# Neural Networks
# Learning the network: Part 1

11-785, Spring 2018

Lecture 3

# Designing a net..

- Input:  An N-D real vector
- Output:  A class (binary classification)

- “Input units”?
- Output units?
- Architecture?
- Output activation?

# Designing a net..

- Input:  An N-D real vector
- Output:  Multi-class classification

- “Input units”?
- Output units?
- Architecture?
- Output activation?

# Designing a net..

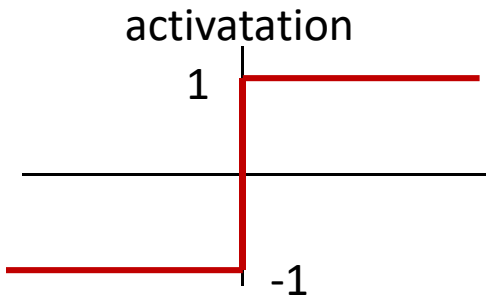
- Input:  An N-D real vector
- Output:  Real-valued output

- “Input units”?
- Output units?
- Architecture?
- Output activation?

# Designing a net..

- Conversion of real number to binary representation
  - Input: A real number
  - Output: The binary sequence for the number

- "Input units"?
- Output units?
- Architecture?
- Output activation?


activatation
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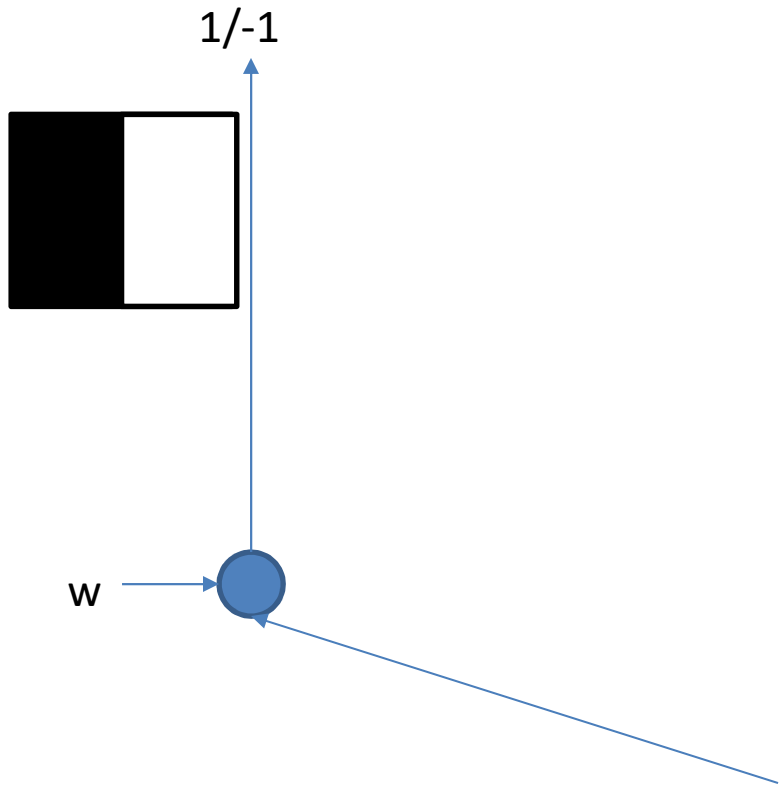
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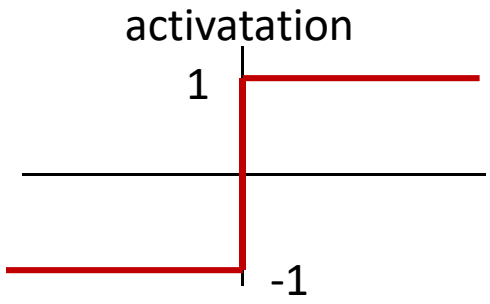
activatation
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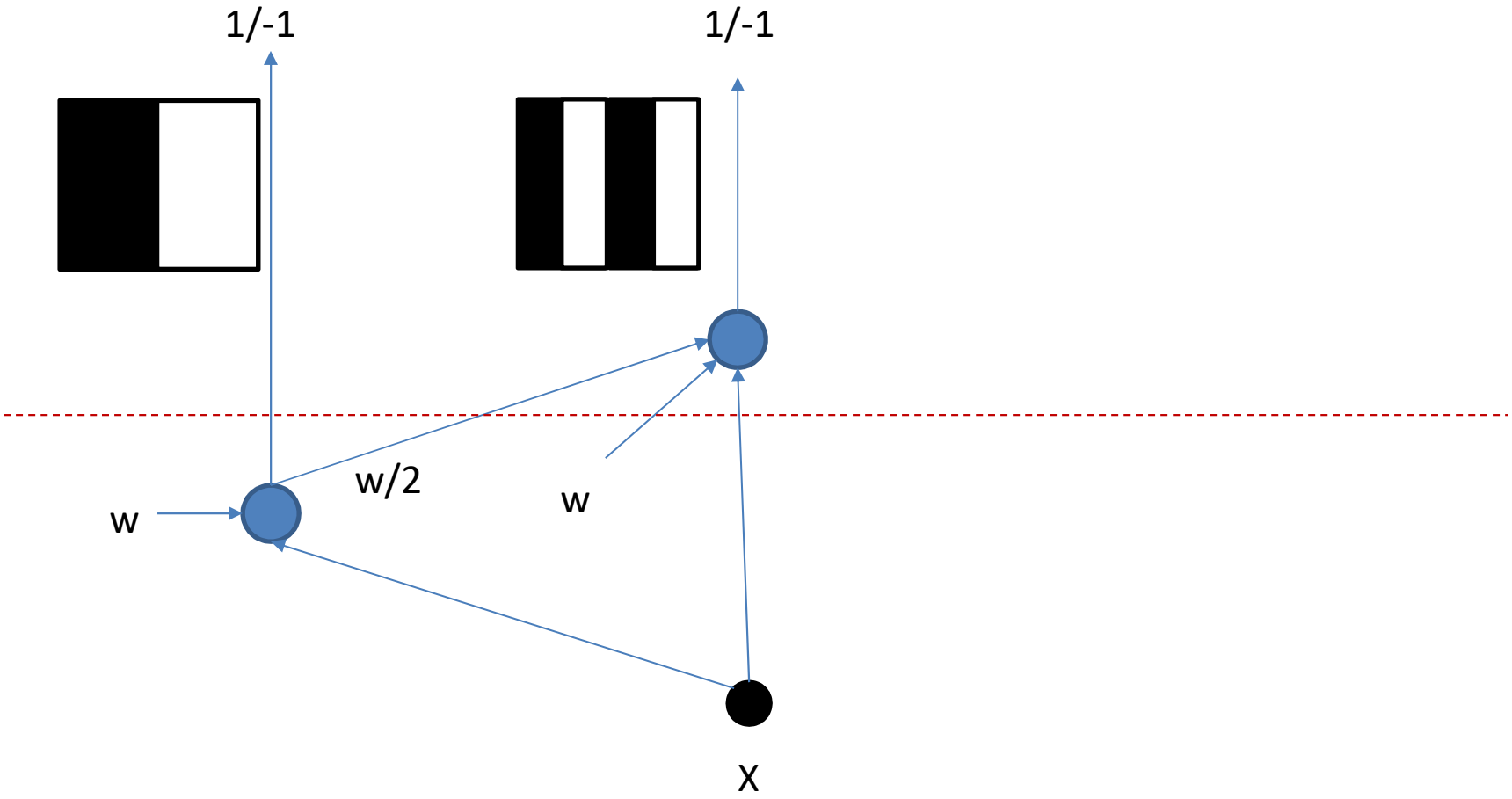
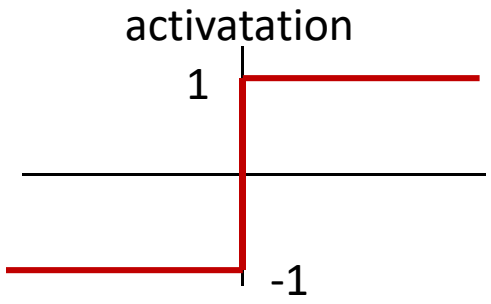

1/-1
1/-1
w
w/2
w
X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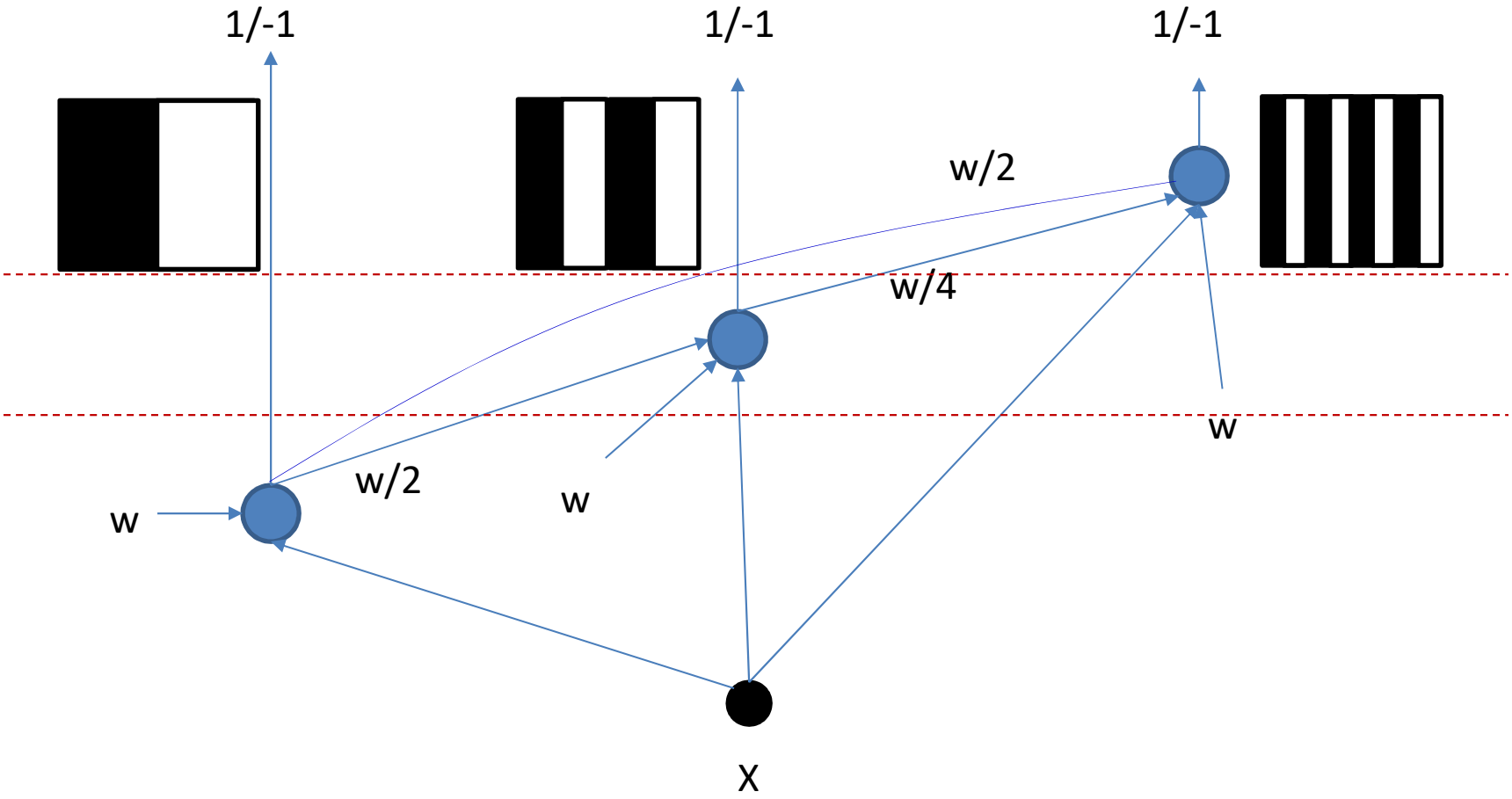

1/-1
1/-1
1/-1
w/2
w/4
w
w/2
w
w
X

# Designing a net..

- Binary addition:
  - Input: Two binary inputs
  - Output:  The binary (bit-sequence) sum

- "Input units"?
- Output units?
- Architecture?
- Output activation?

# Designing a net..

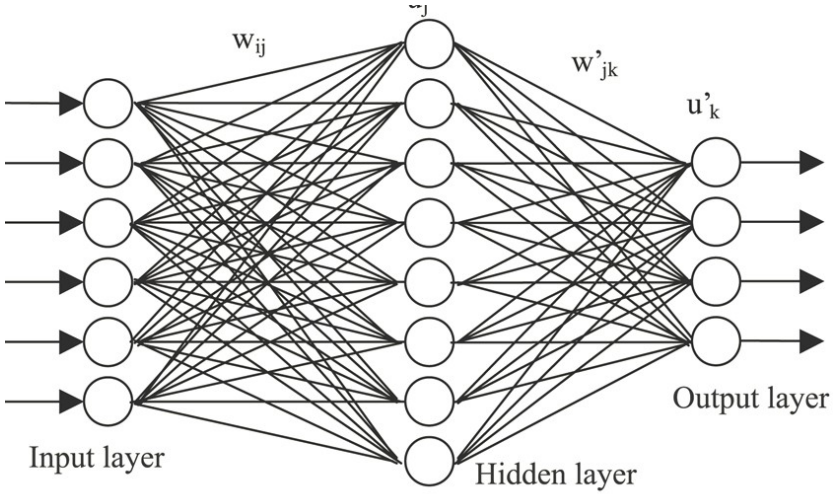
- Clustering:
  - Input: Real-valued vector
  - Output:  Cluster ID

- "Input units"?
- Output units?
- Architecture?
- Output activation?

# Topics for the day

- The problem of learning
- The perceptron rule for perceptrons
  - And its inapplicability to multi-layer perceptrons
- Greedy solutions for classification networks: ADALINE and MADALINE
- Learning through Empirical Risk Minimization
- Intro to function optimization and gradient descent

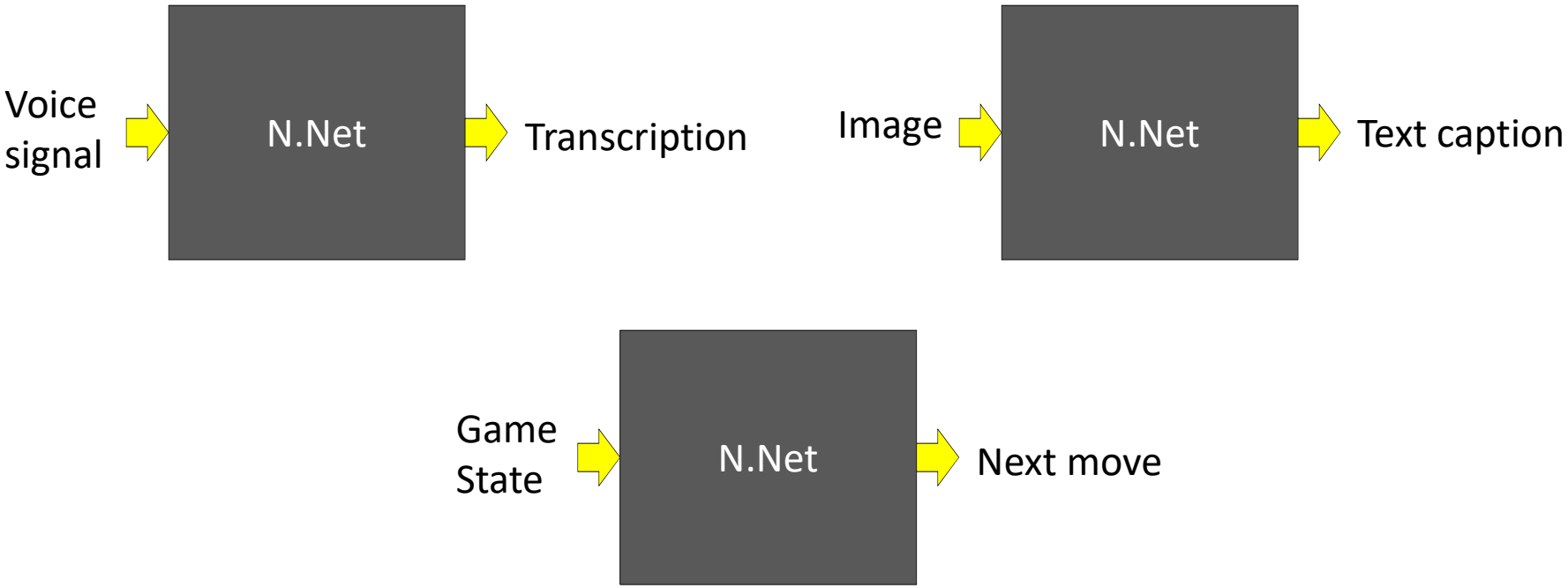
# Recap




- **Neural networks are universal function approximators**
  - Can model any Boolean function
  - Can model any classification boundary
  - Can model any continuous valued function

- *Provided the network satisfies minimal architecture constraints*
  - Networks with fewer than required parameters can be very poor approximators

# These boxes are functions




- Take an input
- Produce an output
- Can be modeled by a neural network!

# Questions

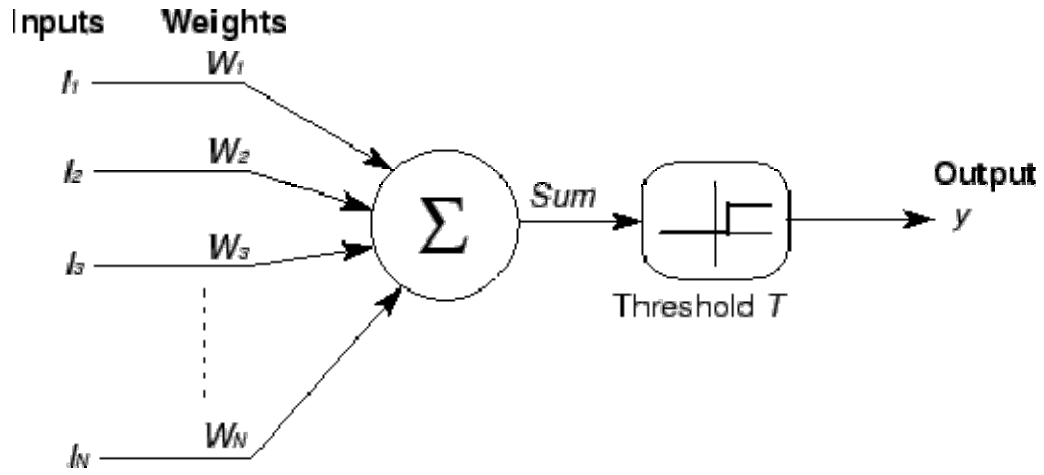

- Preliminaries:
  - How do we represent the input?
  - How do we represent the output?
- How do we compose the network that performs the requisite function?

# Questions


- Preliminaries:
  - How do we represent the input?
  - How do we represent the output?
- *How do we compose the network that performs the requisite function?* ⟵

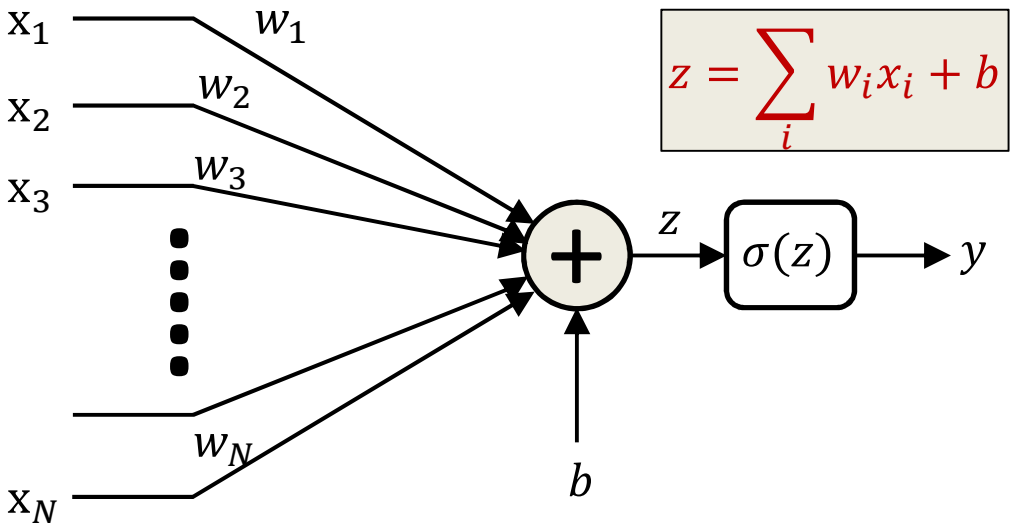
A bit later in the program

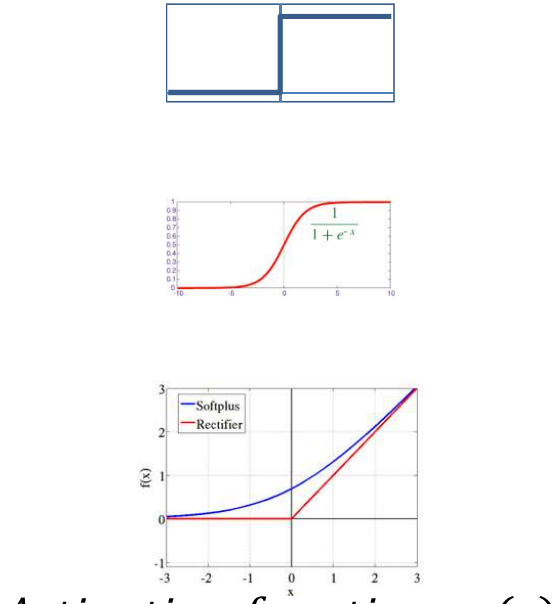
# The original perceptron




- Simple threshold unit
  - Unit comprises a set of weights and a threshold

# Preliminaries: The units in the network

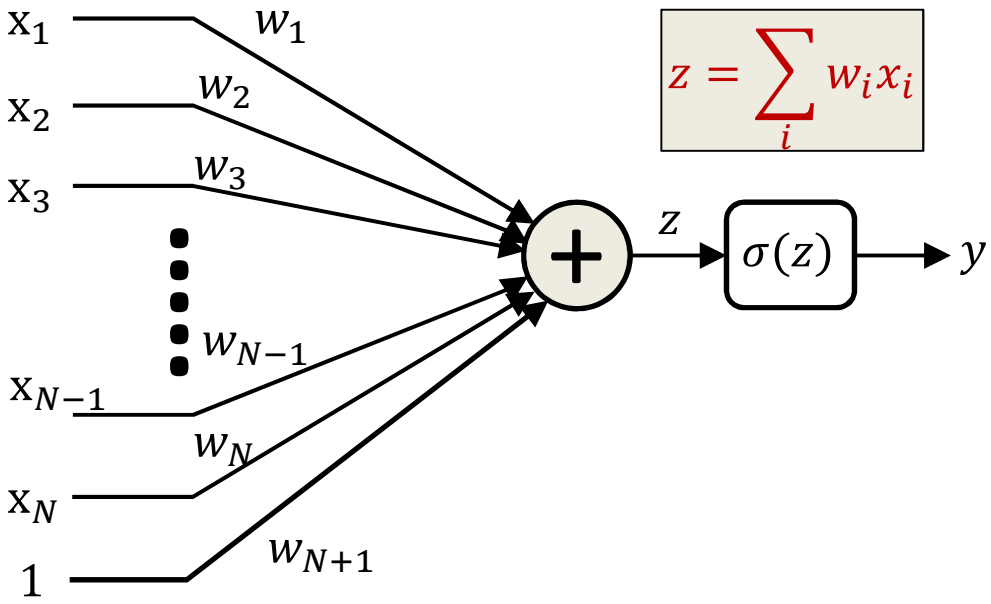


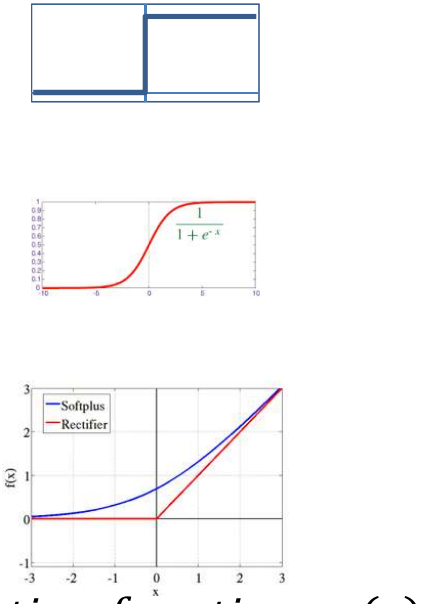




*Activation functions* $\sigma(z)$

- Perceptron
  - General setting, inputs are real valued
  - Activation functions are not necessarily threshold functions
  - A *bias* $b$ representing a threshold to trigger the perceptron

# Preliminaries: Redrawing the neuron

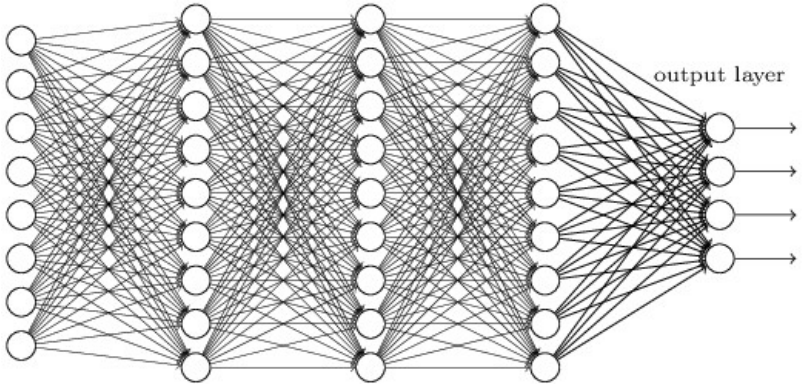


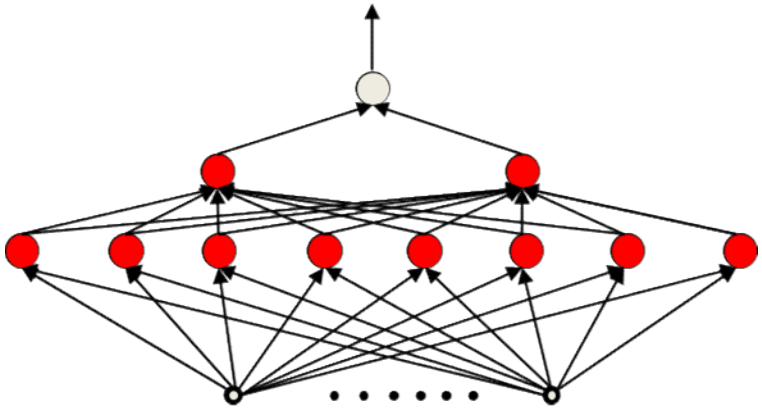




*Activation functions* $\sigma(z)$

- The bias can also be viewed as the weight of another input component that is always set to 1
  - If the bias is not explicitly mentioned, we will implicitly be assuming that every perceptron has an additional input that is always fixed at 1

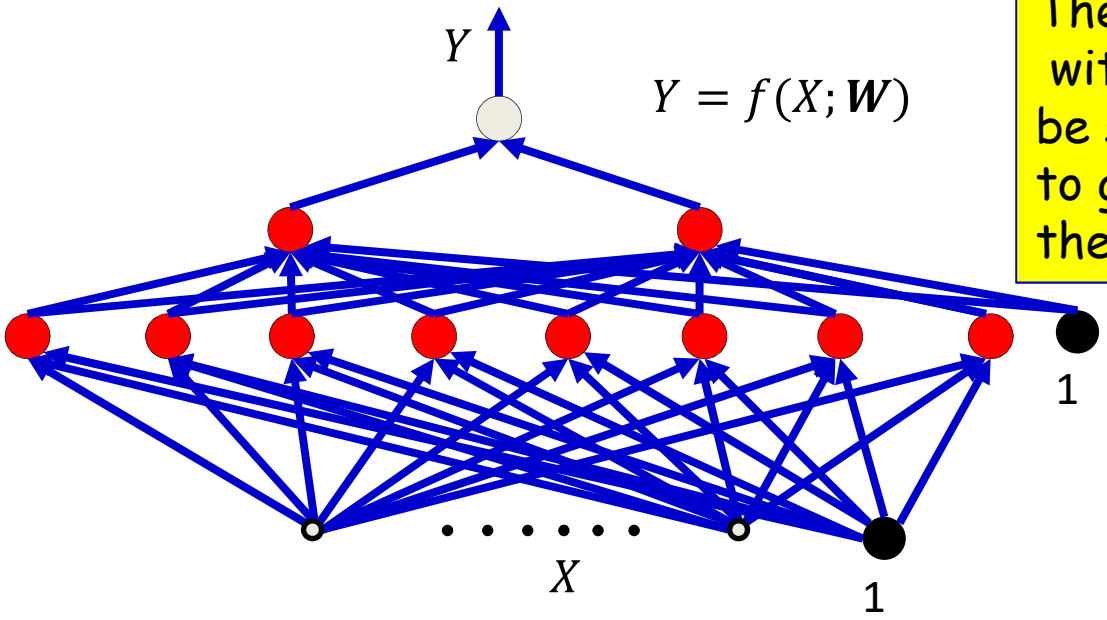
# First: the structure of the network



- We will assume a *feed-forward* network
  - No loops: Neuron outputs do not feed back to their inputs directly or indirectly
  - Loopy networks are a future topic
- **Part of the design of a network: The architecture**
  - How many layers/neurons, which neuron connects to which and how, etc.
- For now, assume the architecture of the network is capable of representing the needed function

# What we learn: The parameters of the network

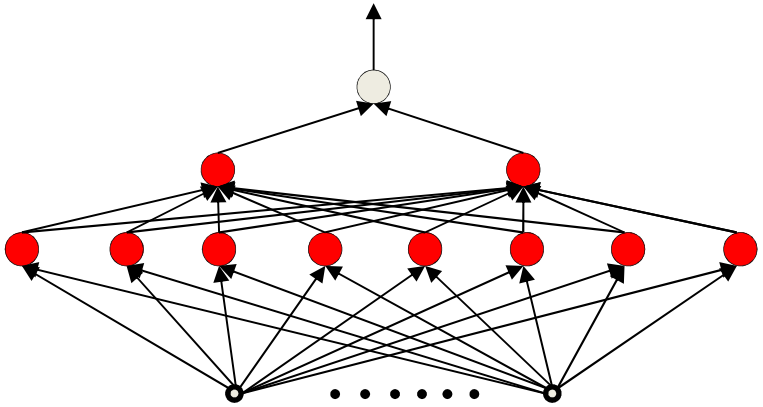


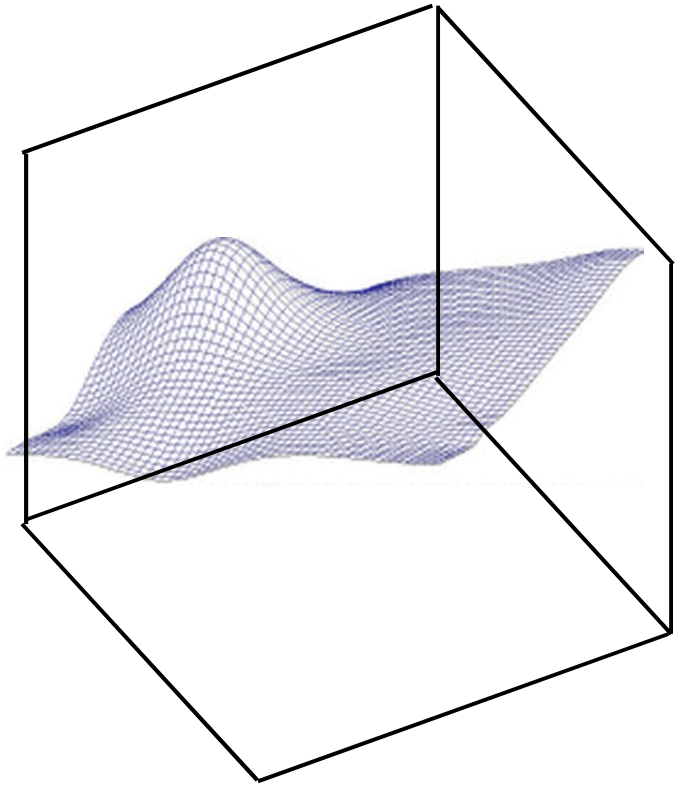

The network is a function f() with parameters W which must be set to the appropriate values to get the desired behavior from the net

- **Given:** the architecture of the network
- The parameters of the network: The weights and biases
  - The weights associated with the blue arrows in the picture
- *Learning the network :* Determining the values of these parameters such that the network computes the desired function

- Moving on..

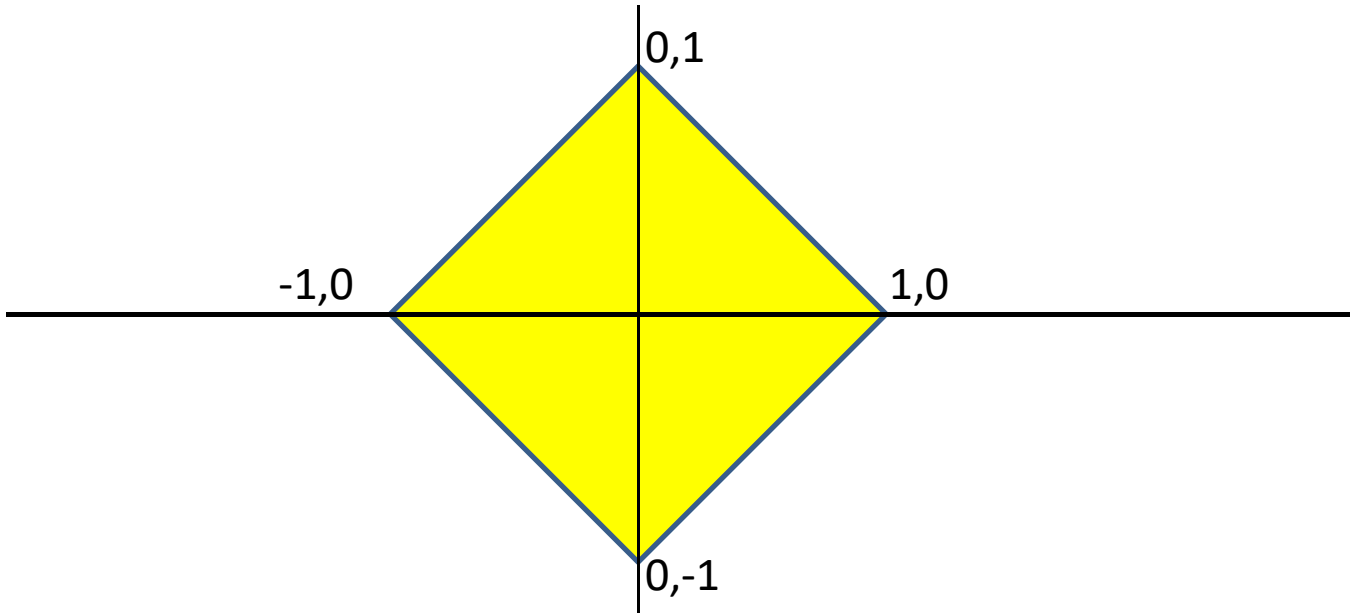
# The MLP *can* represent anything





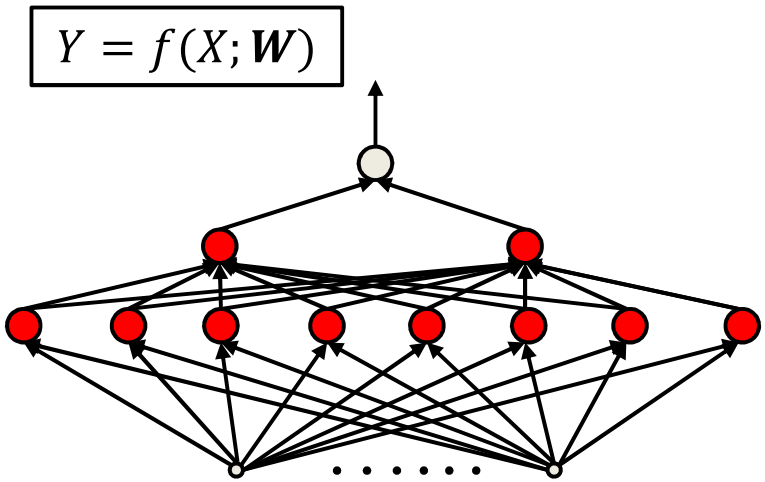
- The MLP *can be constructed* to represent anything
- But *how* do we construct it?

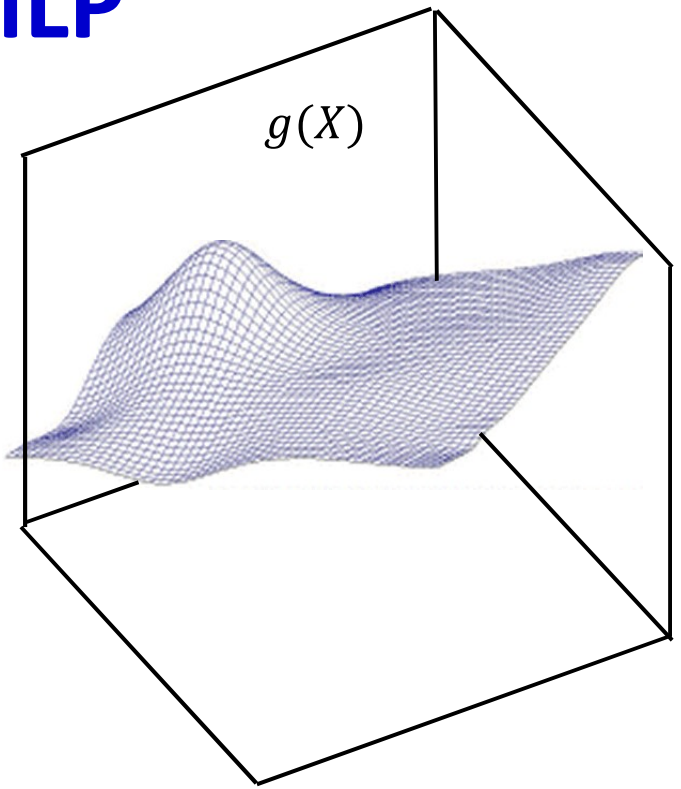
# Option 1: Construct by hand




- Given a function, *handcraft* a network to satisfy it
- E.g.: Build an MLP to classify this decision boundary
- Not possible for all but the simplest problems..

