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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There is no widely-accepted theory for why deep neural networks are so effective

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In modern deep learning, we progress using trial and error

Today we experiment, and maybe tomorrow we discover the theory

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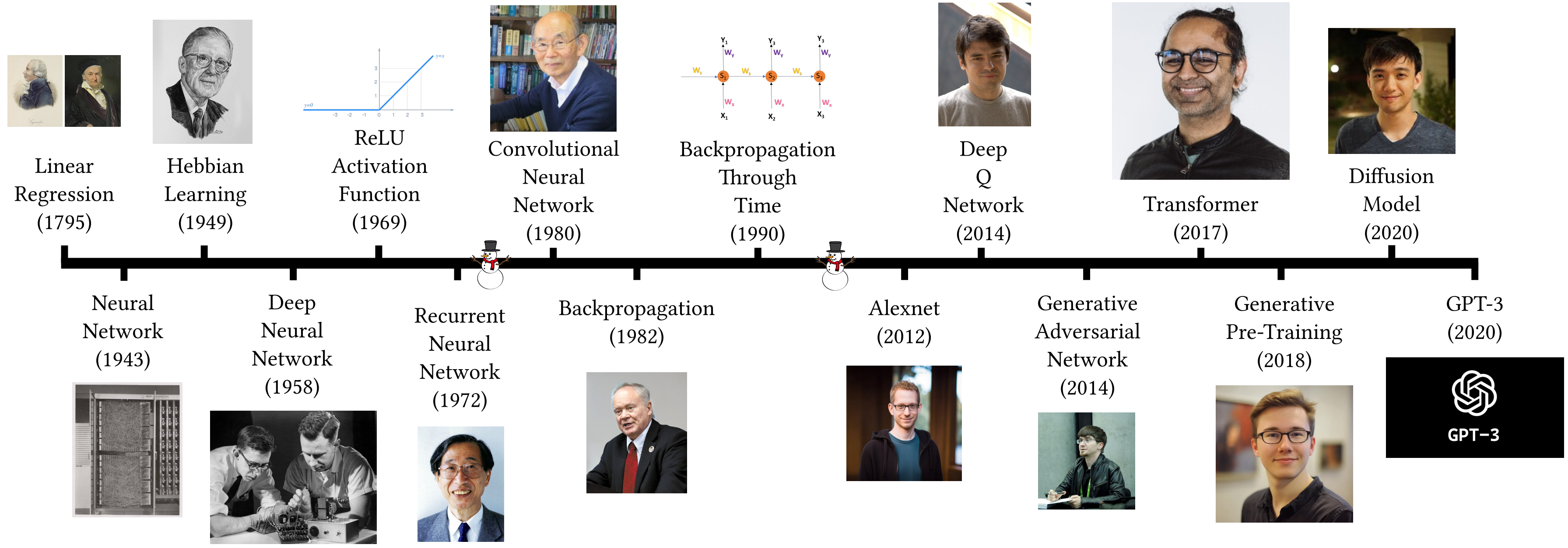

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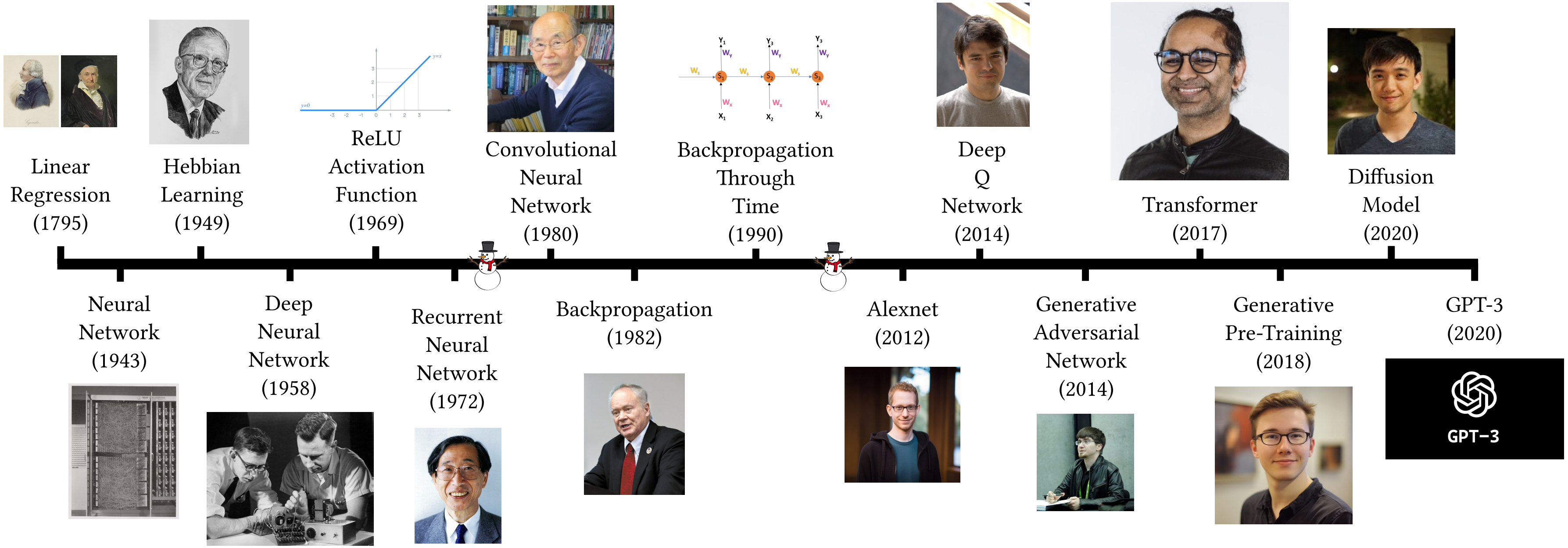

Are modern networks are too complex for humans to understand?

Dirty Secret of Deep Learning

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!

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

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

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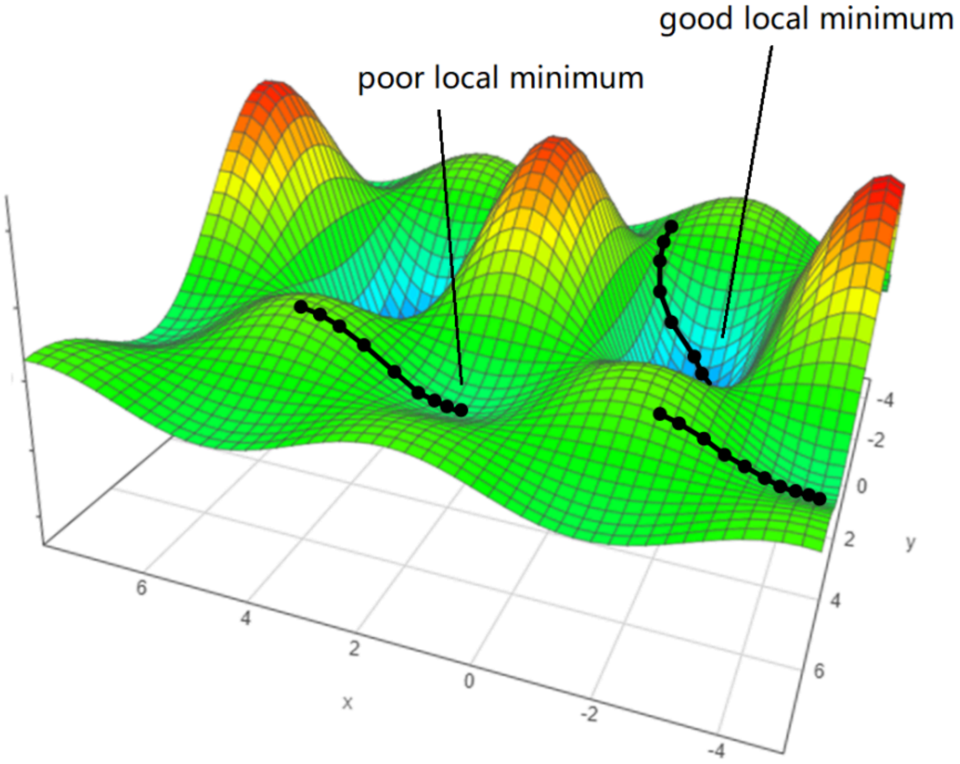

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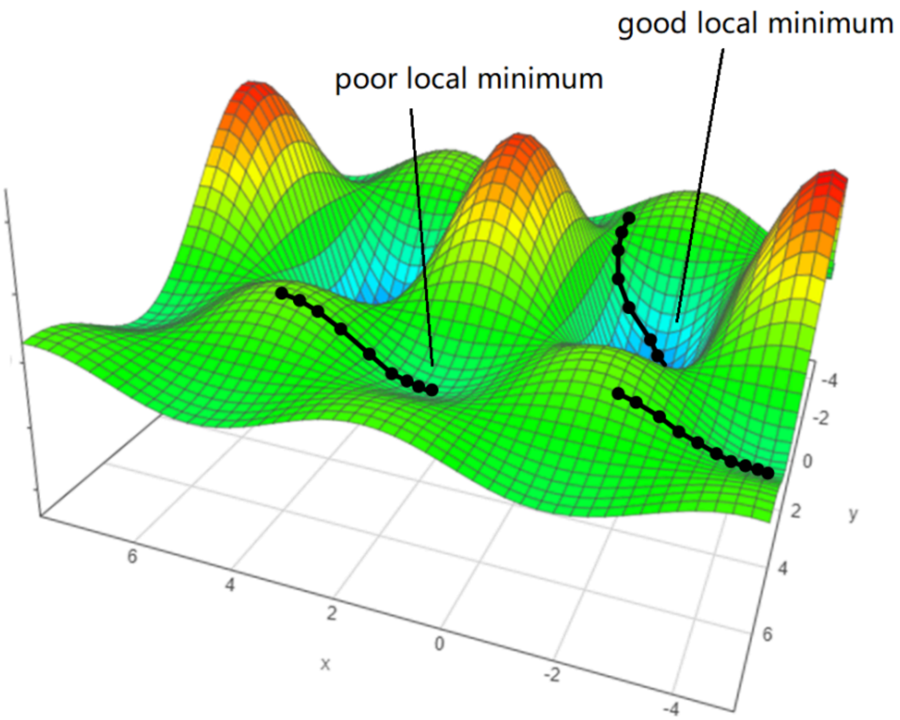

