Neural Networks
Learning the network: Part 1

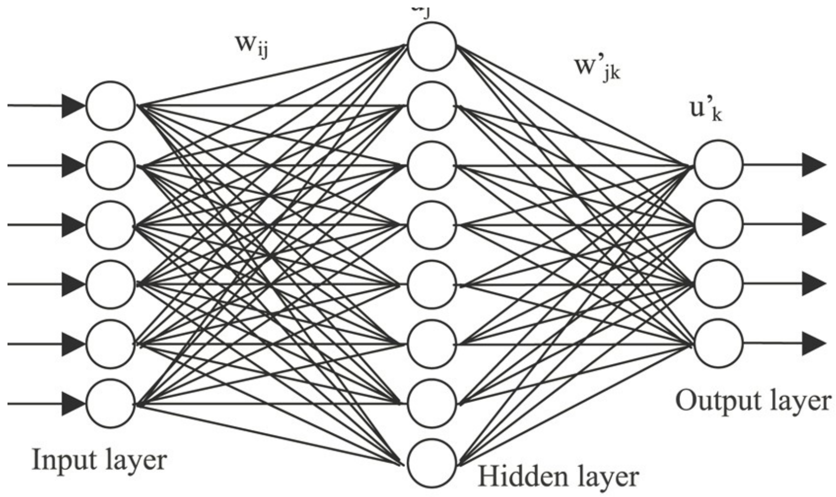
11-785, Fall 2020

Lecture 3

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

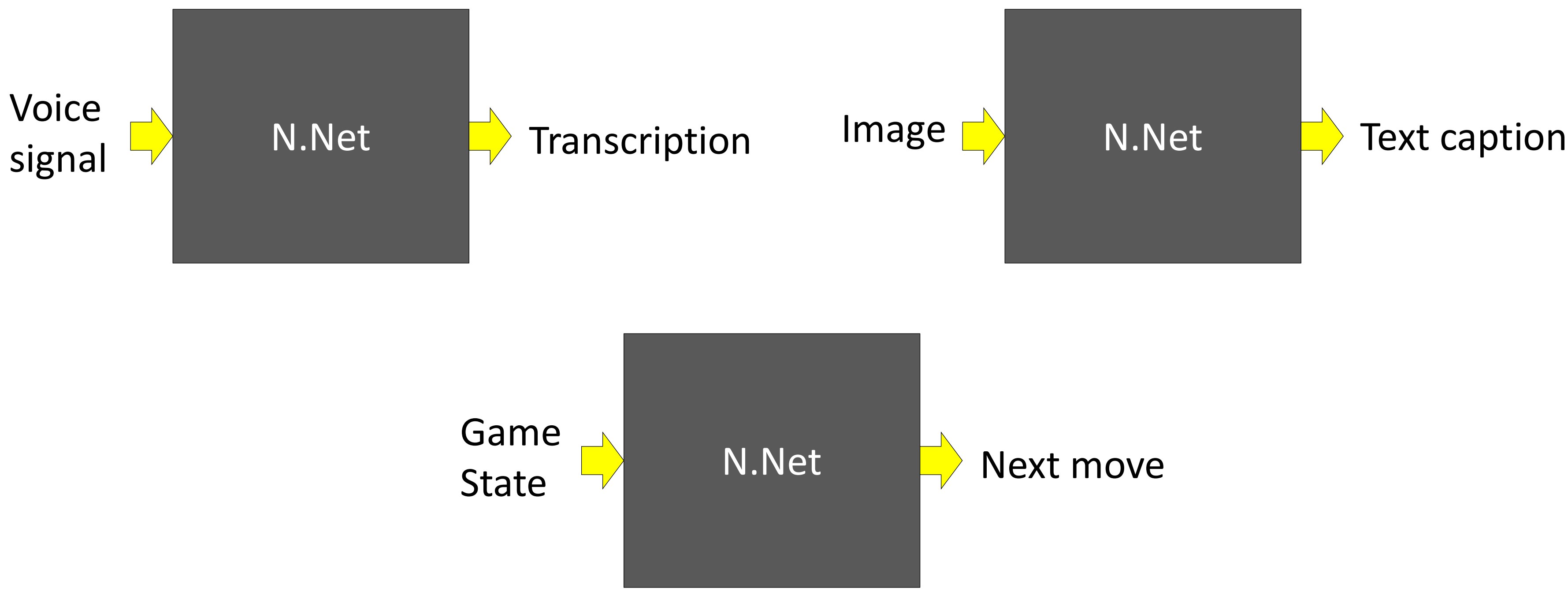
Recap



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

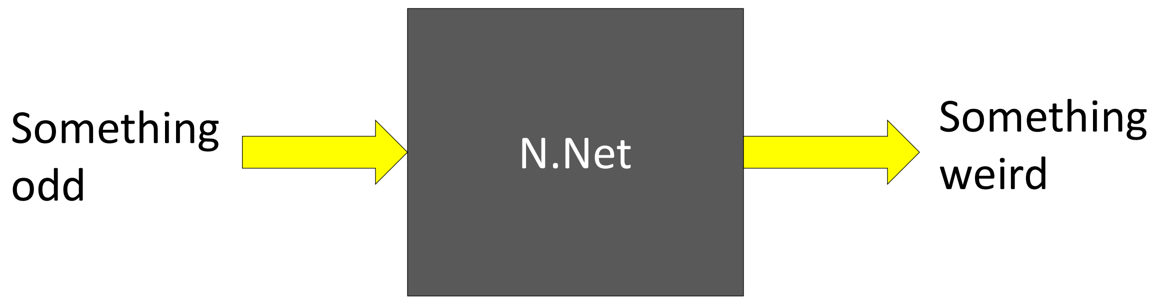
- *Provided the network satisfies minimal architecture constraints*
  - Networks with fewer than the required number of parameters can be very poor approximators

These boxes are functions



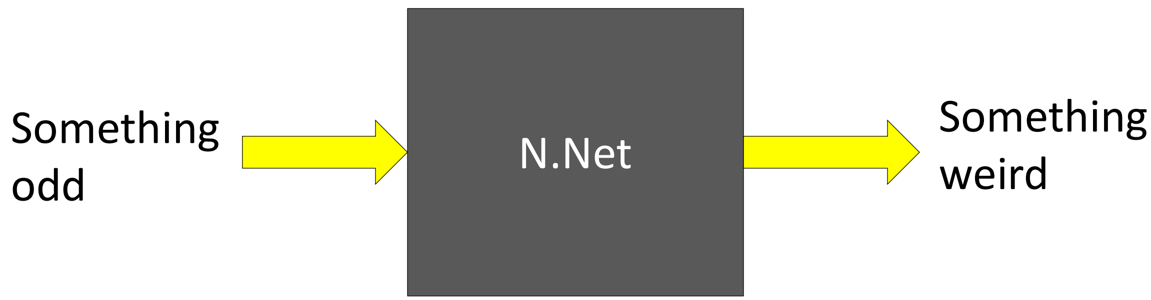
- Take an input
- Produce an output
- Can be modeled by a neural network!

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

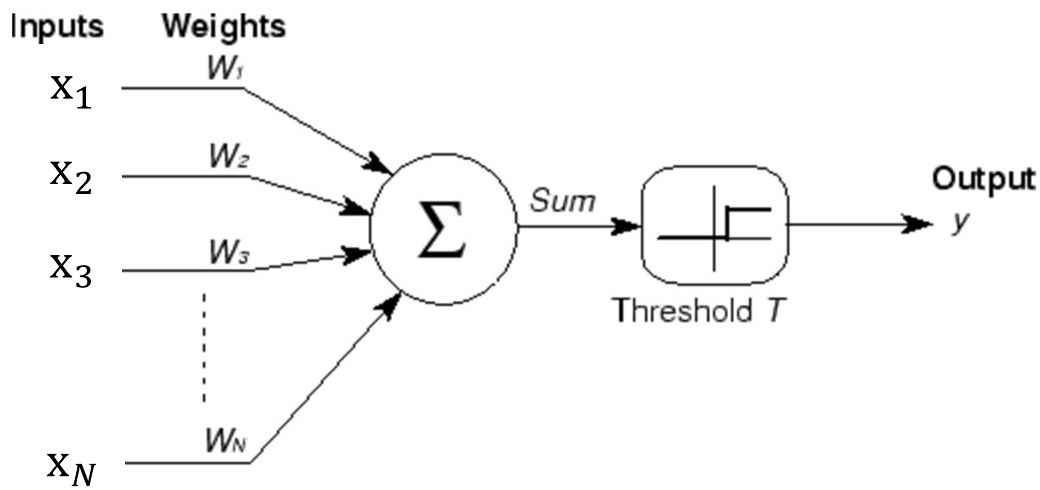


- Preliminaries:
  - How do we represent the input?
  - How do we represent the output?

A bit later in the program

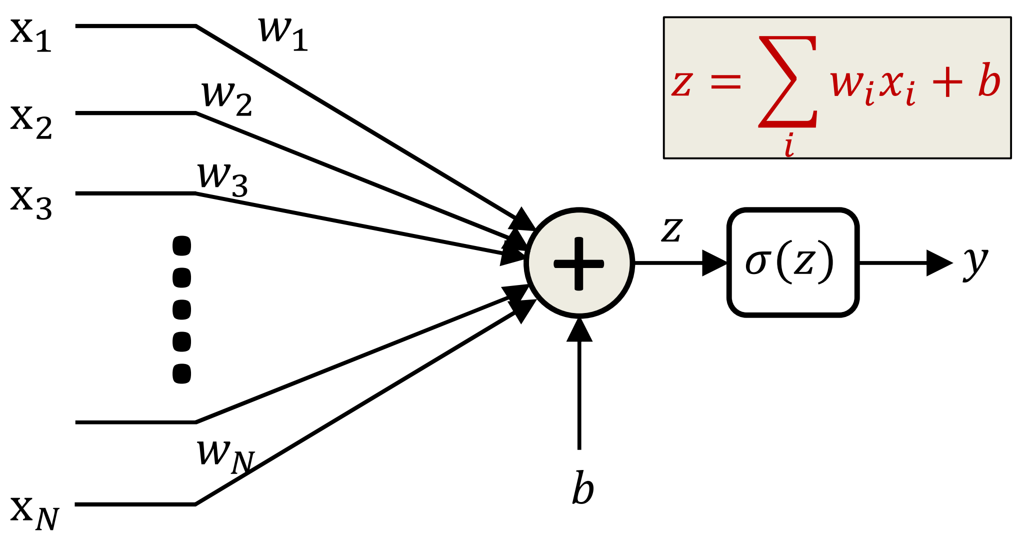
- *How do we compose the network that performs the requisite function?*

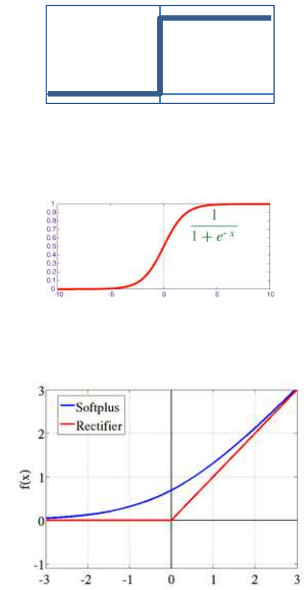
The original perceptron



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

Preliminaries: The units in the network – the perceptron

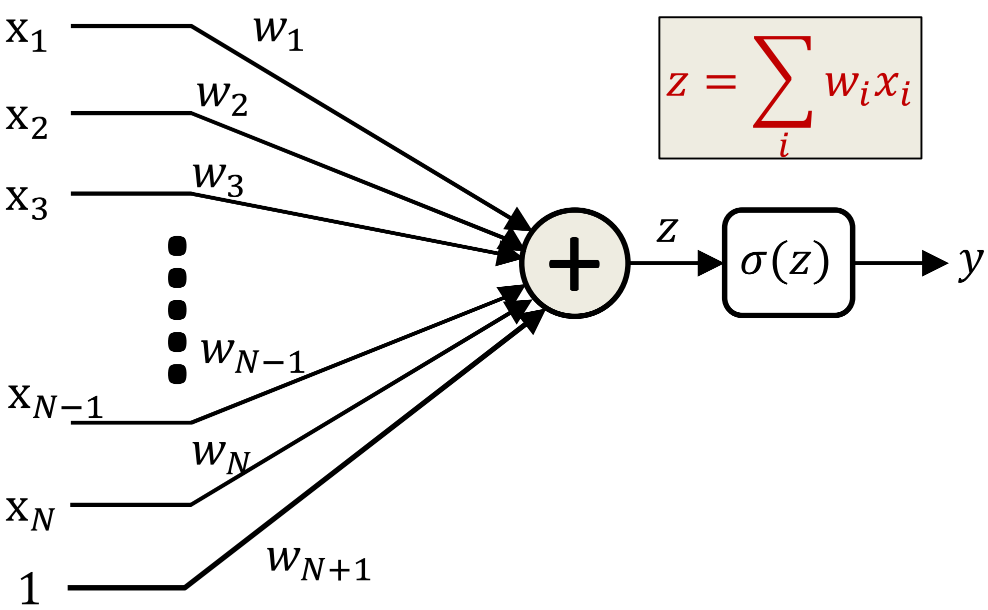


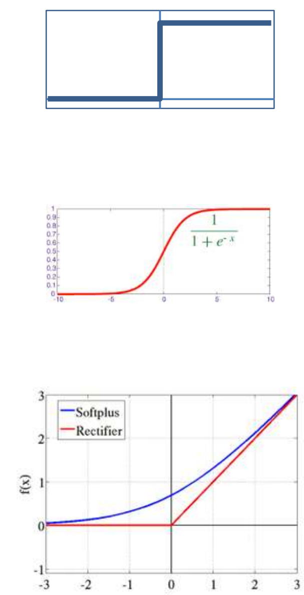


Activation functions $\sigma(z)$

- Perceptron
  - General setting, inputs are real valued
  - A *bias* b representing a threshold to trigger the perceptron
  - Activation functions are not necessarily threshold functions
- The parameters of the perceptron (which determine how it behaves) are its weights and bias

Preliminaries: Redrawing the neuron

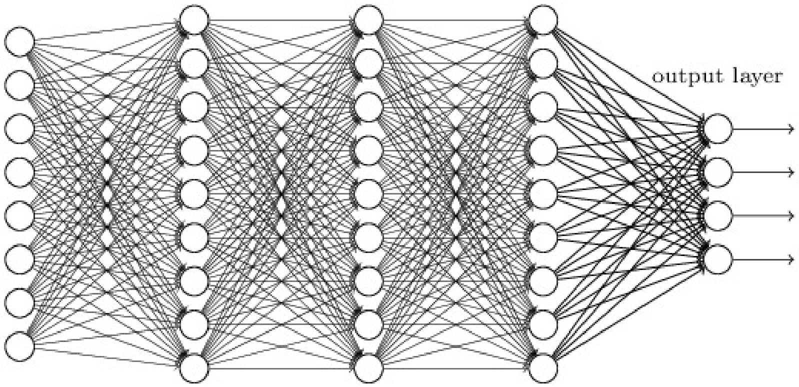


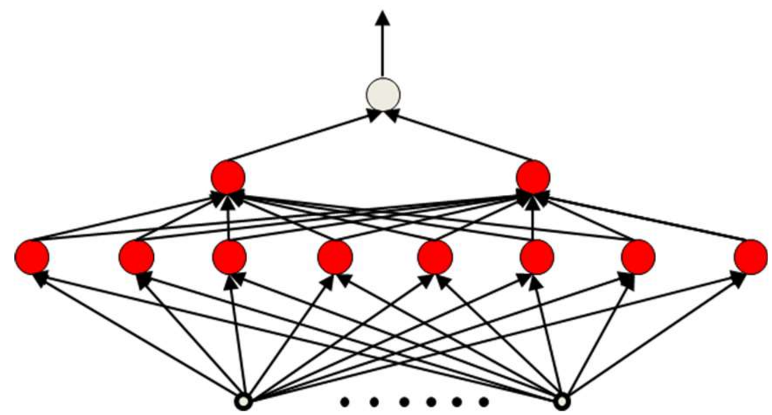


Activation functions $\sigma(z)$

- 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

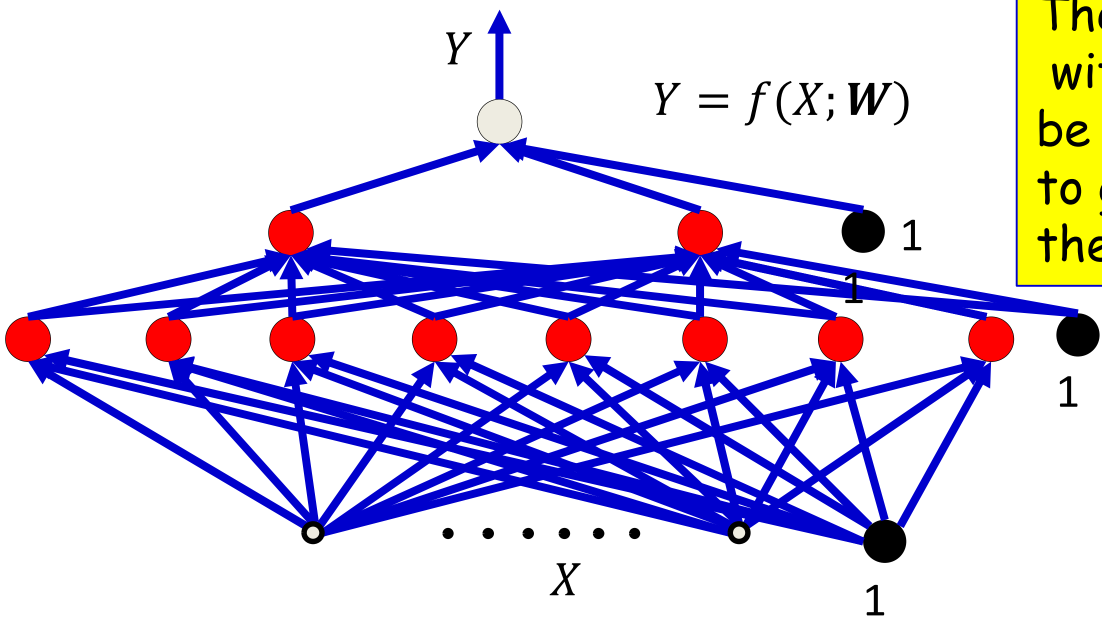
First: the structure of the network





- 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

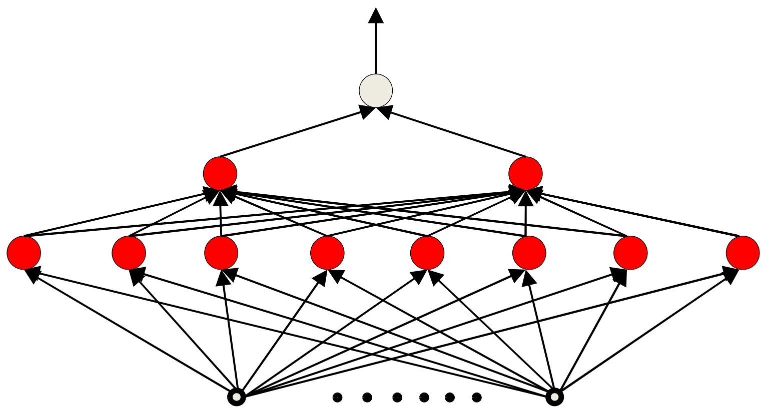


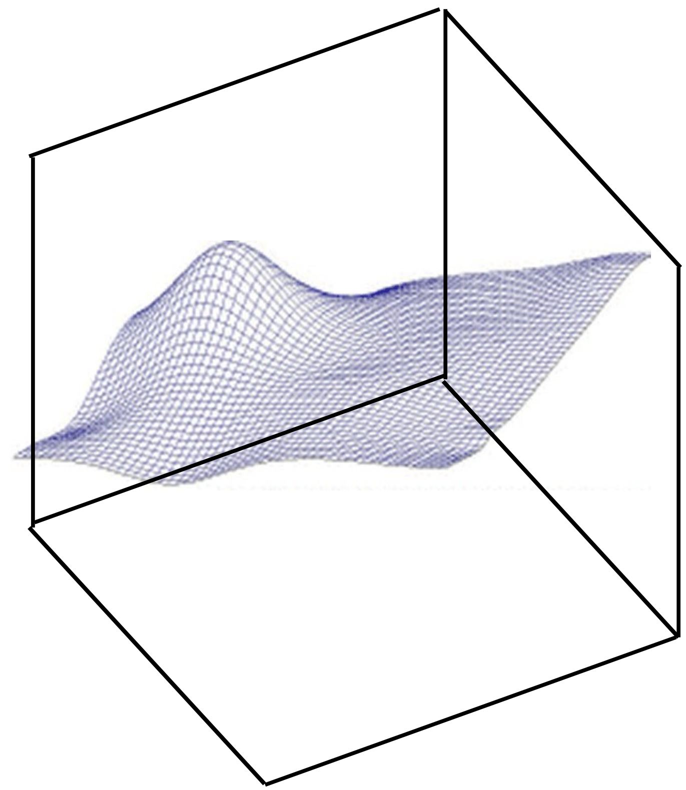
The network is a function f() with parameters W which must be set to the appropriate values to get the desired behavior from the net

- **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..