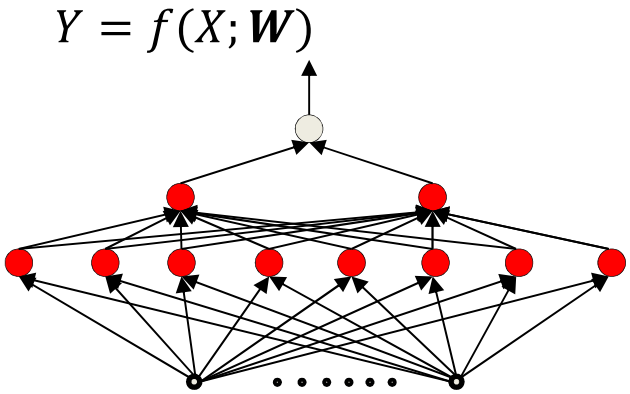
# Option 2: Automatic estimation of an MLP

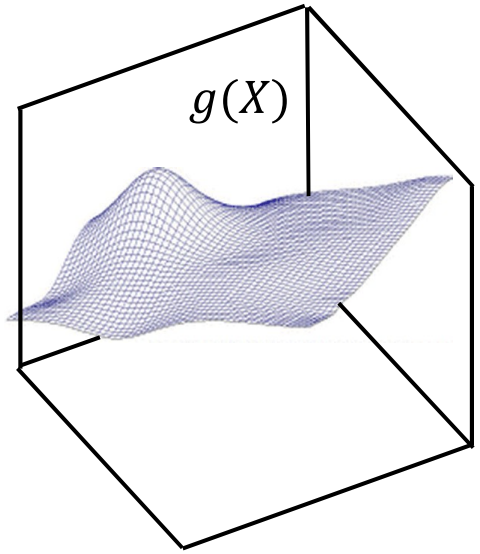



- More generally, *given* the function $g(X)$ to model, we can *derive* the parameters of the network to model it, through computation

# How to learn a network?



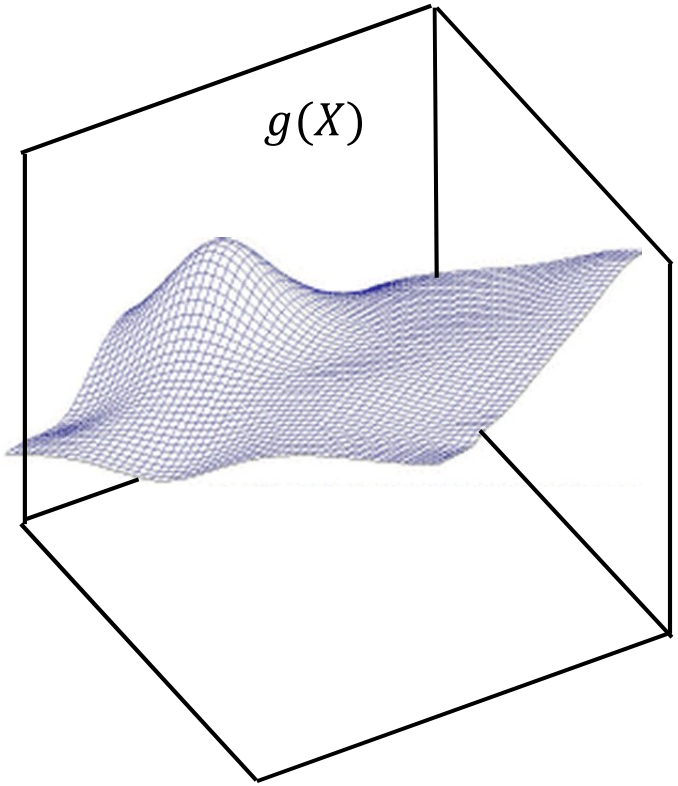




- When $f(X; \boldsymbol{W})$ has the capacity to exactly represent $g(X)$

$$\widehat{\boldsymbol{W}} = \underset{W}{\operatorname{argmin}} \int_X div\big(f(X; W), g(X)\big) dX$$

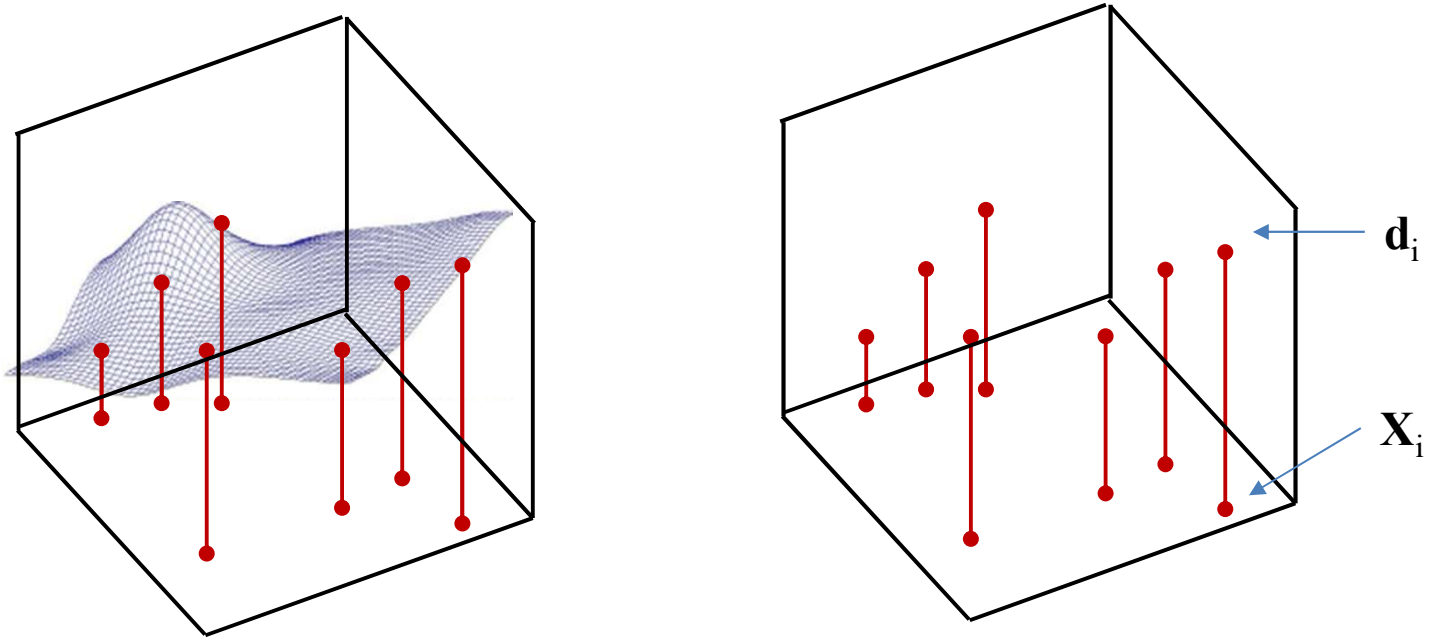
- div() is a *divergence* function that goes to zero when $f(X; W) = g(X)$

# Problem $g(X)$ is unknown



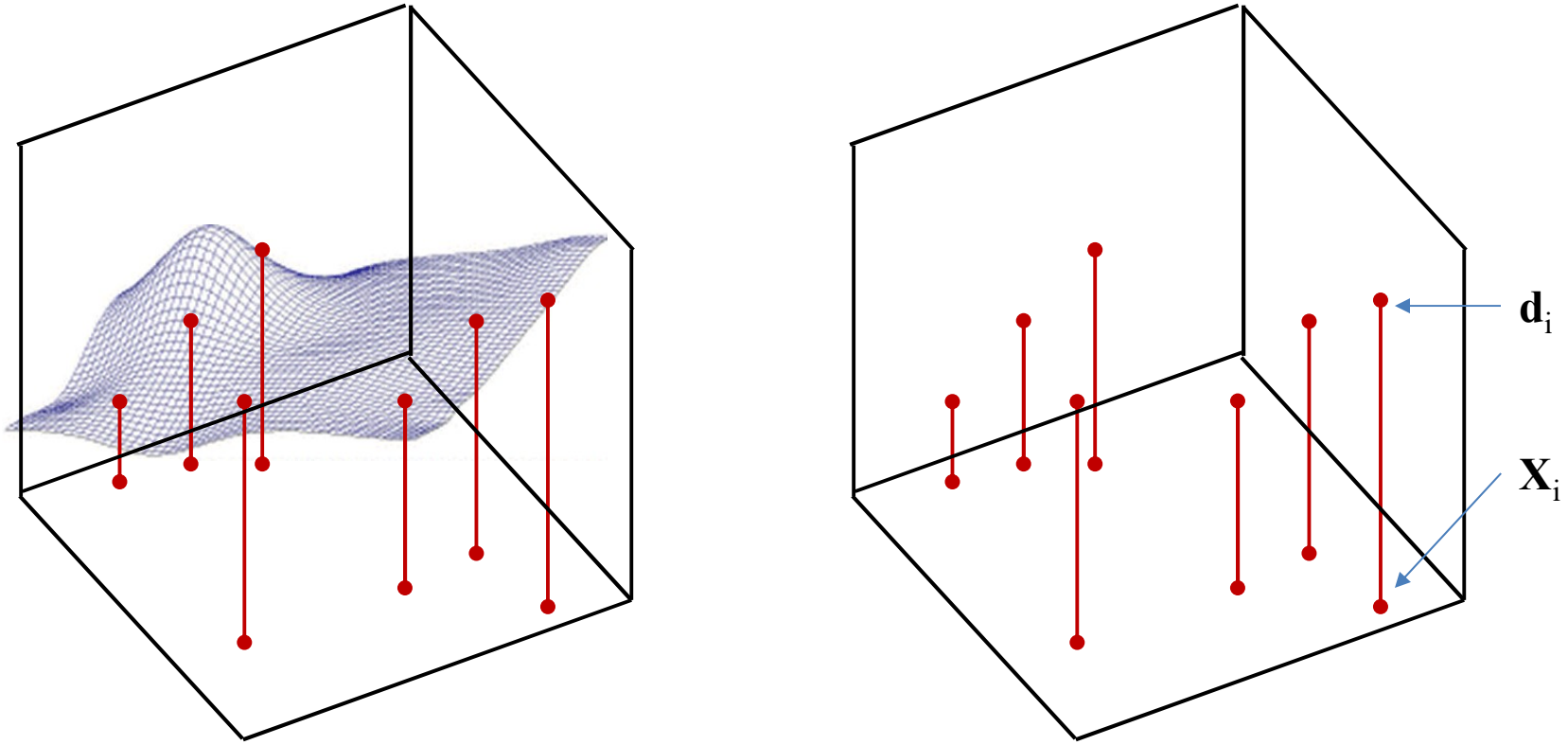

- Function $g(X)$ must be fully specified
  - Known *everywhere,* i.e. for *every* input $X$
- **In practice we will not have such specification**

# Sampling the function




- *Sample* $g(X)$
  - Basically, get input-output pairs for a number of samples of input $X_i$
    - Many samples $(X_i, d_i)$, where $d_i = g(X_i) + noise$
  - Good sampling: the samples of $X$ will be drawn from $P(X)$
- Very easy to do in most problems: just gather training data
  - E.g. set of images and their class labels
  - E.g. speech recordings and their transcription

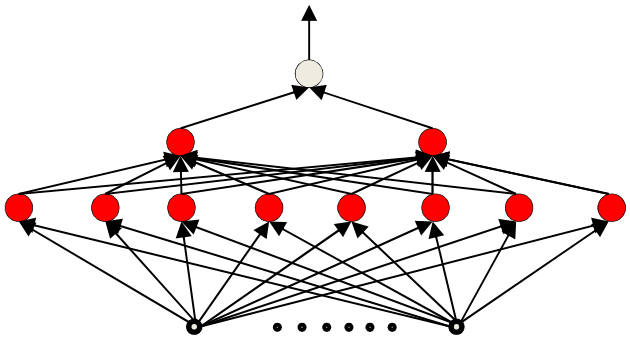
# *Drawing samples*

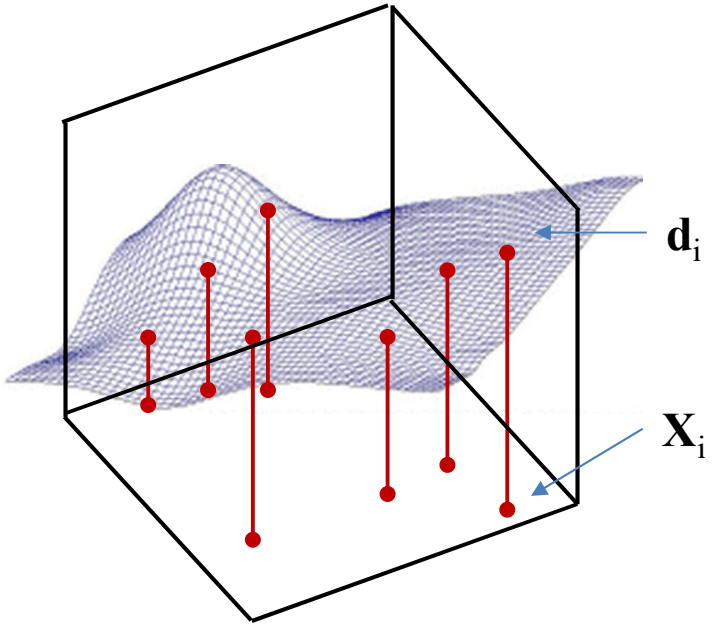



- We must ***learn*** the *entire* function from these few examples
  - The "training" samples

# Learning the function

$Y = f(X; \boldsymbol{W})$



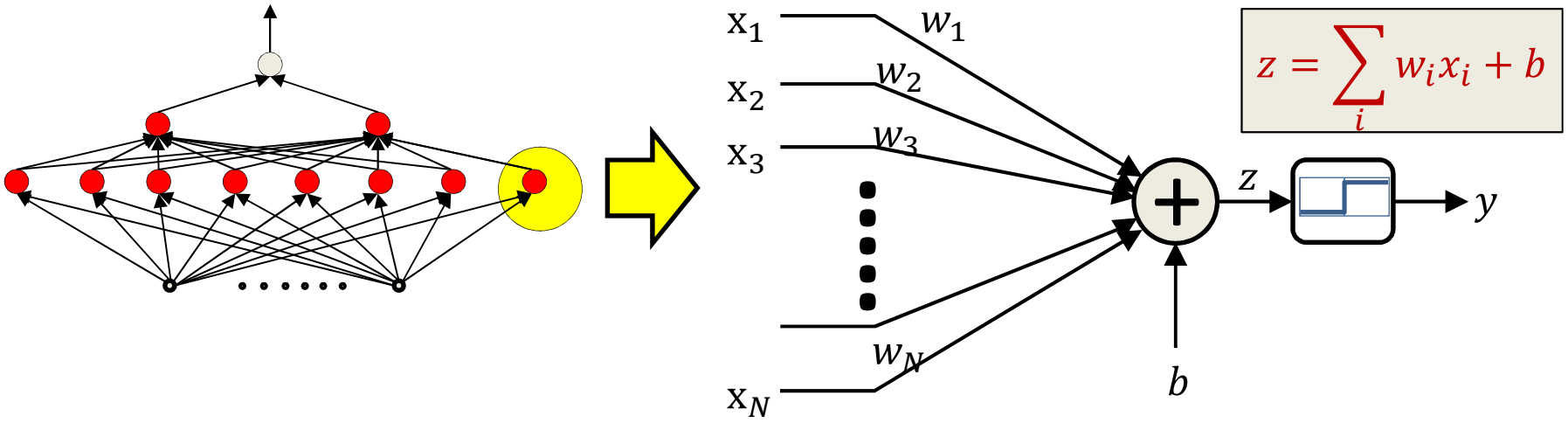



- Estimate the network parameters to "fit" the training points exactly
  - Assuming network architecture is sufficient for such a fit
  - Assuming unique output $d$ at any $\mathbf{X}$
    - And hopefully the resulting function is also correct where we *don't* have training samples

# Lets begin with a simple task

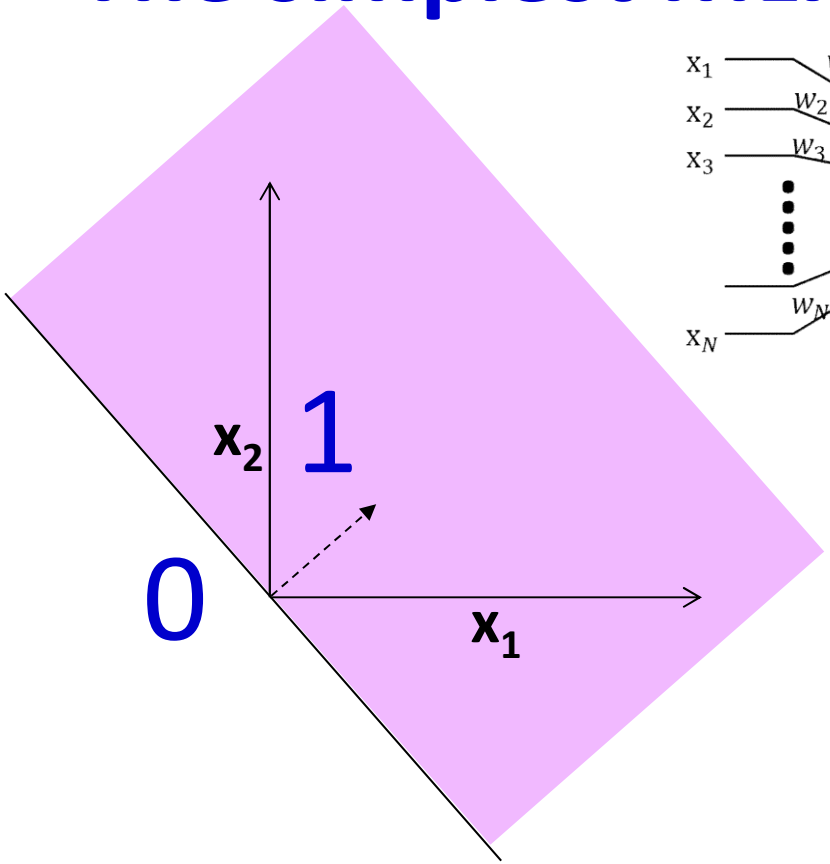
- Learning a *classifier*
  - Simpler than regressions
- This was among the earliest problems addressed using MLPs
- Specifically, consider *binary* classification
  - Generalizes to multi-class

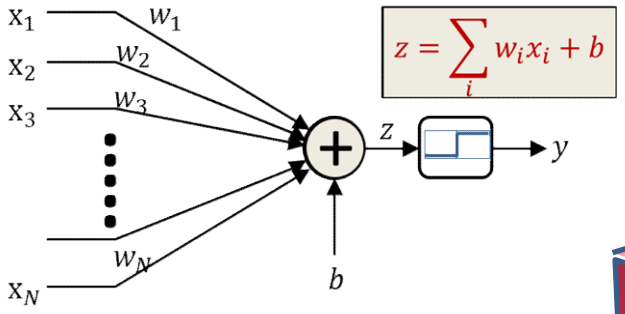
# History: The original MLP

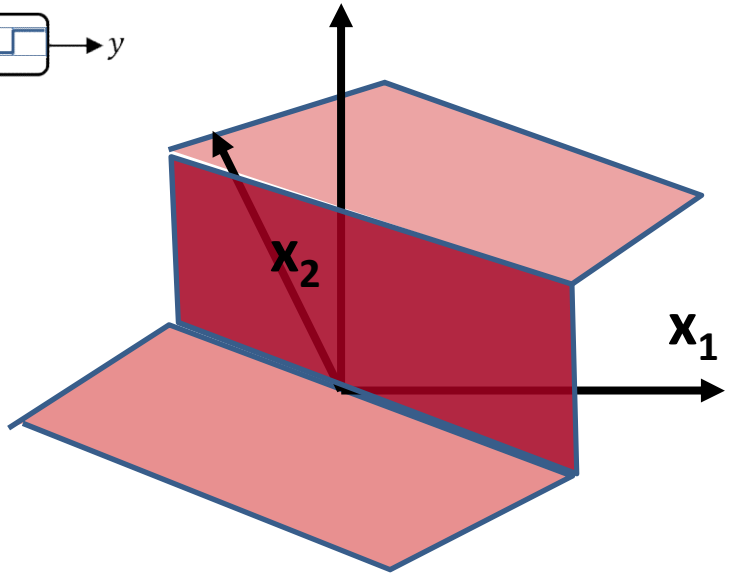



- The original MLP as proposed by Minsky: a network of threshold units
  - But how do you train it?

# The simplest MLP: a single perceptron

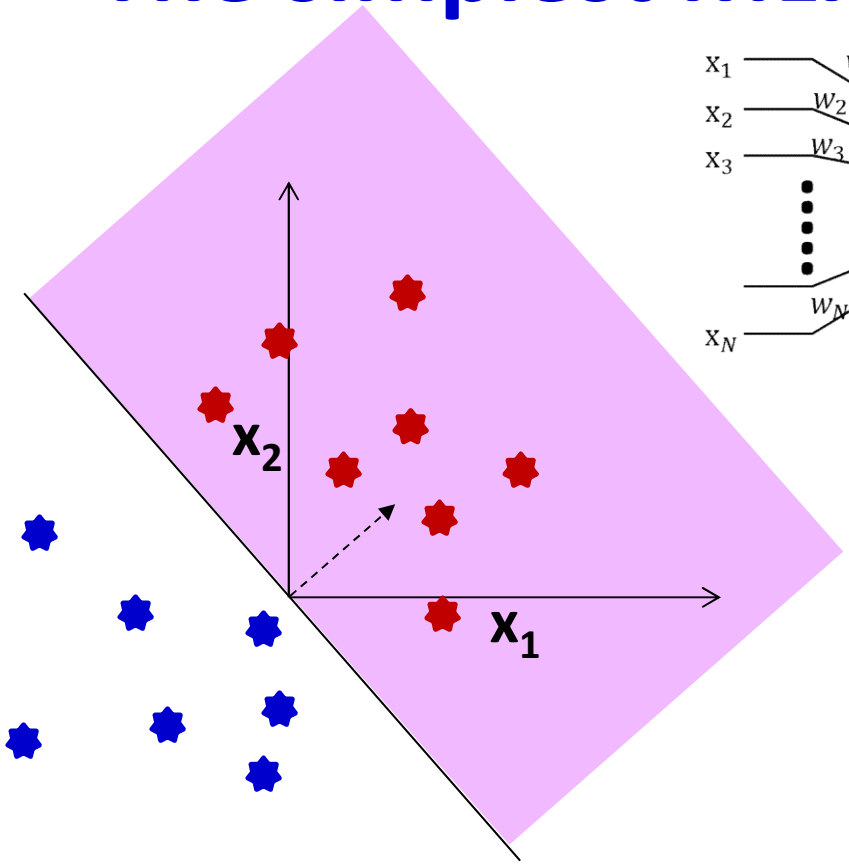


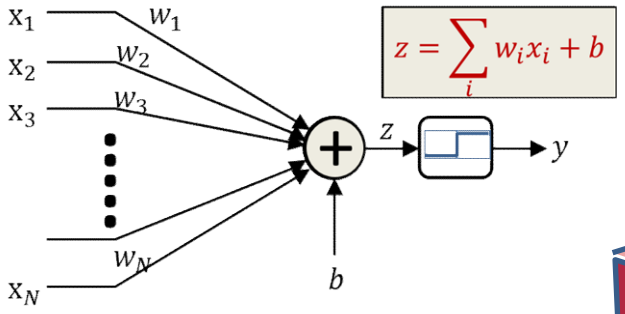



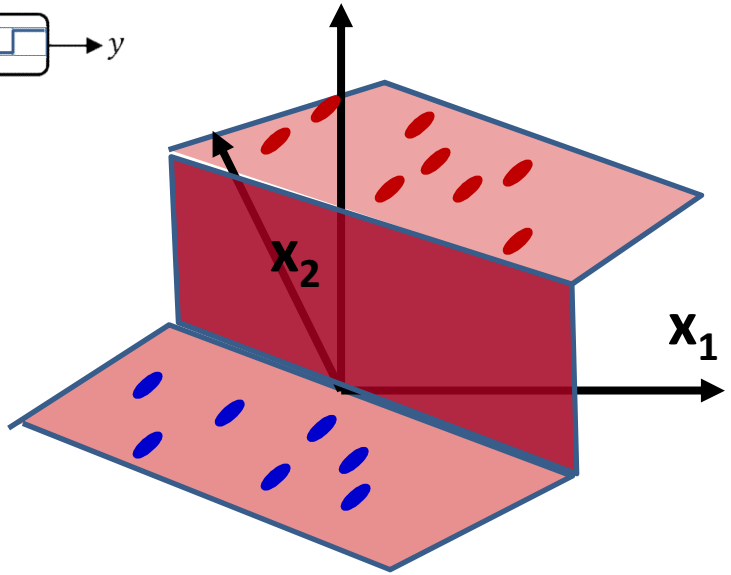




- Learn this function
  - **A step function across a hyperplane**

# The simplest MLP: a single perceptron

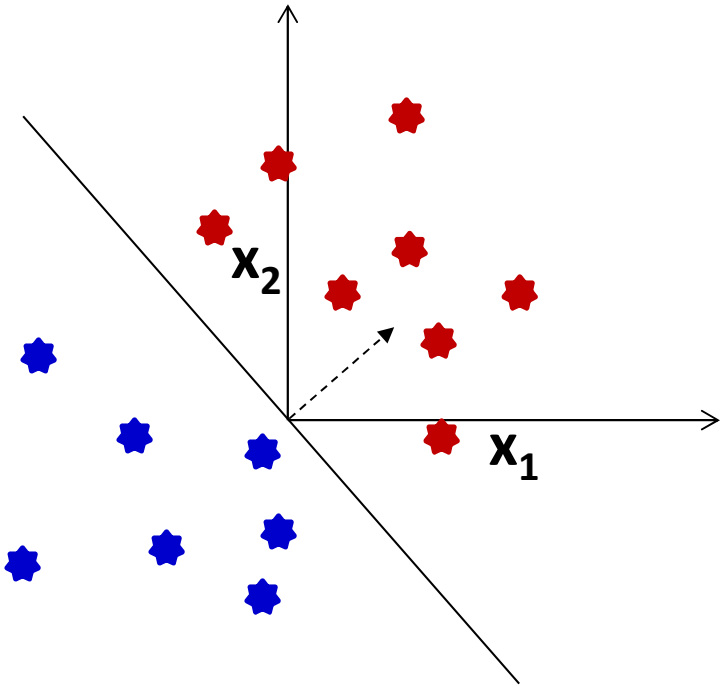


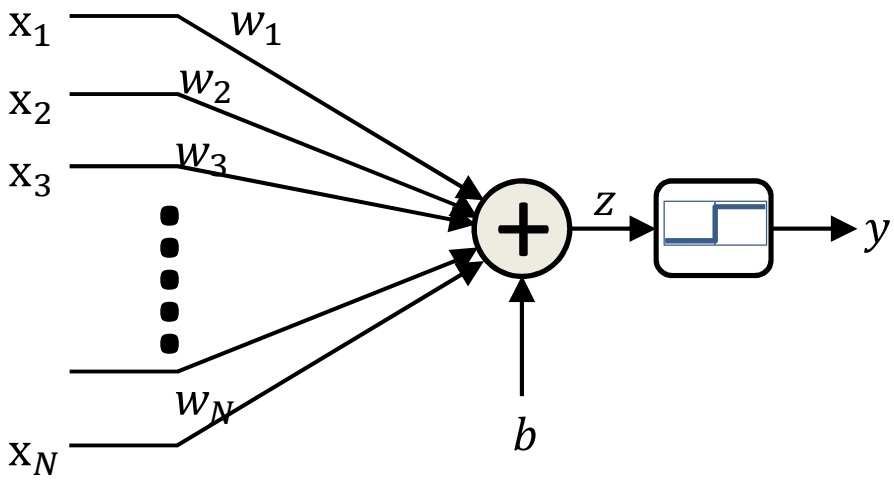




- Learn this function
  - **A step function across a hyperplane**
  - **Given only samples form it**

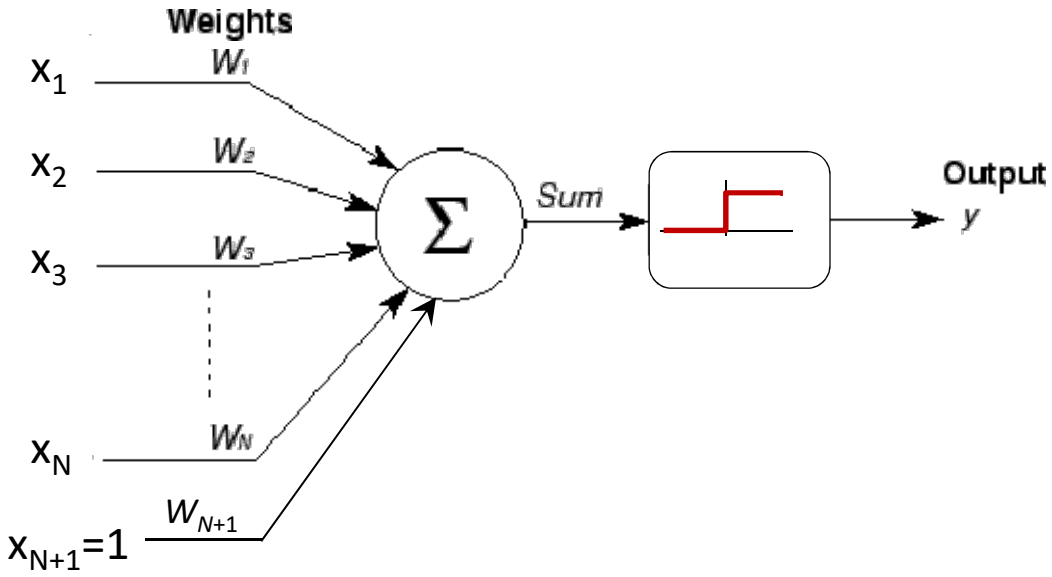
# Learning the perceptron




- Given a number of input output pairs, learn the weights and bias
  - $y = \begin{cases} 1 & if \ \sum_{i=1}^{N} w_i X_i \geq b \\ 0 & otherwise \end{cases}$
  - Learn $W = [w_1 .. w_N]$ and $b$, given several (X, y) pairs

# Restating the perceptron

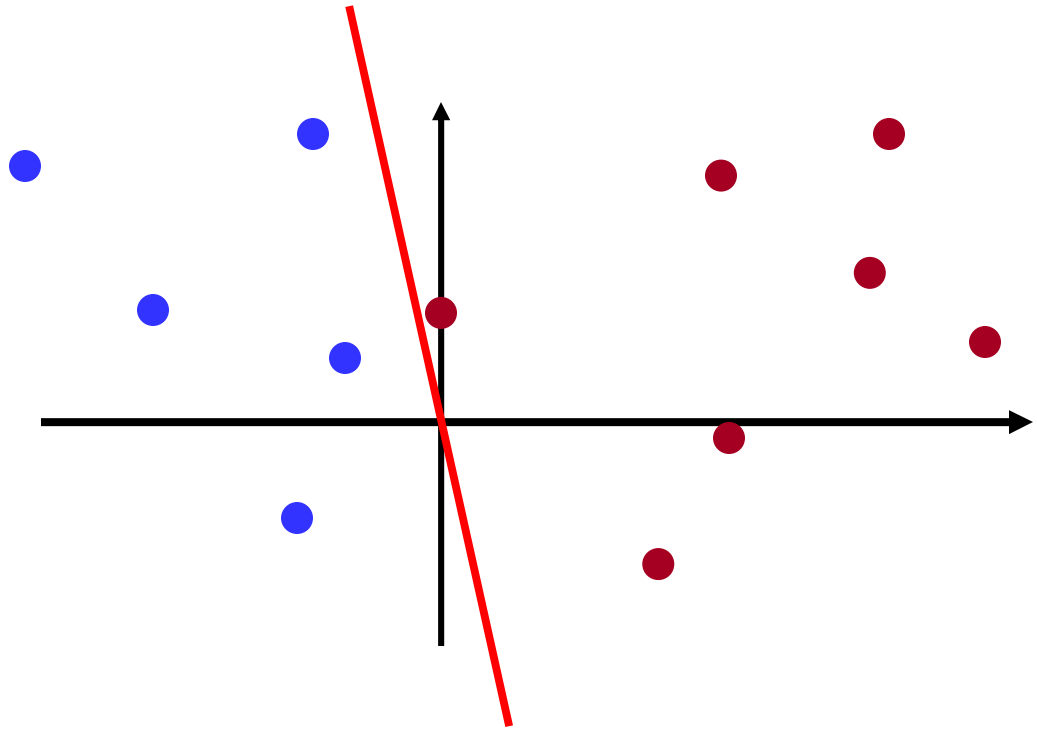



- Restating the perceptron equation by adding another dimension to $X$

$$y = \begin{cases} 1 \;\; if \;\; \sum_{i=1}^{N+1} w_i X_i \geq 0 \\ 0 \;\; otherwise \end{cases}$$

where $X_{N+1} = 1$

# The Perceptron Problem



- Find the hyperplane $\sum_{i=1}^{N+1} w_i X_i = 0$ that perfectly separates the two groups of points

# Perceptron Learning Algorithm

- Given $N$ training instances $(X_1, Y_1), (X_2, Y_2), \ldots, (X_N, Y_N)$
  - $Y_i = +1$ or $-1$

Using a +1/-1 representation for classes to simplify notation

- Initialize $W$
- Cycle through the training instances:
- While more classification errors
  - For $i = 1 \ldots N_{train}$

$$O(X_i) = sign(W^T X_i)$$

    - If $O(X_i) \neq Y_i$

$$W = W + Y_i X_i$$

# Perceptron Algorithm: Summary

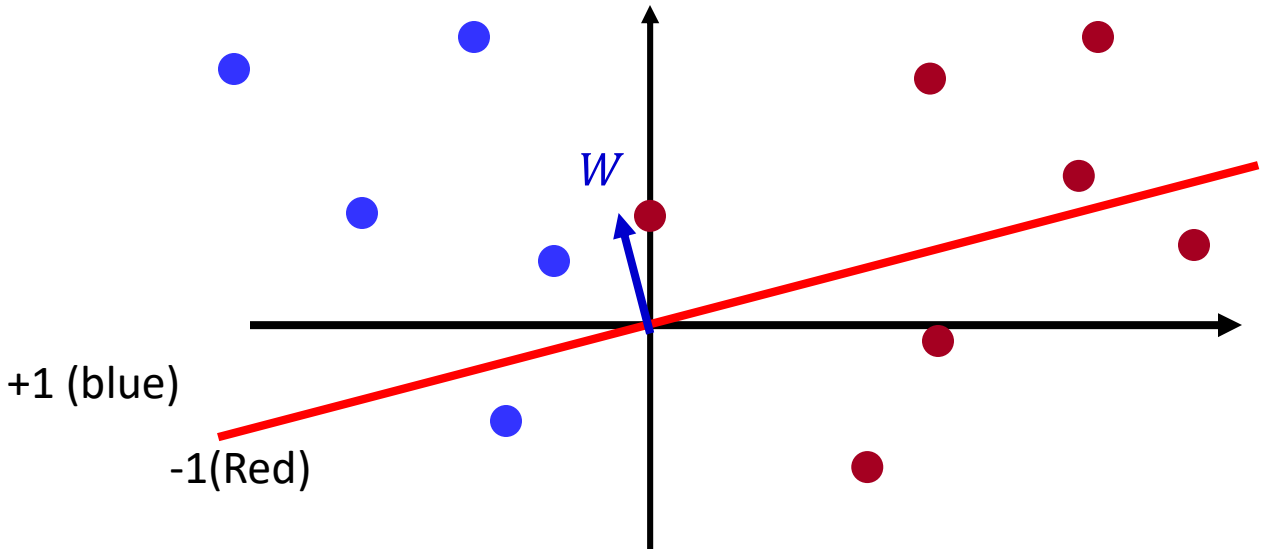
- Cycle through the training instances
- Only update $W$ on misclassified instances
- If instance misclassified:
  - If instance is positive class

$$W = W + X_i$$

  - If instance is negative class

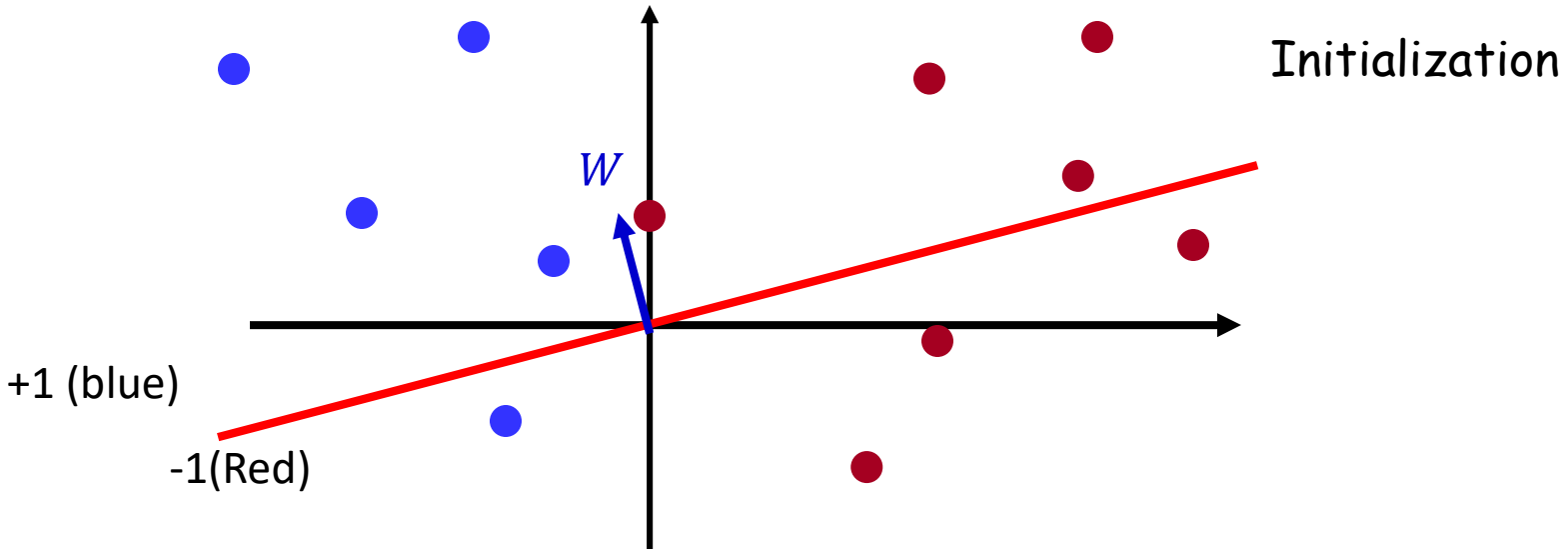
$$W = W - X_i$$

# A Simple Method: The Perceptron Algorithm




- **Initialize:** Randomly initialize the hyperplane
  - I.e. randomly initialize the normal vector $W$
  - Classification rule $sign(W^T X)$
  - The random initial plane will make mistakes

# Perceptron Algorithm



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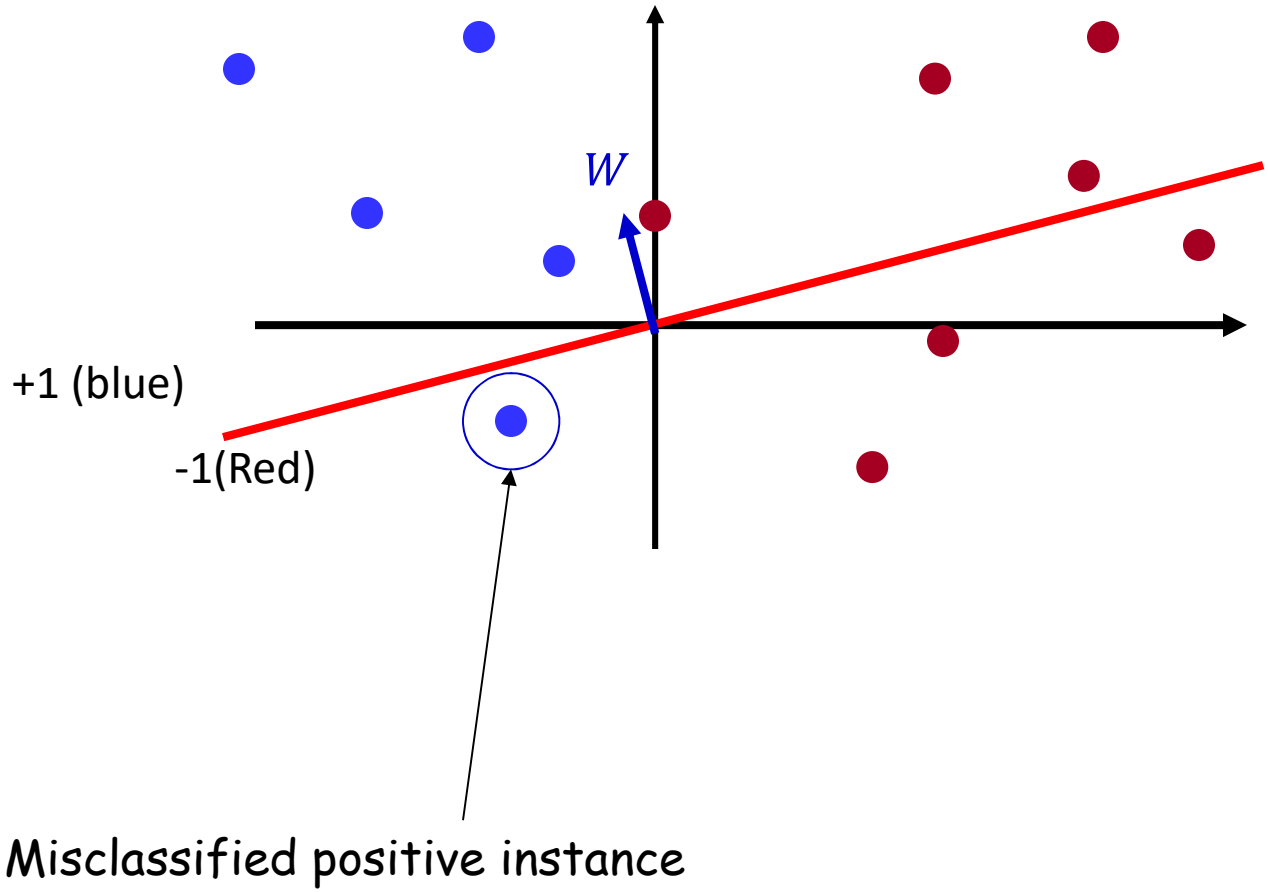

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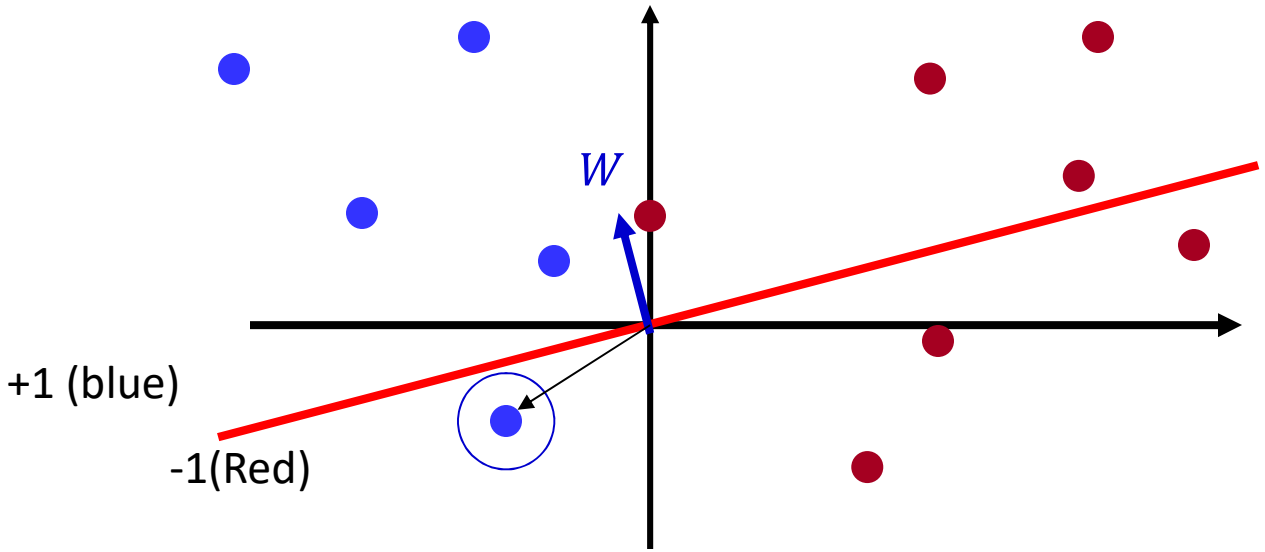
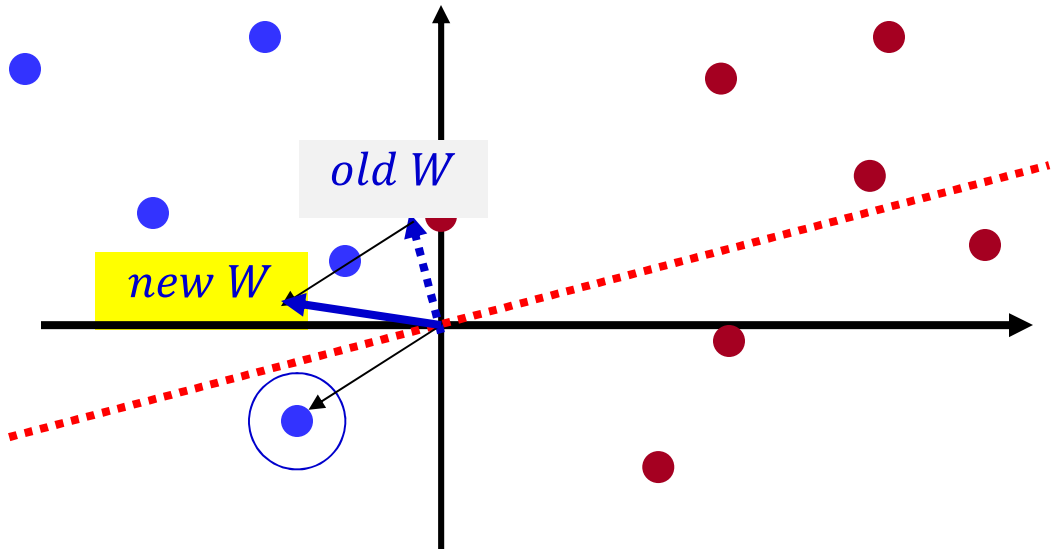