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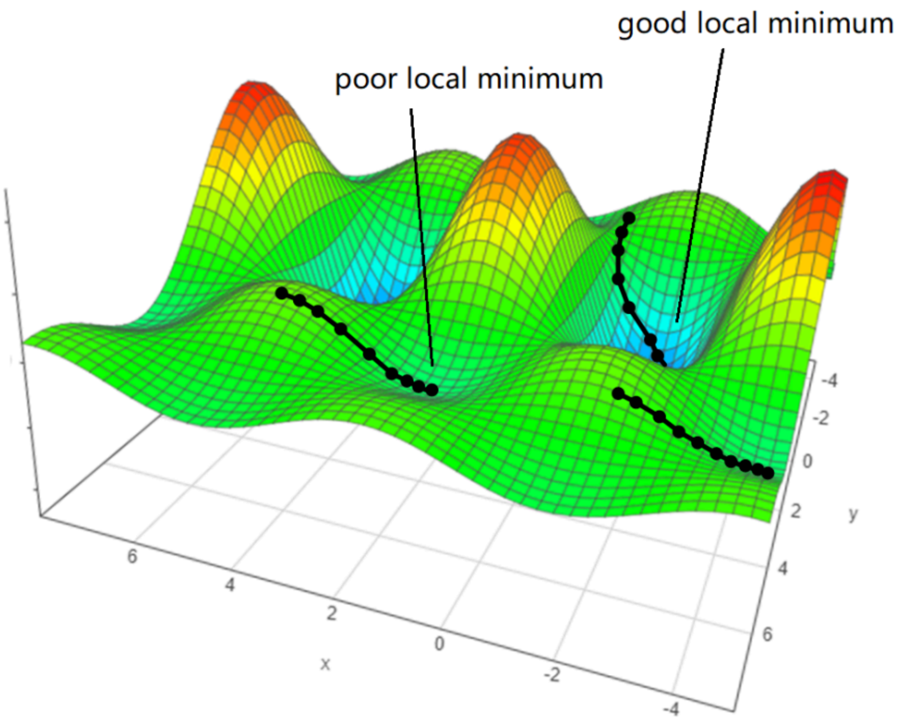

Harder tasks can have millions of local optima, and many of the local optima are not very good!

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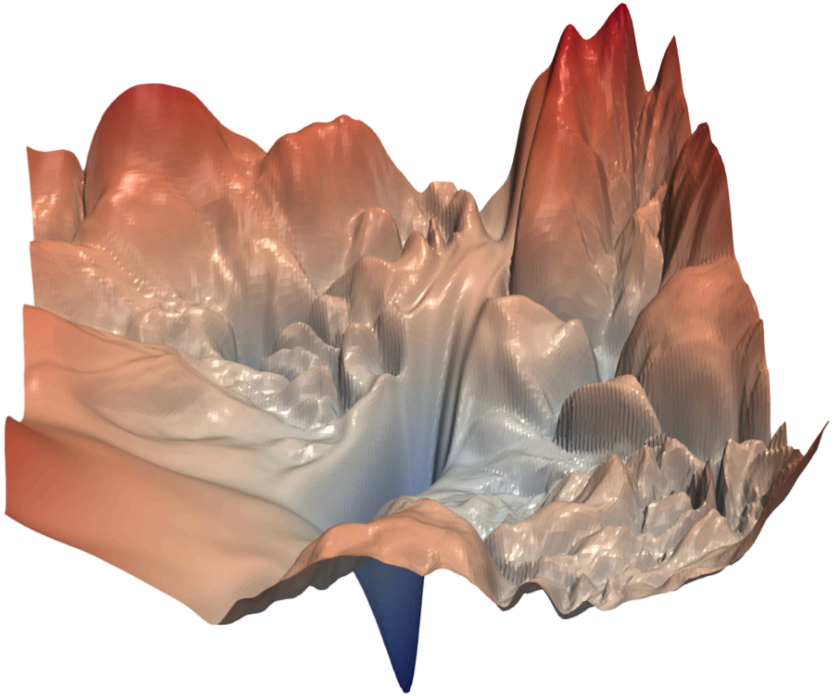

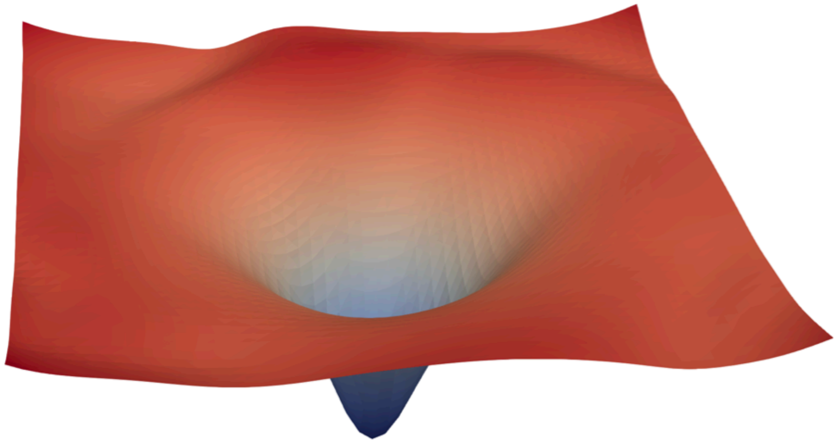

Gradient descent reaches a better optimum more quickly in these cases

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For certain problems, adding one more layer is equivalent to **exponentially** increasing the width

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We need more layers for harder problems

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- "For large-size networks, most local minima are equivalent and yield similar performance on a test set."

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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"

Deeper Neural Networks

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

Deeper Neural Networks

```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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```

```python
# 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)
```

Deeper Neural Networks

```python
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)
```

Deeper Neural Networks

```
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),
    equinox.nn.Lambda(jax.nn.sigmoid),
    ...
    equinox.nn.Linear(d_h, d_y),
])

x = jax.numpy.ones((d_x,))
y = net(x)
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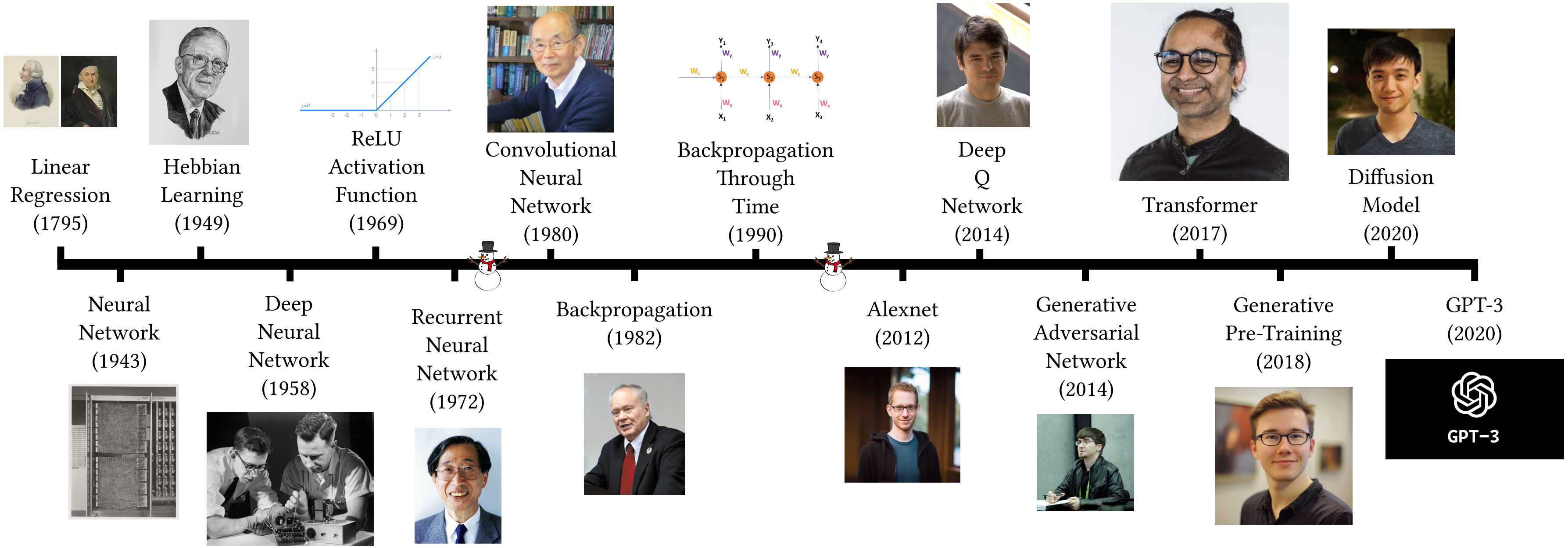

