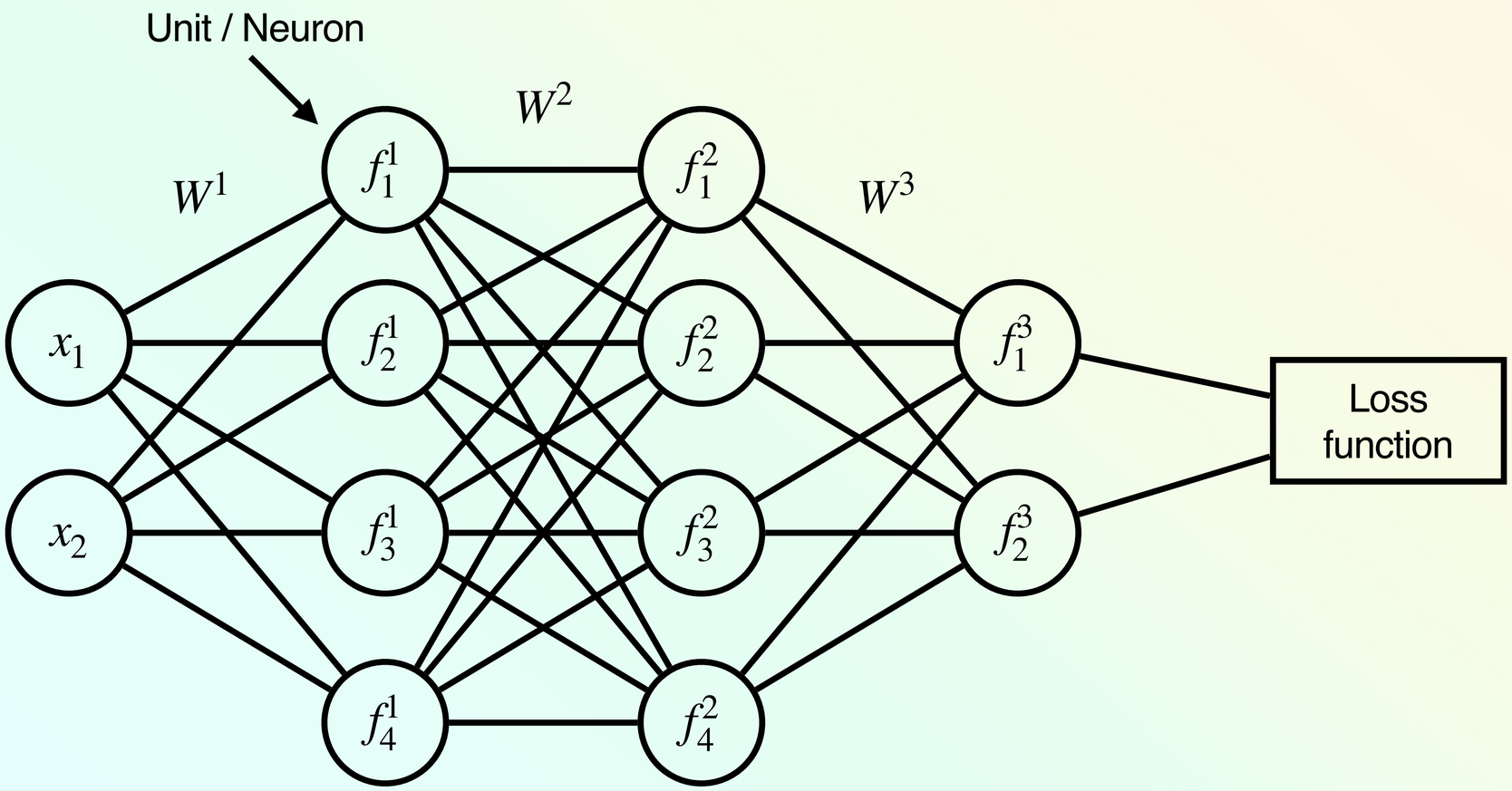
NEURAL NETWORKS

Input Layer Hidden Layers Output Layer



h^0 $h^1 = f^1(h^0, W^1)$ $h^2 = f^2(h^1, W^2)$ $h^3 = f^3(h^2, W^3)$

THE STRUCTURE OF NEURAL NETWORKS

ABSTRACT PROCESS

We can write the neural network outputs as a sequential process.

$$
\begin{aligned}
h^0 &= x \\
h^1 &= f^1(h^0, W^1) \\
h^2 &= f^2(h^1, W^2) \\
&\vdots \\
h^i &= f^i(h^{i-1}, W^i) \\
&\vdots \\
h^k &= f^k(h^{k-1}, W^k)
\end{aligned}
$$

To be concise, we can write the network output as $h^k = f(x, \theta), \theta = \{W^i\}_{i=1}^k$

NEURAL NETWORK LAYERS

MULTILAYER PERCEPTION

$$f^i(h^{i-1}, W^i) = \sigma\left(h^{i-1}W^{i\top}\right)$$

$h_{i-1} \in \mathbb{R}^{1\times n_{i-1}}$, $h_i \in \mathbb{R}^{1\times n_i}$ — row vectors

$W^i \in \mathbb{R}^{n_i \times n_{i-1}}$ each row corresponds to the weights for one output unit

$\sigma\colon \mathbb{R} \to \mathbb{R}$ is a nonlinear function called an *activation function* that is applied elementwise

NOTATION FOR NEURAL NETWORKS

$x \in \mathbb{R}^{m \times n_0}$ is a matrix of m data points containing n_0 features for each data point

Each row is a data point

$$x = \begin{bmatrix} x_{1,1} & x_{1,2} & \cdots & x_{1,n_0} \\ x_{1,1} & x_{1,2} & \cdots & x_{1,n_0} \\ \vdots & \vdots & \ddots & \vdots \\ x_{m,1} & x_{m,2} & \cdots & x_{m,n_0} \end{bmatrix}$$

$h^0 = x$ input to the neural network

NOTATION FOR NEURAL NETWORKS

$$h^1 = f^1(h^0, W^1) = \sigma\left(h^0 {W^1}^\top\right) = \sigma\left(z^1\right)$$

$h^1 \in \mathbb{R}^{m \times n_1}$ outputs of the first layer of the neural network. Each row is a different data point

$$h^0 {W^1}^\top = \begin{bmatrix} h^0_{1,1} & h^0_{1,2} & \cdots & h^0_{1,n_0} \\ h^0_{1,1} & h^0_{1,2} & \cdots & h^0_{1,n_0} \\ \vdots & \vdots & \ddots & \vdots \\ h^0_{m,1} & h^0_{m,2} & \cdots & h^0_{m,n_0} \end{bmatrix} \begin{bmatrix} W^1_{1,1} & W^1_{2,1} & \cdots & W^1_{n_1,1} \\ W^1_{1,2} & W^1_{2,2} & \cdots & W^1_{n_1,2} \\ \vdots & \vdots & \ddots & \vdots \\ W^1_{1,n_0} & hW^1_{2,n_0} & \cdots & W^1_{n_1,n_0} \end{bmatrix} = \begin{bmatrix} z^1_{1,1} & z^1_{1,2} & \cdots & z^1_{1,n_1} \\ z^1_{1,1} & z^1_{1,2} & \cdots & z^1_{1,n_1} \\ \vdots & \vdots & \ddots & \vdots \\ z^1_{m,1} & z^1_{m,2} & \cdots & z^1_{m,n_1} \end{bmatrix} = z^1$$

