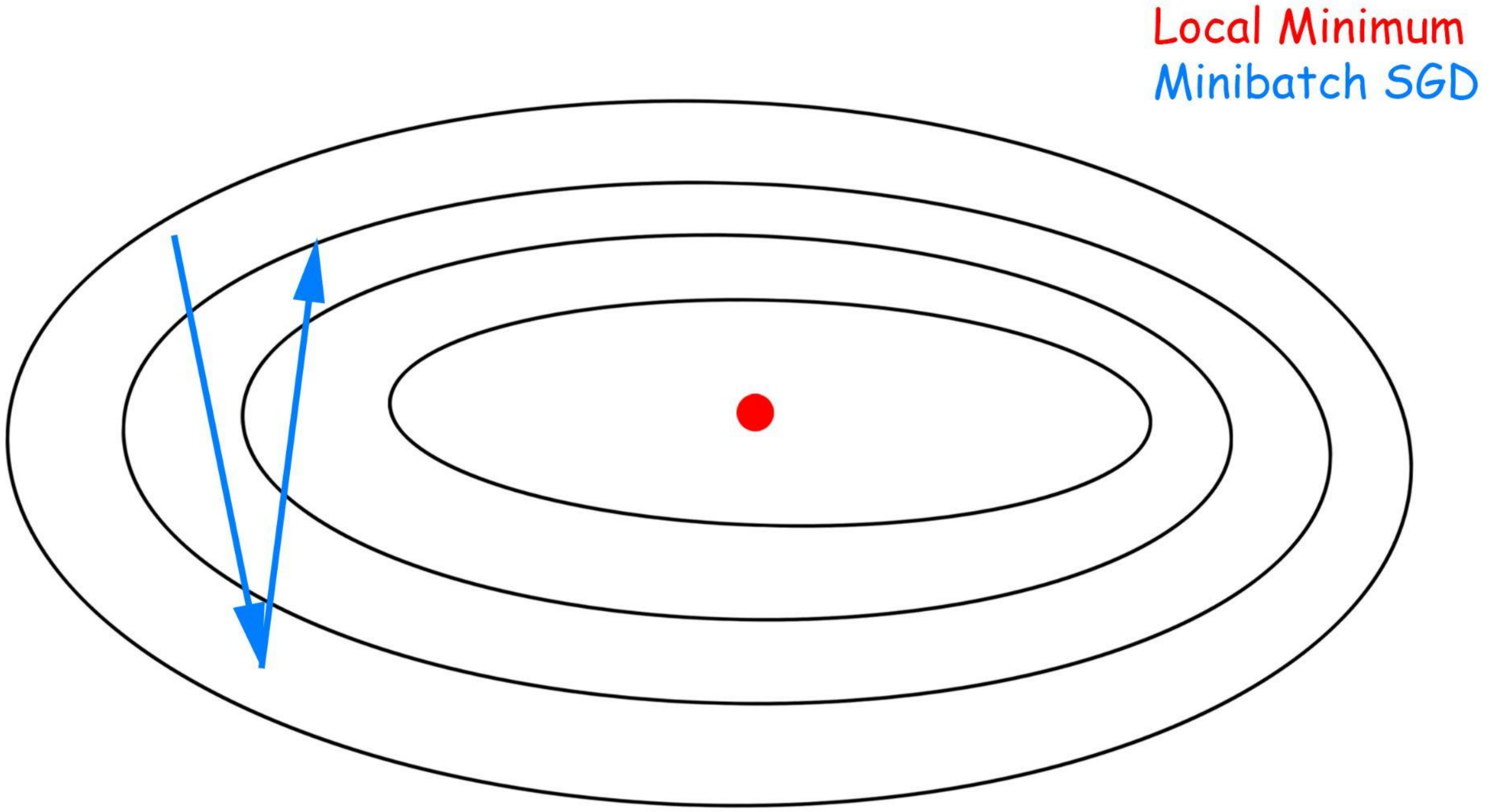
$$\mathbf{w}_{t+1} = \mathbf{w}_t - \alpha \cdot \frac{1}{b} \sum_{i \in \mathcal{B}_t} \nabla \ell(\mathbf{w}_t, \mathbf{x}_i)$$

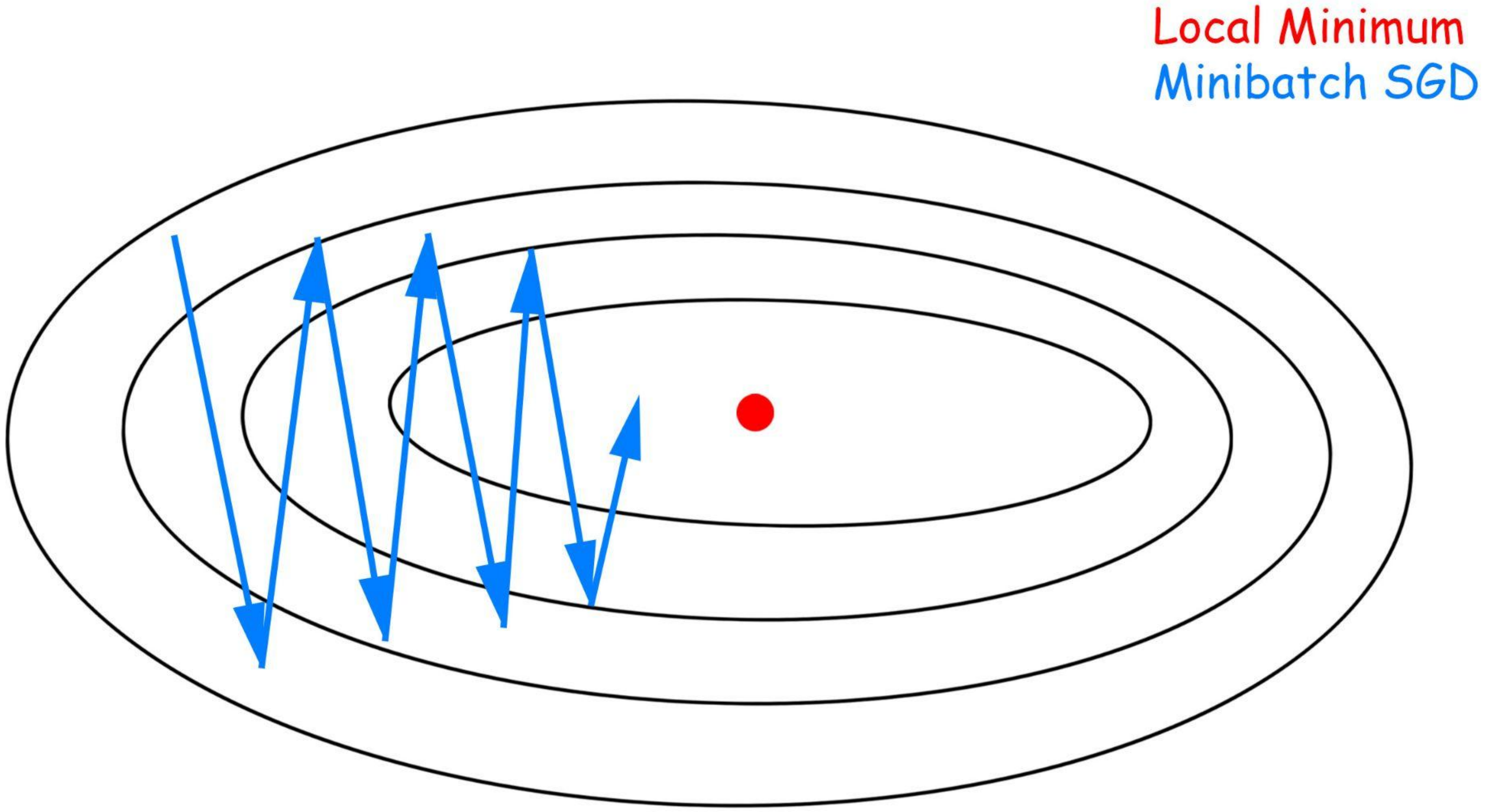
Let's look at an example!