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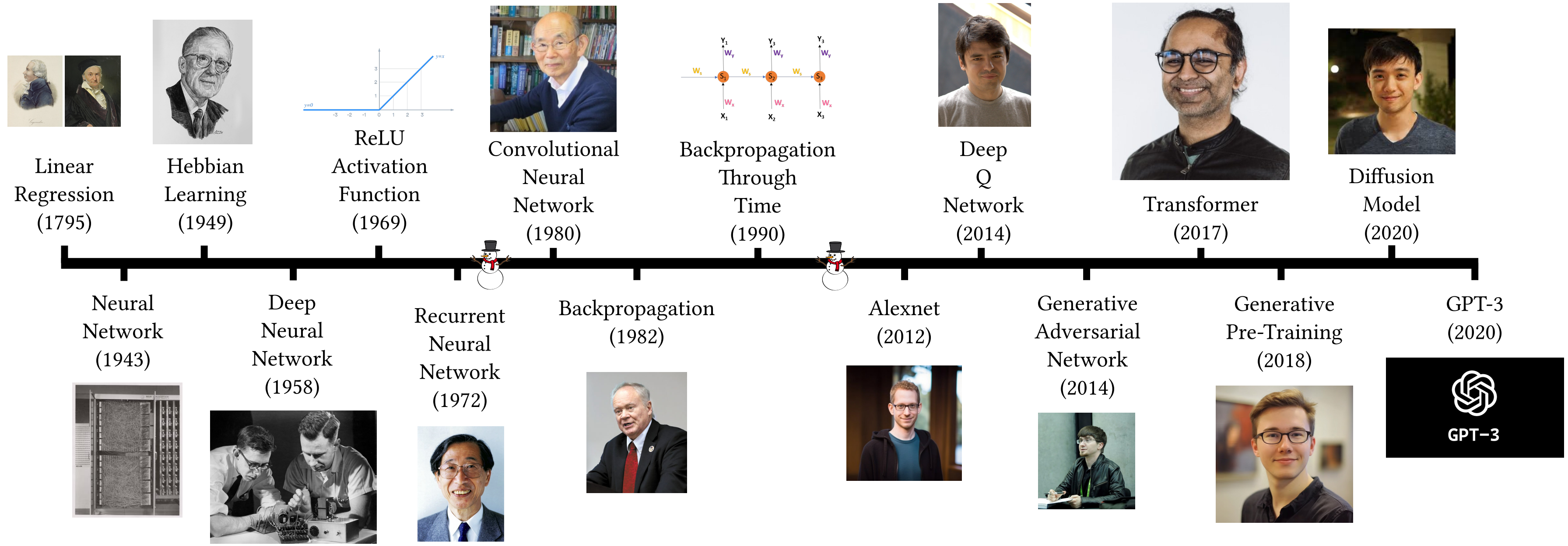
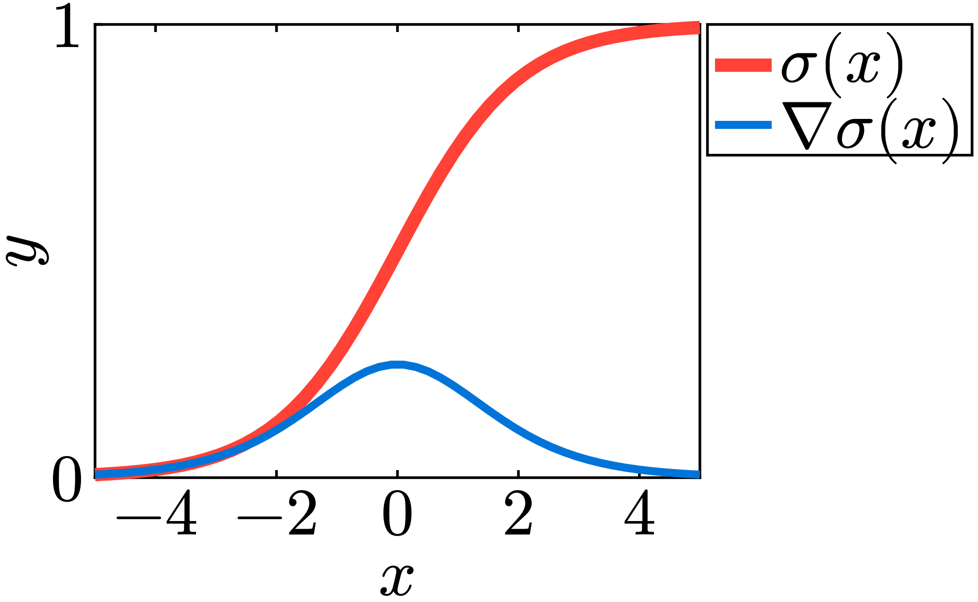


In 2012, people realized that ReLU activation performed much better

Activation Functions



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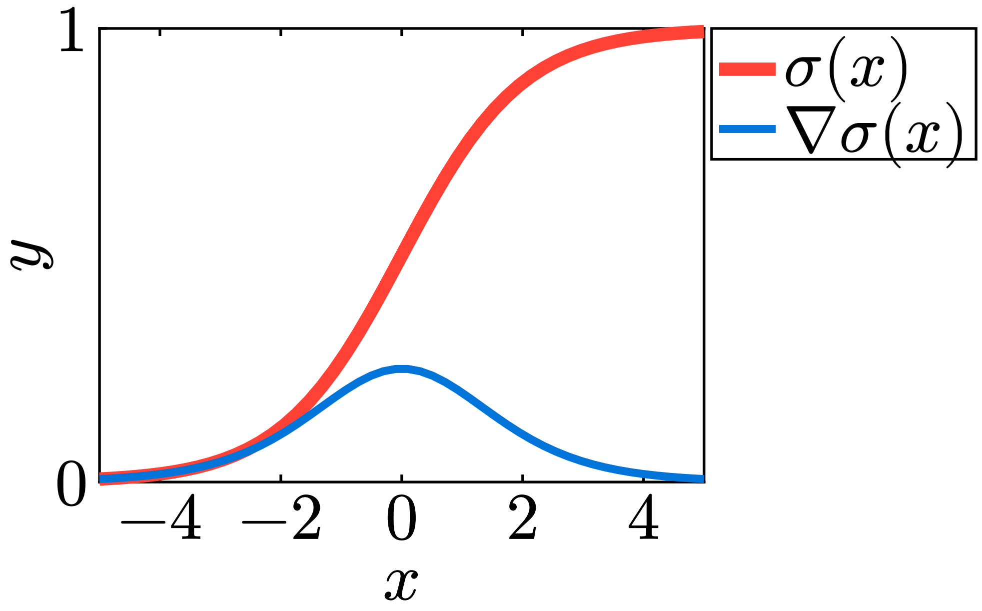

The sigmoid function can result in a **vanishing gradient**

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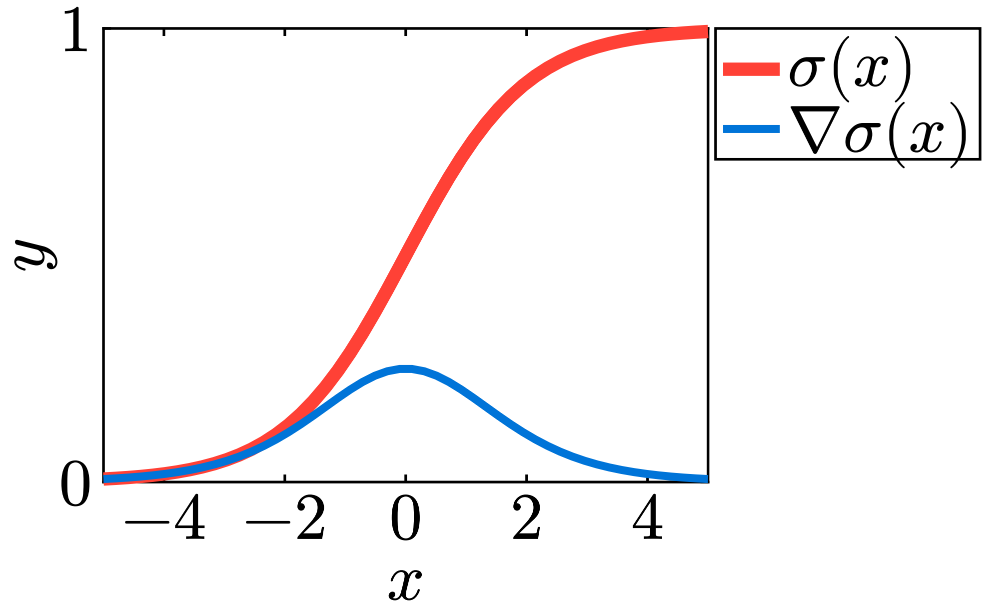

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$$f(\boldsymbol{x}, \boldsymbol{\theta}) = \sigma(\boldsymbol{\theta}_3^\top \sigma(\boldsymbol{\theta}_2^\top \sigma(\boldsymbol{\theta}_1^\top \overline{\boldsymbol{x}})))$$

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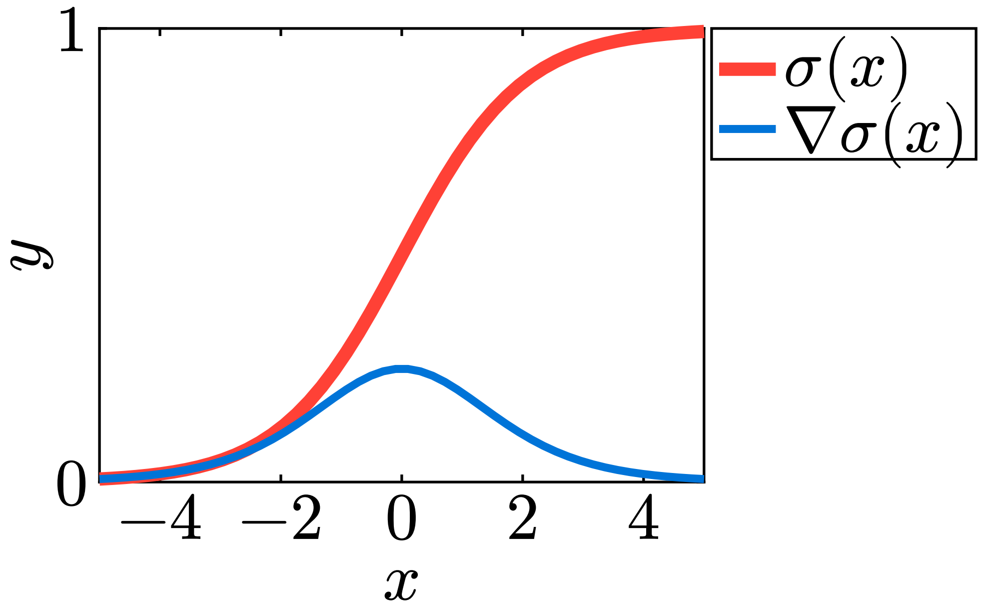