Note the matrix on the right in z^1 is ${W^1}^\top$, $W^1 \in \mathbb{R}^{n_1 \times n_0}$, ${W^1}^\top \in \mathbb{R}^{n_0 \times n_1}$

NOTATION FOR NEURAL NETWORKS

For any layer i

$$h^i = f^i(h^{i-1}, W^i) = \sigma\left(h^{i-1}W^{i^\top}\right) = \sigma\left(z^i\right)$$

$$h^i \in \mathbb{R}^{m \times n_i},\ z^i \in \mathbb{R}^{m \times n_i},\ W^i \in \mathbb{R}^{n_i \times n_{i-1}}$$

NOTATION FOR NEURAL NETWORKS

For the output layer (layer k)

The activation function may be the identify function, e.g., $\sigma(x) = x$

$$h^k = f^i(h^{k-1}, W^k) = h^{k-1}{W^k}^\top = z^k$$

We do this when

Targets $y \in \mathbb{R}$ and loss is mean squared error Regression

sometimes for classification (numerical precision reasons, future lecture)

OUTPUT UNITS

multiple outputs

$y \in \mathbb{R}^{n_y}$ — Mean square error loss and linear output units (one data point (x, y))

The only change is how we calculate this

$$l(x, y, \theta) = \|h^k - y\|_2^2 = \sum_{i=1}^{n_y} (h_i^k - y_i)^2$$

$y \in \{0,1\}$ — negative log-likelihood and sigmoid output units

$$l(x, y, \theta) = -y \ln h^k - (1 - y)\ln(1 - h^k)$$

MULTICLASS CLASSIFICATION

Want to classify cats, dogs, planes, cars, horses, etc

$y \in \{1,2,3,4,\ldots,n\}$ — each number represents a specific class

MULTICLASS CLASSIFICATION

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$y \in \{1,2,3,4,\ldots,n\}$ — each number represents a specific class

Objective function:

Can still minimize the NLL, i.e., $-\ln \Pr(\hat{Y} = y \,|\, X = x)$

How to represent a probability distribution over multiple classes?

GENERALIZING BINARY CLASSIFCATION

Sigmoid $\sigma(z) = \dfrac{1}{1 + e^{-z}}$

$\Pr(\hat{Y} = 1 \,|\, X = x) = \sigma(z), \qquad z = h^{k-1}W^k \;\; z \in \mathbb{R}$

z represents the log odds of $\hat{Y} = 1$, i.e., how likely is the label 1.

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If we increaseed the 1 would $\sigma(z)$ increase?

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If we increaseed the 1 would $\sigma(z)$ increase?

- No, it decreases, and decreasing the 1 makes it increase
- Increasing 1 makes the probability of $Y = 0$ increase

GENERALIZING BINARY CLASSIFCATION

likelihood of class 0

for class 1

$$z = [z_0, z_1]$$

$$\sigma(z) = \frac{e^{z_1}}{e^{z_0} + e^{z_1}}$$

$$\Pr(\hat{Y} = 1 \,|\, X = x) = \sigma(z)$$

$$\Pr(\hat{Y} = 0 \,|\, X = x) = 1 - \sigma(z)$$

GENERALIZING BINARY CLASSIFCATION

$$
\begin{aligned}
\Pr(\hat{Y} = 0 \,|\, X = x) = \;& 1 - \sigma(z) \\
= \;& 1 - \frac{e^{z_1}}{e^{z_0} + e^{z_1}} \\
= \;& \frac{e^{z_0} + e^{z_1}}{e^{z_0} + e^{z_1}} - \frac{e^{z_1}}{e^{z_0} + e^{z_1}} \\
= \;& \frac{e^{z_0}}{e^{z_0} + e^{z_1}}
\end{aligned}
$$

GENERALIZING BINARY CLASSIFCATION

$$\Pr(\hat{Y} = 0 \,|\, X = x) = \frac{e^{z_0}}{e^{z_0} + e^{z_1}}$$

$$\Pr(\hat{Y} = 1 \,|\, X = x) = \frac{e^{z_1}}{e^{z_0} + e^{z_1}}$$

Likelihood

Normalization

CREATING A PROBABILITY DISTRIBUTION

Probability distribution

$\forall x,\ \Pr(X = x) \geq 0$ — all events have a nonnegative probability

$\sum_{x} \Pr(X = x) = 1$ — probability of all events sum to one.

CREATING A PROBABILITY DISTRIBUTION

Probability distribution

$\forall x,\ \Pr(X = x) \geq 0$ — all events have a nonnegative probability

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$z \in \mathbb{R}^n$ — scores representing the likelihood of each class

1. Make those scores positive

2. Normalize so that the total probability sums to 1

SOFTMAX

$z \in \mathbb{R}^n$

$$\Pr(\hat{Y} = i \mid X = x) = \frac{e^{z_i}}{\sum_{j=1}^{n} e^{z_j}}$$

Make positive

Normalize

SOFTMAX

$z \in \mathbb{R}^n$

$$\Pr(\hat{Y} = i \mid X = x) = \frac{e^{z_i}}{\sum_{j=1}^{n} e^{z_j}}$$

Make positive

Normalize

Positivity: $\forall x \in (-\infty, \infty),\ e^x > 0$

Total probability: $\sum_{i=1}^{n} \frac{e^{z_i}}{\sum_{j=1}^{n} e^{z_j}} = \frac{\sum_{i=1}^{n} e^{z_i}}{\sum_{j=1}^{n} e^{z_j}} = 1$

SOFTMAX OUTPUT UNIT

$$z = h^{k-1} W^k \in \mathbb{R}^n$$

$$\sigma(z) = \left[\frac{e^{z_1}}{\sum_{j=1}^{n} e^{z_j}}, \frac{e^{z_2}}{\sum_{j=1}^{n} e^{z_j}}, \cdots, \frac{e^{z_n}}{\sum_{j=1}^{n} e^{z_j}} \right]$$

SOFTMAX OUTPUT UNIT

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$$\sigma(z) = \left[\frac{e^{z_1}}{\sum_{j=1}^{n} e^{z_j}}, \frac{e^{z_1}}{\sum_{j=1}^{n} e^{z_j}}, \cdots, \frac{e^{z_n}}{\sum_{j=1}^{n} e^{z_j}} \right]$$

$$h^k = \sigma(z) = \left[\Pr(\hat{Y} = 1 \,|\, X = x), \Pr(\hat{Y} = 2 \,|\, X = x), \cdots, \Pr(\hat{Y} = n \,|\, X = x) \right]$$