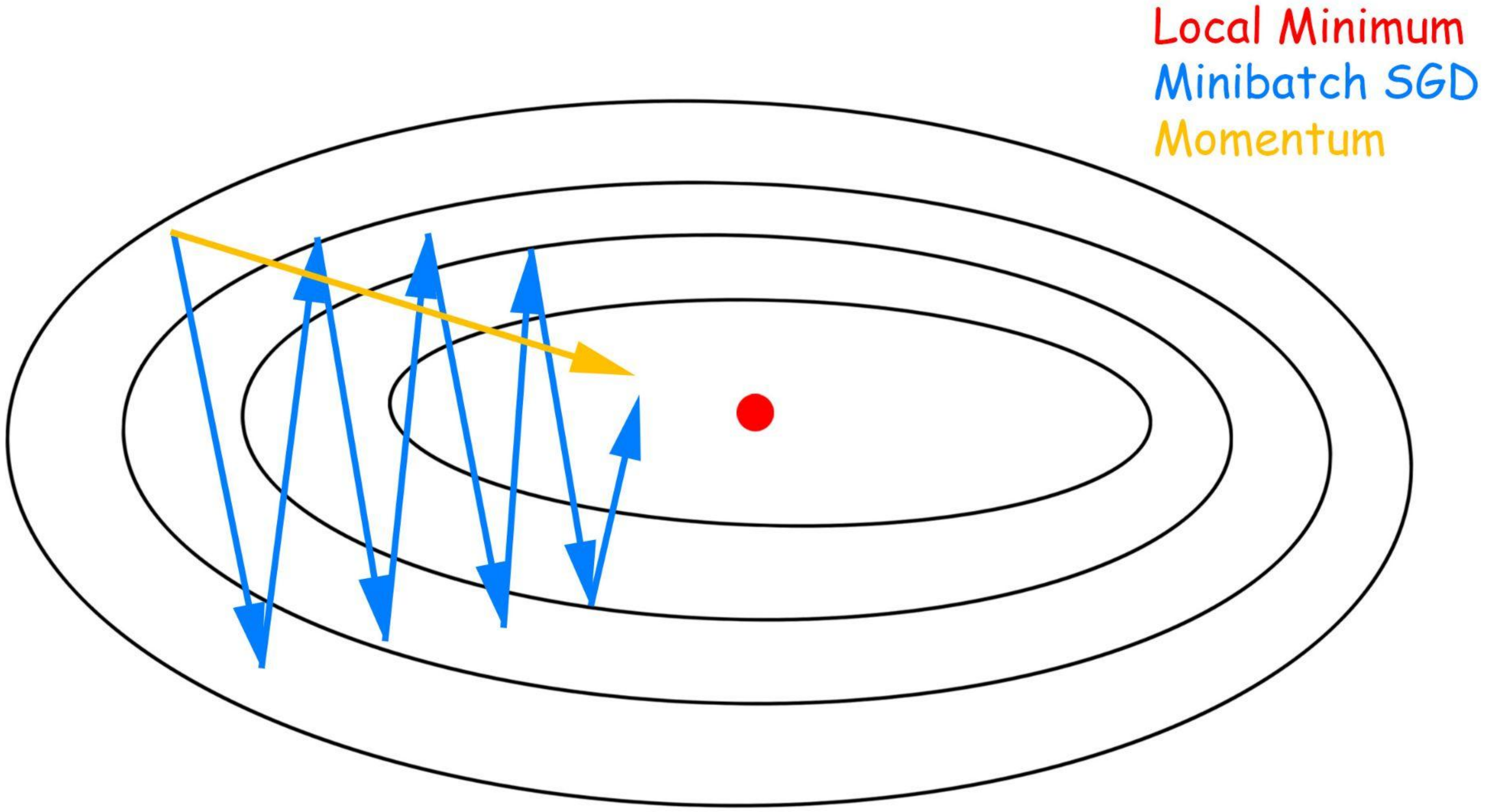
Local Minimum




Local Minimum
Minibatch SGD


Local Minimum
Minibatch SGD


Local Minimum
Minibatch SGD


Local Minimum
Minibatch SGD
Momentum

SGD with Momentum (Polyak, 1964)

*Compute an **Exponentially Weighted Moving Average (EWMA)** of the gradients as **momentum** and use that to update the weight instead.*

SGD with Momentum (Polyak, 1964)

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SGD with Momentum (Polyak, 1964)

*Compute an **Exponentially Weighted Moving Average (EWMA)** of the gradients as **momentum** and use that to update the weight instead.*

SGD Update Rule

$$\mathbf{w}_{t+1} = \mathbf{w}_t - \alpha \nabla \ell(\mathbf{w}_t, \mathbf{x}_i) \longrightarrow \begin{aligned} \mathbf{m}_{t+1} &= \mu \mathbf{m}_t - \alpha \nabla l(\mathbf{w}_t; \mathbf{x}_i) \\ \mathbf{w}_{t+1} &= \mathbf{w}_t + \mathbf{m}_{t+1} \end{aligned}$$

where $\mu \in [0, 1]$ is the momentum coefficient.

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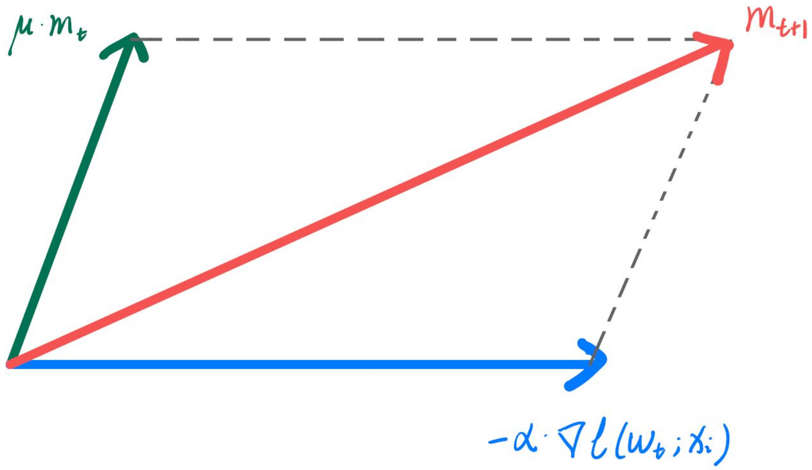
SGD with Momentum (Polyak, 1964)

*Compute an **Exponentially Weighted Moving Average (EWMA)** of the gradients as **momentum** and use that to update the weight instead.*



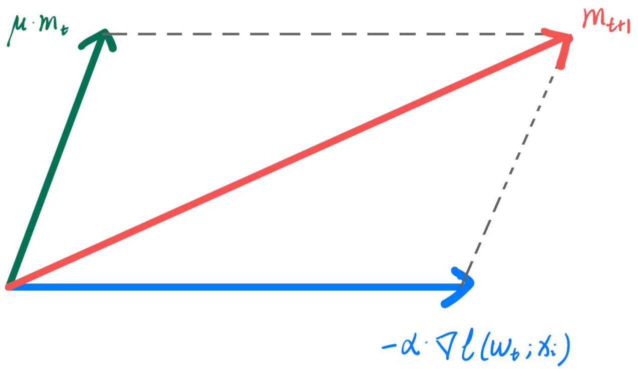
$$\mathbf{m}_{t+1} = \mu \mathbf{m}_t - \alpha \nabla l(\mathbf{w}_t; \mathbf{x}_i)$$
$$\mathbf{w}_{t+1} = \mathbf{w}_t + \mathbf{m}_{t+1}$$

where $\mu \in [0, 1]$ is the momentum coefficient.

SGD with Momentum

Compute an ***Exponentially Weighted Moving Average (EWMA)*** *of the gradients as* ***momentum*** *and use that to update the weight instead.*

$$\mathbf{m}_{t+1} = \mu \mathbf{m}_t - \alpha \nabla l(\mathbf{w}_t; \mathbf{x}_i)$$
$$\mathbf{w}_{t+1} = \mathbf{w}_t + \mathbf{m}_{t+1}$$



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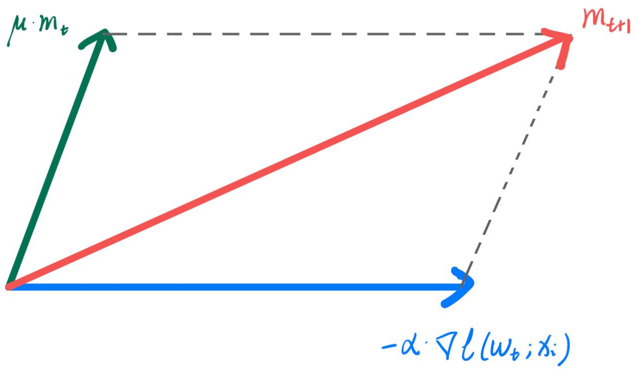
SGD with Momentum

*Compute an **Exponentially Weighted Moving Average (EWMA)** of the gradients as **momentum** and use that to update the weight instead.*

$$\mathbf{g}_t = \nabla l(\mathbf{w}_t; \mathbf{x}_i)$$
$$\mathbf{m}_{t+1} = \mu \mathbf{m}_t - \alpha \mathbf{g}_t$$
$$\mathbf{w}_{t+1} = \mathbf{w}_t + \mathbf{m}_{t+1}$$



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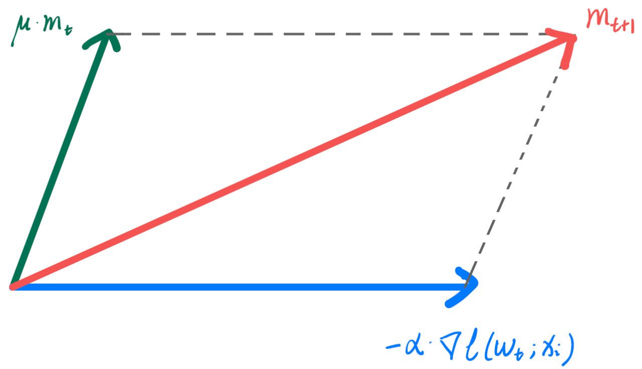
SGD with Momentum

*Compute an **Exponentially Weighted Moving Average (EWMA)** of the gradients as **momentum** and use that to update the weight instead.*

$$\mathbf{g}_t = \nabla l(\mathbf{w}_t; \mathbf{x}_i)$$
$$\mathbf{m}_{t+1} = \mu \mathbf{m}_t - \alpha \mathbf{g}_t$$
$$\mathbf{w}_{t+1} = \mathbf{w}_t + \mu \mathbf{m}_t - \alpha \mathbf{g}_t$$



Cornell Bowers C·IS

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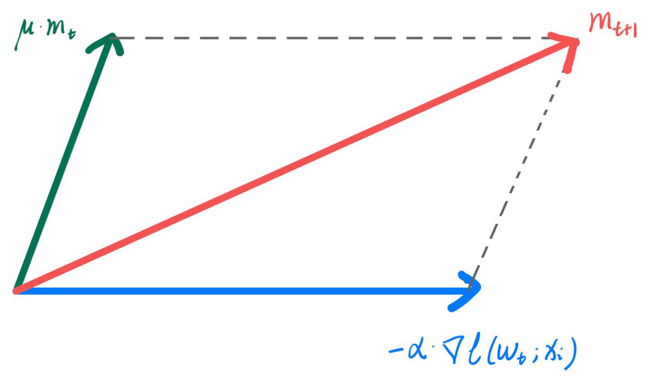
$$
\begin{aligned}
\mathbf{g}_t &= \nabla l(\mathbf{w}_t; \mathbf{x}_i) \\
\mathbf{m}_{t+1} &= \mu \mathbf{m}_t - \alpha \mathbf{g}_t \\
\mathbf{w}_{t+1} &= \mathbf{w}_t + \mu \mathbf{m}_t - \alpha \mathbf{g}_t \\
&= \mathbf{w}_t + \mu(\mu \mathbf{m}_{t-1} - \alpha \mathbf{g}_{t-1}) - \alpha \mathbf{g}_t
\end{aligned}
$$



