Modern Techniques

CISC 7026: Introduction to Deep Learning

University of Macau

Agenda

1. Review
2. Dirty secret of deep learning
3. Optimization is hard
4. Deeper neural networks
5. Activation functions
6. Parameter initialization
7. Stochastic gradient descent
8. Modern optimization
9. Coding

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So far, we only looked at regression. Now, let us look at classification

Task: Given a picture of clothes, predict the text description

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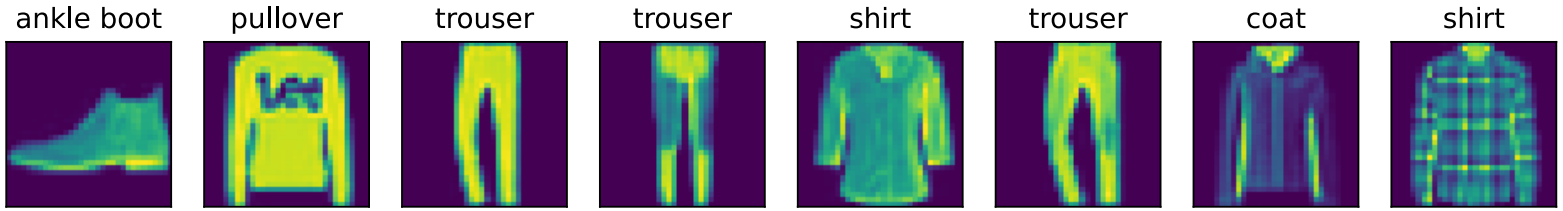
$$X : \mathbb{Z}_{0,255}^{32\times32}$$



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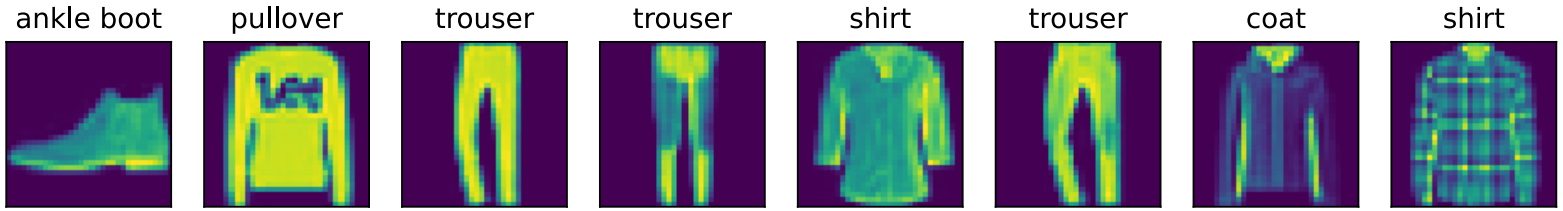

$Y : \{\text{T-shirt, Trouser, Pullover, Dress, Coat,}$

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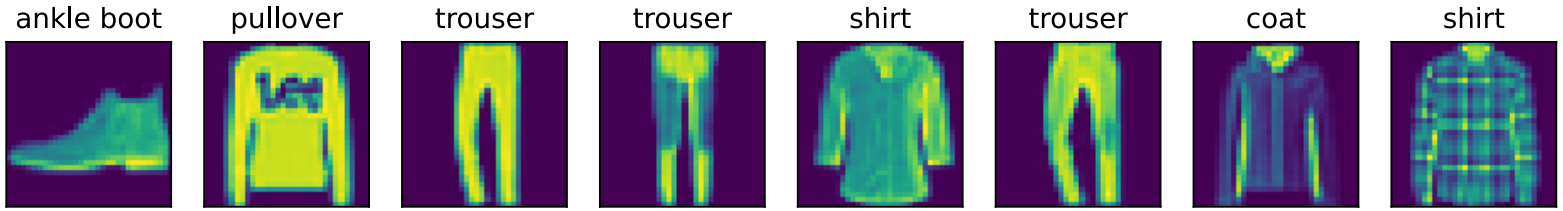

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Approach: Learn $\boldsymbol{\theta}$ that produce **conditional probabilities**

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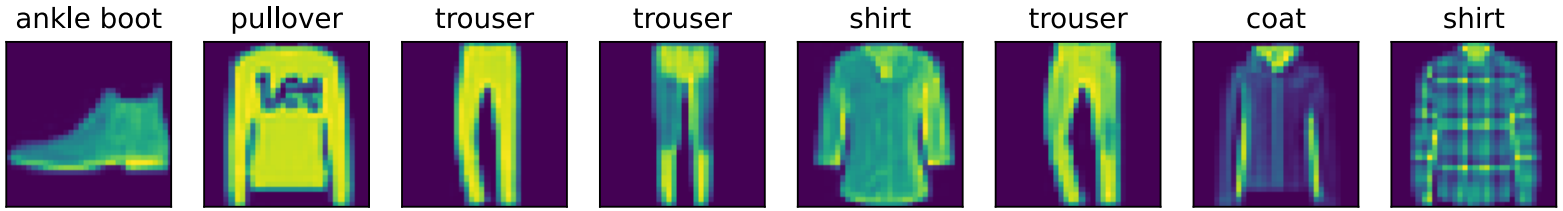

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Approach: Learn $\boldsymbol{\theta}$ that produce **conditional probabilities**

$$f(\boldsymbol{x}, \boldsymbol{\theta}) = P(\boldsymbol{y} \mid \boldsymbol{x}) = P\left(\begin{bmatrix} \text{T-Shirt} \\ \text{Trouser} \\ \vdots \end{bmatrix} \middle| \quad \right) = \begin{bmatrix} 0.2 \\ 0.01 \\ \vdots \end{bmatrix}$$

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$$P(A \mid B) = \frac{P(A \cap B)}{P(B)}$$

$$P(\text{Rain} \cap \text{Cloud}) = 0.1$$

Walk outside

$$P(\text{Cloud}) = 0.2$$

$$P(\text{Rain} \mid \text{Cloud}) = \frac{0.1}{0.2} = 0.5$$

How can we represent a probability distribution for a neural network?

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$$\boldsymbol{v} = \left\{ \begin{bmatrix} v_1 \\ \vdots \\ v_{d_y} \end{bmatrix} \middle| \quad \sum_{i=1}^{d_y} v_i = 1; \quad v_i \in (0, 1) \right\}$$

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$$\Delta^{d_y - 1}$$

The simplex Δ^k is an $k-1$-dimensional triangle in k-dimensional space

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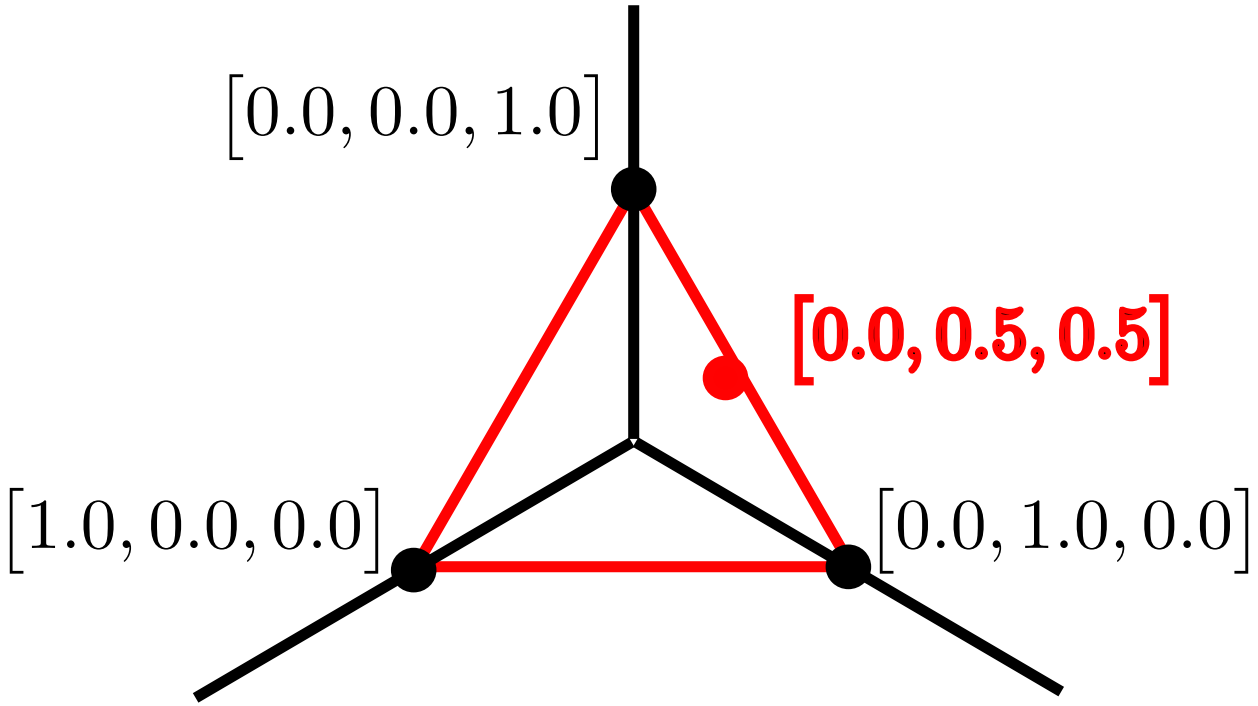

It has only $k-1$ free variables, because $x_k = 1 - \sum_{i=1}^{k-1} x_i$

The softmax function maps real numbers to the simplex (probabilities)

$$\text{softmax} : \mathbb{R}^k \mapsto \Delta^{k-1}$$

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$$\text{softmax}\left(\begin{bmatrix} x_1 \\ \vdots \\ x_k \end{bmatrix}\right) = \frac{e^{\boldsymbol{x}}}{\sum_{i=1}^{k} e^{x_i}} = \begin{bmatrix} \frac{e^{x_1}}{e^{x_1}+e^{x_2}+\ldots e^{x_k}} \\ \frac{e^{x_2}}{e^{x_1}+e^{x_2}+\ldots e^{x_k}} \\ \vdots \\ \frac{e^{x_k}}{e^{x_1}+e^{x_2}+\ldots e^{x_k}} \end{bmatrix}$$

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If we attach it to our linear model, we can output probabilities!

$$f(\boldsymbol{x}, \boldsymbol{\theta}) = \text{softmax}(\boldsymbol{\theta}^\top \boldsymbol{x})$$

Question: Why do we output probabilities instead of a binary values

$$f(\boldsymbol{x}, \boldsymbol{\theta}) = \begin{bmatrix} P\Big(\text{Shirt} \mid \text{  }\Big) \\ P\Big(\text{Bag} \mid \text{  }\Big) \\ \vdots \end{bmatrix} = \begin{bmatrix} 0.25 \\ 0.08 \\ \vdots \end{bmatrix}; \quad f(\boldsymbol{x}, \boldsymbol{\theta}) = \begin{bmatrix} 1 \\ 0 \\ \vdots \end{bmatrix}$$

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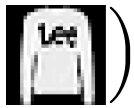
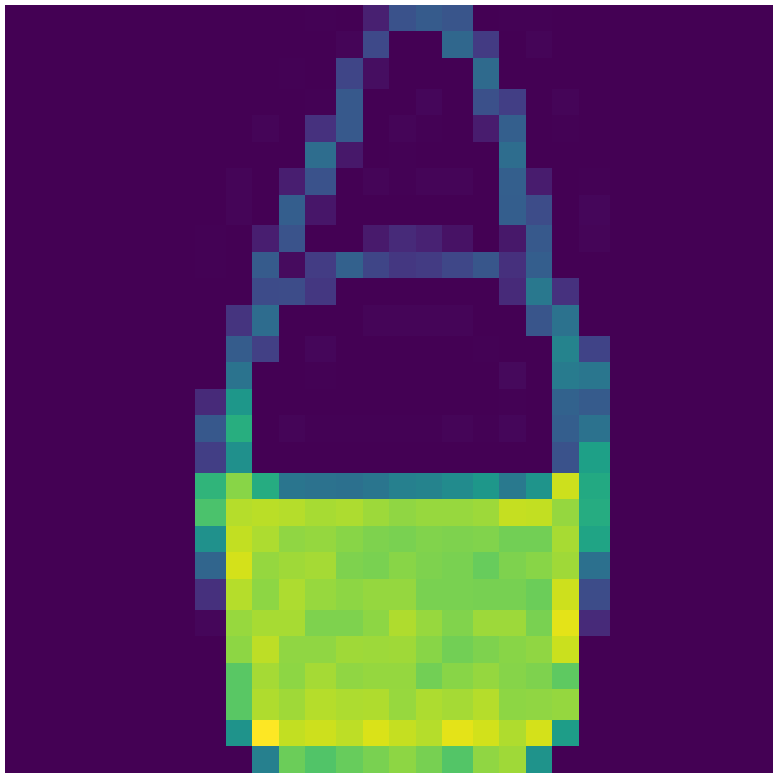
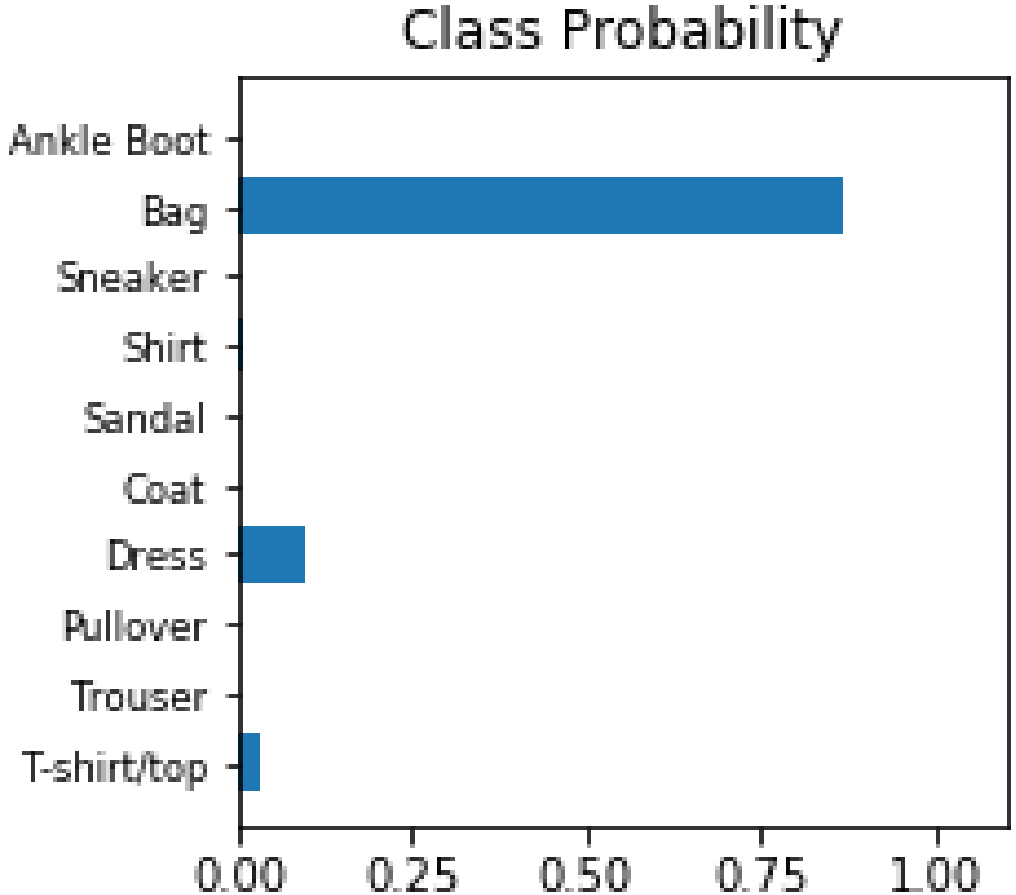
$$f(\boldsymbol{x}, \boldsymbol{\theta}) = \begin{bmatrix} P\big(\text{Shirt} \mid \text{  }\big) \\ P\big(\text{Bag} \mid \text{  }\big) \\ \vdots \end{bmatrix} = \begin{bmatrix} 0.25 \\ 0.08 \\ \vdots \end{bmatrix}; \quad f(\boldsymbol{x}, \boldsymbol{\theta}) = \begin{bmatrix} 1 \\ 0 \\ \vdots \end{bmatrix}$$