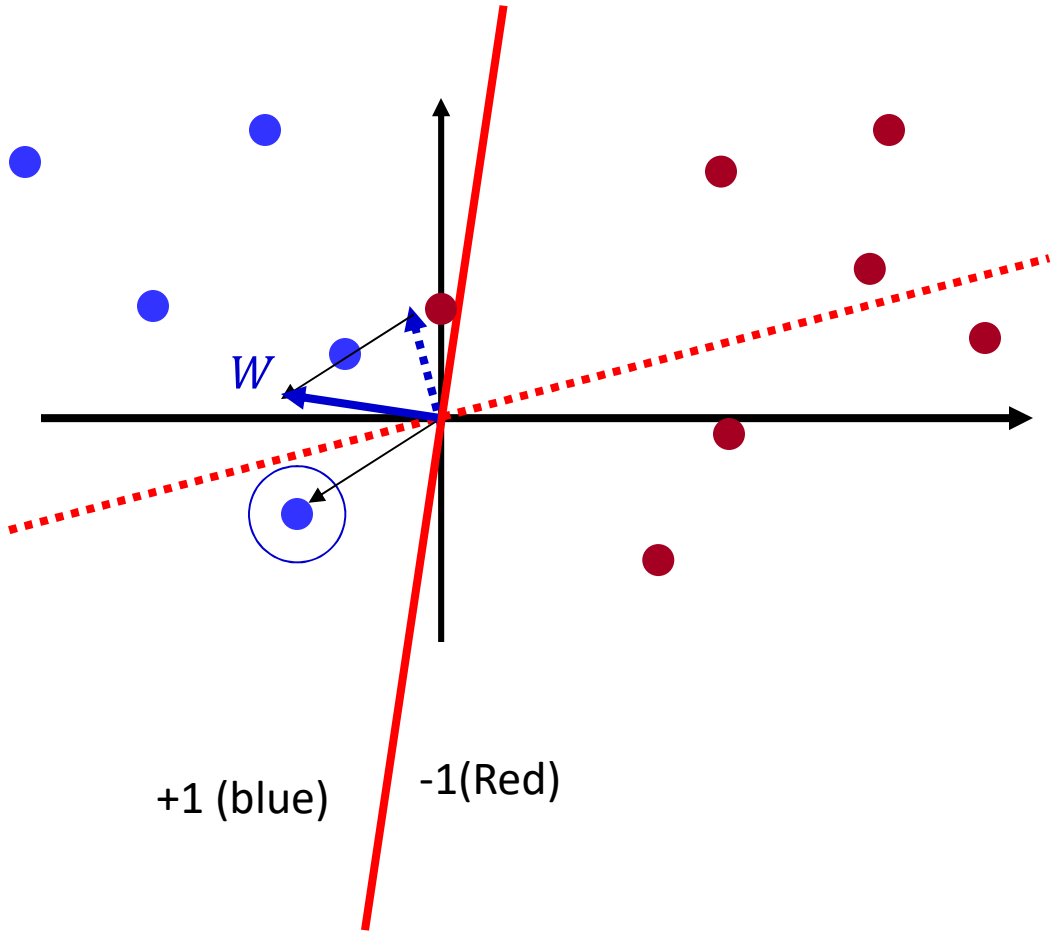
# Perceptron Algorithm



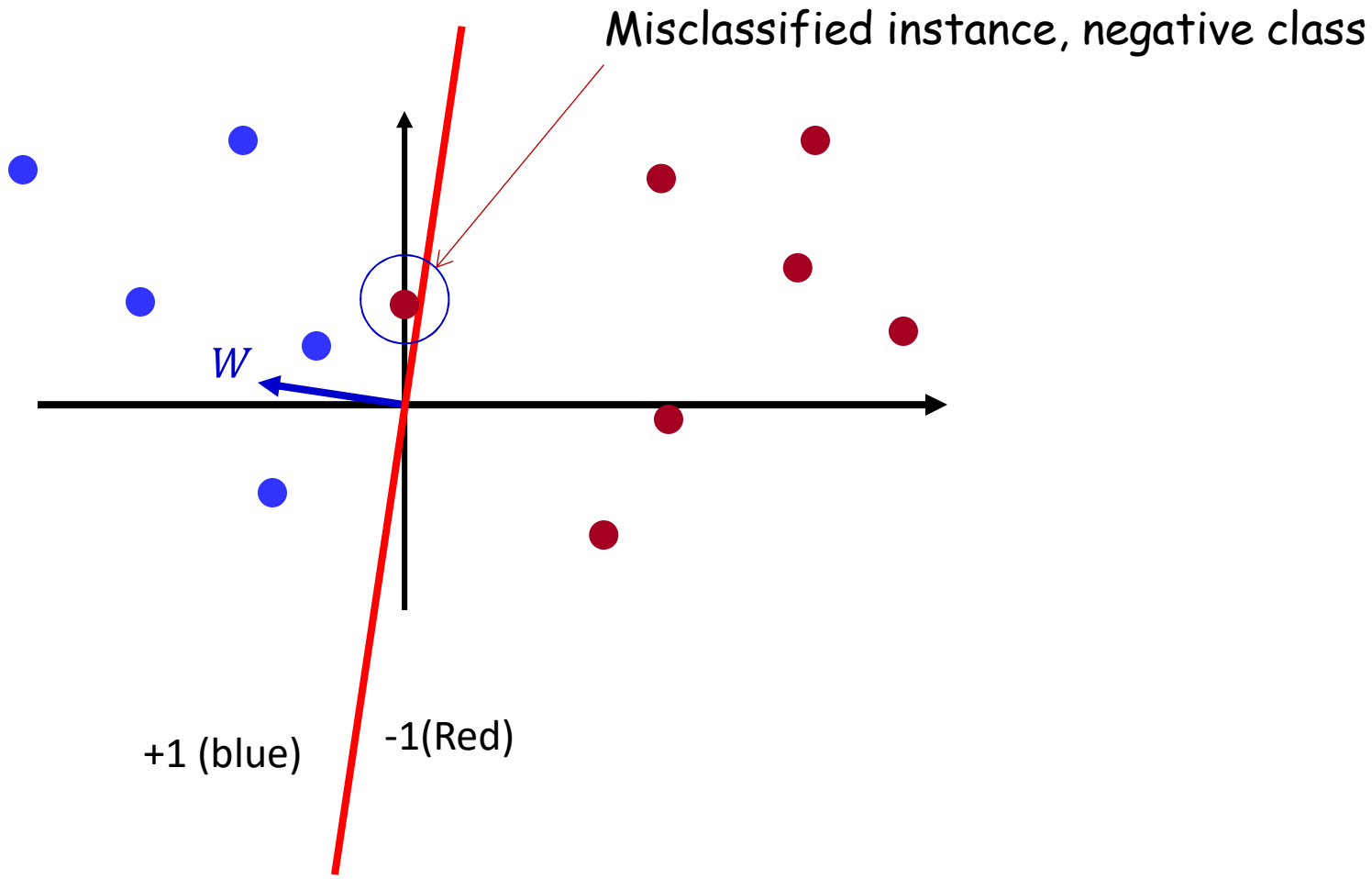

Updated weight vector

Misclassified *positive* instance, *add* it to W

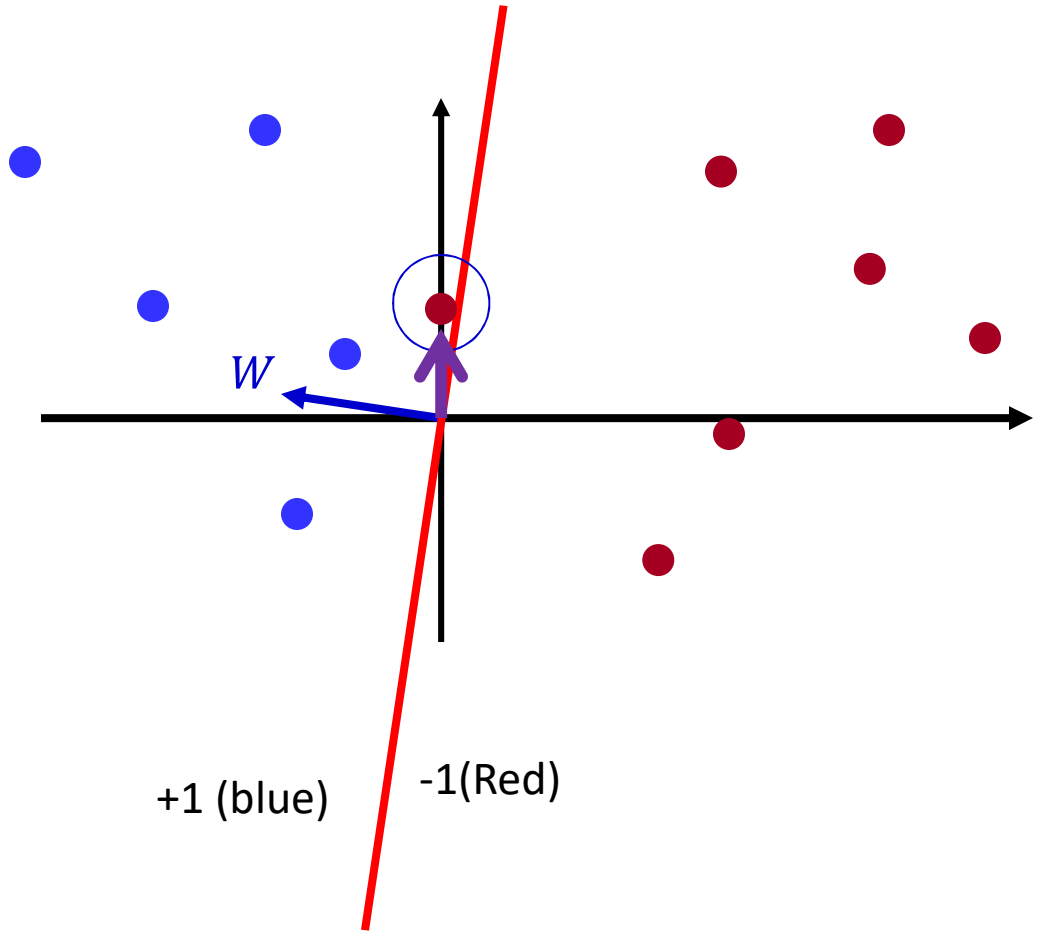
# Perceptron Algorithm



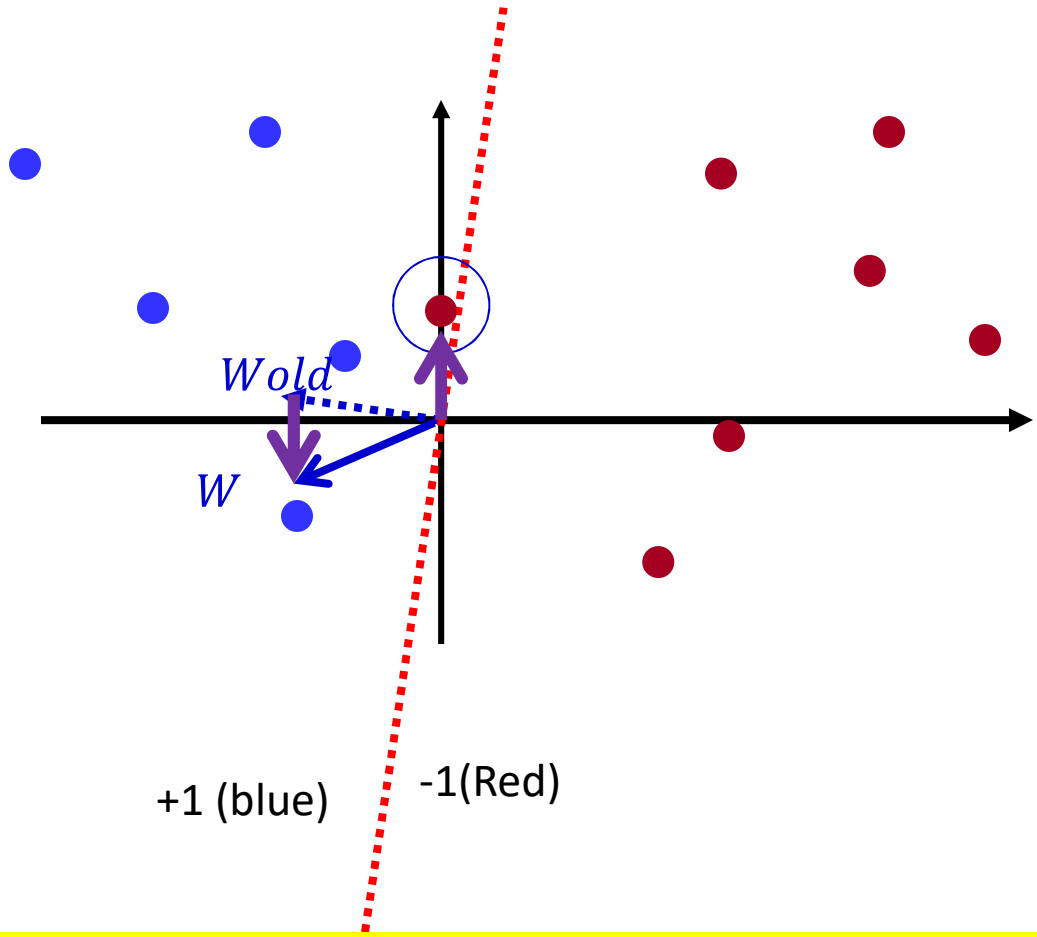
# Perceptron Algorithm



# Perceptron Algorithm

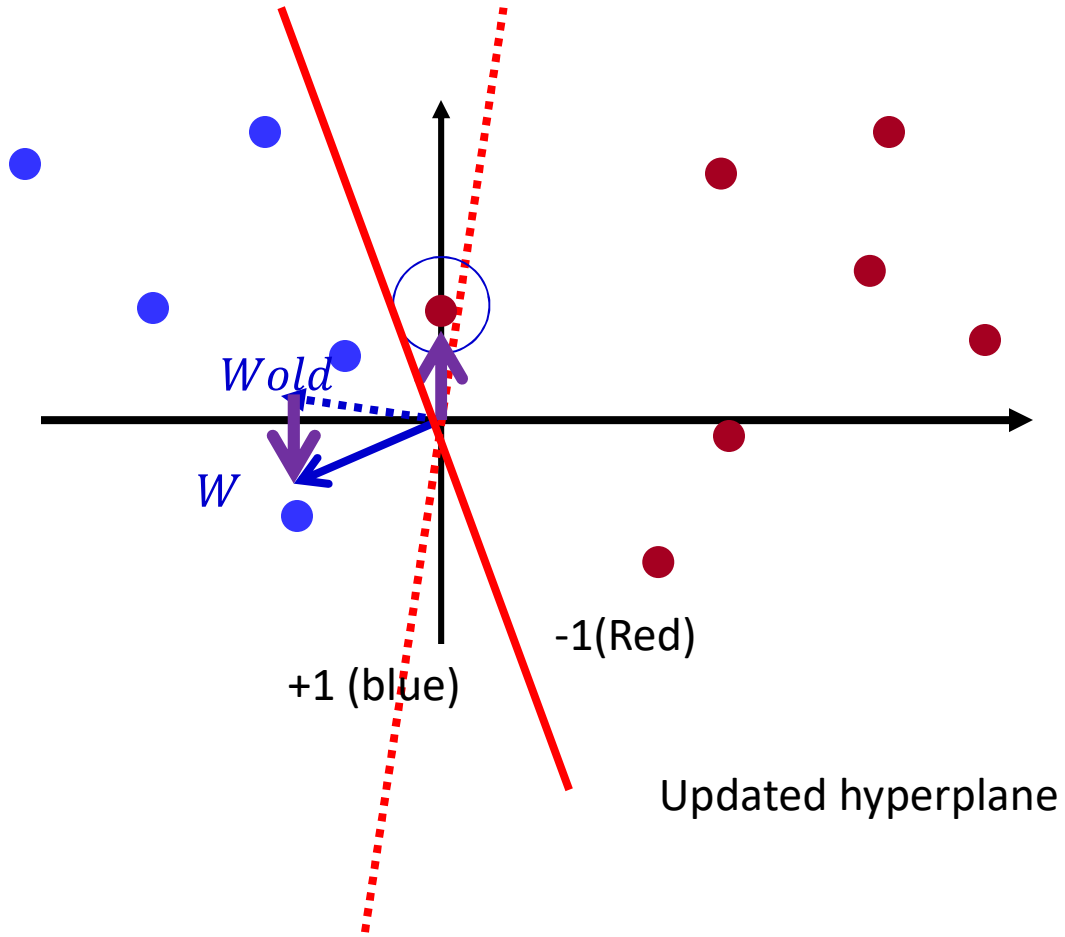


# Perceptron Algorithm

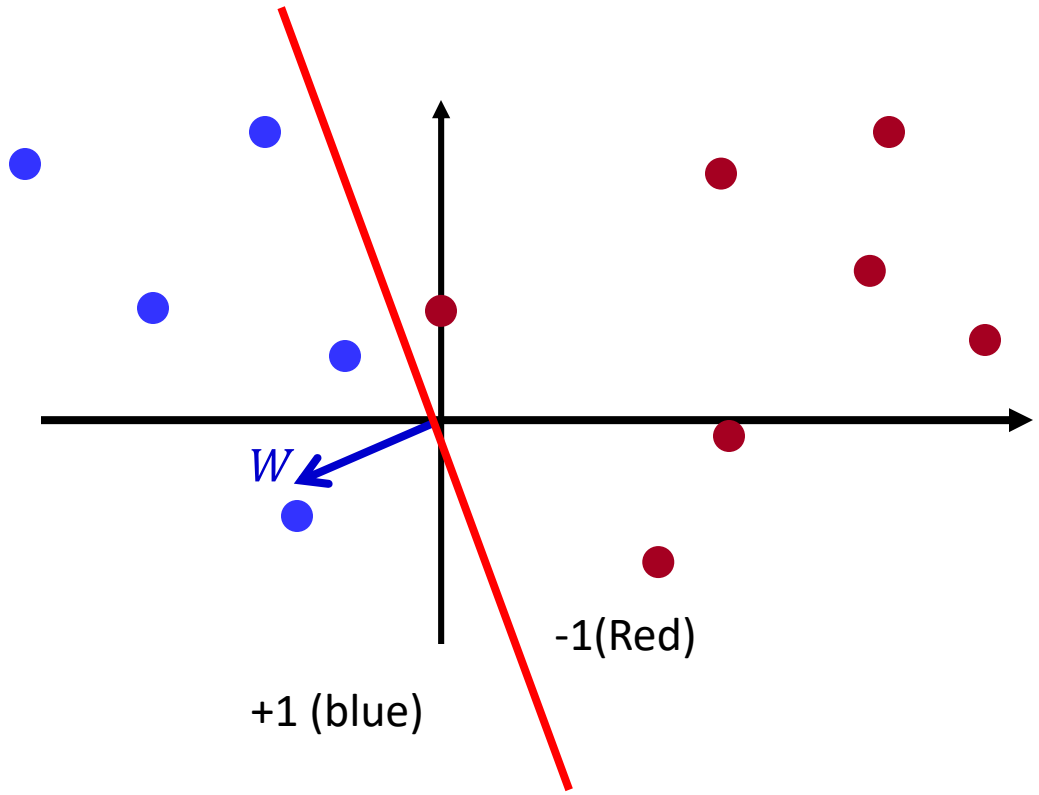



Misclassified *negative* instance, *subtract* it from W

# Perceptron Algorithm



# Perceptron Algorithm

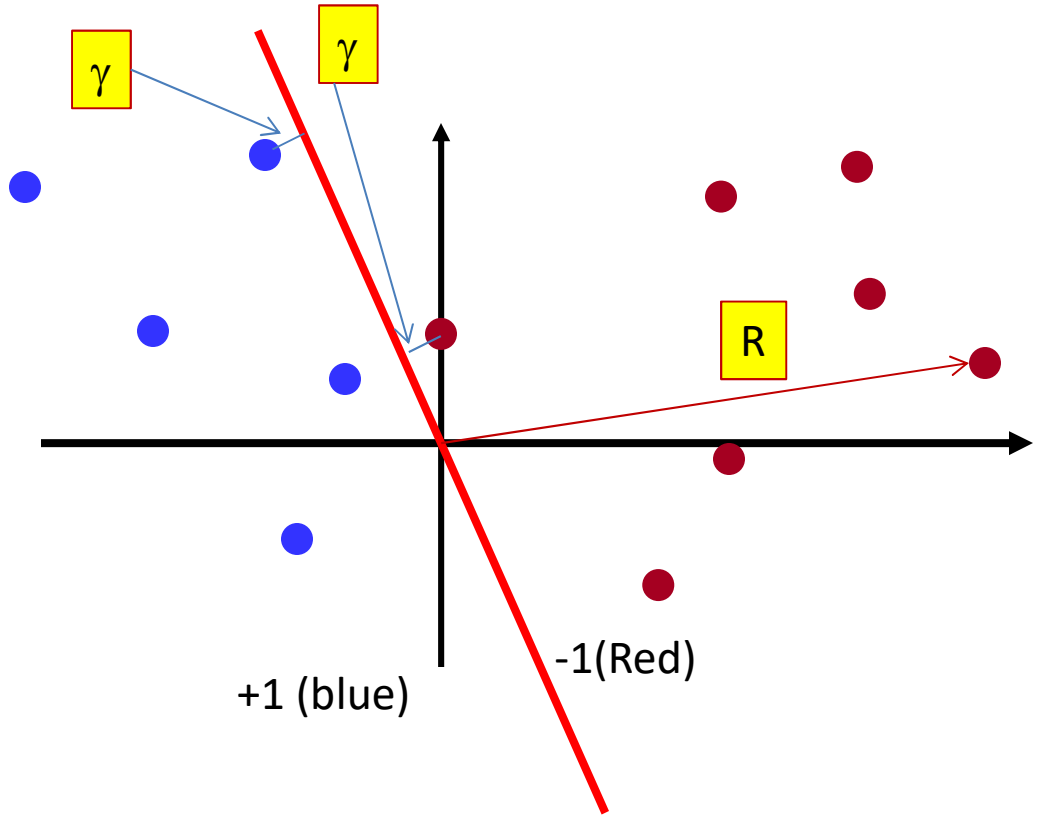



Perfect classification, no more updates

# Convergence of Perceptron Algorithm

- Guaranteed to converge if classes are linearly separable
  - After no more than $\left(\frac{R}{\gamma}\right)^2$ misclassifications
    - Specifically when W is initialized to 0
  - $R$ is length of longest training point
  - $\gamma$is the *best case* closest distance of a training point from the classifier
    - Same as the margin in an SVM
  - Intuitively – takes many increments of size $\gamma$ to undo an error resulting from a step of size $R$

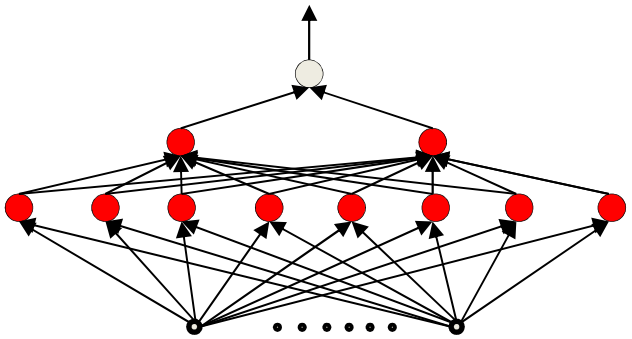
# Perceptron Algorithm

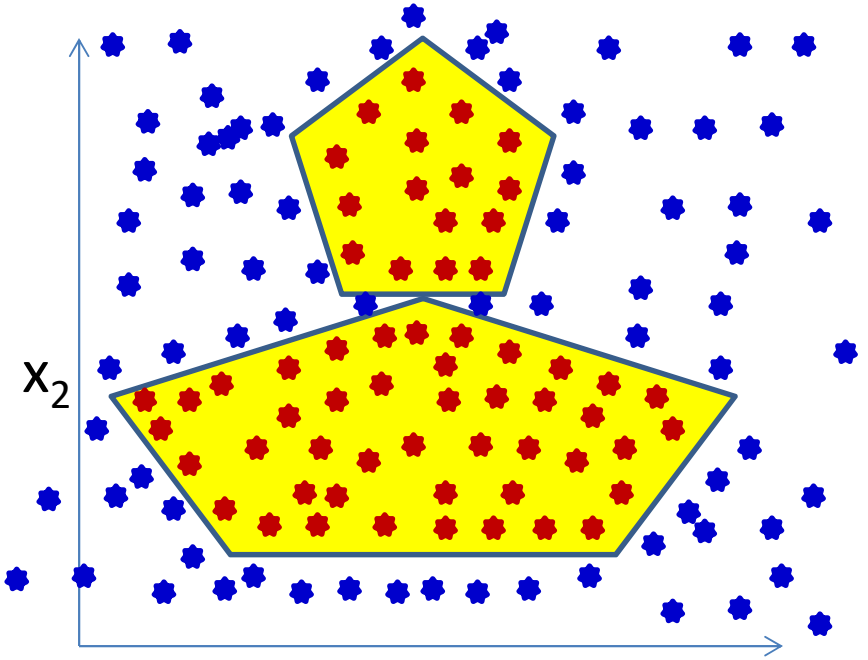



$\gamma$ is the best-case margin

R is the length of the longest vector

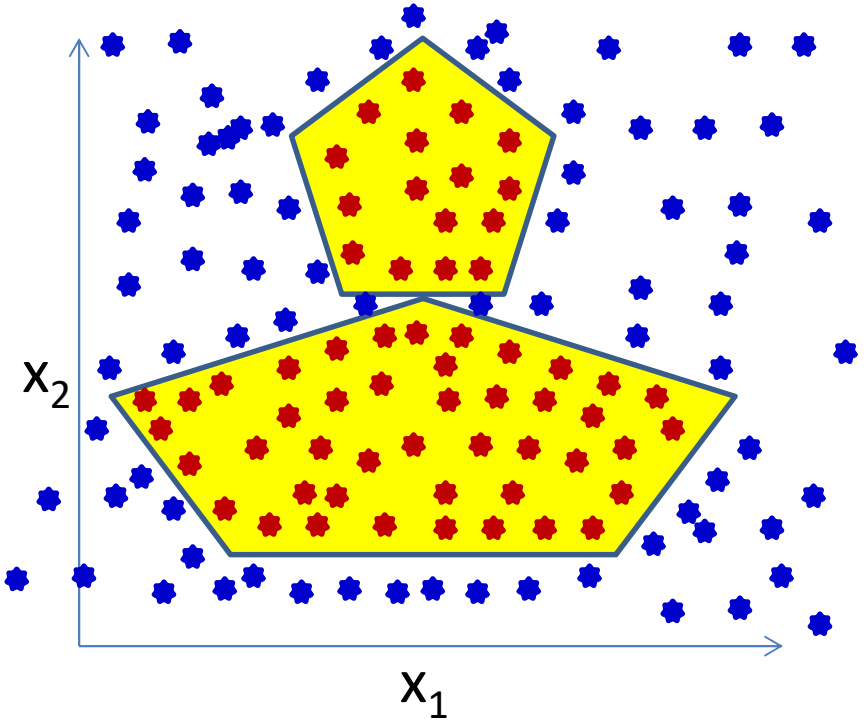
# History: A more complex problem

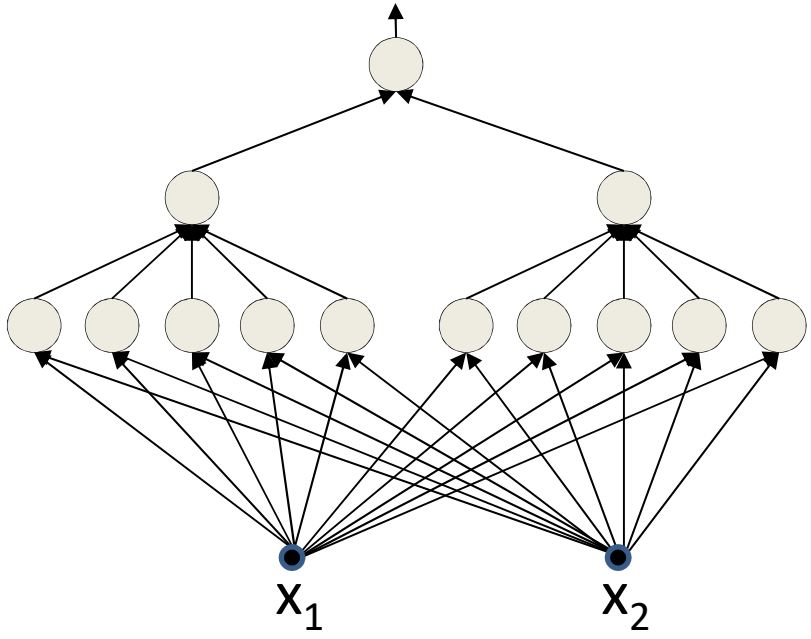





- Learn an *MLP* for this function
  - 1 in the yellow regions, 0 outside
- Using just the samples
- We know this can be perfectly represented using an MLP

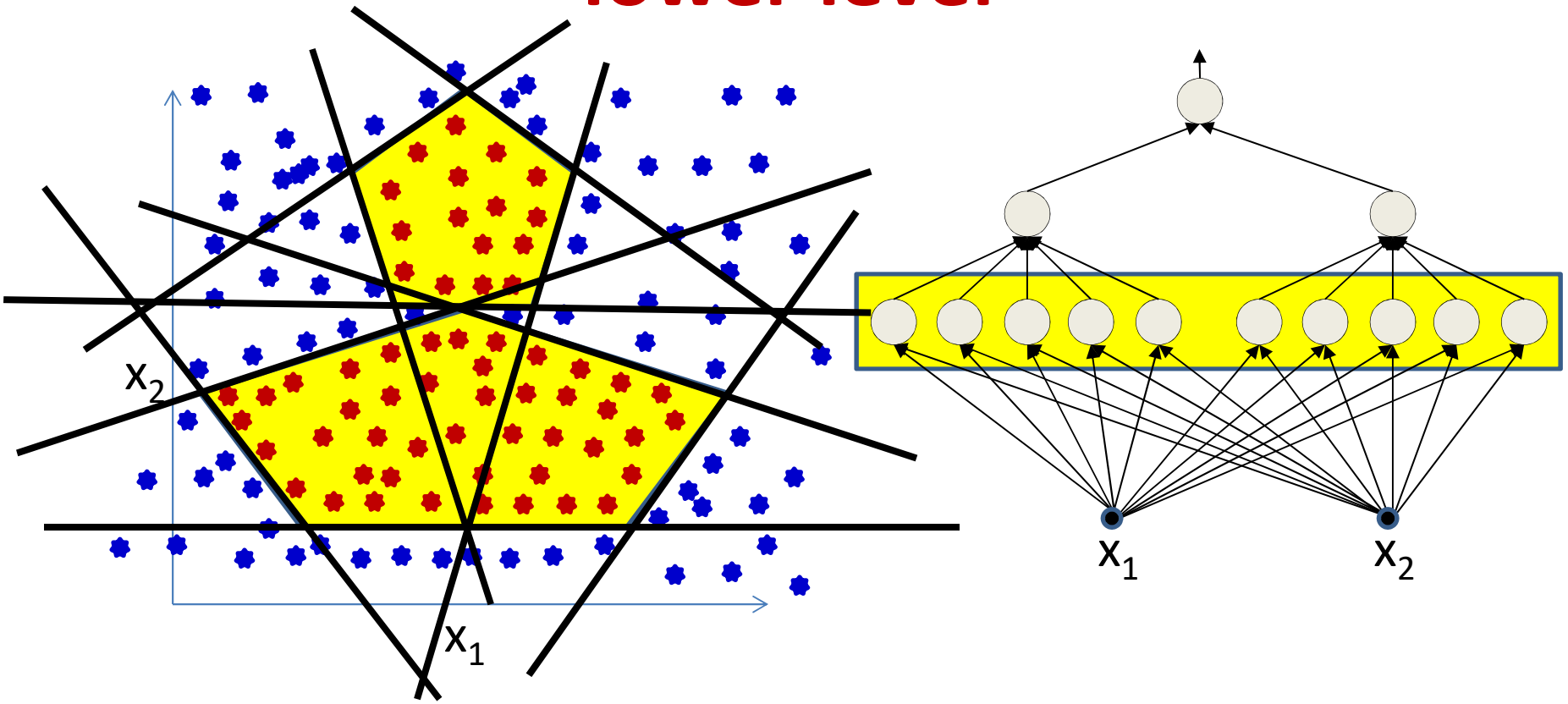
# More complex decision boundaries



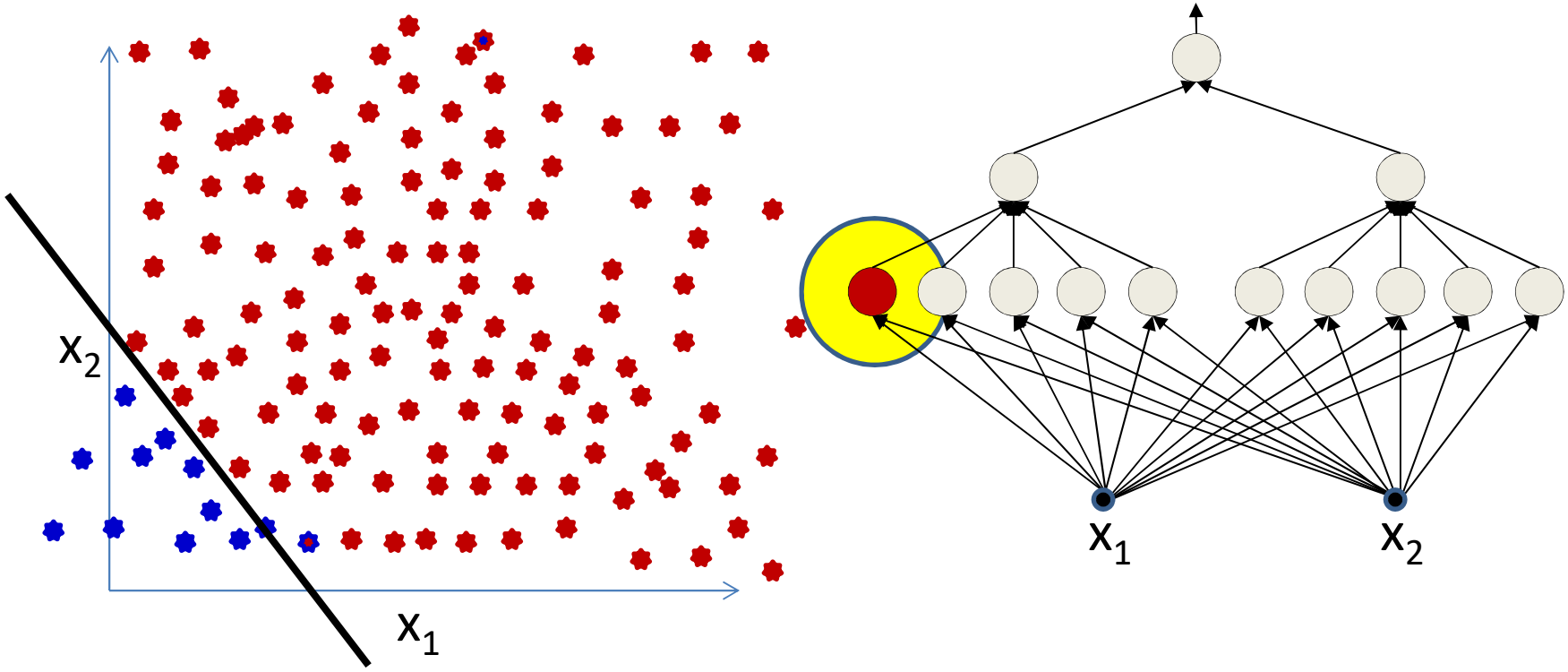

- Even using the perfect architecture
- Can we use the perceptron algorithm?

# The pattern to be learned at the lower level



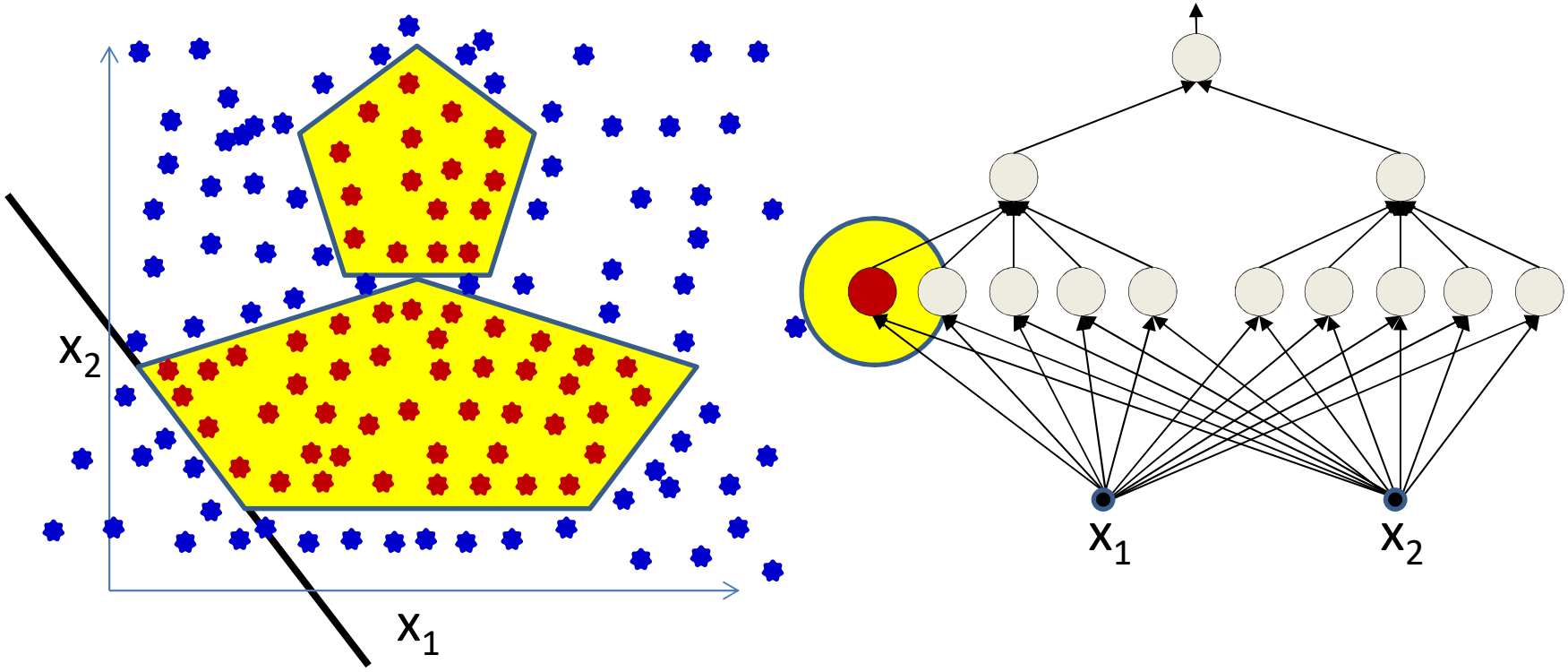

- The lower-level neurons are linear classifiers

# The pattern to be learned at the lower level



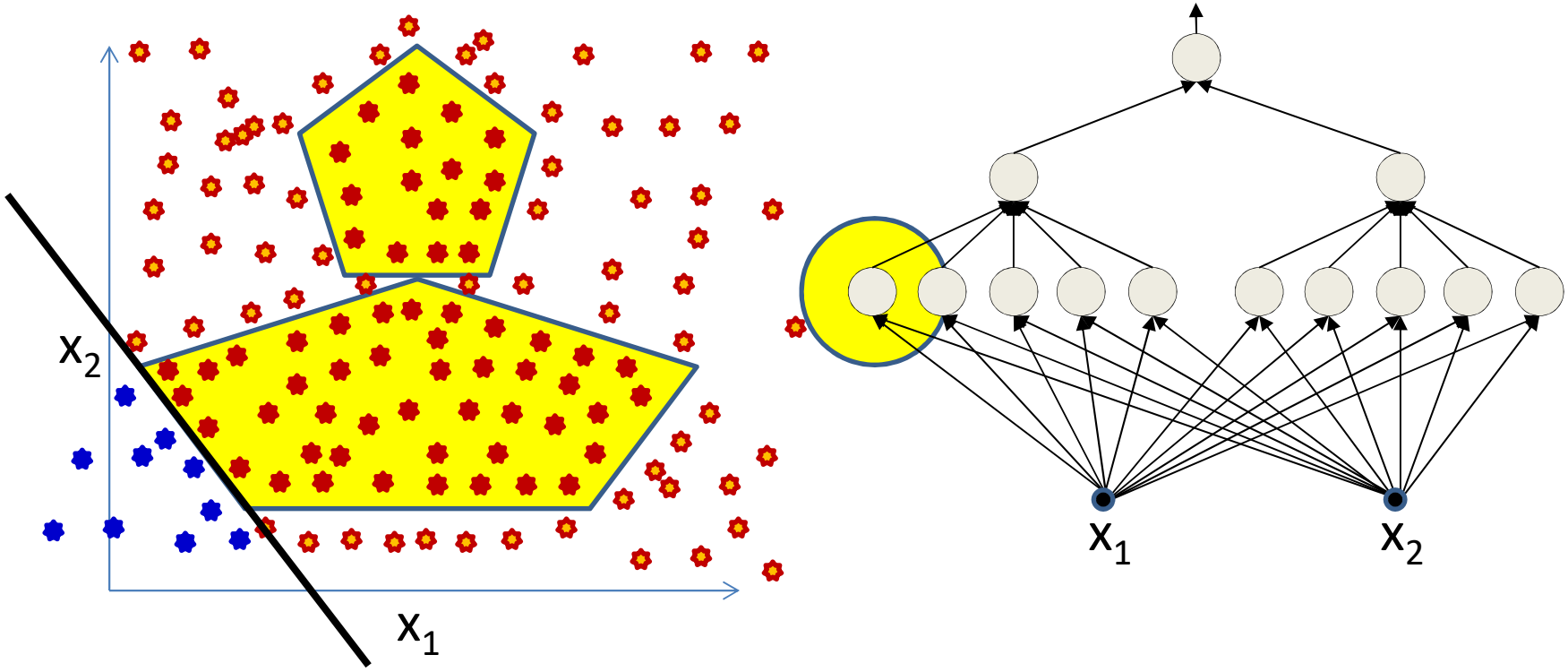

- The lower-level neurons are linear classifiers
  - They require linearly separated labels to be learned

# The pattern to be learned at the lower level



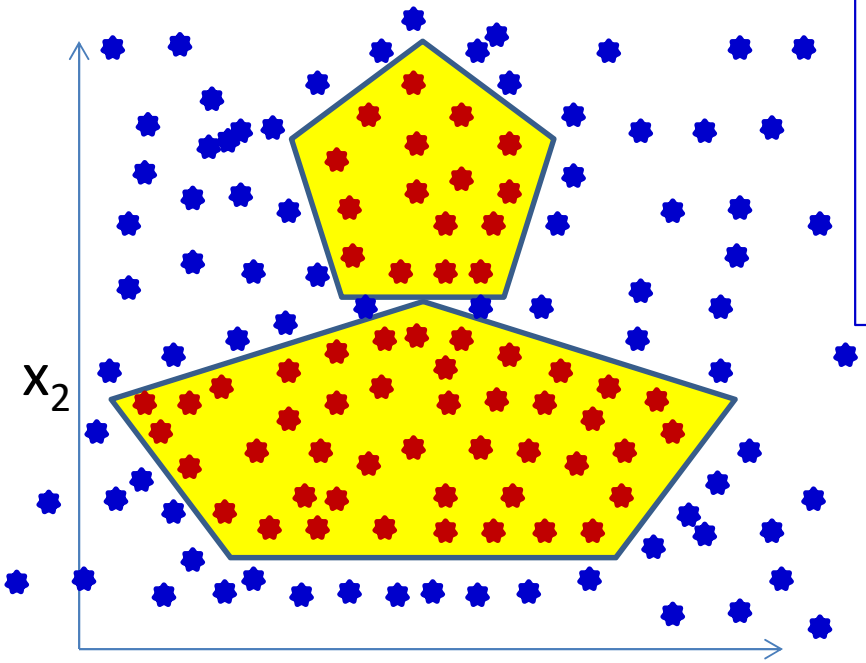

- The lower-level neurons are linear classifiers
  - They require linearly separated labels to be learned
  - The actually provided labels are not linearly separated

# The pattern to be learned at the lower level




- The lower-level neurons are linear classifiers
  - They require linearly separated labels to be learned
  - The actually provided labels are not linearly separated
  - Challenge: *Must also learn the labels for the lowest units!*

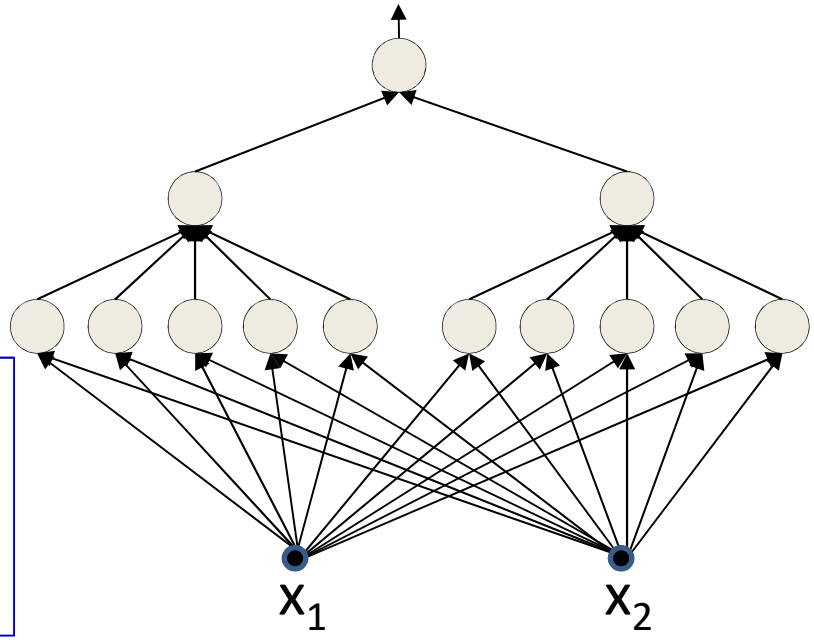
Individual neurons represent one of the lines that compose the figure (linear classifiers)




Must know the output of every neuron for *every* training instance, in order to learn this neuron

The outputs should be such that the neuron individually has a linearly separable task

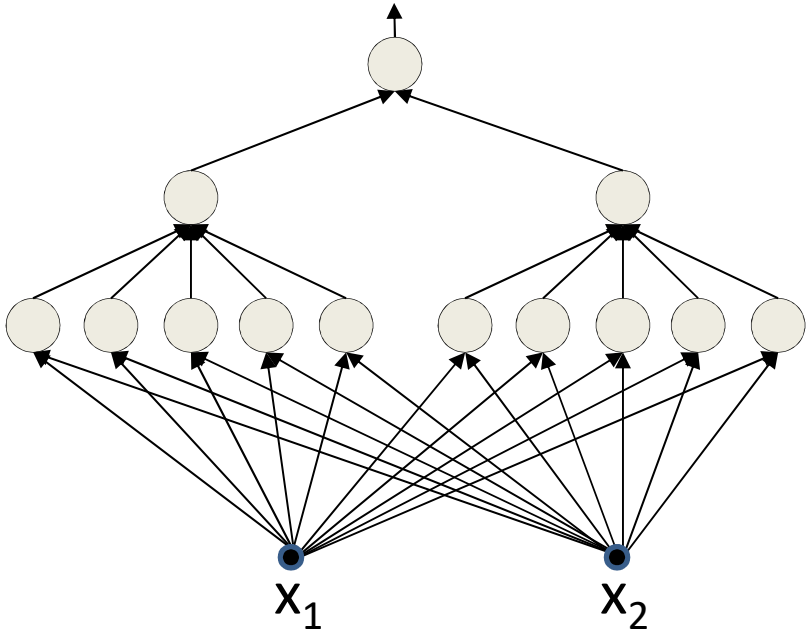
The linear separators must combine to form the desired boundary




This must be done for *every* neuron

Getting any of them wrong will result in incorrect output!