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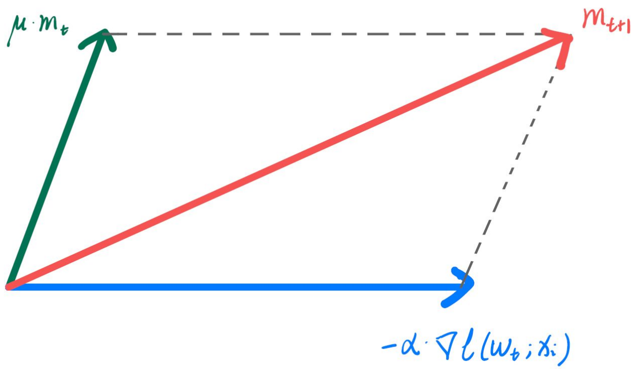

$$
\begin{aligned}
\mathbf{g}_t &= \nabla l(\mathbf{w}_t; \mathbf{x}_i) \\
\mathbf{m}_{t+1} &= \mu \mathbf{m}_t - \alpha \mathbf{g}_t \\
\mathbf{w}_{t+1} &= \mathbf{w}_t + \mu \mathbf{m}_t - \alpha \mathbf{g}_t \\
&= \mathbf{w}_t + \mu(\mu \mathbf{m}_{t-1} - \alpha \mathbf{g}_{t-1}) - \alpha \mathbf{g}_t \\
&= \mathbf{w}_t + \mu(\mu(\mu \mathbf{m}_{t-2} - \alpha \mathbf{g}_{t-2}) - \alpha \mathbf{g}_{t-1}) - \alpha \mathbf{g}_t \\
&= \mathbf{w}_t - \alpha \mathbf{g}_t - \mu \alpha \mathbf{g}_{t-1} - \mu^2 \alpha \mathbf{g}_{t-2} - \mu^3 \alpha \mathbf{g}_{t-3} - \ldots
\end{aligned}
$$

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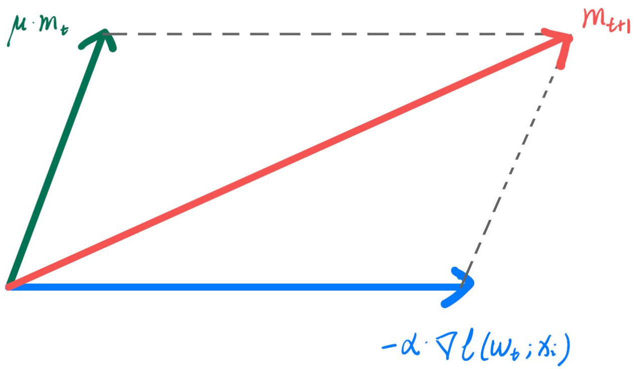
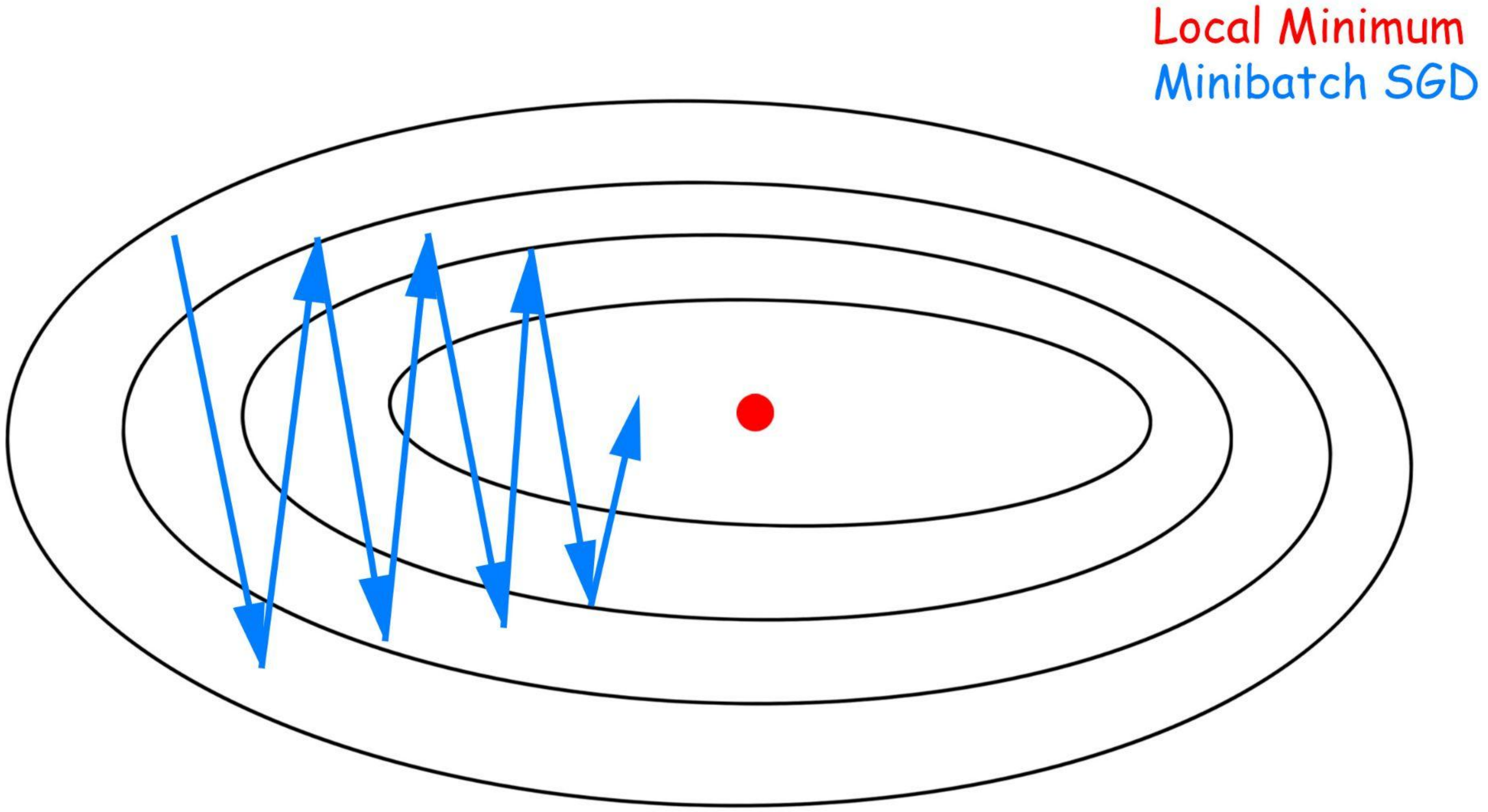
SGD with Momentum

*Compute an **Exponentially Weighted Moving Average (EWMA)** of the gradients as **momentum** and use that to update the weight instead.*

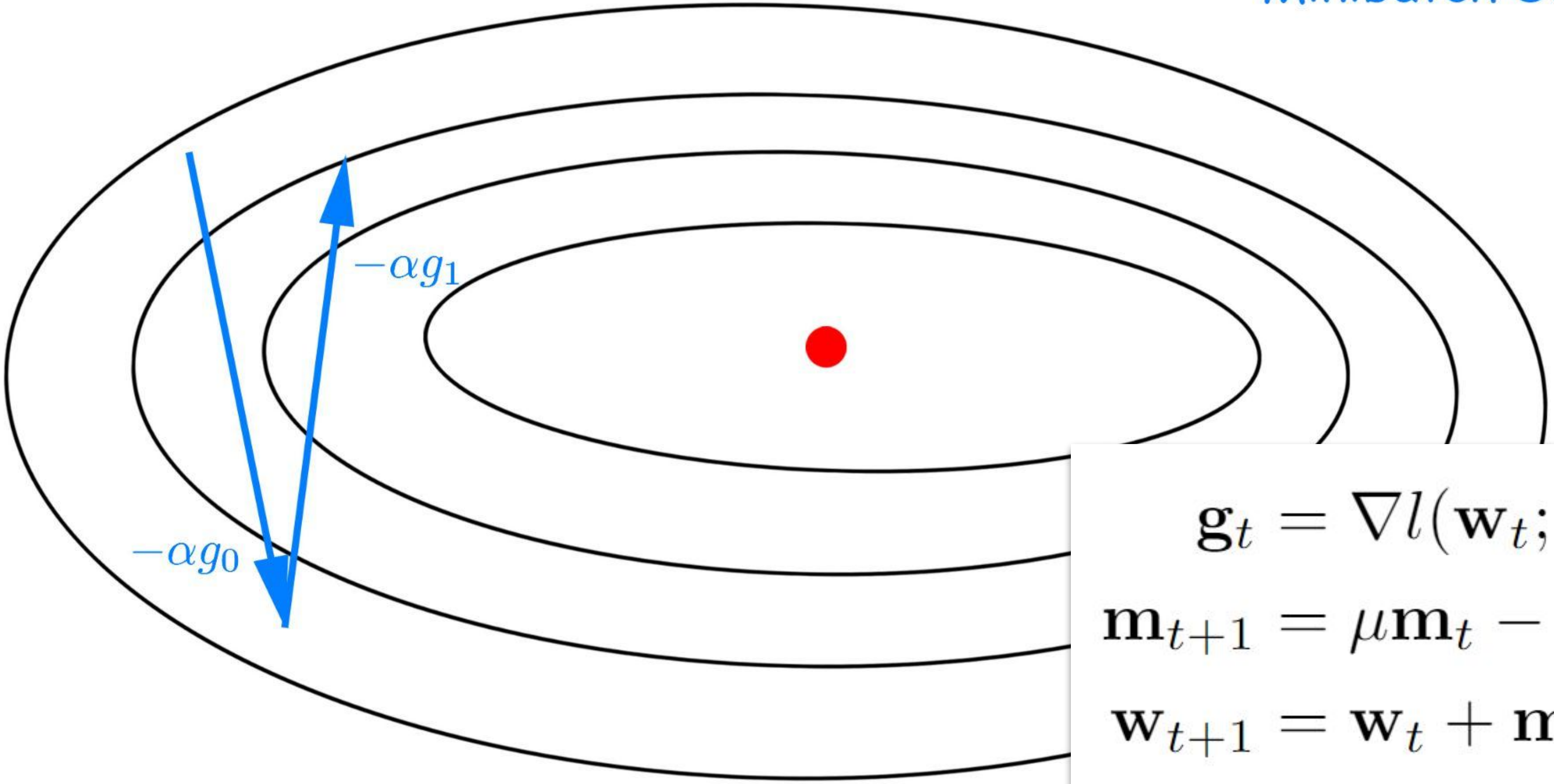
$$
\begin{aligned}
\mathbf{g}_t &= \nabla l(\mathbf{w}_t; \mathbf{x}_i) \\
\mathbf{m}_{t+1} &= \mu \mathbf{m}_t - \alpha \mathbf{g}_t \\
\mathbf{w}_{t+1} &= \mathbf{w}_t + \mu \mathbf{m}_t - \alpha \mathbf{g}_t \\
&= \mathbf{w}_t + \mu(\mu \mathbf{m}_{t-1} - \alpha \mathbf{g}_{t-1}) - \alpha \mathbf{g}_t \\
&= \mathbf{w}_t + \mu(\mu(\mu \mathbf{m}_{t-2} - \alpha \mathbf{g}_{t-2}) - \alpha \mathbf{g}_{t-1}) - \alpha \mathbf{g}_t \\
&= \mathbf{w}_t - \alpha \mathbf{g}_t - \mu \alpha \mathbf{g}_{t-1} - \mu^2 \alpha \mathbf{g}_{t-2} - \mu^3 \alpha \mathbf{g}_{t-3} - \dots \\
&= \mathbf{w}_t - \alpha \sum_{i=0}^{t} \mu^i \mathbf{g}_{t-i}
\end{aligned}
$$