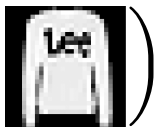
Answer 1: Outputting probabilities results in differentiable functions

Answer 2: We report uncertainty, which is useful in many applications




Class Probability
Ankle Boot
Bag
Sneaker
Shirt
Sandal
Coat
Dress
Pullover
Trouser
T-shirt/top
0.00
0.25
0.50
0.75
1.00

We consider the label $\boldsymbol{y}_{[i]}$ as a conditional distribution

$$P\left(\boldsymbol{y}_{[i]} \mid \boldsymbol{x}_{[i]}\right) = \begin{bmatrix} P\left(\text{Shirt} \mid \text{  }\right) \\ P\left(\text{Bag} \mid \text{  }\right) \end{bmatrix} = \begin{bmatrix} 1 \\ 0 \end{bmatrix}$$

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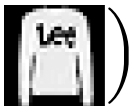
$$P\left(\boldsymbol{y}_{[i]} \mid \boldsymbol{x}_{[i]}\right) = \begin{bmatrix} P\left(\text{Shirt} \mid \text{  }\right) \\ P\left(\text{Bag} \mid \text{  }\right) \end{bmatrix} = \begin{bmatrix} 1 \\ 0 \end{bmatrix}$$

What loss function should we use for classification?

Since $f(\boldsymbol{x}, \boldsymbol{\theta})$ and $P(\boldsymbol{y} \mid \boldsymbol{x})$ are both distributions, we want to measure the difference between distributions

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One measurement is the **Kullback-Leibler Divergence (KL)**

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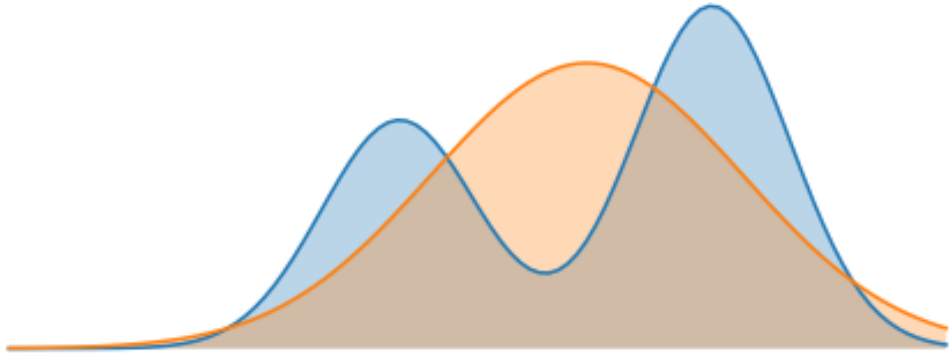

From the KL divergence, we derived the **cross-entropy loss** function, which we use for classification

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$$\mathcal{L}(\boldsymbol{x}, \boldsymbol{y}, \boldsymbol{\theta}) = \left[-\sum_{j=1}^{n} \sum_{i=1}^{d_y} P\left(y_{[j],i} \mid \boldsymbol{x}_{[j]}\right) \log f\left(\boldsymbol{x}_{[j]}, \boldsymbol{\theta}\right)_i \right]$$

Finish coding exercise

https://colab.research.google.com/drive/1BGMIE2CjlLJOH-D2r9AariPDVgxjWlqG#scrollTo=AnHP-PHVhpW_

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Today we experiment, and maybe tomorrow we discover the theory

Similar to using neural networks for 40 years without knowing how to train them

Dirty secret of deep learning

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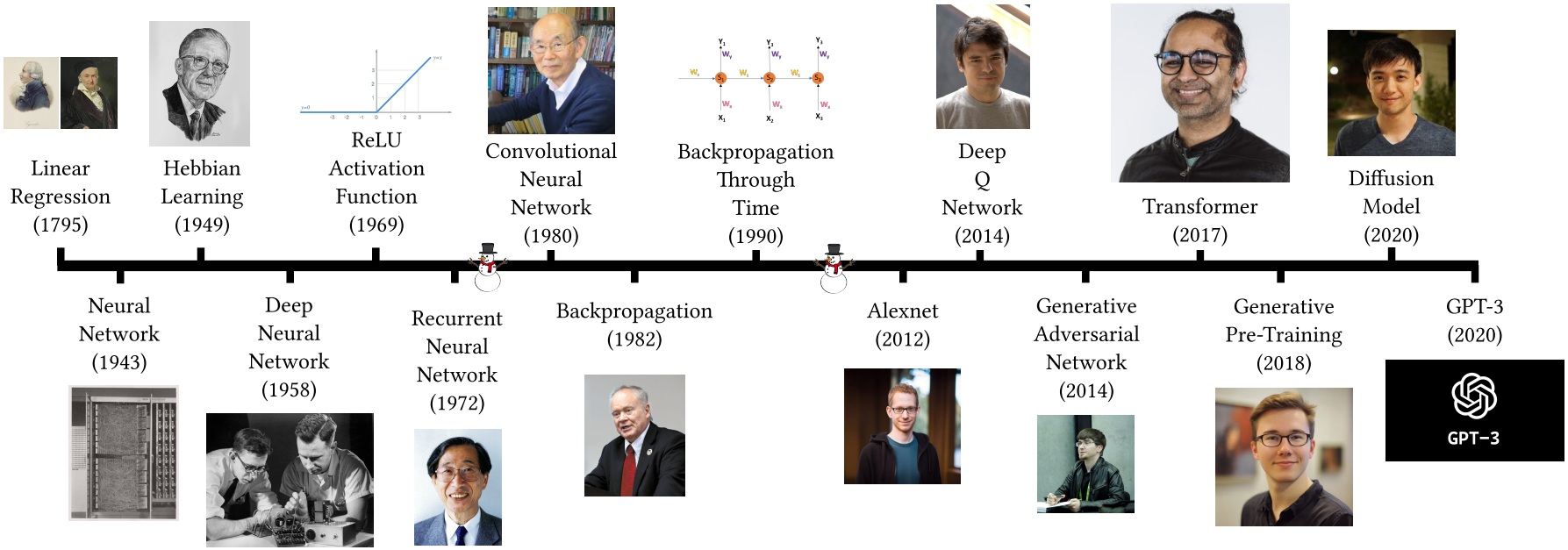

Dirty secret of deep learning

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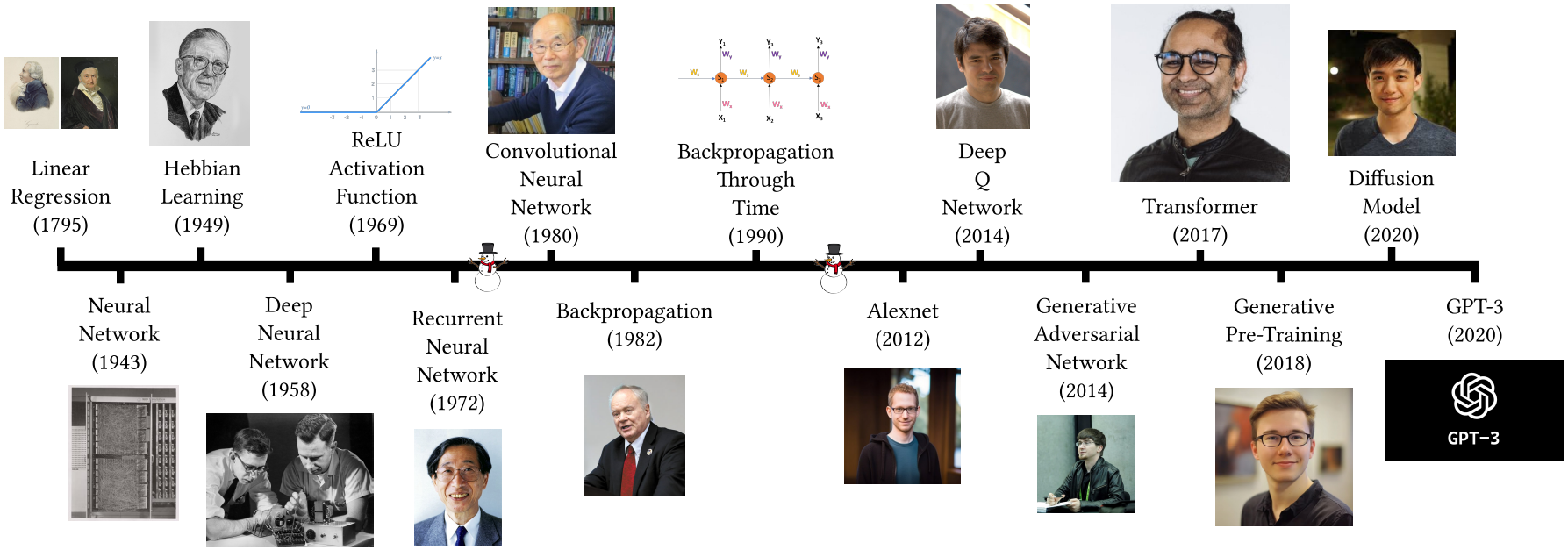

Are modern networks are too complex for humans to understand?

Scientific method:

Dirty secret of deep learning

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1. Collect observations

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Scientific method:

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However, there is a second part:

1. Find theory
2. Find counterexample
3. Publish counterexample
4. Falsify theory

Deep learning is new, so much of part 2 has not happened yet!

For many concepts, the **observations** are stronger than the **theory**

Dirty secret of deep learning

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Observe that a concept improves many types of neural networks

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This is how medicine works (e.g., Anesthetics)!

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$$\lim_{d_h \to \infty} \varepsilon = 0$$

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$$\mid f(\boldsymbol{x}, \boldsymbol{\theta}) - g(\boldsymbol{x}) \mid < \varepsilon$$

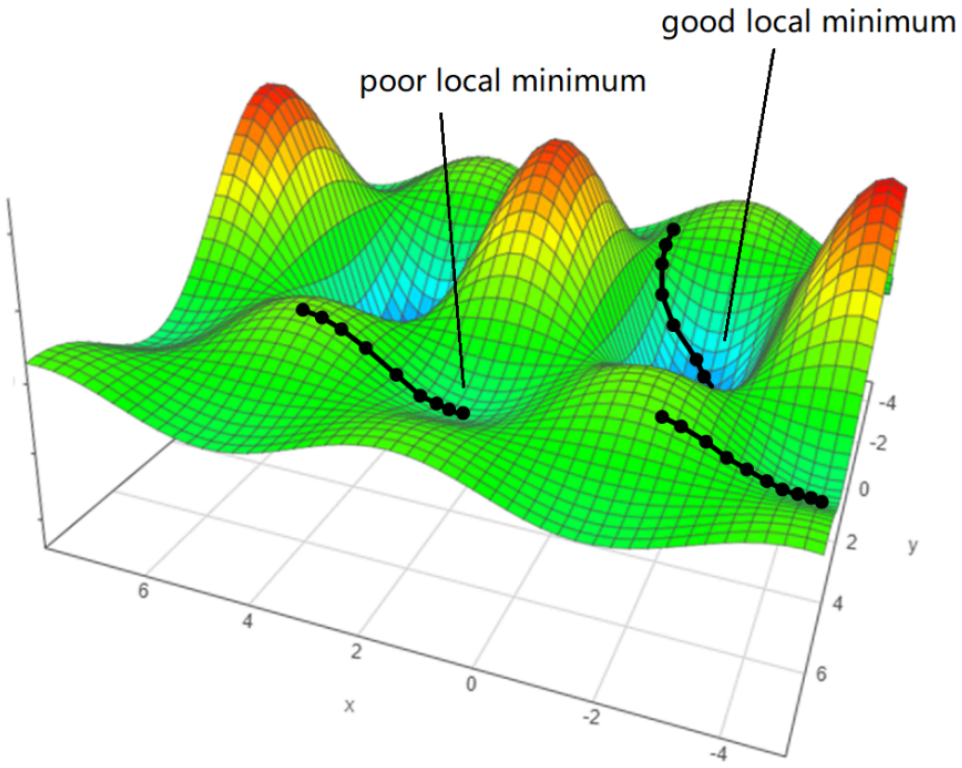
$$\lim_{d_h \to \infty} \varepsilon = 0$$