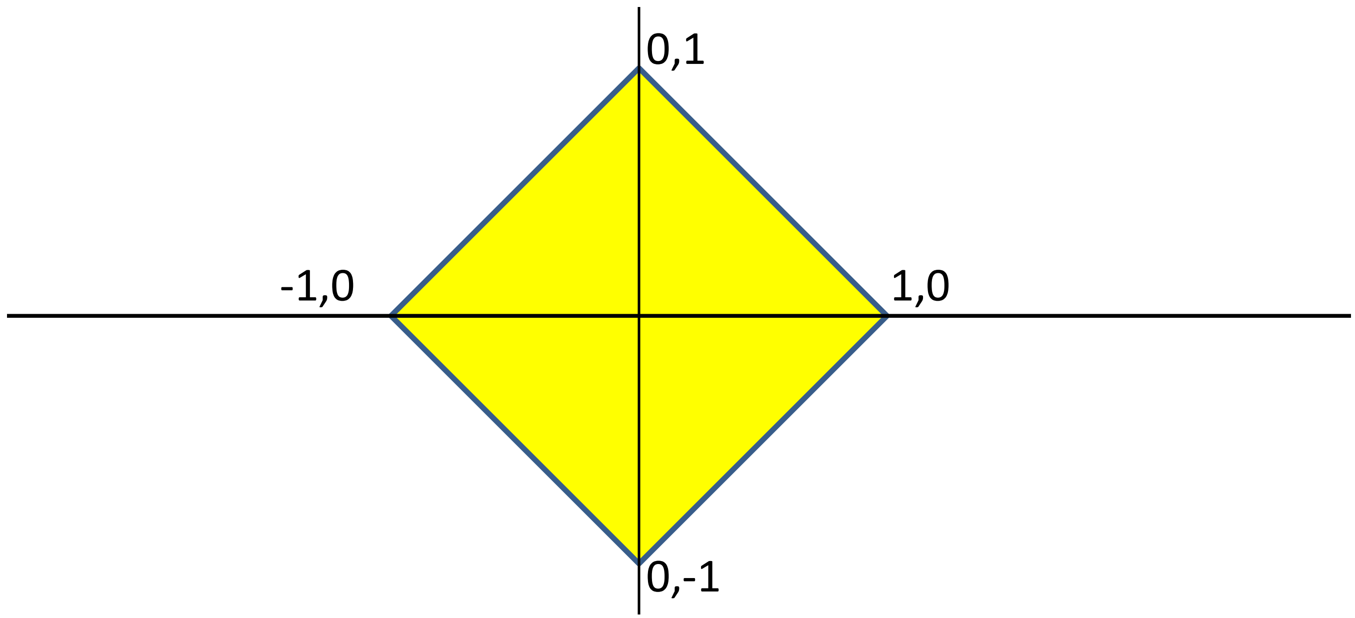
The MLP *can* represent anything





- 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

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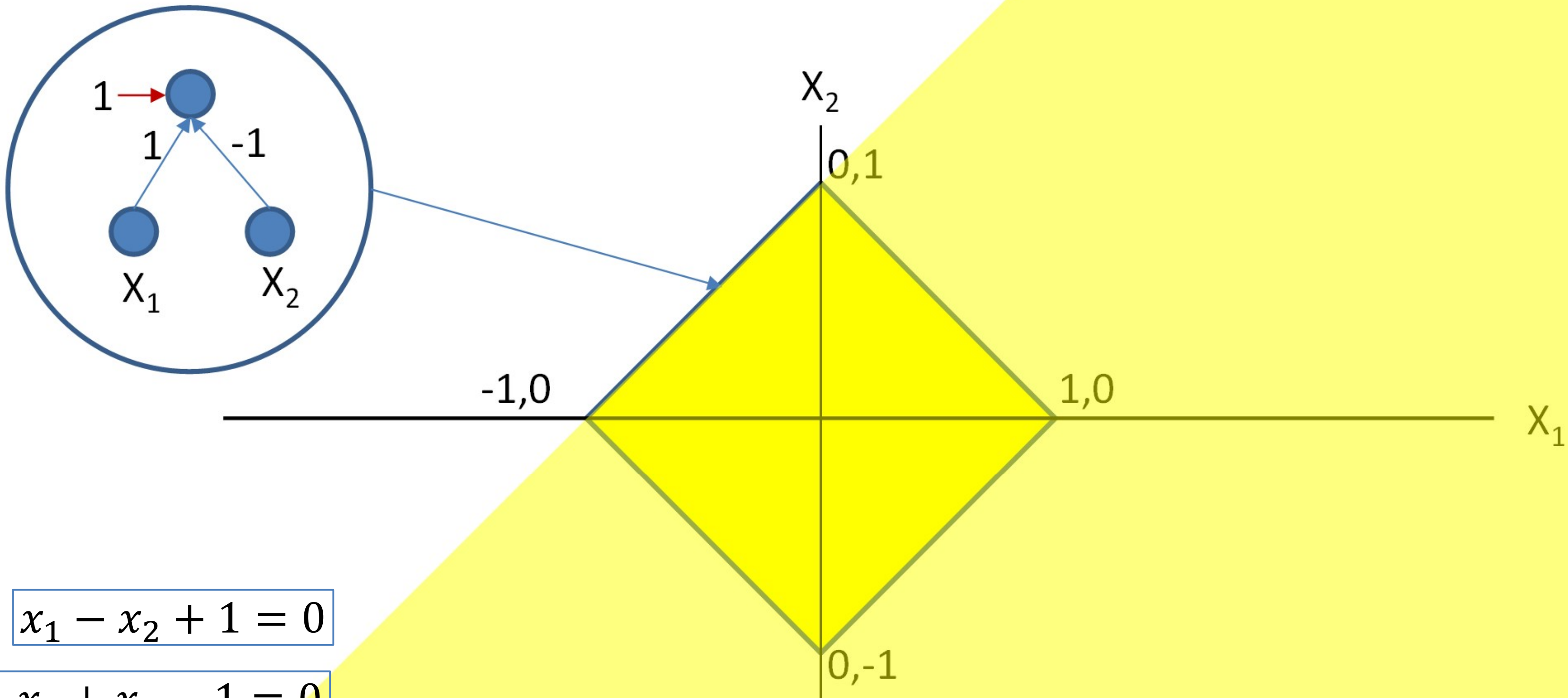

$$x_1 - x_2 + 1 = 0$$

$$-x_1 + x_2 - 1 = 0$$

Assuming simple perceptrons:
output = 1 if $\sum_i w_i x_i + b_i \geq 0, else\ 0$

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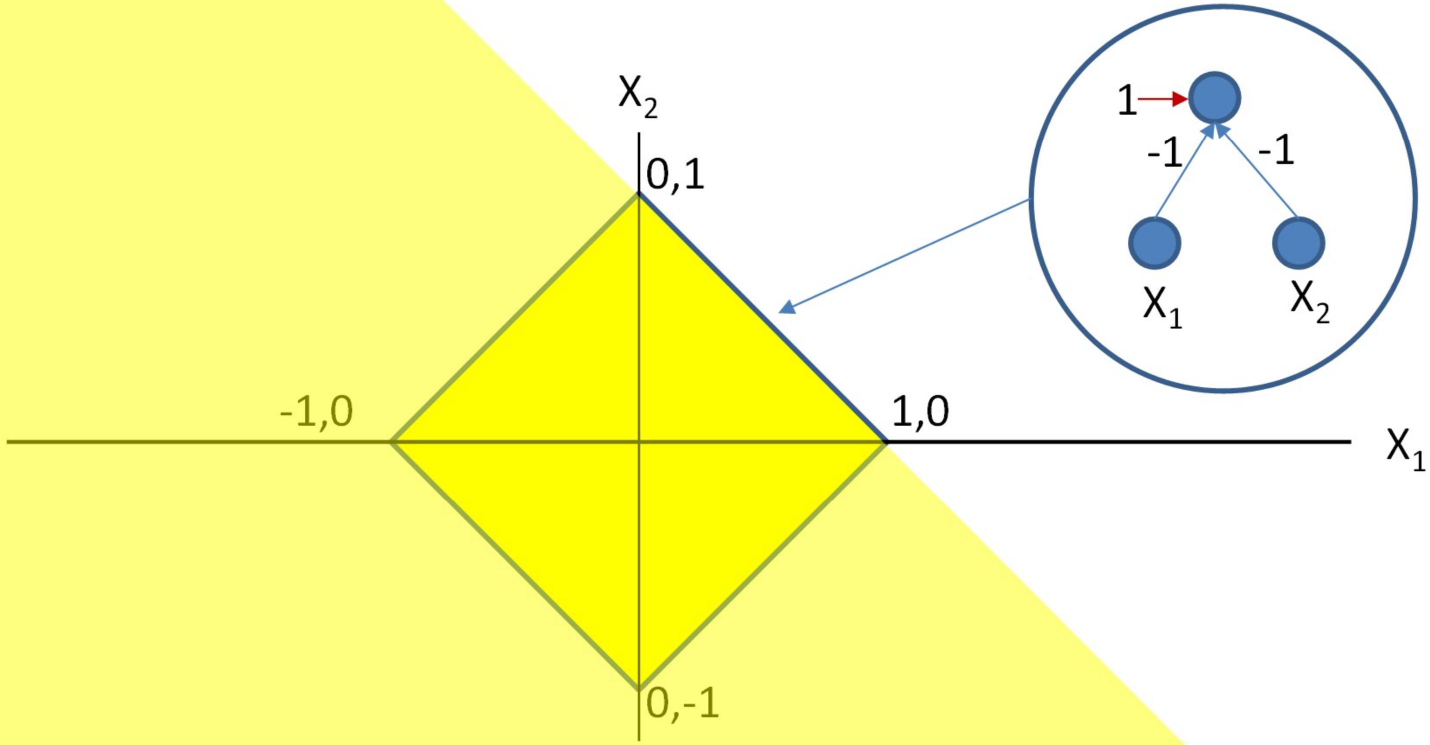

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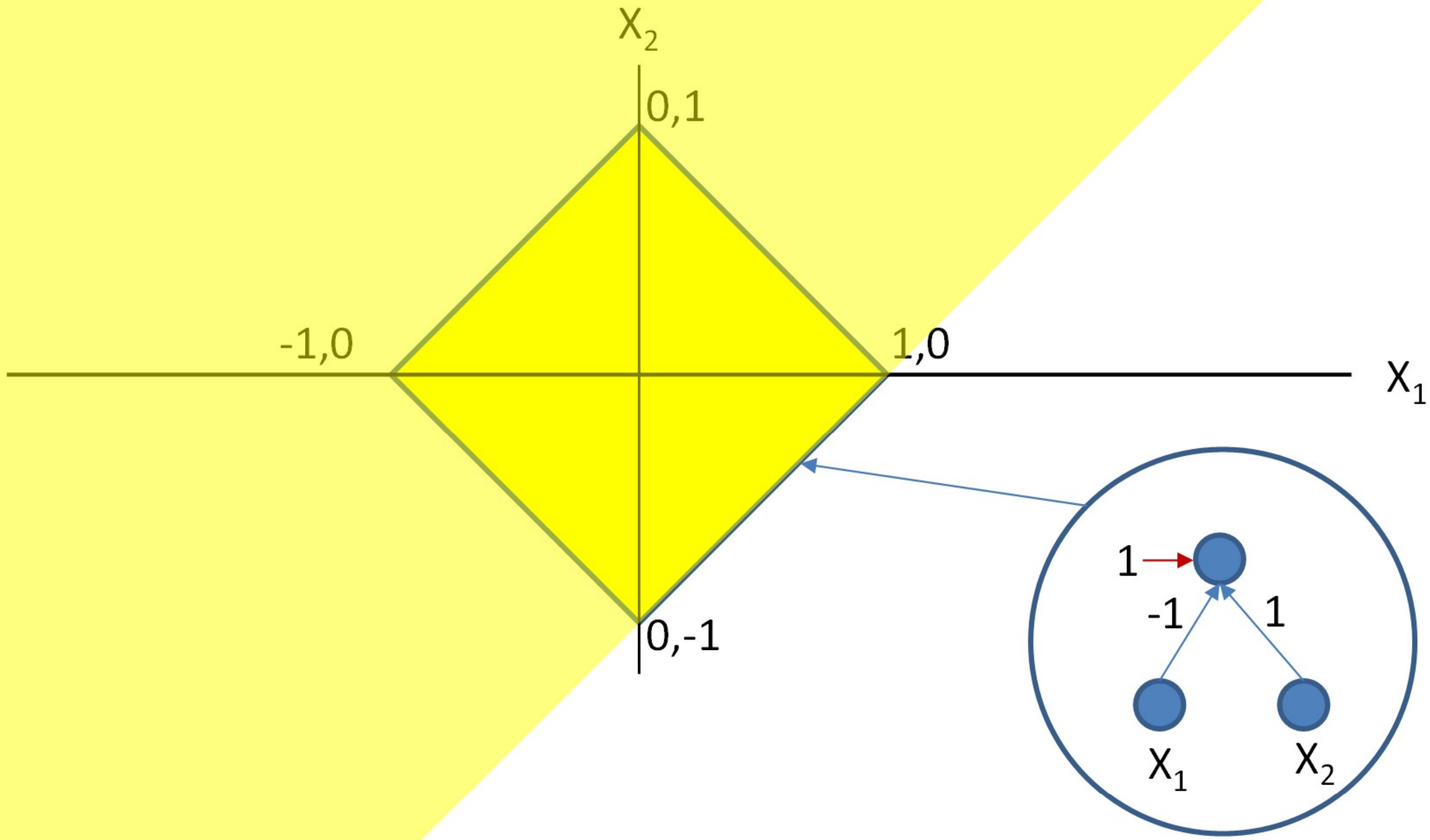

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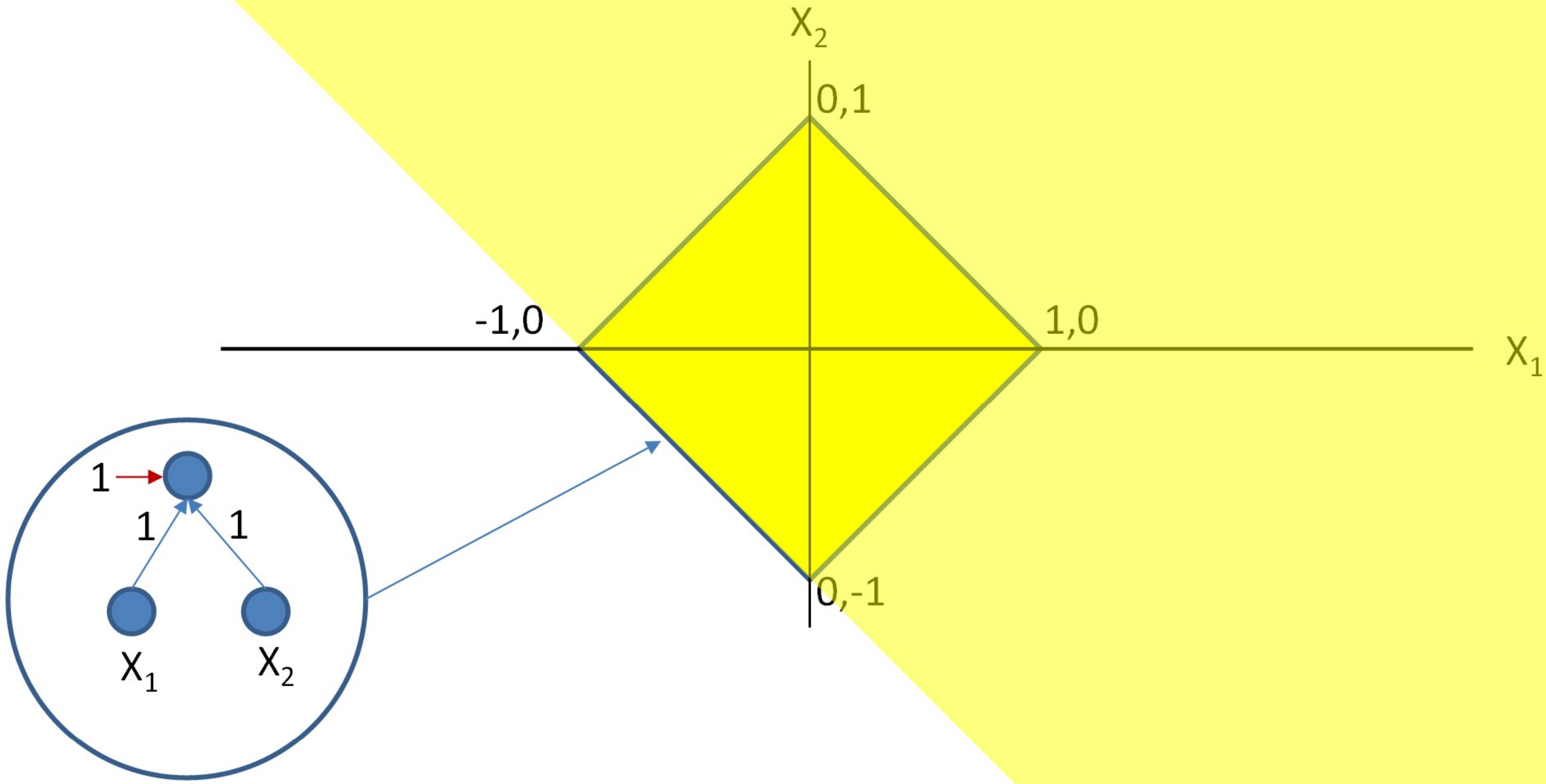

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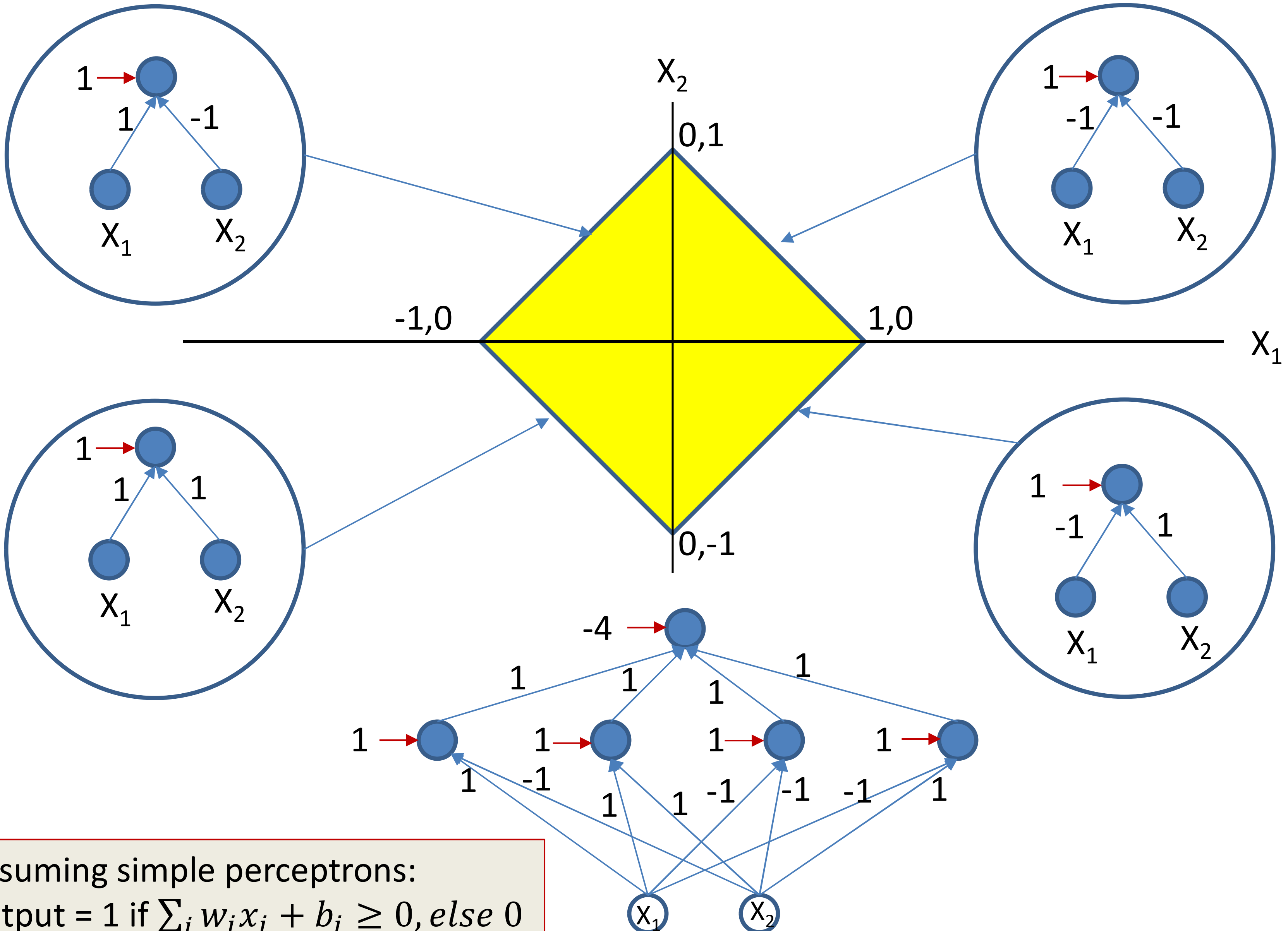