Local Minimum
Minibatch SGD

Local Minimum

Minibatch SGD



$$\mathbf{g}_t = \nabla l(\mathbf{w}_t; \mathbf{x}_i)$$

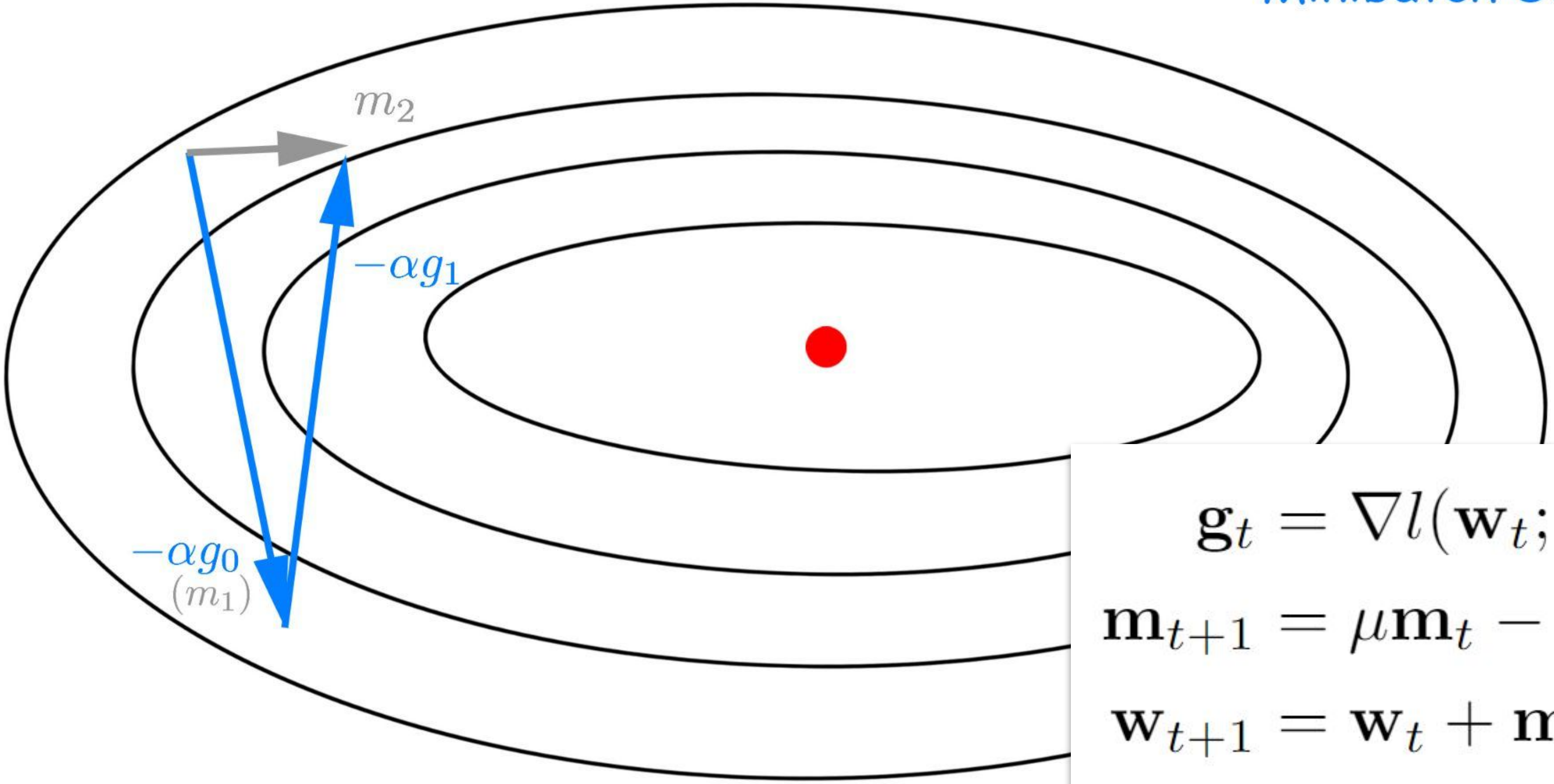
$$\mathbf{m}_{t+1} = \mu \mathbf{m}_t - \alpha \mathbf{g}_t$$

$$\mathbf{w}_{t+1} = \mathbf{w}_t + \mathbf{m}_{t+1}$$

$$\mathbf{m}_2 = \mu \mathbf{m}_1 - \alpha \mathbf{g}_1$$

Local Minimum

Minibatch SGD



$$\mathbf{g}_t = \nabla l(\mathbf{w}_t; \mathbf{x}_i)$$

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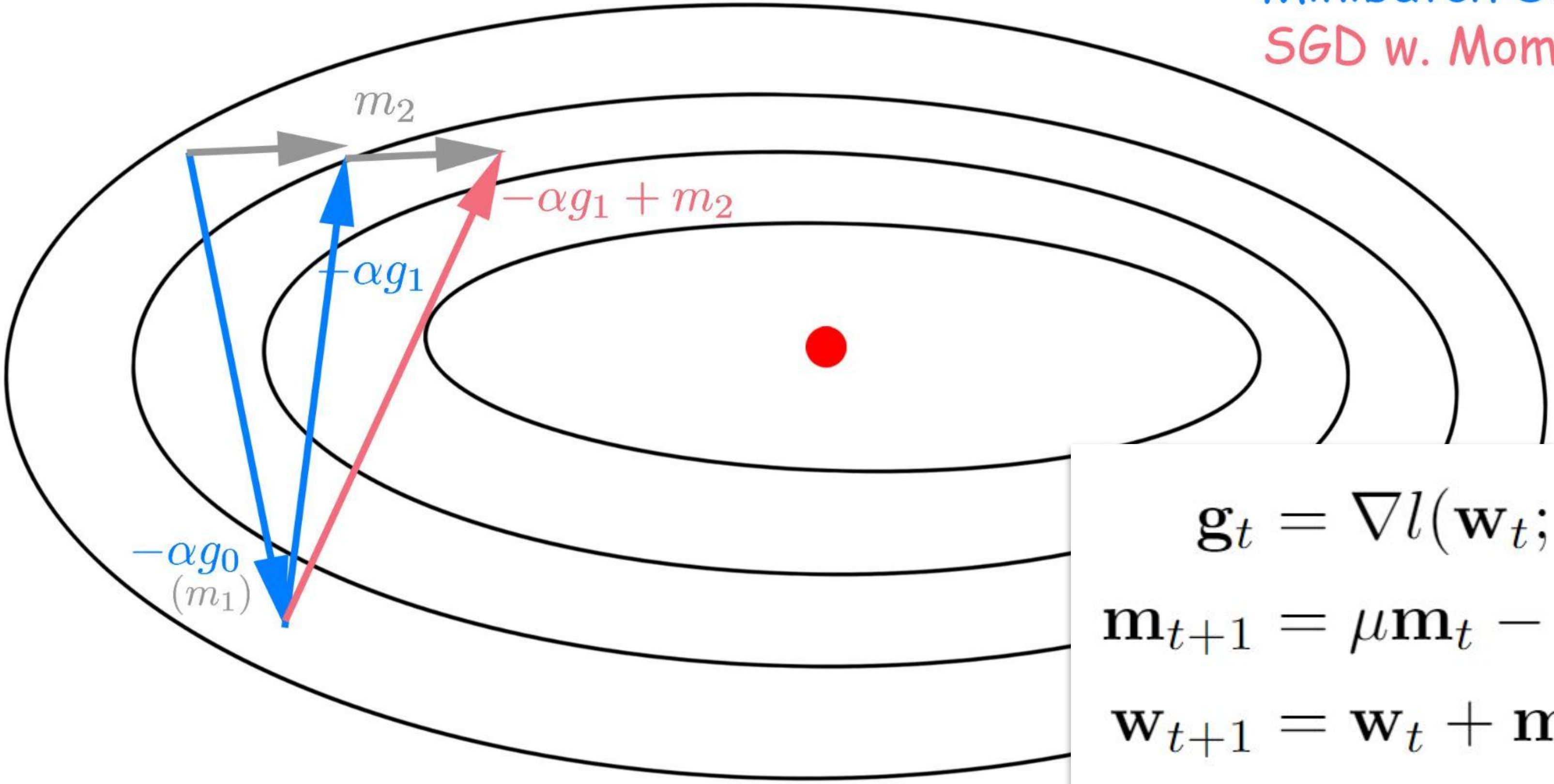
Local Minimum
Minibatch SGD
SGD w. Momentum