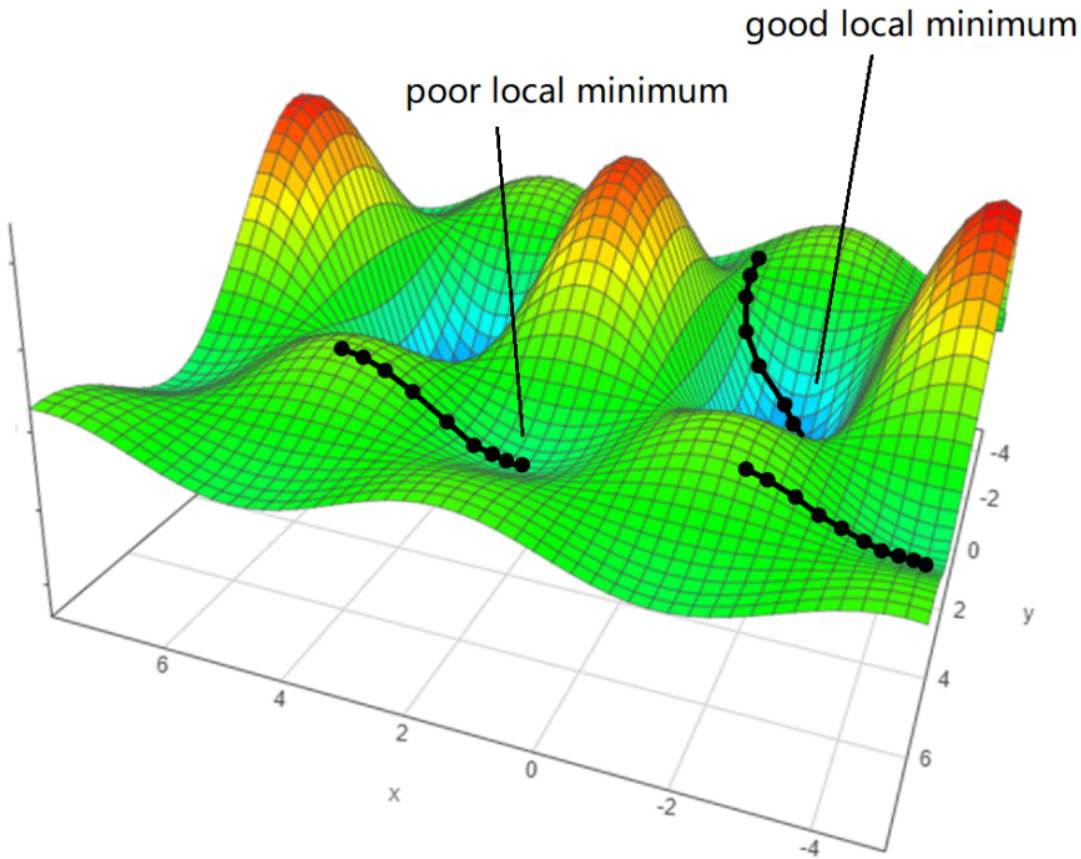
However, finding such $\boldsymbol{\theta}$ is a much harder problem

Gradient descent only guarantees convergence to a **local** optima

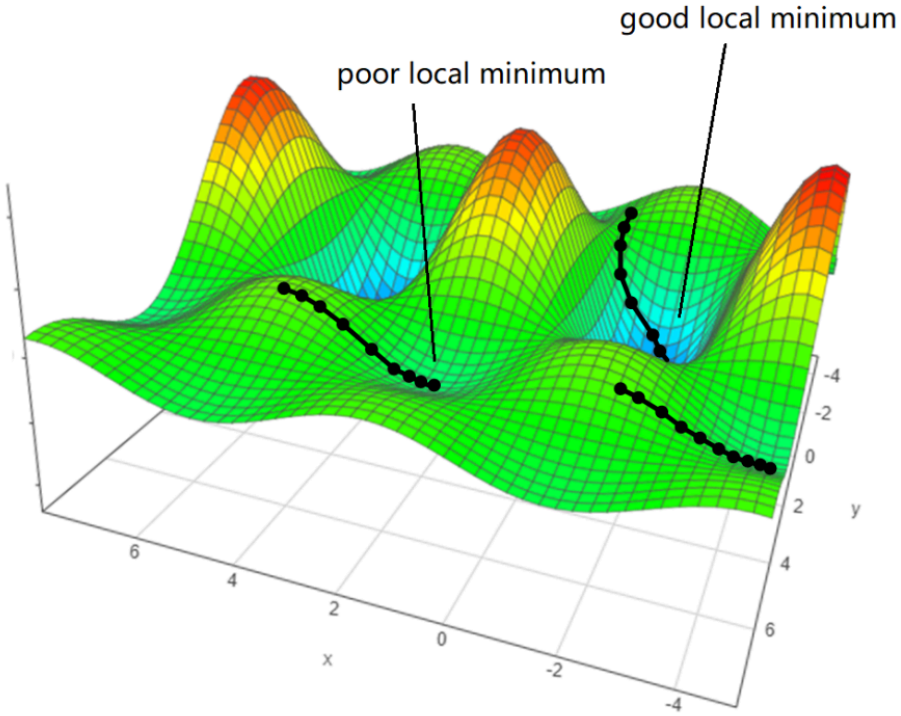
Optimization is hard

Gradient descent only guarantees convergence to a **local** optima




good local minimum
poor local minimum
6
4
2
0
-2
-4
x
-4
-2
0
2
4
6
y

Optimization is hard

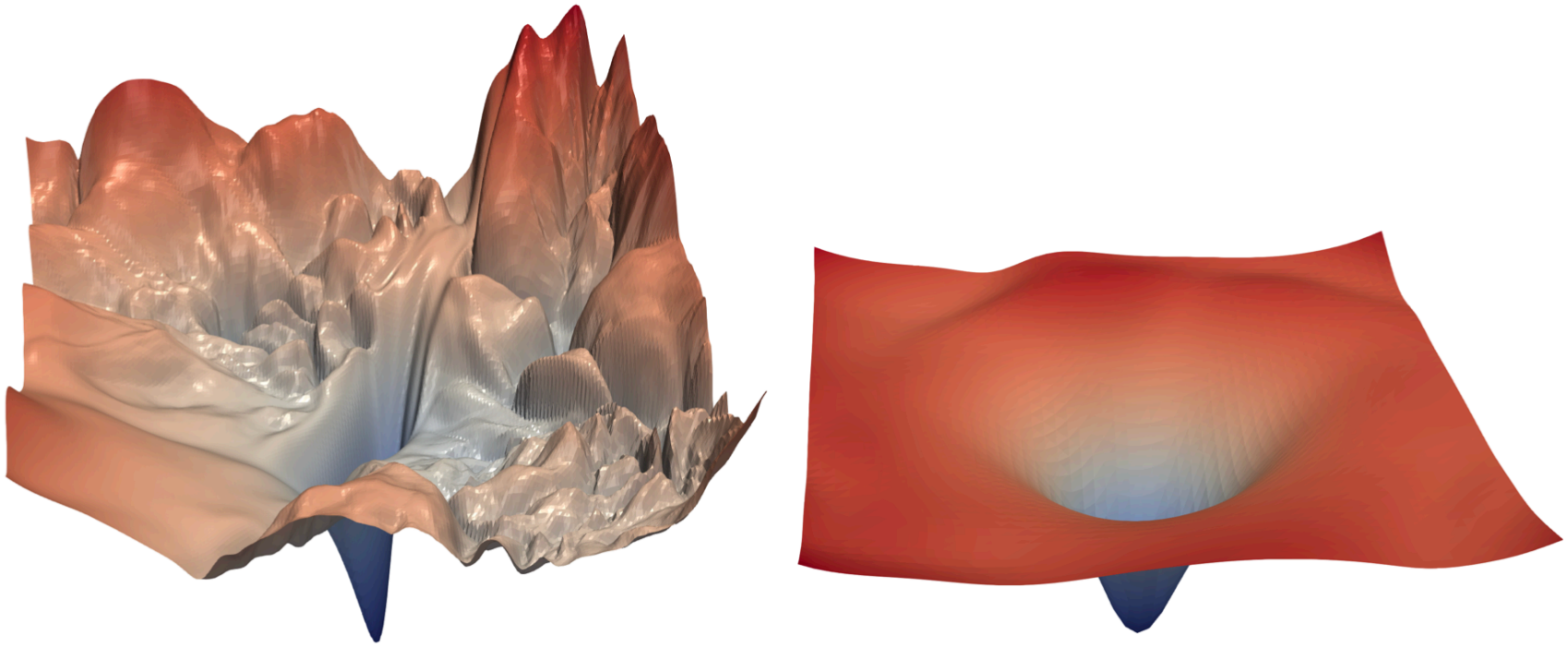


Harder tasks can have millions of local optima, and many of the local optima are not very good!

Many of the concepts today create a **flat** loss landscape

Optimization is hard

Many of the concepts today create a **flat** loss landscape



Gradient descent reaches a better optimum more quickly in these cases

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2. Dirty secret of deep learning
3. **Optimization is hard**
4. Deeper neural networks
5. Activation functions
6. Parameter initialization
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9. Coding

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We need more layers for harder problems

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From Choromanska, Anna, et al. “The loss surfaces of multilayer networks.”:

- “For large-size networks, most local minima are equivalent and yield similar performance on a test set."
- “The probability of finding a “bad” (high value) local minimum is non-zero for small-size networks and decreases quickly with network size”

To summarize, deeper and wider neural networks tend to produce better results

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Add more layers to your network

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Add more layers to your network