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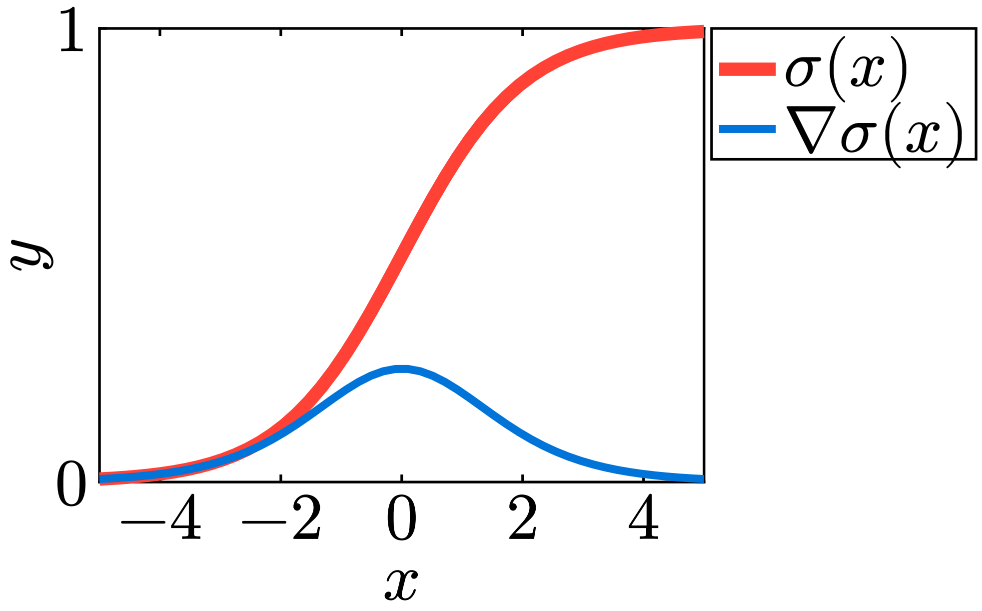

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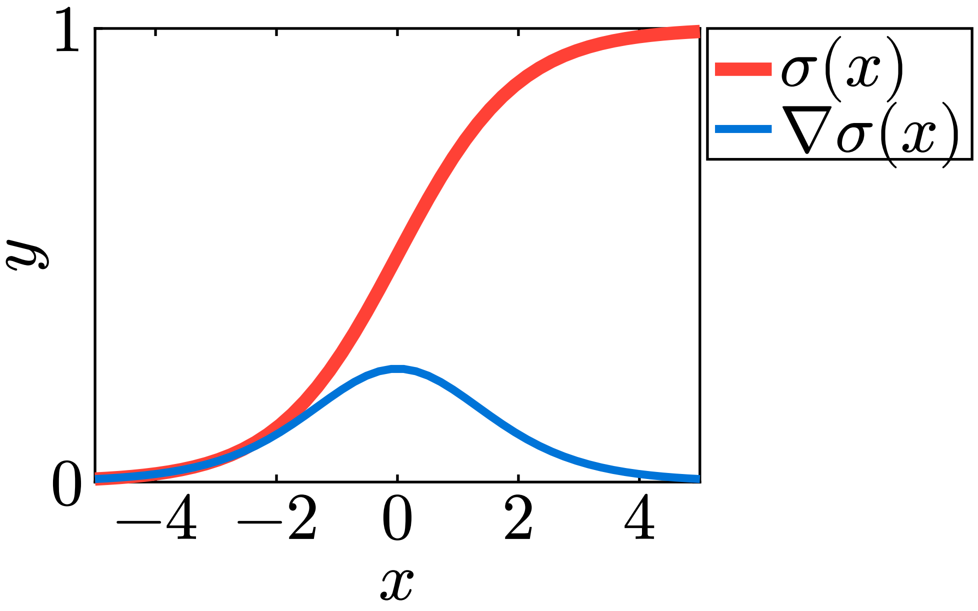

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$$\nabla_{\boldsymbol{\theta}} f(\boldsymbol{x}, \boldsymbol{\theta}) \approx 0$$

Activation Functions

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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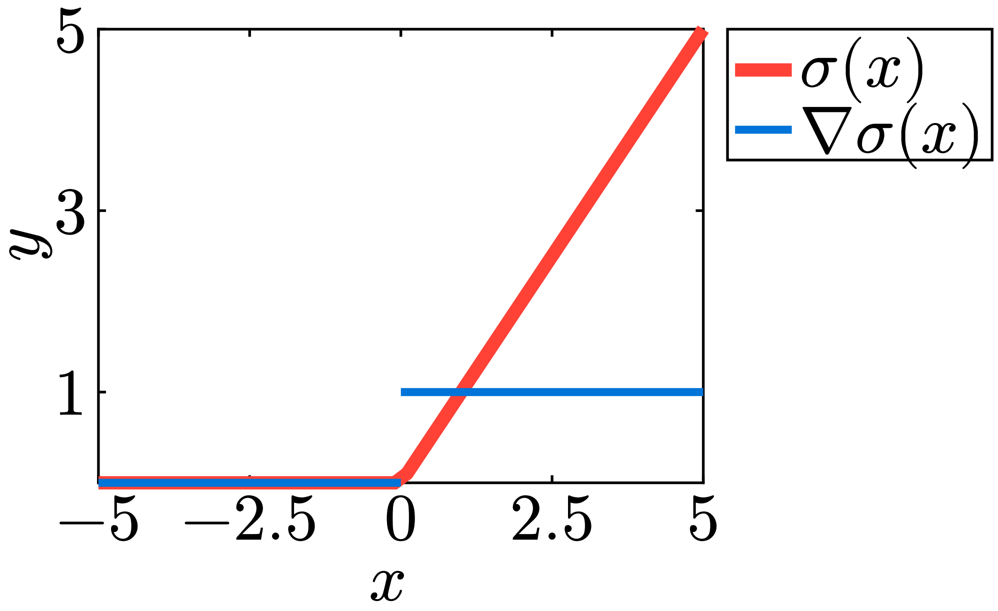

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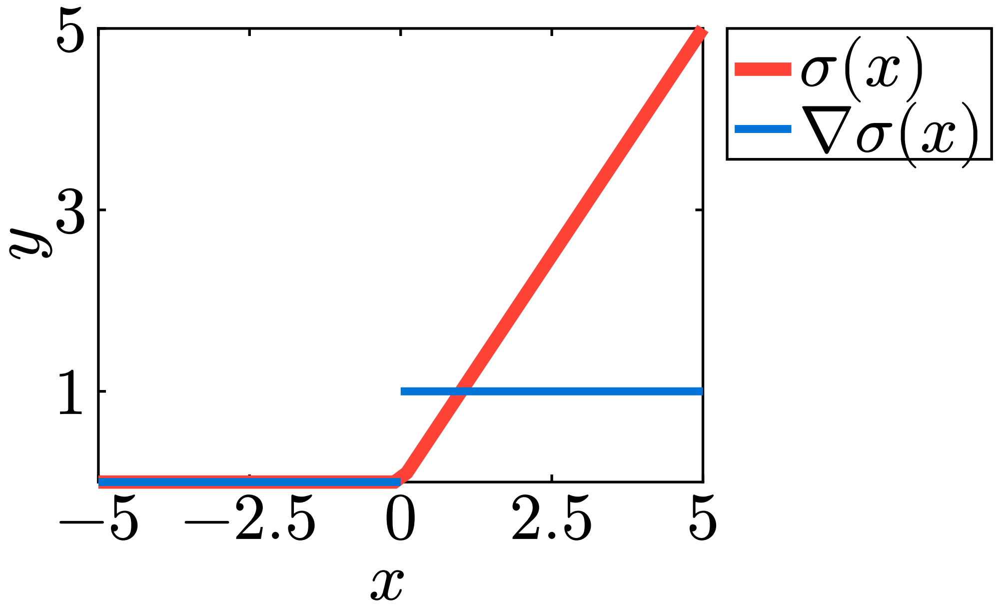

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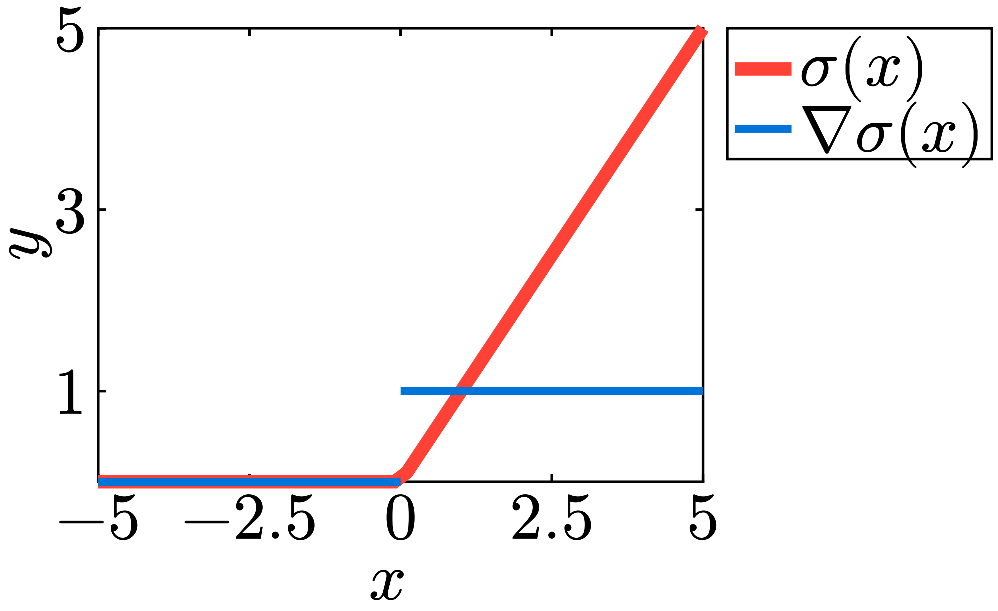

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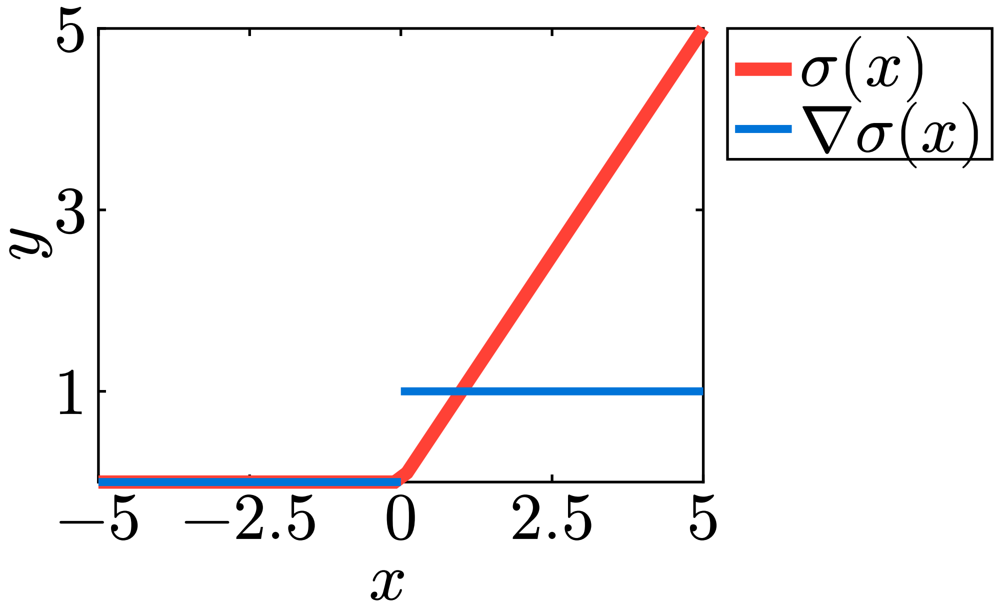