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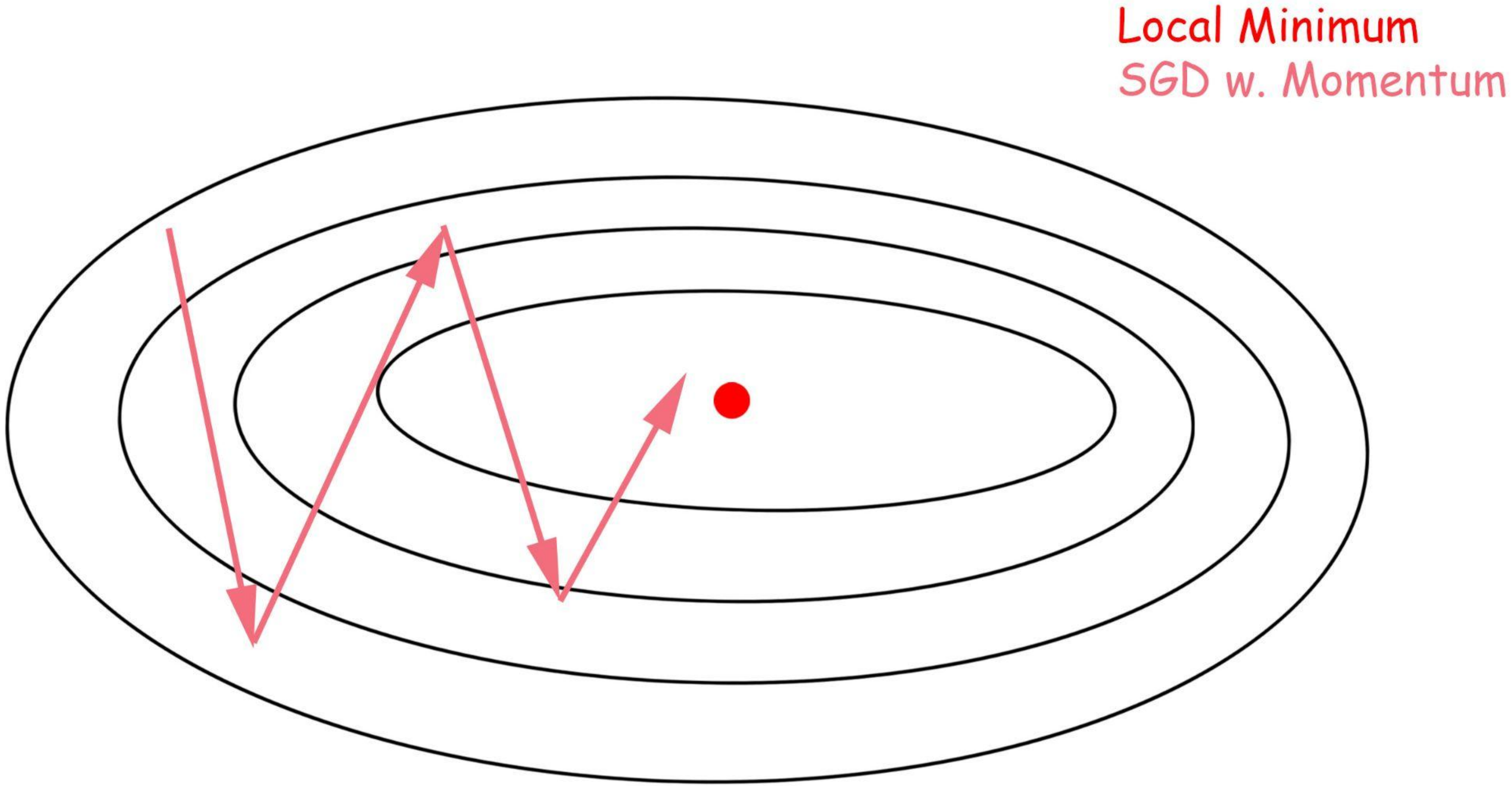
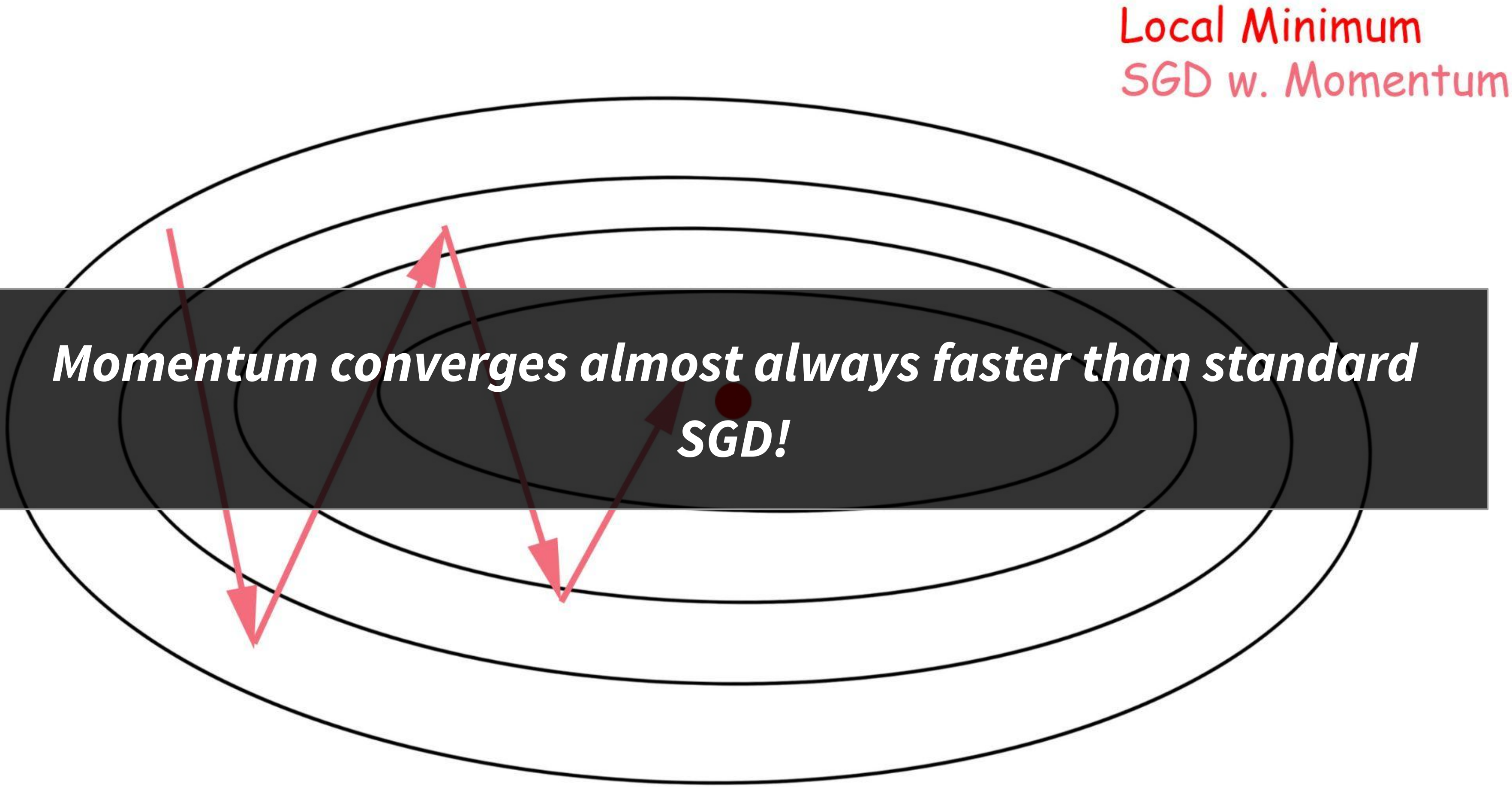

Local Minimum
SGD w. Momentum



Momentum converges almost always faster than standard SGD!

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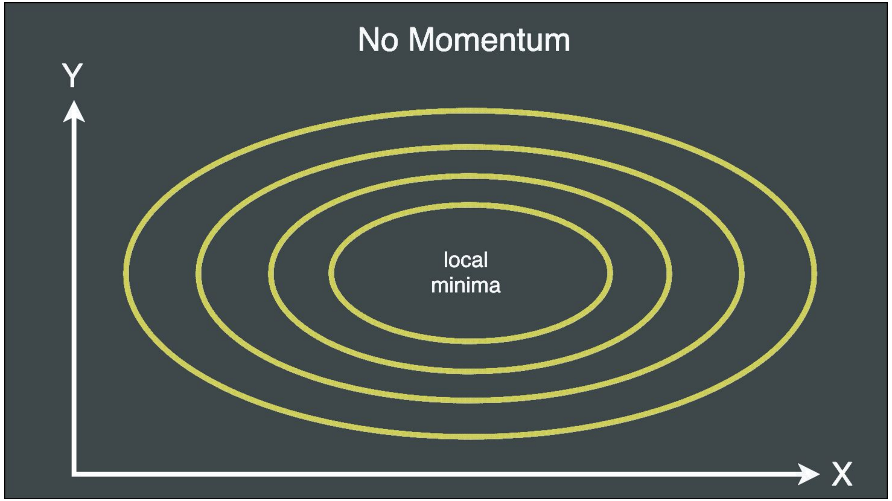

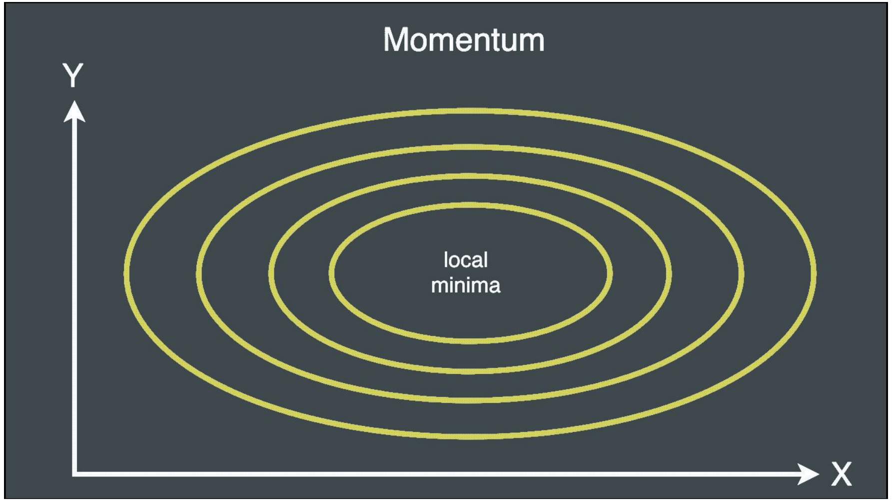

Momentum converges almost always faster than standard SGD!