Increase the width of each layer

```python
# Deep neural network
from torch import nn

d_x, d_y, d_h = 1, 1, 16
# Linear(input, output)
l1 = nn.Linear(d_x, d_h)
l2 = nn.Linear(d_h, d_y)
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```
# Deeper and wider neural
network
from torch import nn

d_x, d_y, d_h = 1, 1, 256
# Linear(input, output)
l1 = nn.Linear(d_x, d_h)
l2 = nn.Linear(d_h, d_h)
l3 = nn.Linear(d_h, d_h)
...
l6 = nn.Linear(d_h, d_y)
```

```
import torch
d_x, d_y, d_h = 1, 1, 256
net = torch.nn.Sequential([
    torch.nn.Linear(d_x, d_h),
    torch.nn.Sigmoid(),
    torch.nn.Linear(d_h, d_h),
    torch.nn.Sigmoid(),
    ...
    torch.nn.Linear(d_h, d_y),
])

x = torch.ones((d_x,))
y = net(x)
```

```
import jax, equinox
d_x, d_y, d_h = 1, 1, 256
net = equinox.nn.Sequential([
    equinox.nn.Linear(d_x, d_h),
    equinox.nn.Lambda(jax.nn.sigmoid),
    equinox.nn.Linear(d_h, d_h),
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    ...
    equinox.nn.Linear(d_h, d_y),
])

x = jax.numpy.ones((d_x,))
y = net(x)
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The sigmoid function was the standard activation function until ~ 2012

Activation functions

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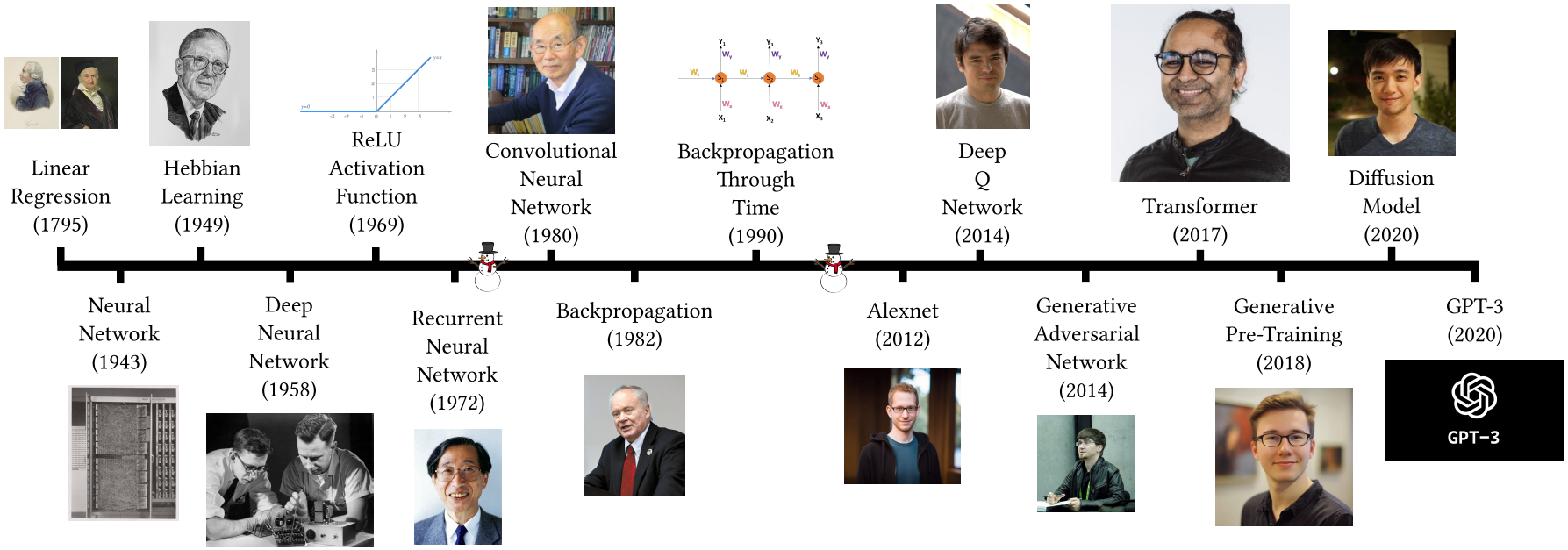

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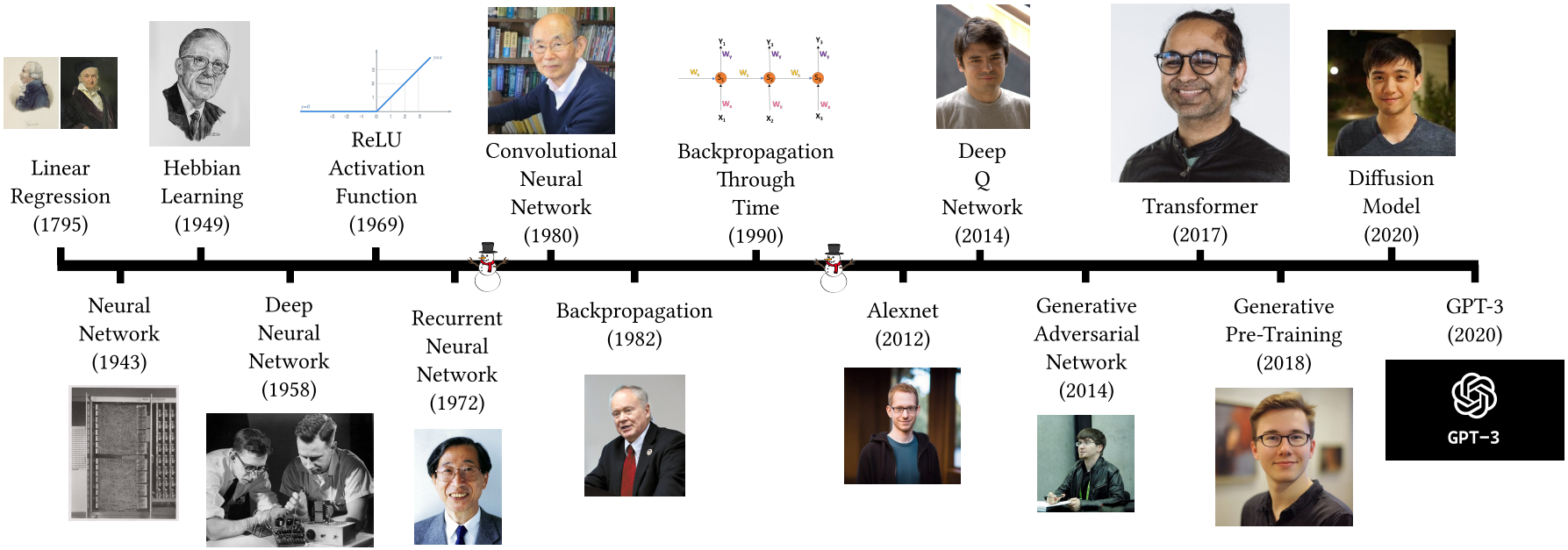
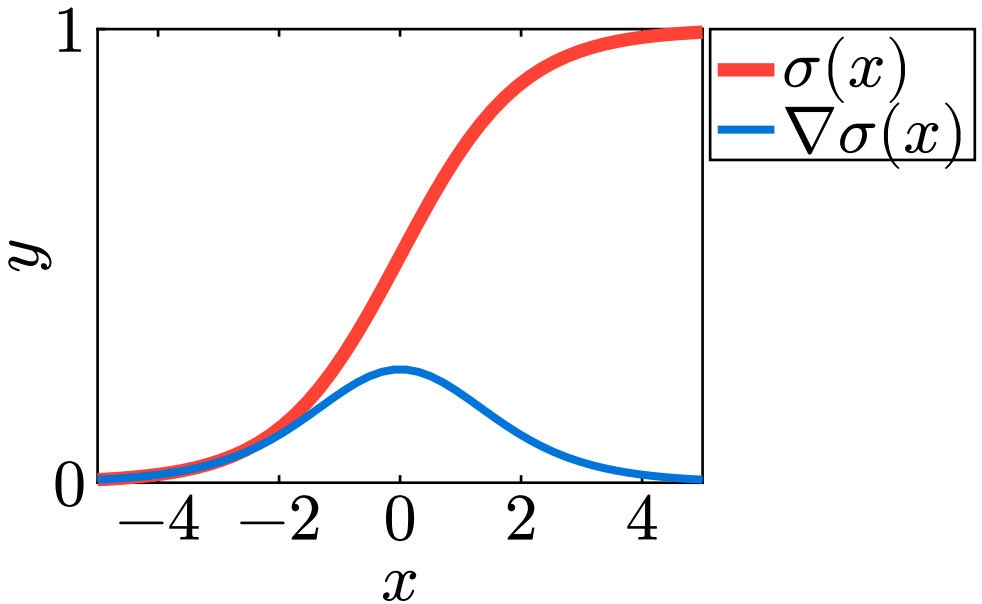
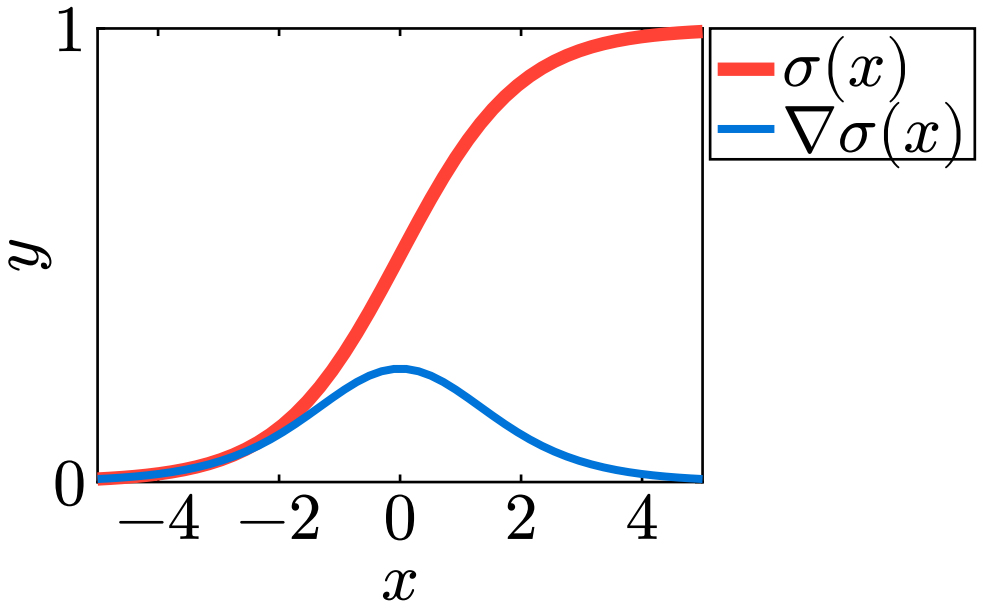


In 2012, people realized that ReLU activation performed much better

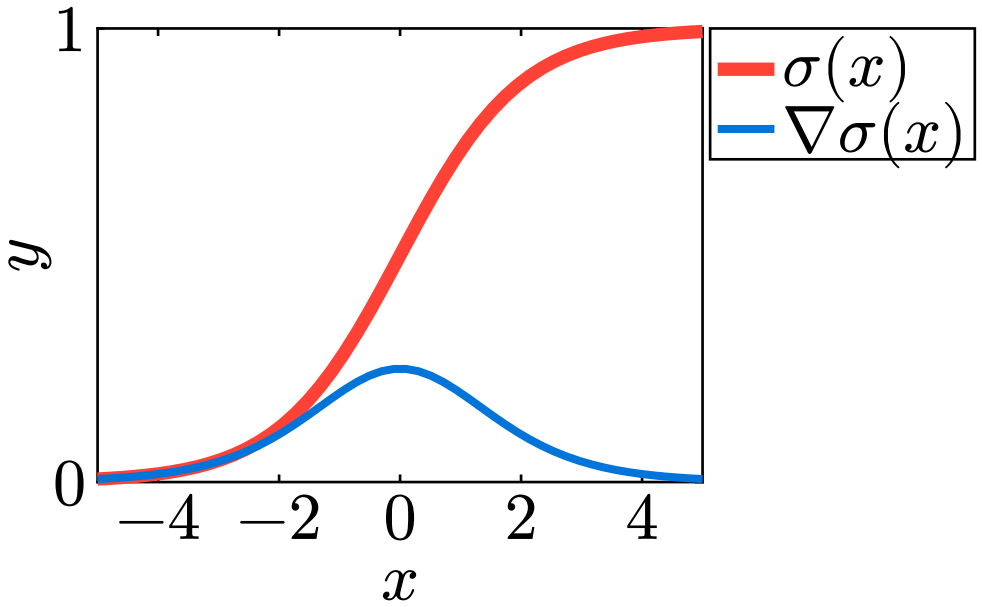

1
0
y
−4
−2
0
2
4
x
σ(x)
∇σ(x)

Activation functions



The sigmoid function can result in a **vanishing gradient**

Activation functions



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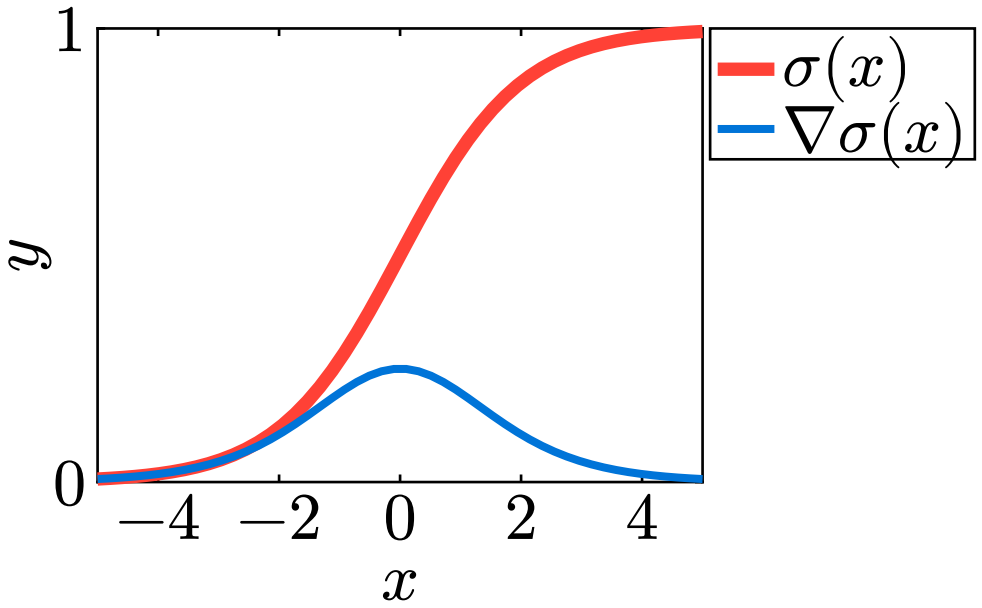
$$f(\boldsymbol{x}, \boldsymbol{\theta}) = \sigma(\boldsymbol{\theta}_3^\top \sigma(\boldsymbol{\theta}_2^\top \sigma(\boldsymbol{\theta}_1^\top \overline{\boldsymbol{x}})))$$

Activation functions



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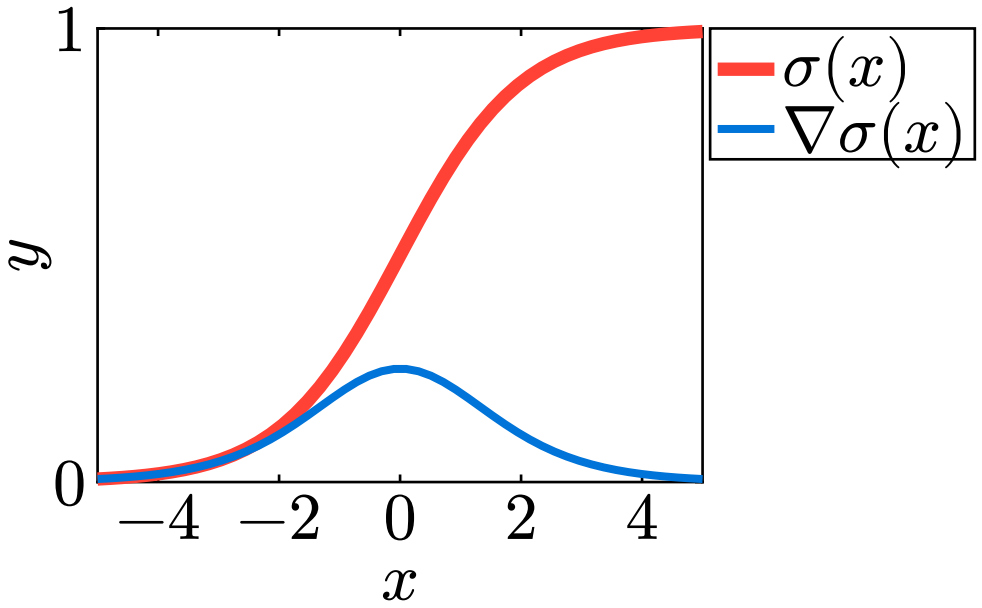

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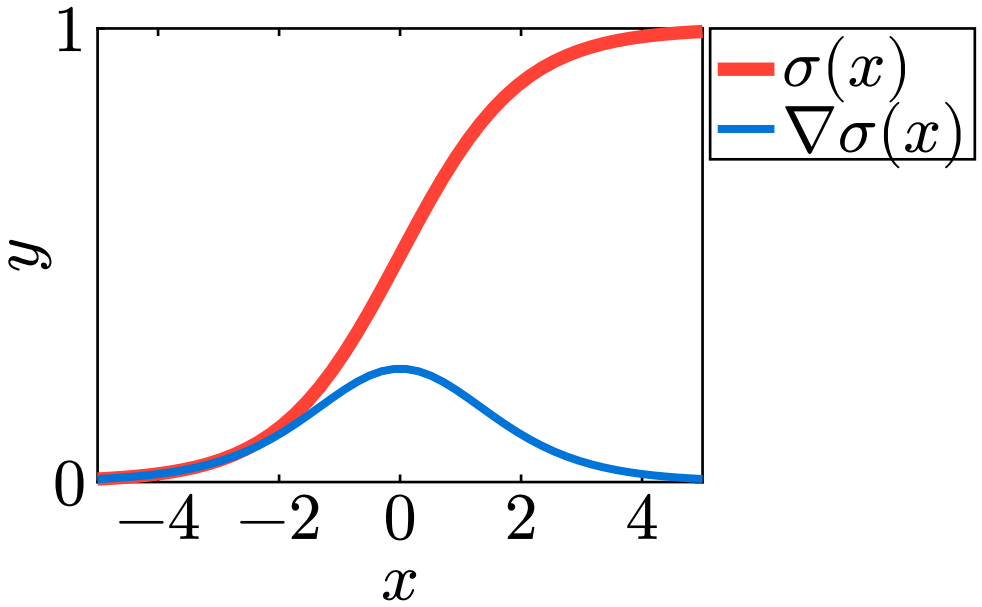

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$$\nabla_{\boldsymbol{\theta}} f(\boldsymbol{x}, \boldsymbol{\theta}) \approx 0$$

To fix the vanishing gradient, researchers use the **rectified linear unit (ReLU)**

$$\sigma(x) = \max(0, x)$$

$$\nabla\sigma(x) = \begin{cases} 0 \text{ if } x < 0 \\ 1 \text{ if } x \geq 0 \end{cases}$$

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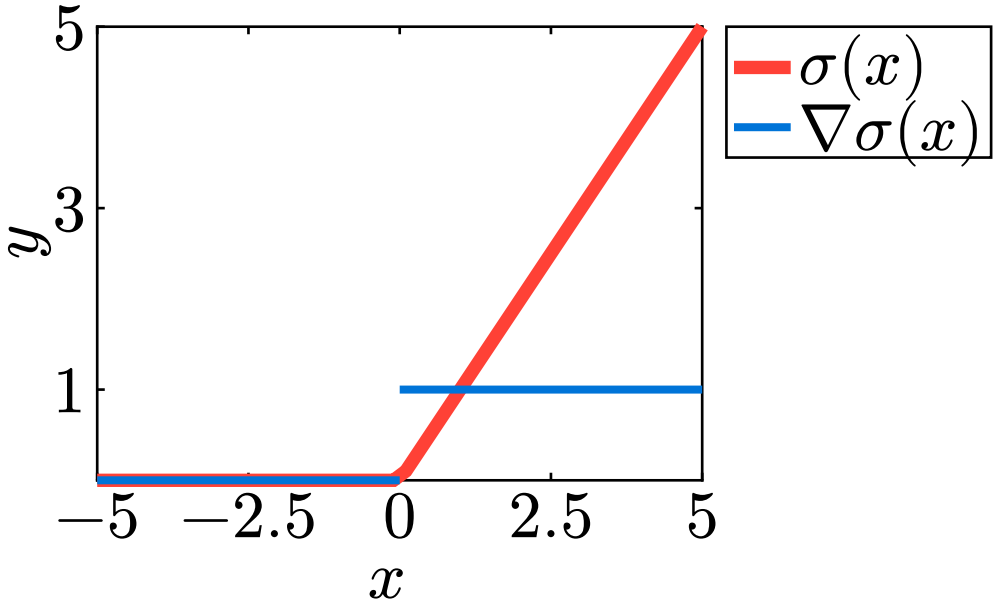

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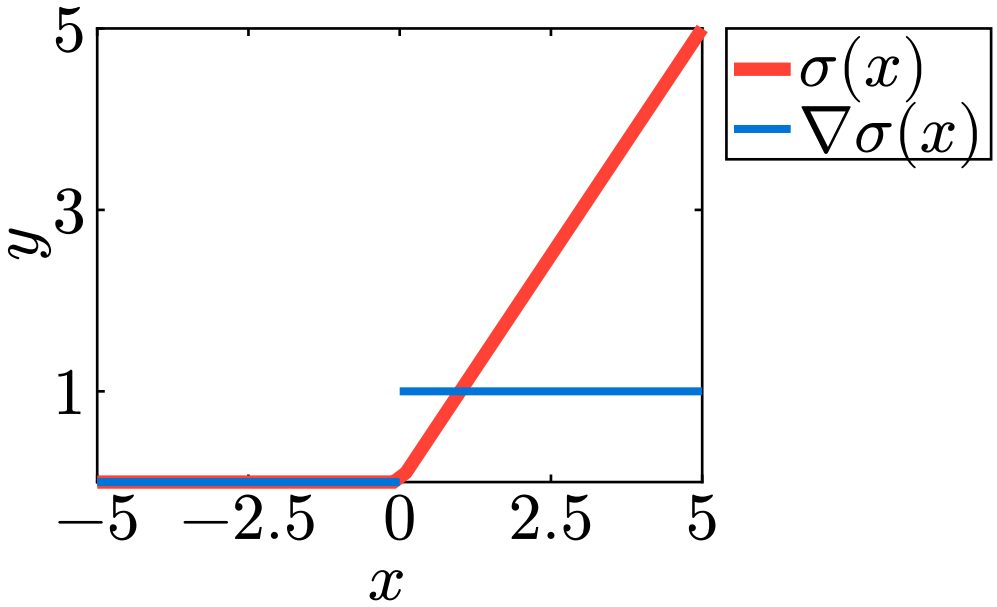

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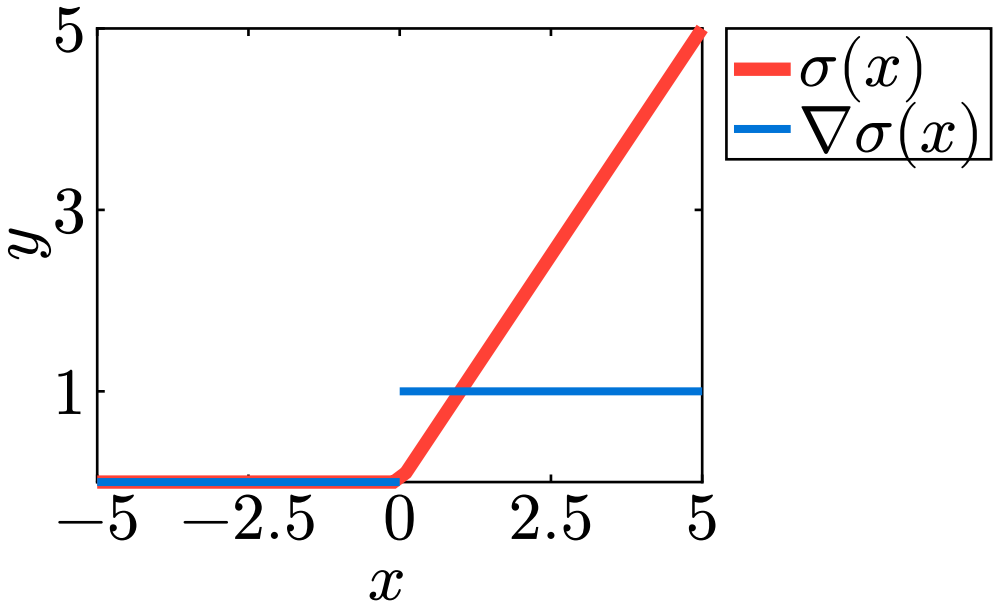

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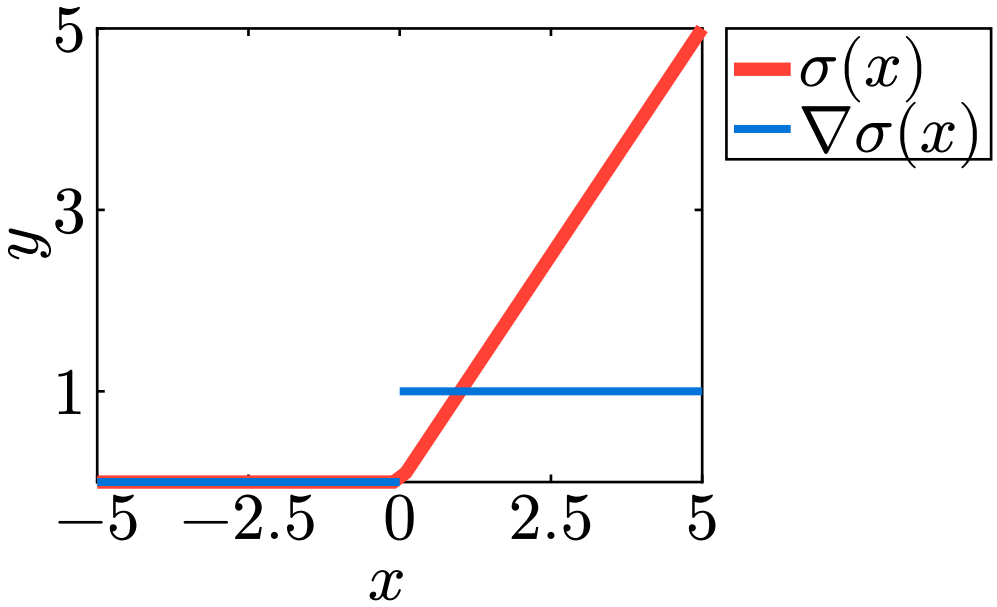

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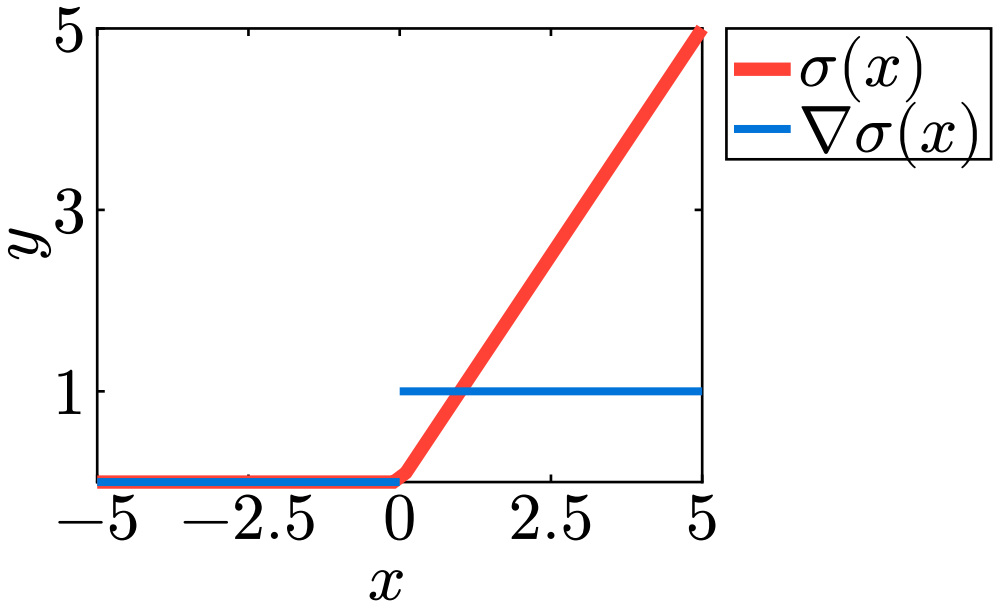

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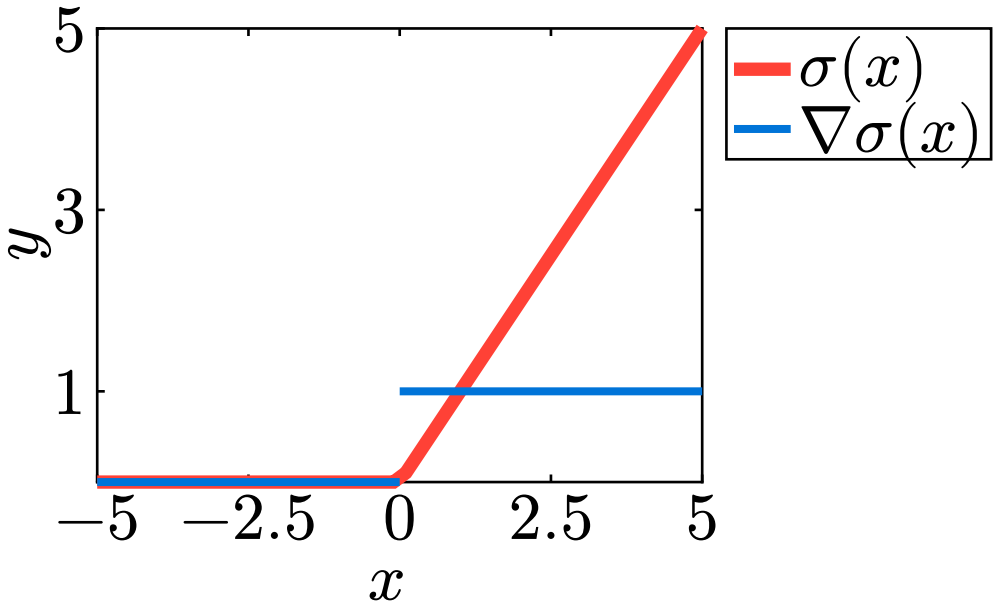

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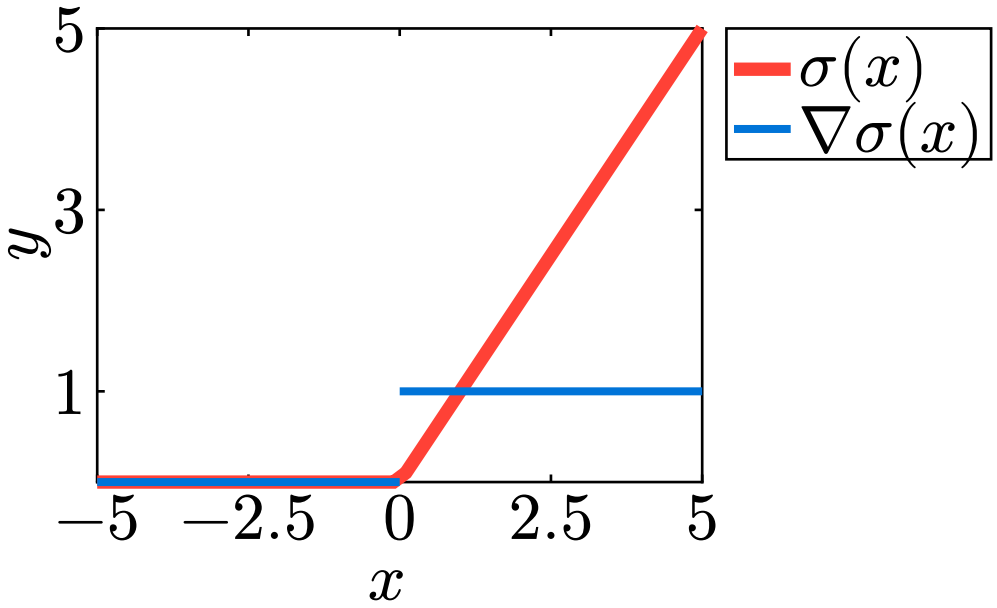

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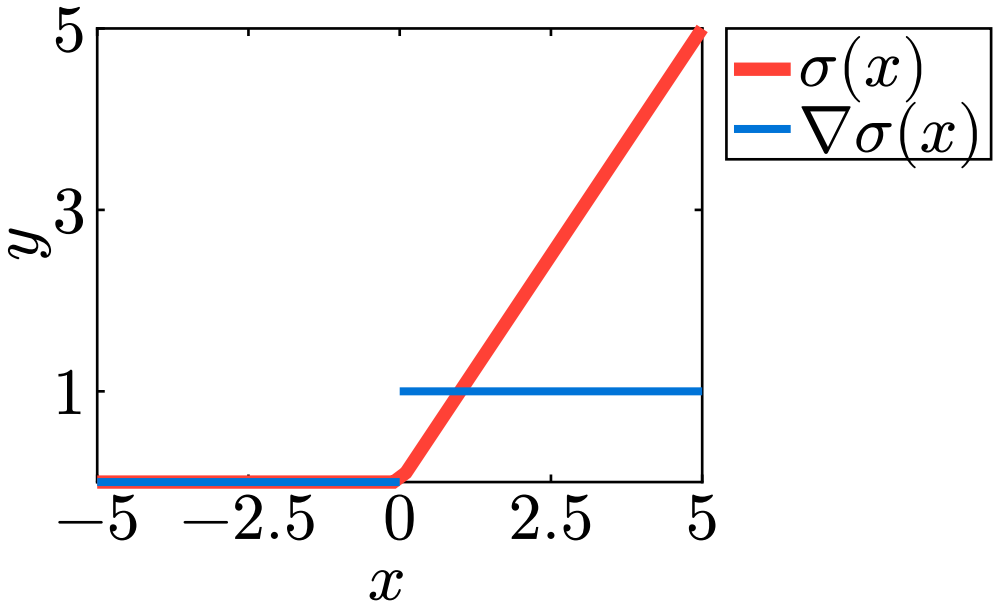