LOSS FUNCTION FOR SOFTMAX

$$-\ln \Pr(\hat{Y} = y \mid X = x) = -\sum_{i=1}^{n} \mathbf{1}_{y=i} \ln h_{1,i}^{k}$$

Just choose the ones that corresponds to class i

LOSS FUNCTION FOR SOFTMAX

$$-\ln \Pr(\hat{Y} = y \mid X = x) = -\sum_{i=1}^{n} \mathbf{1}_{y=i} \ln h_{1,i}^{k}$$

Instead of for loops

$y = [0,\cdots,1,\cdots,0]$ — One-hot vector, the i^{th} element is 1 if $y = i$, all others are 0

$$l(x, y, \theta) = -y(\ln h^{k})^{\top} = -\sum_{i=1}^{n} y_i \ln h_{1,i}^{k}$$

QUIZ

SOFTMAX PROPERTIES

Softmax is has n parameters for n probabilities

Only need $n - 1$ parameters to define the probability distribution.

$$\Pr(X = 1) \doteq p_1,\ \Pr(X = 2) \doteq p_2,\ \cdots,\ \Pr(X = n-1) \doteq p_{n-1},\ \Pr(X = n) \doteq 1 - \sum_{i=1}^{n-1} p_i$$

Pr of the last term

we only need (n-1) parameters

SOFTMAX PROPERTIES

Softmax is has n parameters for n probabilities

Only need $n - 1$ parameters to define the probability distribution.

$$\Pr(X = 1) \doteq p_1,\ \Pr(X = 2) \doteq p_2,\ \cdots,\ \Pr(X = n - 1) \doteq p_{n-1},\ \Pr(X = n) \doteq 1 - \sum_{i=1}^{n-1} p_i$$

A distribution with $\geq n$ parameters and n possible outcomes is called *over parameterized*

Multiple ways to represent the same probability distribution

SOFTMAX PROPERTIES

Softmax is over-parameterized:

Can set $z_n = 0$ and still represent probabilities for each class

$$i < n, \Pr(\hat{Y} = i \mid X = x) = \frac{e^{z_i}}{1 + \sum_{j=1}^{n-1} e^{z_j}} \qquad \Pr(\hat{Y} = n \mid X = x) = \frac{1}{1 + \sum_{j=1}^{n-1} e^{z_j}}$$

In practice, both forms work equally well. Easier to do an over-parameterized version

SOFTMAX PROPERTIES

Invariance to translation

For $c \in \mathbb{R}$, $\sigma(z) = \sigma(z + c)$

In practice, we often subtract off the largest value to prevent numerical instability, e.g.,

$$\sigma(z - \max_i z_i)$$ avoids numerical stability

SOFTMAX PROPERTIES

Not invariant to rescaling:

$\alpha > 0, \sigma(z) \neq \sigma(\alpha z)$

$\alpha \to 0$ — probabilities become uniform, e.g., $1/n$

$\alpha \to \infty$ — probabilities become 0 except for the largest i, which has a probability 1

α is called the temperature of the softmax

$$\Pr\left(\hat{Y} = i \,|\, X = x\right) = \frac{e^{\alpha z_i}}{\sum_j e^{\alpha z_j}}$$

ACTIVATION FUNCTIONS

FOR HIDDEN LAYERS

Sigmoid: $\sigma(x) = \frac{1}{1 + e^{-x}}$

ACTIVATION FUNCTIONS

FOR HIDDEN LAYERS

Sigmoid: $\sigma(x) = \dfrac{1}{1 + e^{-x}}$ ← close

Tanh: $\sigma(x) = \dfrac{e^{x} - e^{-x}}{e^{x} + e^{-x}} = 2\dfrac{1}{1 + e^{-2x}} - 1$

RELU (Rectified Linear Unit): $\sigma(x) = \max(0,x)$ ← Always +ve

Softplus: $\sigma(x) = \ln(1 + e^{x})$

ACTIVATION FUNCTIONS

FOR HIDDEN LAYERS

Sigmoid: $\sigma(x) = \dfrac{1}{1 + e^{-x}}$

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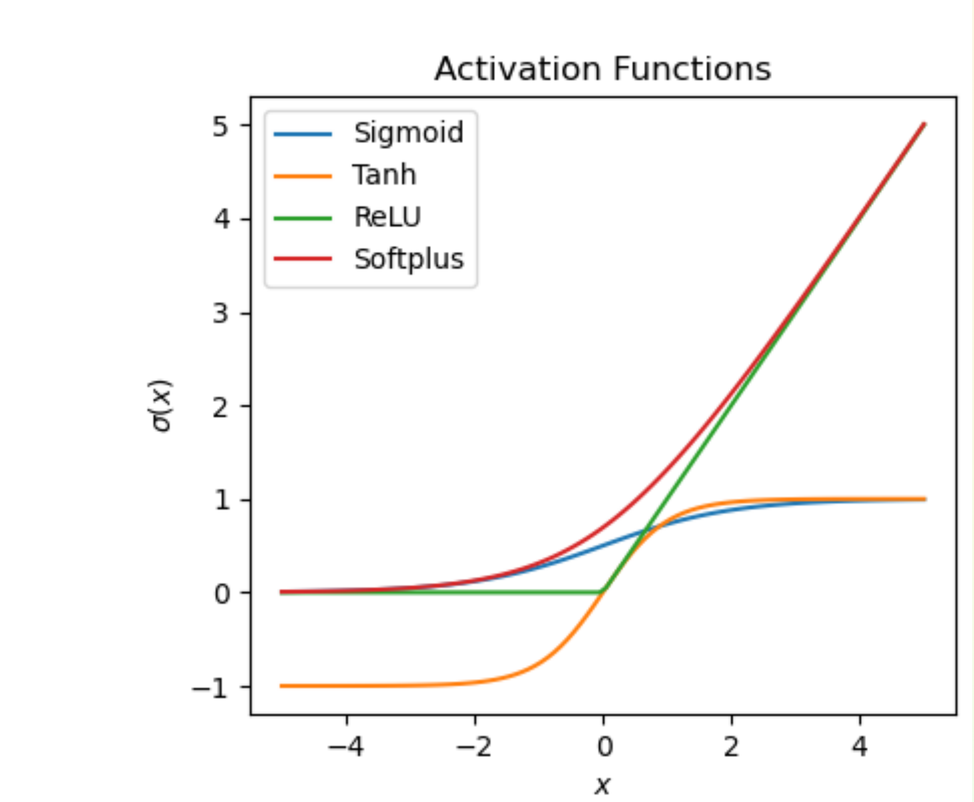

ACTIVATION FUNCTIONS

FOR HIDDEN LAYERS

Sigmoid: $\sigma(x) = \dfrac{1}{1+e^{-x}}$

Which should we use?