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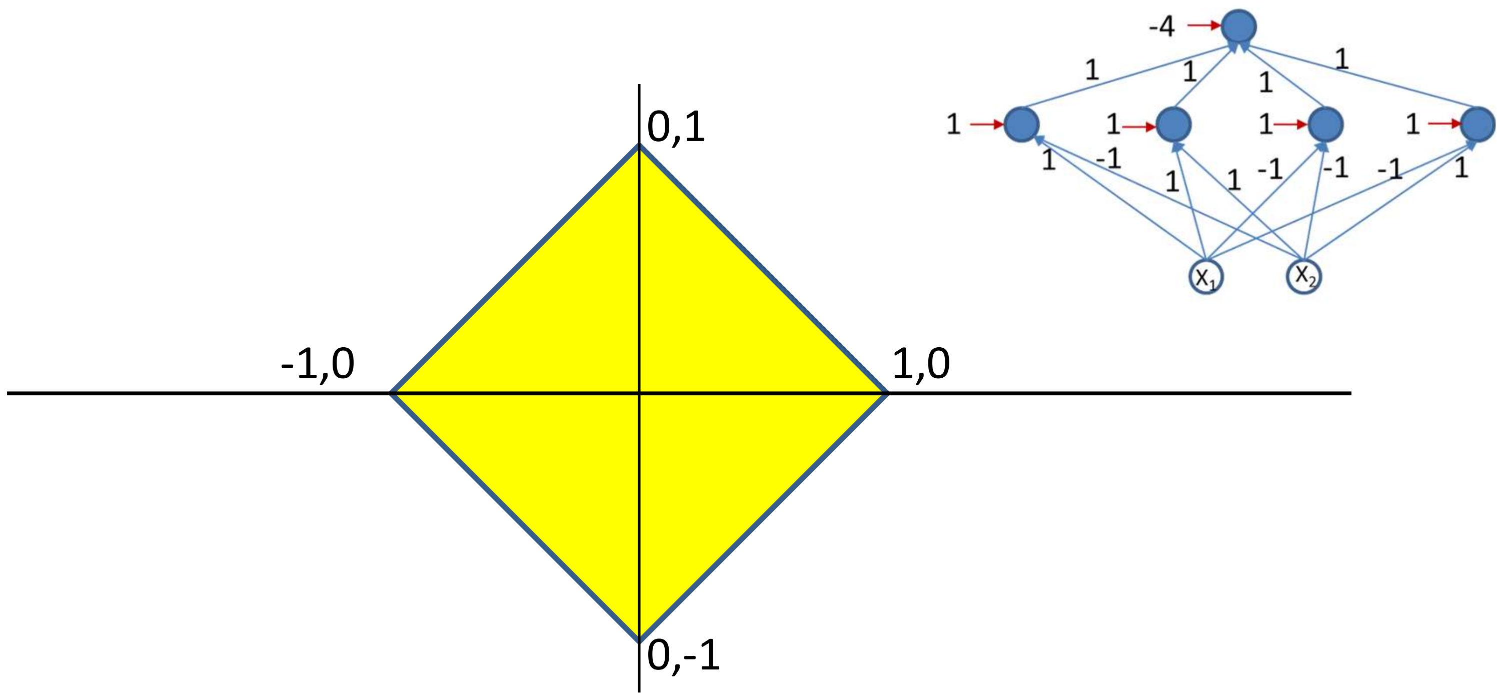
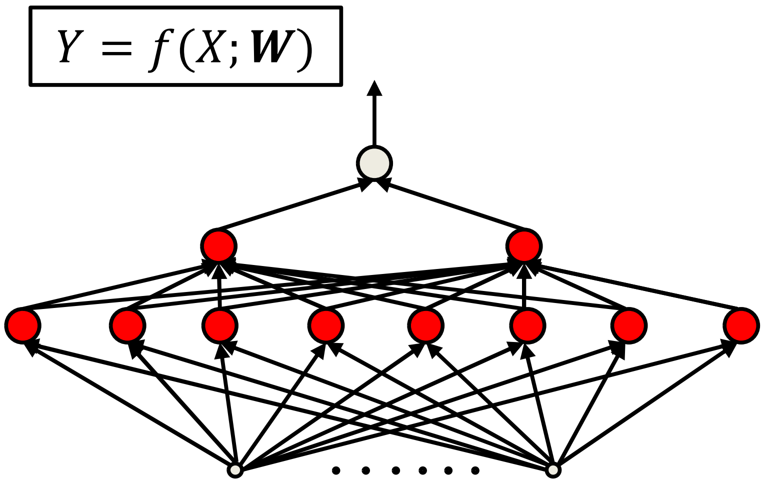
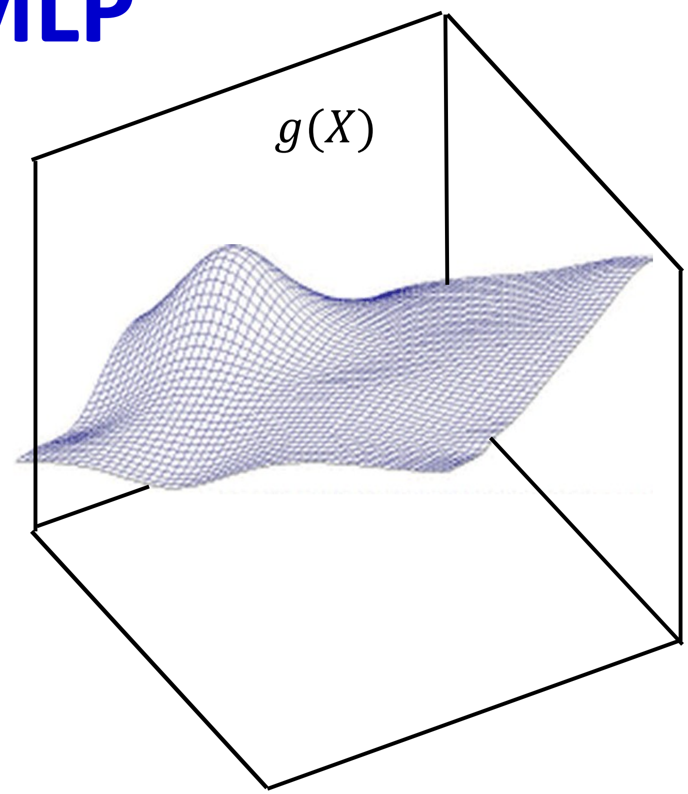


- Given a function, *handcraft* a network to satisfy it
- E.g.: Build an MLP to classify this decision boundary
- Not possible for all but the simplest problems..

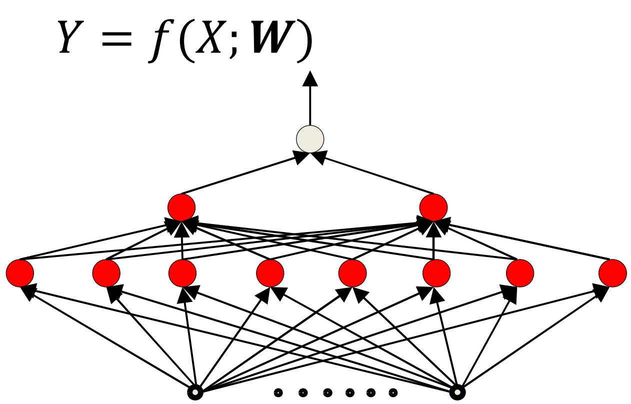
Option 2: Automatic estimation of an MLP

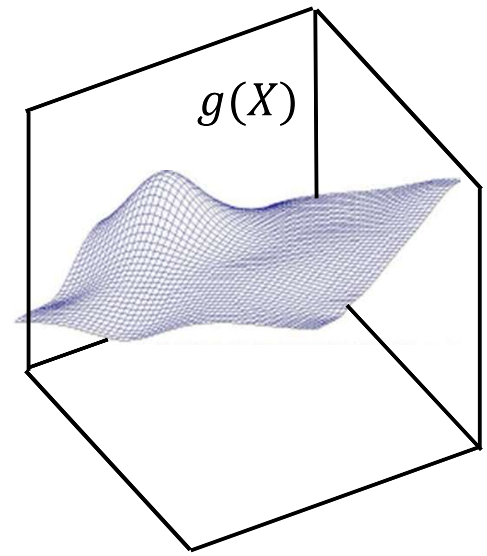




- More generally, *given* the function $g(X)$ to model, we can *derive* the parameters of the network to model it, through computation

How to learn a network?



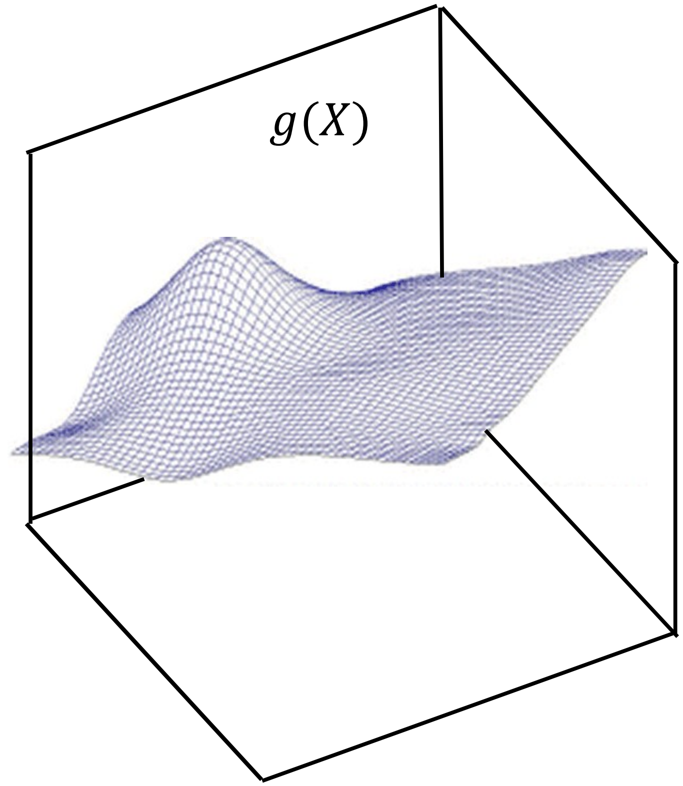


- When $f(X; \boldsymbol{W})$ has the capacity to exactly represent $g(X)$

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

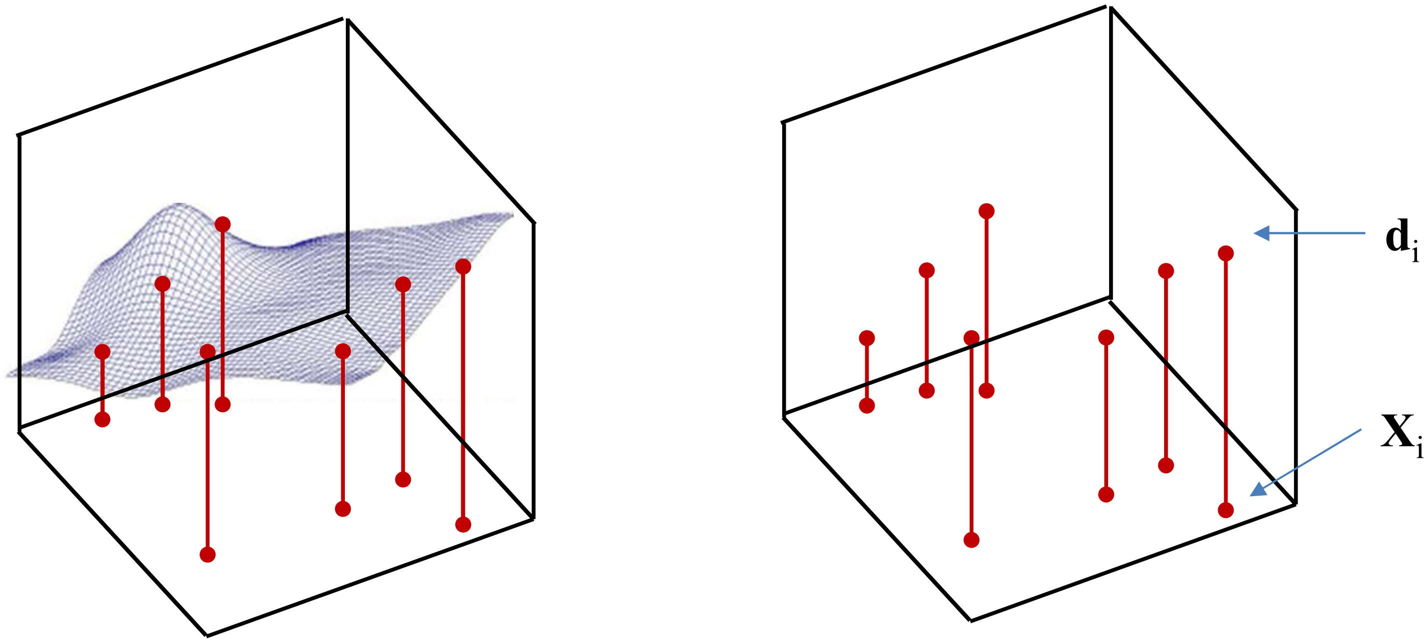
- $div()$ is a *divergence* function that goes to zero when $f(X; W) = g(X)$

Problem $g(X)$ is unknown



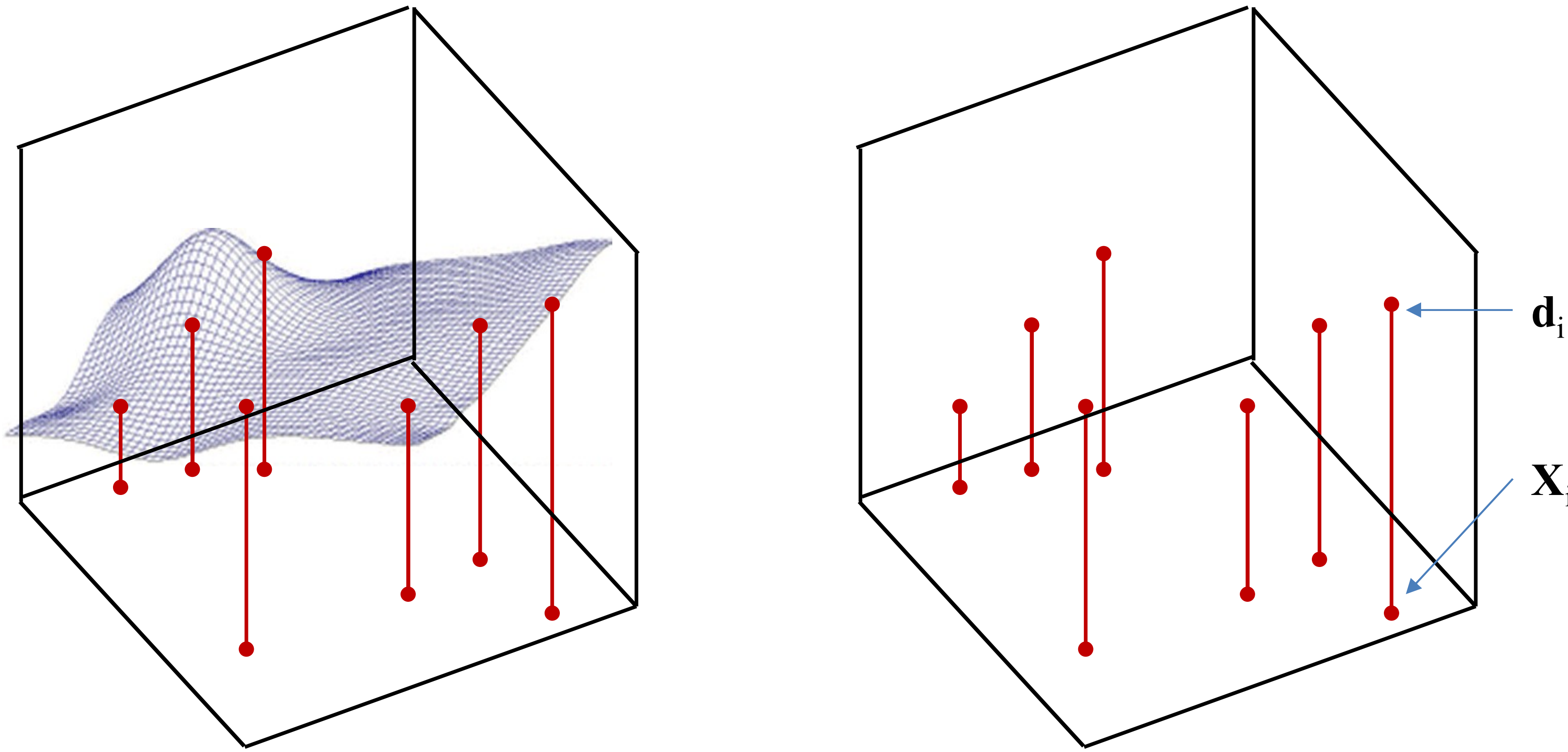
- Function $g(X)$ must be fully specified
  - Known *everywhere,* i.e. for *every* input X
- **In practice we will not have such specification**

Sampling the function



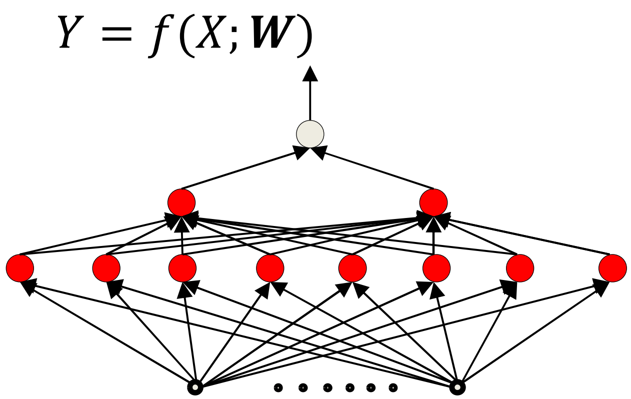
- *Sample* $g(X)$
  - Basically, get input-output pairs for a number of samples of input X_i
    - Many samples (X_i, d_i), where $d_i = g(X_i) + noise$
  - Good sampling: the samples of X will be drawn from $P(X)$
- Very easy to do in most problems: just gather training data
  - E.g. set of images and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

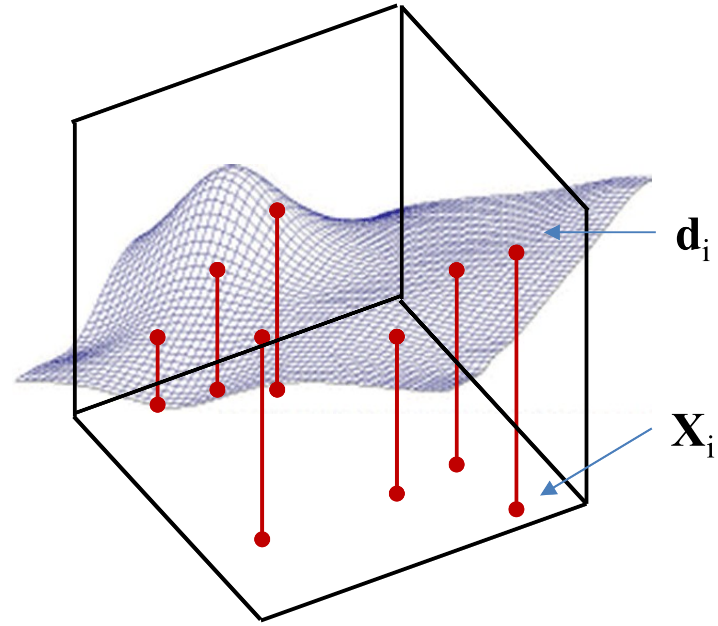
Drawing samples



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

Learning the function





- 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

Story so far

- "Learning" a neural network == determining the parameters of the network (weights and biases) required for it to model a desired function
  - The network must have sufficient capacity to model the function

- Ideally, we would like to optimize the network to represent the desired function everywhere
- However this requires knowledge of the function everywhere
- Instead, we draw "input-output" *training* instances from the function and estimate network parameters to "fit" the input-output relation at these instances
  - And hope it fits the function elsewhere as well