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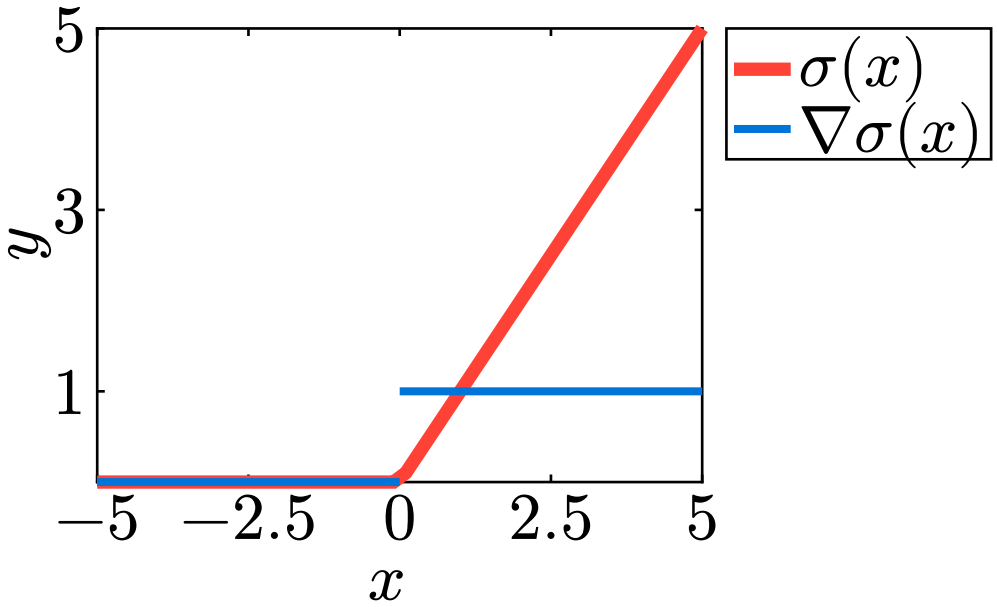

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These neurons cannot recover, they are **dead neurons**

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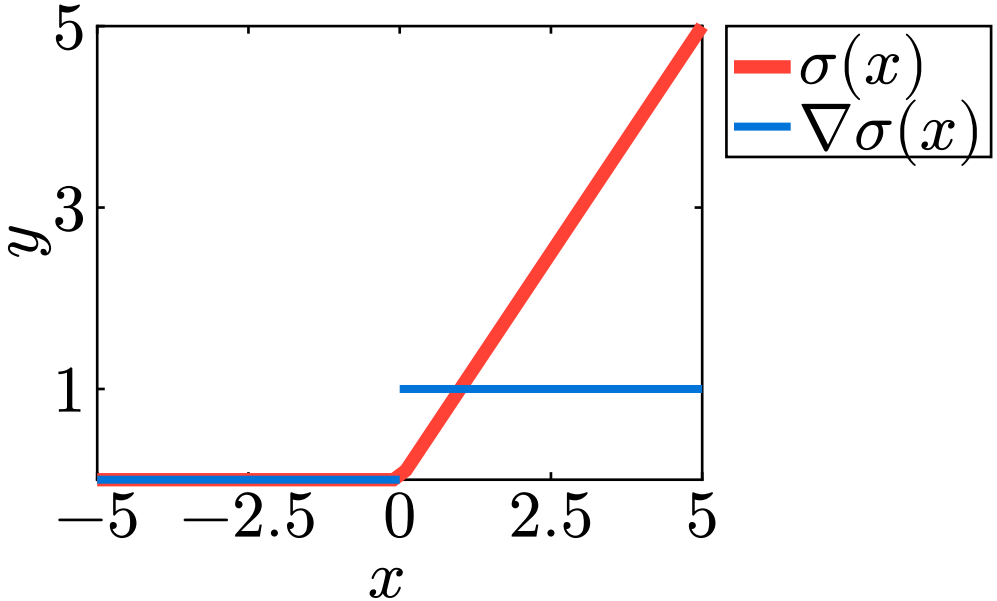

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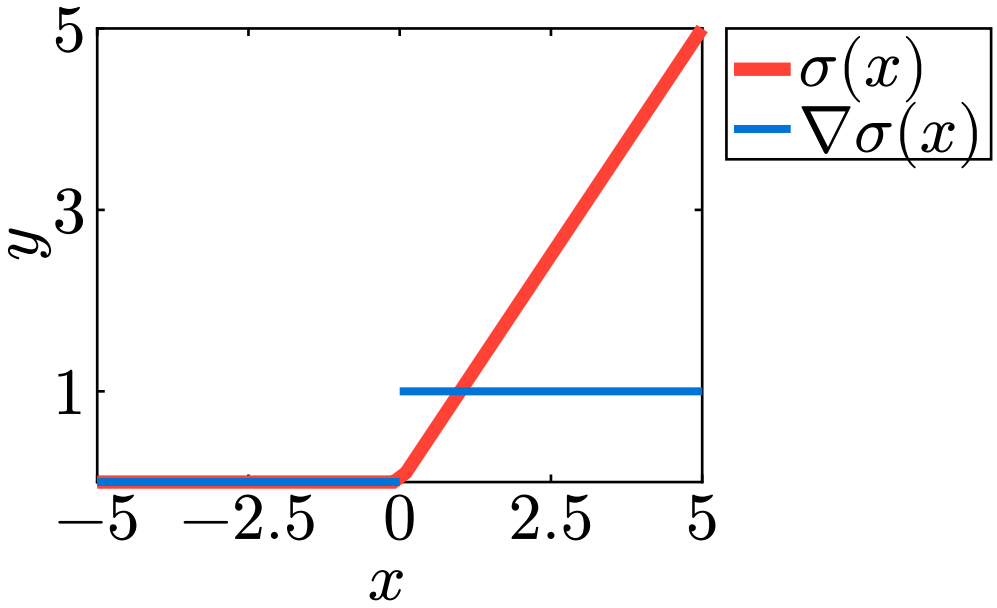

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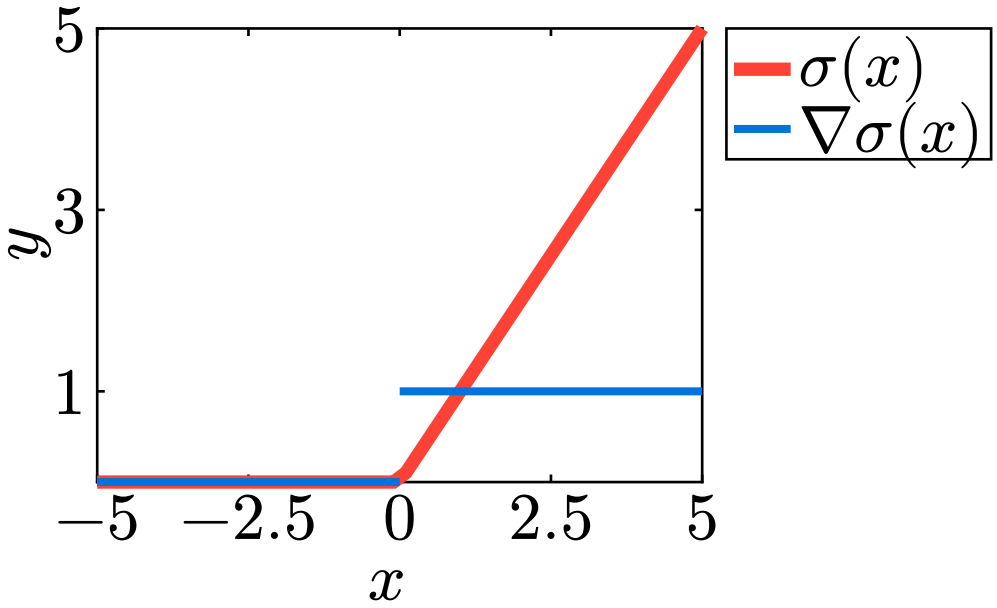

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Dead neurons hurt your network!

To fix dying neurons, use **leaky ReLU**

Activation functions

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$$\sigma(x) = \max(0.1x, x)$$

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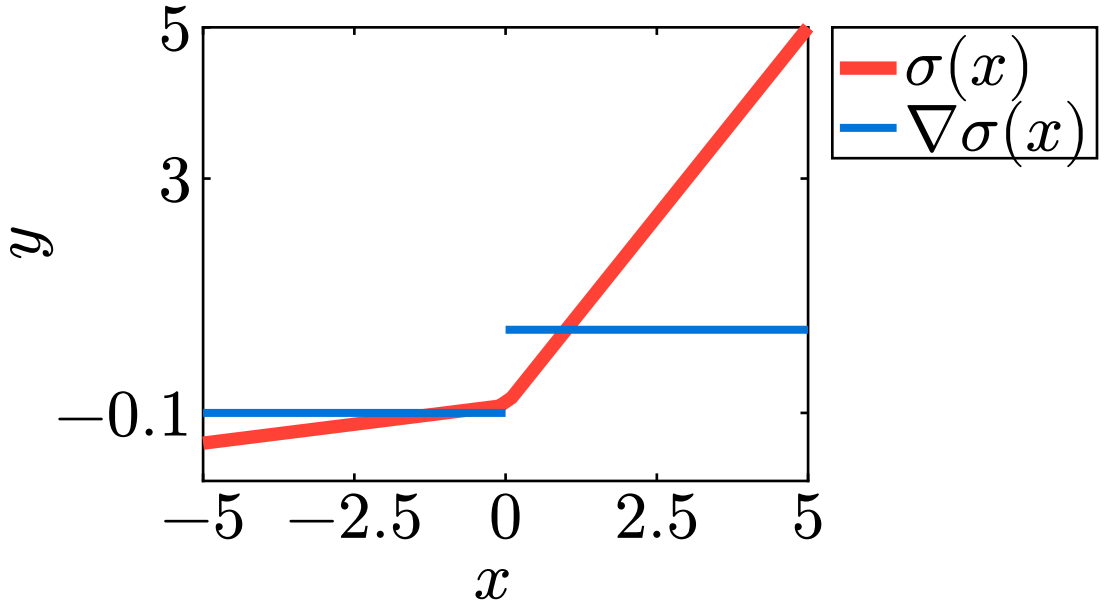

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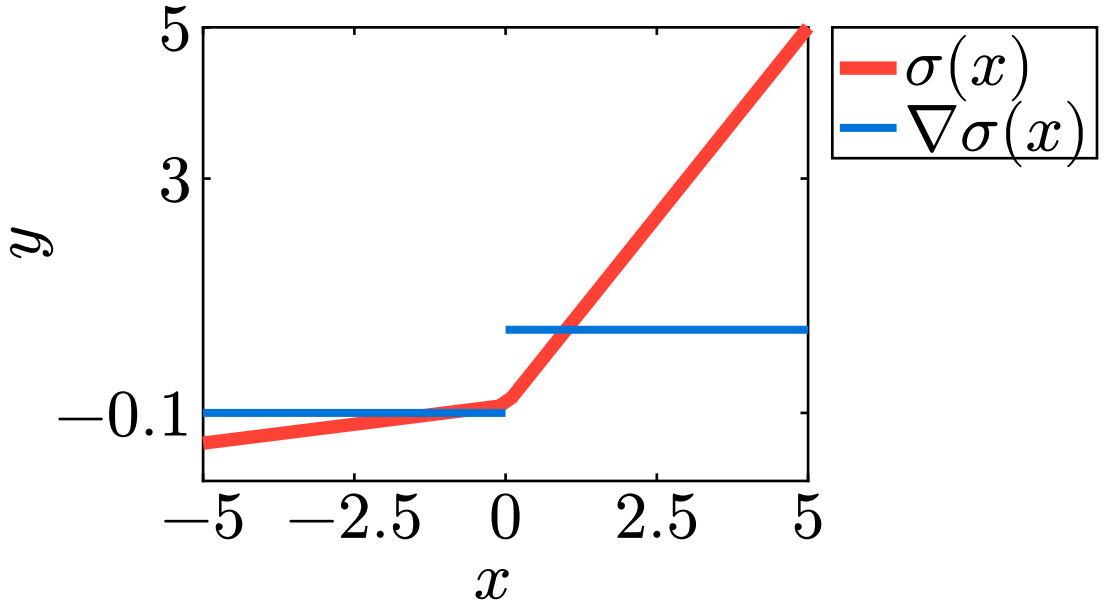

Small negative slope allows dead neurons to recover

There are other activation functions that are better than leaky ReLU

Activation functions

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Activation functions

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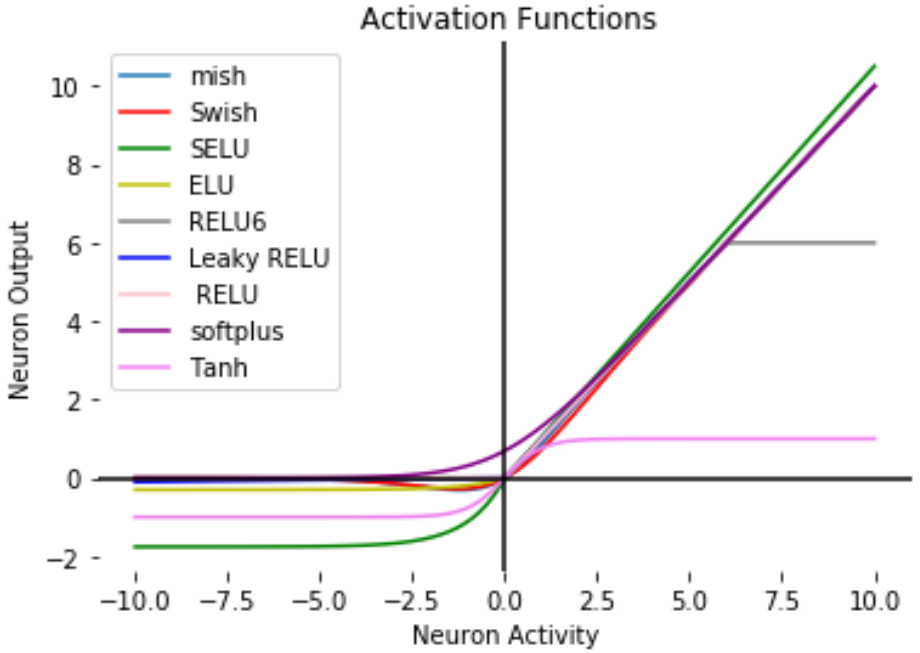

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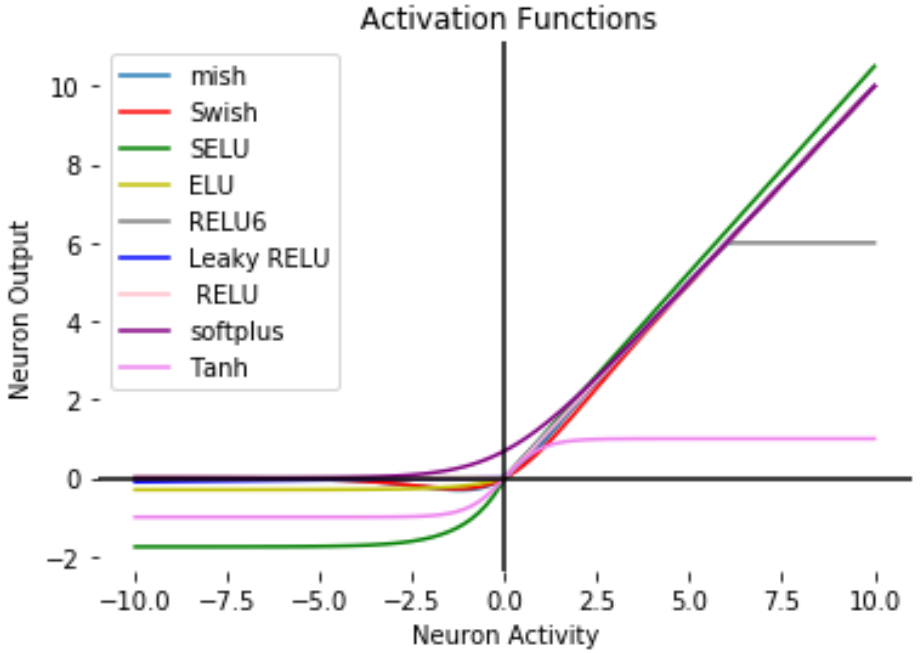

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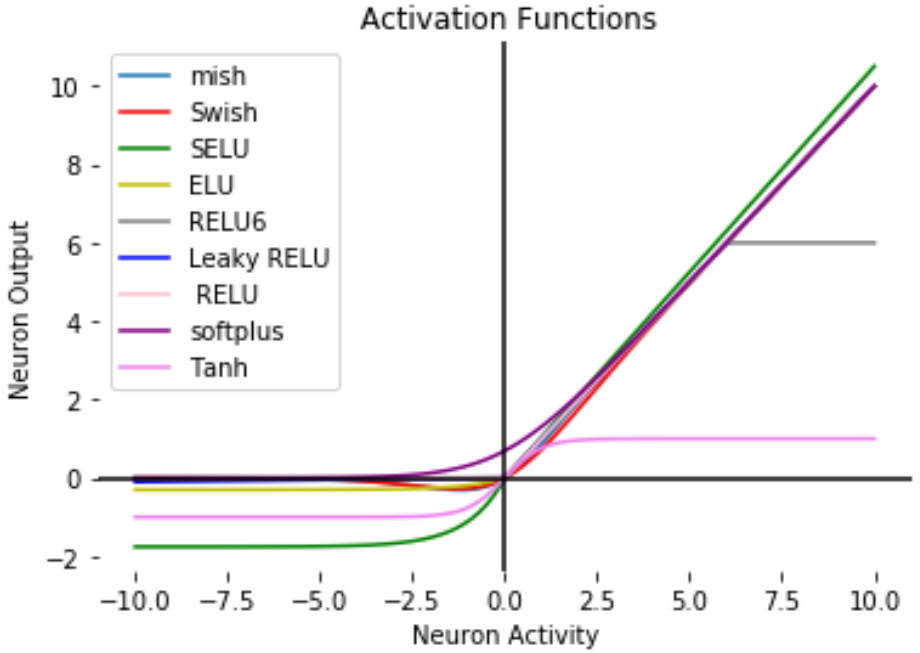

They are all very similar

I usually use leaky ReLU because it works well enough

https://pytorch.org/docs/stable/nn.html#non-linear-activations-weighted-sum-nonlinearity

https://jax.readthedocs.io/en/latest/jax.nn.html#activation-functions

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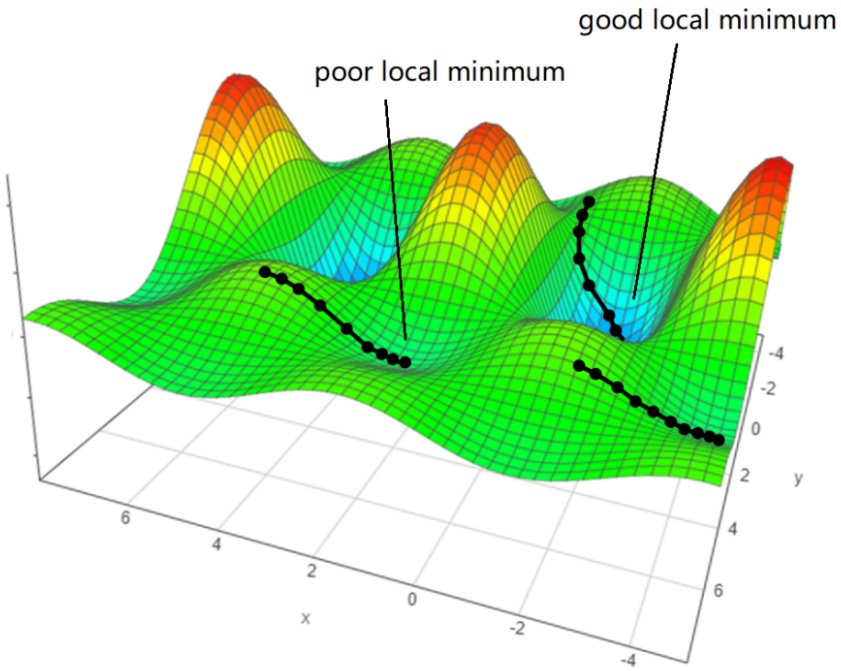
Recall the gradient descent algorithm

1: **function** GRADIENT DESCENT($\boldsymbol{X}$, $\boldsymbol{Y}$, $\mathcal{L}$, t, α)
2: ▷ Randomly initialize parameters
3: $\boldsymbol{\theta} \leftarrow \mathcal{N}(0, 1)$
4: **for** $i \in 1...t$ **do**
5: ▷ Compute the gradient of the loss
6: $\boldsymbol{J} \leftarrow \nabla_{\boldsymbol{\theta}} \mathcal{L}(\boldsymbol{X}, \boldsymbol{Y}, \boldsymbol{\theta})$
7: ▷ Update the parameters using the negative gradient
8: $\boldsymbol{\theta} \leftarrow \boldsymbol{\theta} - \alpha \boldsymbol{J}$
9: **return** $\boldsymbol{\theta}$

Initial θ is starting position for gradient descent

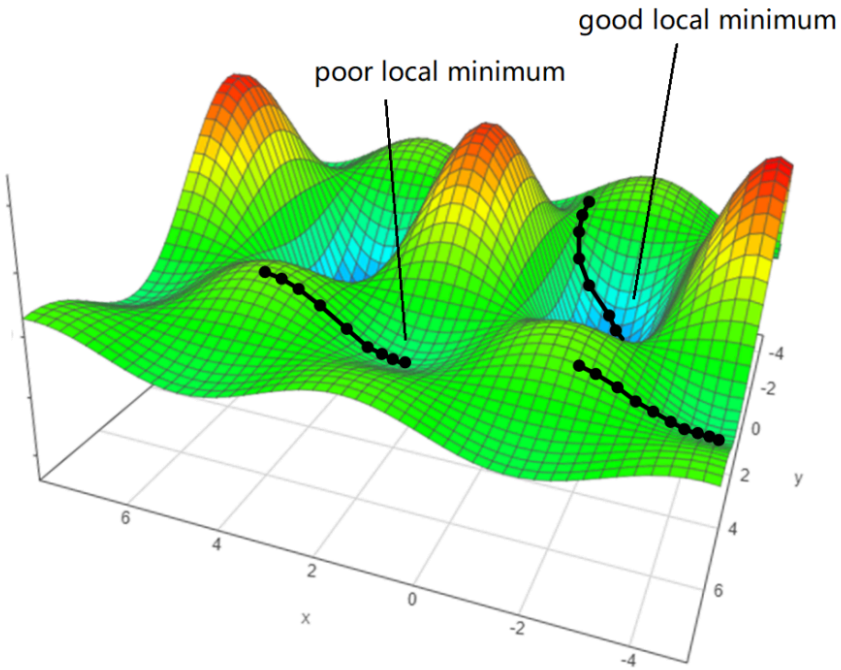
Parameter initialization

Initial θ is starting position for gradient descent



Parameter initialization

Initial θ is starting position for gradient descent



Pick θ that results in good local minima

Start simple, initialize all parameters to 0

$$\boldsymbol{\theta} = \begin{bmatrix} 0 & \dots & 0 \\ \vdots & \ddots & \vdots \\ 0 & \dots & 0 \end{bmatrix}, \begin{bmatrix} 0 & \dots & 0 \\ \vdots & \ddots & \vdots \\ 0 & \dots & 0 \end{bmatrix}, \dots$$

Parameter initialization

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$$\boldsymbol{\theta} = \begin{bmatrix} 0 & \dots & 0 \\ \vdots & \ddots & \vdots \\ 0 & \dots & 0 \end{bmatrix}, \begin{bmatrix} 0 & \dots & 0 \\ \vdots & \ddots & \vdots \\ 0 & \dots & 0 \end{bmatrix}, \dots$$

Question: Any issues?

Parameter initialization

Start simple, initialize all parameters to 0

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Question: Any issues?