Tanh: $\sigma(x) = \dfrac{e^{x}-e^{-x}}{e^{x}+e^{-x}} = 2\dfrac{1}{1+e^{-2x}} - 1$

RELU (Rectified Linear Unit): $\sigma(x) = \max(0,x)$

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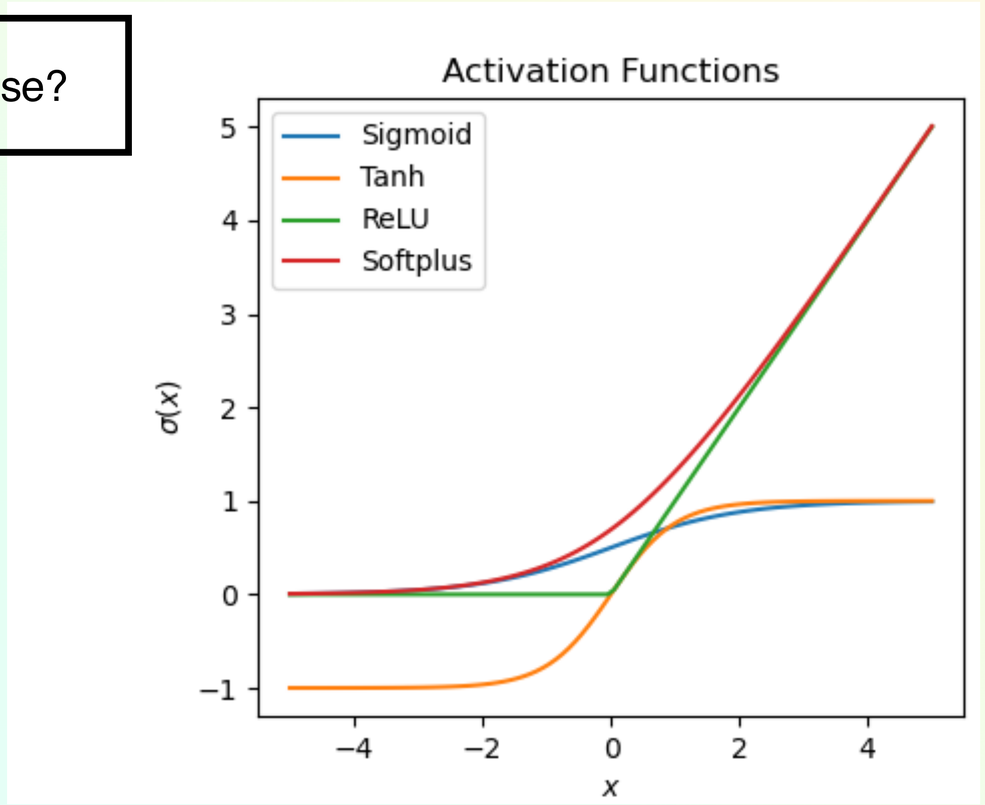


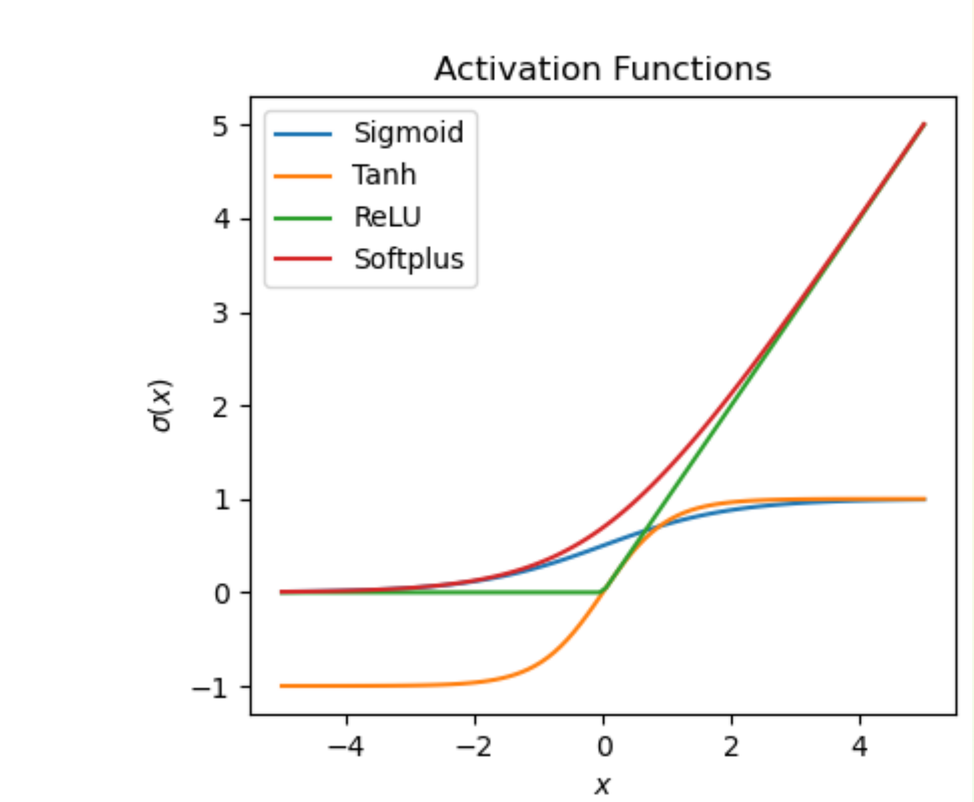
ACTIVATION FUNCTIONS

FOR HIDDEN LAYERS

With enough hidden units, they all can represent similar functions

We want to choose one that makes learning easy

— Derivative for weights at each hidden layer should not be flat



PARTIAL DERIVATIVES

FOR EACH HIDDEN LAYER

will do this in the 3rd homework

For a single data point x, y

$$\frac{\partial l(x, y, \theta)}{\partial W^i} = ? =$$

chain rule

$$\frac{\partial L(X,Y,\theta)}{\partial h^K} \frac{\partial h^K}{\partial w_i} \Rightarrow \frac{\partial L(X,Y,\theta)}{\partial h^K} \frac{\partial f^K(h^{K-1}, w^K)}{\partial w_i}$$

$$= \frac{\partial L(X,Y,\theta)}{\partial h^K} \frac{\partial f^K(h^{K-1}, w^K)}{\partial h^{K-1}} \frac{\partial h^{K-1}}{\partial w_i}$$

$$\frac{\partial f^{K-1}(h^{K-2}, w^{K-1})}{\partial w_i}$$

$$\frac{\partial f^{K-1}(h^{K-2}, w^{K-1})}{\partial h^{K-2}} \frac{\partial h^{K-2}}{\partial w_i}$$