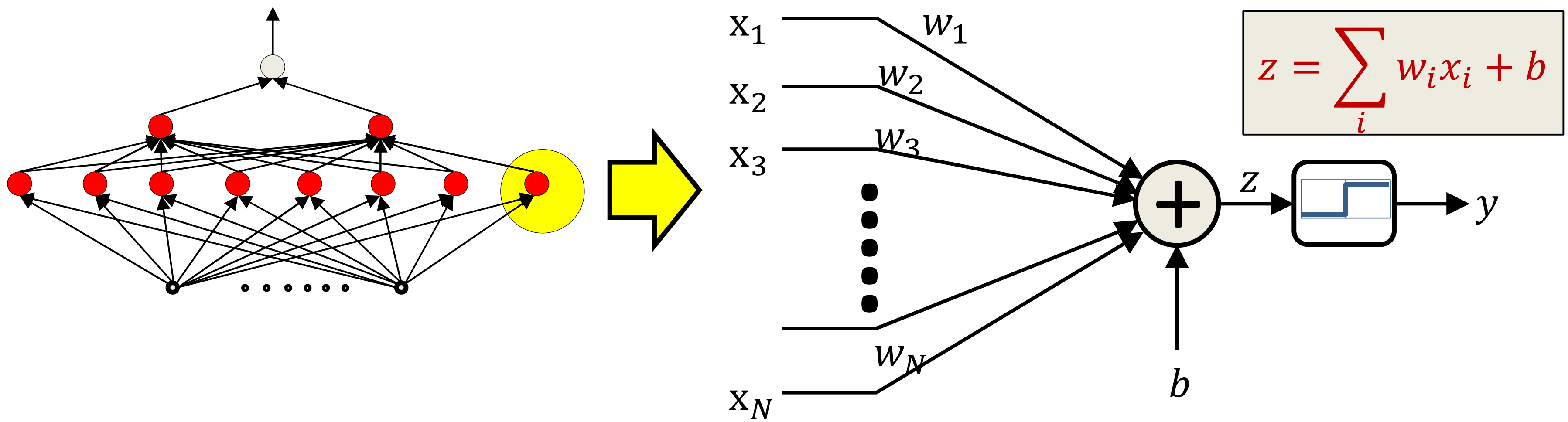
Let's begin with a simple task

- Learning a *classifier*
  - Simpler than regressions

- This was among the earliest problems addressed using MLPs

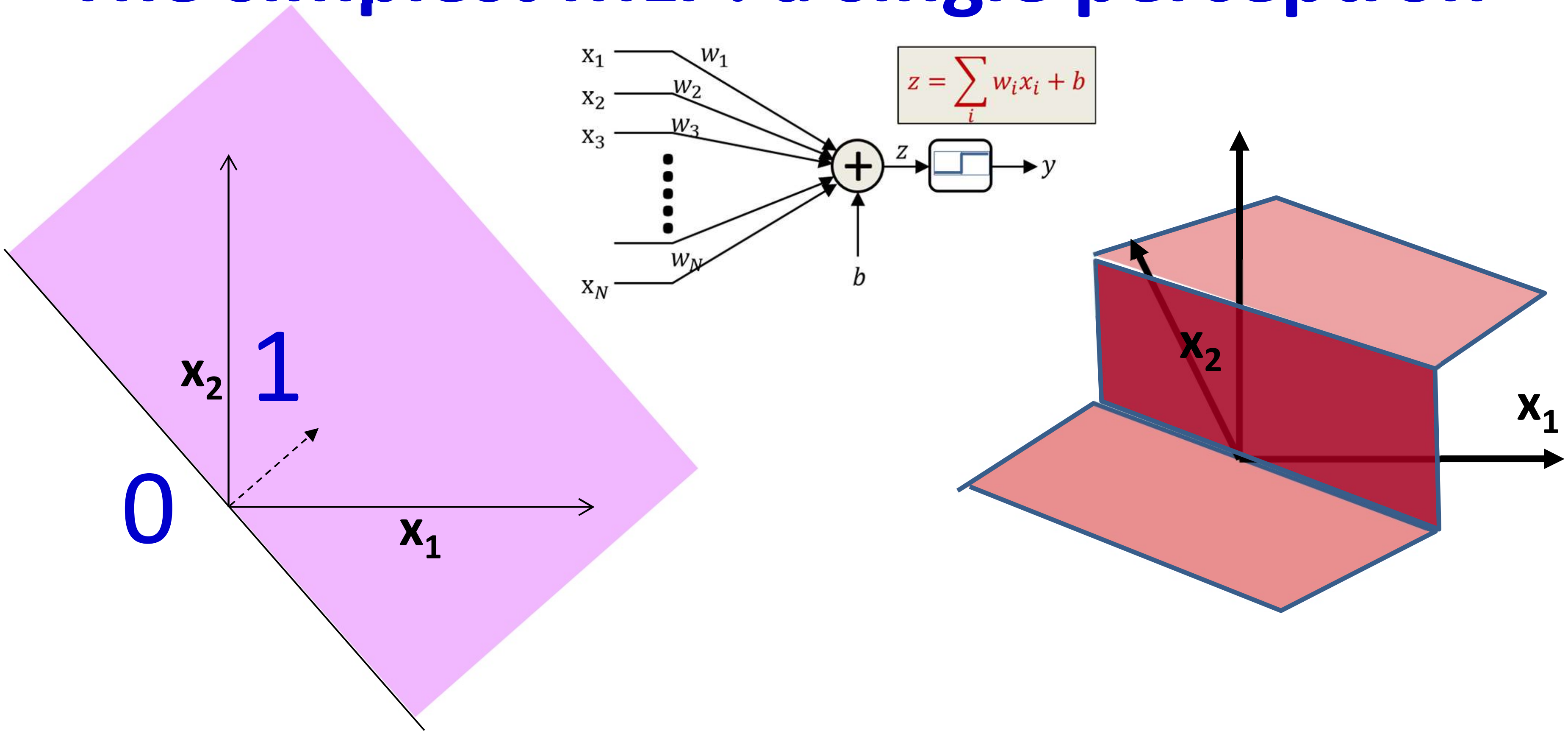
- Specifically, consider *binary* classification
  - Generalizes to multi-class

History: The original MLP



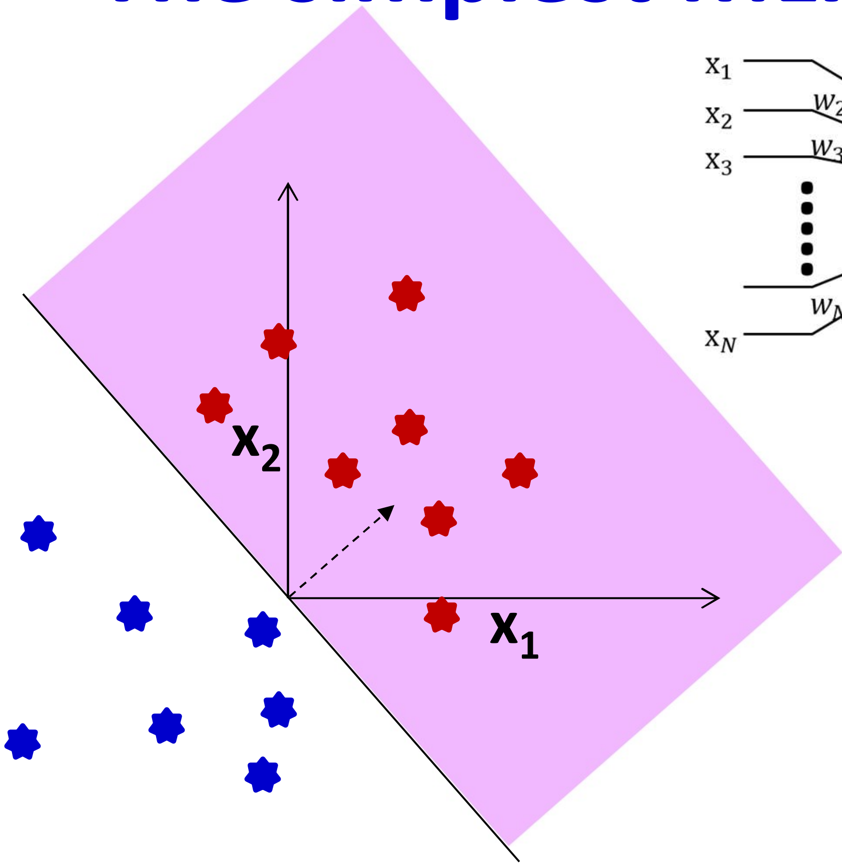
- The original MLP as proposed by Minsky: a network of threshold units
  - But how do you train it?
    - Given only “training” instances of input-output pairs

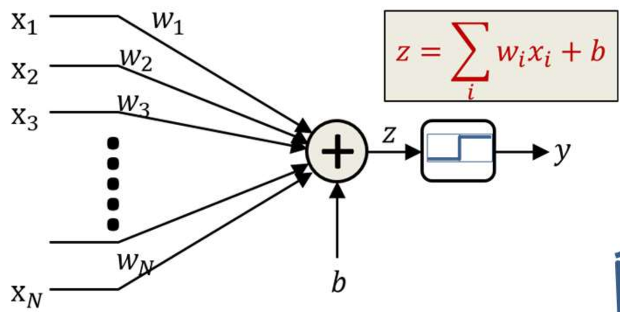
The simplest MLP: a single perceptron

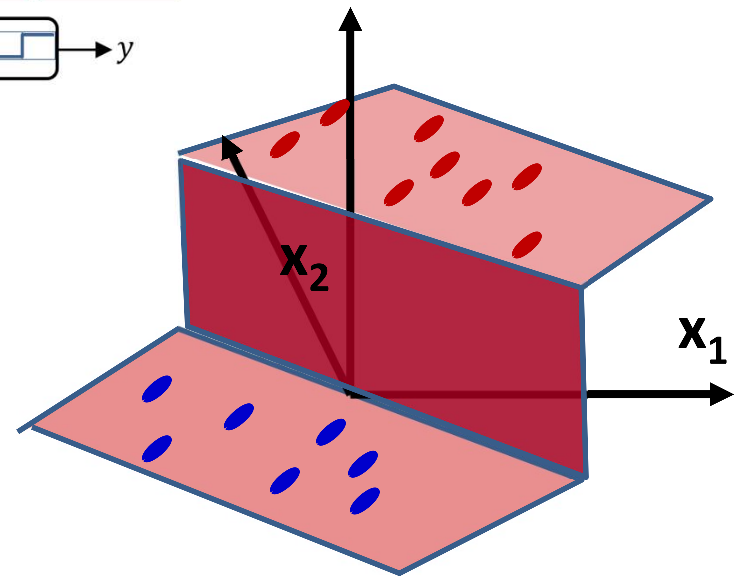


- Learn this function
  - **A step function across a hyperplane**

The simplest MLP: a single perceptron

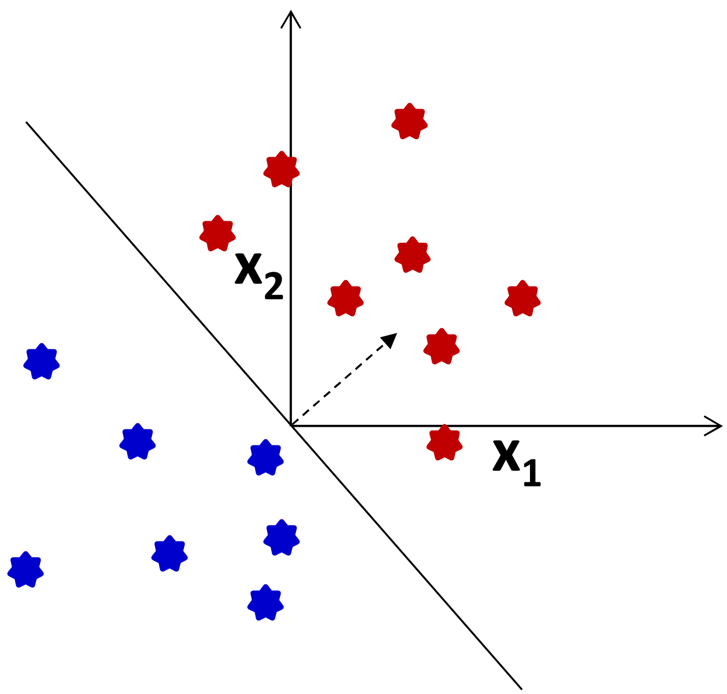


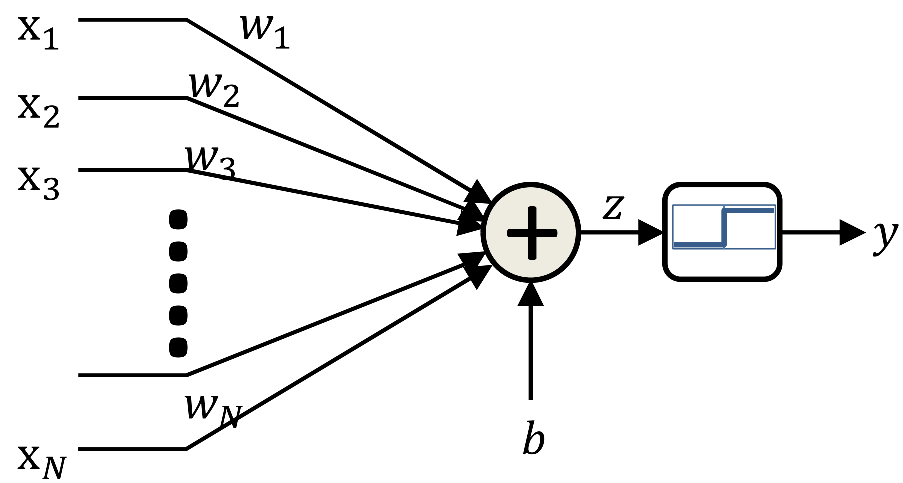




- Learn this function
  - **A step function across a hyperplane**
  - **Given only samples from it**

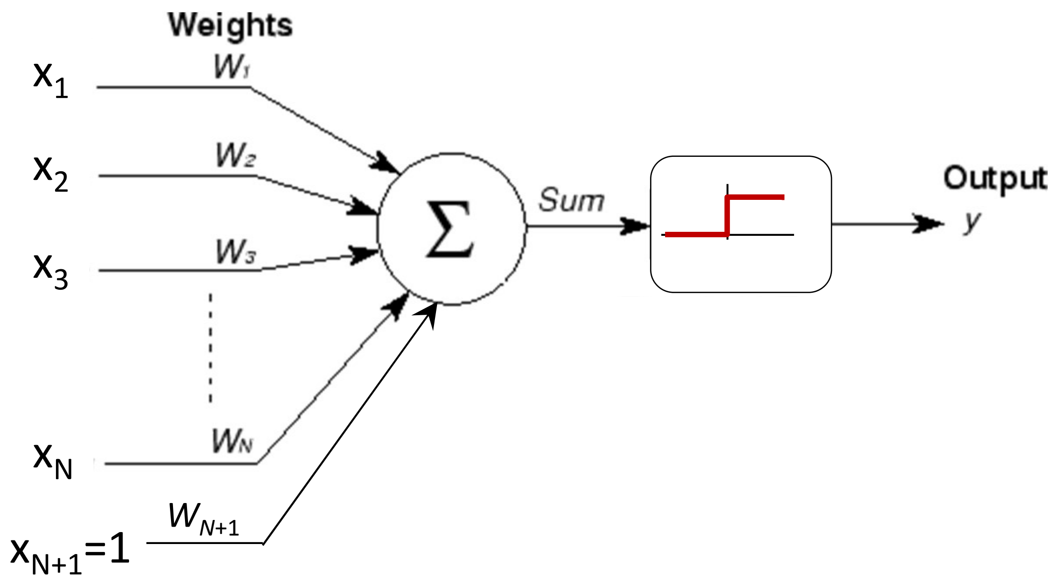
Learning the perceptron





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

Restating the perceptron



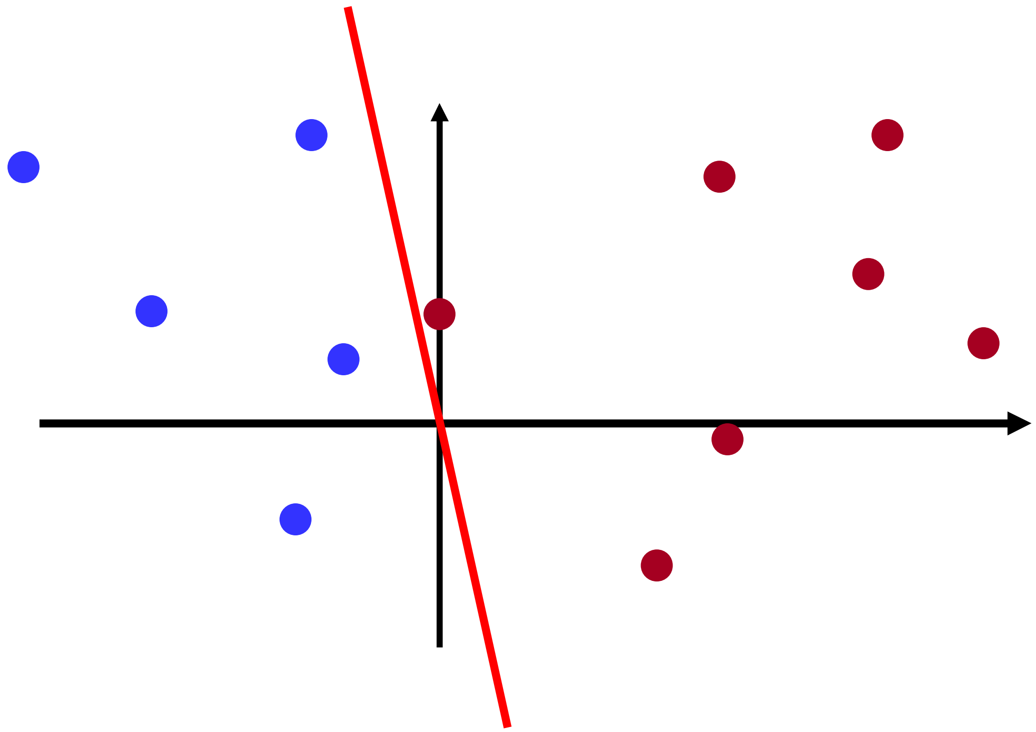
- Restating the perceptron equation by adding another dimension to X

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

where $X_{N+1} = 1$

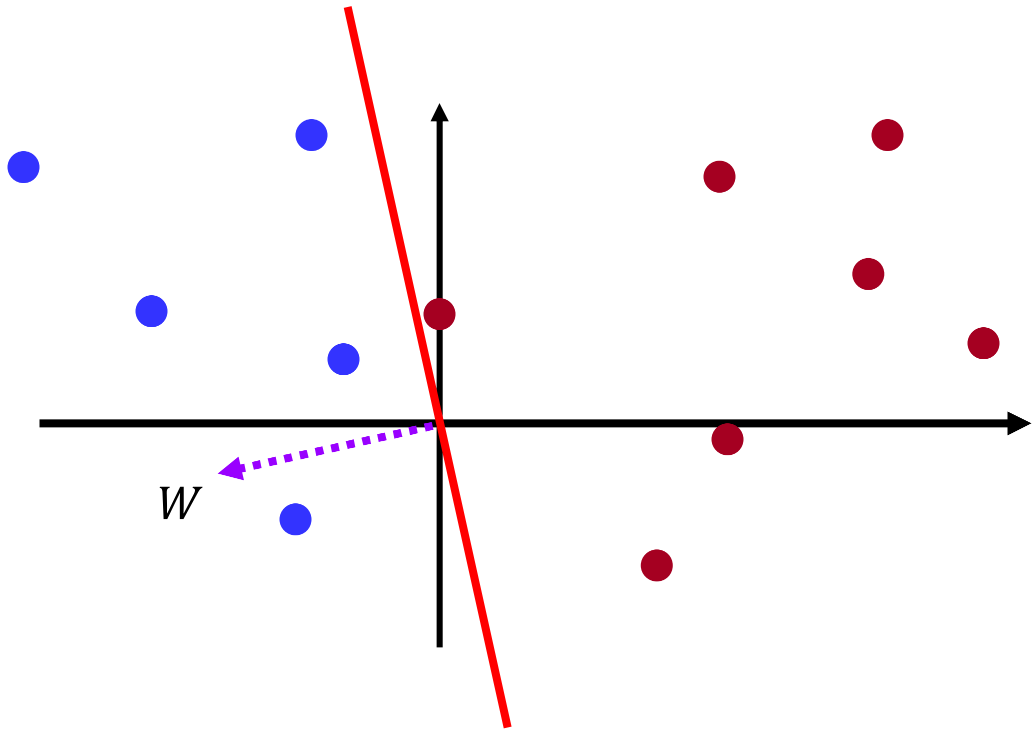
- Note that the boundary $\sum_{i=1}^{N+1} w_i X_i \geq 0$ is now a hyperplane through origin