Answer: The gradient will always be zero

$$\nabla_{\boldsymbol{\theta}_1} f = \sigma\left(\boldsymbol{\theta}_2^\top \sigma\left(\boldsymbol{\theta}_1^\top \overline{\boldsymbol{x}}\right)\right) \, \sigma\left(\boldsymbol{\theta}_1^\top \overline{\boldsymbol{x}}\right) \, \overline{\boldsymbol{x}}$$

Parameter initialization

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$$\nabla_{\boldsymbol{\theta}_1} f = \sigma\left(\mathbf{0}^\top \sigma\left(\boldsymbol{\theta}_1^\top \overline{\boldsymbol{x}}\right)\right) \sigma\left(\boldsymbol{\theta}_1^\top \overline{\boldsymbol{x}}\right) \overline{\boldsymbol{x}} = 0$$

Ok, so initialize $\boldsymbol{\theta} = \mathbf{1}$

Parameter initialization

Ok, so initialize $\boldsymbol{\theta} = \mathbf{1}$

$$\boldsymbol{\theta} = \begin{bmatrix} 1 & \dots & 1 \\ \vdots & \ddots & \vdots \\ 1 & \dots & 1 \end{bmatrix}, \begin{bmatrix} 1 & \dots & 1 \\ \vdots & \ddots & \vdots \\ 1 & \dots & 1 \end{bmatrix}, \dots$$

Parameter initialization

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$$\boldsymbol{\theta} = \begin{bmatrix} 1 & \dots & 1 \\ \vdots & \ddots & \vdots \\ 1 & \dots & 1 \end{bmatrix}, \begin{bmatrix} 1 & \dots & 1 \\ \vdots & \ddots & \vdots \\ 1 & \dots & 1 \end{bmatrix}, \dots$$

Question: Any issues?

All neurons in a layer will have the same gradient, and so they will always be the same (useless)

$$z_i = \sigma\left(\sum_{j=1}^{d_x} \theta_j \cdot \overline{x}_j\right) = \sigma\left(\sum_{j=1}^{d_x} \overline{x}_j\right)$$

$\boldsymbol{\theta}$ must be randomly initialized for neurons

$$\boldsymbol{\theta} = \begin{bmatrix} -0.5 & \dots & 2 \\ \vdots & \ddots & \vdots \\ 0.1 & \dots & 0.6 \end{bmatrix}, \begin{bmatrix} 1.3 & \dots & 1.2 \\ \vdots & \ddots & \vdots \\ -0.8 & \dots & -1.1 \end{bmatrix}, \dots$$

Parameter initialization

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But what scale? If $\boldsymbol{\theta} \ll 0$ the gradients will vanish to zero, if $\boldsymbol{\theta} \gg 0$ the gradients explode to infinity

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Parameter initialization

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Almost everyone initializes following a single paper from 2010:

- Glorot, Xavier, and Yoshua Bengio. “Understanding the difficulty of training deep feedforward neural networks."
- Maybe there are better options?

Here is the magic equation, given the input and output size of the layer is d_h

$$\boldsymbol{\theta} \sim \mathcal{U}\left[-\frac{\sqrt{6}}{\sqrt{2d_h}}, \frac{\sqrt{6}}{\sqrt{2d_h}}\right]$$

Parameter initialization

Here is the magic equation, given the input and output size of the layer is d_h

$$\boldsymbol{\theta} \sim \mathcal{U}\left[-\frac{\sqrt{6}}{\sqrt{2d_h}}, \frac{\sqrt{6}}{\sqrt{2d_h}}\right]$$

If you have different input or output sizes, such as d_x, d_y, then the equation is

$$\boldsymbol{\theta} \sim \mathcal{U}\left[-\frac{\sqrt{6}}{\sqrt{d_x + d_y}}, \frac{\sqrt{6}}{\sqrt{d_x + d_y}}\right]$$

These equations are designed for ReLU and similar activation functions

Parameter initialization

These equations are designed for ReLU and similar activation functions

They prevent vanishing or exploding gradients

Usually `torch` and `jax/equinox` will automatically use this initialization when you create `nn.Linear`