$$\frac{\partial f^i(h^i, w^i)}{\partial w_i}$$

PARTIAL DERIVATIVES

FOR EACH HIDDEN LAYER

$$
\begin{aligned}
\frac{\partial l(x,y,\theta)}{\partial W^i} &= \frac{\partial l(x,y,\theta)}{\partial h^k}\frac{\partial h^k}{\partial W^i} \\
&= \frac{\partial l(x,y,\theta)}{\partial h^k}\frac{\partial f(h^{k-1},W^k)}{\partial W^i} \\
&= \frac{\partial l(x,y,\theta)}{\partial h^k}\frac{\partial f^k(h^{k-1},W^k)}{\partial h^{k-1}}\frac{\partial h^{k-1}}{\partial W^i} \\
&= \frac{\partial l(x,y,\theta)}{\partial h^k}\frac{\partial f^k(h^{k-1},W^k)}{\partial h^{k-1}}\frac{\partial f^{k-1}(h^{k-2},W^{k-1})}{\partial W^i} \\
&= \frac{\partial l(x,y,\theta)}{\partial h^k}\frac{\partial f^k(h^{k-1},W^k)}{\partial h^{k-1}}\frac{\partial f^{k-1}(h^{k-2},W^{k-1})}{\partial h^{k-2}}\frac{\partial h^{k-2}}{\partial W^i} \\
&\vdots \\
&= \frac{\partial l(x,y,\theta)}{\partial h^k}\frac{\partial f^k(h^{k-1},W^k)}{\partial h^{k-1}}\frac{\partial f^{k-1}(h^{k-2},W^{k-1})}{\partial h^{k-2}}\cdots\frac{\partial f^i(h^{i-1},W^i)}{\partial W^i}
\end{aligned}
$$

PARTIAL DERIVATIVES

FOR EACH HIDDEN LAYER

$$\frac{\partial f^i(h^{i-1}, W^i)}{\partial W^i} = \frac{\partial \sigma(h^{i-1}W^{i\top})}{\partial W^i}$$

$$= \frac{\partial \sigma(h^{i-1}W^{i\top})}{\partial h^{i-1}W^{i\top}}^{\top} \frac{\partial h^{i-1}W^{i\top}}{\partial W^i}$$

output

output

& weight

input

PARTIAL DERIVATIVES

FOR EACH HIDDEN LAYER

$$\frac{\partial f^i(h^{i-1}, W^i)}{\partial W^i} = \frac{\partial \sigma(z^i)}{\partial W^i}$$

$$= \frac{\partial \sigma(z^i)}{\partial z^i}^\top \frac{\partial z^i}{\partial W^i}$$

PARTIAL DERIVATIVES

FOR EACH HIDDEN LAYER

$$\frac{\partial f^i(h^{i-1}, W^i)}{\partial W^i} = \frac{\partial \sigma(z^i)}{\partial W^i}$$

$$= \frac{\partial \sigma(z^i)}{\partial z^i} \top \frac{\partial z^i}{\partial W^i}$$

$$= \begin{bmatrix} \frac{\partial \sigma(z^i_{1,1})}{\partial z^i_1} \\ \frac{\partial \sigma(z^i_{1,2})}{\partial z^i_2} \\ \vdots \\ \frac{\partial \sigma(z^i_{1,n_i})}{\partial z^i_{1,n_i}} \end{bmatrix} \top \quad h^{i-1}$$

PARTIAL DERIVATIVES

FOR EACH HIDDEN LAYER

$$\frac{\partial f^i(h^{i-1}, W^i)}{\partial W^i} = \begin{bmatrix} \frac{\partial \sigma(z^i_{1,1})}{\partial z^i_1} \\ \frac{\partial \sigma(z^i_{1,2})}{\partial z^i_2} \\ \vdots \\ \frac{\partial \sigma(z^i_{1,n_i})}{\partial z^i_{1,n_i}} \end{bmatrix}^\top h^{i-1}$$

If $\frac{\partial \sigma(z^i_{1,j})}{\partial z^i_{1,j}}$ is near zero, then the derivative is also near zero.

Want an activation function that does not have small derivatives

ACTIVATION FUNCTIONS

FOR HIDDEN LAYERS

Sigmoid: $\sigma = \dfrac{1}{1 + e^{-x}}$

Tanh: $\sigma(x) = \dfrac{e^{x} - e^{-x}}{e^{x} + e^{-x}} = 2\dfrac{1}{1 + e^{-2x}} - 1$

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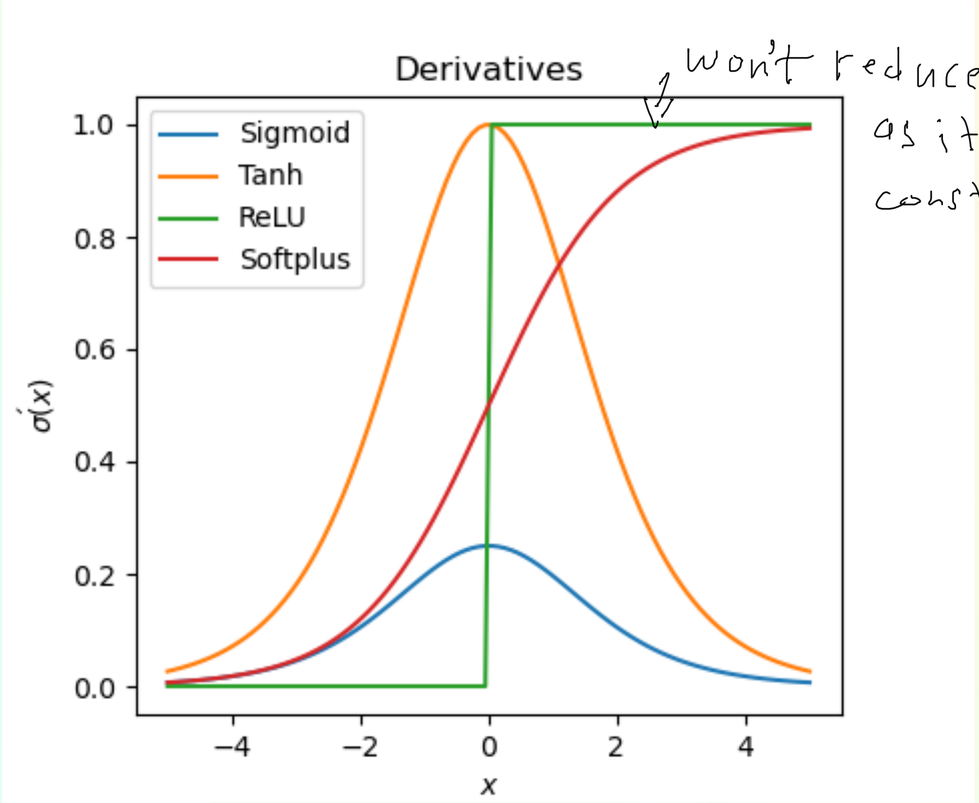