# Learning a *multilayer* perceptron




Training data only specifies input and output of network

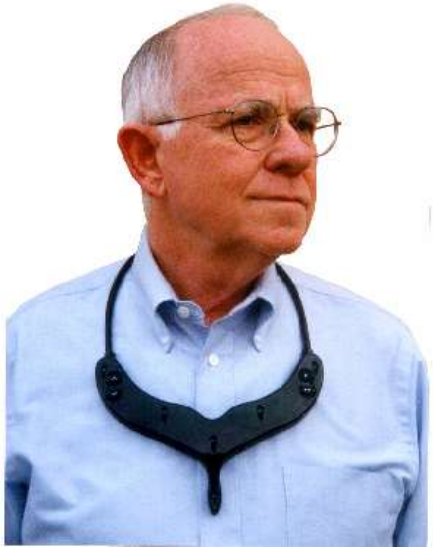
Intermediate outputs (outputs of individual neurons) are not specified

- Training this network using the perceptron rule is a combinatorial optimization problems
- We don't know the outputs of the individual intermediate neurons in the network for any training input
- **Must also determine the correct output for *each* neuron for *every* training instance**
- **NP! Exponential complexity**

# Greedy algorithms: Adaline and Madaline

- The perceptron learning algorithm cannot directly be used to learn an MLP
  - Exponential complexity of assigning intermediate labels
    - Even worse when classes are not actually separable
- Can we use a *greedy* algorithm instead?
  - Adaline / Madaline
  - On slides, will skip in class (check the quiz)

# A little bit of History: Widrow



Bernie Widrow

- Scientist, Professor, Entrepreneur
- Inventor of most useful things in signal processing and machine learning!

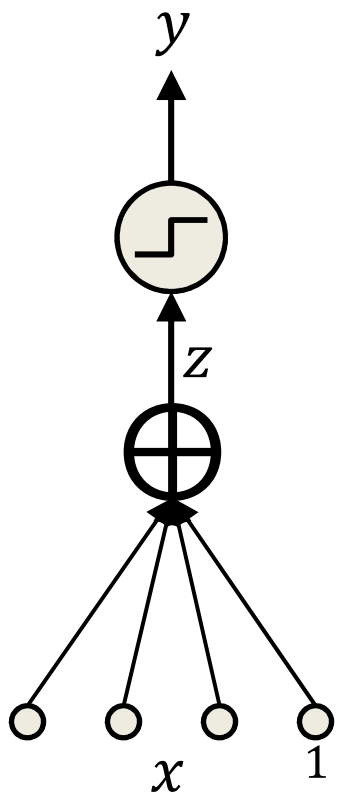
- First known attempt at an analytical solution to training the perceptron and the MLP
- Now famous as the LMS algorithm
  - Used everywhere
  - Also known as the “delta rule”

# History: ADALINE

$$z = \sum_t w_i x_i$$

Using 1-extended vector notation to account for bias

$$y = \begin{cases} 0, & z < 0 \\ 1, & z \geq 0 \end{cases}$$



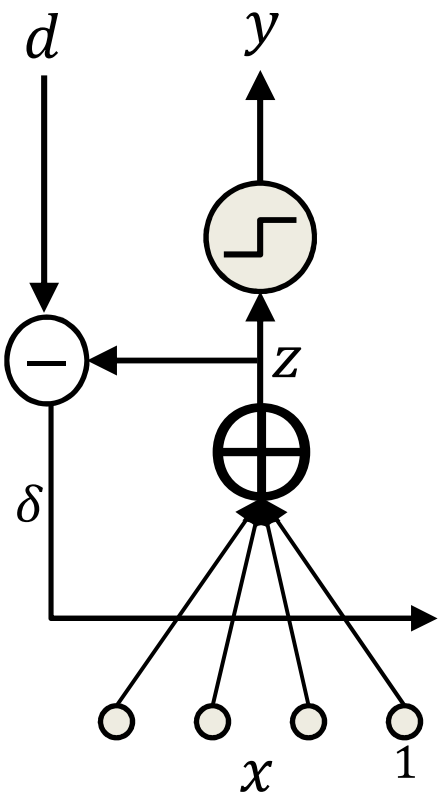

- Adaptive *linear* element (Hopf and Widrow, 1960)
- Actually just a regular perceptron
  - Weighted sum on inputs and bias passed through a thresholding function
- ADALINE differs in the *learning rule*

# History: Learning in ADALINE

$$z = \sum_t w_i x_i$$

$$out = \begin{cases} 0, & z < 0 \\ 1, & z \geq 0 \end{cases}$$

- During learning, minimize the squared error assuming $z$ to be real output
- The desired output is still binary!




$$Err(x) = \frac{1}{2}(d - z)^2$$

Error for a single input

$$\frac{dErr(x)}{dw_i} = -(d - z)x_i$$

# History: Learning in ADALINE

$$z = \sum_t w_i x_i$$

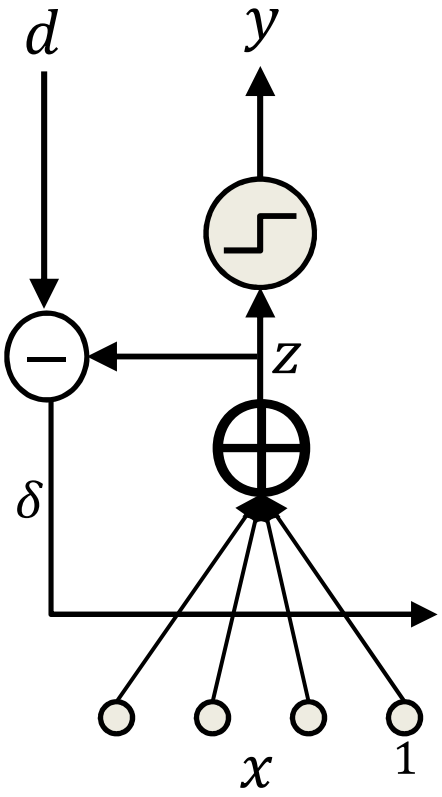
$$Err(x) = \frac{1}{2}(d - z)^2$$

Error for a single input

$$\frac{dErr(x)}{dw_i} = -(d - z)x_i$$

- If we just have a single training input, the gradient descent update rule is

$$w_i = w_i + \eta(d - z)x_i$$



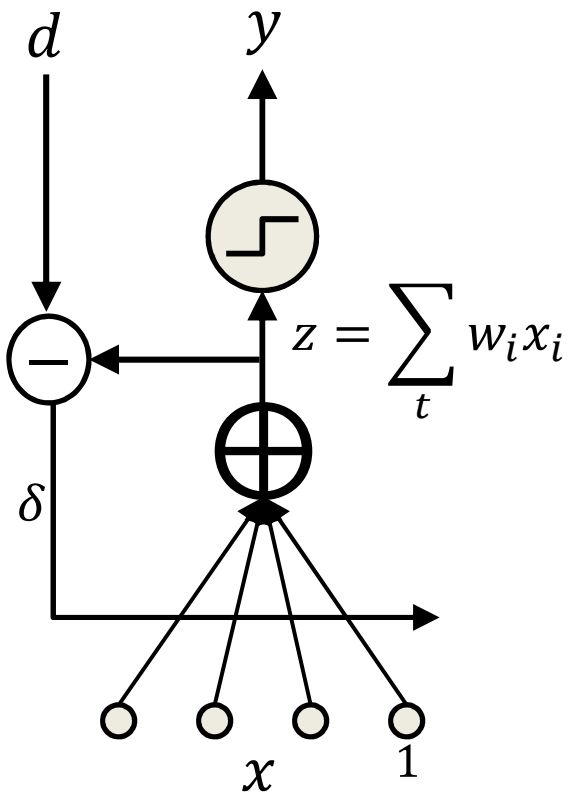
# The ADALINE learning rule

- Online learning rule
- **After each input x**, that has target (binary) output $d$, compute and update:

$$\delta = d - z$$

$$w_i = w_i + \eta \delta x_i$$

- This is the famous *delta rule*
  - Also called the LMS update rule

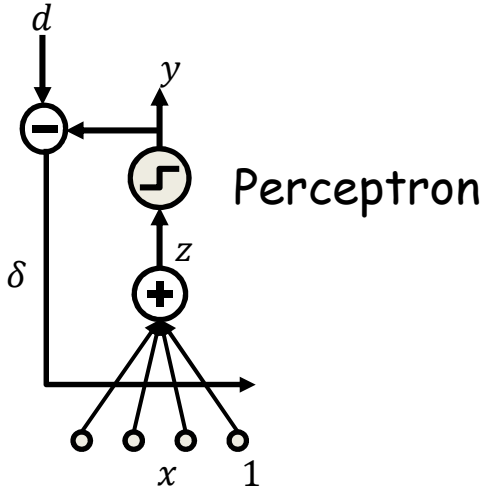


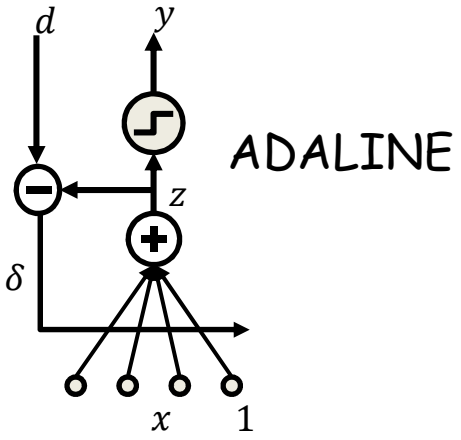
# The Delta Rule

- In fact both the Perceptron and ADALINE use variants of the delta rule!
  - Perceptron: Output used in delta rule is $y$
  - ADALINE: Output used to estimate weights is $z$

$$\delta = d - ??$$

$$w_i = w_i + \eta \delta x_i$$



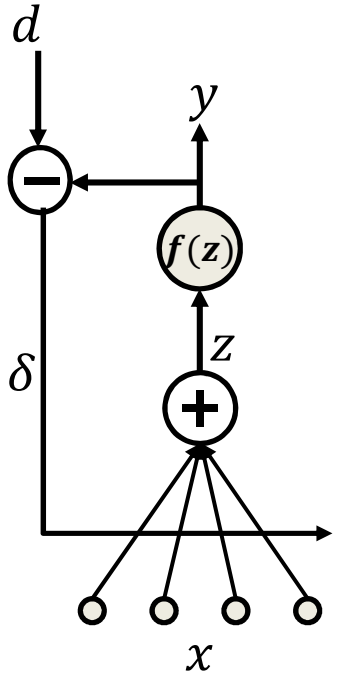



# Aside: Generalized delta rule

- For any differentiable activation function the following update rule is used

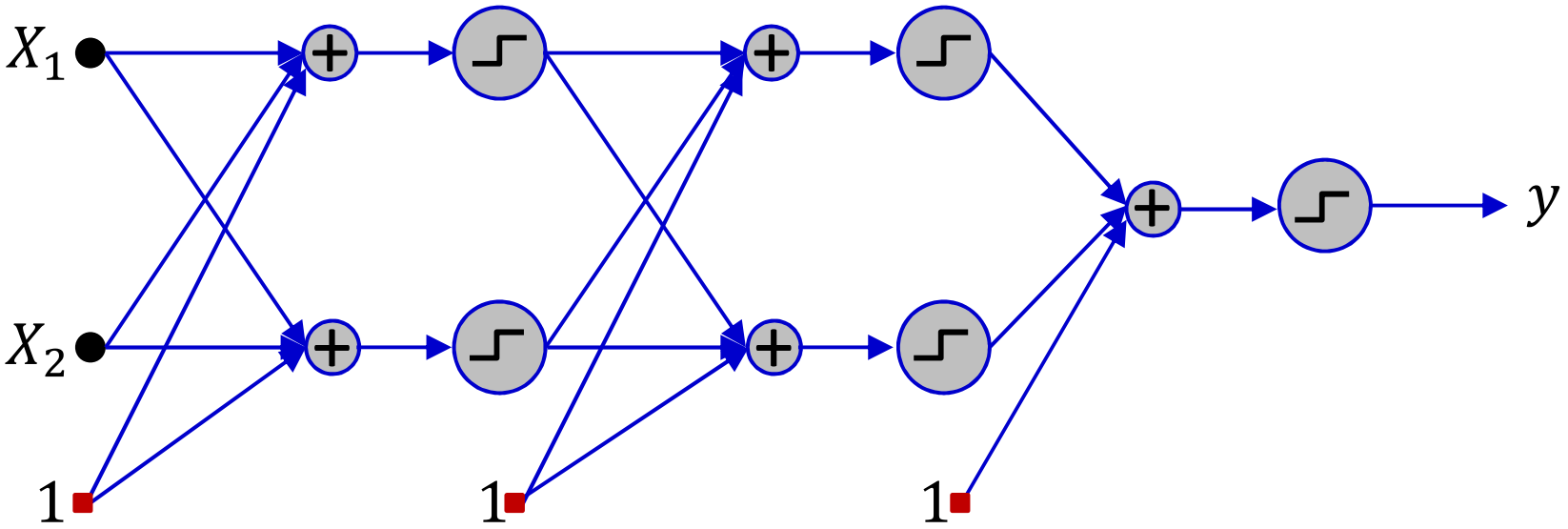
$$\delta = d - y$$

$$w_i = w_i + \eta \delta f'(z) x_i$$



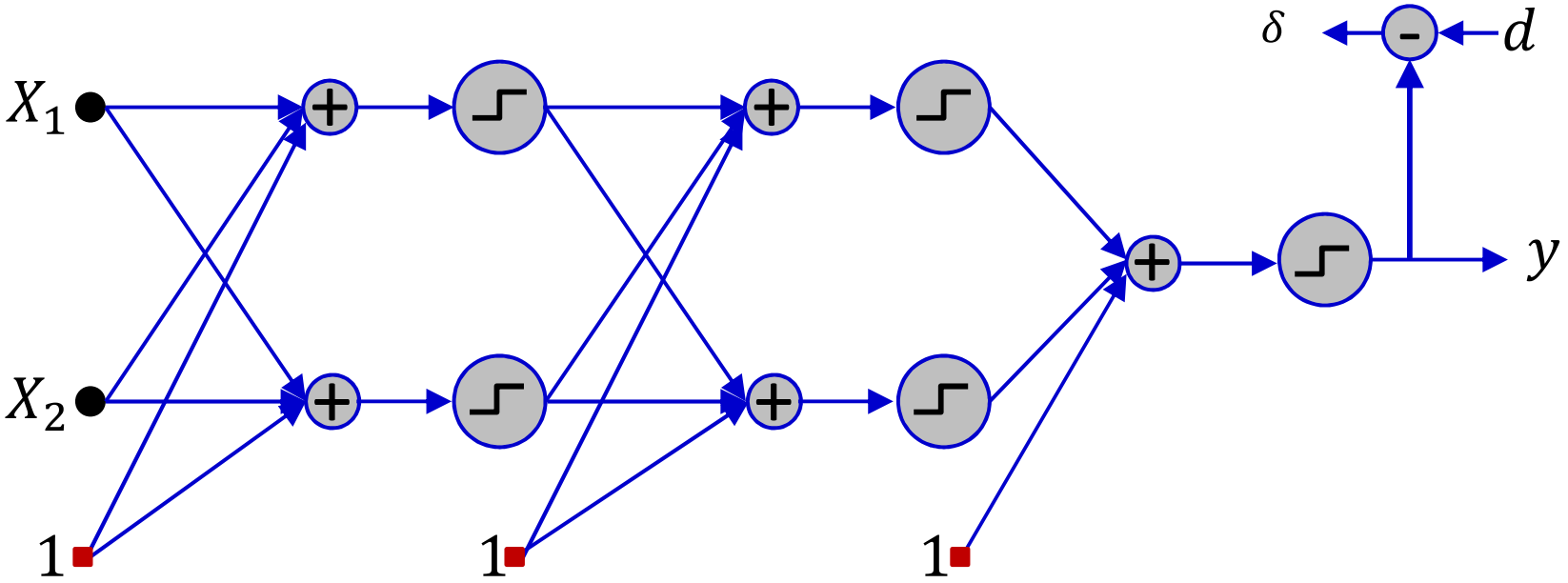

- This is the famous Widrow-Hoff update rule
  - Lookahead: Note that this is *exactly* backpropagation in multilayer nets if we let $f(z)$ represent the entire network between $z$ and $y$
- It is possibly the most-used update rule in machine learning and signal processing
  - Variants of it appear in almost every problem

# *Multilayer perceptron*: MADALINE



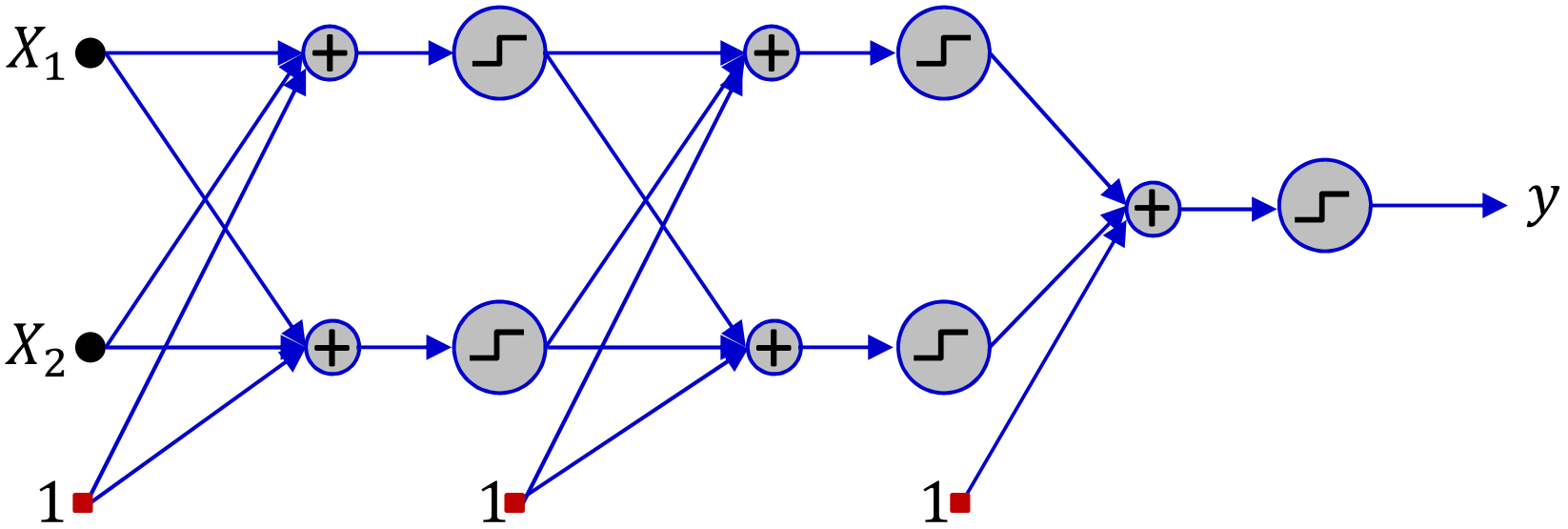

- *Multiple* Adaline
  - A multilayer perceptron with threshold activations
  - The MADALINE

# MADALINE Training



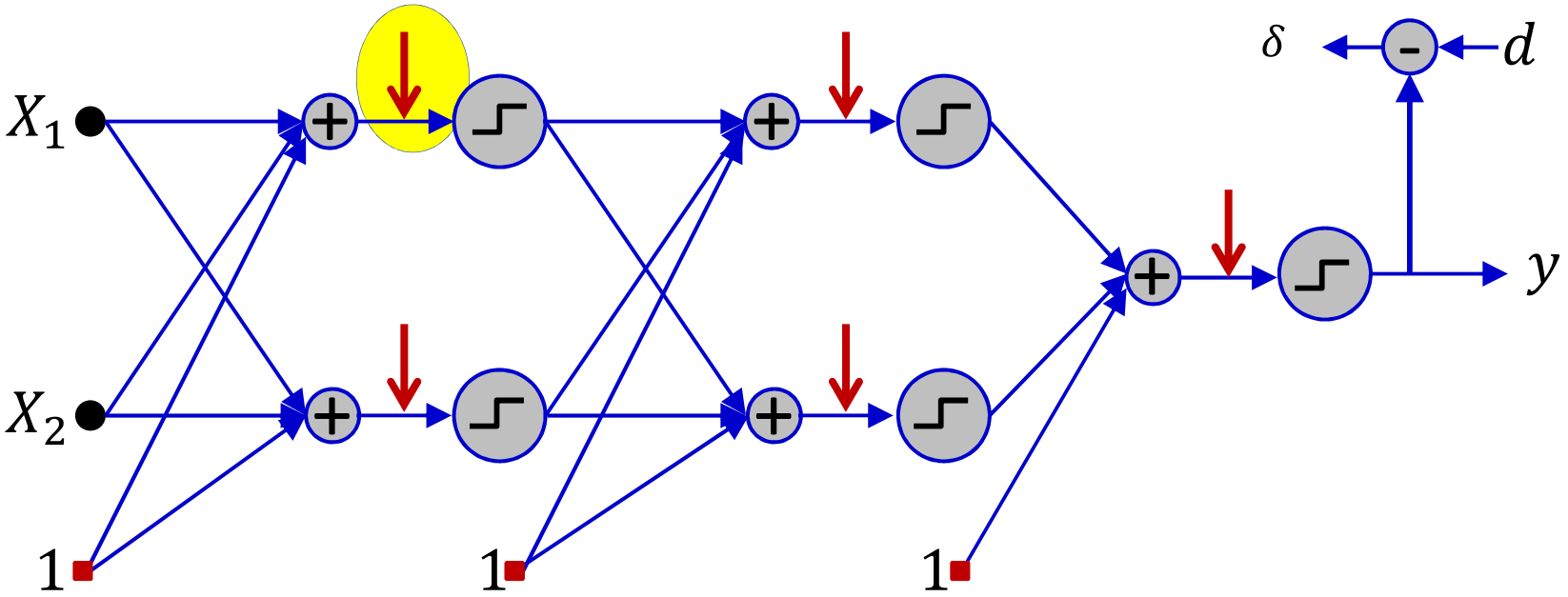

- *Update only on error*
  - $\delta \neq 0$
  - On inputs for which output and target values differ

# MADALINE Training



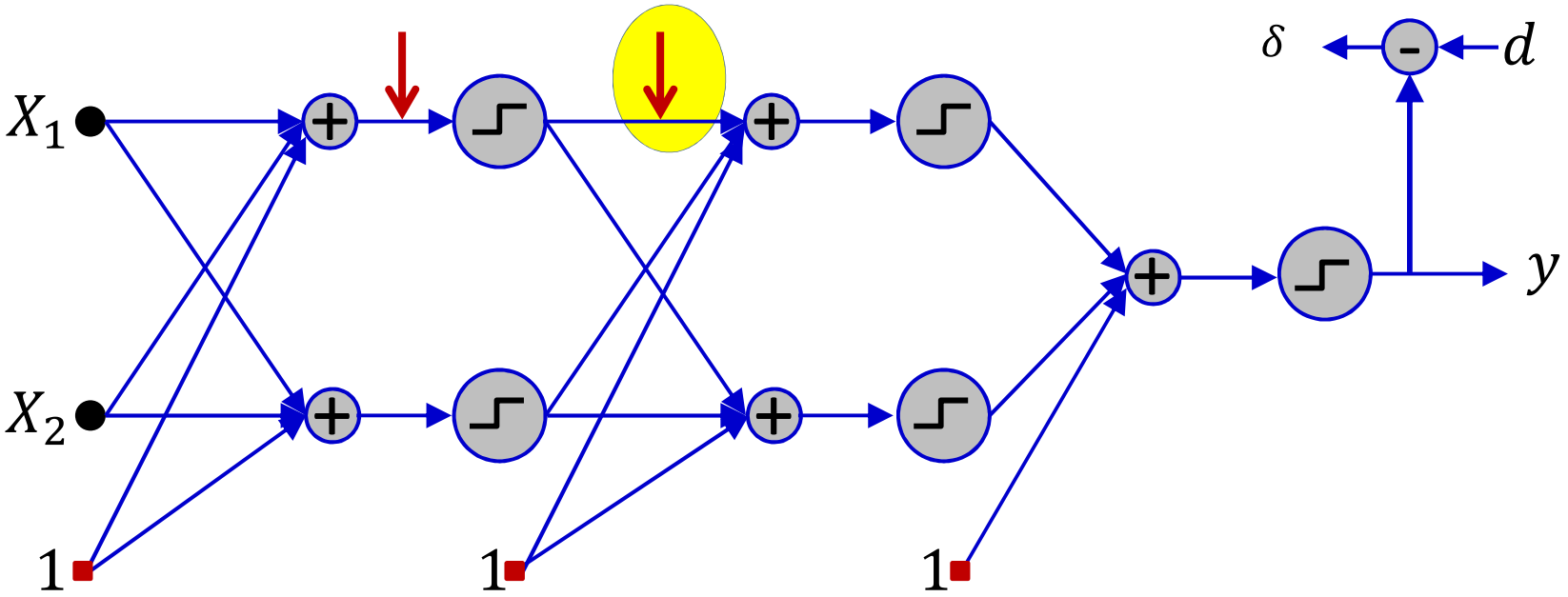

- While stopping criterion not met do:
  - Classify an input

# MADALINE Training



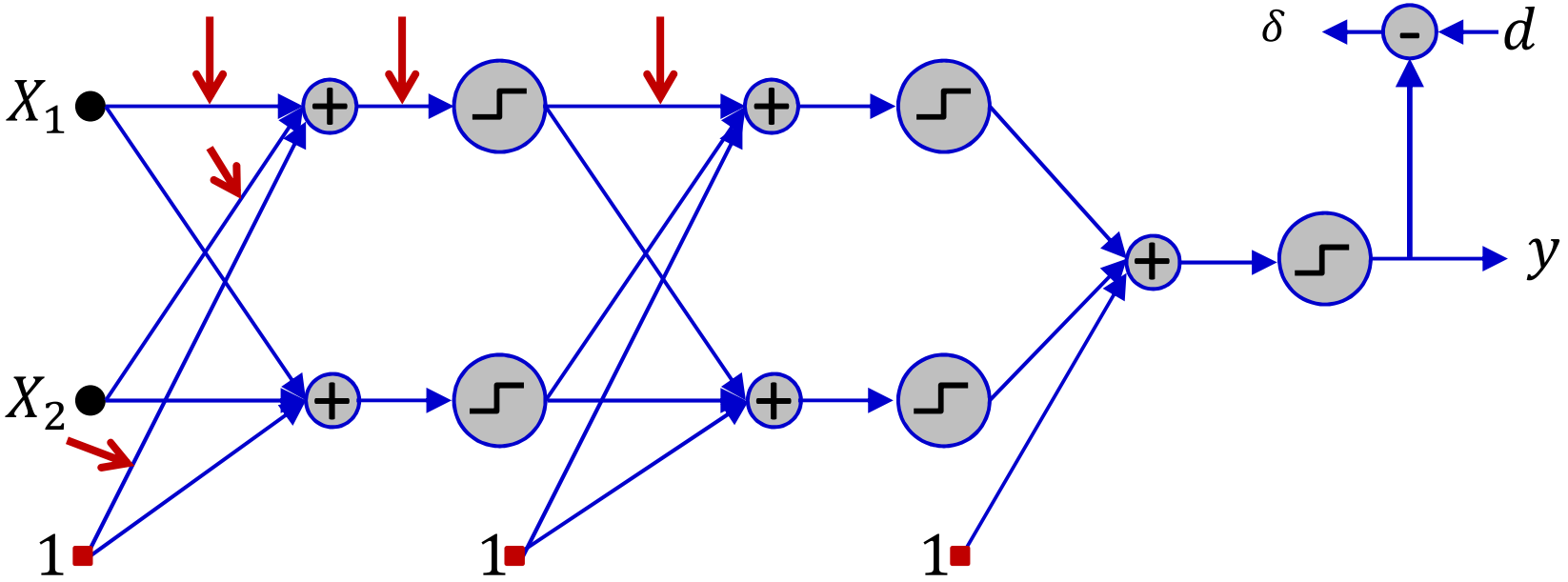

- While stopping criterion not met do:
  - Classify an input
  - If error, find the z that is closest to 0

# MADALINE Training




- While stopping criterion not met do:
  - Classify an input
  - If error, find the z that is closest to 0
  - Flip the output of corresponding unit and compute new output

# MADALINE Training




- While stopping criterion not met do:
  - Classify an input
  - If error, find the z that is closest to 0
  - Flip the output of corresponding unit and compute new output
  - If error reduces:
    - Set the desired output of the unit to the flipped value
    - Apply ADALINE rule to update weights of the unit

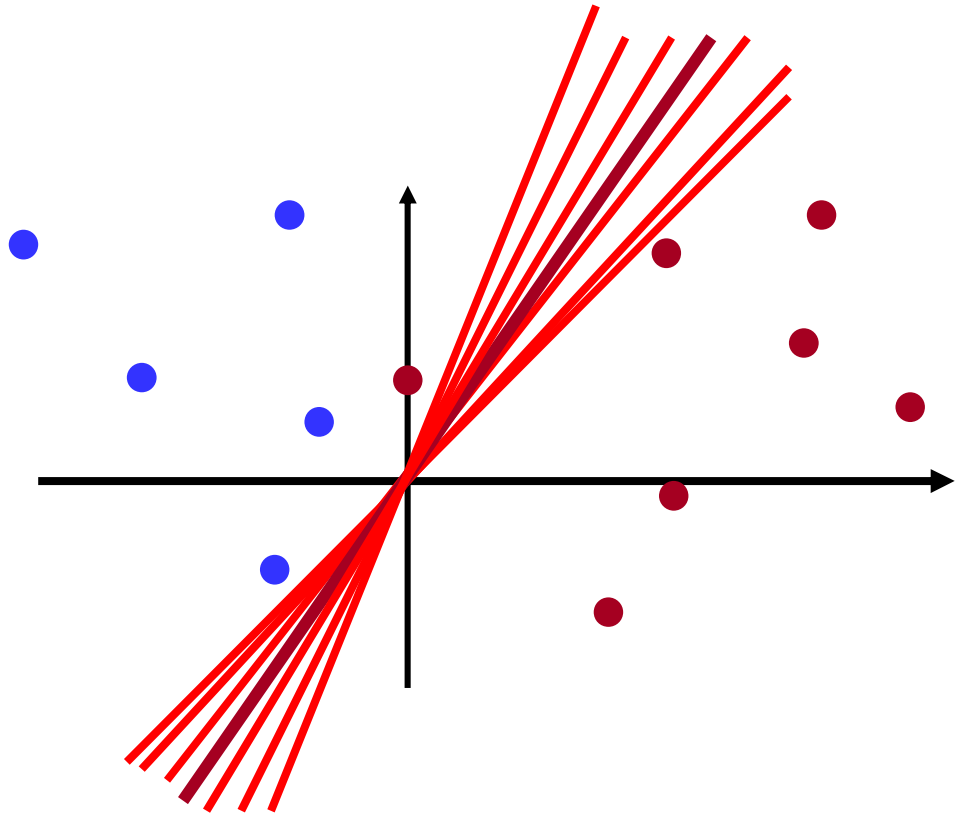
# MADALINE

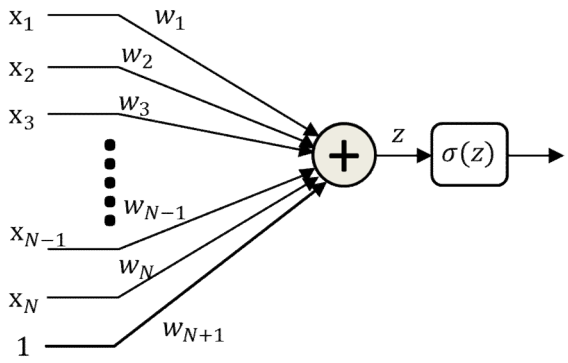
- Greedy algorithm, effective for small networks
- Not very useful for large nets
  - Too expensive
  - Too greedy

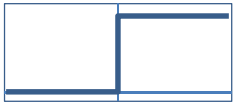
# History..

- The realization that training an entire MLP was a combinatorial optimization problem stalled development of neural networks for well over a decade!

# Why this problem?

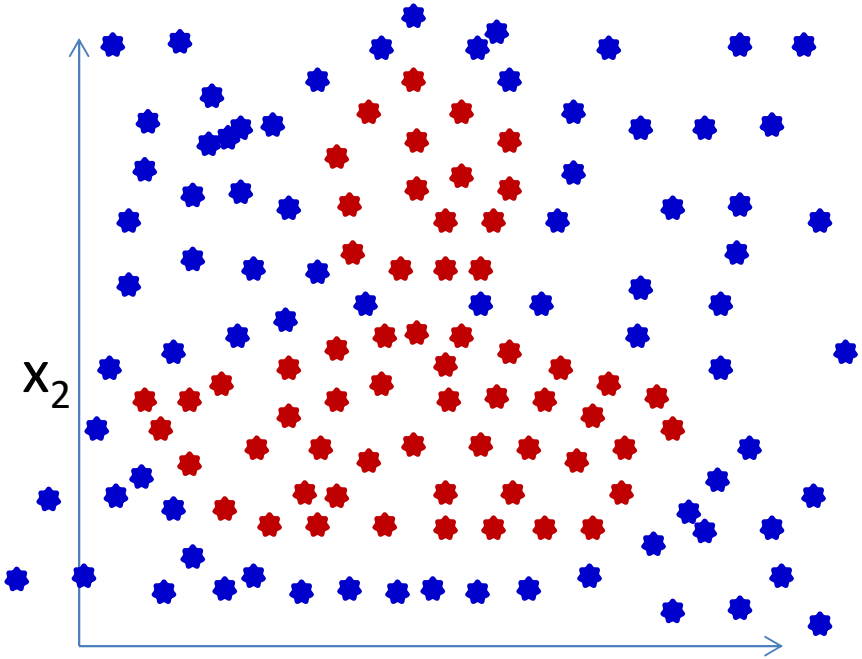


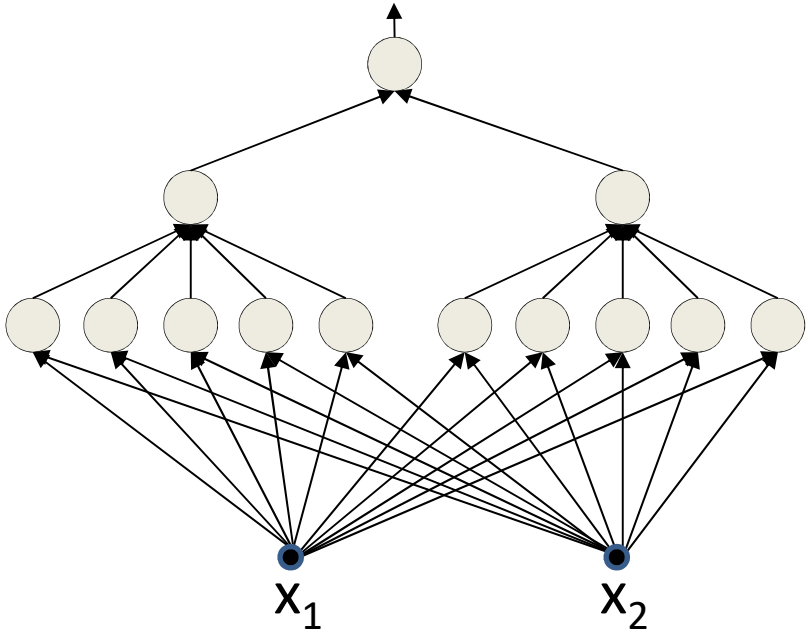



$\sigma(z) =$ 

- The perceptron is a flat function with zero derivative everywhere, except at 0 where it is non-differentiable
  - You can vary the weights a *lot* without changing the error
  - There is no indication of which direction to change the weights to reduce error

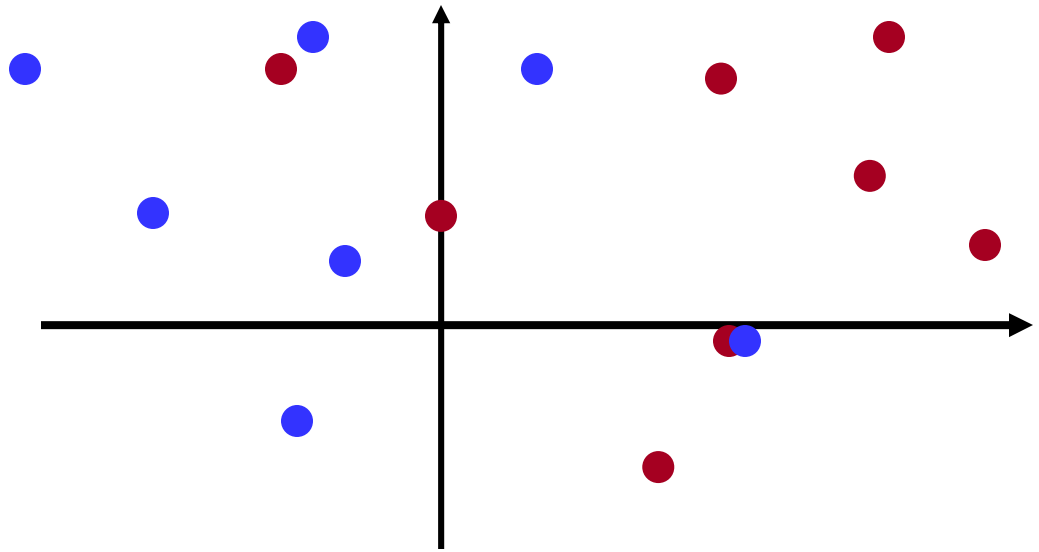
# This only compounds on larger problems



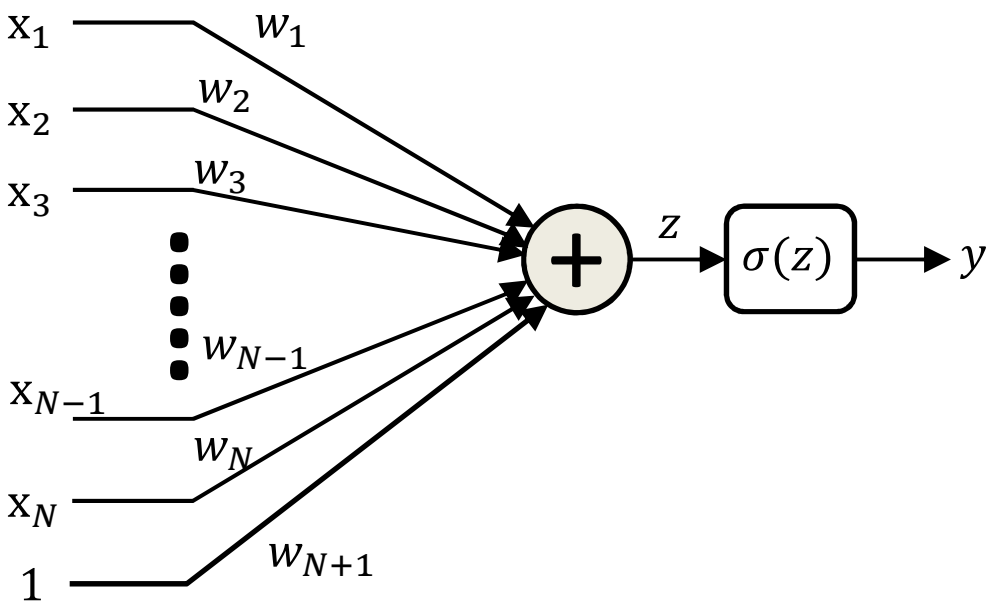

- Individual neurons' weights can change significantly without changing overall error
- The simple MLP is a flat, non-differentiable function

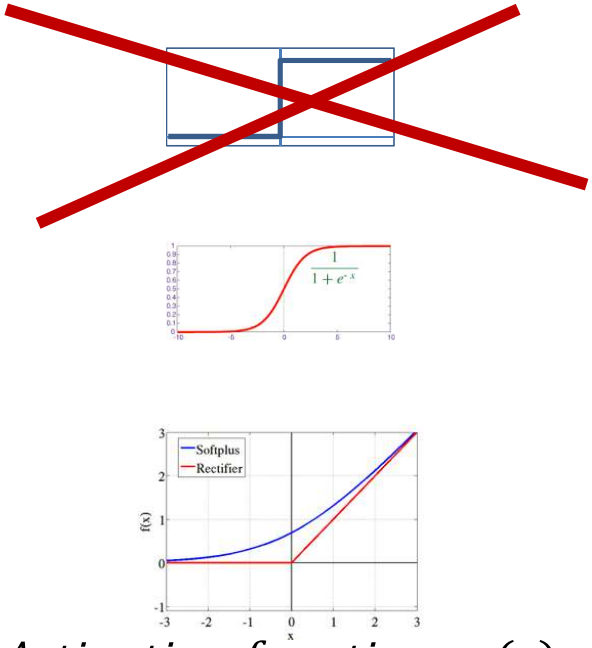
# A second problem: What we *actually* model