The Perceptron Problem



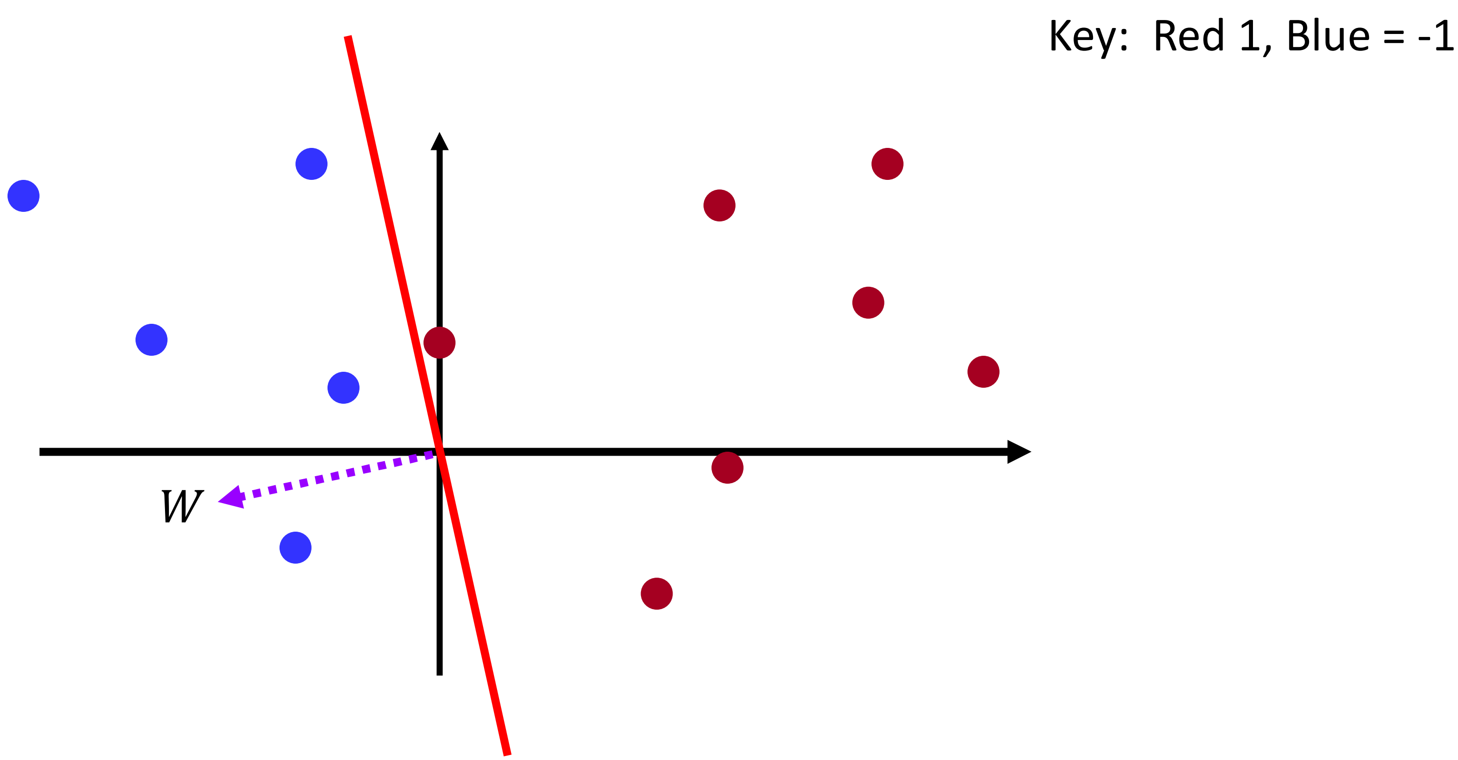
- Find the hyperplane $\sum_{i=1}^{N+1} w_i X_i = 0$ that perfectly separates the two groups of points

The Perceptron Problem



- Find the hyperplane $\sum_{i=1}^{N+1} w_i X_i = 0$ that perfectly separates the two groups of points
  - Note: $W = [w_1, w_2, \dots, w_{N+1}]^T$ is a vector that is orthogonal to the hyperplane
    - In fact the equation for the hyperplane itself means "the set of all Xs that are orthogonal to W" ($\sum_{i=1}^{N+1} w_i X_i = W^T X = 0$)

The Perceptron Problem



- Learning the perceptron: Find the weights vector W such that $W^T X$ is positive for all blue dots and negative for all red ones

Perceptron Algorithm: Summary

- Cycle through the training instances
- Only update W on misclassified instances
- If instance misclassified:
  - If instance is positive class (positive misclassified as negative)

$$W = W + X_i$$

  - If instance is negative class (negative misclassified as positive)

$$W = W - X_i$$

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:
- do
  - For $i = 1..N_{train}$

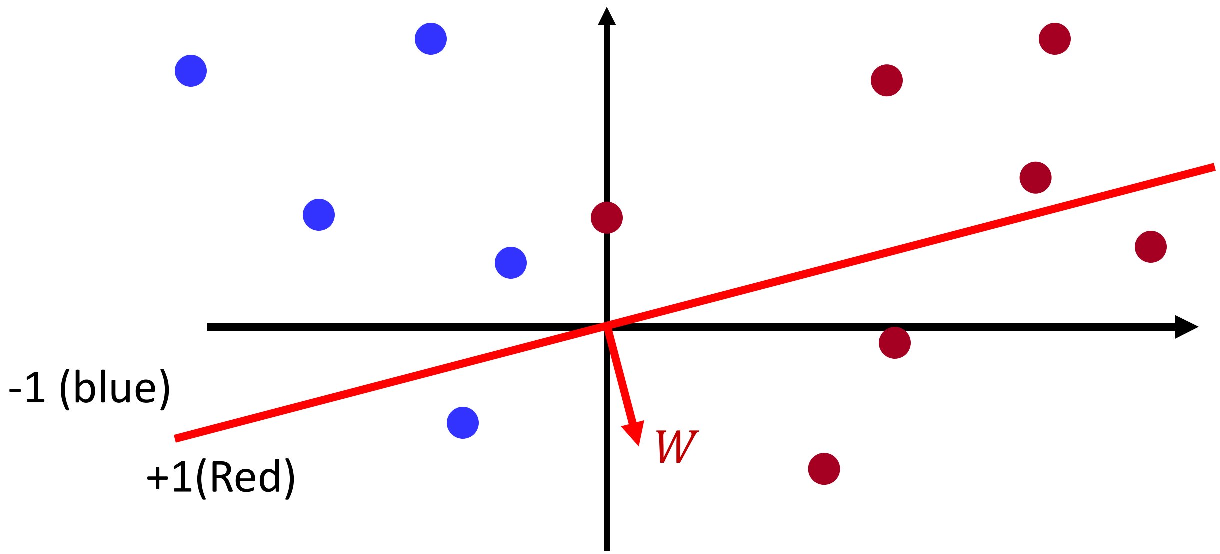
$$O(X_i) = sign(W^T X_i)$$

    - If $O(X_i) \neq y_i$

$$W = W + y_i X_i$$

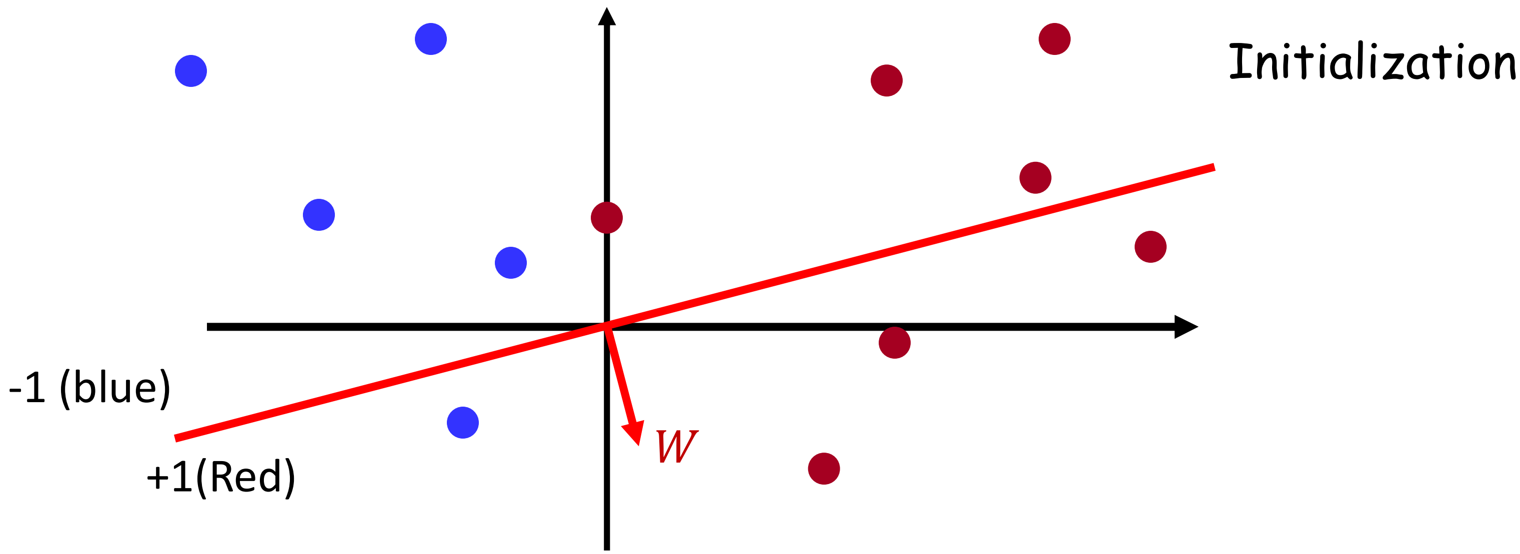
- until no more classification errors

A Simple Method: The Perceptron Algorithm

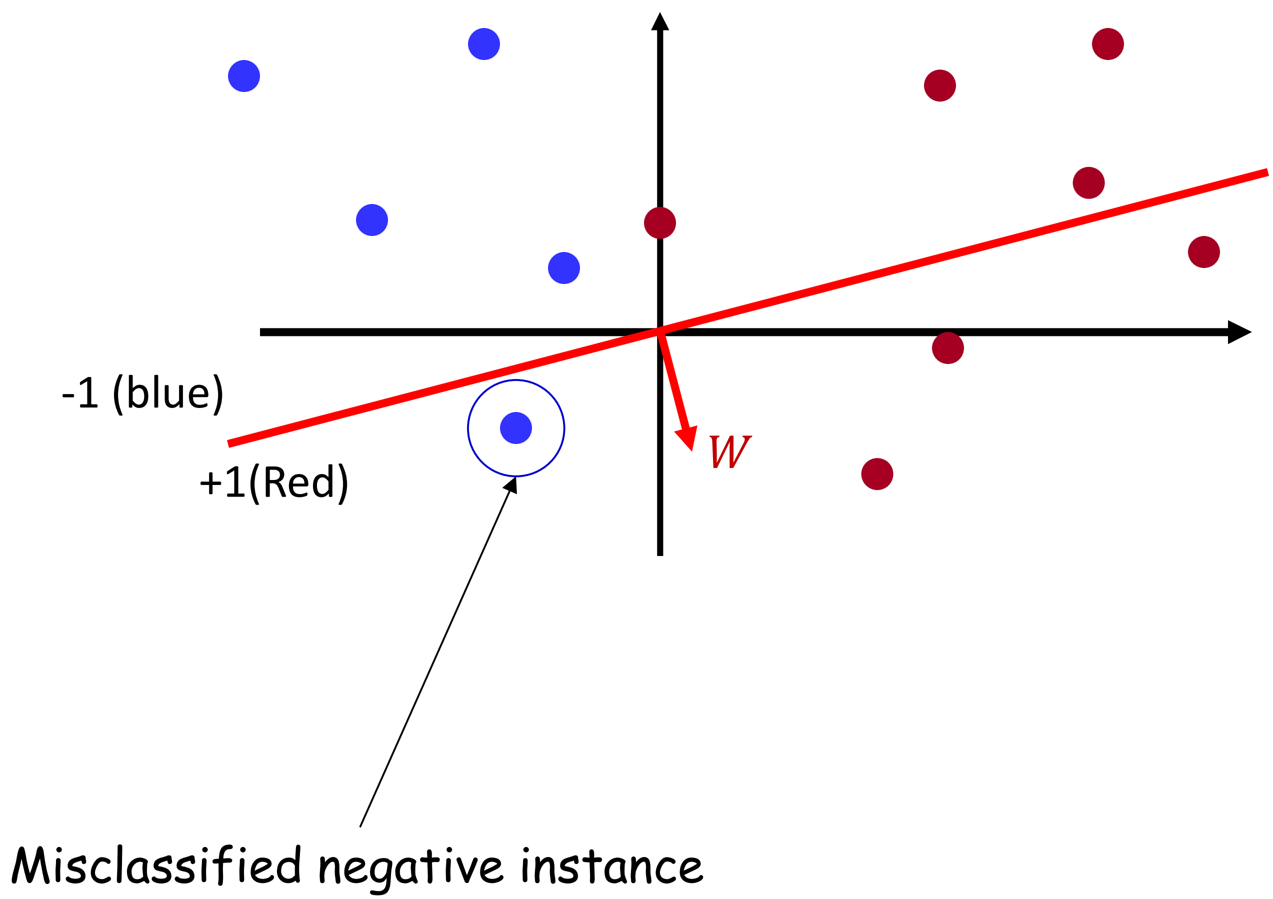


- **Initialize:** Randomly initialize the hyperplane
  - I.e. randomly initialize the normal vector W
- **Classification rule** $sign(W^T X)$
  - Vectors on the same side of the hyperplane as W will be assigned +1 class, and those on the other side will be assigned -1
- The random initial plane will make mistakes

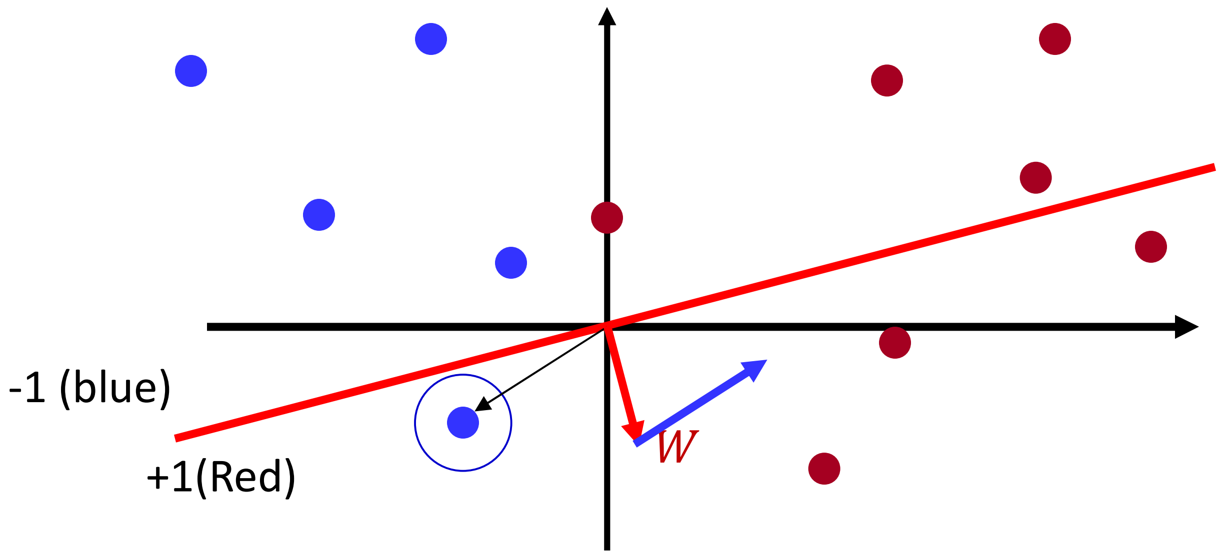
Perceptron Algorithm



Perceptron Algorithm

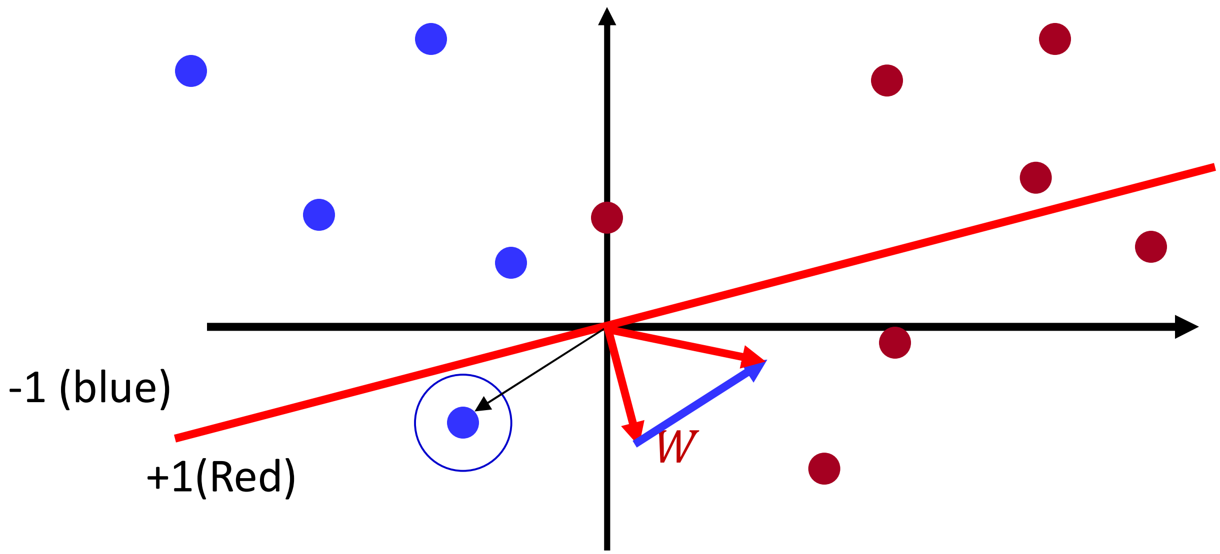


Perceptron Algorithm



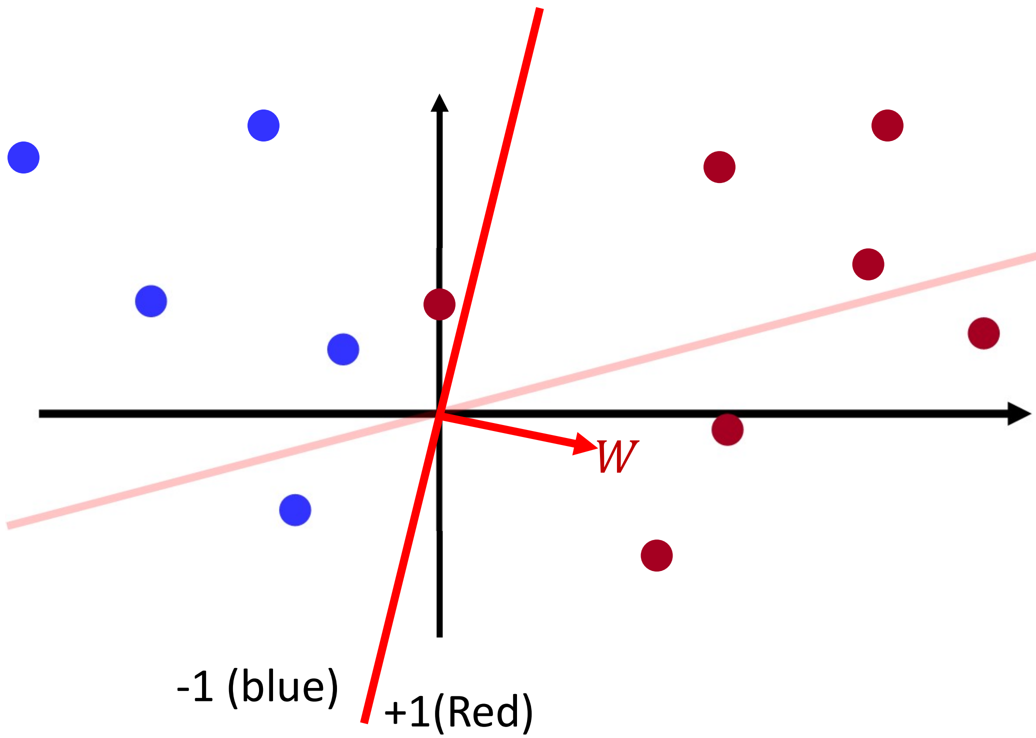
Misclassified *negative* instance, *subtract* it from W