ACTIVATION FUNCTIONS

FOR HIDDEN LAYERS

important

Sigmoid: makes gradient smaller

Tanh: better than sigmoid near 0

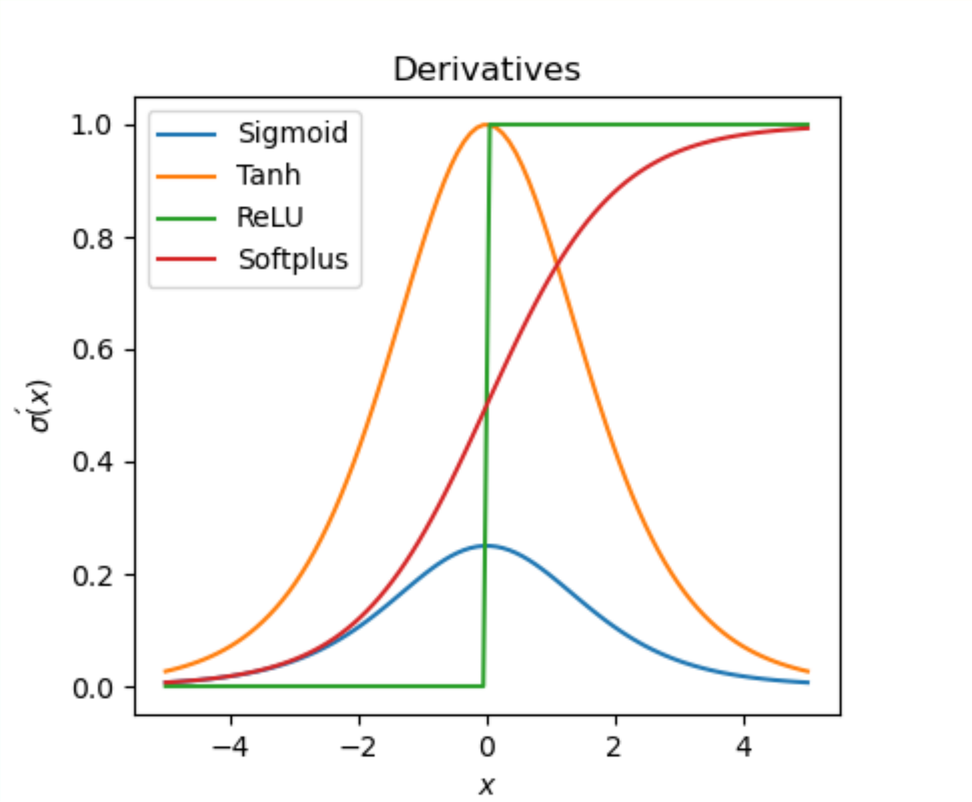
— can initialize weights so z is close to zero

RELU: Great when x > 0!

— if x is always < 0, then it will be a useless unit

Softplus: Like RELU but smooth

— still shrinks gradients at each layer



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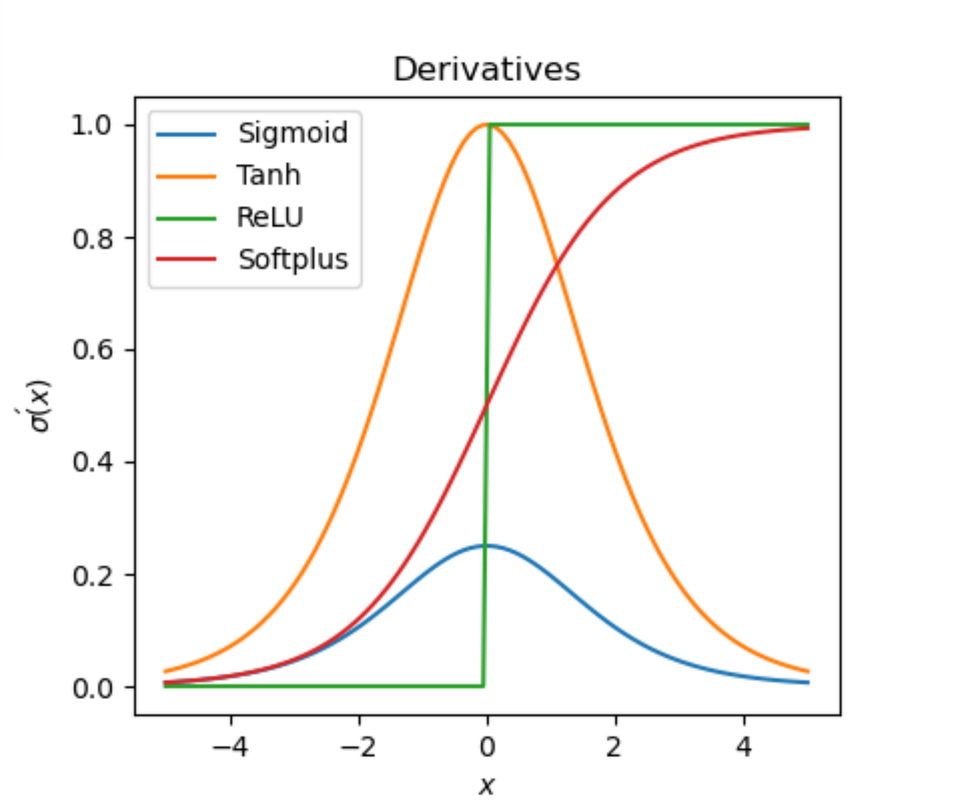


PARTIAL DERIVATIVES

FOR EACH HIDDEN LAYER

$$\frac{\partial l(x,y,\theta)}{\partial W^i} = \frac{\partial l(x,y,\theta)}{\partial h^k}\frac{\partial f^k(h^{k-1},W^k)}{\partial h^{k-1}}\frac{\partial f^{k-1}(h^{k-2},W^{k-1})}{\partial h^{k-2}}\cdots\frac{\partial f^i(h^{i-1},W^i)}{\partial W^i}$$

Each layer has the potential to increase or decrease the magnitude of the derivatives

PARTIAL DERIVATIVES

FOR EACH HIDDEN LAYER

$$\frac{\partial l(x,y,\theta)}{\partial W^i} = \frac{\partial l(x,y,\theta)}{\partial h^k}\frac{\partial f^k(h^{k-1},W^k)}{\partial h^{k-1}}\frac{\partial f^{k-1}(h^{k-2},W^{k-1})}{\partial h^{k-2}}\cdots\frac{\partial f^i(h^{i-1},W^i)}{\partial W^i}$$

Each layer has the potential to increase or decrease the magnitude of the derivatives

Let $A^i = \frac{\partial f^i(h^{i-1},W^i)}{\partial h^{i-1}}$ ← derivative with respect to the input

$$\frac{\partial l(x,y,\theta)}{\partial W^i} = \frac{\partial l(x,y,\theta)}{\partial h^k}\left(\prod_{j=i+1}^{k} A^j\right)\frac{\partial f^i(h^{i-1},W^i)}{\partial W^i}$$

PARTIAL DERIVATIVES

FOR EACH HIDDEN LAYER

$$\frac{\partial l(x,y,\theta)}{\partial W^i} = \frac{\partial l(x,y,\theta)}{\partial h^k}\frac{\partial f^k(h^{k-1},W^k)}{\partial h^{k-1}}\frac{\partial f^{k-1}(h^{k-2},W^{k-1})}{\partial h^{k-2}}\cdots\frac{\partial f^i(h^{i-1},W^i)}{\partial W^i}$$

Each layer has the potential to increase or decrease the magnitude of the derivatives