Quick Recap

Gradient Descent

$$\mathbf{w}_{t+1} = \mathbf{w}_t - \alpha \cdot \frac{1}{n} \sum_{i=1}^{n} \nabla \ell(\mathbf{w}_t, \mathbf{x}_i)$$

Stochastic Gradient Descent

$$\mathbf{w}_{t+1} = \mathbf{w}_t - \alpha \nabla \ell(\mathbf{w}_t, \mathbf{x}_i)$$

Minibatch SGD

$$\mathbf{w}_{t+1} = \mathbf{w}_t - \alpha \cdot \frac{1}{b} \sum_{i \in \mathcal{B}_t} \nabla \ell(\mathbf{w}_t, \mathbf{x}_i)$$

SGD w. Momentum

$$m_{t+1} = \mu m_t - \alpha \nabla l(w_t; x_i)$$

$$w_{t+1} = w_t + m_{t+1}$$

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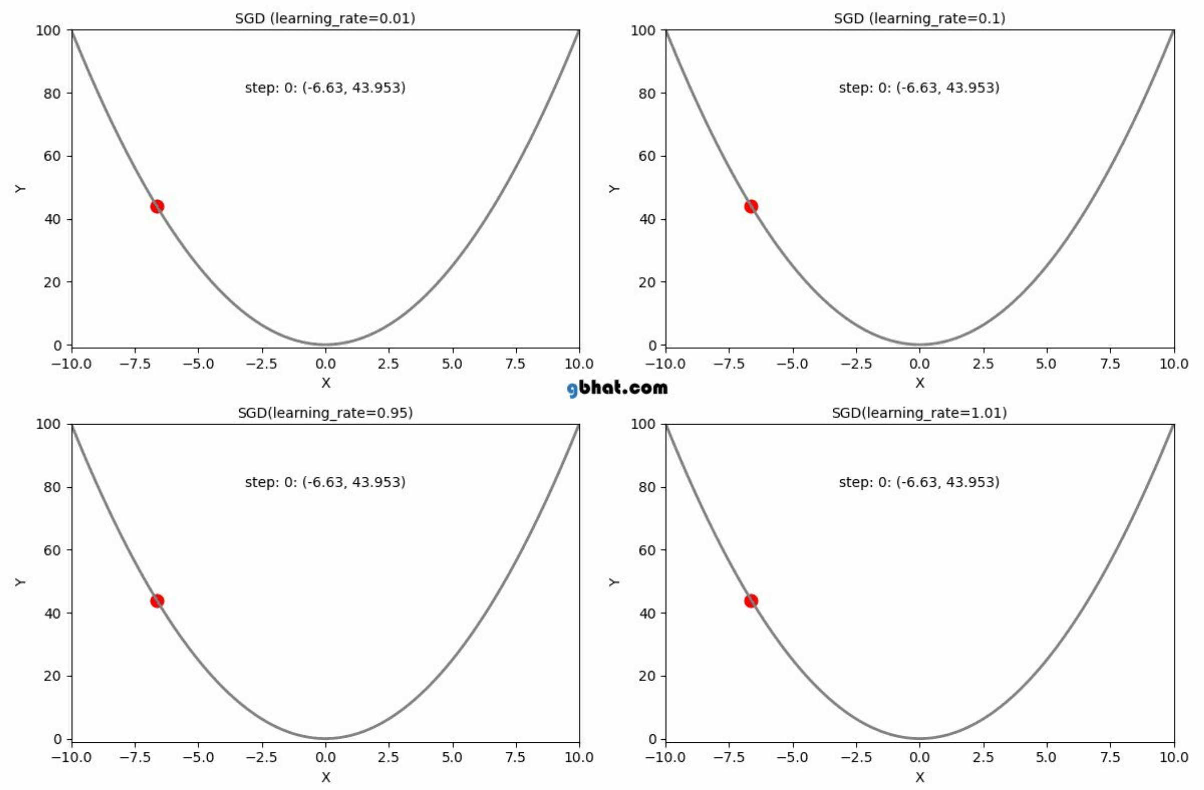
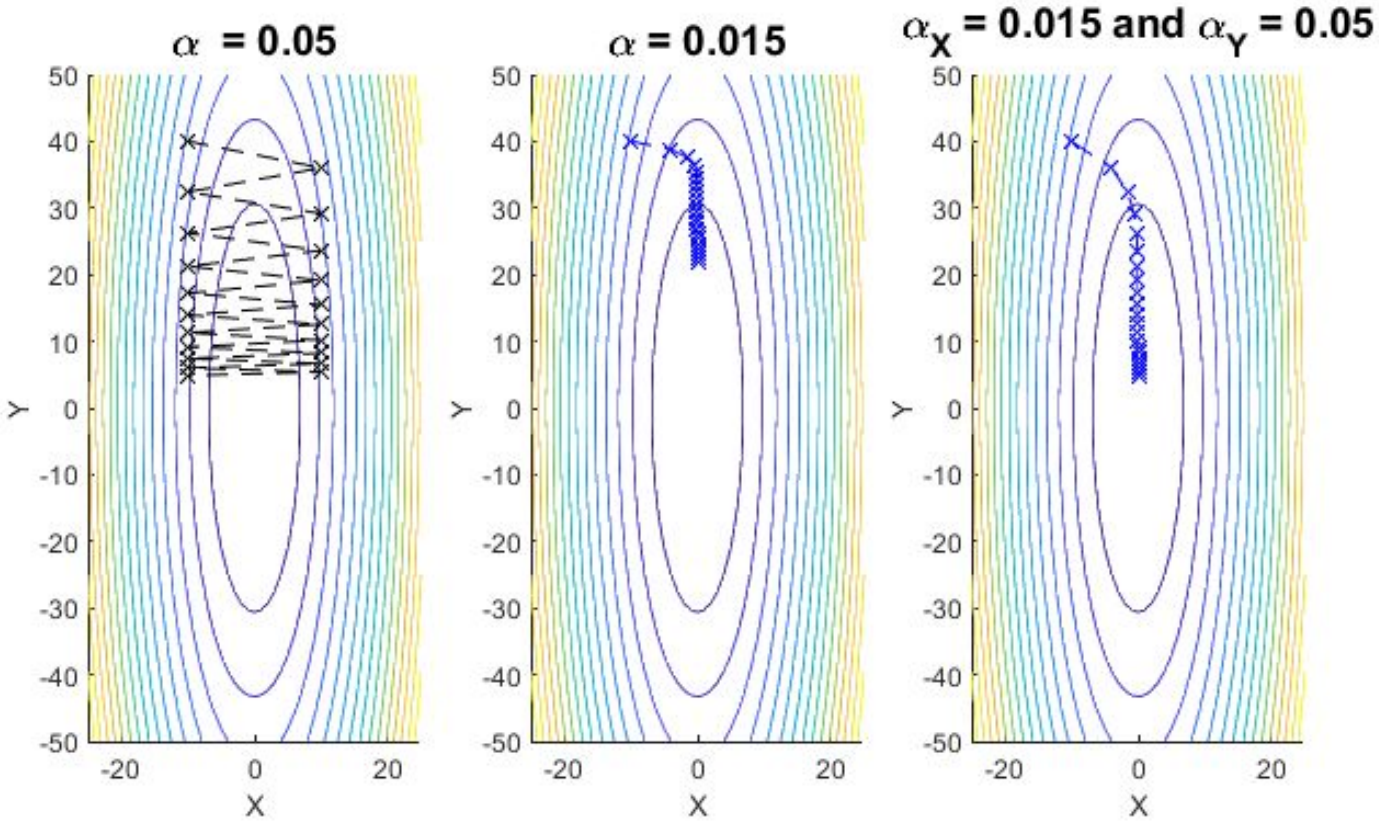
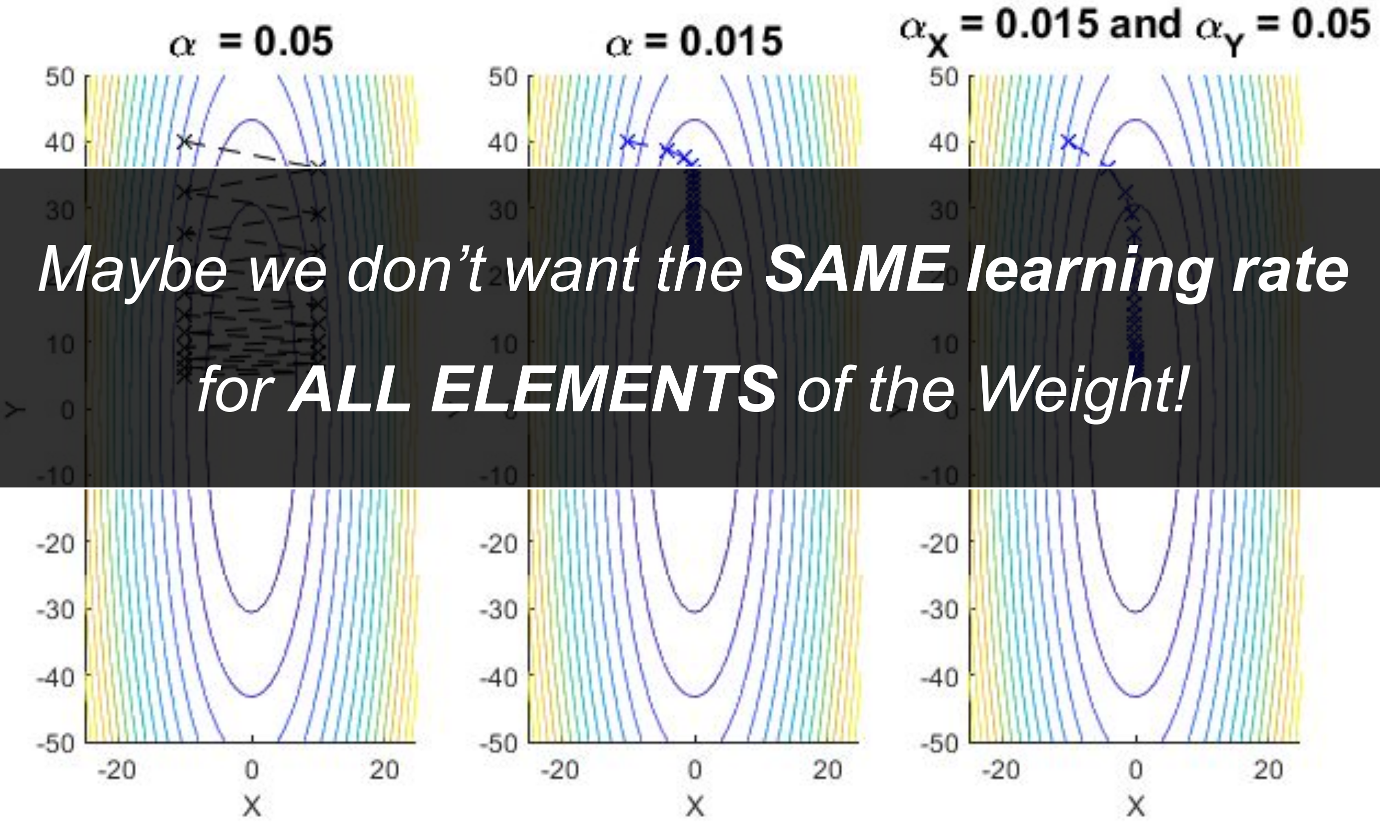
Importance of Learning Rate