Perceptron Algorithm



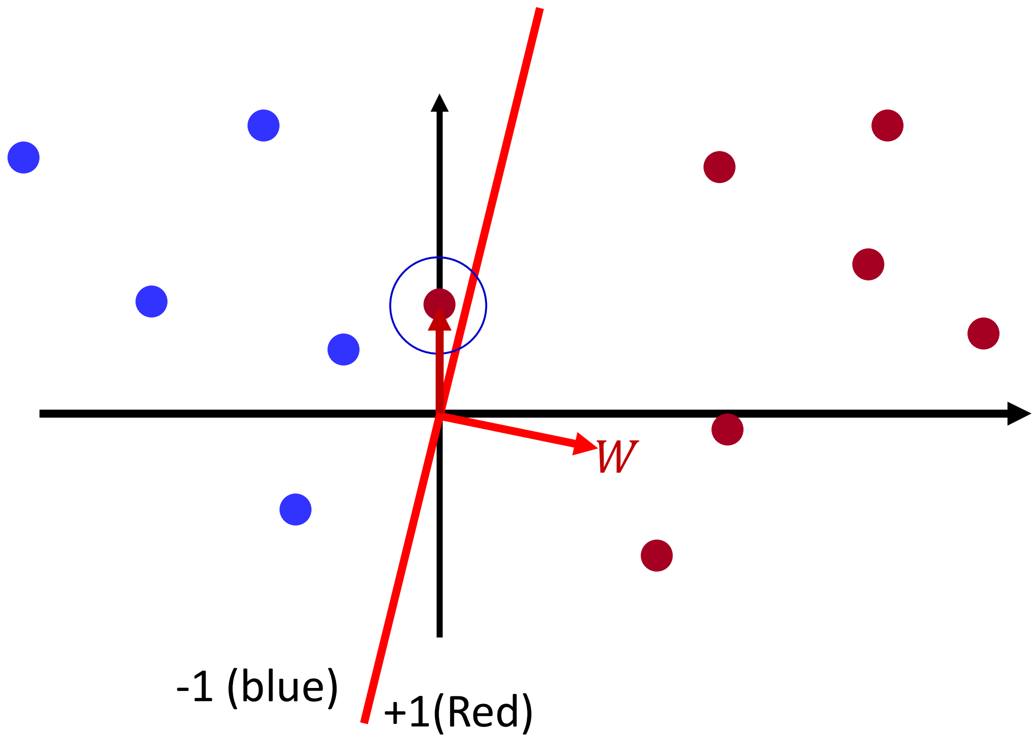
The new weight

Perceptron Algorithm



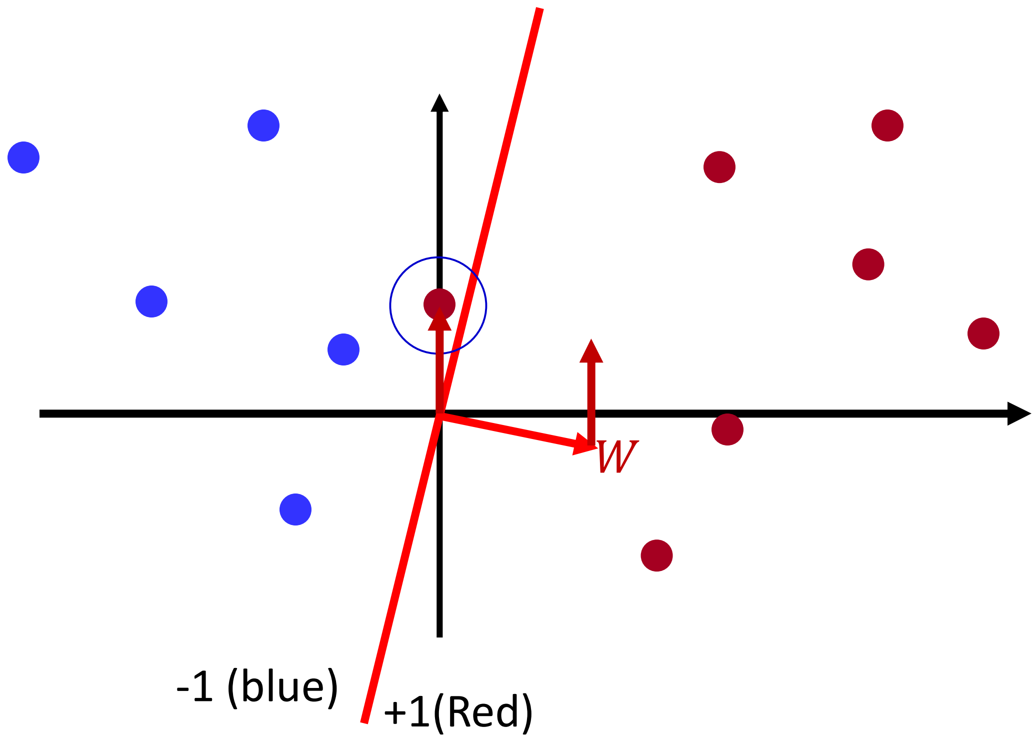
The new weight (and boundary)

Perceptron Algorithm



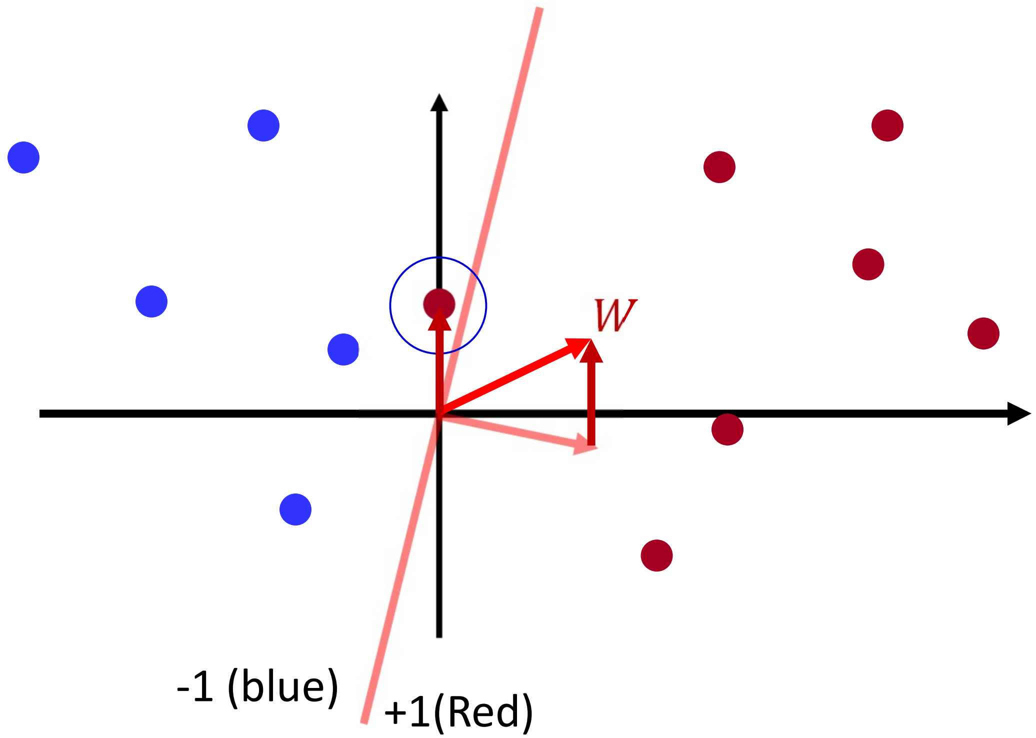
Misclassified *positive* instance

Perceptron Algorithm



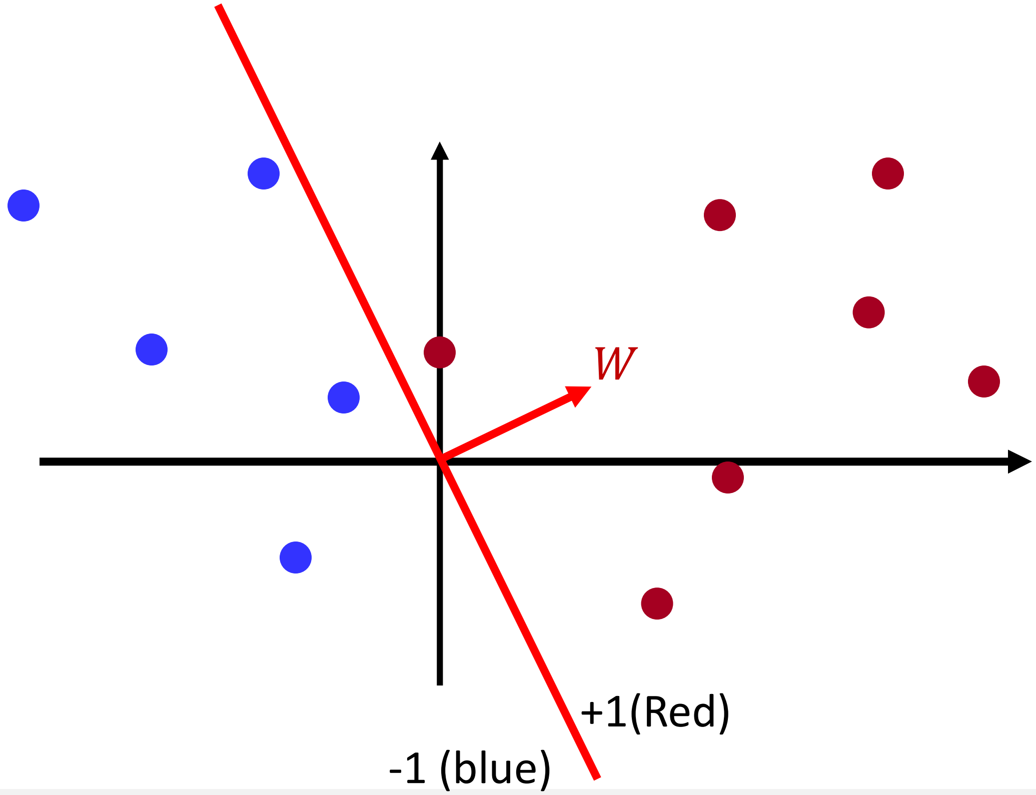
Misclassified *positive* instance, *add* it to W

Perceptron Algorithm



The new weight vector

Perceptron Algorithm



The new decision boundary

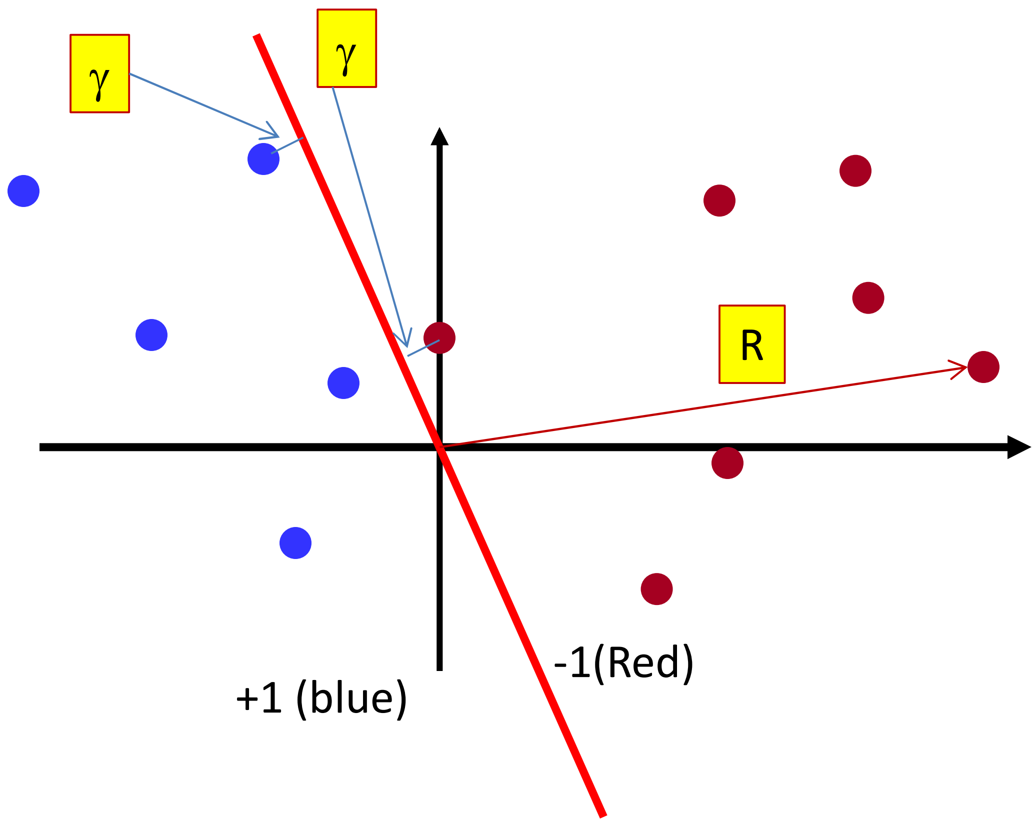
Perfect classification, no more updates, we are done

If the classes are linearly separable, guaranteed to converge in a finite number of steps

Convergence of Perceptron Algorithm

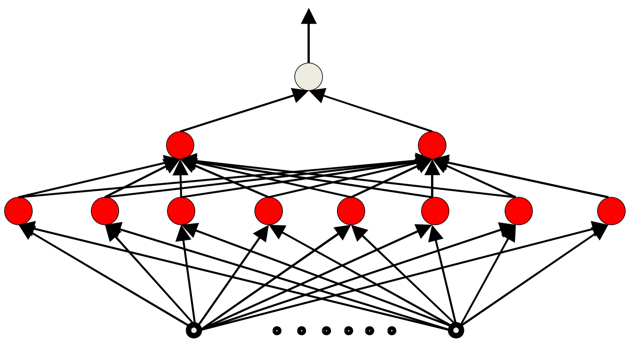
- Guaranteed to converge if classes are linearly separable
  - After no more than $\left(\frac{R}{\gamma}\right)^2$ misclassifications
    - Specifically when W is initialized to 0
  - R is length of longest training point
  - γ is the *best case* closest distance of a training point from the classifier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

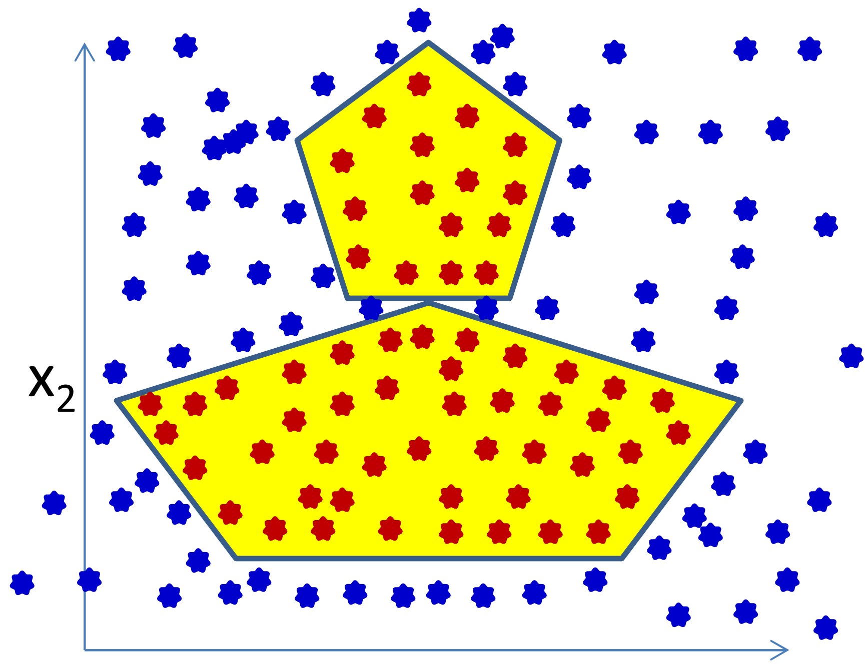
Perceptron Algorithm



γ is the best-case margin
R is the length of the longest vector

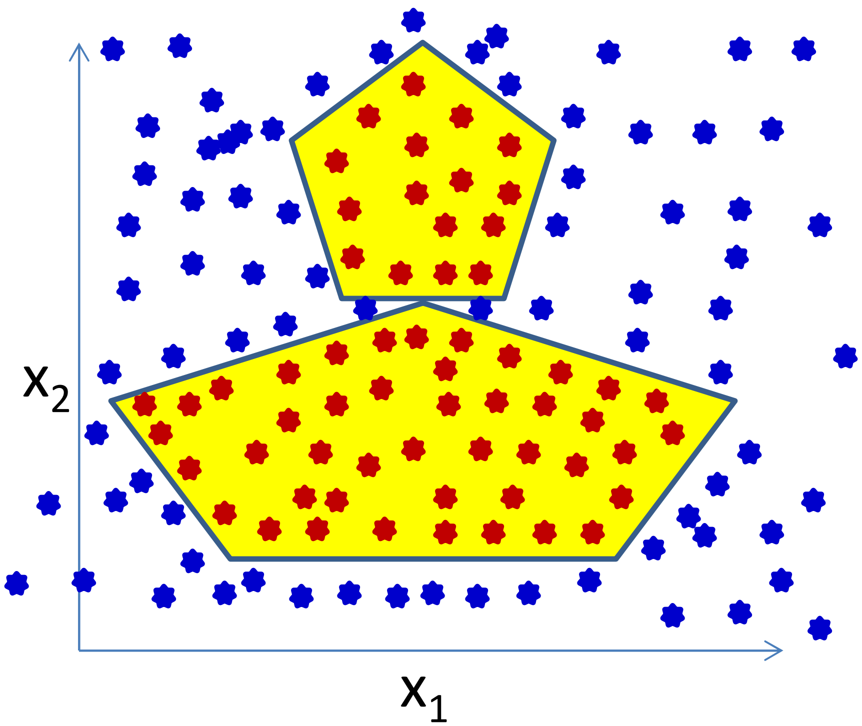
History: A more complex problem

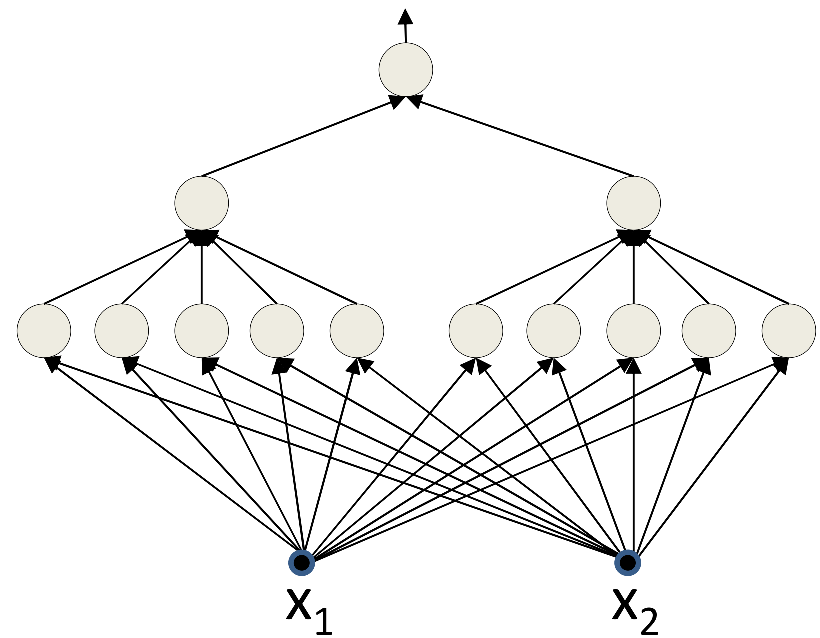




- Learn an *MLP* for this function
  - 1 in the yellow regions, 0 outside
- Using just the samples
- We know this can be perfectly represented using an MLP