Let $A^i = \frac{\partial f^i(h^{i-1},W^i)}{\partial h^{i-1}}$

$$\frac{\partial l(x,y,\theta)}{\partial W^i} = \frac{\partial l(x,y,\theta)}{\partial h^k}\left(\prod_{j=i+1}^{k} A^j\right)\frac{\partial f^i(h^{i-1},W^i)}{\partial W^i}$$

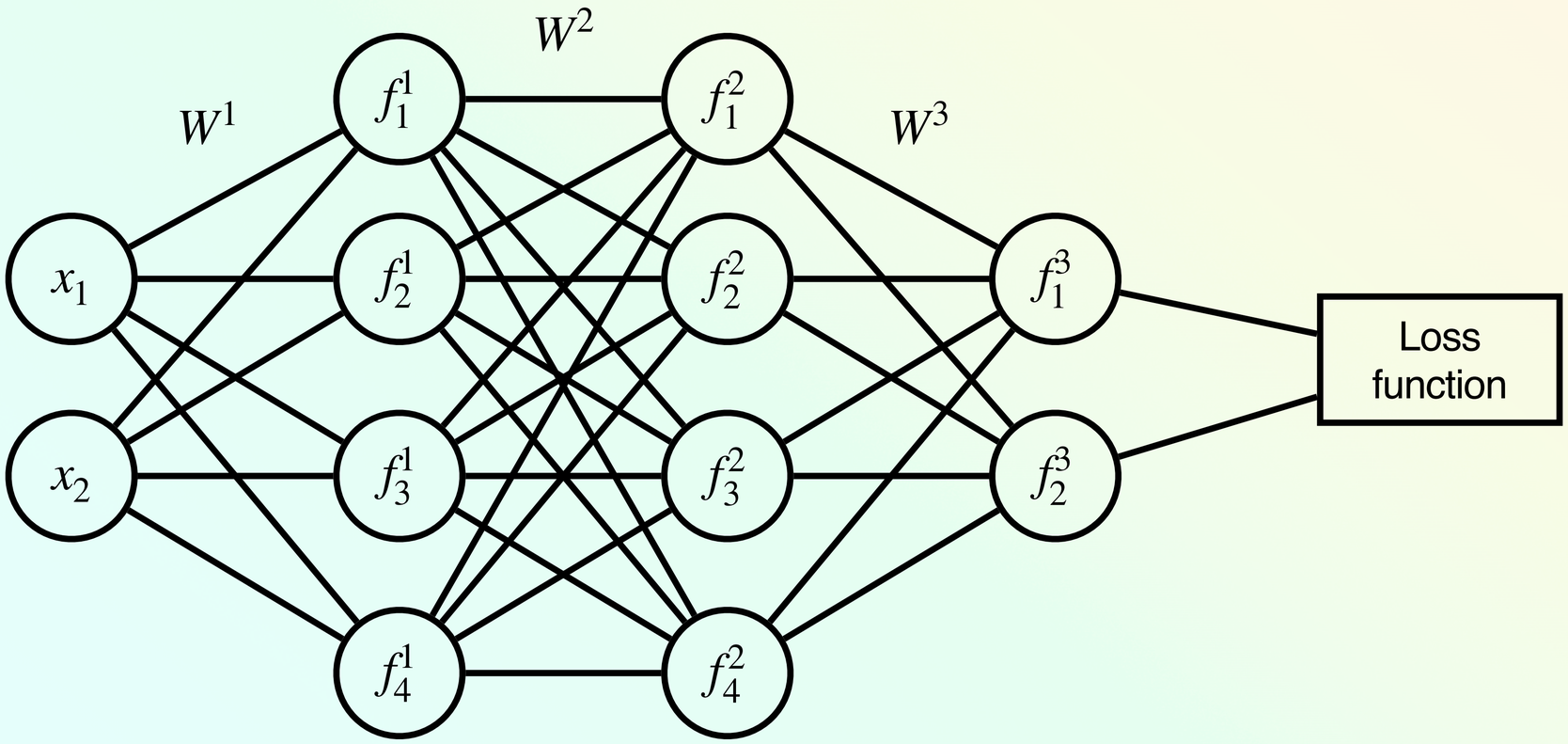
The product of A^js can quickly go to 0 or grow much greater than 1 — exploding or vanishing gradients

Deep networks can be harder to train because of this property. (Used to)

QUIZ

Input Layer Hidden Layers Output Layer

How wide?
How deep?



h^0 $h^1 = f^1(h^0, W^1)$ $h^2 = f^2(h^1, W^2)$ $h^3 = f^3(h^2, W^3)$

UNIVERSAL FUNCTION APPROXIMATON

THEOREM-ISH

For some function f on a compact set $\mathcal{X}$ there exists a neural network with a single hidden layer that can approximate f to an arbitrarily small precision

— hidden layer may need to be infinitely wide

— other results for infinite depth (see Wikipedia)

Does not say how to find that network, only that it exists.

CHOOSING WIDTH

GENERAL INSIGHTS

Width controls how many linear functions that layer can represent

- Decreasing the width over the layers or keeping them the same is the general strategy
- A wide layer after a narrow layer provides no value

Adding depth allows for identifying and repeating patterns

- more depth is usually more helpful
- the number of functions that can be represented grows faster with depth than width

ACTIVATION FUNCTIONS

WHAT THEY REPRESENT

$$z^i = h^{i-1} {W^{i-1}}^\top + b^i$$

$$\sigma(x) = \frac{1}{1 + e^{-z^i}}$$

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W — controls direction of a hyperplane