- Real-life data are rarely clean
  - Not linearly separable
  - Rosenblatt's perceptron wouldn't work in the first place

# Solution

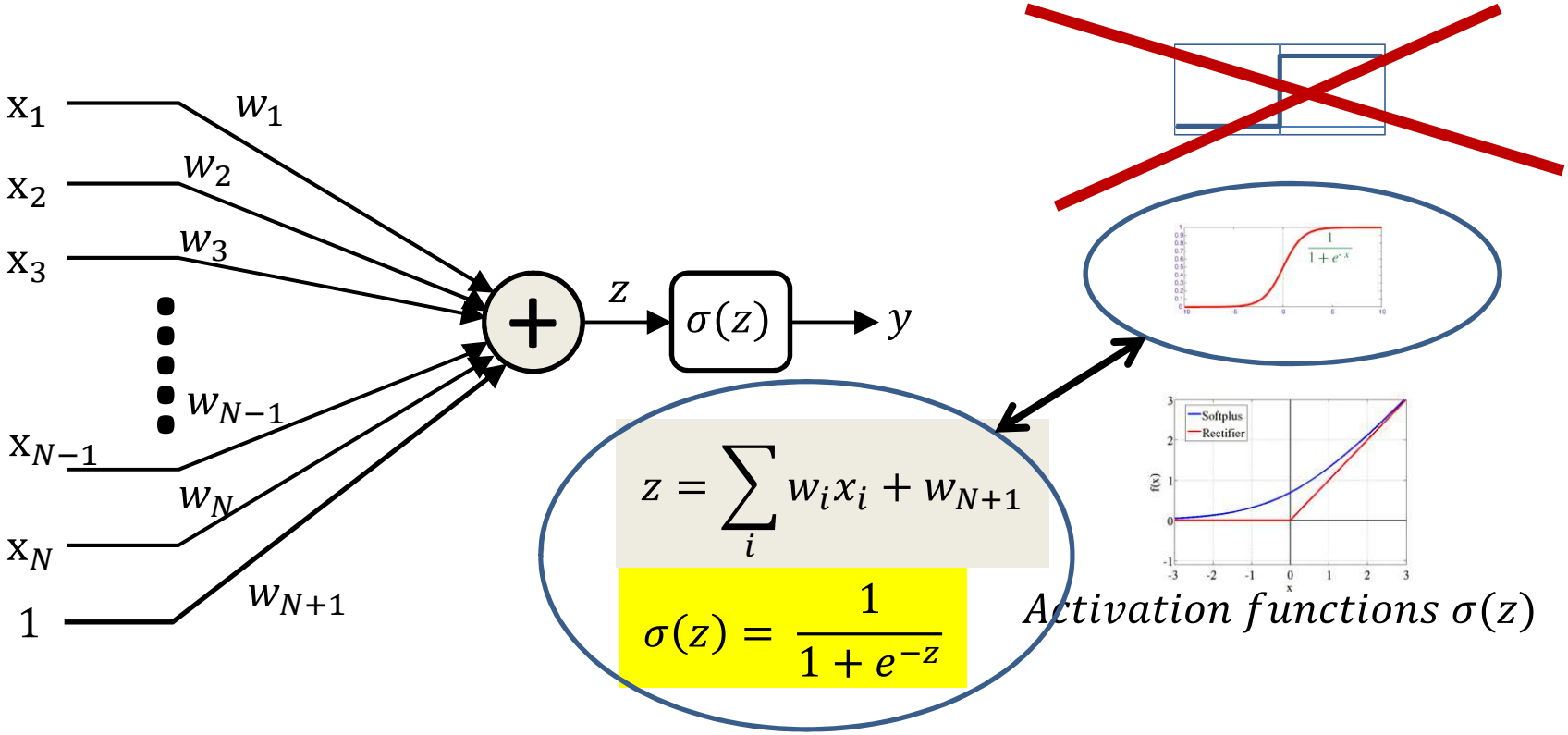



*Activation functions* $\sigma(z)$

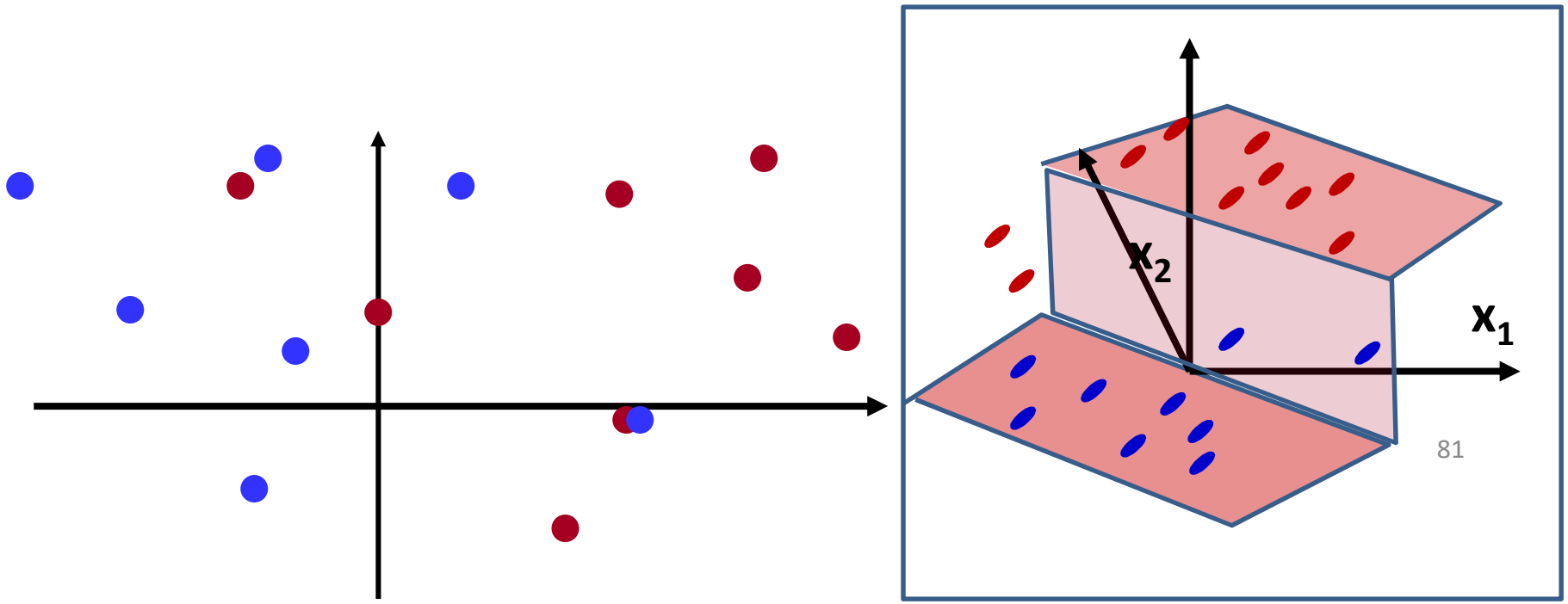
- Lets make the neuron differentiable
  - Small changes in weight can result in non-negligible changes in output
  - This enables us to estimate the parameters using gradient descent techniques..

# Differentiable Activations: An aside



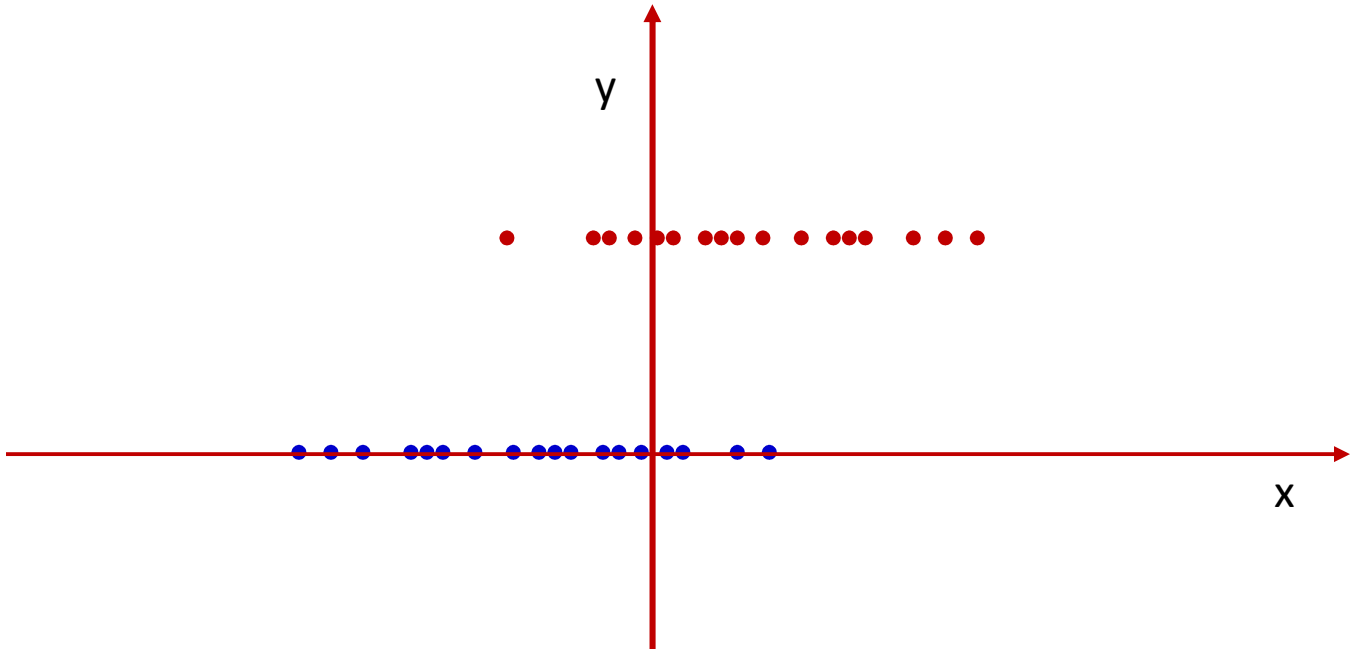

- This particular one has a nice interpretation

# Non-linearly separable data



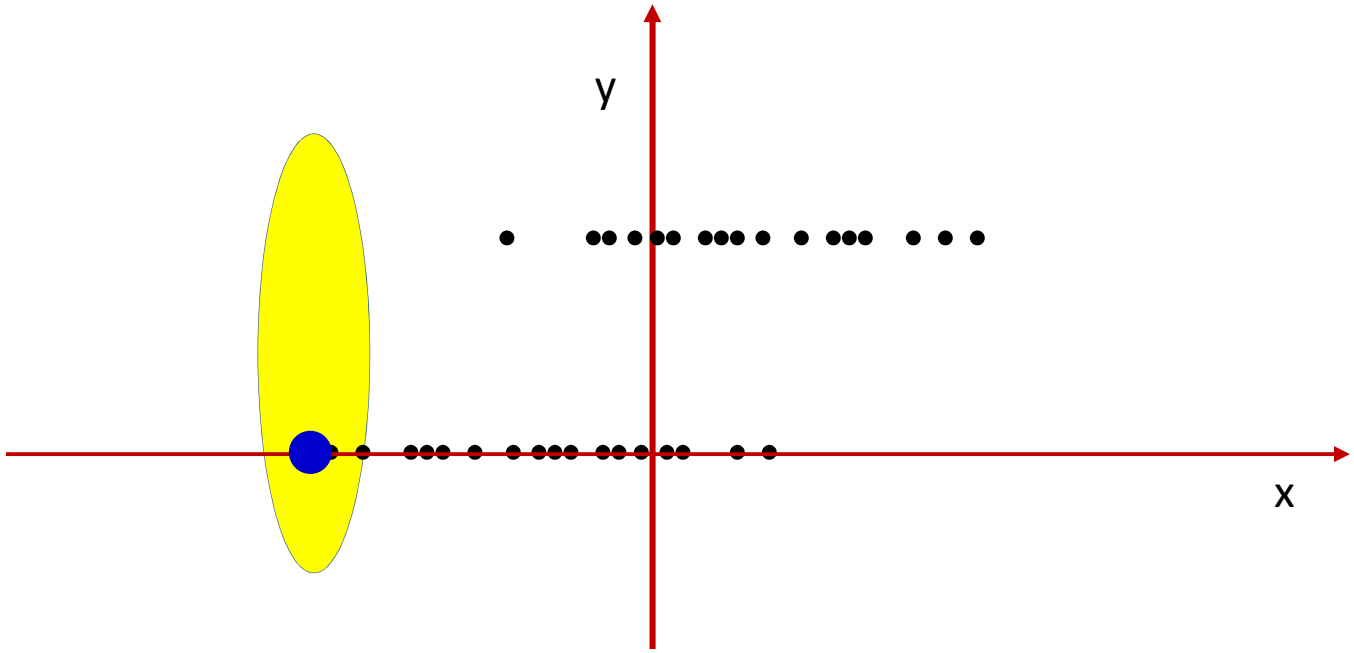

- Two-dimensional example
  - Blue dots (on the floor) on the “red” side
  - Red dots (suspended at Y=1) on the “blue” side
  - No line will cleanly separate the two colors

# Non-linearly separable data: 1-D example



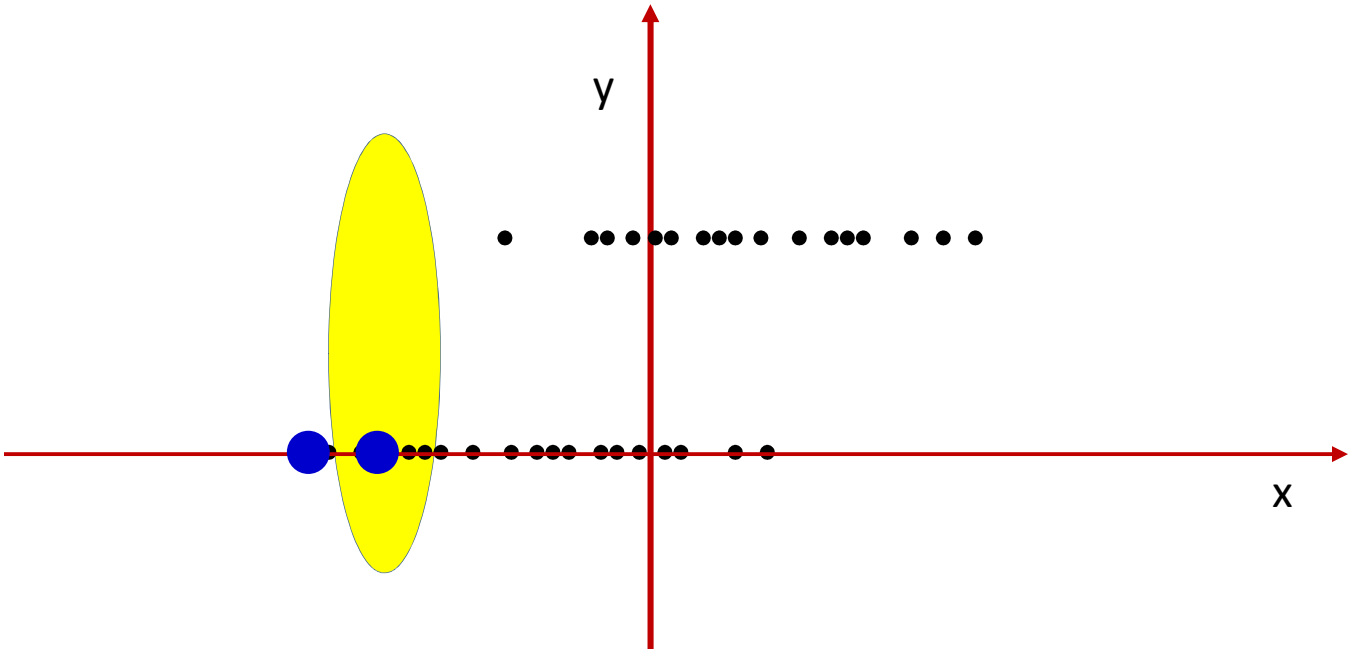

- One-dimensional example for visualization
  - All (red) dots at Y=1 represent instances of class Y=1
  - All (blue) dots at Y=0 are from class Y=0
  - The data are not linearly separable
    - In this 1-D example, a linear separator is a threshold
    - No threshold will cleanly separate red and blue dots

# The *probability* of y=1




- Consider this differently: at each point look at a small window around that point
- Plot the average value within the window
  - This is an approximation of the *probability* of Y=1 at that point

# The *probability* of y=1

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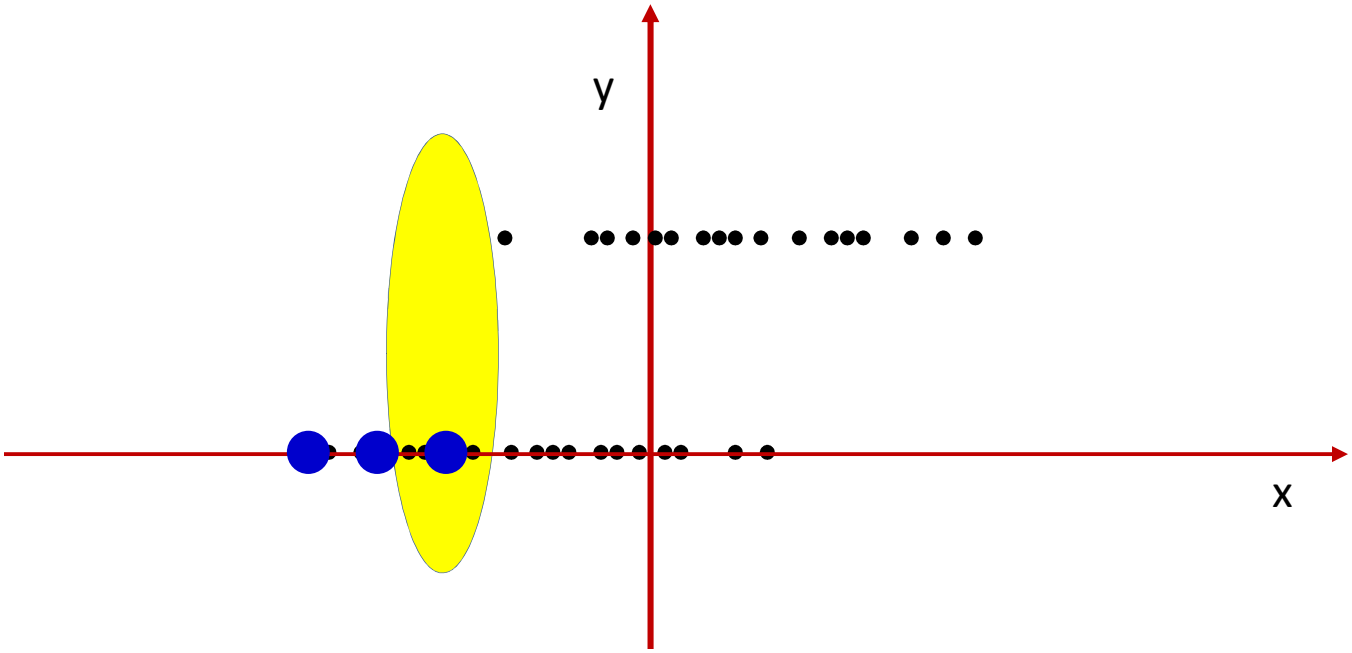


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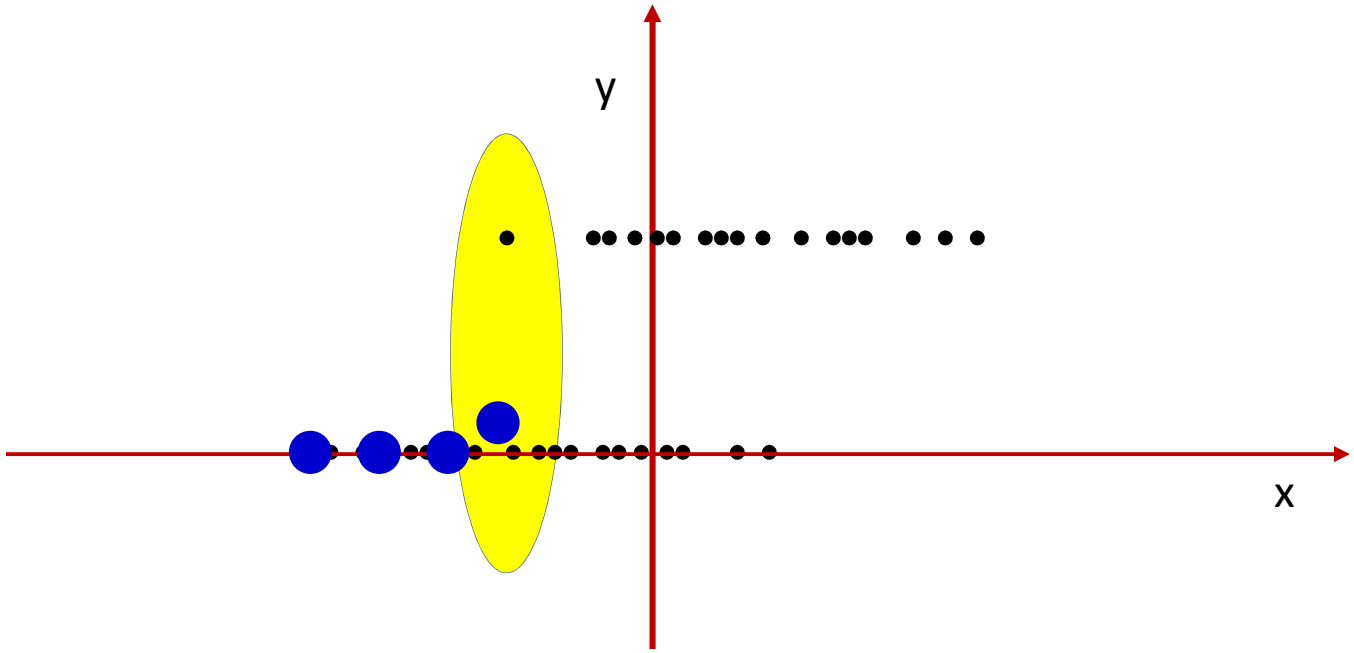


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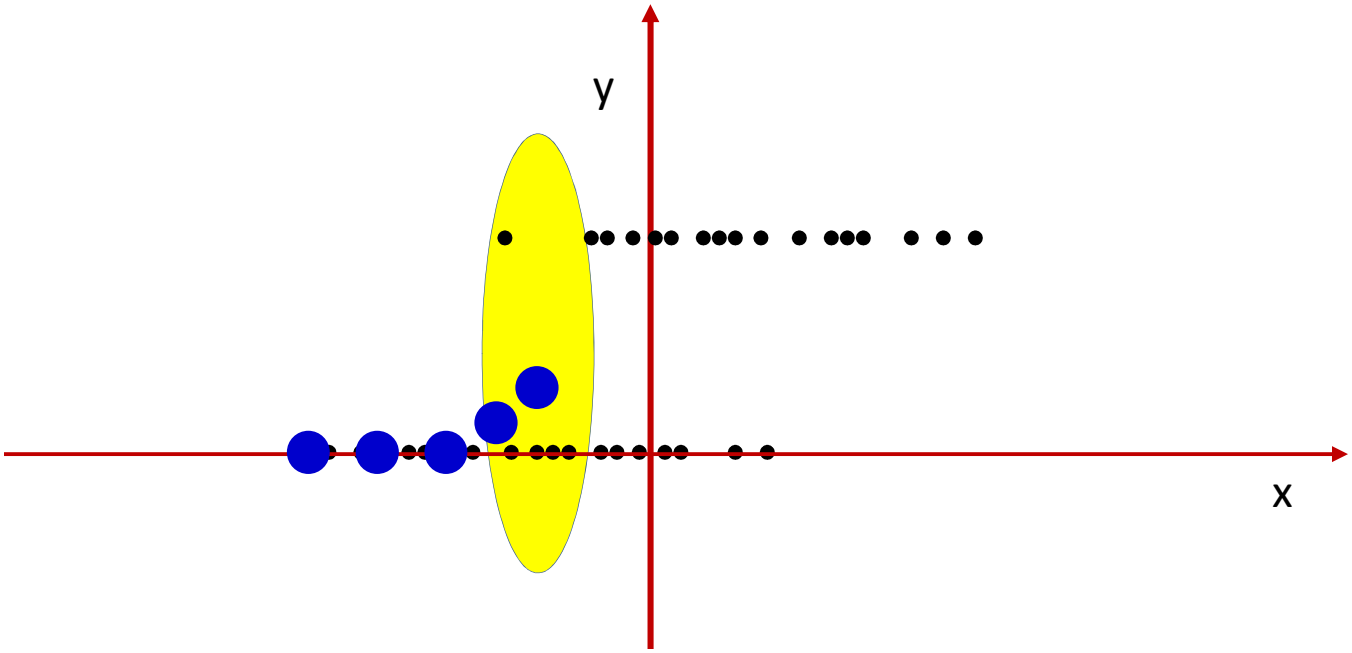


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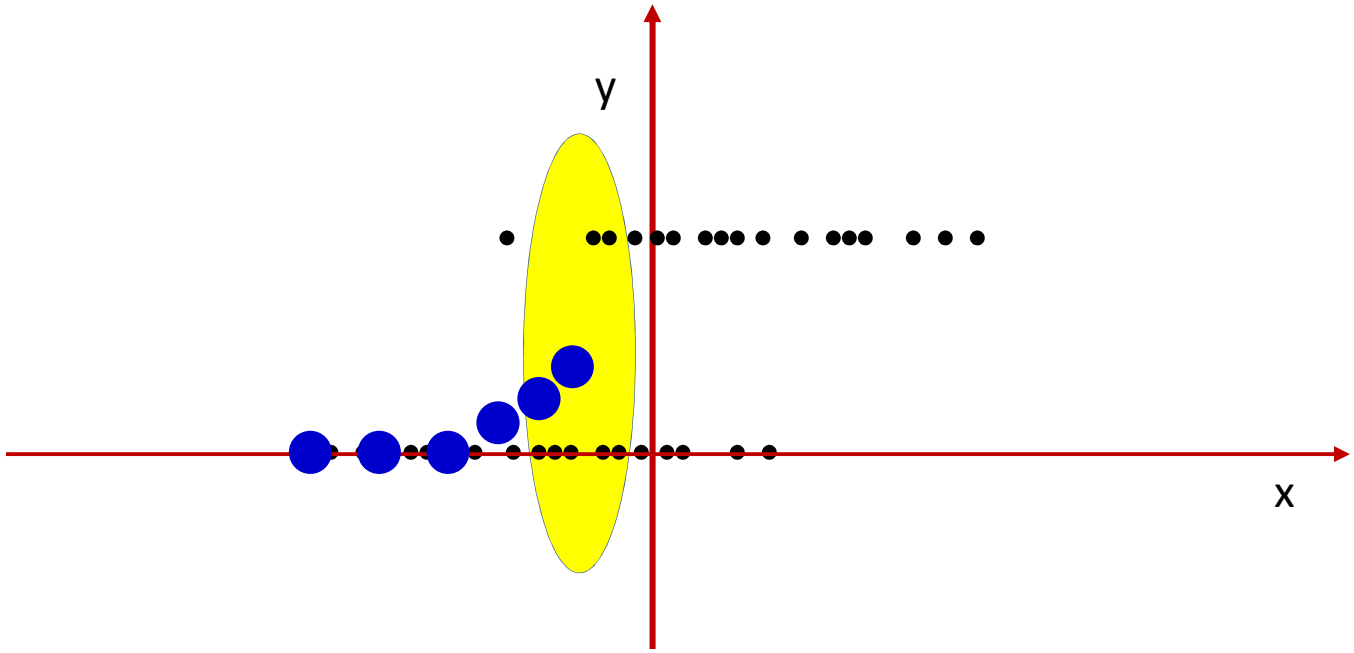


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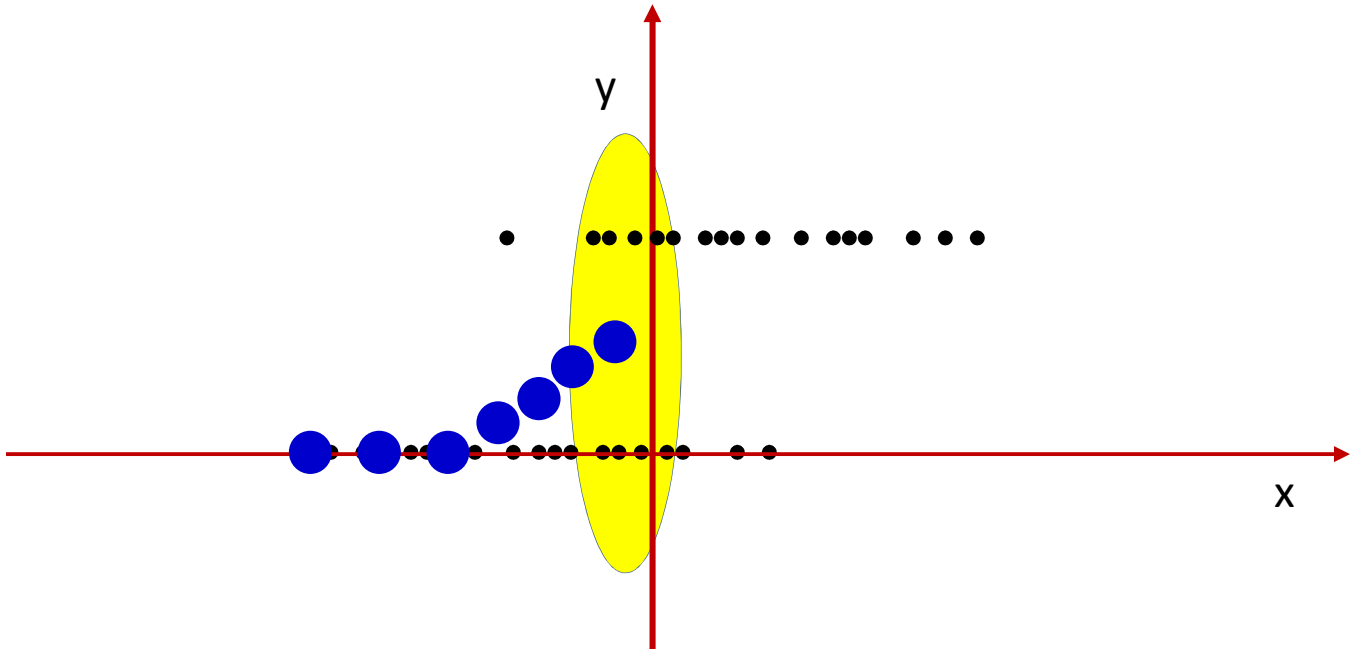


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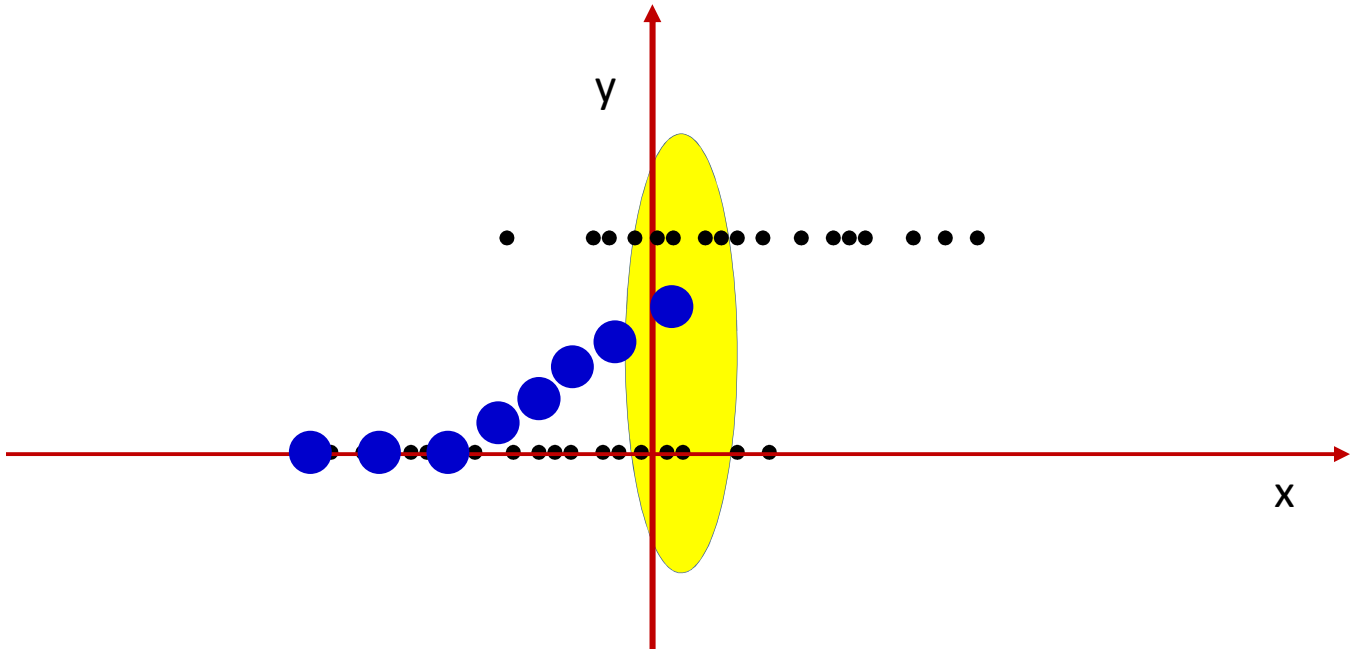


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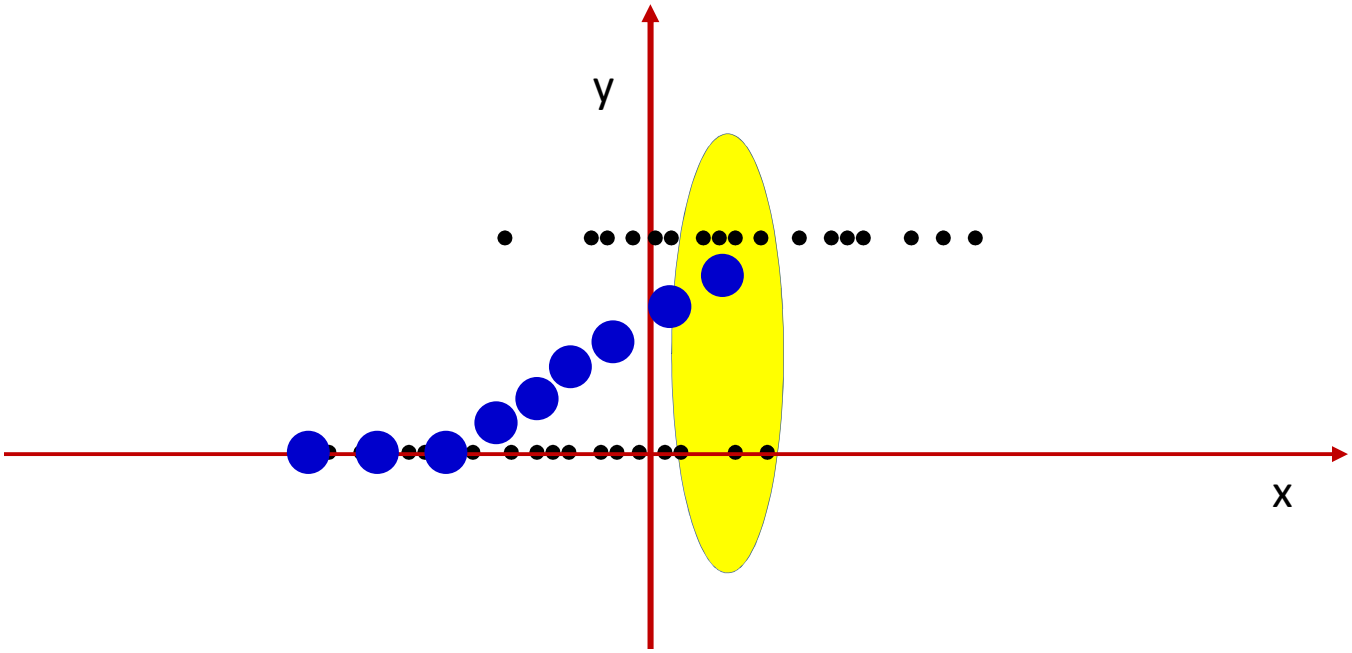


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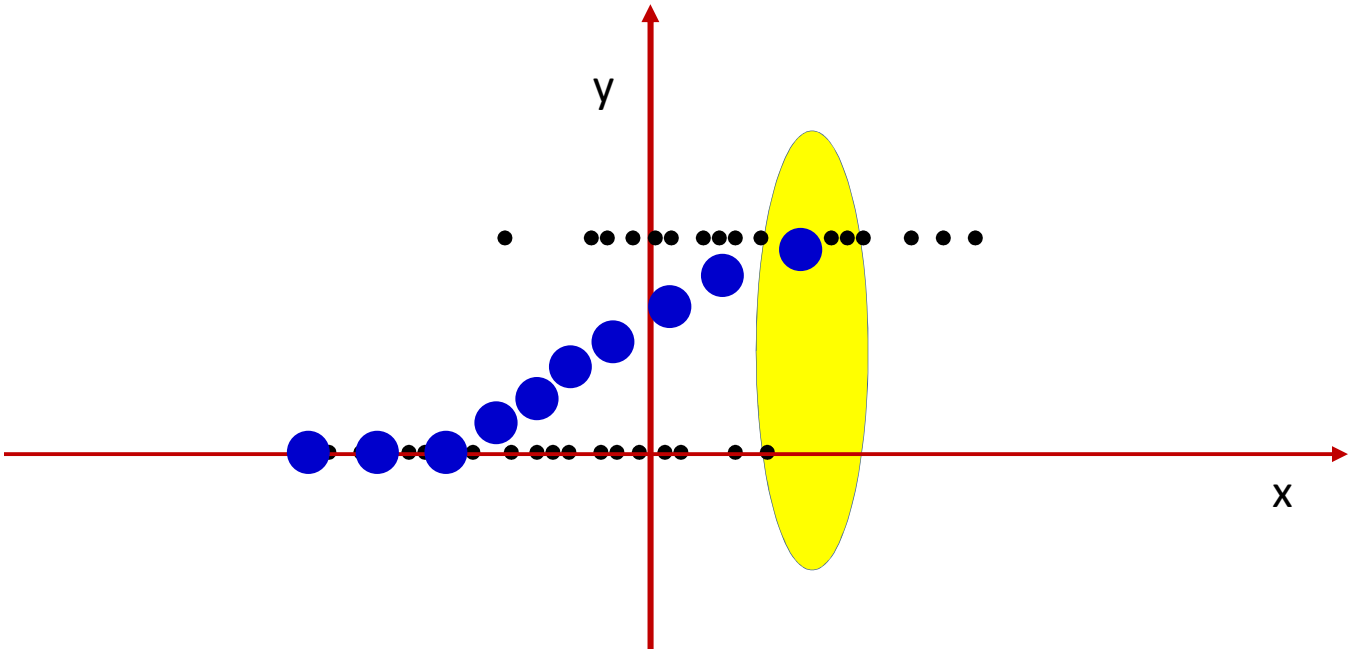


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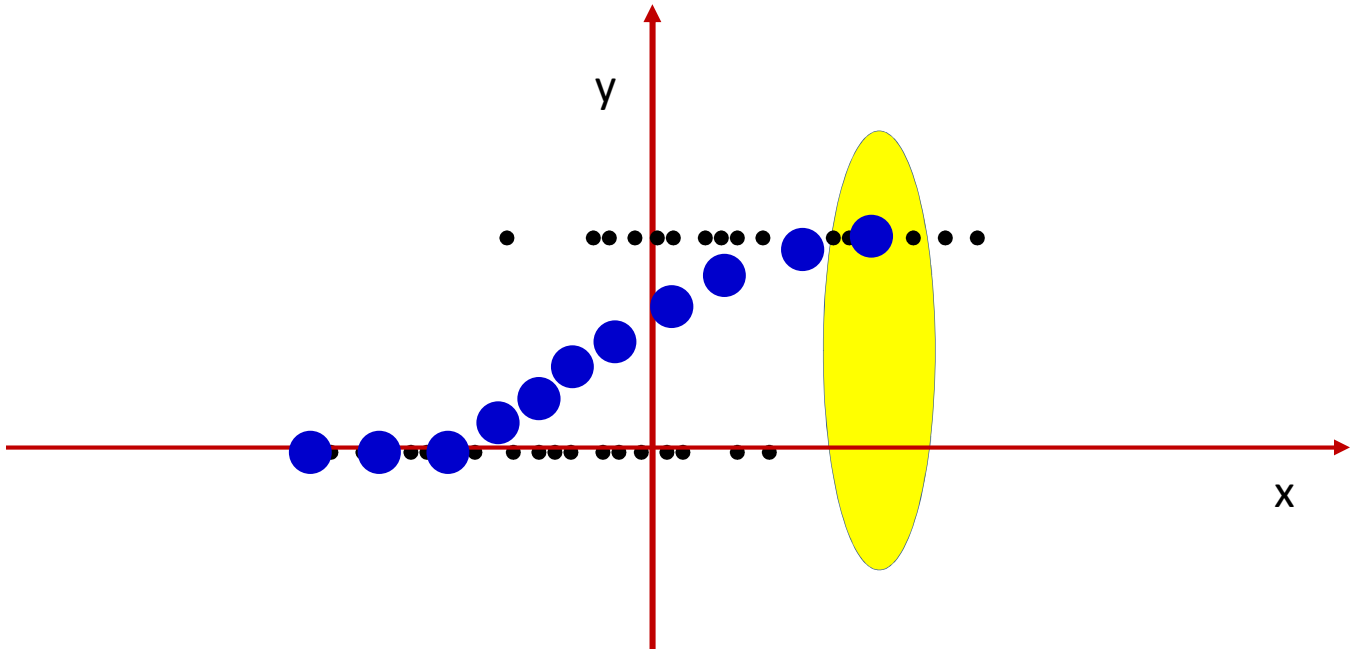