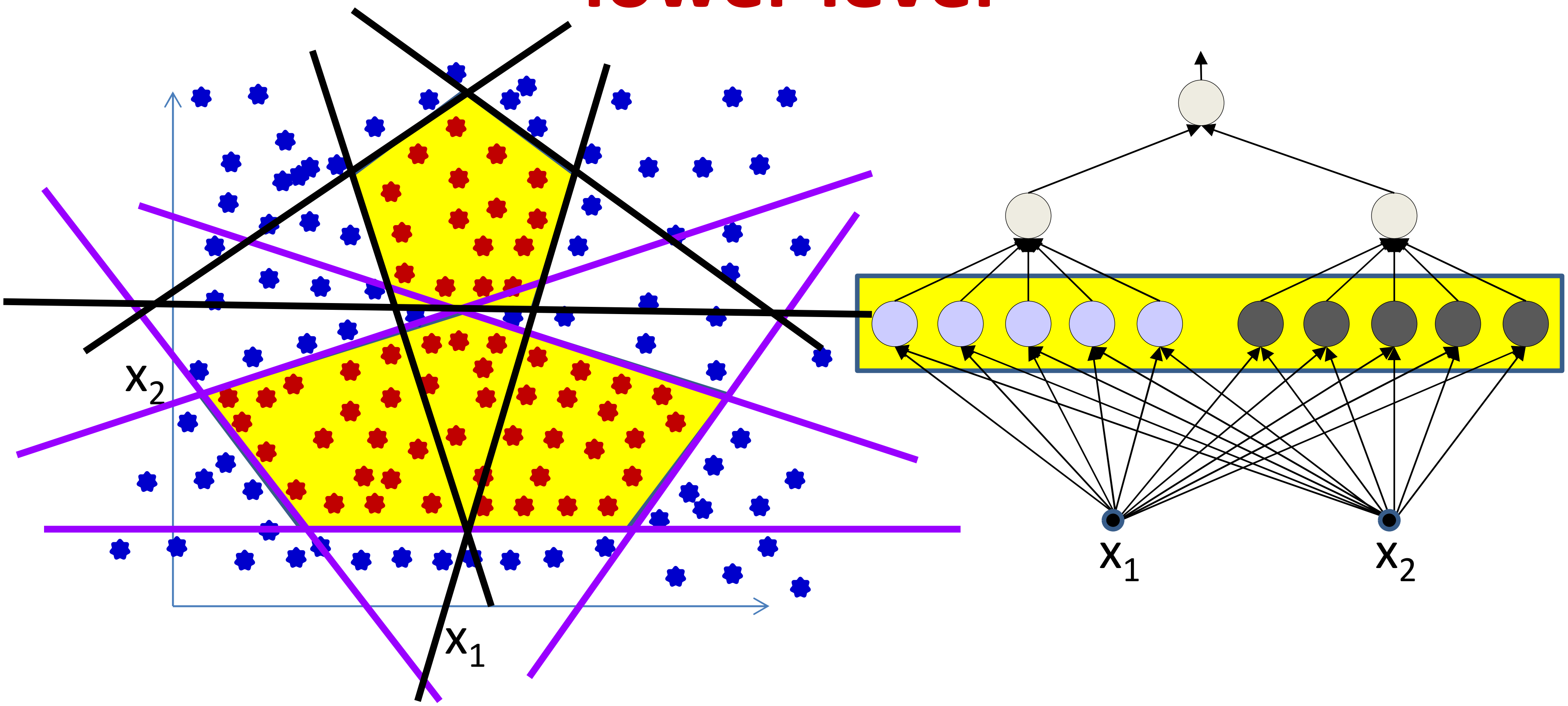
More complex decision boundaries





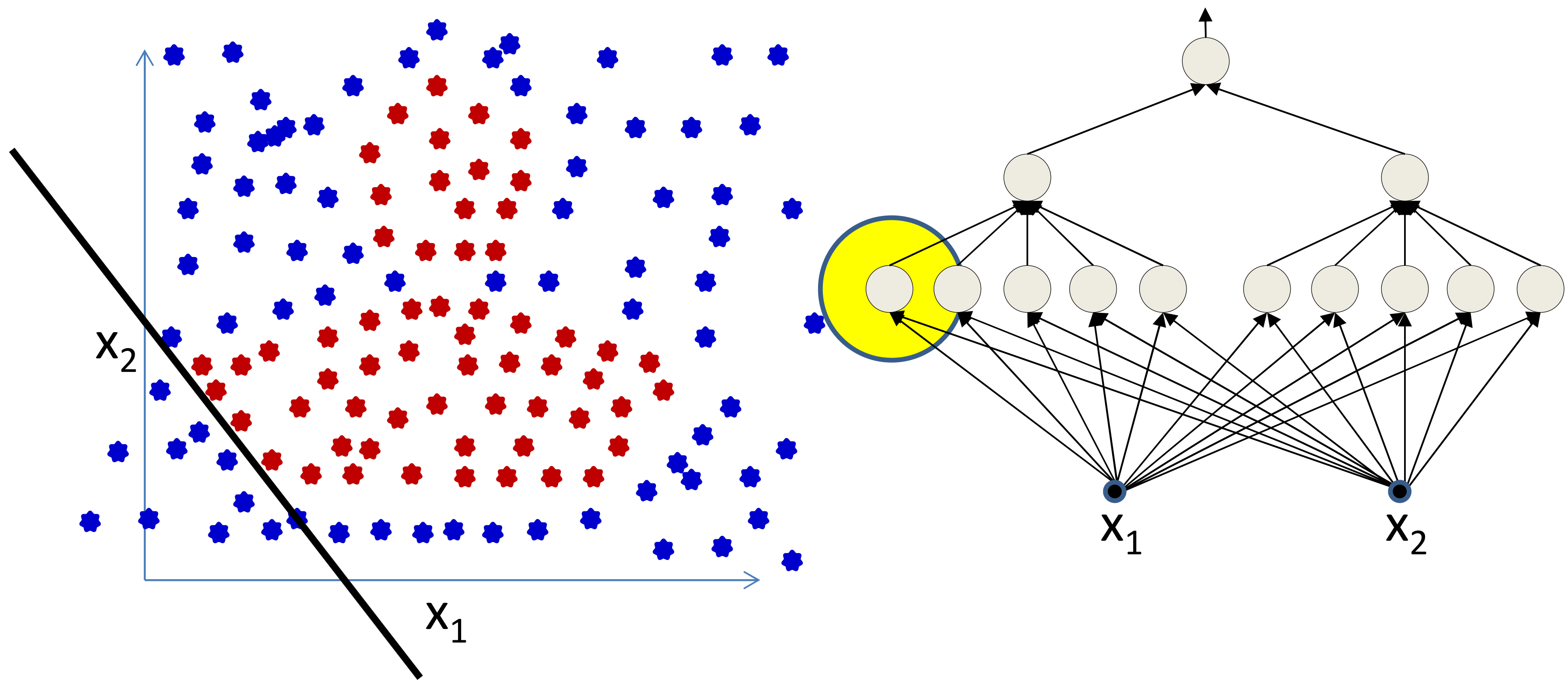
- Even using the perfect architecture
- Can we use the perceptron algorithm?
  - Making incremental corrections every time we encounter an error

The pattern to be learned at the lower level



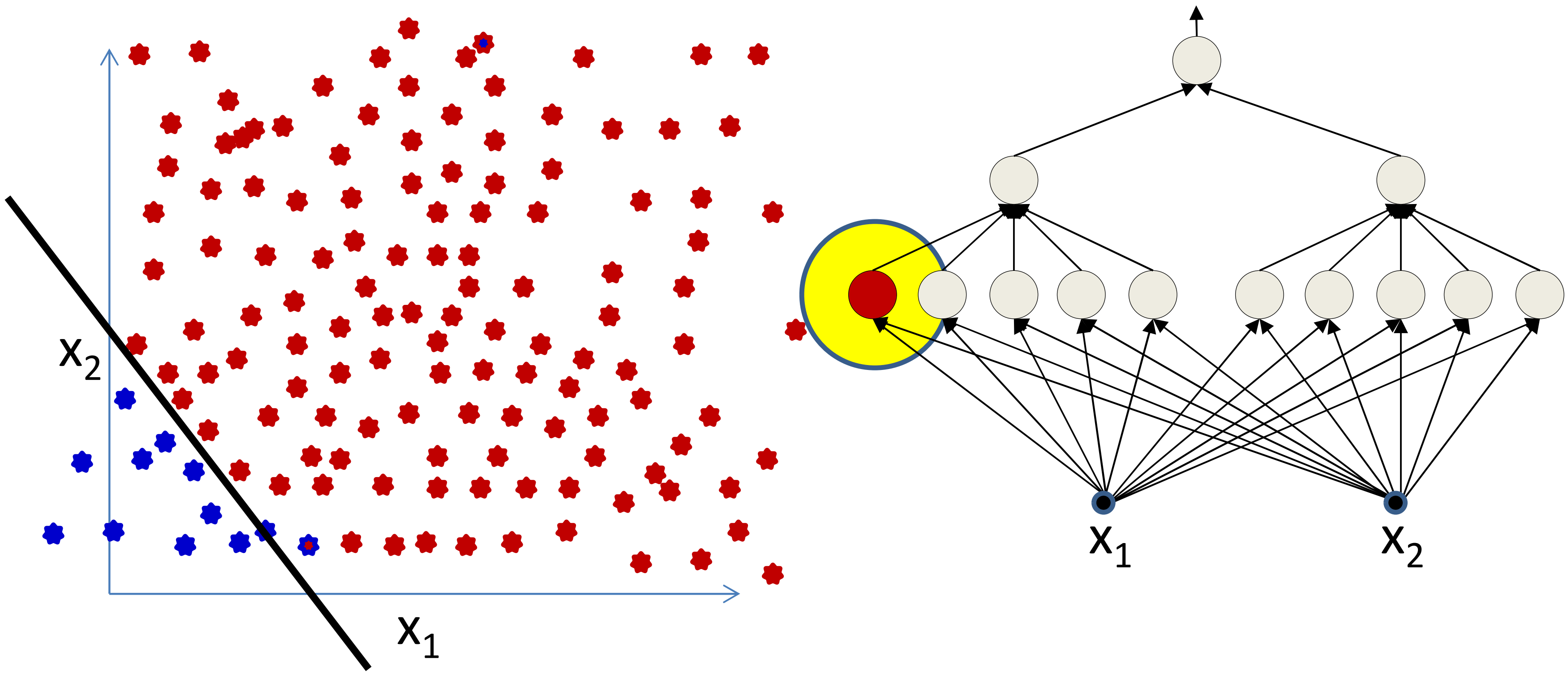
- The lower-level neurons are linear classifiers
  - They require linearly separated labels to be learned
  - The actually provided labels are not linearly separated
  - Challenge: *Must also learn the labels for the lowest units!*

The pattern to be learned at the lower level



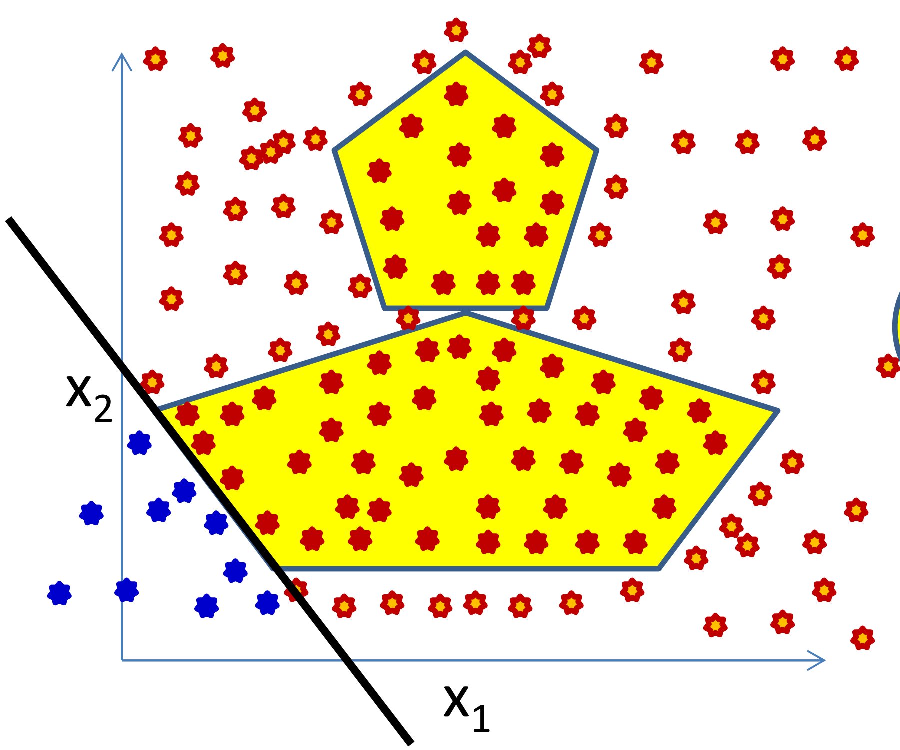
- Consider a single linear classifier that must be learned from the training data
  - Can it be learned from this data?

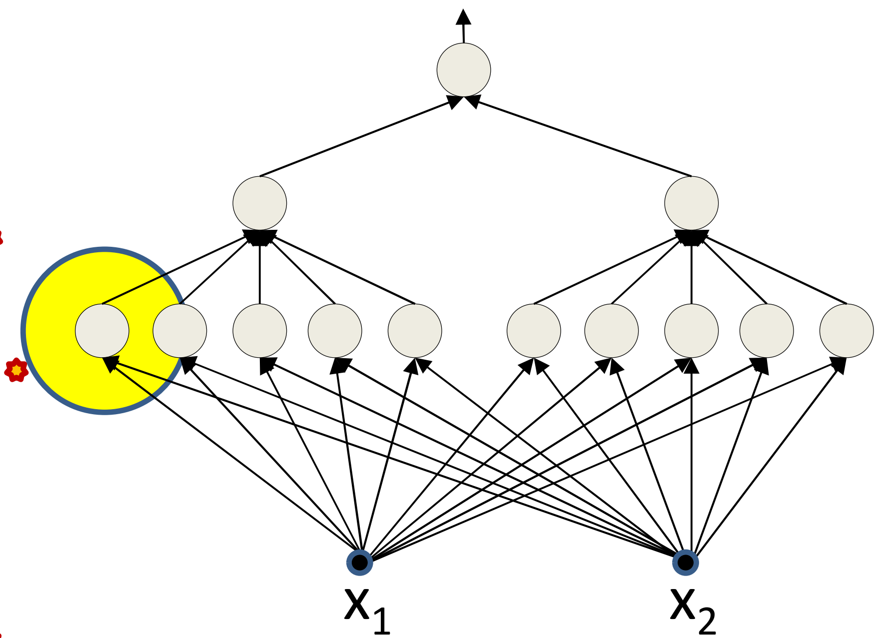
The pattern to be learned at the lower level



- Consider a single linear classifier that must be learned from the training data
  - Can it be learned from this data?
  - The individual classifier actually requires the kind of labelling shown here
    - Which is *not* given!!

The pattern to be learned at the lower level





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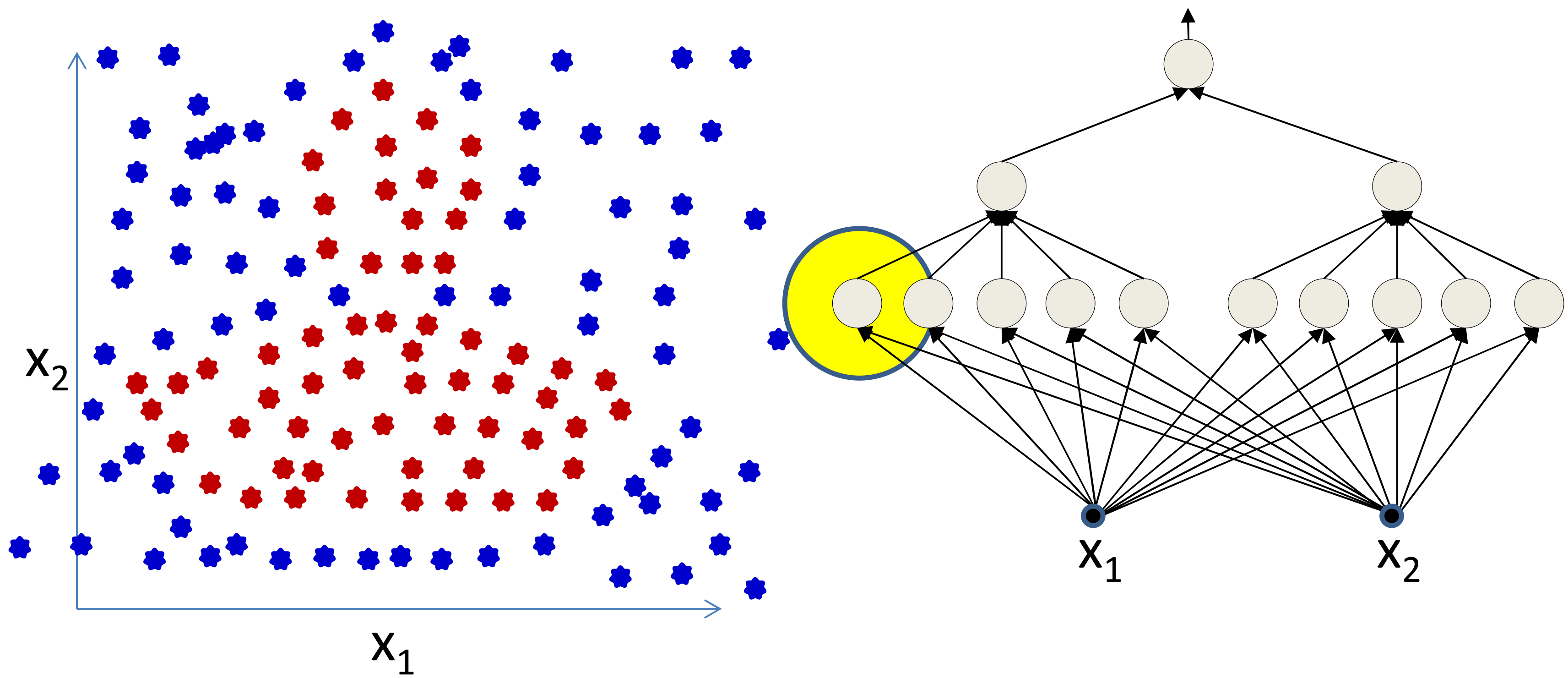
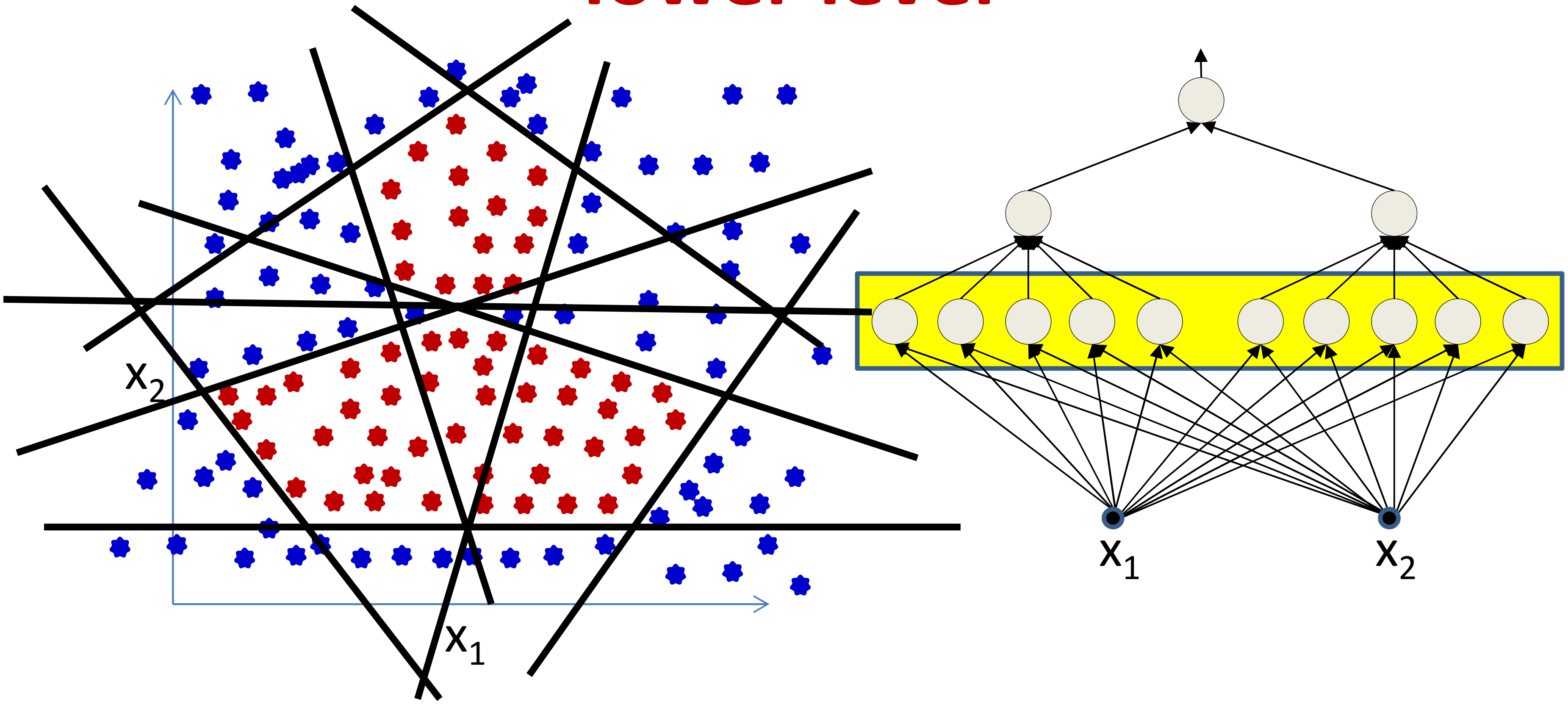
The pattern to be learned at the lower level



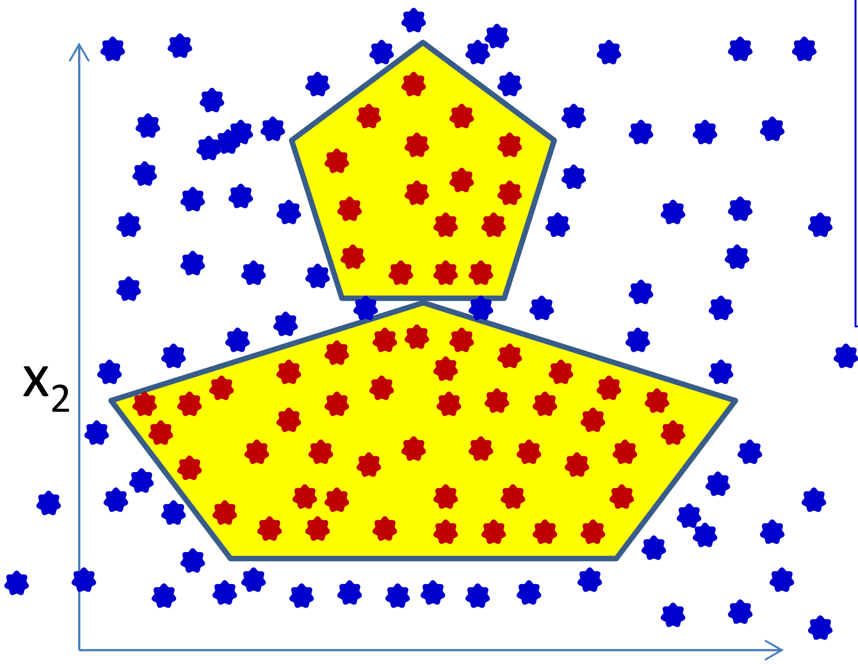
- For a single line:
  - Try out *every possible way of relabeling the blue dots such that we can learn a line that keeps all the red dots on one side!*

The pattern to be learned at the lower level



- This must be done for *each* of the lines (perceptrons)
- Such that, when all of them are combined by the higher-level perceptrons we get the desired pattern
  – Basically an exponential search over inputs