Another example



Adaptive Learning Rate



*Maybe we don't want the **SAME learning rate***

*for **ALL ELEMENTS** of the Weight!*

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Adaptive Optimizers

Different Learning Rate *for* ***each element*** *of the* ***Model Weights!***

AdaGrad (Duchi et al. 2011)

More updates -> more decay

- Handle sparse gradients well
  - *Sparse: The vector has 0 in most of the entries*

Element-wise product

$$\mathbf{w}_{t+1} = \mathbf{w}_t - \alpha \nabla \mathcal{L}(\mathbf{w}_t)$$

SGD

$$\mathbf{v}_{t+1} = \mathbf{v}_t + \mathbf{g}_t^2$$

$$\mathbf{w}_{t+1} = \mathbf{w}_t - \frac{\alpha}{\sqrt{\mathbf{v}_{t+1} + \epsilon}} \odot \mathbf{g}_t$$

Adagrad

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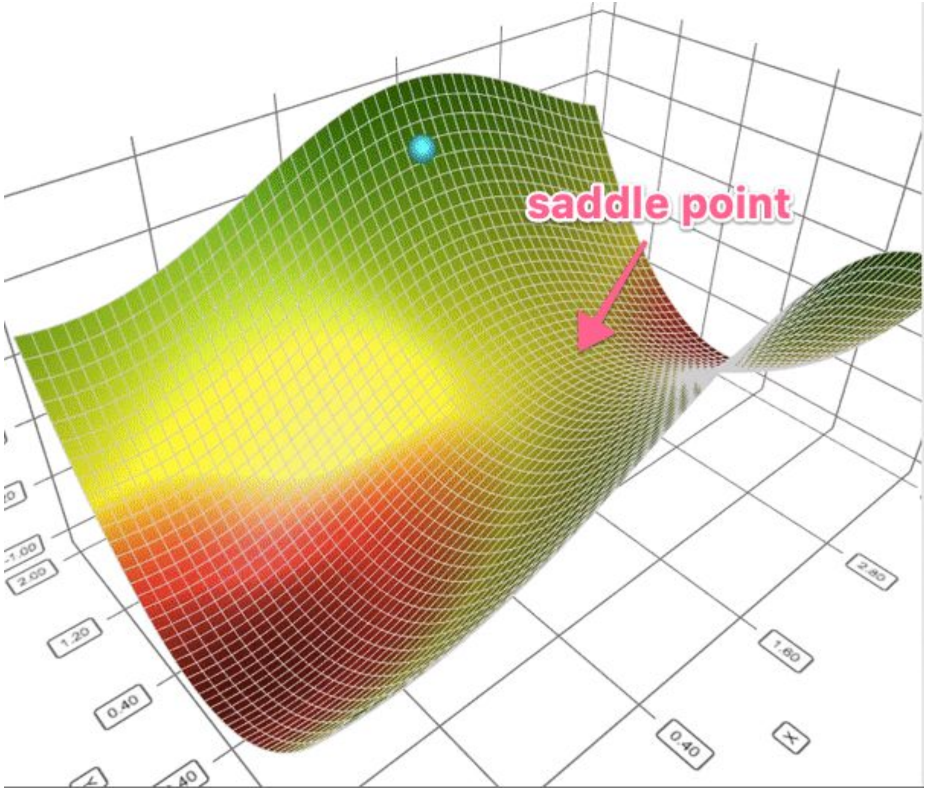

Gradient Descent
AdaGrad

AdaGrad (Duchi et al. 2011)

More updates → more decay

- Handle sparse gradients well
  - *Sparse: The vector has 0 in most of the entries*

$$\mathbf{w}_{t+1} = \mathbf{w}_t - \alpha \nabla \mathcal{L}(\mathbf{w}_t)$$

GD

Element-wise product

$$\mathbf{v}_{t+1} = \mathbf{v}_t + \mathbf{g}_t^2$$

$$\mathbf{w}_{t+1} = \mathbf{w}_t - \frac{\alpha}{\sqrt{\mathbf{v}_{t+1} + \epsilon}} \odot \mathbf{g}_t$$

Adagrad

Exercise:

What's could be wrong with this optimizator?

(What would happen to the denominator.)

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AdaGrad (Duchi et al. 2011)

More updates → more decay

- Handle sparse gradients well
  - *Sparse: The vector has 0 in most of the entries*

$$\boxed{\mathbf{w}_{t+1} = \mathbf{w}_t - \alpha \nabla \mathcal{L}(\mathbf{w}_t)}$$

GD

Element-wise product

$$\mathbf{v}_{t+1} = \mathbf{v}_t + \mathbf{g}_t^2$$

$$\mathbf{w}_{t+1} = \mathbf{w}_t - \frac{\alpha}{\sqrt{\mathbf{v}_{t+1} + \epsilon}} \odot \mathbf{g}_t$$

Adagrad

***Issue**: decays too aggressively!*

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RMSProp (Graves, 2013)

Keep an **exponential moving average** of the squared gradient for each element

$$\mathbf{v}_{t+1} = \mathbf{v}_t + \mathbf{g}_t^2$$
$$\mathbf{w}_{t+1} = \mathbf{w}_t - \frac{\alpha}{\sqrt{\mathbf{v}_{t+1} + \epsilon}} \odot \mathbf{g}_t$$

Adagrad

$$\mathbf{v}_{t+1} = \boxed{\beta}\mathbf{v}_t + \boxed{(1-\beta)}\mathbf{g}_t^2$$
$$\mathbf{w}_{t+1} = \mathbf{w}_t - \frac{\alpha}{\sqrt{\mathbf{v}_{t+1} + \epsilon}} \odot \mathbf{g}_t$$

RmsProp

where $\beta \in [0, 1]$ the exponential moving average constant.

$$\mathbf{m}_{t+1} = \mu \mathbf{m}_t - \alpha \nabla l(\mathbf{w}_t; \mathbf{x}_i)$$
$$\mathbf{w}_{t+1} = \mathbf{w}_t + \mathbf{m}_{t+1}$$

Momentum

$$\mathbf{v}_{t+1} = \beta \mathbf{v}_t + (1-\beta)\mathbf{g}_t^2$$
$$\mathbf{w}_{t+1} = \mathbf{w}_t - \frac{\alpha}{\sqrt{\mathbf{v}_{t+1} + \epsilon}} \odot \mathbf{g}_t$$

RMSProp

$$\boxed{\begin{aligned} \mathbf{m}_{t+1} &= \mu \mathbf{m}_t - \alpha \nabla l(\mathbf{w}_t; \mathbf{x}_i) \\ \mathbf{w}_{t+1} &= \mathbf{w}_t + \mathbf{m}_{t+1} \end{aligned}}$$

Momentum

$$\boxed{\begin{aligned} \mathbf{v}_{t+1} &= \beta \mathbf{v}_t + (1-\beta)\mathbf{g}_t^2 \\ \mathbf{w}_{t+1} &= \mathbf{w}_t - \frac{\alpha}{\sqrt{\mathbf{v}_{t+1} + \epsilon}} \odot \mathbf{g}_t \end{aligned}}$$

RMSProp

$$\mathbf{v}_{t+1} = \beta \mathbf{v}_t + (1-\beta)\mathbf{g}_t^2$$

$$\mathbf{w}_{t+1} = \mathbf{w}_t - \frac{\alpha}{\boxed{\sqrt{\mathbf{v}_{t+1} + \epsilon}}} \odot \mathbf{g}_t$$

RMSProp

$$\mathbf{v}_{t+1} = \beta_2 \mathbf{v}_t + (1-\beta_2)\mathbf{g}_t^2$$

$$\mathbf{w}_{t+1} = \mathbf{w}_t - \frac{\alpha}{\boxed{\sqrt{\widehat{\mathbf{v}}_{t+1} + \epsilon}}} \odot \widehat{\mathbf{m}}_{t+1}$$

ADAM

(**Ada**ptive **M**oment Estimate)

$$\mathbf{m}_{t+1} = \mu \mathbf{m}_t - \alpha \nabla l(\mathbf{w}_t; \mathbf{x}_i)$$
$$\mathbf{w}_{t+1} = \mathbf{w}_t + \mathbf{m}_{t+1}$$

Momentum

$$\mathbf{v}_{t+1} = \beta \mathbf{v}_t + (1-\beta)\mathbf{g}_t^2$$
$$\mathbf{w}_{t+1} = \mathbf{w}_t - \frac{\alpha}{\sqrt{\mathbf{v}_{t+1} + \epsilon}} \odot \mathbf{g}_t$$

RMSProp

$$\boxed{\mathbf{m}_{t+1} = \beta_1 \mathbf{m}_t + (1-\beta_1)\mathbf{g}_t}$$
$$\mathbf{v}_{t+1} = \beta_2 \mathbf{v}_t + (1-\beta_2)\mathbf{g}_t^2$$
$$\mathbf{w}_{t+1} = \mathbf{w}_t - \frac{\alpha}{\sqrt{\widehat{\mathbf{v}}_{t+1} + \epsilon}} \odot \widehat{\mathbf{m}}_{t+1}$$

ADAM
(**Ada**ptive **M**oment Estimate)

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$$\mathbb{E}[\widehat{\mathbf{m}}_{t+1}]$$

$$\mathbb{E}[\widehat{\mathbf{v}}_{t+1}]$$

$$\mathbf{m}_{t+1} = \beta_1 \mathbf{m}_t + (1-\beta_1)\mathbf{g}_t$$

$$\mathbf{v}_{t+1} = \beta_2 \mathbf{v}_t + (1-\beta_2)\mathbf{g}_t^2$$

$$\boxed{\widehat{\mathbf{m}}_{t+1}} = \frac{\mathbf{m}_{t+1}}{1-\beta_1^{t+1}}$$

$$\boxed{\widehat{\mathbf{v}}_{t+1}} = \frac{\mathbf{v}_{t+1}}{1-\beta_2^{t+1}}$$

$$\mathbf{w}_{t+1} = \mathbf{w}_t - \frac{\alpha}{\sqrt{\widehat{\mathbf{v}}_{t+1}} + \epsilon} \odot \widehat{\mathbf{m}}_{t+1}$$

ADAM

(**Ada**ptive **M**oment Estimate)