```
layer = nn.Linear(d_x, d_h) # Uses Glorot init
```

You can find many initialization functions at https://pytorch.org/docs/stable/nn.init.html

For JAX it is https://jax.readthedocs.io/en/latest/jax.nn.initializers.html

```python
import torch
d_h = 10
# Manually
theta = torch.zeros((d_h + 1, d_h))
torch.nn.init.xavier_uniform_(theta)
theta = torch.nn.Parameter(theta)

# Using nn.Linear
layer = torch.nn.Linear(d_h, d_h)
# USe .data, to bypass autograd security
torch.nn.init.xavier_uniform_(layer.weight.data)
torch.nn.init.xavier_uniform_(layer.bias.data)
```

```
import jax
d_h = 10

init = jax.nn.initializers.glorot_uniform()
theta = init(jax.random.key(0), (d_h + 1, d_h))
```

```python
import jax, equinox
d_h = 10

layer = equinox.nn.Linear(d_h, d_h, key=jax.random.key(0))
# Create new bias and weight
new_weight = init(jax.random.key(1), (d_h, d_h))
new_bias = init(jax.random.key(2), (d_h,))

# Use a lambda function to save space
# tree_at creates a new layer with the new weight
layer = equinox.tree_at(lambda l: l.weight, layer,
new_weight)
layer = equinox.tree_at(lambda l: l.bias, layer, new_weight)
```

Remember, in `equinox` and `torch`, `nn.Linear` will already be initialized correctly!

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```
function GRADIENT DESCENT(X, Y, 𝓛, t, α)
    ▷ Randomly initialize parameters
    θ ← Glorot()
    for i ∈ 1...t do
        ▷ Compute the gradient of the loss
        J ← ∇_θ 𝓛(X, Y, θ)
        ▷ Update the parameters using the negative gradient
        θ ← θ − αJ
    return θ
```

Stochastic gradient descent

1: **function** GRADIENT DESCENT($\boldsymbol{X}$, $\boldsymbol{Y}$, $\mathcal{L}$, t, α)
2: ▷ Randomly initialize parameters
3: $\boldsymbol{\theta} \leftarrow \text{Glorot}()$
4: **for** $i \in 1...t$ **do**
5: ▷ Compute the gradient of the loss
6: $\boldsymbol{J} \leftarrow \nabla_{\boldsymbol{\theta}} \mathcal{L}(\boldsymbol{X}, \boldsymbol{Y}, \boldsymbol{\theta})$
7: ▷ Update the parameters using the negative gradient
8: $\boldsymbol{\theta} \leftarrow \boldsymbol{\theta} - \alpha \boldsymbol{J}$
9: **return** $\boldsymbol{\theta}$

Gradient descent computes $\nabla \mathcal{L}$ over all $\boldsymbol{X}$

This works for our small datasets, where $n = 1000$

Stochastic gradient descent

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Question: How many GB are the LLM datasets?