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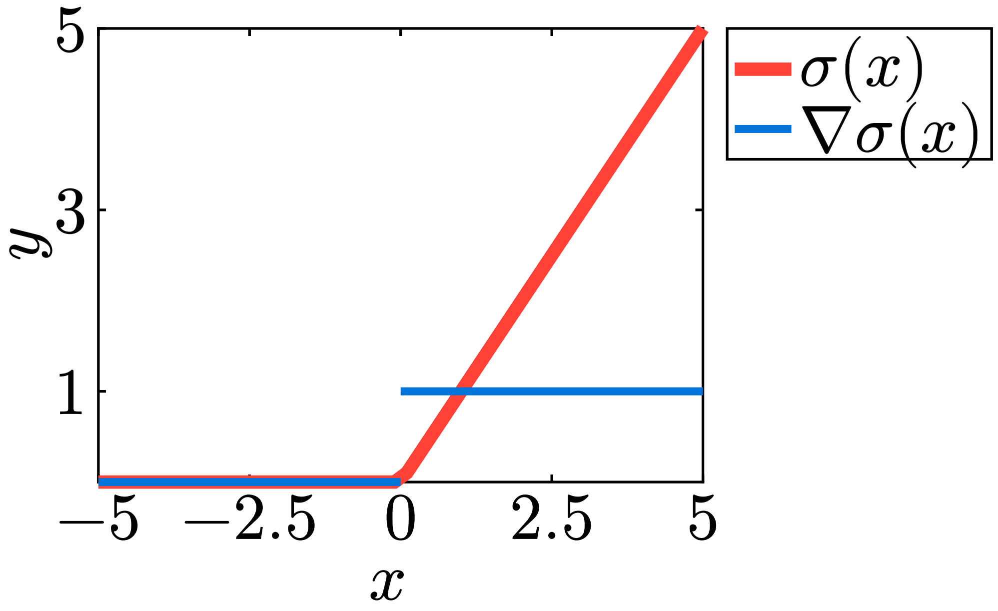

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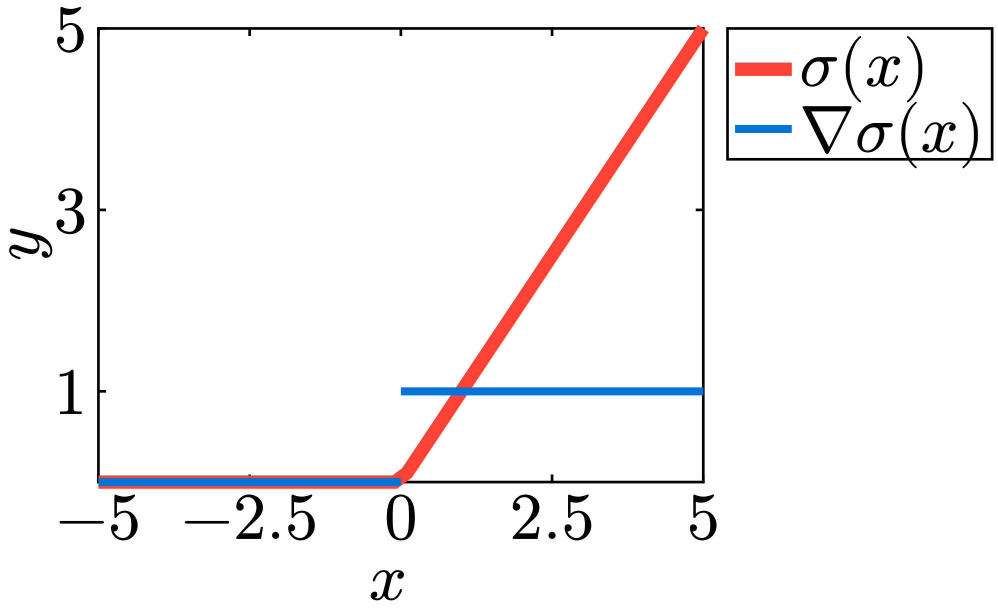

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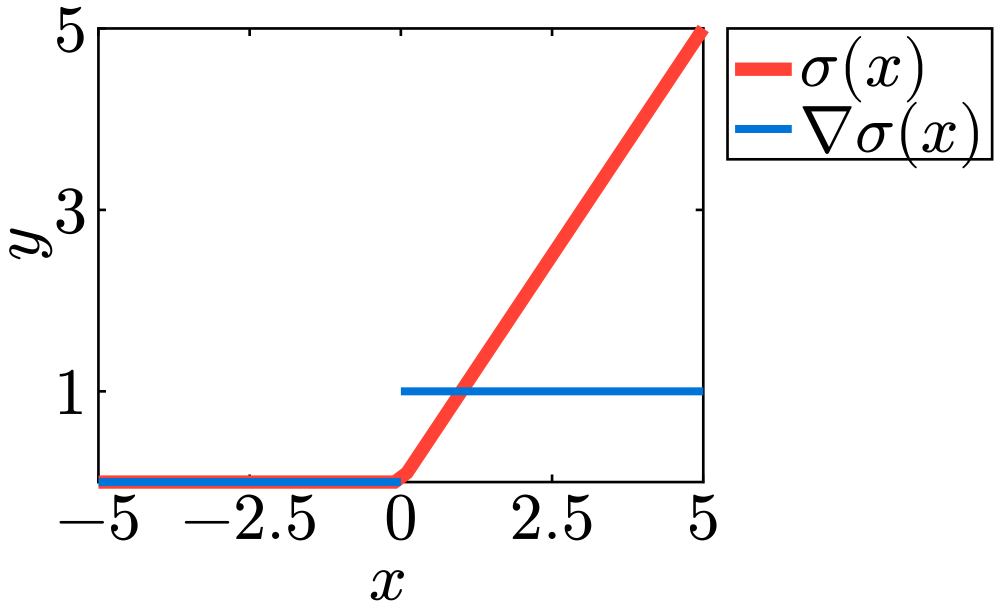

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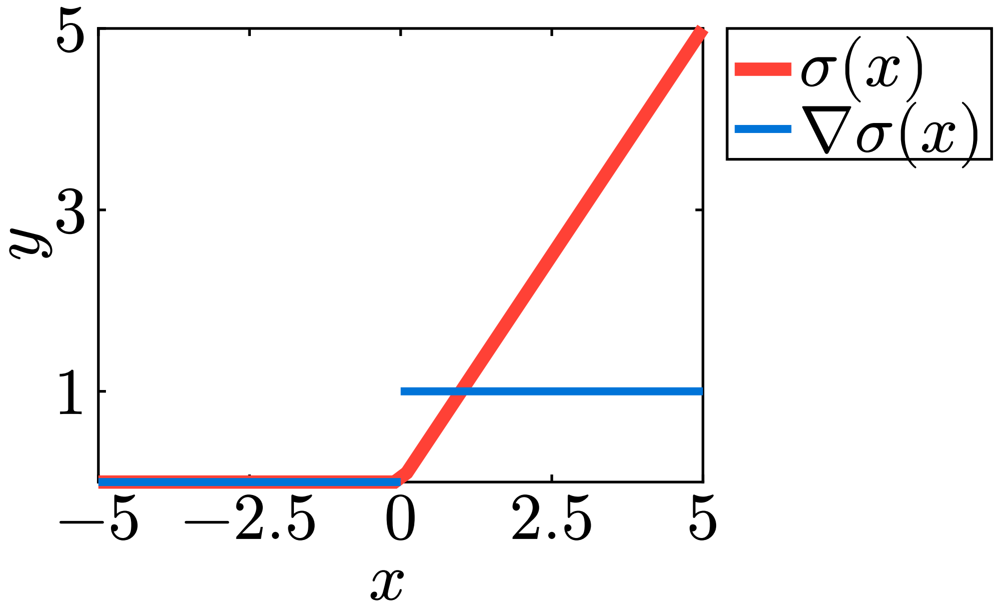

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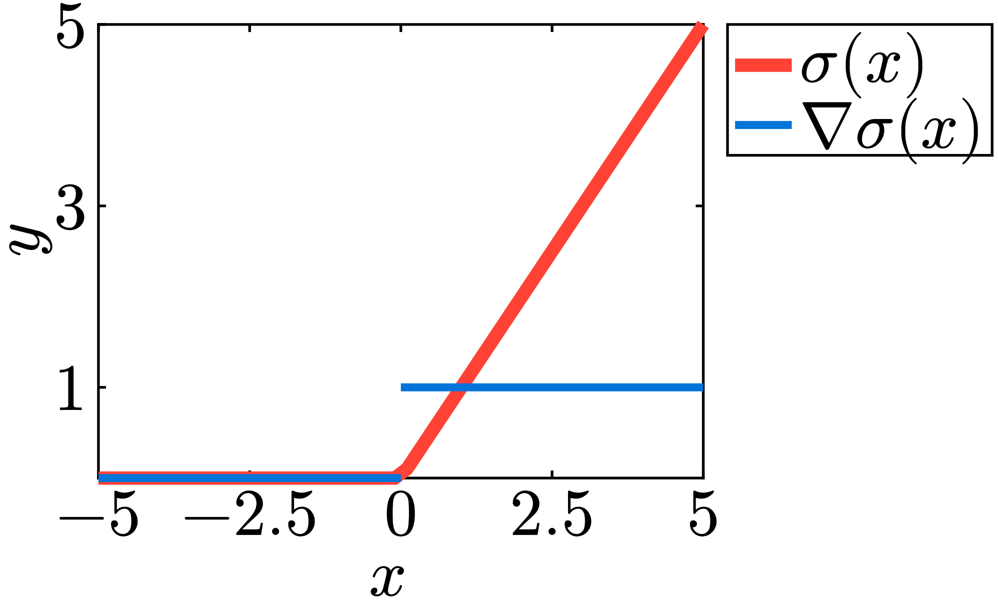