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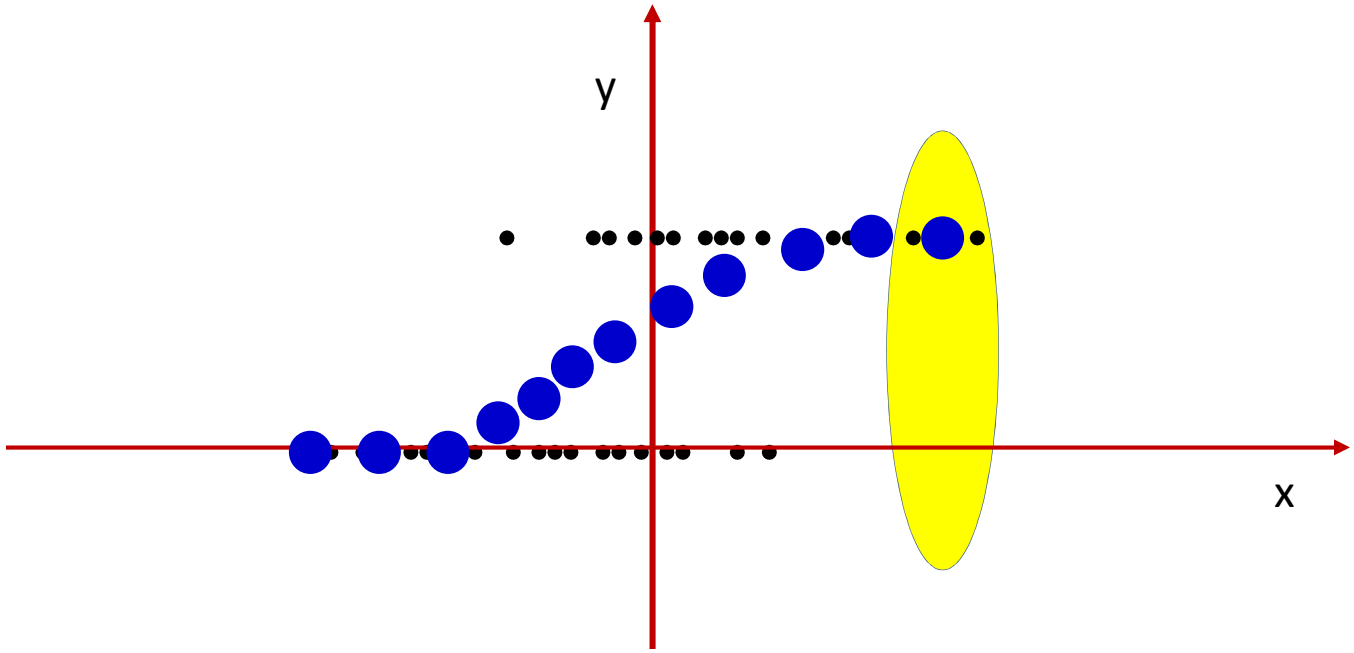


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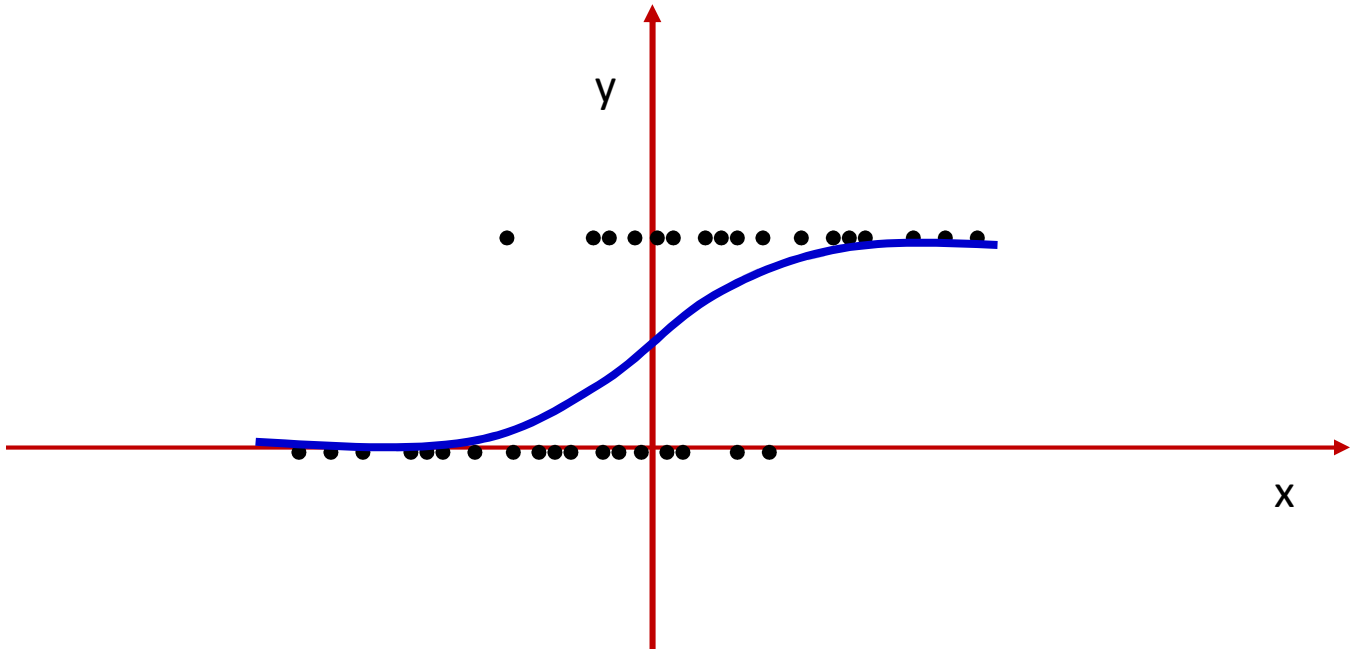


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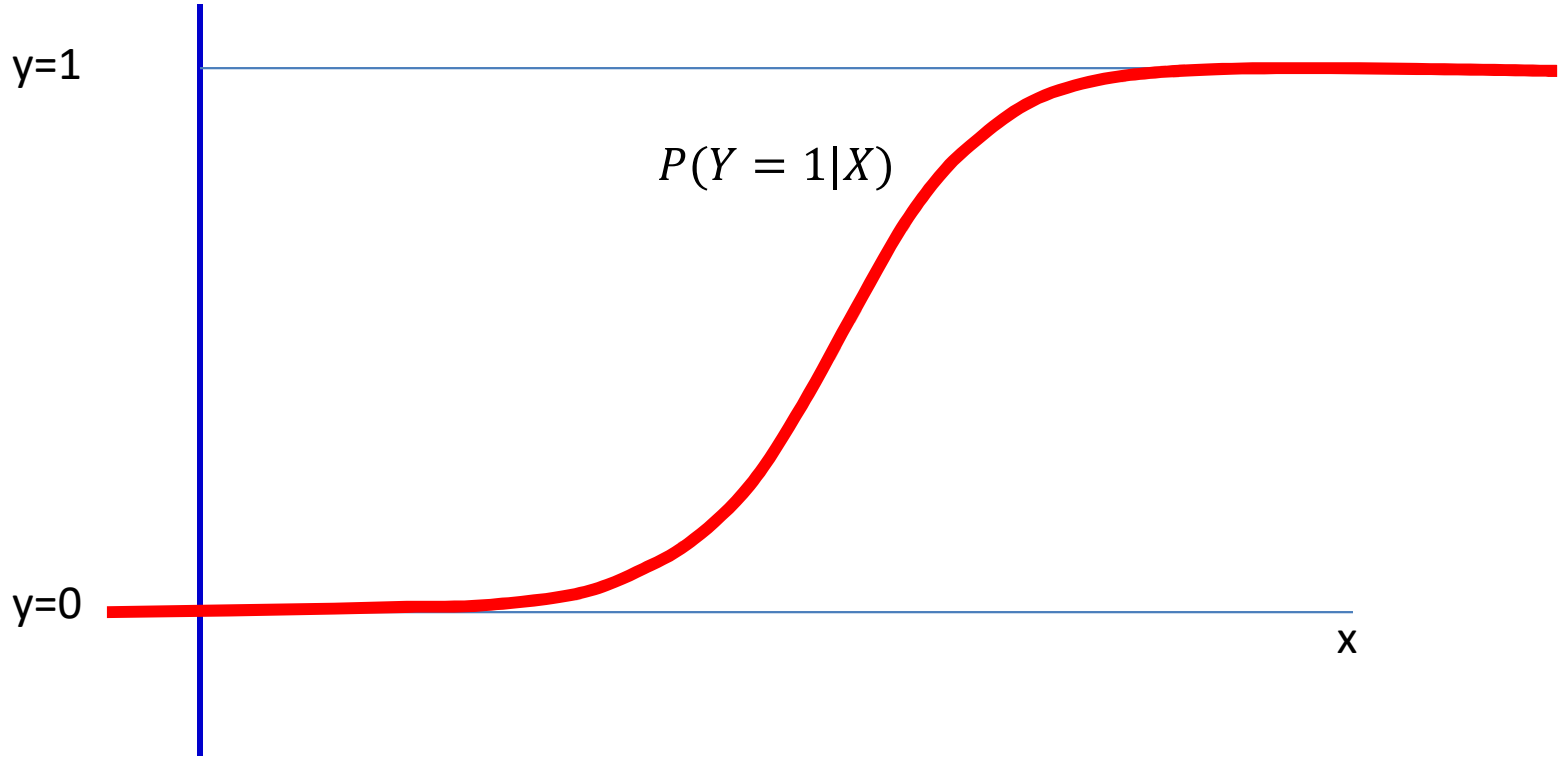
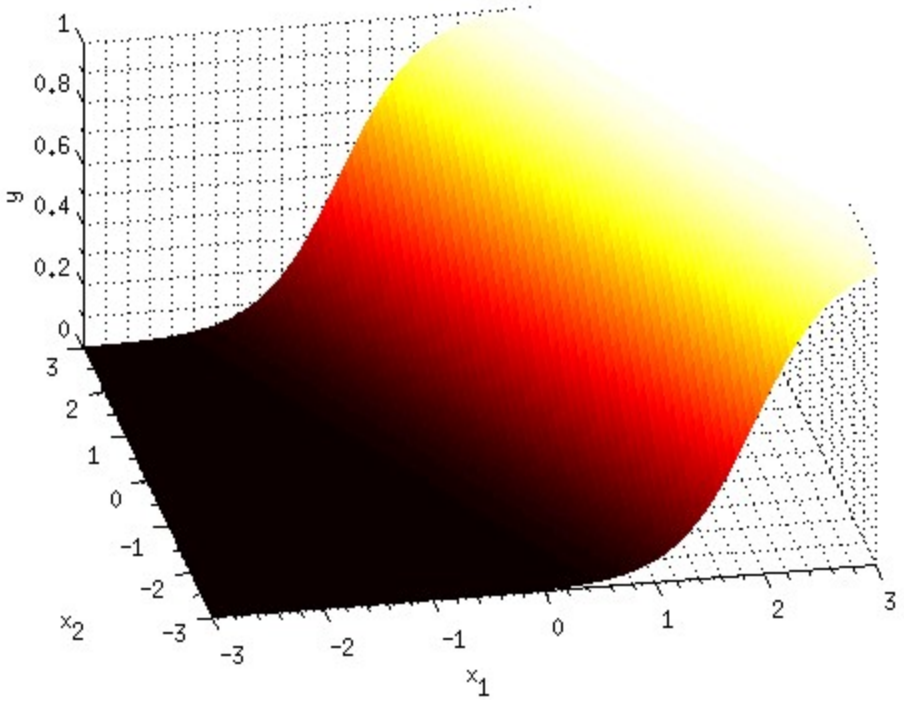
# The logistic regression model



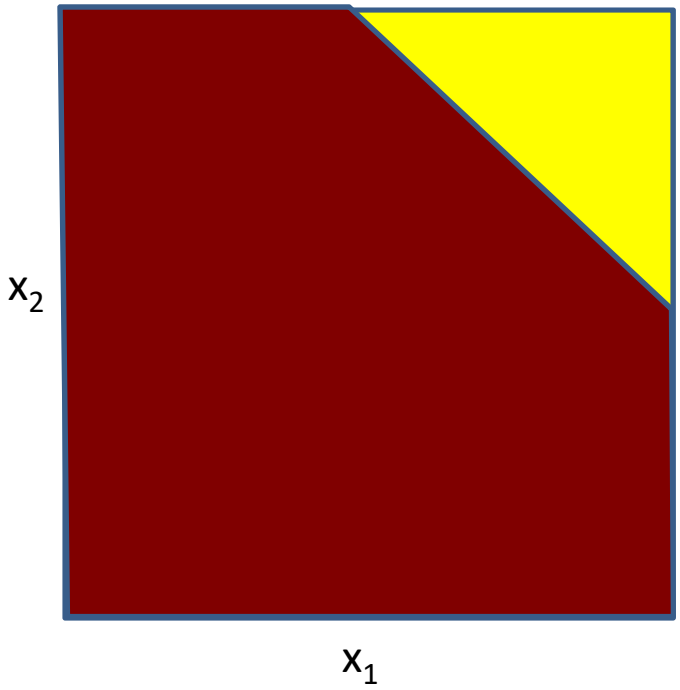

- Class 1 becomes increasingly probable going left to right
  - Very typical in many problems

# Logistic regression




When X is a 2-D variable

Decision: y > 0.5?




$$P(Y = 1|X) = \frac{1}{1 + \exp\left(-\sum_i w_i x_i - b\right)}$$

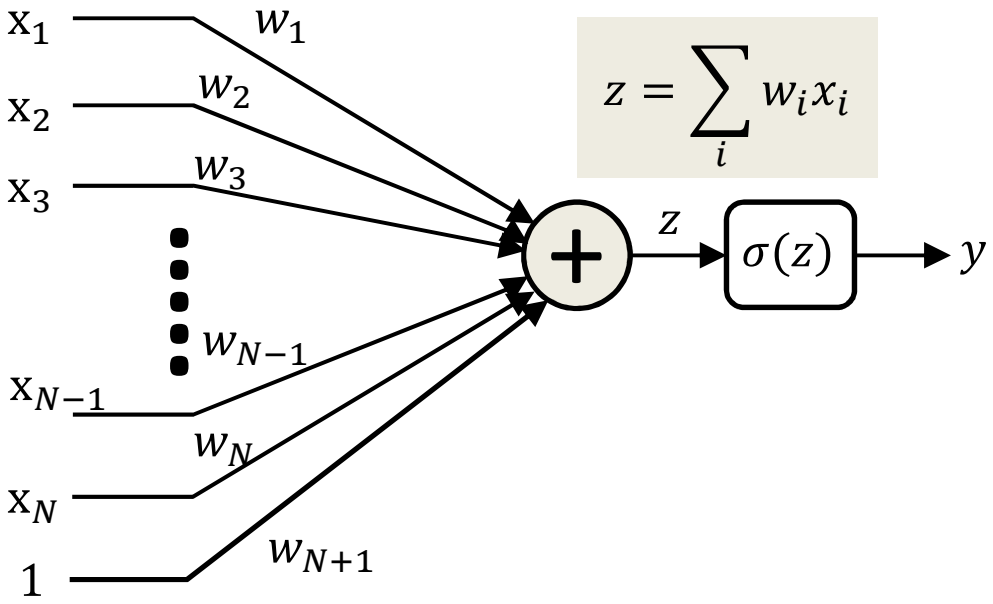
- This the perceptron with a sigmoid activation
  - It actually computes the *probability* that the input belongs to class 1

# Perceptrons and probabilities

- We will return to the fact that perceptrons with sigmoidal activations actually model class probabilities in a later lecture

- But for now moving on..

# Perceptrons with differentiable activation functions



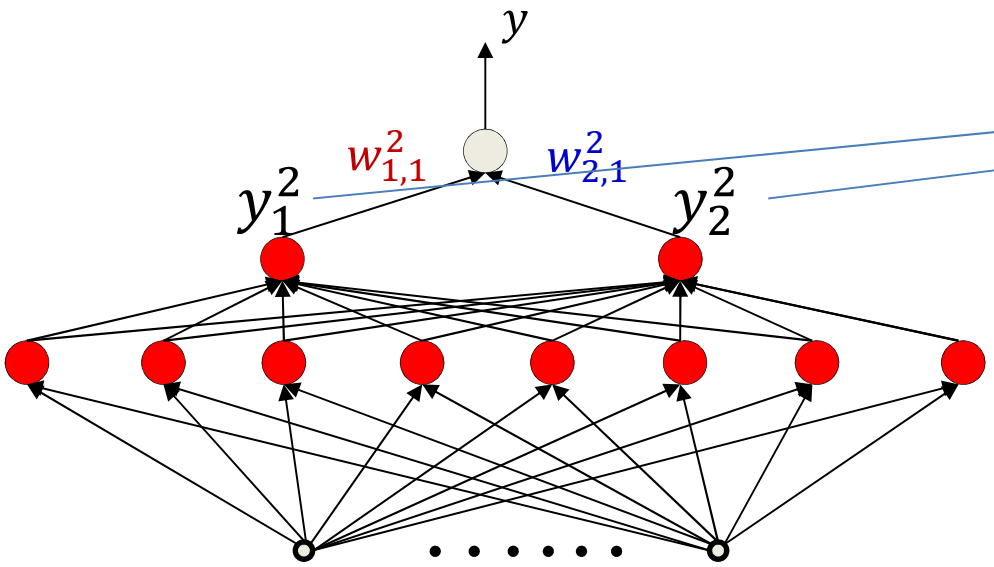

$$z = \sum_i w_i x_i$$

$$\frac{dy}{dw_i} = \frac{dy}{dz}\frac{dz}{dw_i} = \sigma'(z)x_i$$

$$\frac{dy}{dx_i} = \frac{dy}{dz}\frac{dz}{dx_i} = \sigma'(z)w_i$$

- **$\sigma(z)$is a differentiable function of $z$**
  - $\frac{d\sigma(z)}{dz}$ is well-defined and finite for all $z$
- **Using the chain rule, $y$ is a differentiable function of both inputs $x_i$ and weights $w_i$**
- **This means that we can compute the change in the output for *small* changes in either the input or the weights**

# Overall network is differentiable




$$y = \sigma(w^2_{1,1}y^2_1 + w^2_{2,1}y^2_2 + w^2_{3,1})$$

$y$ = output of overall network

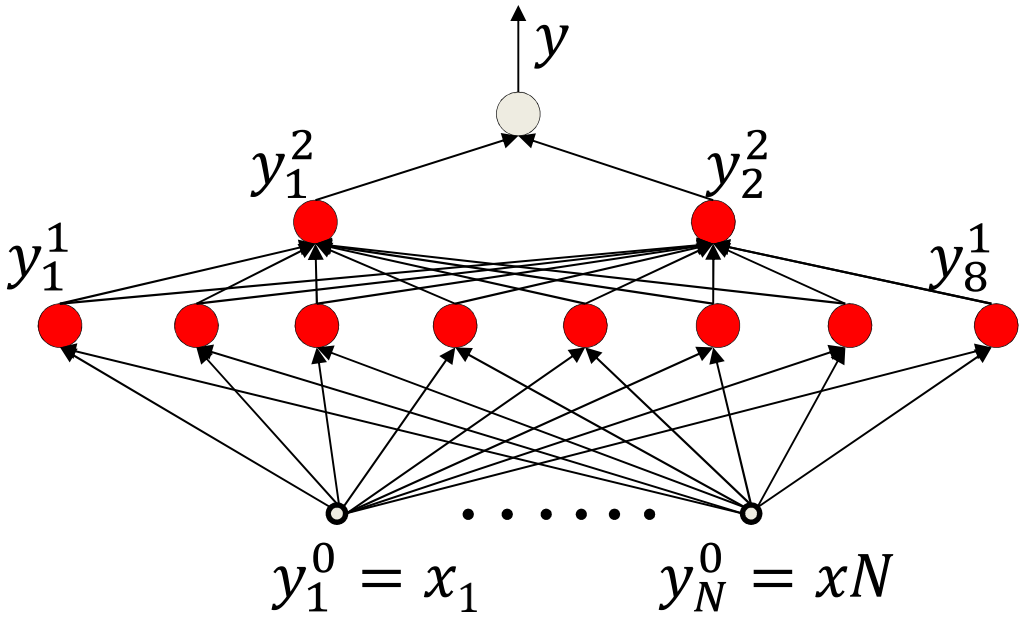
$w^k_{i,j}$ = weight connecting the ith unit of the kth layer to the jth unit of the k+1-th layer

$y^k_i$ = output of the ith unit of the kth layer

$\sigma()$ is differentiable w.r.t both $w$ and $y^k_i$

- Every individual perceptron is differentiable w.r.t its inputs and its weights (including "bias" weight)
- By the chain rule, the overall function is differentiable w.r.t every parameter (weight or bias)
  - Small changes in the parameters result in measurable changes in output

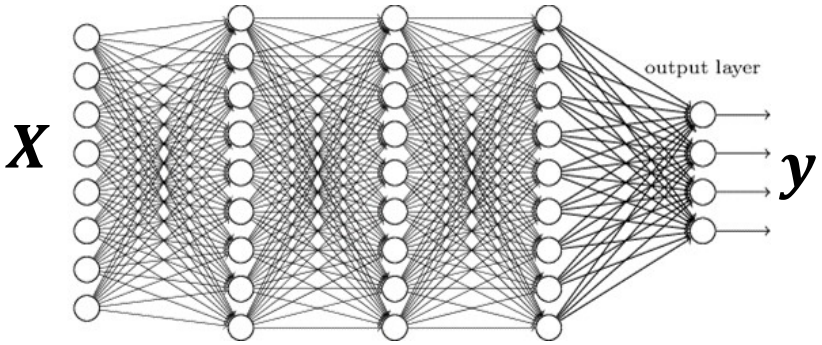
# Overall function is differentiable

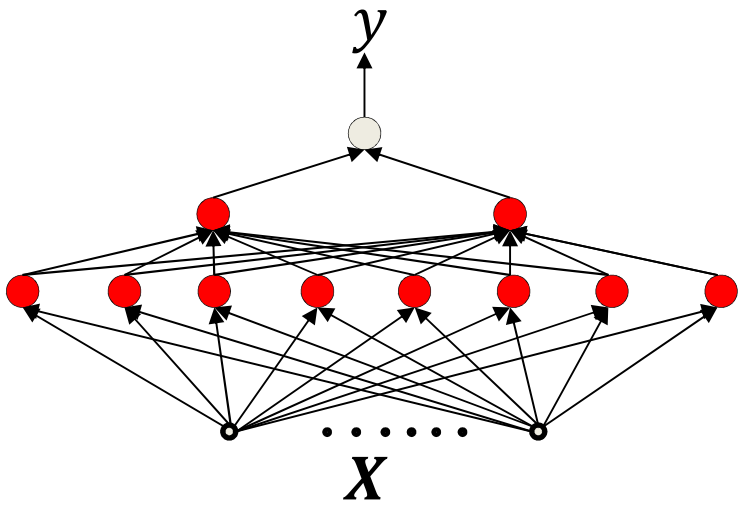



$$y_j^k = \sigma\left(\sum_i w_{i,j}^{k-1} y_i^{k-1}\right)$$

- The overall function is differentiable w.r.t every parameter
  - Small changes in the parameters result in measurable changes in the output
  - We will derive the actual derivatives using the chain rule later

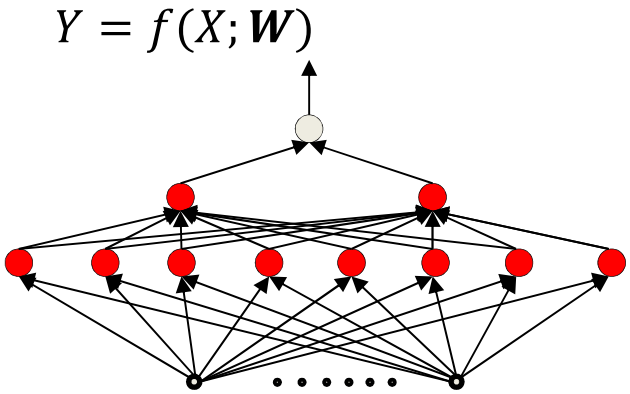
# Overall setting for "Learning" the MLP

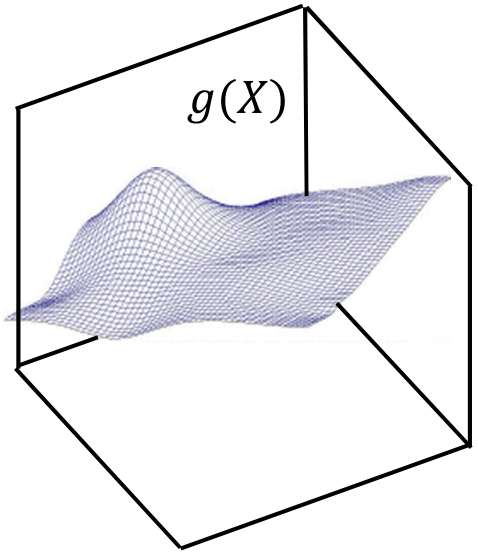



- Given a training set of input-output pairs $(\boldsymbol{X}_1, \boldsymbol{d}_1), (\boldsymbol{X}_2, \boldsymbol{d}_2), \ldots, (\boldsymbol{X}_N, \boldsymbol{d}_N)$ …
  - $\boldsymbol{d}$ is the *desired output* of the network in response to $\boldsymbol{X}$
  - $\boldsymbol{X}$ and $\boldsymbol{d}$ may both be vectors
- …we must find the network parameters such that the network produces the desired output for each training input
  - Or a close approximation of it
  - **The *architecture* of the network must be specified by us**

# Recap: Learning the function



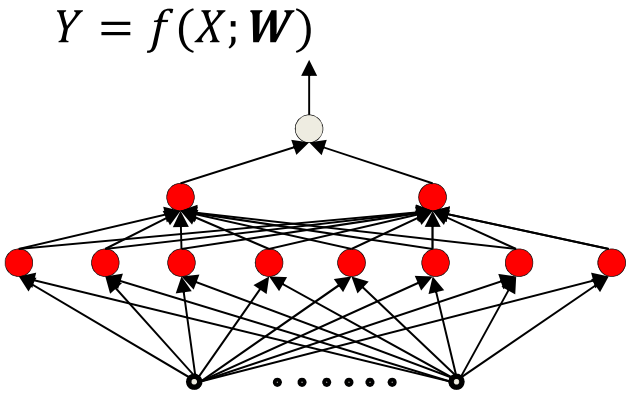



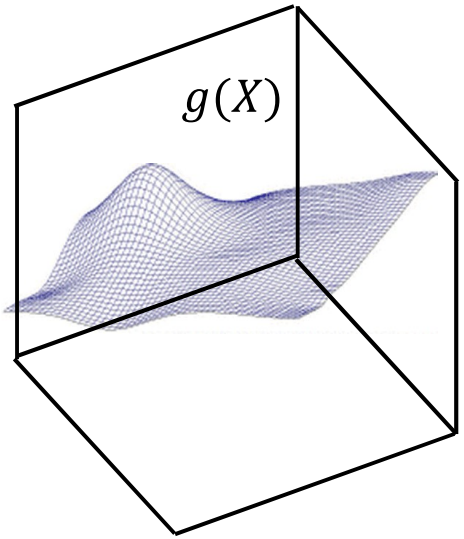

- When $f(X; \boldsymbol{W})$ has the capacity to exactly represent $g(X)$

$$\widehat{\boldsymbol{W}} = \underset{W}{\operatorname{argmin}} \int_X div\big(f(X; W), g(X)\big) dX$$

- div() is a divergence function that goes to zero when $f(X; W) = g(X)$

# Minimizing *expected* error



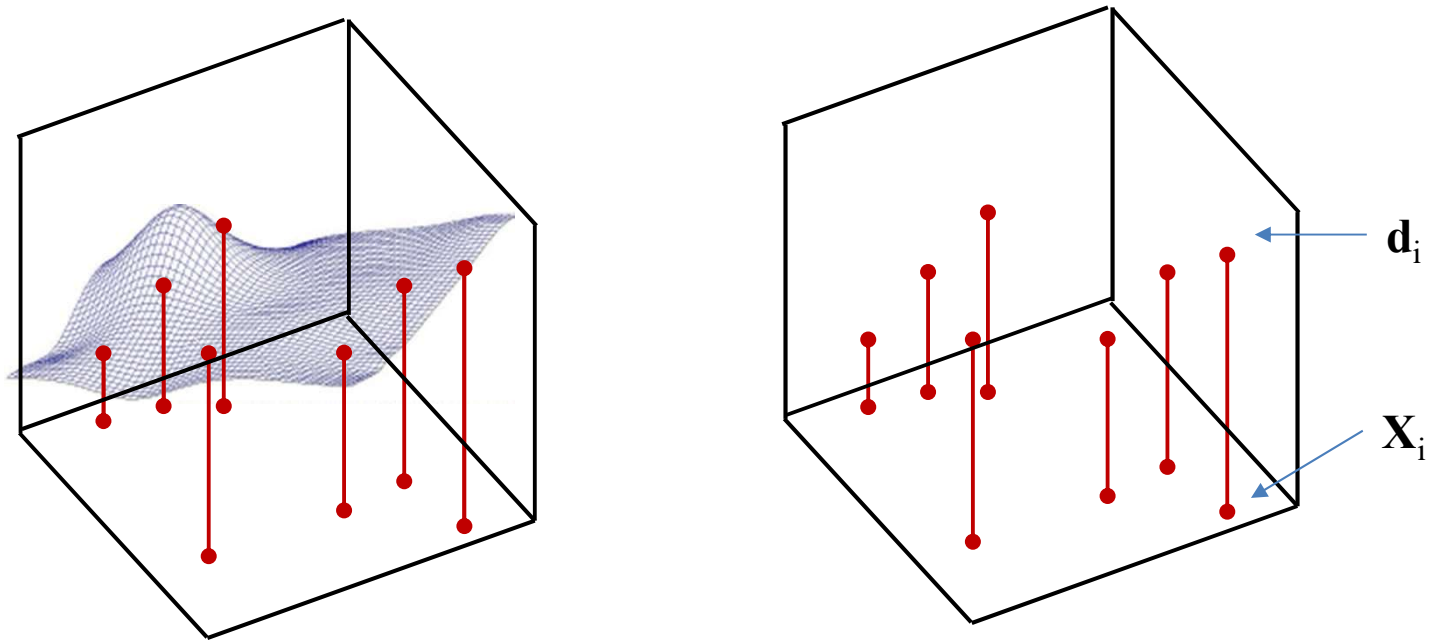




- More generally, assuming $X$ is a random variable

$$\widehat{\boldsymbol{W}} = \underset{W}{\operatorname{argmin}} \int_X div\big(f(X;W), g(X)\big) P(X) dX$$

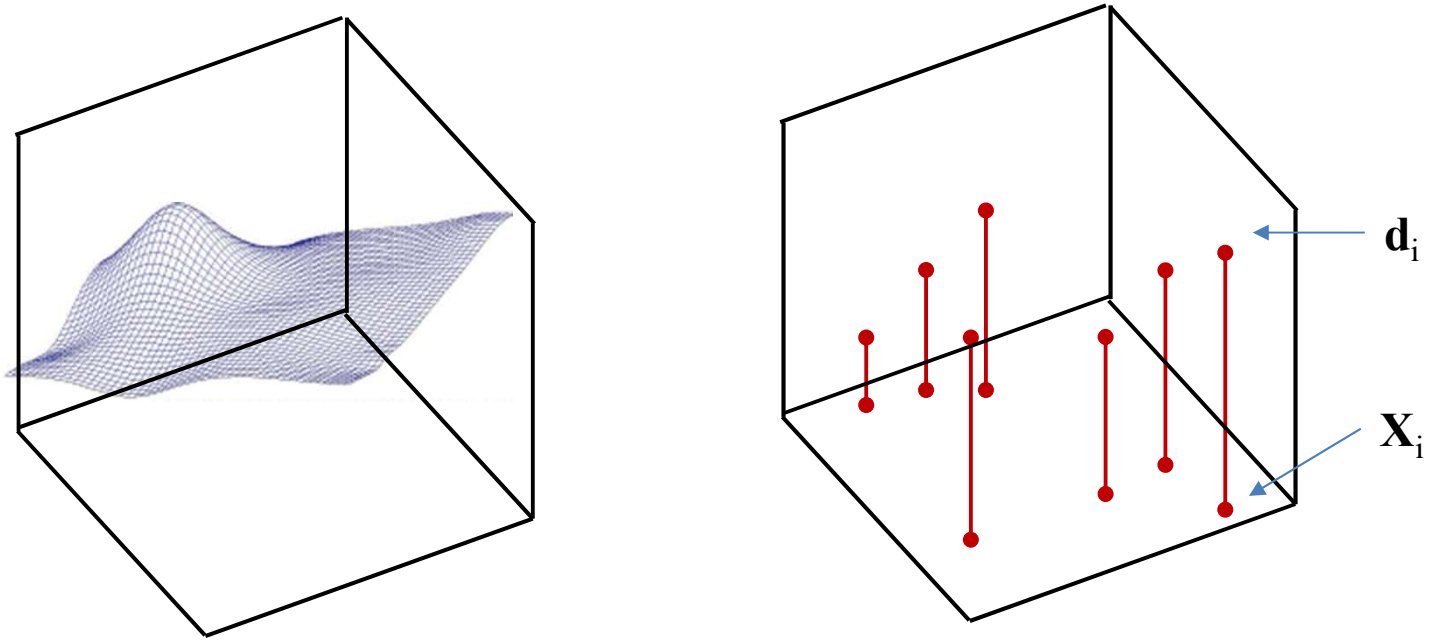
$$= \underset{W}{\operatorname{argmin}}\, E\big[div\big(f(X;W), g(X)\big)\big]$$

# Recap: Sampling the function




- *Sample* $g(X)$
  - Basically, get input-output pairs for a number of samples of input $X_i$
    - Many samples $(X_i, d_i)$, where $d_i = g(X_i) + noise$
  - Good sampling: the samples of $X$ will be drawn from $P(X)$
- Estimate function from the samples

# The *Empirical* risk



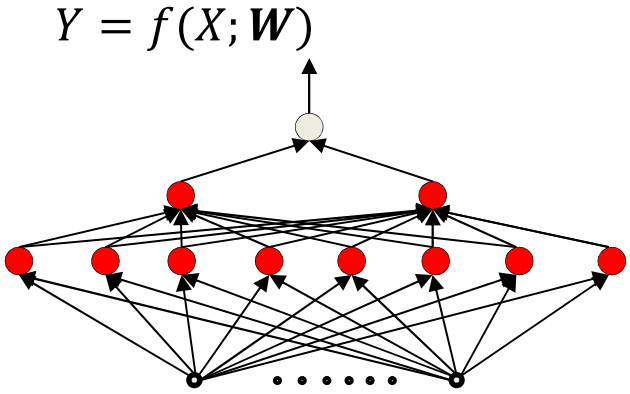

- The *expected* error is the average error over the entire input space

$$E\big[div\big(f(X;W),g(X)\big)\big] = \int_X div\big(f(X;W),g(X)\big)P(X)dX$$

- The *empirical estimate* of the expected error is the *average* error over the samples

$$E\big[div\big(f(X;W),g(X)\big)\big] \approx \frac{1}{N}\sum_{i=1}^{N} div(f(X_i;W),d_i)$$

# Empirical Risk Minimization




- Given a training set of input-output pairs $(\boldsymbol{X}_1, \boldsymbol{d}_1), (\boldsymbol{X}_2, \boldsymbol{d}_2), \ldots, (\boldsymbol{X}_N, \boldsymbol{d}_N)$
  - Error on the ith instance: $div(f(X_i; W), d_i)$
  - Empirical average error on all training data:

$$Err(W) = \frac{1}{N} \sum_i div(f(X_i; W), d_i)$$

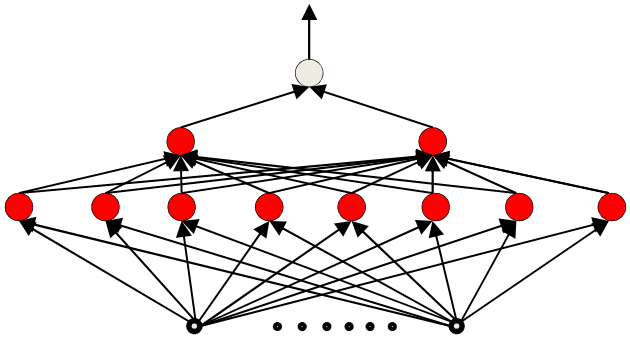
- Estimate the parameters to minimize the empirical estimate of expected error

$$\widehat{\boldsymbol{W}} = \underset{W}{\operatorname{argmin}}\, Err(W)$$

  - I.e. minimize the *empirical error* over the drawn samples

# Empirical Risk Minimization

$$Y = f(X; \boldsymbol{W})$$



- Note: The empirical risk $Err(W)$ is only an empirical approximation to the true risk $E\left[div\left(f(X;W), g(X)\right)\right]$ which is our *actual* minimization objective

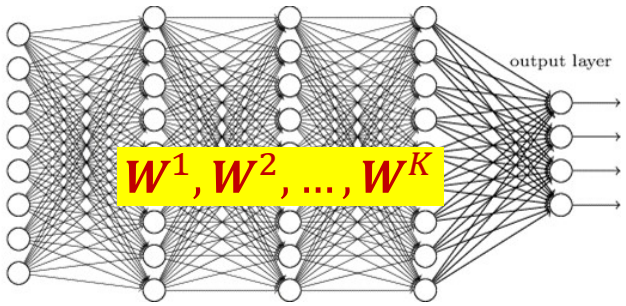
$$Err(W) = \frac{1}{N}\sum_{i} div(f(X_i; W), d_i)$$

- Estimate the parameters to minimize the empirical estimate of expected error

$$\widehat{\boldsymbol{W}} = \underset{W}{\operatorname{argmin}}\, Err(W)$$

  - I.e. minimize the *empirical error* over the drawn samples

# ERM for neural networks




**Actual output of network:**

$$Y_i = net\left(X_i; \{w_{i,j}^k \forall i,j,k\}\right)$$
$$= net(X_i; W^1, W^2, \ldots, W^K)$$

**Desired output of network:** $d_i$

**Error on i-th training input:** $Div(Y_i, d_i; W^1, W^2, \ldots, W^K)$

**Total training error:**

$$Err(W^1, W^2, \ldots, W^K) = \frac{1}{N}\sum_{i=1}^{N} Div(Y_i, d_i; W^1, W^2, \ldots, W^K)$$

– What is the exact form of Div()? More on this later

- Optimize network parameters to minimize the total error over all training inputs

# Problem Statement

- Given a training set of input-output pairs $(\boldsymbol{X}_1, \boldsymbol{d}_1), (\boldsymbol{X}_2, \boldsymbol{d}_2), \ldots, (\boldsymbol{X}_N, \boldsymbol{d}_N)$
- Minimize the following function

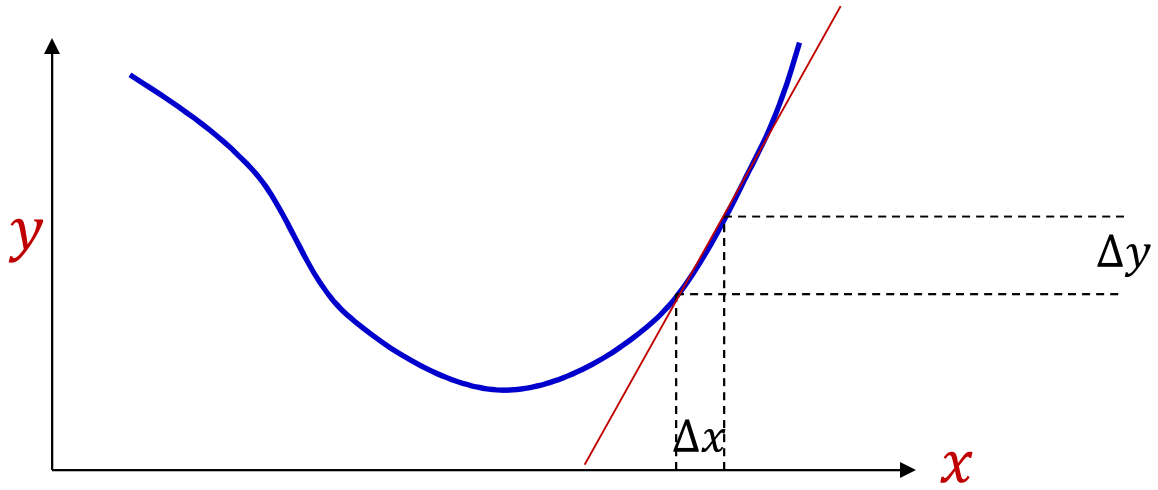
$$Err(W) = \frac{1}{N} \sum_i div(f(X_i; W), d_i)$$

w.r.t $W$

- This is problem of function minimization
  - An instance of optimization

- **A CRASH COURSE ON FUNCTION OPTIMIZATION**

# A brief note on derivatives..



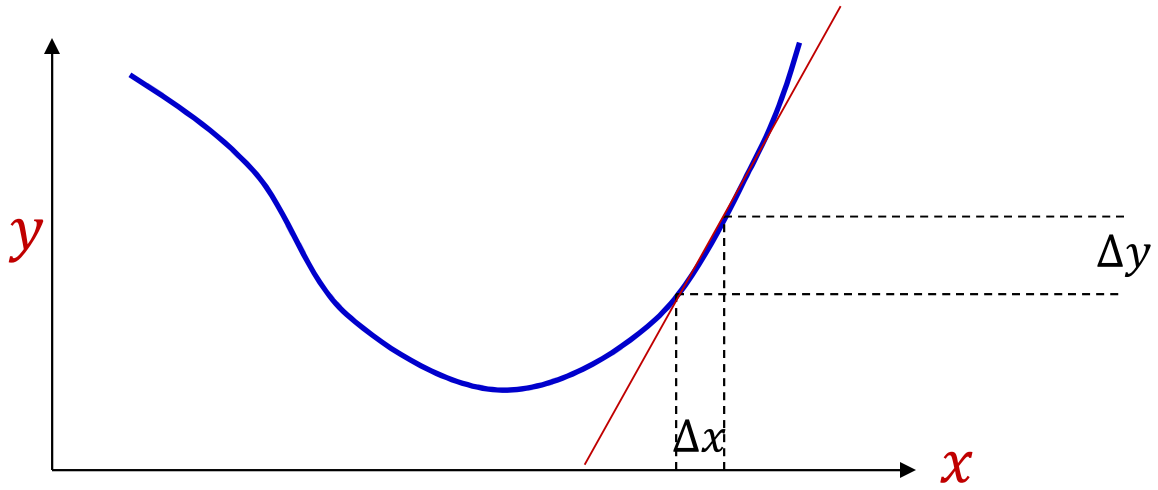

derivative

- A derivative of a function at any point tells us how much a minute increment to the *argument* of the function will increment the *value* of the function
  - For any $y = f(x)$, expressed as a multiplier $\alpha$ to a tiny increment $\Delta x$ to obtain the increments $\Delta y$ to the output

$$\Delta y = \alpha \Delta x$$

  - Based on the fact that at a fine enough resolution, any smooth, continuous function is locally linear at any point

# Scalar function of scalar argument




- When $x$ and $y$ are scalar

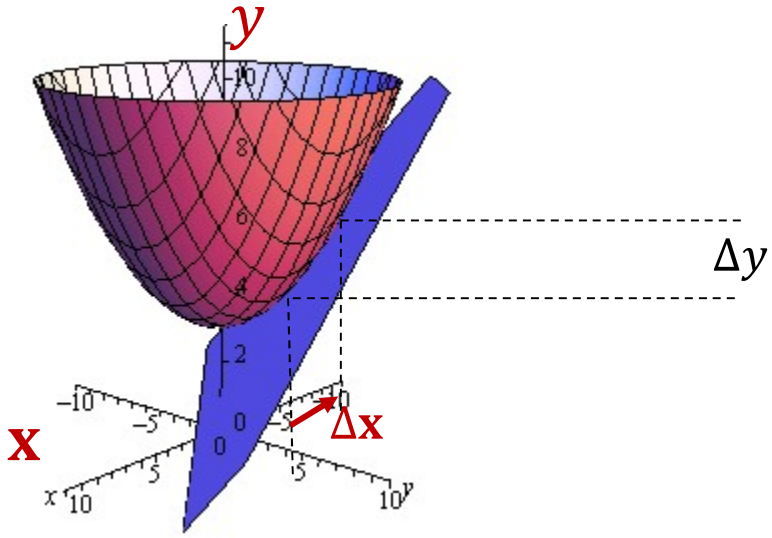
$$y = f(x)$$

  - Derivative:

$$\Delta y = \alpha \Delta x$$

  - Often represented (using somewhat inaccurate notation) as $\frac{dy}{dx}$
  - Or alternately (and more reasonably) as $f'(x)$