Stochastic gradient descent

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Answer: About 774,000 GB according to *Datasets for Large Language Models: A Comprehensive Survey*

Stochastic gradient descent

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Question: How many GB are the LLM datasets?

Answer: About 774,000 GB according to *Datasets for Large Language Models: A Comprehensive Survey*

This is just the dataset size, the gradient is orders of magnitude larger

$$\nabla_{\boldsymbol{\theta}} \mathcal{L}\Big(\boldsymbol{x}_{[i]}, \boldsymbol{y}_{[i]}, \boldsymbol{\theta}\Big) = \begin{bmatrix} \frac{\partial f_1}{\partial x_1} & \cdots & \frac{\partial f_\ell}{\partial x_1} \\ \vdots & \ddots & \vdots \\ \frac{\partial f_n}{\partial x_1} & \cdots & \frac{\partial f_\ell}{\partial x_1} \end{bmatrix}_{[i]}$$

Question: We do not have enough memory to compute the gradient. What can we do?

Stochastic gradient descent

Question: We do not have enough memory to compute the gradient. What can we do?

Answer: We approximate the gradient using a subset of the data

First, we sample random datapoint indices

$$i, j, k, \ldots \sim \mathcal{U}[1, n]$$

Stochastic gradient descent

First, we sample random datapoint indices

$$i, j, k, \ldots \sim \mathcal{U}[1, n]$$

Then construct a **batch** of training data

$$\begin{bmatrix} \boldsymbol{x}_{[i]} \\ \boldsymbol{x}_{[j]} \\ \boldsymbol{x}_{[k]} \\ \vdots \end{bmatrix}; \quad \begin{bmatrix} \boldsymbol{y}_{[i]} \\ \boldsymbol{y}_{[j]} \\ \boldsymbol{y}_{[k]} \\ \vdots \end{bmatrix}$$

Stochastic gradient descent

First, we sample random datapoint indices

$$i, j, k, \ldots \sim \mathcal{U}[1, n]$$

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We call this **stochastic gradient descent**

1: **function** STOCHASTIC GRADIENT DESCENT($\boldsymbol{X}$, $\boldsymbol{Y}$, $\mathcal{L}$, t, α)
2: $\quad\boldsymbol{\theta} \leftarrow \text{Glorot}()$
3: $\quad$**for** $i \in 1...t$ **do**
4: $\quad\quad\boldsymbol{X}, \boldsymbol{Y} \leftarrow \text{Shuffle}(\boldsymbol{X}), \text{Shuffle}(\boldsymbol{Y})$
5: $\quad\quad$**for** $j \in 0...\frac{n}{B} - 1$ **do**
6: $\quad\quad\quad\boldsymbol{X}_j \leftarrow \begin{bmatrix}\boldsymbol{x}_{[jB]} & \boldsymbol{x}_{[jB+1]} & \cdots & \boldsymbol{x}_{[(j+1)B]}\end{bmatrix}$
7: $\quad\quad\quad\boldsymbol{Y}_j \leftarrow \begin{bmatrix}\boldsymbol{y}_{[jB]} & \boldsymbol{y}_{[jB+1]} & \cdots & \boldsymbol{y}_{[(j+1)B]}\end{bmatrix}$
8: $\quad\quad\quad\boldsymbol{J} \leftarrow \nabla_{\boldsymbol{\theta}}\mathcal{L}\left(\boldsymbol{X}_j, \boldsymbol{Y}_j, \boldsymbol{\theta}\right)$
9: $\quad\quad\quad\boldsymbol{\theta} \leftarrow \boldsymbol{\theta} - \alpha\boldsymbol{J}$
10: $\quad$**return** $\boldsymbol{\theta}$

Stochastic gradient descent (SGD) is useful for saving memory

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But it can also improve performance

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Since the “dataset” changes every update, so does the loss manifold

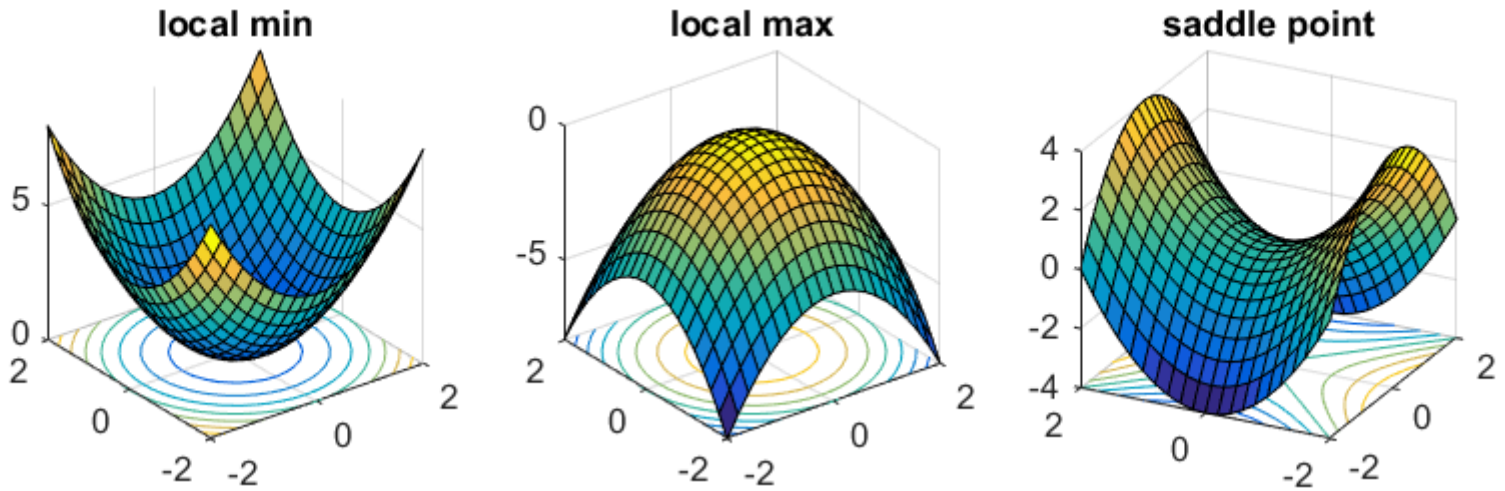
Stochastic gradient descent

Stochastic gradient descent (SGD) is useful for saving memory

But it can also improve performance

Since the "dataset" changes every update, so does the loss manifold

This makes it less likely we get stuck in bad optima



There is `torch.utils.data.DataLoader` to help

Stochastic gradient descent

There is `torch.utils.data.DataLoader` to help

```
import torch
dataloader = torch.utils.data.DataLoader(
    training_data,
    batch_size=32, # How many datapoints to sample
    shuffle=True, # Randomly shuffle each epoch
)
for epoch in number_of_epochs:
    for batch in dataloader:
        X_j, Y_j = batch
        loss = L(X_j, Y_j, theta)
        ...
```

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Gradient descent is a powerful tool, but it has issues

Modern optimization

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Many researchers work on improving gradient descent to converge more quickly, while also preventing premature convergence

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It is hard to teach adaptive optimization through math

Modern optimization

Gradient descent is a powerful tool, but it has issues

1. It can be slow to converge
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Many researchers work on improving gradient descent to converge more quickly, while also preventing premature convergence

It is hard to teach adaptive optimization through math

So first, I want to show you a video to prepare you

https://www.youtube.com/watch?v=MD2fYip6QsQ&t=77s

The video simulations provide an intuitive understanding of adaptive optimizers

Modern optimization

The video simulations provide an intuitive understanding of adaptive optimizers

The key behind modern optimizers is two concepts:

- Momentum

Modern optimization

The video simulations provide an intuitive understanding of adaptive optimizers

The key behind modern optimizers is two concepts:

- Momentum
- Adaptive learning rate

Modern optimization

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The key behind modern optimizers is two concepts:

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Let us discuss the algorithms more slowly

Review gradient descent again, because we will be making changes to it

Modern optimization

Review gradient descent again, because we will be making changes to it

function GRADIENT DESCENT($\boldsymbol{X}$, $\boldsymbol{Y}$, $\mathcal{L}$, t, α)
    ▷ Randomly initialize parameters
    $\boldsymbol{\theta} \leftarrow \text{Glorot}()$
    for $i \in 1...t$ **do**
        ▷ Compute the gradient of the loss
        $\boldsymbol{J} \leftarrow \nabla_{\boldsymbol{\theta}} \mathcal{L}(\boldsymbol{X}, \boldsymbol{Y}, \boldsymbol{\theta})$
        ▷ Update the parameters using the negative gradient
        $\boldsymbol{\theta} \leftarrow \boldsymbol{\theta} - \alpha \boldsymbol{J}$
    return $\boldsymbol{\theta}$

Introduce **momentum** first

Modern optimization

Introduce **momentum** first

1: **function** Momentum Gradient Descent($\boldsymbol{X}$, $\boldsymbol{Y}$, $\mathcal{L}$, t, α, β)
2: $\boldsymbol{\theta} \leftarrow \text{Glorot}()$
3: $\boldsymbol{M} \leftarrow \boldsymbol{0}$ # Init momentum
4: **for** $i \in 1...t$ **do**
5: $\boldsymbol{J} \leftarrow \nabla_{\boldsymbol{\theta}} \mathcal{L}(\boldsymbol{X}, \boldsymbol{Y}, \boldsymbol{\theta})$ # Represents acceleration
6: $\boldsymbol{M} \leftarrow \beta \cdot \boldsymbol{M} + (1 - \beta) \cdot \boldsymbol{J}$ # Momentum and acceleration
7: $\boldsymbol{\theta} \leftarrow \boldsymbol{\theta} - \alpha \boldsymbol{M}$
8: **return** $\boldsymbol{\theta}$

Now **adaptive learning rate**

Modern optimization

Now **adaptive learning rate**

1: **function** RMSProp($\boldsymbol{X}, \boldsymbol{Y}, \mathcal{L}, t, \alpha, \beta, \varepsilon$)
2: $\quad\boldsymbol{\theta} \leftarrow \text{Glorot}()$
3: $\quad\boldsymbol{V} \leftarrow \boldsymbol{0}$ # Init variance
4: $\quad$**for** $i \in 1...t$ **do**
5: $\quad\quad\boldsymbol{J} \leftarrow \nabla_{\boldsymbol{\theta}}\mathcal{L}(\boldsymbol{X}, \boldsymbol{Y}, \boldsymbol{\theta})$ # Represents acceleration
6: $\quad\quad\boldsymbol{V} \leftarrow \beta \cdot \boldsymbol{V} + (1-\beta) \cdot \boldsymbol{J} \odot \boldsymbol{J}$ # Magnitude
7: $\quad\quad\boldsymbol{\theta} \leftarrow \boldsymbol{\theta} - \alpha \boldsymbol{J} \oslash \sqrt[\odot]{\boldsymbol{V} + \varepsilon}$ # Rescale grad by prev updates
8: $\quad$**return** $\boldsymbol{\theta}$

Combine **momentum** and **adaptive learning rate** to create **Adam**

Modern optimization

Combine **momentum** and **adaptive learning rate** to create **Adam**

function ADAPTIVE MOMENT ESTIMATION($\boldsymbol{X}$, $\boldsymbol{Y}$, $\mathcal{L}$, t, α, β_1, β_2, ε)
    $\boldsymbol{\theta} \leftarrow \text{Glorot}()$
    $\boldsymbol{M}, \boldsymbol{V} \leftarrow \boldsymbol{0}$
    for $i \in 1...t$ **do**
        $\boldsymbol{J} \leftarrow \nabla_{\boldsymbol{\theta}} \mathcal{L}(\boldsymbol{X}, \boldsymbol{Y}, \boldsymbol{\theta})$
        $\boldsymbol{M} \leftarrow \beta_1 \boldsymbol{M} + (1 - \beta_1)\boldsymbol{J}$ # Compute momentum
        $\boldsymbol{V} \leftarrow \beta_2 \cdot \boldsymbol{V} + (1 - \beta_2) \cdot \boldsymbol{J} \odot \boldsymbol{J}$ # Magnitude
        $\boldsymbol{\theta} \leftarrow \boldsymbol{\theta} - \alpha \boldsymbol{M} \oslash \sqrt[\circ]{\boldsymbol{V} + \varepsilon}$ # Adaptive param update
    return $\boldsymbol{\theta}$ # Note, we use biased $\boldsymbol{M}, \boldsymbol{V}$ for clarity

```
import torch
betas = (0.9, 0.999)
net = ...
theta = net.parameters()

sgd = torch.optim.SGD(theta, lr=alpha)
momentum = torch.optim.SGD(
    theta, lr=alpha, momentum=betas[0])
rmsprop = torch.optim.RMSprop(
    theta, lr=alpha, momentum=betas[1])
adam = torch.optim.Adam(theta, lr=alpha, betas=betas)
...
sgd.step(), momentum.step(), rmsprop.step(), adam.step()
```

```
import optax
betas = (0.9, 0.999)
theta = ...

sgd = optax.sgd(lr=alpha)
momentum = optax.sgd(lr=alpha, momentum=betas[0])
rmsprop = optax.rmsprop(lr=alpha, decay=betas[1])
adam = optax.adam(lr=alpha, b1=betas[0], b2=betas[1])

v = rmsprop.init(theta)
theta, v = rmsprop.update(J, v, theta)
mv = adam.init(theta) # contains M and V
theta, mv = mv.update(J, mv, theta)
```

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https://colab.research.google.com/drive/1qTNSvB_JEMnMJfcAwsLJTuIlfxa_kyTD#scrollTo=YVkCyz78x4Rp