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These neurons cannot recover, they are **dead neurons**

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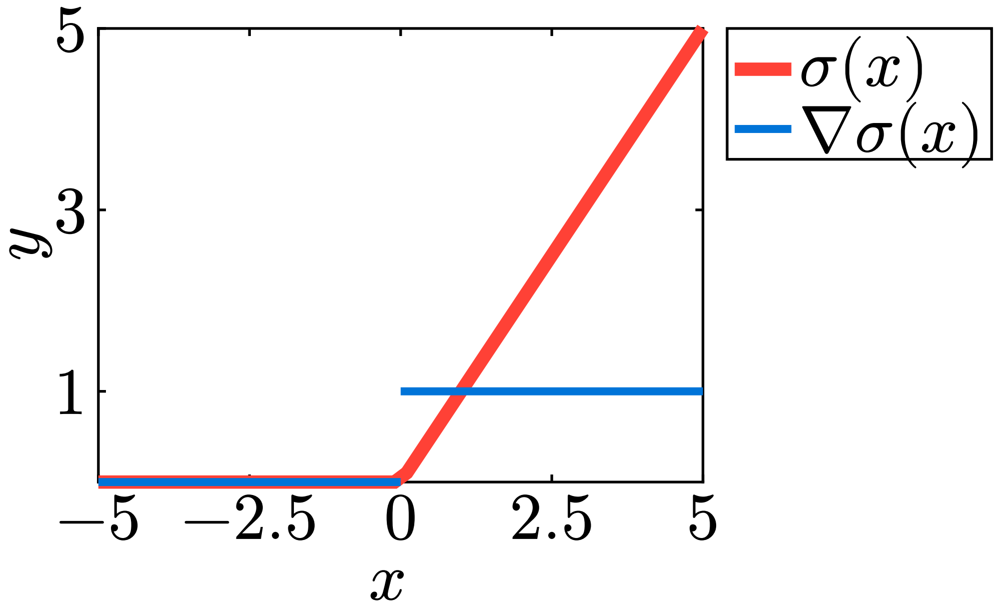

These neurons cannot recover, they are **dead neurons**

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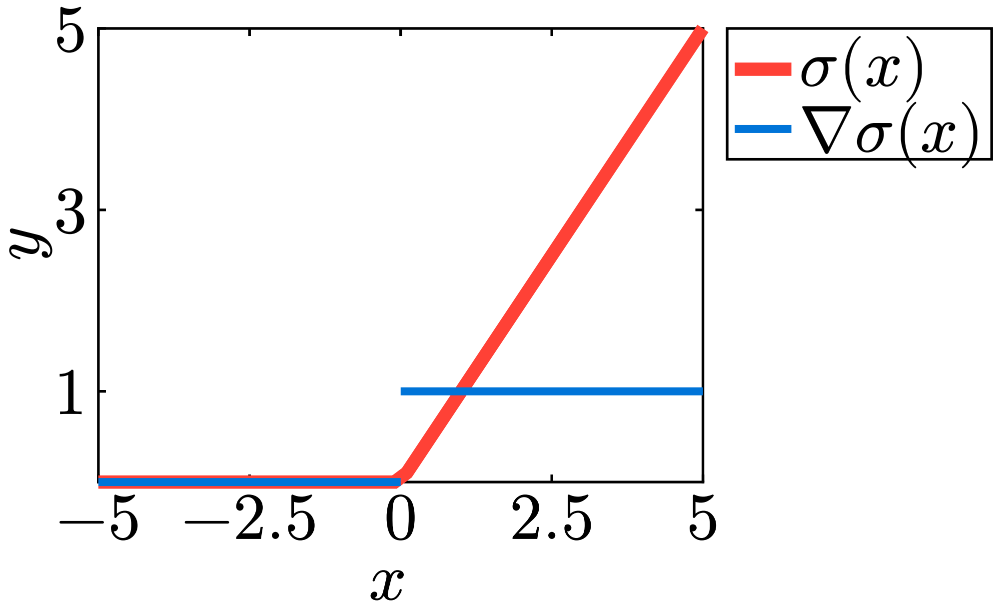

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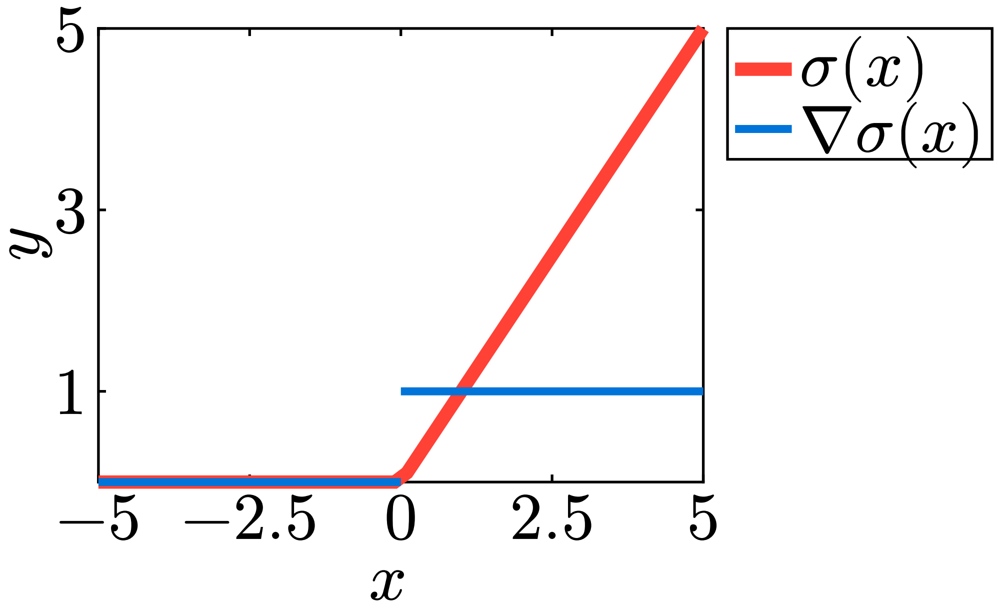

These neurons cannot recover, they are **dead neurons**

Training for longer results in more dead neurons

Dead neurons hurt your network!

Activation Functions

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

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

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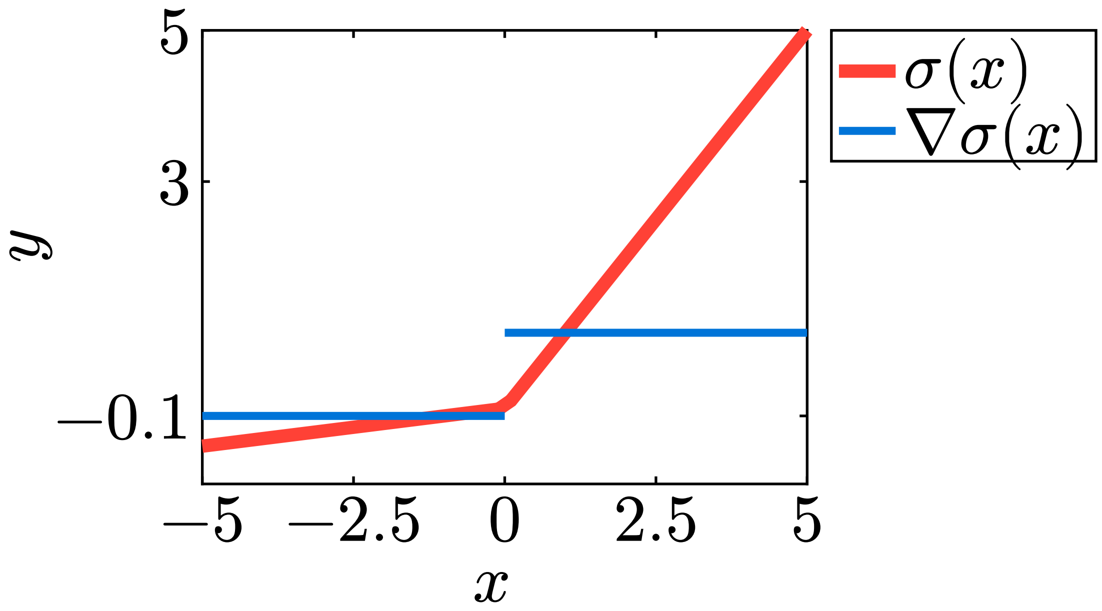

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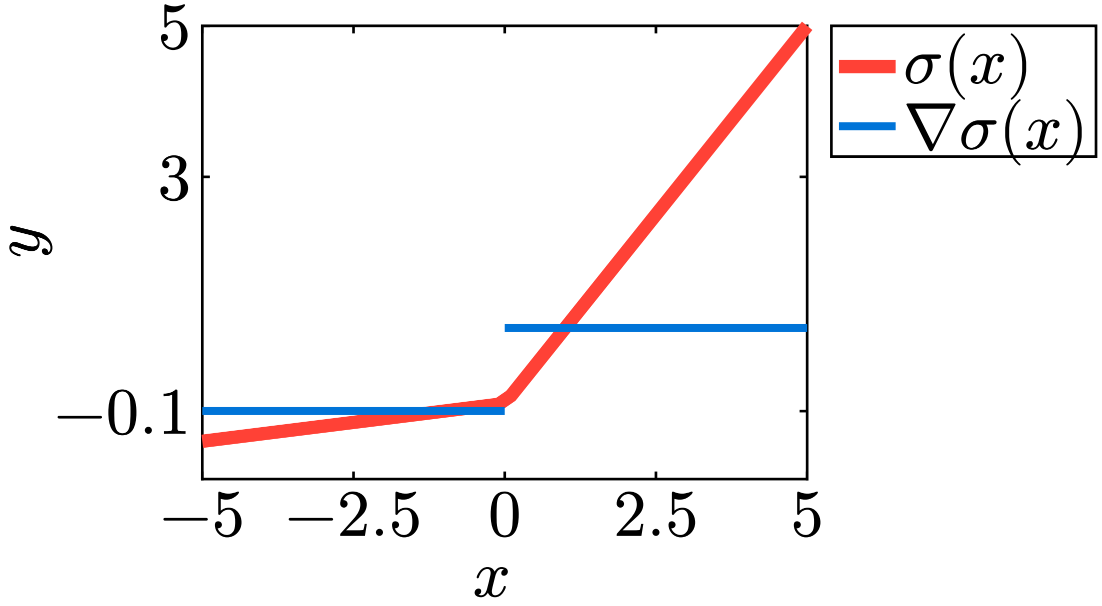