# Multivariate scalar function:
# Scalar function of *vector* argument




Note: $\Delta\mathbf{x}$ is now a vector

$$\Delta\mathbf{x} = \begin{bmatrix} \Delta x_1 \\ \vdots \\ \Delta x_D \end{bmatrix}$$

$$\Delta y = \alpha \Delta\mathbf{x}$$

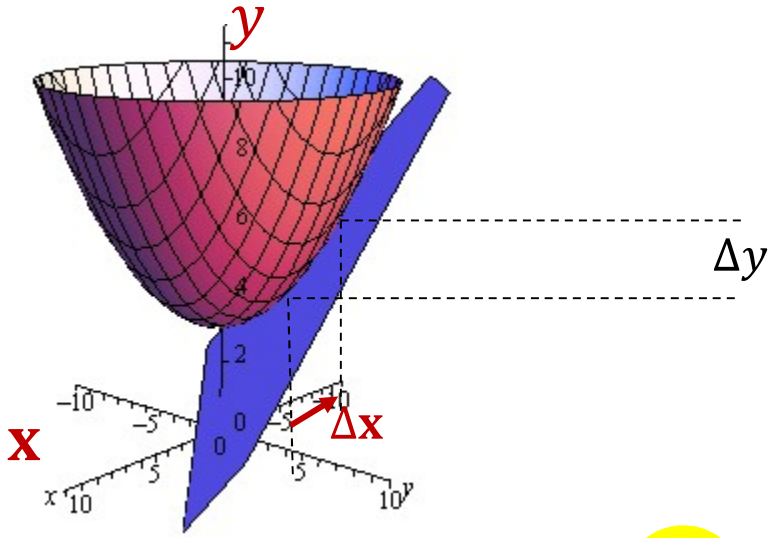
- Giving us that $\alpha$ is a row vector: $\alpha = [\alpha_1 \quad \cdots \quad \alpha_D]$

$$\Delta y = \alpha_1 \Delta x_1 + \alpha_2 \Delta x_2 + \cdots + \alpha_D \Delta x_D$$

- The *partial* derivative $\alpha_i$ gives us how $y$ increments when *only* $x_i$ is incremented
- Often represented as $\frac{\partial y}{\partial x_i}$

$$\Delta y = \frac{\partial y}{\partial x_1}\Delta x_1 + \frac{\partial y}{\partial x_2}\Delta x_2 + \cdots + \frac{\partial y}{\partial x_D}\Delta x_D$$

# Multivariate scalar function: Scalar function of *vector* argument




Note: $\Delta\mathbf{x}$ is now a vector

$$\Delta\mathbf{x} = \begin{bmatrix} \Delta x_1 \\ \vdots \\ \Delta x_D \end{bmatrix}$$

$$\Delta y = \nabla_{\mathbf{x}} y \Delta\mathbf{x}$$

Gradient

- Where

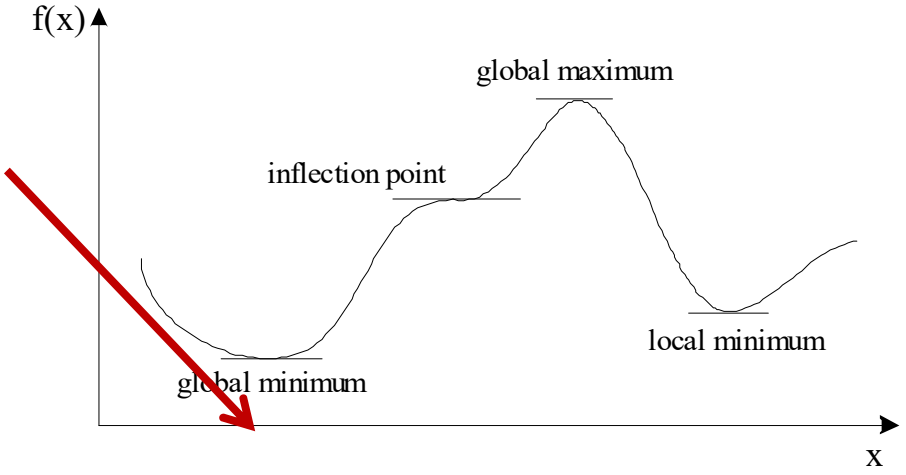
$$\nabla_{\mathbf{x}} y = \begin{bmatrix} \frac{\partial y}{\partial x_1} & \cdots & \frac{\partial y}{\partial x_D} \end{bmatrix}$$

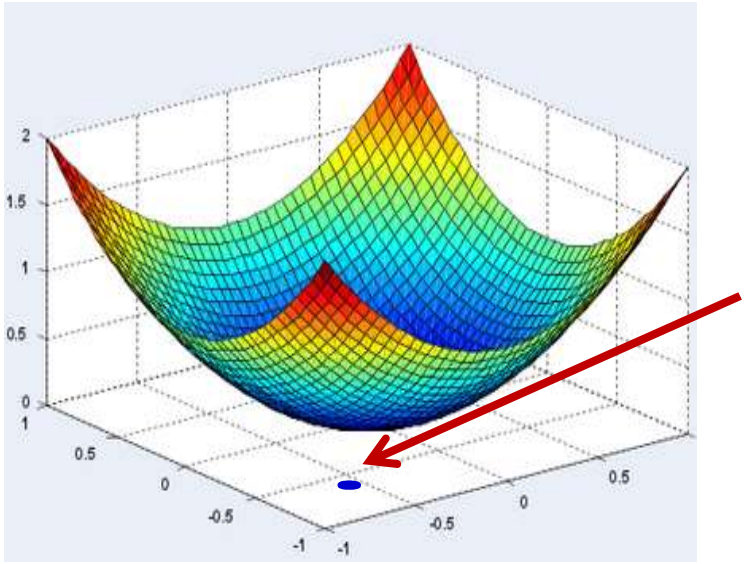
- Sometimes also written with a *transpose* in which case the gradient becomes a column vector

# Caveat about following slides

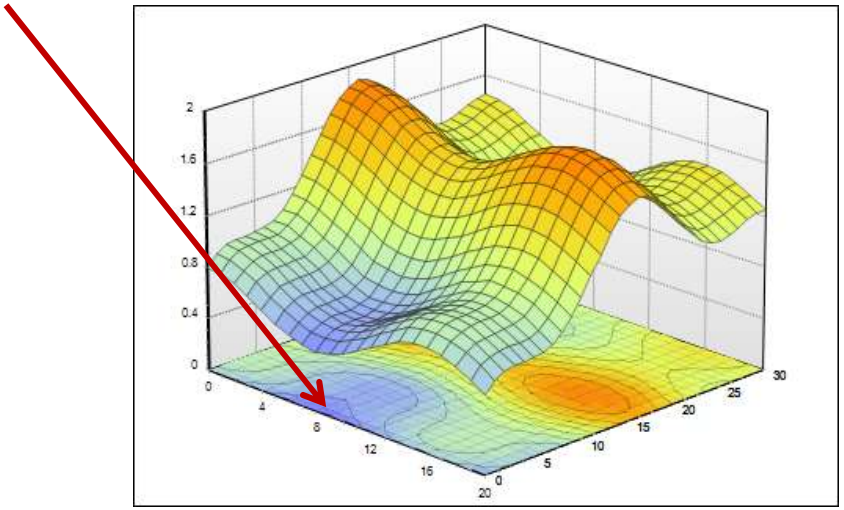
- The following slides speak of optimizing a function w.r.t a variable “x”
- This is only mathematical notation. In our actual network optimization problem we would be optimizing w.r.t. network weights “w”
- To reiterate – “x” in the slides represents the variable that we’re optimizing a function over and not the input to a neural network
- **Do not get confused!**

# The problem of optimization

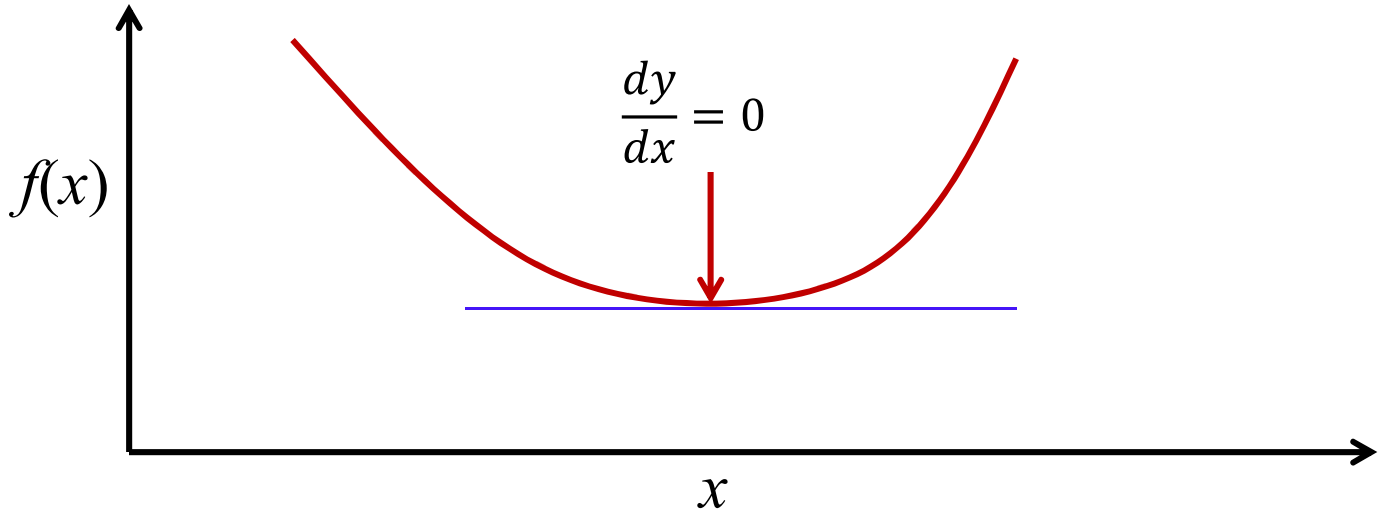


- General problem of optimization: find the value of $\boldsymbol{x}$ where $\mathbf{f}(\boldsymbol{x})$ is minimum



# Finding the minimum of a function

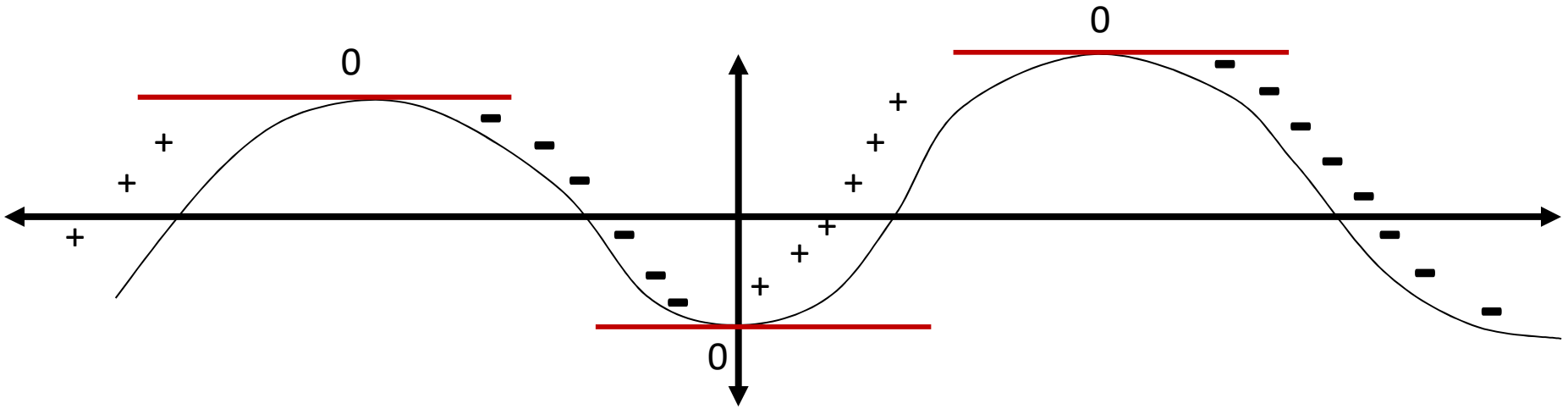



- Find the value $x$ at which $f'(x) = 0$
  - Solve

$$\frac{df(x)}{dx} = 0$$

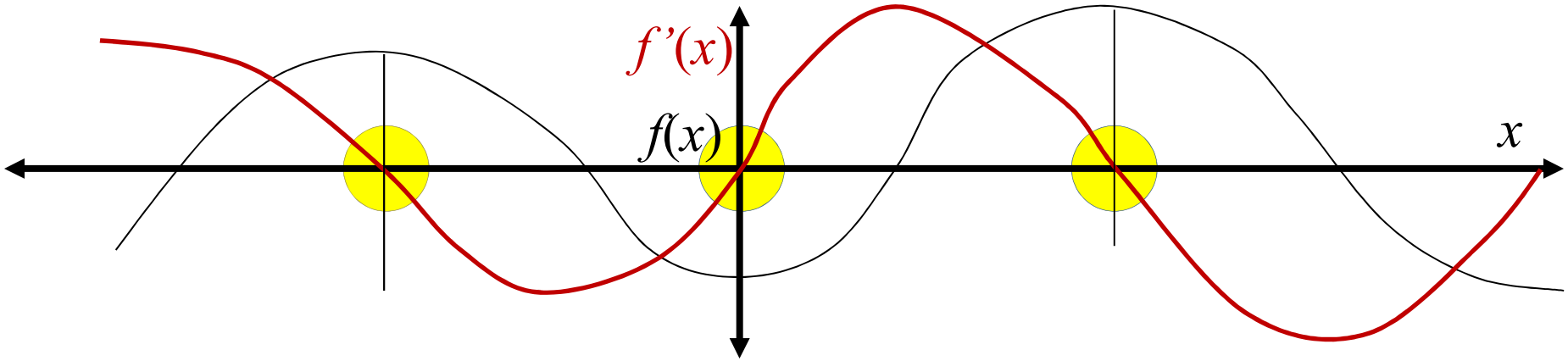
- The solution is a "turning point"
  - Derivatives go from positive to negative or vice versa at this point
- But is it a minimum?

# Turning Points



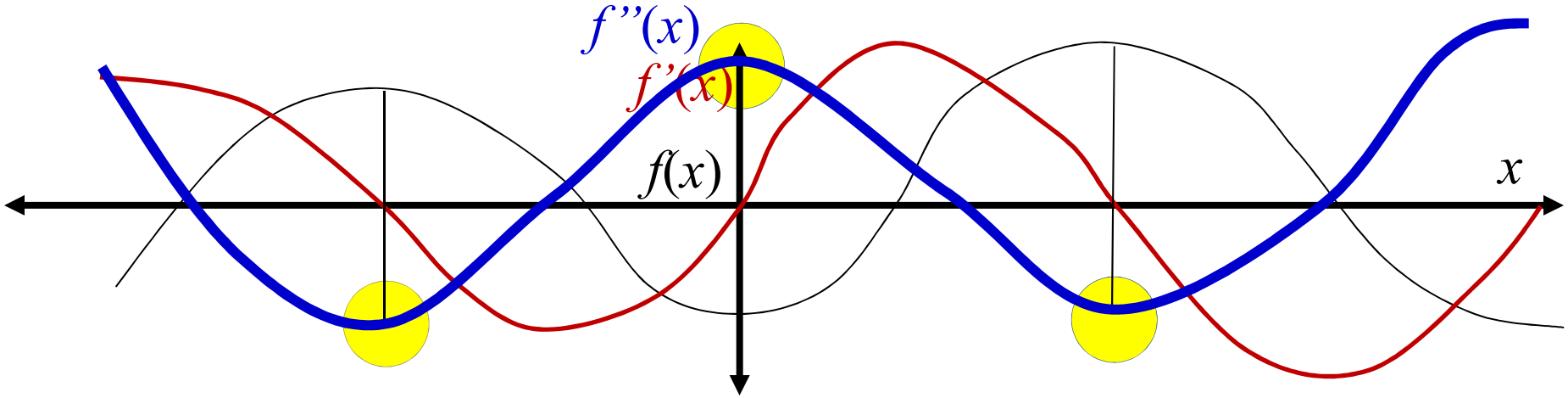

- Both *maxima* and *minima* have zero derivative
- Both are turning points

# Derivatives of a curve




- Both *maxima* and *minima* are turning points
- Both *maxima* and *minima* have zero derivative

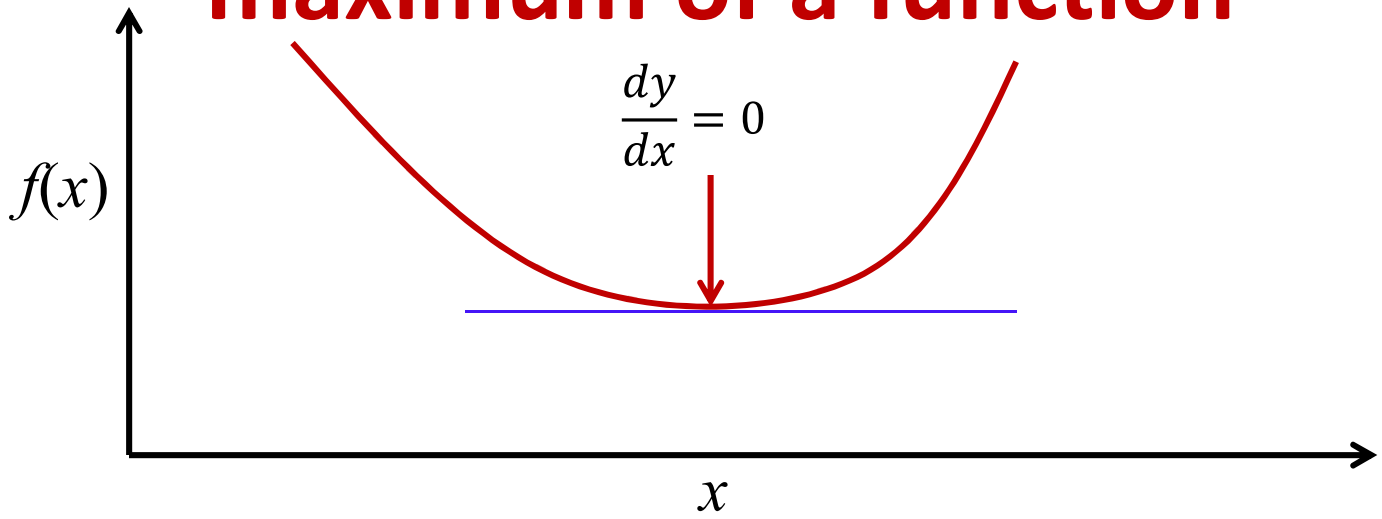
# Derivative of the derivative of the curve




- Both *maxima* and *minima* are turning points
- Both *maxima* and *minima* have zero derivative

- The *second derivative f''*(*x*) is –ve at maxima and +ve at minima!

# Soln: Finding the minimum or maximum of a function




- Find the value $x$ at which $f'(x) = 0$: Solve

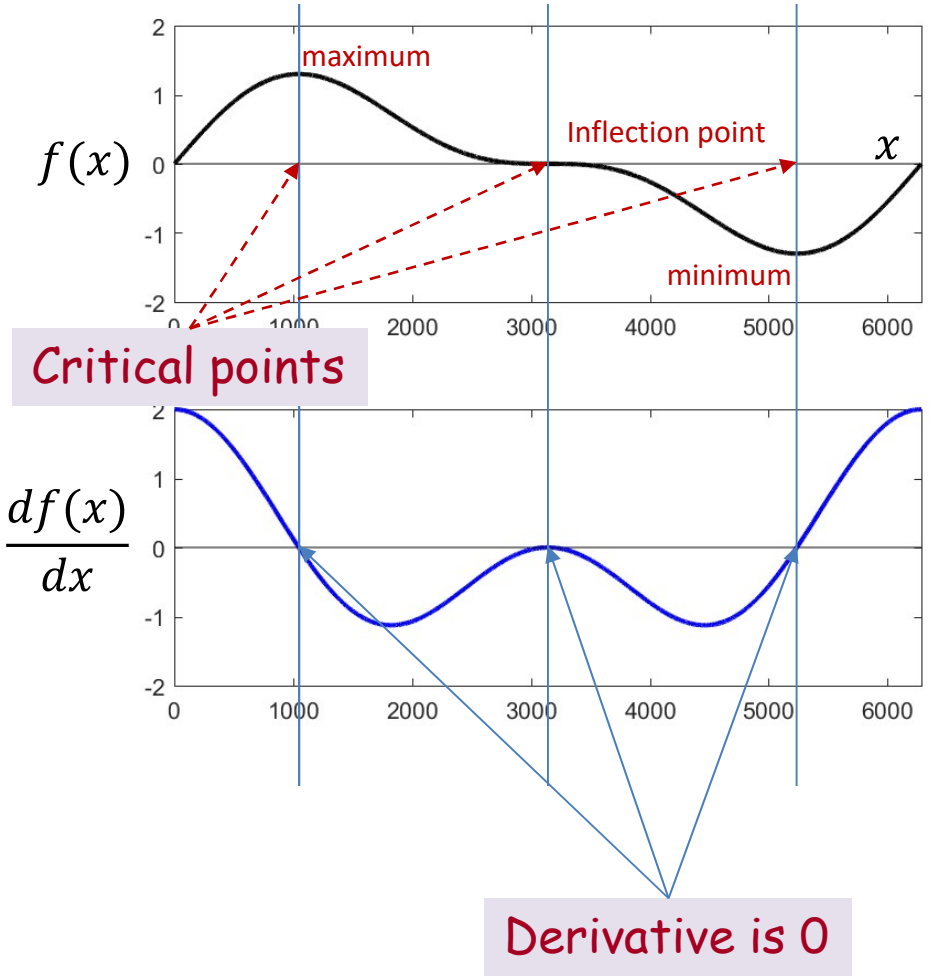
$$\frac{df(x)}{dx} = 0$$

- The solution $x_{soln}$ is a turning point
- Check the double derivative at $x_{soln}$ : compute

$$f''(x_{soln}) = \frac{df'(x_{soln})}{dx}$$

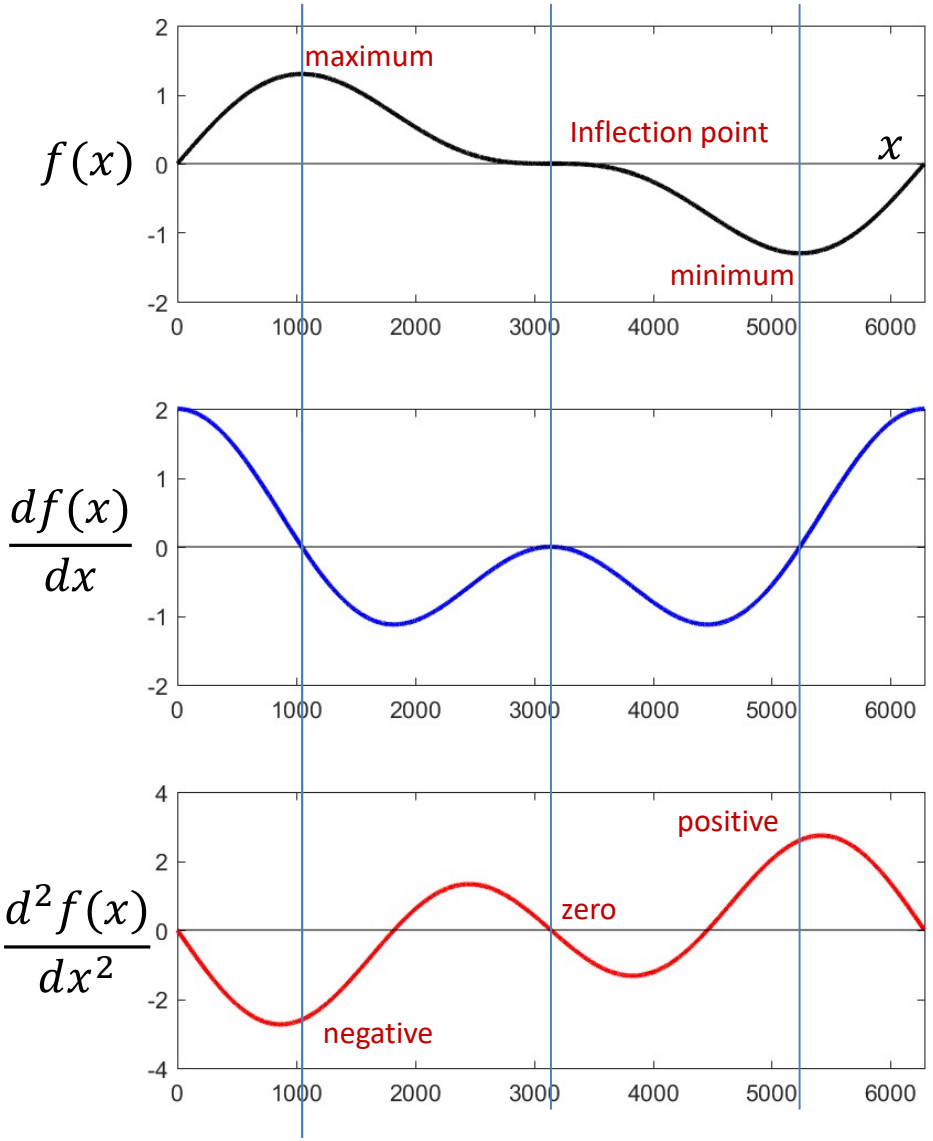
- If $f''(x_{soln})$ is positive $x_{soln}$ is a minimum, otherwise it is a maximum

# A note on derivatives of functions of single variable



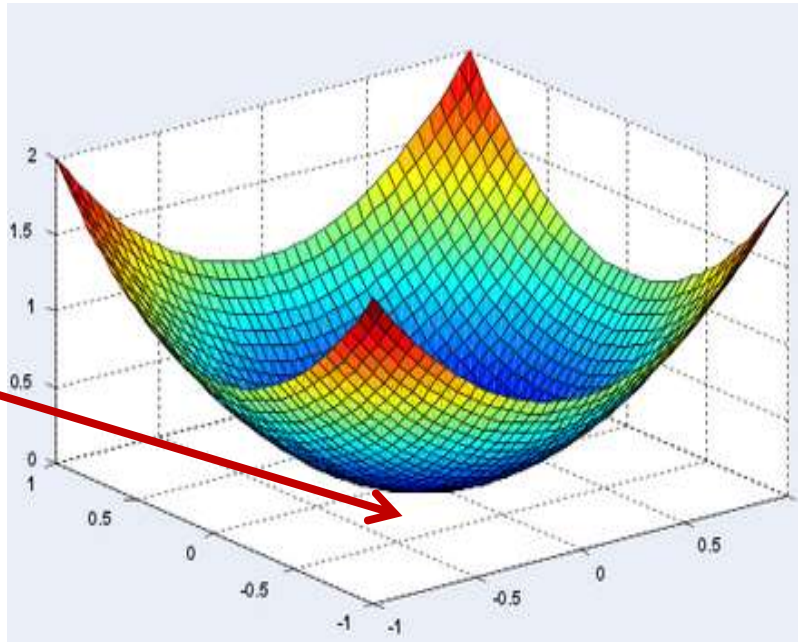

- All locations with zero derivative are *critical* points
  - These can be local maxima, local minima, or inflection points

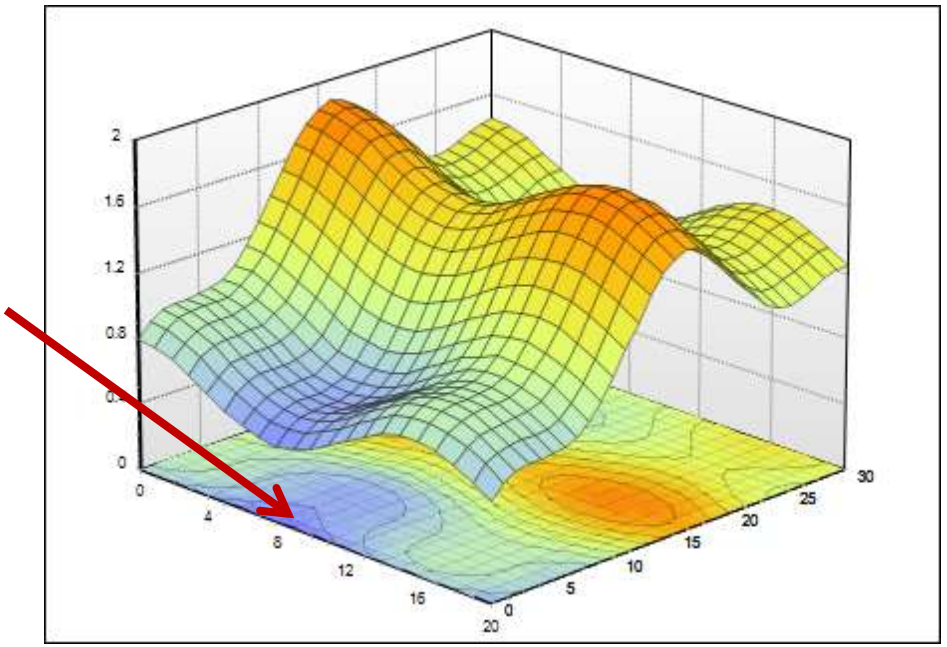
# A note on derivatives of functions of single variable




- All locations with zero derivative are *critical* points
  - These can be local maxima, local minima, or inflection points
- The *second* derivative is
  - $\geq 0$ at minima
  - $\leq 0$ at maxima
  - Zero at inflection points
- It's a little more complicated for functions of multiple variables..

# What about functions of multiple variables?

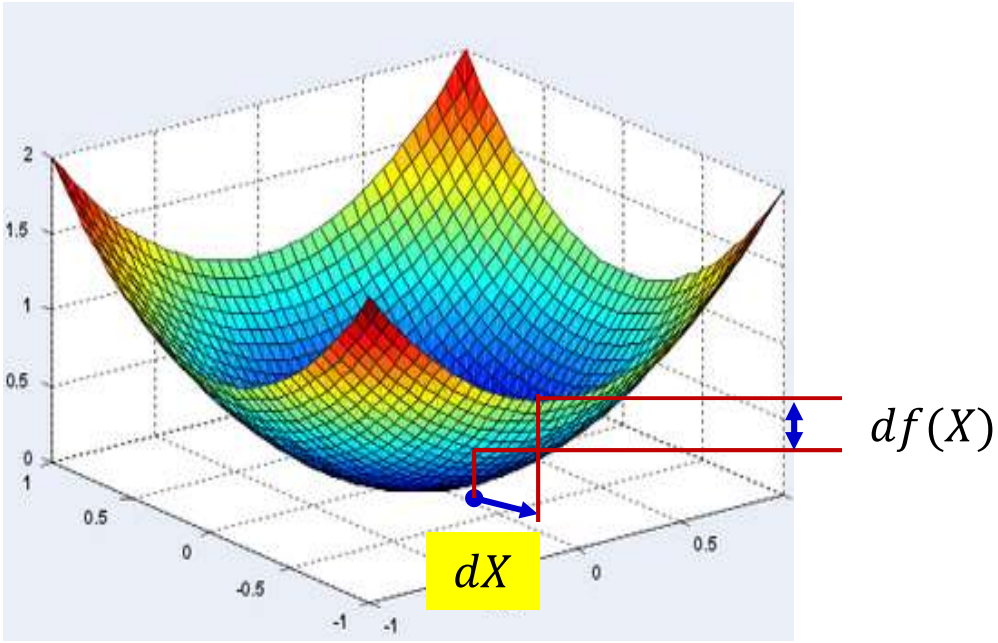



- The optimum point is still "turning" point
  - Shifting in any direction will increase the value
  - For smooth functions, miniscule shifts will not result in any change at all
- We must find a point where shifting in any direction by a microscopic amount will not change the value of the function

# A brief note on derivatives of multivariate functions

# The *Gradient* of a scalar function

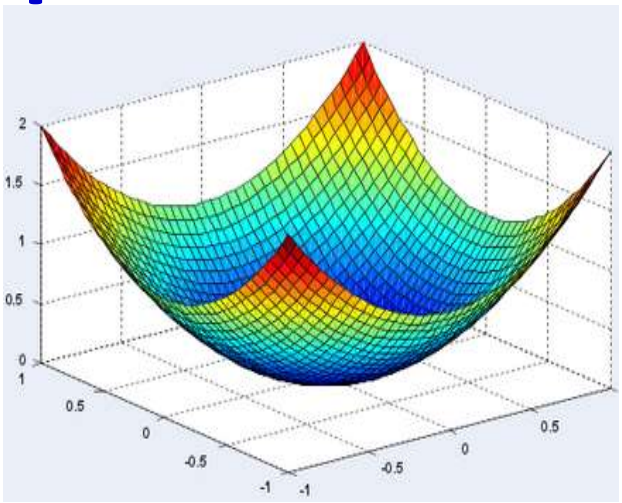



- The *Gradient* $\nabla f(X)$ of a scalar function $f(X)$ of a multi-variate input $X$ is a multiplicative factor that gives us the change in $f(X)$ for tiny variations in $X$

$$df(X) = \nabla f(X) dX$$

# Gradients of scalar functions with multi-variate inputs

- Consider $f(X) = f(x_1, x_2, \dots, x_n)$



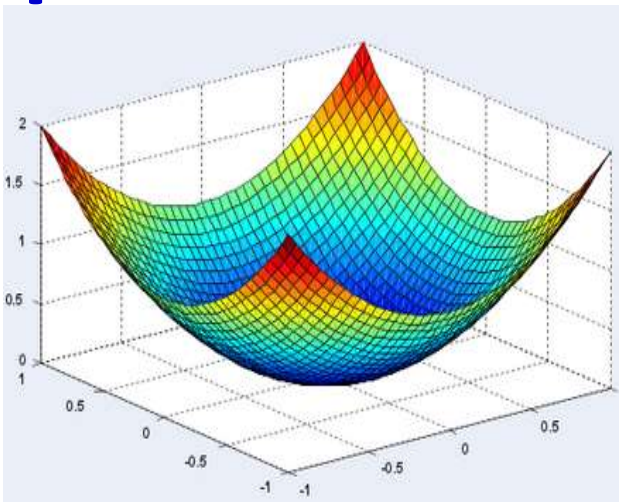
$$\nabla f(X) = \left[\frac{\partial f(X)}{\partial x_1} \quad \frac{\partial f(X)}{\partial x_2} \quad \cdots \quad \frac{\partial f(X)}{\partial x_n}\right]$$

- Check:

$$df(X) = \nabla f(X) dX$$
$$= \frac{\partial f(X)}{\partial x_1} dx_1 + \frac{\partial f(X)}{\partial x_2} dx_2 + \cdots + \frac{\partial f(X)}{\partial x_n} dx_n$$

# Gradients of scalar functions with multi-variate inputs

- Consider $f(X) = f(x_1, x_2, \ldots, x_n)$



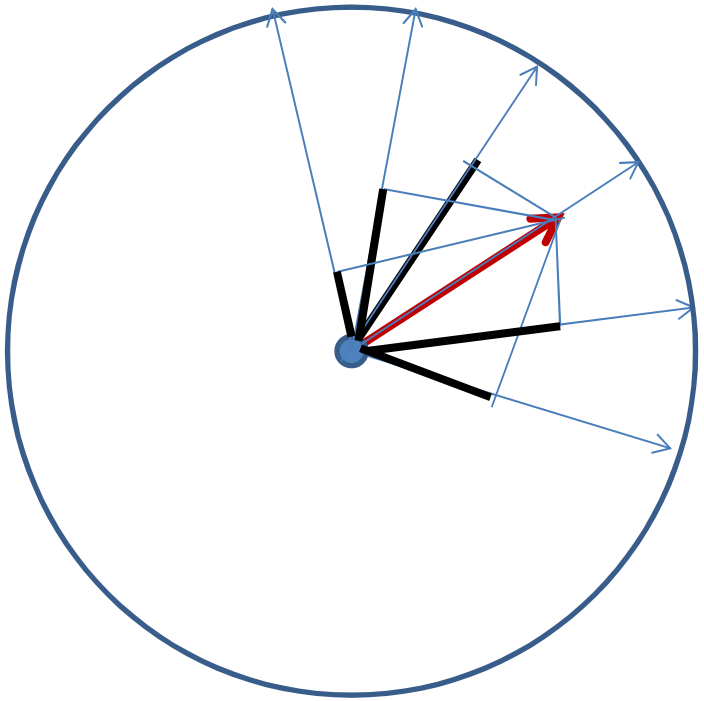
$$\nabla f(X) = \left[\frac{\partial f(X)}{\partial x_1} \quad \frac{\partial f(X)}{\partial x_2} \quad \ldots \quad \frac{\partial f(X)}{\partial x_n}\right]$$

- Check:

$$df(X) = \nabla f(X) dX$$

This is a vector inner product. To understand its behavior lets consider a well-known property of inner products

# A well-known vector property



$$\mathbf{u}^{\mathrm{T}}\mathbf{v} = |\mathbf{u}||\mathbf{v}|cos\theta$$

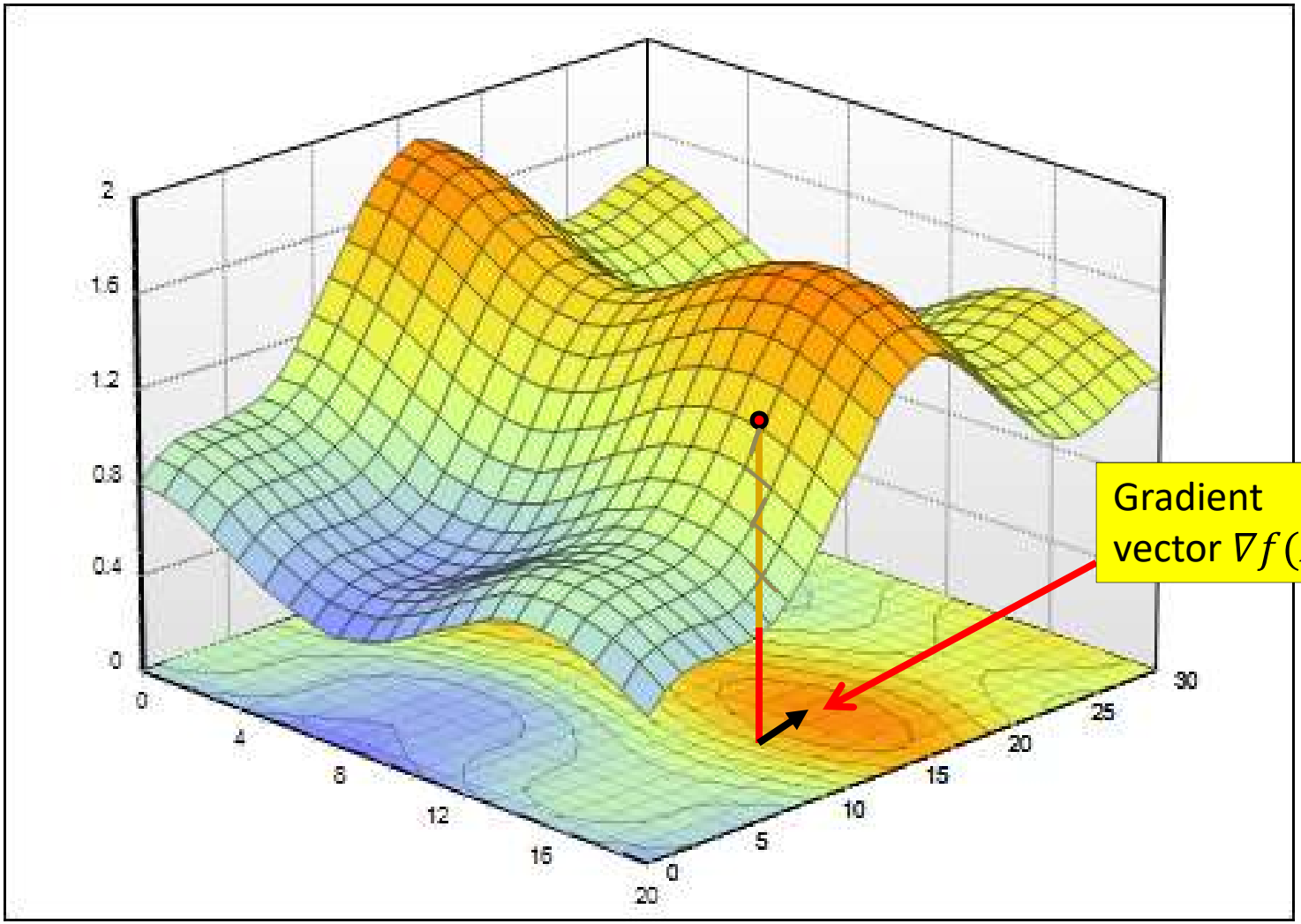
- The inner product between two vectors of fixed lengths is maximum when the two vectors are aligned
  - i.e. when $\theta = 0$

# Properties of Gradient

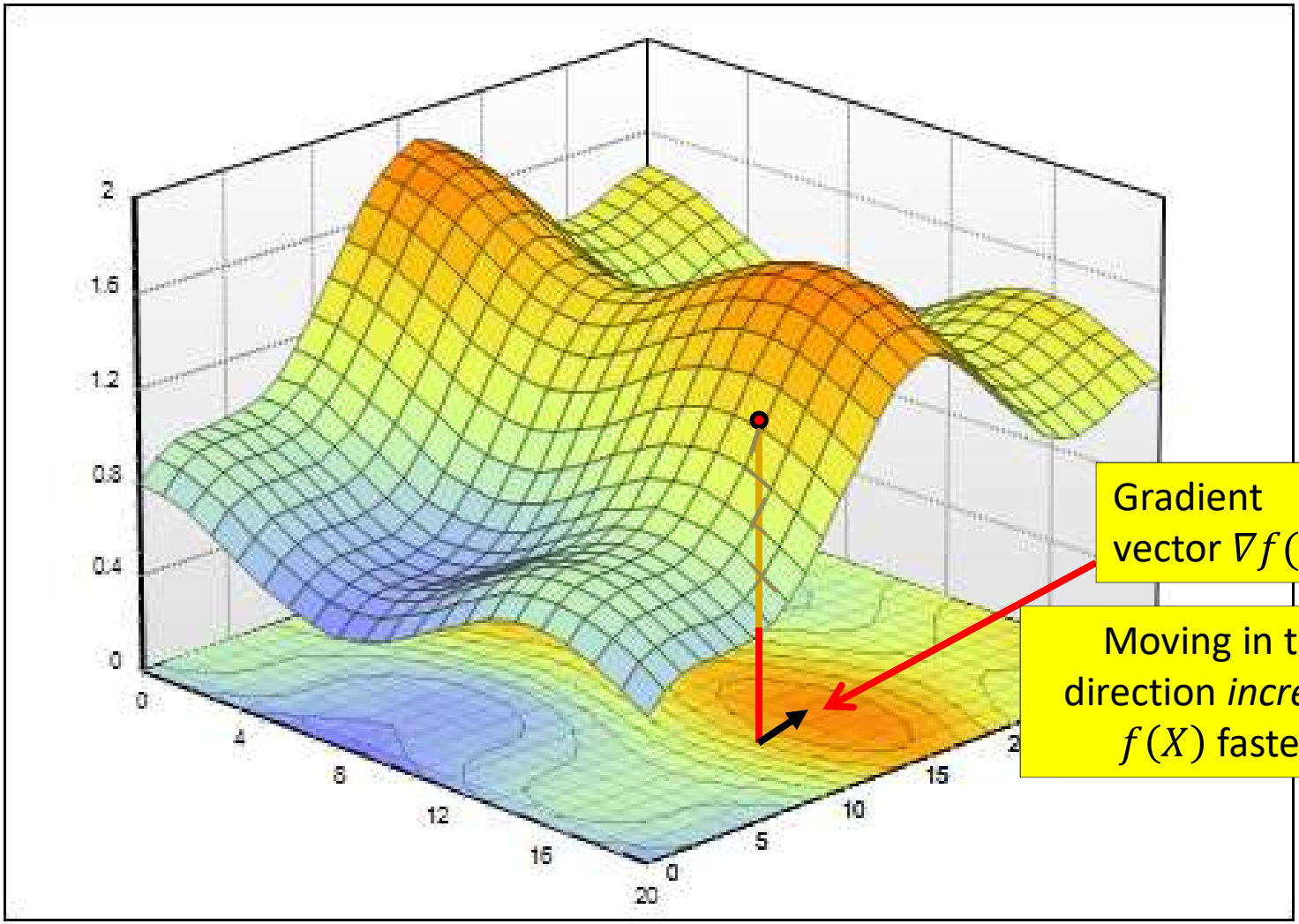
- $df(X) = \nabla f(X) dX$
  - The inner product between $\nabla f(X)$ and $dX$
- Fixing the length of $dX$
  - E.g. $|dX| = 1$
- $df(X)$ is max if $dX$ is aligned with $\nabla f(X)$
  - $\angle \nabla f(X), dX = 0$
  - The function $f(X)$ increases most rapidly if the input increment $dX$ is perfectly aligned to $\nabla f(X)$
- The gradient is the direction of fastest increase in $f(X)$