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Optimizers Recap

- Gradient Descent
  - *Vanilla, costly, but for best convergence rate*
- Stochastic Gradient Descent
  - *Simple, lightweight*
- **Mini-batch SGD**
  - *balanced between SGD and GD*
  - ***1st choice for small, simple models***

- SGD w. Momentum
  - *Faster, capable to jump out local minimum*

- AdaGrad
- RMSProp
- **ADAM**
  - **JUST USE ADAM IF YOU DON'T KNOW WHAT TO USE IN DEEP LEARNING**

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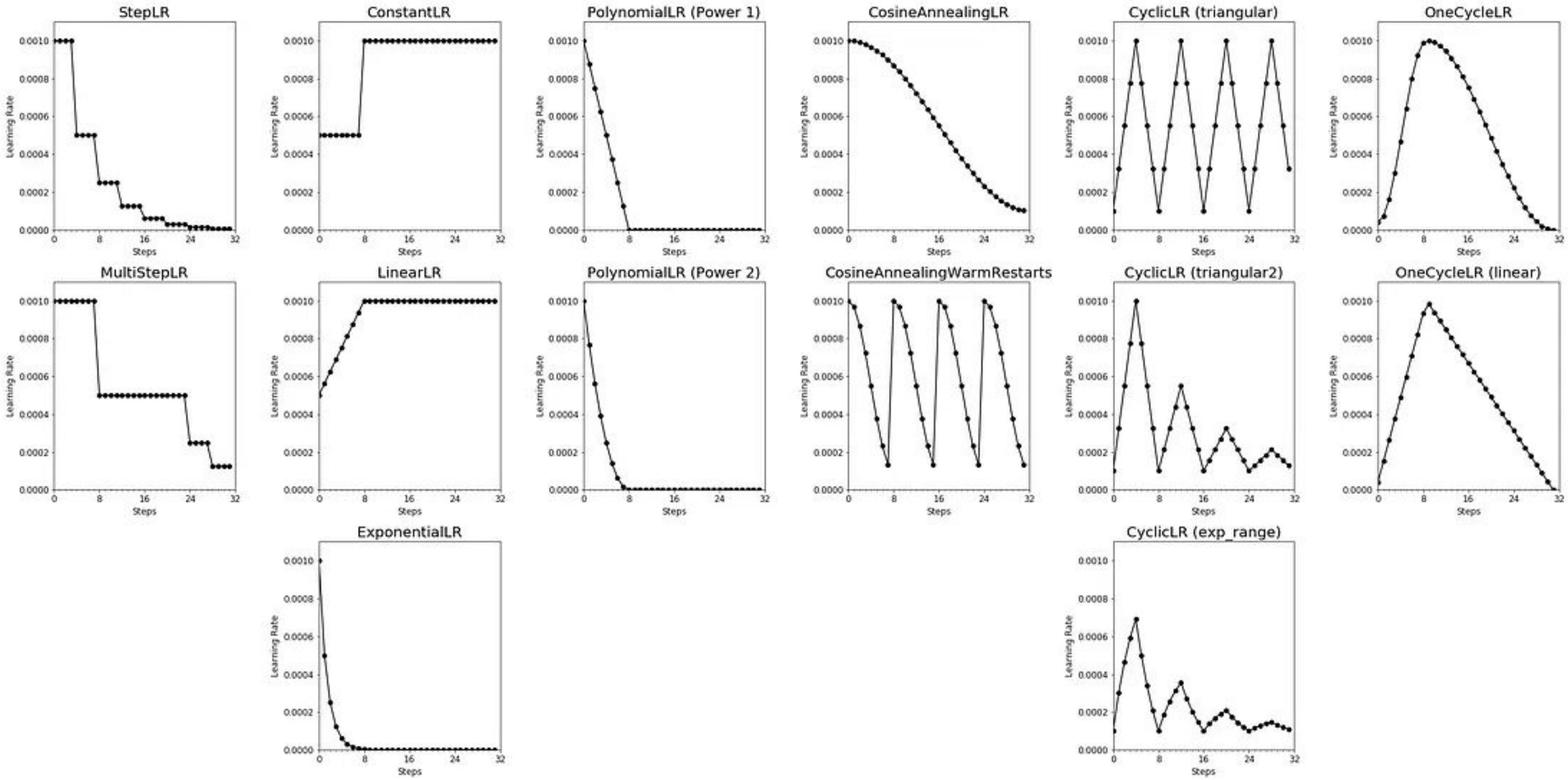
But are they equivalent somehow?

No!

There are *many* minimizers of the training loss

The **optimizer** determines which minimizer you converge to

Learning Rate Scheduling



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OPT: Open Pre-trained Transformer Language Models

OPT is an open source LLM like GPT-4 from Meta.

For large models like OPT-175B, more engineering efforts are needed.

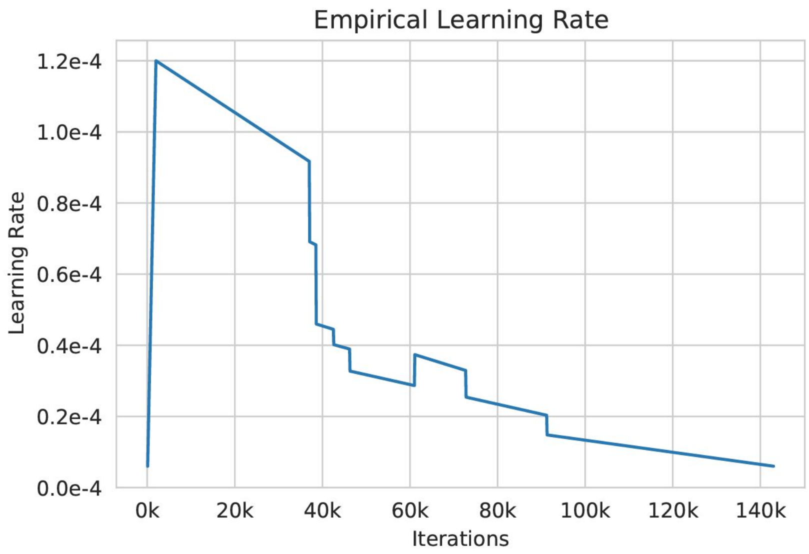

Figure 1: **Empirical LR schedule.** We found that lowering learning rate was helpful for avoiding instabilities.

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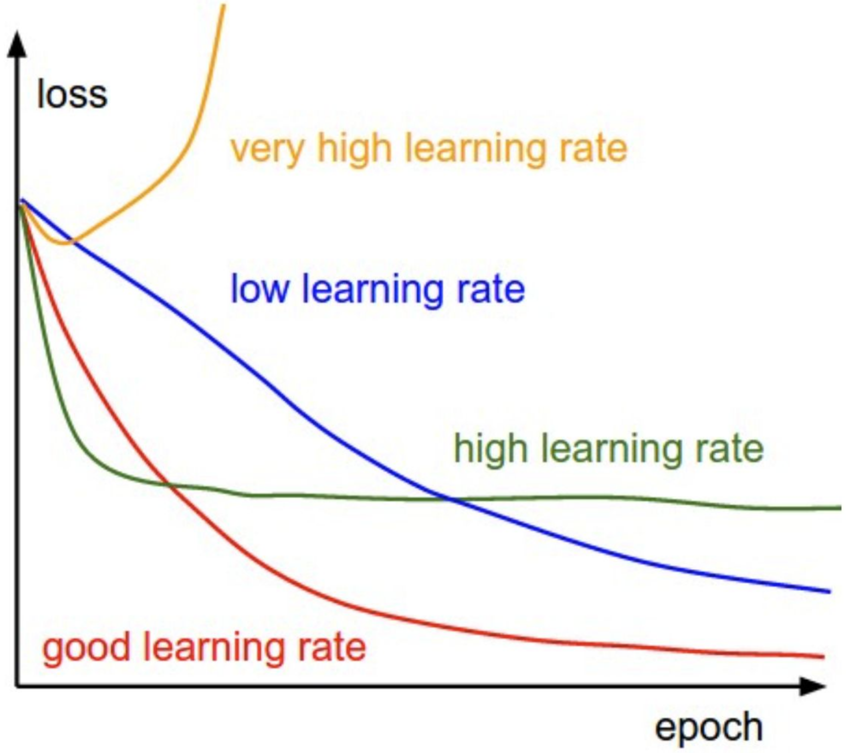
Hyperparameters

- Learning rate
- Batch size
- Beta1 & beta2 of adam
- Regularization strength

These are all hyperparameters that affect performance!



Source: https://cs231n.github.io/neural-networks-3/

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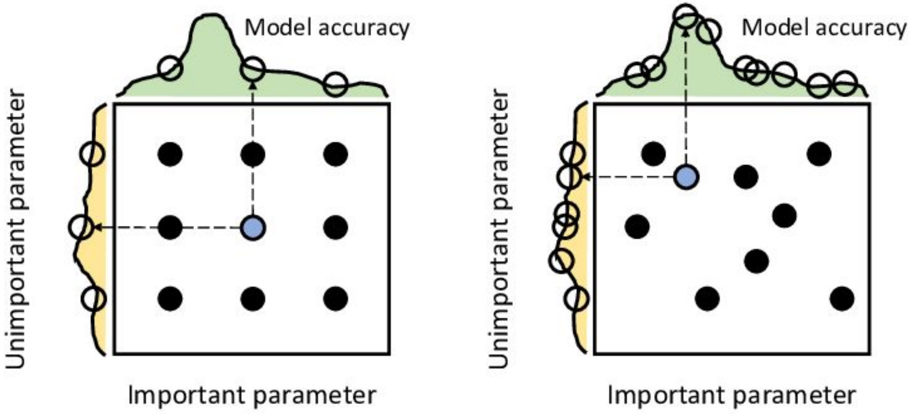
Hyperparameter Optimization (HPO)

- Learning rate
- Batch size
- Beta1 & beta2 of adam
- Regularization strength

These are all hyperparameters that affects performance!

Random search HPO is the efficient and simple way to start!



(a) Grid Search

(b) Random Search

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Summary

- **Optimization** tries to obtain the model weights that **minimize the loss function**.
- **Adam** is often a good default optimizer in deep learning
- The learning rate usually needs to be tuned carefully
- A monotonically **decreasing learning rate scheduler** with a **warmup** is a good default choice
- ***Random search*** *HPO is the* ***efficient*** *and* ***simple*** *way to start!*