Small negative slope allows dead neurons to recover

Activation Functions

There are other activation functions that are better than leaky ReLU

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- Mish

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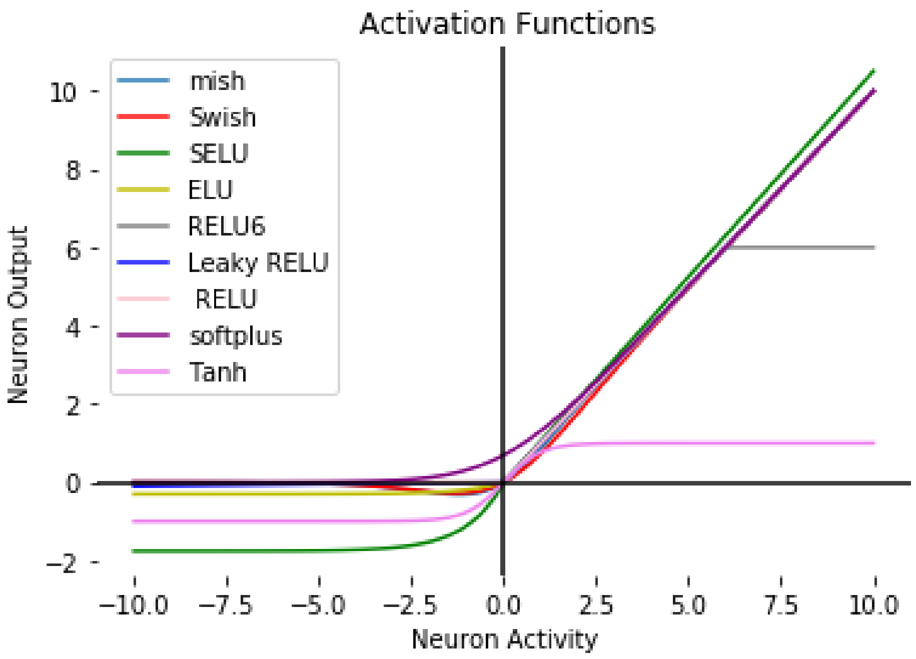

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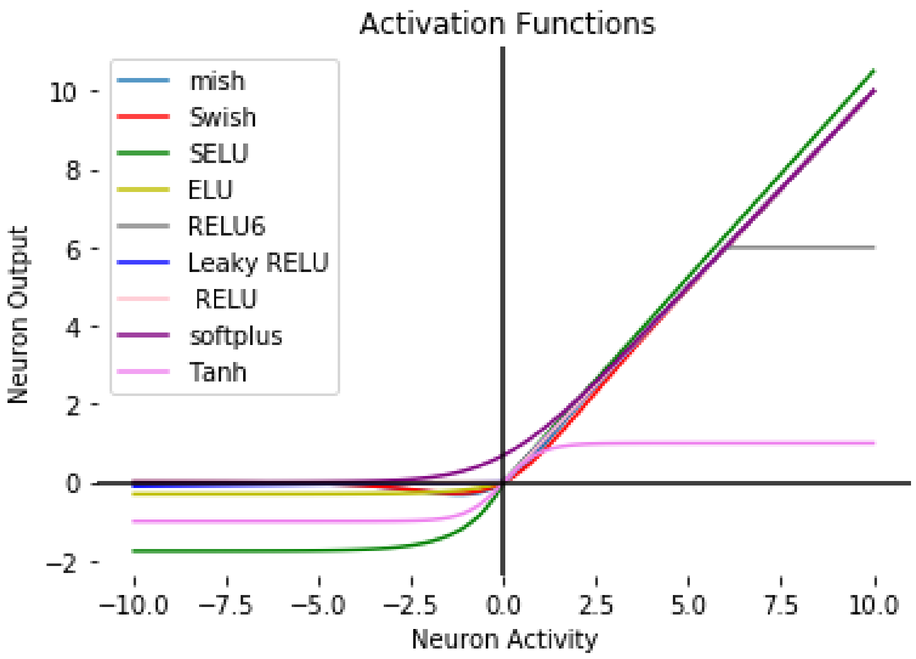
They are all very similar



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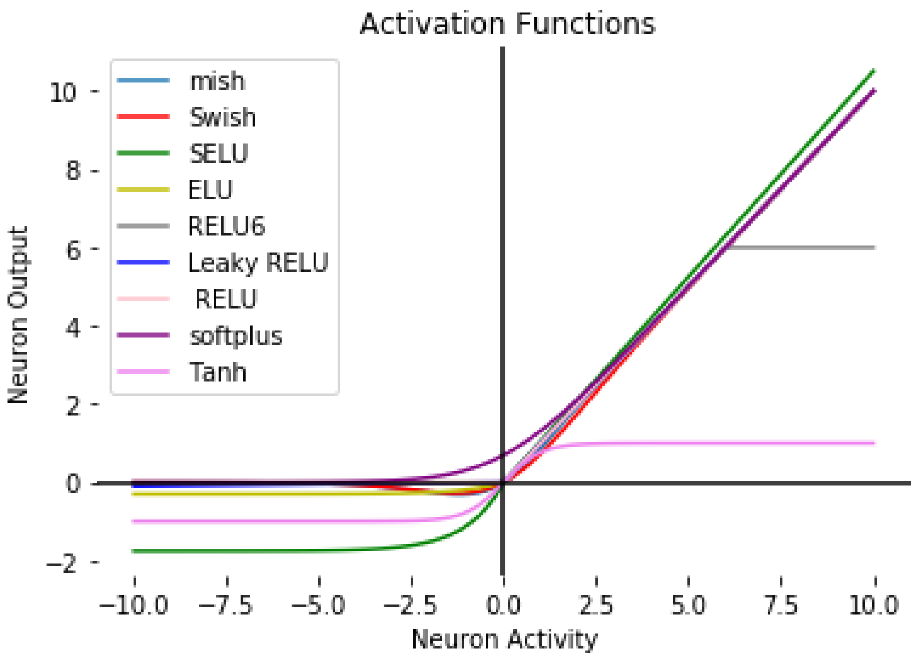

They are all very similar

I usually use leaky ReLU because it works well enough

Activation Functions

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

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

Agenda

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3. Optimization is hard
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5. **Activation functions**
6. Parameter initialization
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Parameter Initialization

Recall the gradient descent algorithm

function Gradient Descent($\boldsymbol{X}, \boldsymbol{Y}, \mathcal{L}, t, \alpha$)
    ▷ Randomly initialize parameters
    $\boldsymbol{\theta} \leftarrow \mathcal{N}(0, 1)$
    for $i \in 1 \ldots t$ **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 $\boldsymbol{\theta}$

Parameter Initialization

Initial $\boldsymbol{\theta}$ is starting position for gradient descent

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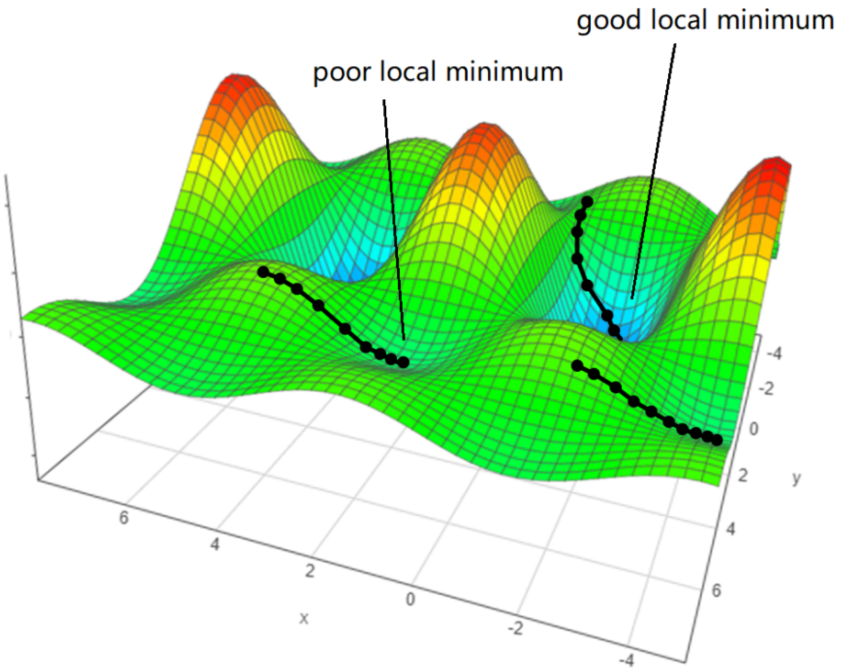
Initial θ is starting position for gradient descent



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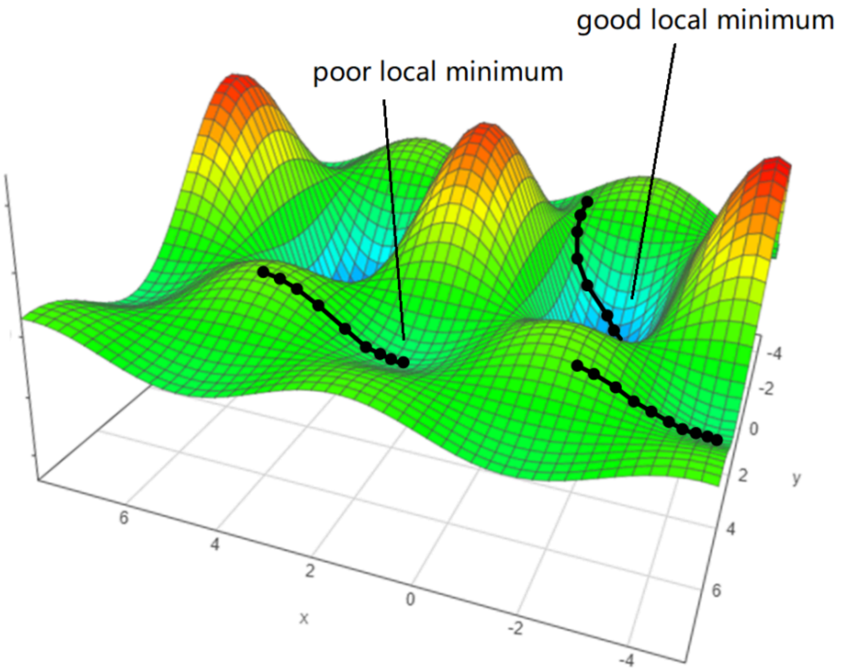
Initial $\boldsymbol{\theta}$ is starting position for gradient descent



Pick $\boldsymbol{\theta}$ that results in good local minima

Parameter Initialization

Start simple, initialize all parameters to 0

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

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Question: Any issues?