Some sloppy maths here, with apology – comparing row and column vectors

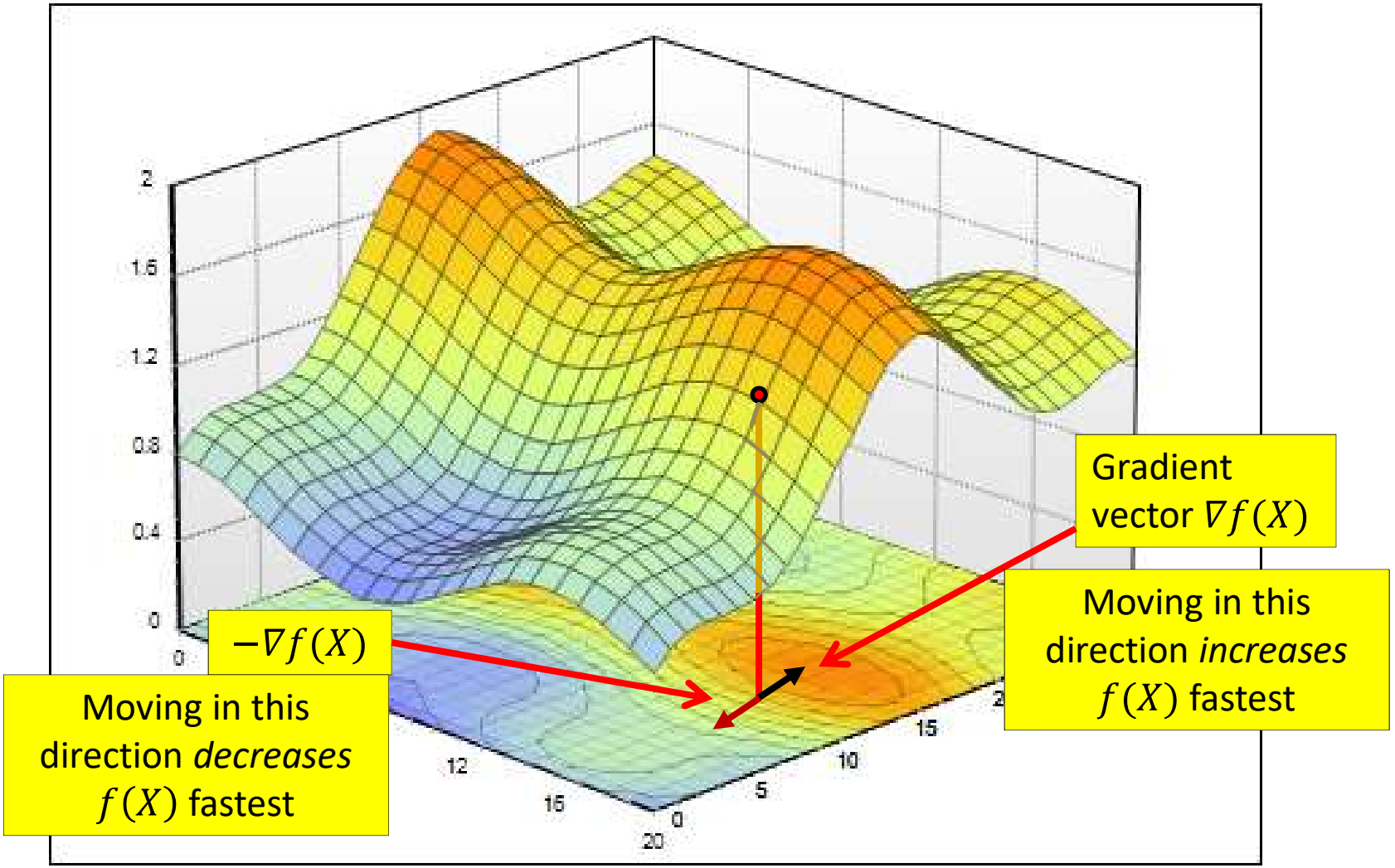
# Gradient


2
1.6
1.2
0.8
0.4
0
0
4
8
12
16
20
0
5
10
15
20
25
30
Gradient vector $\nabla f(X)$

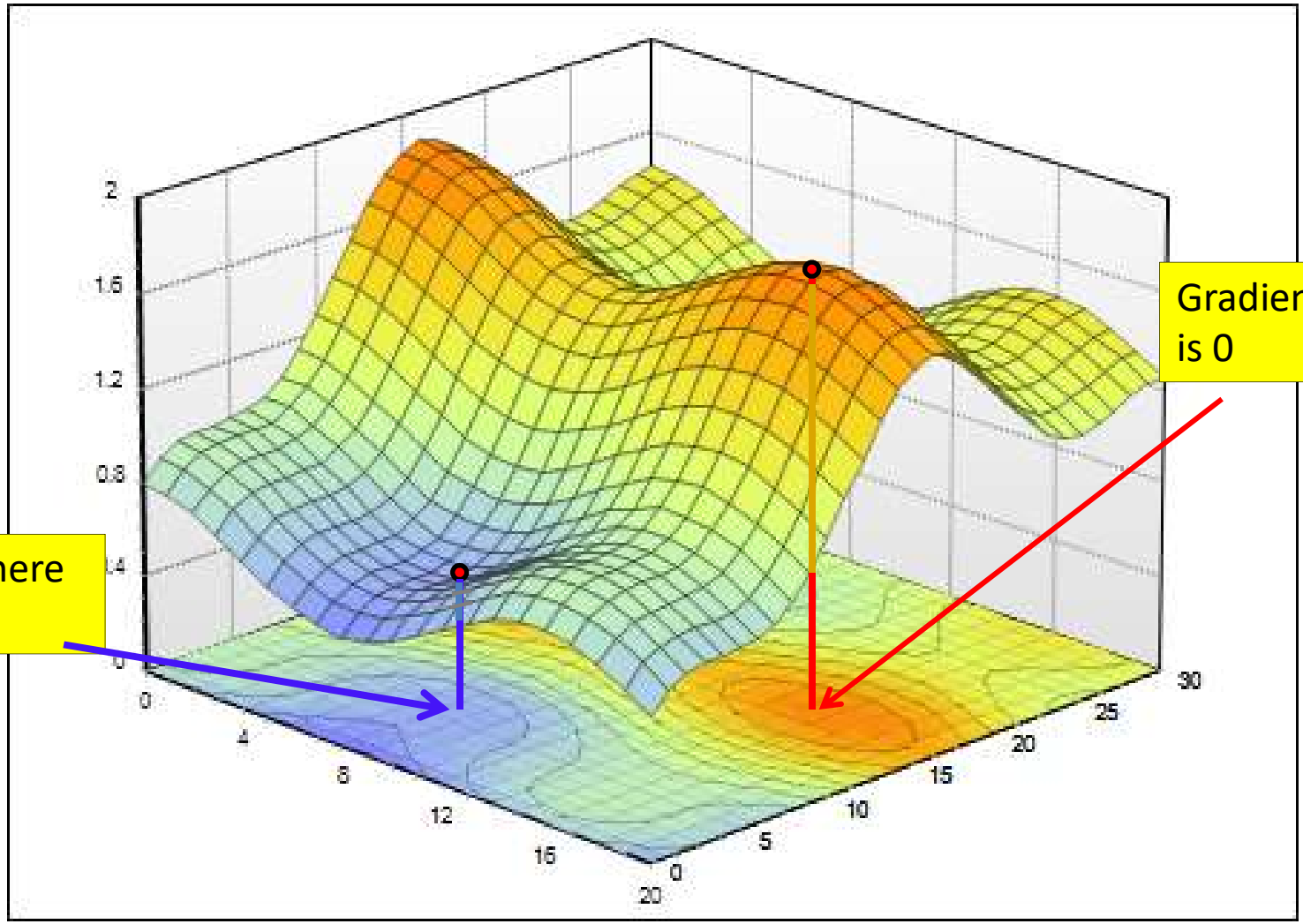
# Gradient


2
1.6
1.2
0.8
0.4
0
0
4
8
12
16
20
0
5
10
15
Gradient vector $\nabla f(X)$
Moving in this direction *increases* $f(X)$ fastest

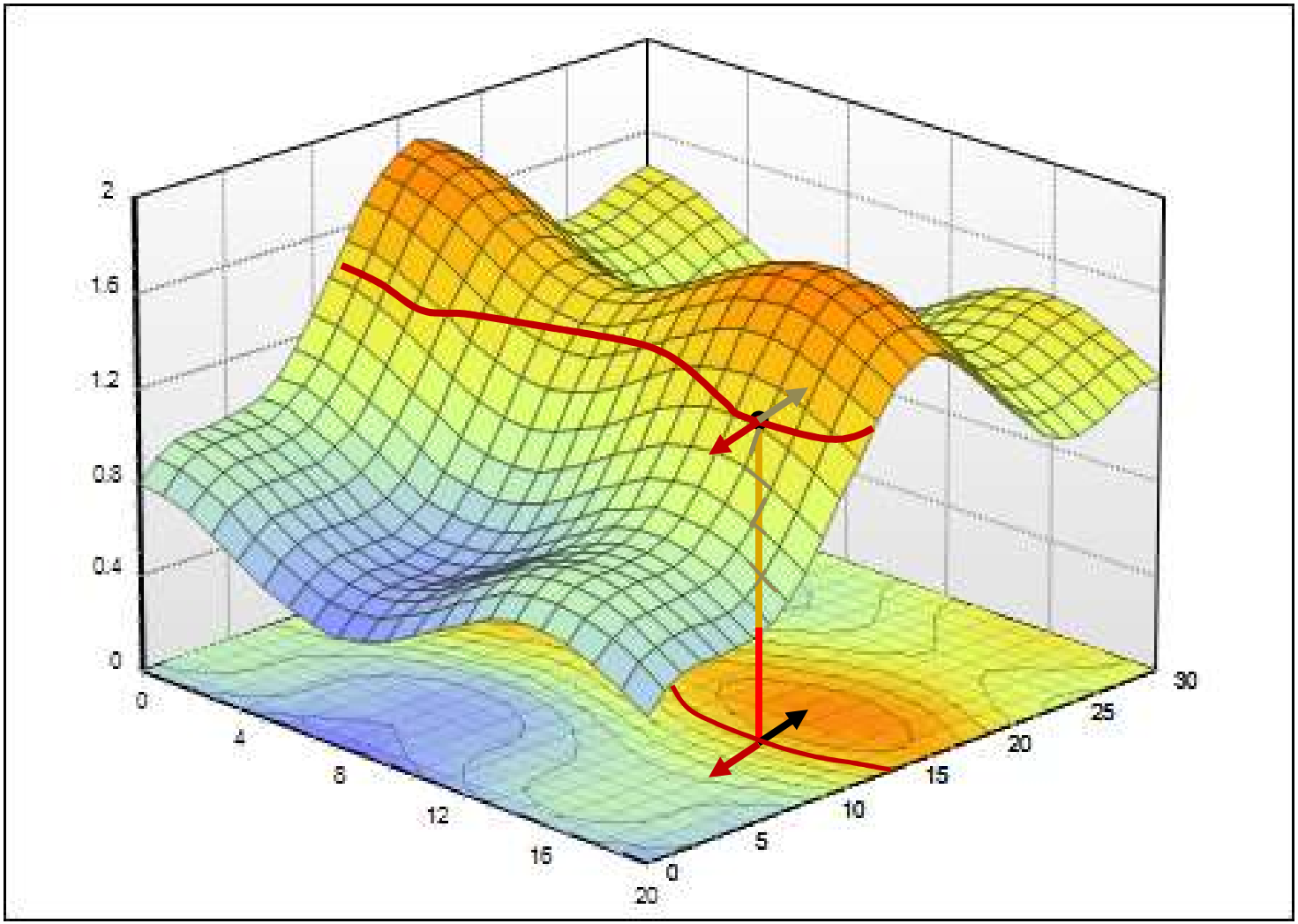
# Gradient


Gradient vector $\nabla f(X)$
Moving in this direction *increases* $f(X)$ fastest
$-\nabla f(X)$
Moving in this direction *decreases* $f(X)$ fastest

# Gradient


Gradient here is 0
Gradient here is 0
2
1.6
1.2
0.8
0
4
8
12
16
20
0
5
10
15
20
25
30

# Properties of Gradient: 2




- The gradient vector $\nabla f(X)$ is perpendicular to the level curve

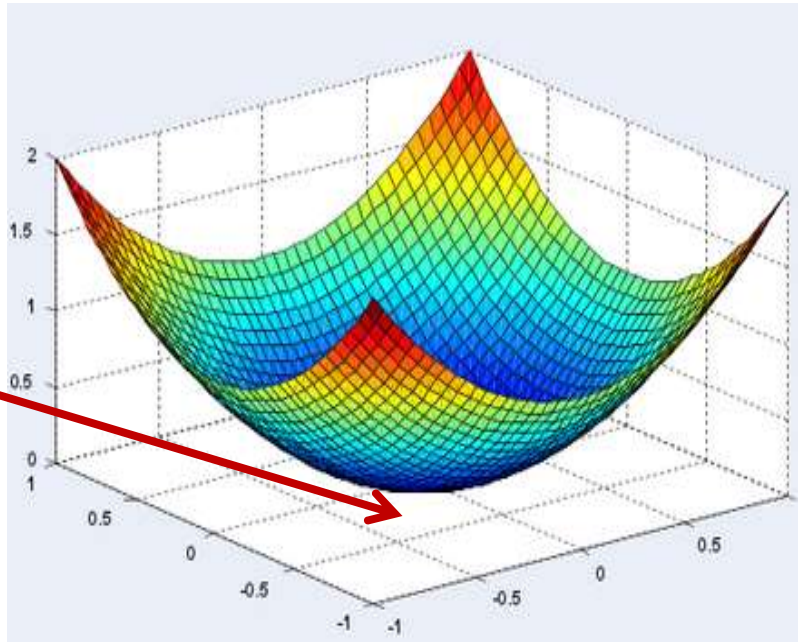
# The Hessian

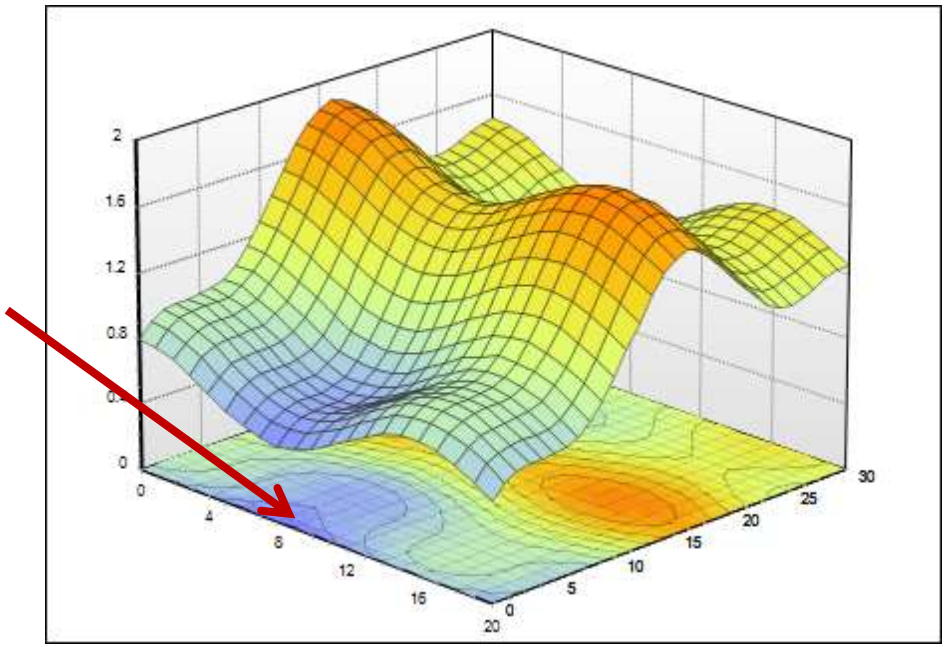
- The Hessian of a function $f(x_1, x_2, \ldots, x_n)$ is given by the second derivative

$$\nabla^2 f(x_1,\ldots,x_n) := \begin{bmatrix} \frac{\partial^2 f}{\partial x_1^2} & \frac{\partial^2 f}{\partial x_1 \partial x_2} & \cdots & \frac{\partial^2 f}{\partial x_1 \partial x_n} \\ \frac{\partial^2 f}{\partial x_2 \partial x_1} & \frac{\partial^2 f}{\partial x_2^2} & \cdots & \frac{\partial^2 f}{\partial x_2 \partial x_n} \\ \vdots & \vdots & \ddots & \vdots \\ \frac{\partial^2 f}{\partial x_n \partial x_1} & \frac{\partial^2 f}{\partial x_n \partial x_2} & \cdots & \frac{\partial^2 f}{\partial x_n^2} \end{bmatrix}$$

# Returning to direct optimization…

# Finding the minimum of a scalar function of a multi-variate input




- The optimum point is a turning point – the gradient will be 0

# Unconstrained Minimization of function (Multivariate)

1. Solve for the $X$ where the gradient equation equals to zero

$$\nabla f(X) = 0$$

2. Compute the Hessian Matrix $\nabla^2 f(X)$ at the candidate solution and verify that
   - Hessian is positive definite (eigenvalues positive) -> to identify local minima
   - Hessian is negative definite (eigenvalues negative) -> to identify local maxima

# Unconstrained Minimization of function (Example)

- Minimize

$$f(x_1, x_2, x_3) = (x_1)^2 + x_1(1 - x_2) - (x_2)^2 - x_2 x_3 + (x_3)^2 + x_3$$

- Gradient

$$\nabla f = \begin{bmatrix} 2x_1 + 1 - x_2 \\ -x_1 + 2x_2 - x_3 \\ -x_2 + 2x_3 + 1 \end{bmatrix}^T$$

# Unconstrained Minimization of function (Example)

- Set the gradient to null

$$\nabla f = 0 \Rightarrow \begin{bmatrix} 2x_1 + 1 - x_2 \\ -x_1 + 2x_2 - x_3 \\ -x_2 + 2x_3 + 1 \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \\ 0 \end{bmatrix}$$

- Solving the 3 equations system with 3 unknowns

$$x = \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} = \begin{bmatrix} -1 \\ -1 \\ -1 \end{bmatrix}$$

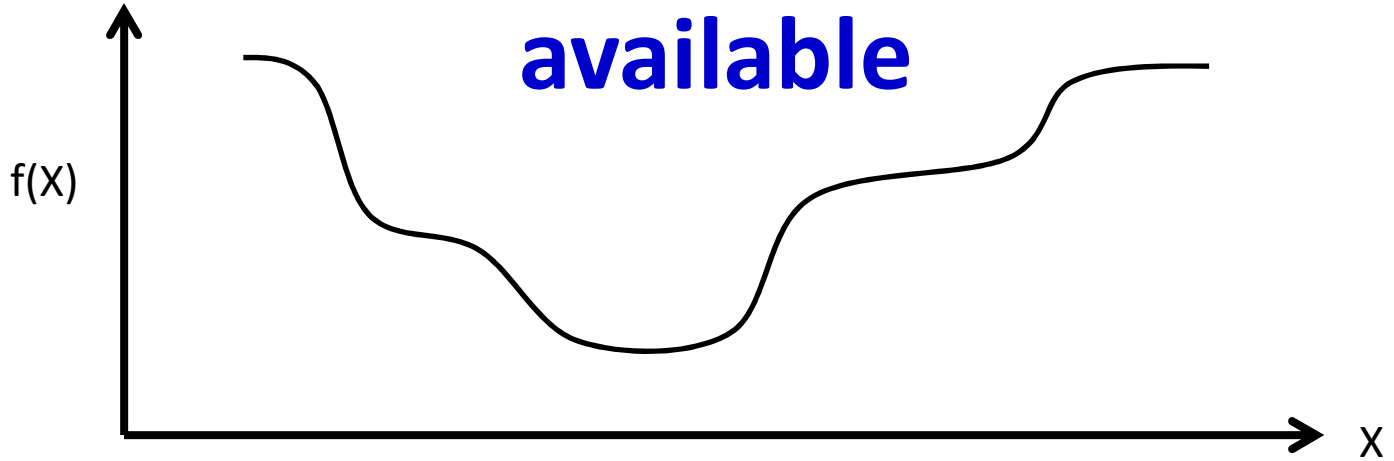
# Unconstrained Minimization of function (Example)

- Compute the Hessian matrix $\nabla^2 f = \begin{bmatrix} 2 & -1 & 0 \\ -1 & 2 & -1 \\ 0 & -1 & 2 \end{bmatrix}$
- Evaluate the eigenvalues of the Hessian matrix

$$\lambda_1 = 3.414, \quad \lambda_2 = 0.586, \quad \lambda_3 = 2$$

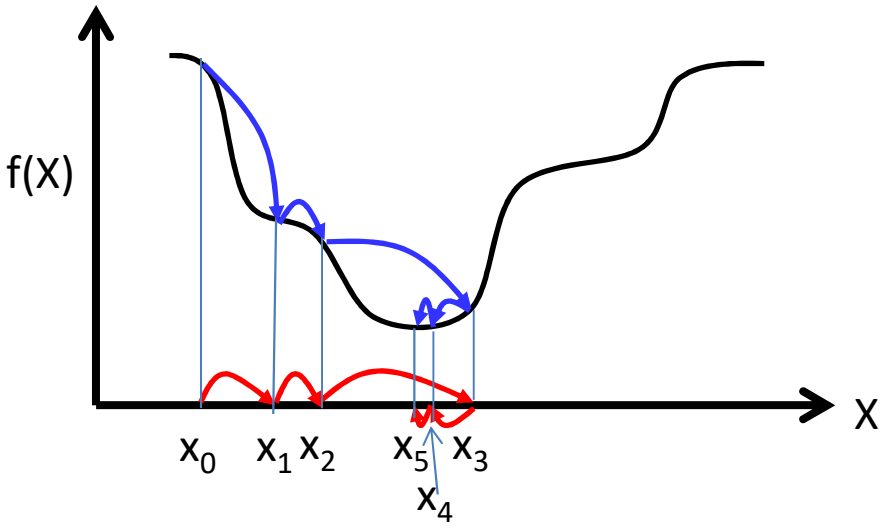
- All the eigenvalues are positives => the Hessian matrix is positive definite
- The point $x = \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} = \begin{bmatrix} -1 \\ -1 \\ -1 \end{bmatrix}$ is a minimum

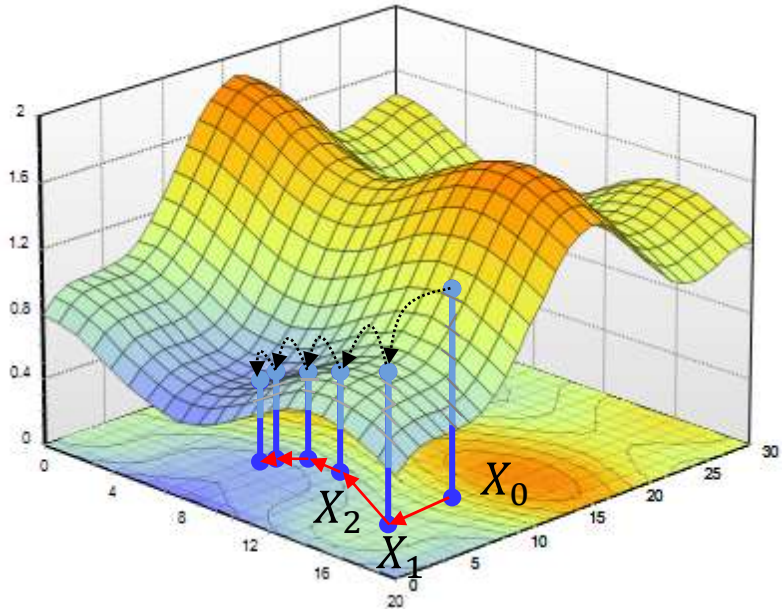
# Closed Form Solutions are not always available




- Often it is not possible to simply solve $\nabla f(X) = 0$
  - The function to minimize/maximize may have an intractable form
- In these situations, iterative solutions are used
  - Begin with a "guess" for the optimal $X$ and refine it iteratively until the correct value is obtained

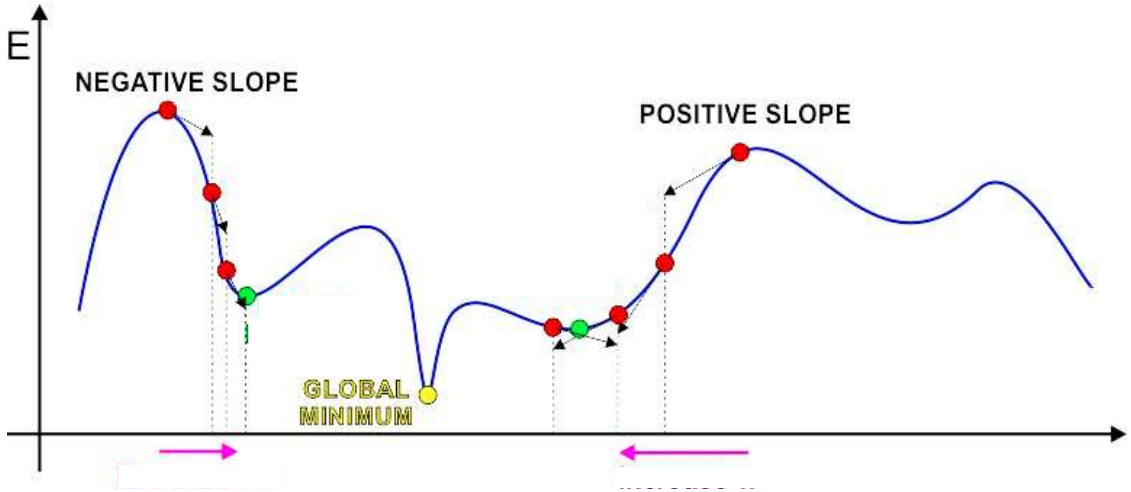
# Iterative solutions



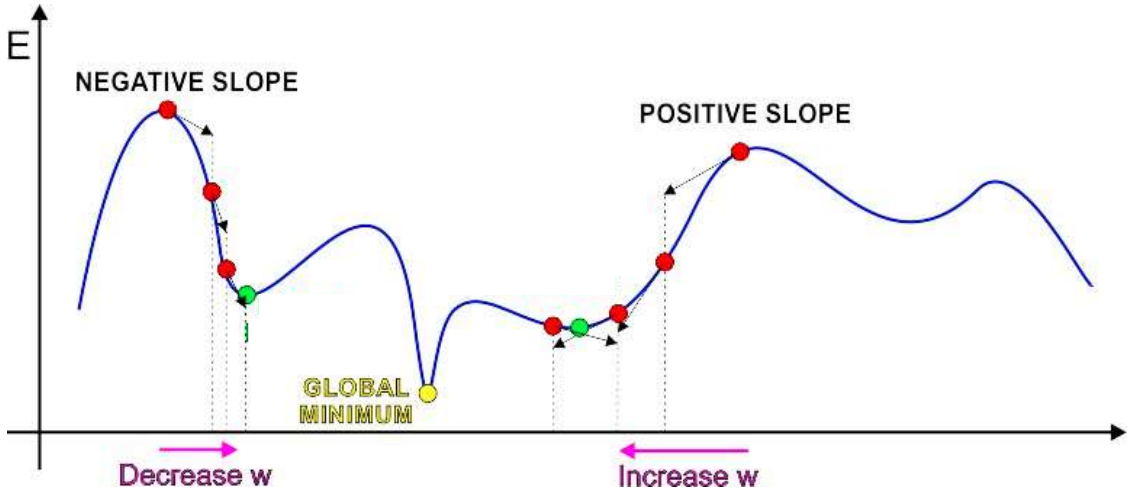

- Iterative solutions
  - Start from an initial guess $X_0$ for the optimal $X$
  - Update the guess towards a (hopefully) "better" value of $\mathrm{f}(X)$
  - Stop when $\mathrm{f}(X)$ no longer decreases
- Problems:
  - Which direction to step in
  - How big must the steps be

# The Approach of Gradient Descent




- Iterative solution:
  - Start at some point
  - Find direction in which to shift this point to decrease error
    - This can be found from the derivative of the function
      - A positive derivative → moving left decreases error
      - A negative derivative → moving right decreases error
  - Shift point in this direction

# The Approach of Gradient Descent




- Iterative solution: Trivial algorithm
  - Initialize $x^0$
  - While $f'(x^k) \neq 0$
    - If $sign\left(f'(x^k)\right)$ is positive:

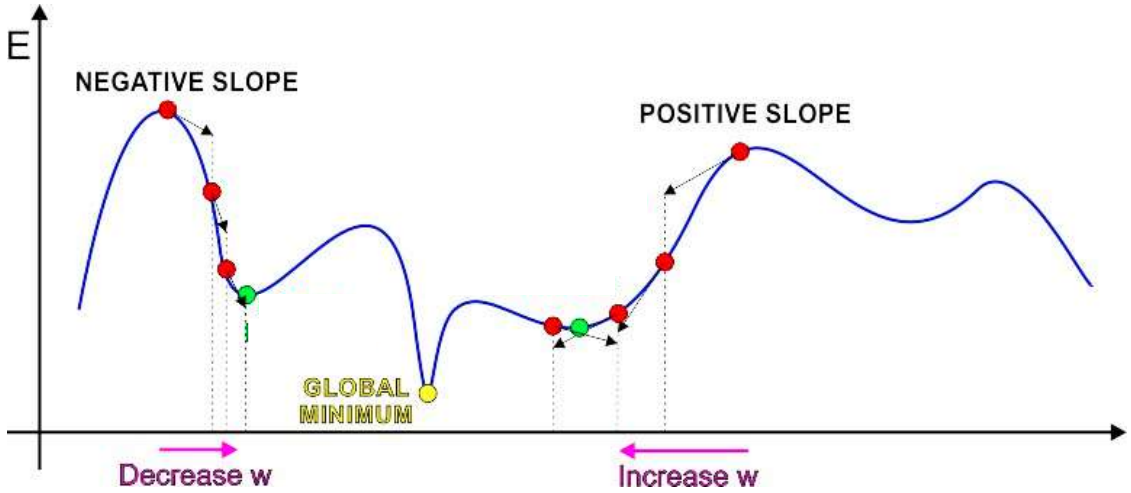
$$x^{k+1} = x^k - step$$

    - Else

$$x^{k+1} = x^k + step$$

  - What must step be to ensure we actually get to the optimum?

# The Approach of Gradient Descent

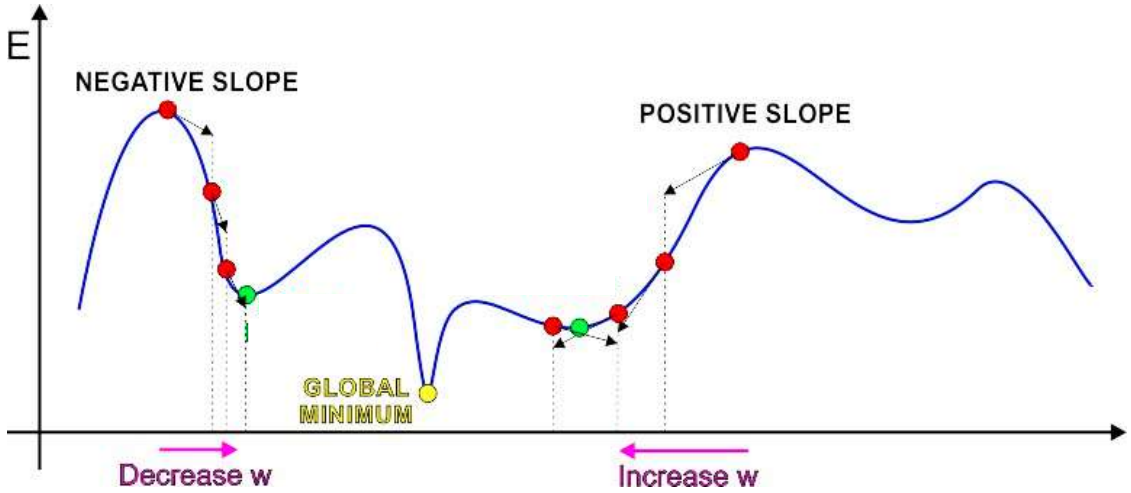



- Iterative solution: Trivial algorithm
  - Initialize $x^0$
  - While $f'(x^k) \neq 0$

$$x^{k+1} = x^k - sign\left(f'(x^k)\right).step$$

- Identical to previous algorithm

# The Approach of Gradient Descent




- Iterative solution: Trivial algorithm
  - Initialize $x^0$
  - While $f'(x^k) \neq 0$

$$x^{k+1} = x^k - \eta^k f'(x^k)$$

- $\eta^k$ is the "step size"

# Gradient descent/ascent (multivariate)

- The gradient descent/ascent method to find the minimum or maximum of a function $f$ iteratively
  - To find a *maximum* move *in the direction of the gradient*

$$x^{k+1} = x^k + \eta^k \nabla f\left(x^k\right)^T$$

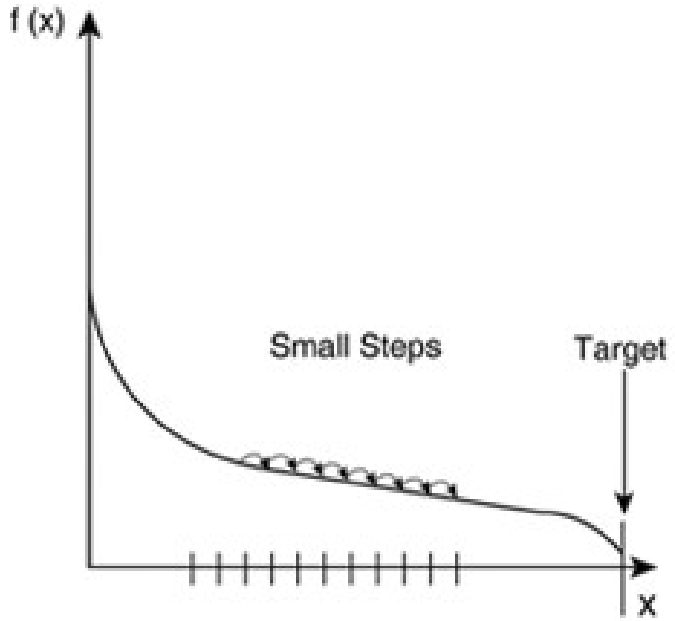
  - To find a *minimum* move *exactly opposite the direction of the gradient*

$$x^{k+1} = x^k - \eta^k \nabla f\left(x^k\right)^T$$

- Many solutions to choosing step size $\eta^k$

# 1. Fixed step size

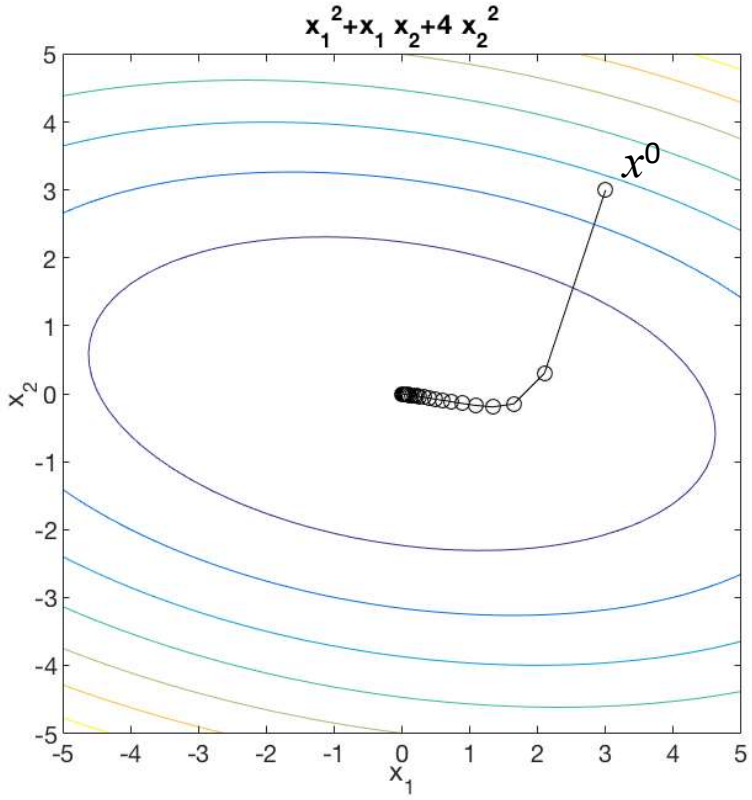
- Fixed step size
  - Use fixed value for $\eta^k$



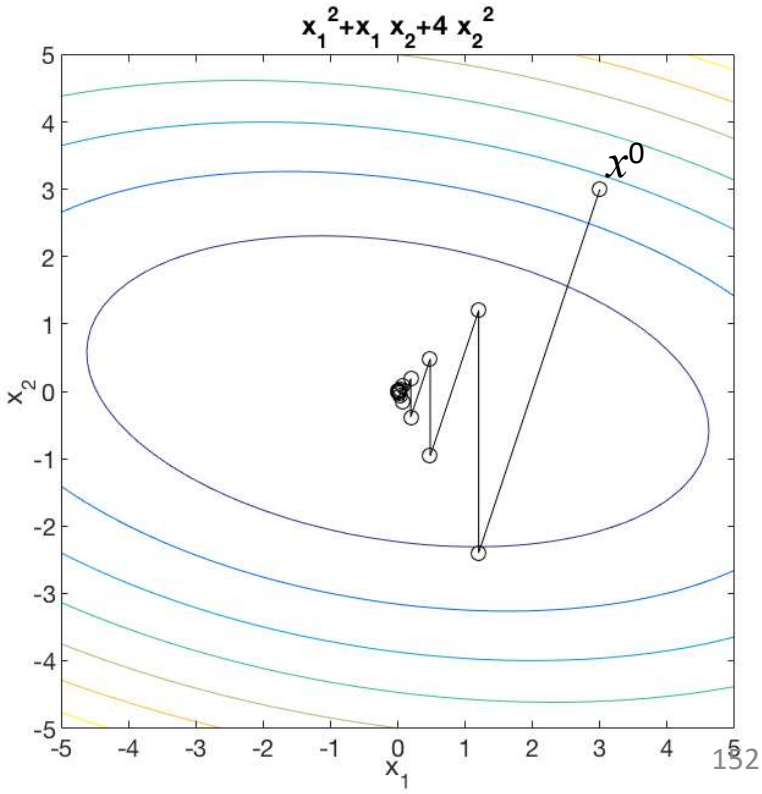
# Influence of step size example (constant step size)

$$f(x_1, x_2) = (x_1)^2 + x_1 x_2 + 4(x_2)^2 \qquad x^{initial} = \begin{bmatrix} 3 \\ 3 \end{bmatrix}$$

$\eta = 0.1$




$\eta = 0.2$



# What is the optimal step size?

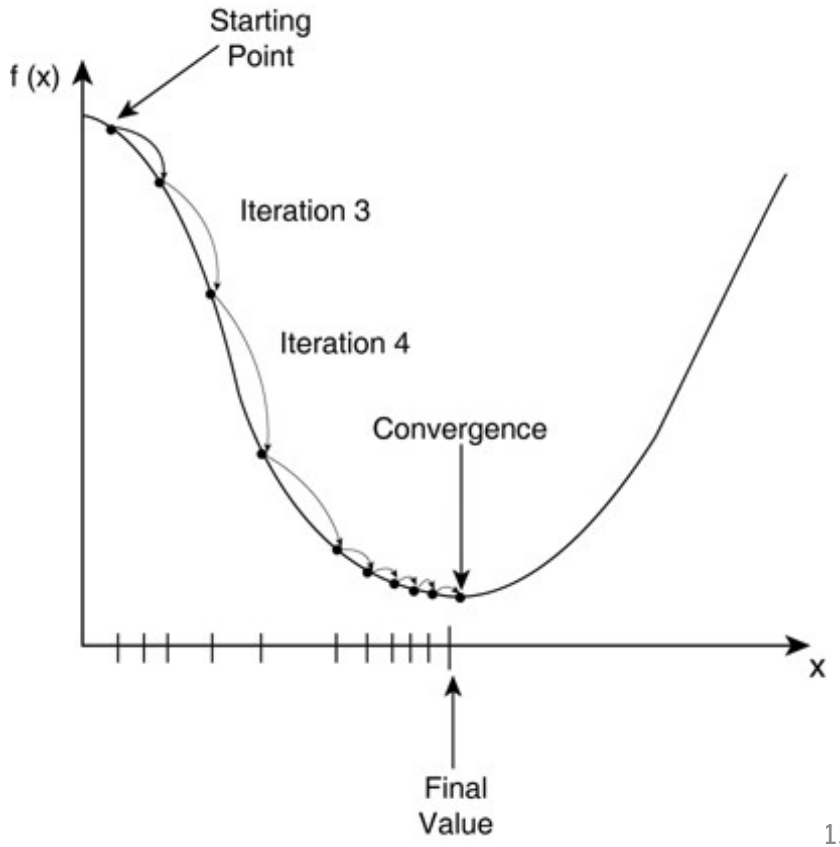
- Step size is critical for fast optimization
- Will revisit this topic later
- For now, simply assume a potentially-iteration-dependent step size

# Gradient descent convergence criteria

- The gradient descent algorithm converges when one of the following criteria is satisfied

$$\left| f(x^{k+1}) - f(x^k) \right| < \varepsilon_1$$

- Or $\left\| \nabla f(x^k) \right\| < \varepsilon_2$



# Overall Gradient Descent Algorithm

- Initialize:
  - $x^0$
  - $k = 0$

- While $\left|f\left(x^{k+1}\right) - f\left(x^k\right)\right| > \varepsilon$
  - $x^{k+1} = x^k - \eta^k \nabla f\left(x^k\right)^T$
  - $k = k + 1$

# Next up

- Gradient descent to train neural networks
- A.K.A.  Back propagation