b — controls position of that plane relative to the origin

ACTIV

WHAT THEY REPF

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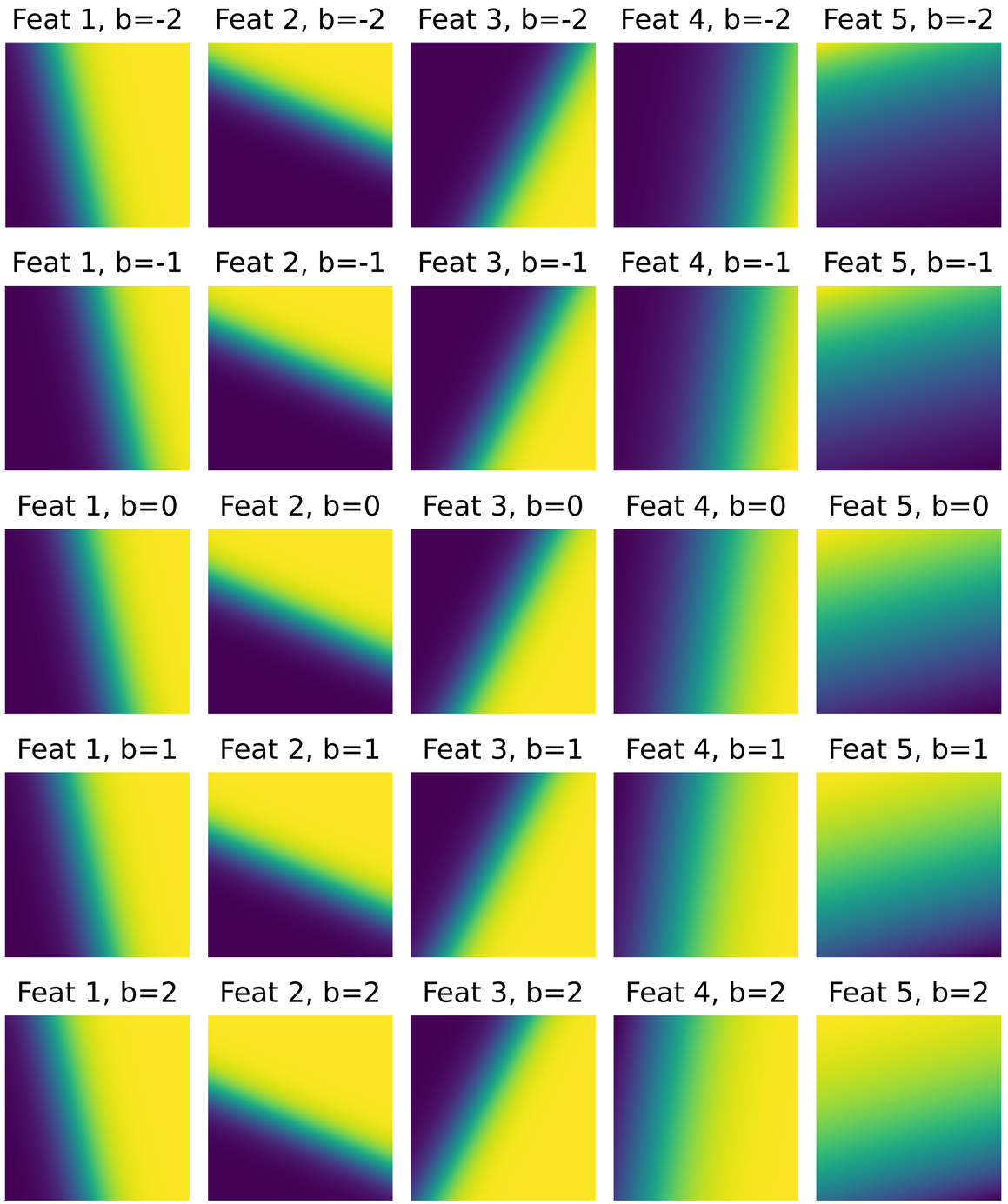
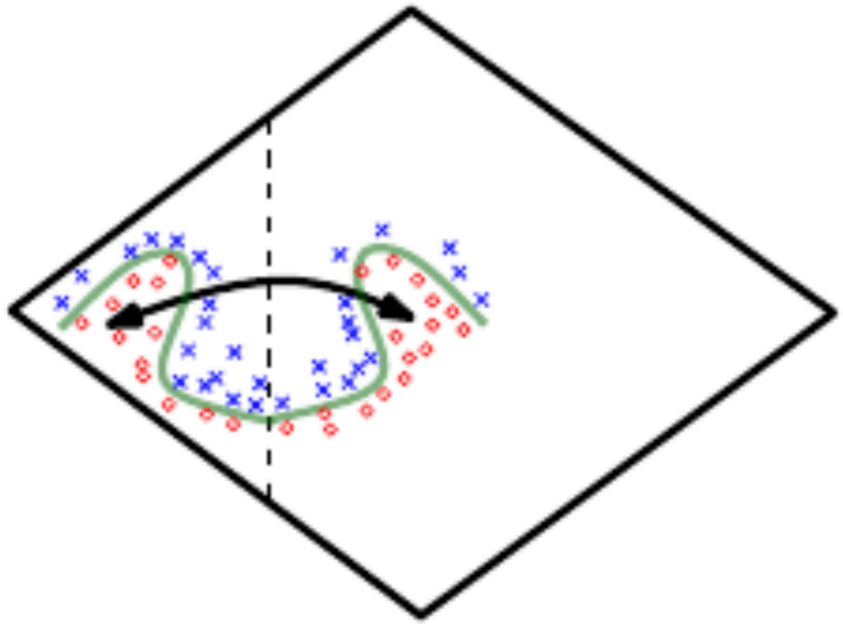
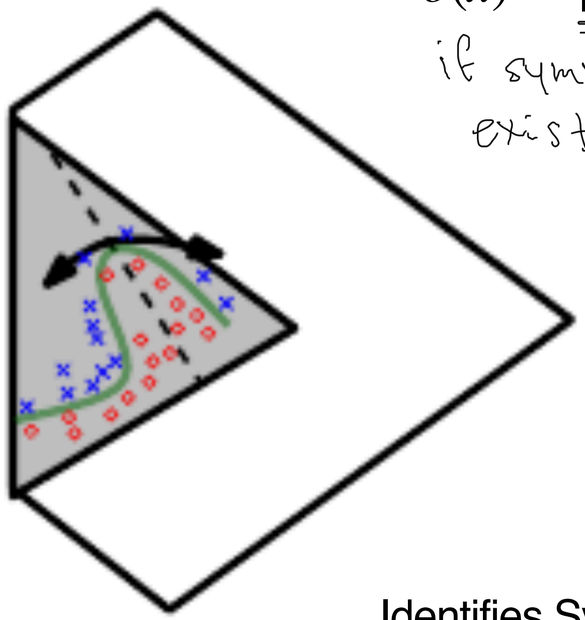


Each column, different w
& row is different offset

ACTIVATION FUNCTIONS

WHAT THEY REPRESENT . what they do

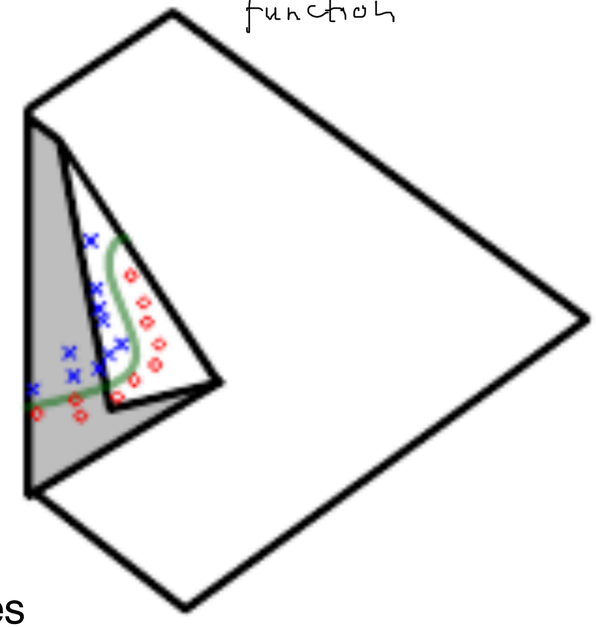




$\sigma(x) = |x|$

if symmetries exist

much simpler function



Identifies Symmetries

NEXT CLASS

Next Class — Training Neural Networks