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Question: Any issues?

Answer: The gradient will always be zero

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

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Question: Any issues?

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

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

Parameter Initialization

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

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

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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?

Parameter Initialization

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

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

Parameter Initialization

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

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

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

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

Parameter Initialization

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

Parameter Initialization

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

Parameter Initialization

```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)
```

Parameter Initialization

```
import jax
d_h = 10

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

Parameter Initialization

```
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)
```

Parameter Initialization

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

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Stochastic Gradient Descent

function GRADIENT DESCENT($\boldsymbol{X}$, $\boldsymbol{Y}$, $\mathcal{L}$, t, α)

$\quad \triangleright$ Randomly initialize parameters

$\quad \boldsymbol{\theta} \leftarrow \text{Glorot}()$

$\quad$ **for** $i \in 1...t$ **do**

$\quad\quad \triangleright$ Compute the gradient of the loss

$\quad\quad \boldsymbol{J} \leftarrow \nabla_{\boldsymbol{\theta}} \mathcal{L}(\boldsymbol{X}, \boldsymbol{Y}, \boldsymbol{\theta})$

$\quad\quad \triangleright$ Update the parameters using the negative gradient

$\quad\quad \boldsymbol{\theta} \leftarrow \boldsymbol{\theta} - \alpha \boldsymbol{J}$

$\quad$ **return** $\boldsymbol{\theta}$

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

Stochastic Gradient Descent

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

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Question: How many GB are the LLM datasets?

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

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

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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

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

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Question: We do not have enough memory to compute the gradient

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First, we sample random datapoint indices

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Then construct a **batch** of training data

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

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We call this **stochastic gradient descent**

Stochastic Gradient Descent

function $\textsc{Stochastic Gradient Descent}(\boldsymbol{X}, \boldsymbol{Y}, \mathcal{L}, t, \alpha)$

$\quad \boldsymbol{\theta} \leftarrow \mathrm{Glorot}()$

$\quad$ **for** $i \in 1...t$ **do**

$\quad\quad \boldsymbol{X}, \boldsymbol{Y} \leftarrow \mathrm{Shuffle}(\boldsymbol{X}), \mathrm{Shuffle}(\boldsymbol{Y})$

$\quad\quad$ **for** $j \in 0...\frac{n}{B} - 1$ **do**

$\quad\quad\quad \boldsymbol{X}_j \leftarrow \begin{bmatrix} \boldsymbol{x}_{[jB]} & \boldsymbol{x}_{[jB+1]} & \dots & \boldsymbol{x}_{[(j+1)B]} \end{bmatrix}$

$\quad\quad\quad \boldsymbol{Y}_j \leftarrow \begin{bmatrix} \boldsymbol{y}_{[jB]} & \boldsymbol{y}_{[jB+1]} & \dots & \boldsymbol{y}_{[(j+1)B]} \end{bmatrix}$

$\quad\quad\quad \boldsymbol{J} \leftarrow \nabla_{\boldsymbol{\theta}} \mathcal{L}(\boldsymbol{X}_j, \boldsymbol{Y}_j, \boldsymbol{\theta})$

$\quad\quad\quad \boldsymbol{\theta} \leftarrow \boldsymbol{\theta} - \alpha \boldsymbol{J}$

$\quad$ **return** $\boldsymbol{\theta}$

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Stochastic gradient descent (SGD) is useful for saving memory

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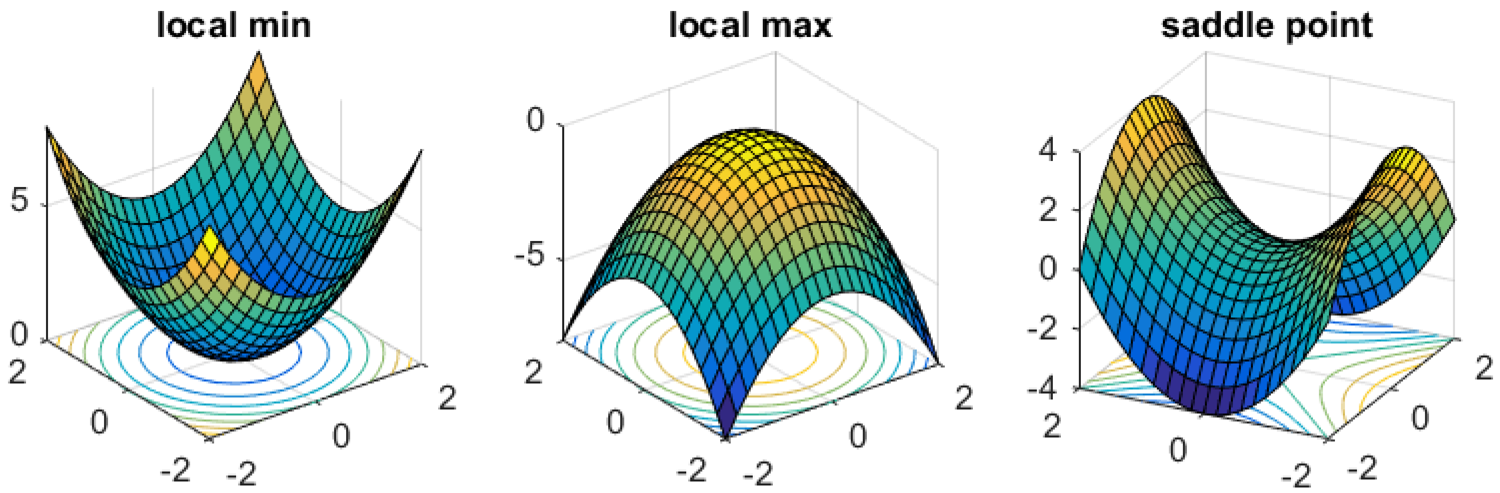
But it can also improve performance

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

This makes it less likely we get stuck in bad optima



Stochastic Gradient Descent

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

Stochastic Gradient Descent

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```
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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Modern Optimization

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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

Modern Optimization

The video simulations provide an intuitive understanding of adaptive optimizers

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The key behind modern optimizers is two concepts:

- Momentum

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Let us discuss the algorithms more slowly

Modern Optimization

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

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function $\textsc{Gradient Descent}(\boldsymbol{X}, \boldsymbol{Y}, \mathcal{L}, t, \alpha)$

  $\triangleright$ Randomly initialize parameters

  $\boldsymbol{\theta} \leftarrow \text{Glorot}()$

  for $i \in 1...t$ **do**

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Modern Optimization

Introduce **momentum** first

Modern Optimization

Introduce **momentum** first

function Momentum $\textsc{Gradient Descent}(\boldsymbol{X}, \boldsymbol{Y}, \mathcal{L}, t, \alpha, \beta)$

$\boldsymbol{\theta} \leftarrow \text{Glorot}()$

$\boldsymbol{M} \leftarrow \boldsymbol{0}$ # Init momentum

for $i \in 1...t$ **do**

$\boldsymbol{J} \leftarrow \nabla_{\boldsymbol{\theta}} \mathcal{L}(\boldsymbol{X}, \boldsymbol{Y}, \boldsymbol{\theta})$ # Represents acceleration

$\boldsymbol{M} \leftarrow \beta \cdot \boldsymbol{M} + (1 - \beta) \cdot \boldsymbol{J}$ # Momentum and acceleration

$\boldsymbol{\theta} \leftarrow \boldsymbol{\theta} - \alpha \boldsymbol{M}$

return $\boldsymbol{\theta}$

Modern Optimization

Now **adaptive learning rate**

Now **adaptive learning rate**

function RMSProp$(\boldsymbol{X}, \boldsymbol{Y}, \mathcal{L}, t, \alpha, \beta, \varepsilon)$

$\quad \boldsymbol{\theta} \leftarrow \mathrm{Glorot}()$

$\quad \boldsymbol{V} \leftarrow \boldsymbol{0}$ # Init variance

$\quad$ **for** $i \in 1...t$ **do**

$\quad\quad \boldsymbol{J} \leftarrow \nabla_{\boldsymbol{\theta}} \mathcal{L}(\boldsymbol{X}, \boldsymbol{Y}, \boldsymbol{\theta})$ # Represents acceleration

$\quad\quad \boldsymbol{V} \leftarrow \beta \cdot \boldsymbol{V} + (1 - \beta) \cdot \boldsymbol{J} \odot \boldsymbol{J}$ # Magnitude

$\quad\quad \boldsymbol{\theta} \leftarrow \boldsymbol{\theta} - \alpha \boldsymbol{J} \oslash \sqrt[\circ]{\boldsymbol{V} + \varepsilon}$ # Rescale grad by prev updates

$\quad$ **return** $\boldsymbol{\theta}$

Adaptive Optimization

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

Adaptive Optimization

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

function Adaptive Moment Estimation($\boldsymbol{X}, \boldsymbol{Y}, \mathcal{L}, t, \alpha, \beta_1, \beta_2, \varepsilon$)

$\boldsymbol{\theta} \leftarrow \text{Glorot}()$

$\boldsymbol{M}, \boldsymbol{V} \leftarrow \boldsymbol{0}$

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

$\boldsymbol{\theta} \leftarrow \boldsymbol{\theta} - \alpha \boldsymbol{M} \oslash \sqrt[\odot]{\boldsymbol{V} + \varepsilon}$ # Adaptive param update

return $\boldsymbol{\theta}$ # Note, we use biased $\boldsymbol{M}, \boldsymbol{V}$ for clarity

Adaptive Optimization

```python
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()
```

Adaptive Optimization

```python
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)
```

Agenda

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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

Agenda

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