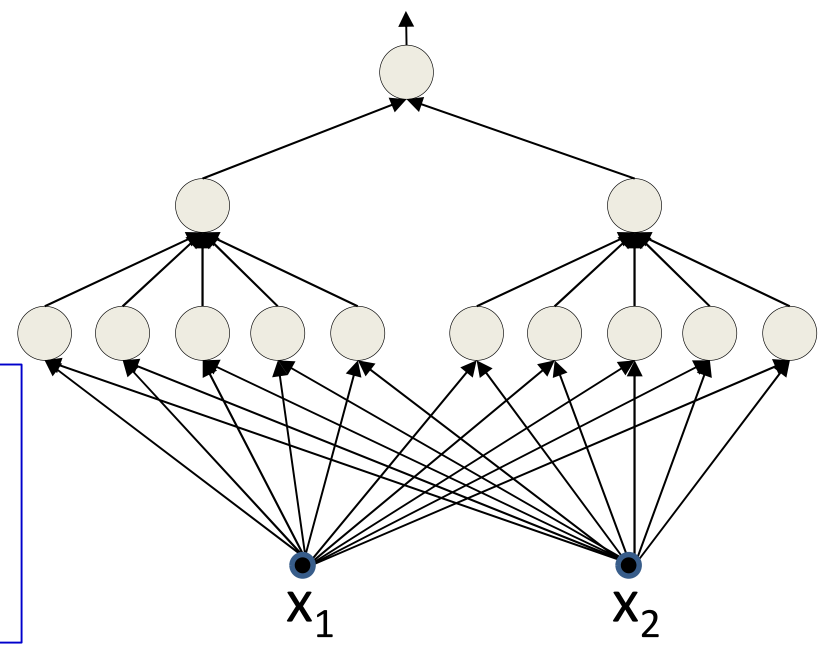
Individual neurons represent one of the lines that compose the figure (linear classifiers)



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

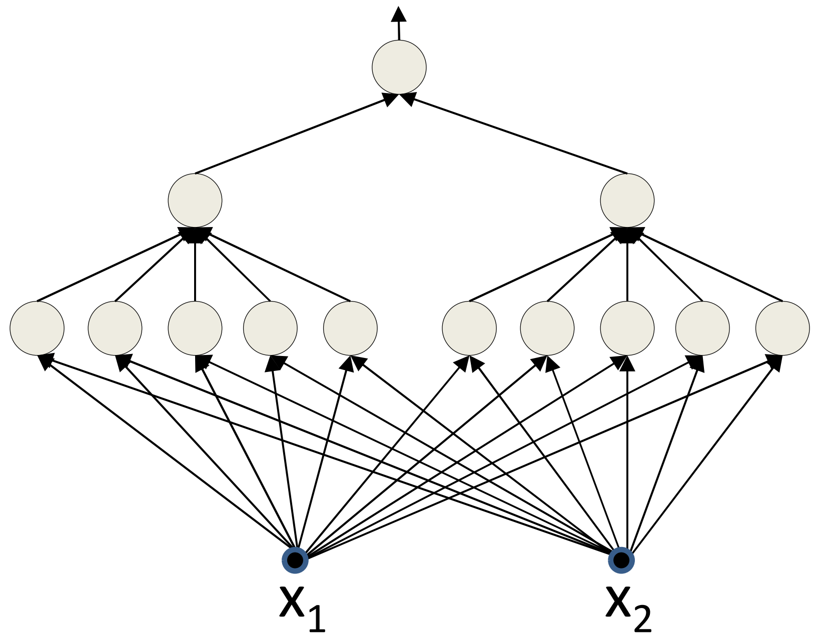
The linear separators must combine to form the desired boundary



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

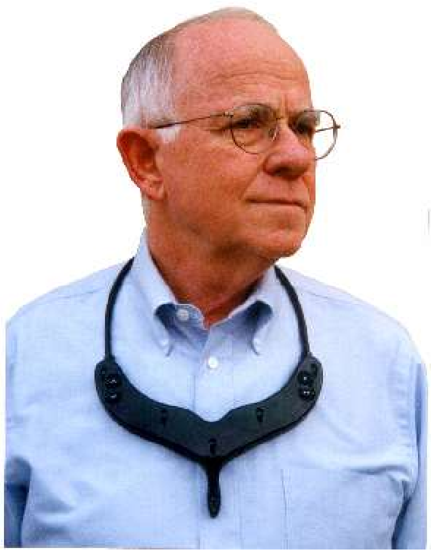
- Training this network using the perceptron rule is a combinatorial optimization problem
- We don't know the outputs of the individual intermediate neurons in the network for any training input
- **Must also determine the correct output for *each* neuron for *every* training instance**
- **NP! Exponential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

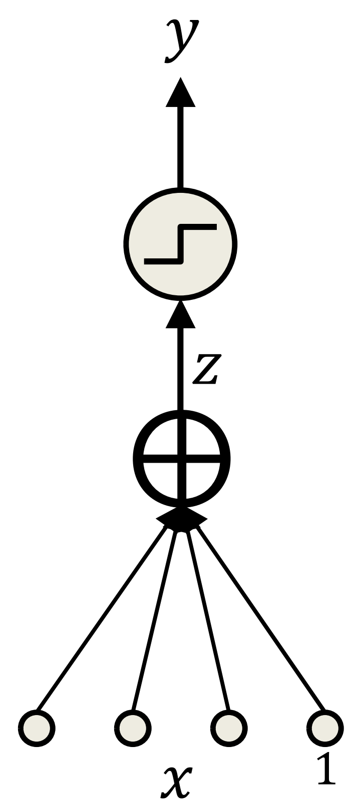
- First known attempt at an analytical solution to training the perceptron and the MLP
- Now famous as the LMS algorithm
  - Used everywhere
  - Also known as the "delta rule"

History: ADALINE

$$z = \sum_t w_i x_i$$

Using 1-extended vector notation to account for bias

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

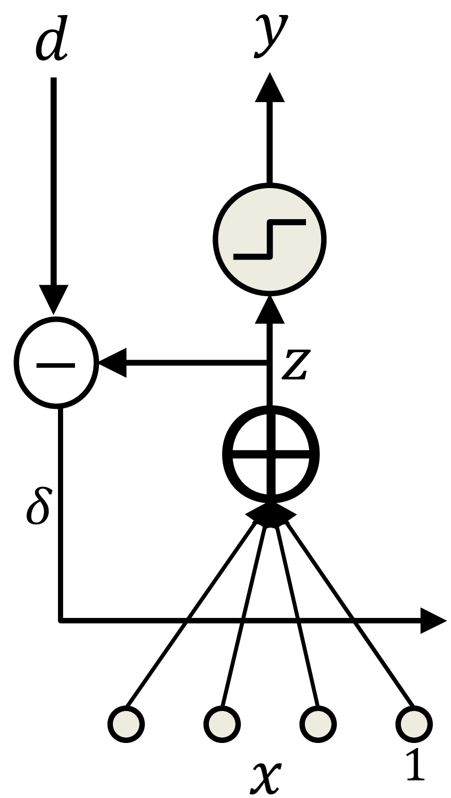


- Adaptive *linear* element (Hopf and Widrow, 1960)
- Actually just a regular perceptron
  - Weighted sum on inputs and bias passed through a thresholding function
- ADALINE differs in the *learning rule*

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

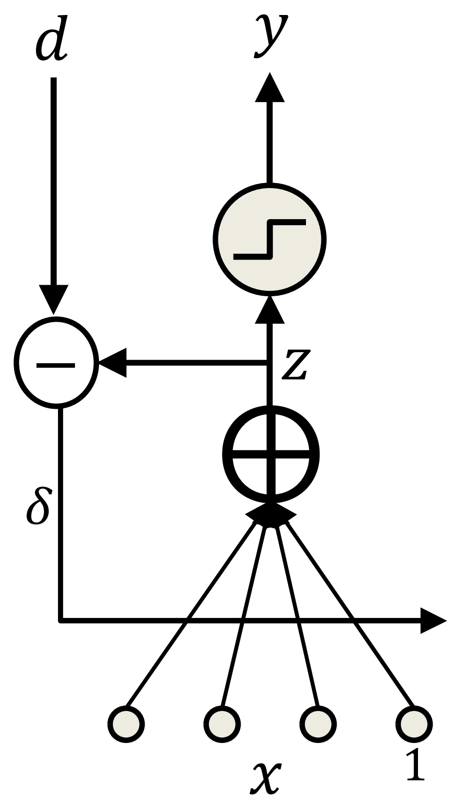
$$\frac{dErr(x)}{dw_i} = -(d - z)x_i$$

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

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

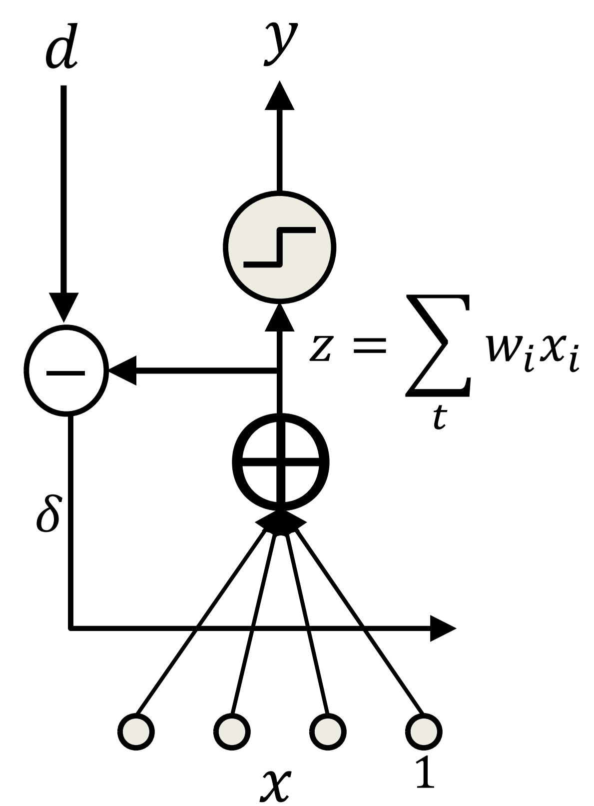
The ADALINE learning rule

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

$$\delta = d - z$$

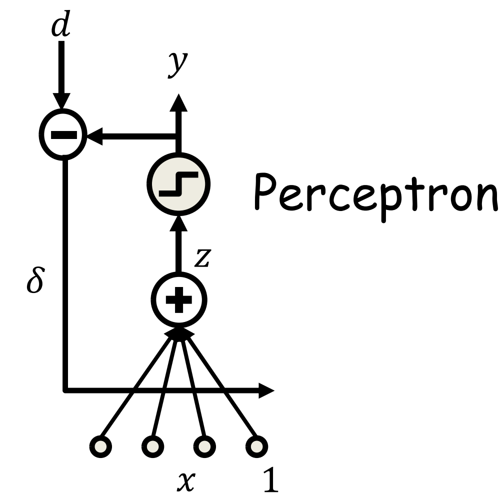
$$w_i = w_i + \eta \delta x_i$$

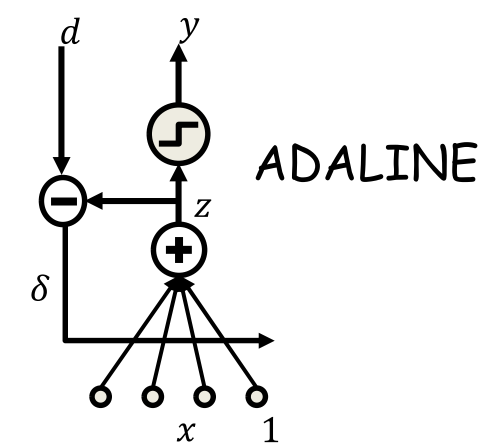
- This is the famous *delta rule*
  - Also called the LMS update rule



The Delta Rule

- In fact both the Perceptron and ADALINE use variants of the delta rule!
  - Perceptron: Output used in delta rule is y
  $$\delta = d - y$$
  - ADALINE: Output used to estimate weights is z
  $$\delta = d - z$$
- For both
$$w_i = w_i + \eta\delta x_i$$



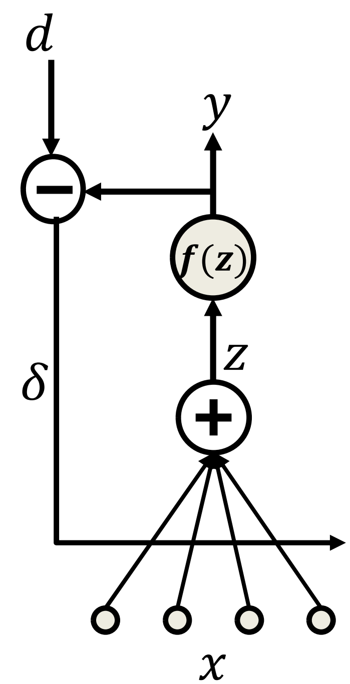


Aside: Generalized delta rule

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

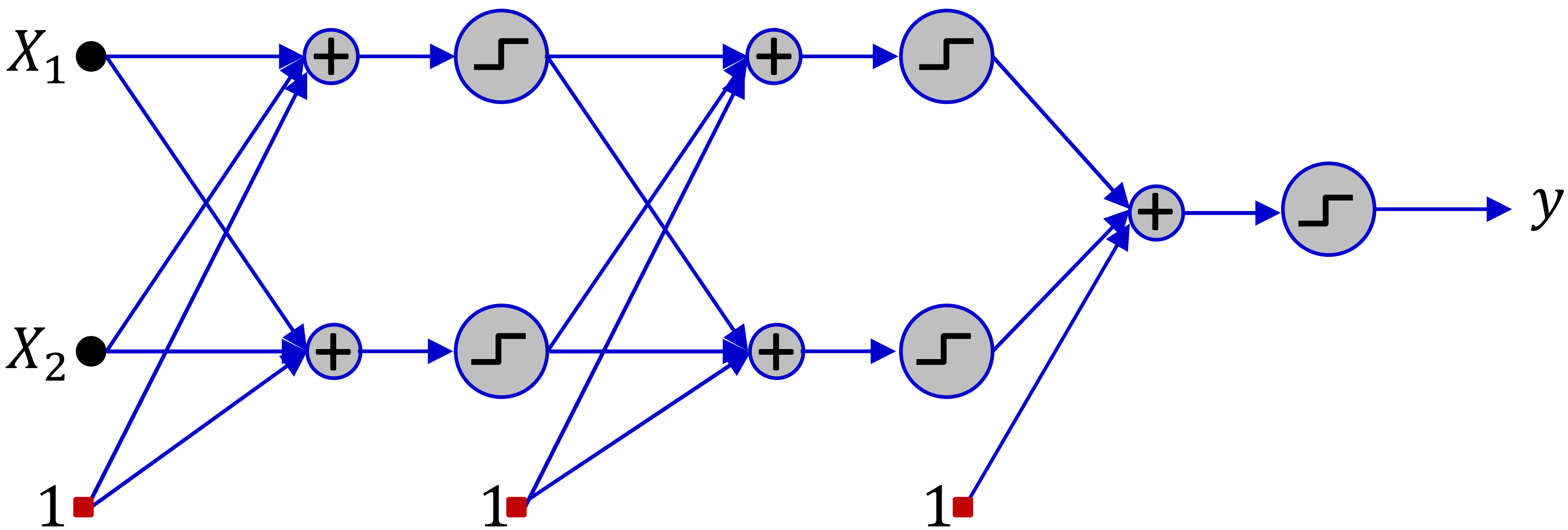
$$\delta = d - y$$

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



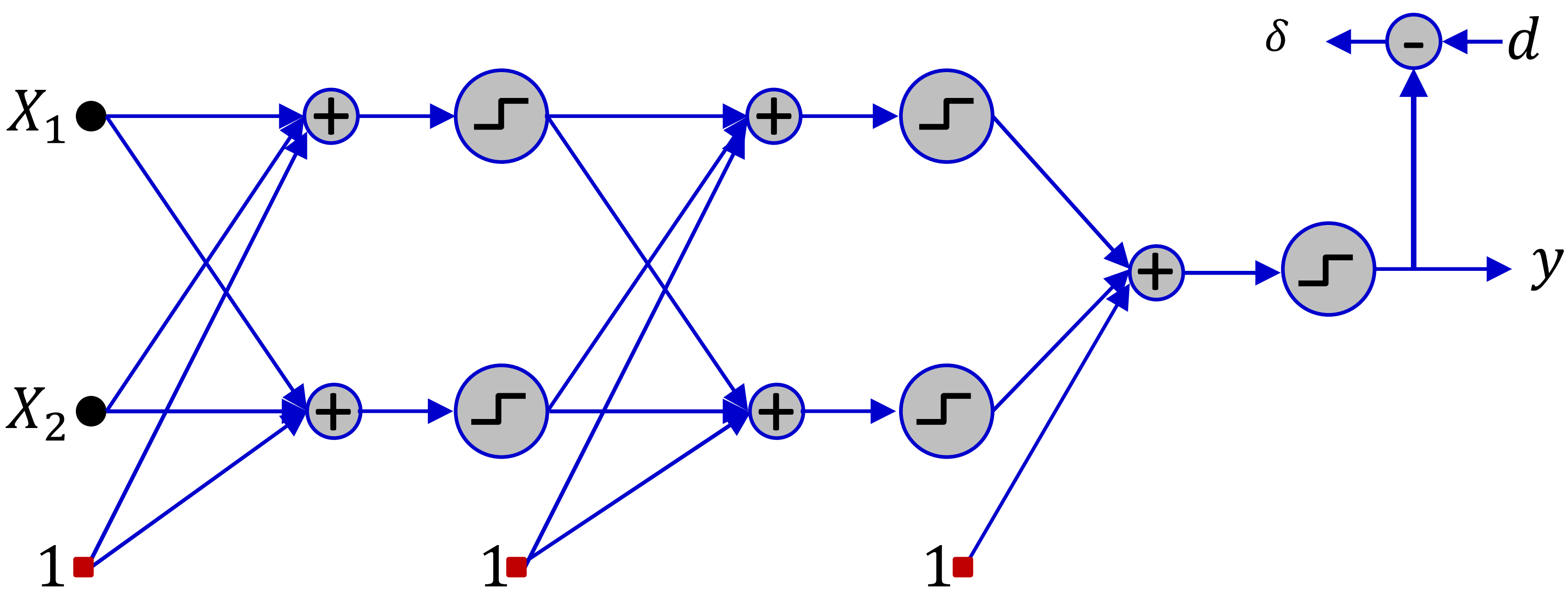
- This is the famous Widrow-Hoff update rule
  - Lookahead: Note that this is *exactly* backpropagation in multilayer nets if we let $f(z)$ represent the entire network between z and y
- It is possibly the most-used update rule in machine learning and signal processing
  - Variants of it appear in almost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

Multilayer perceptron: MADALINE



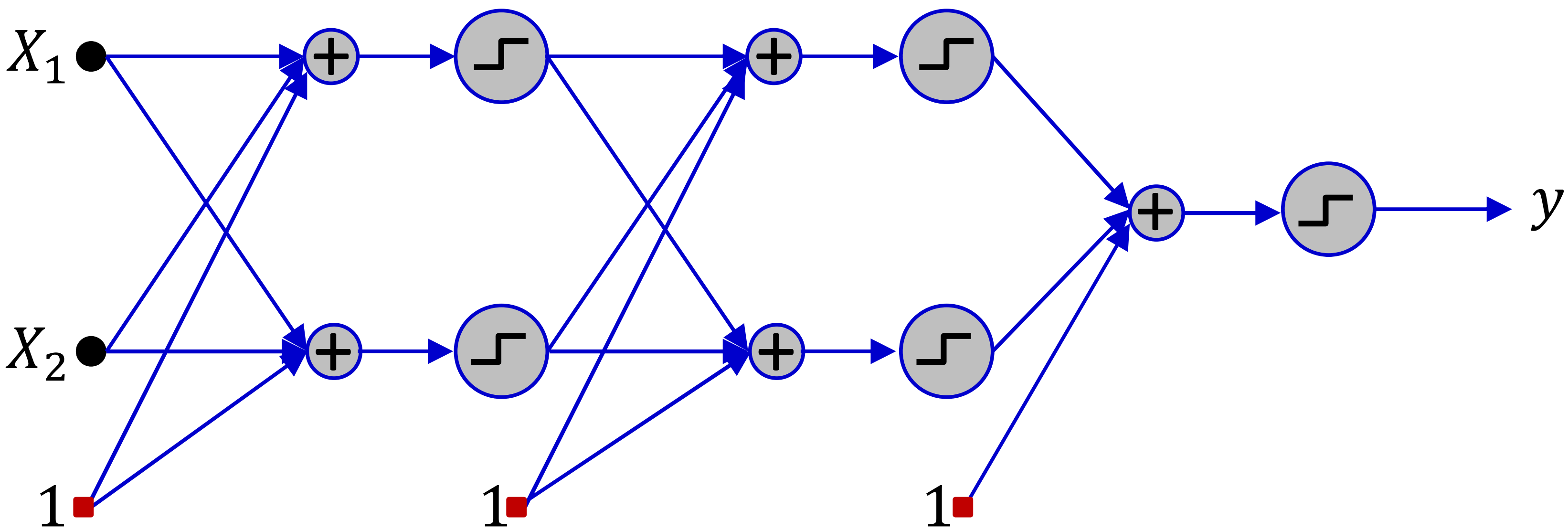
- *Multiple* Adaline
  - A multilayer perceptron with threshold activations
  - The MADALINE

MADALINE Training



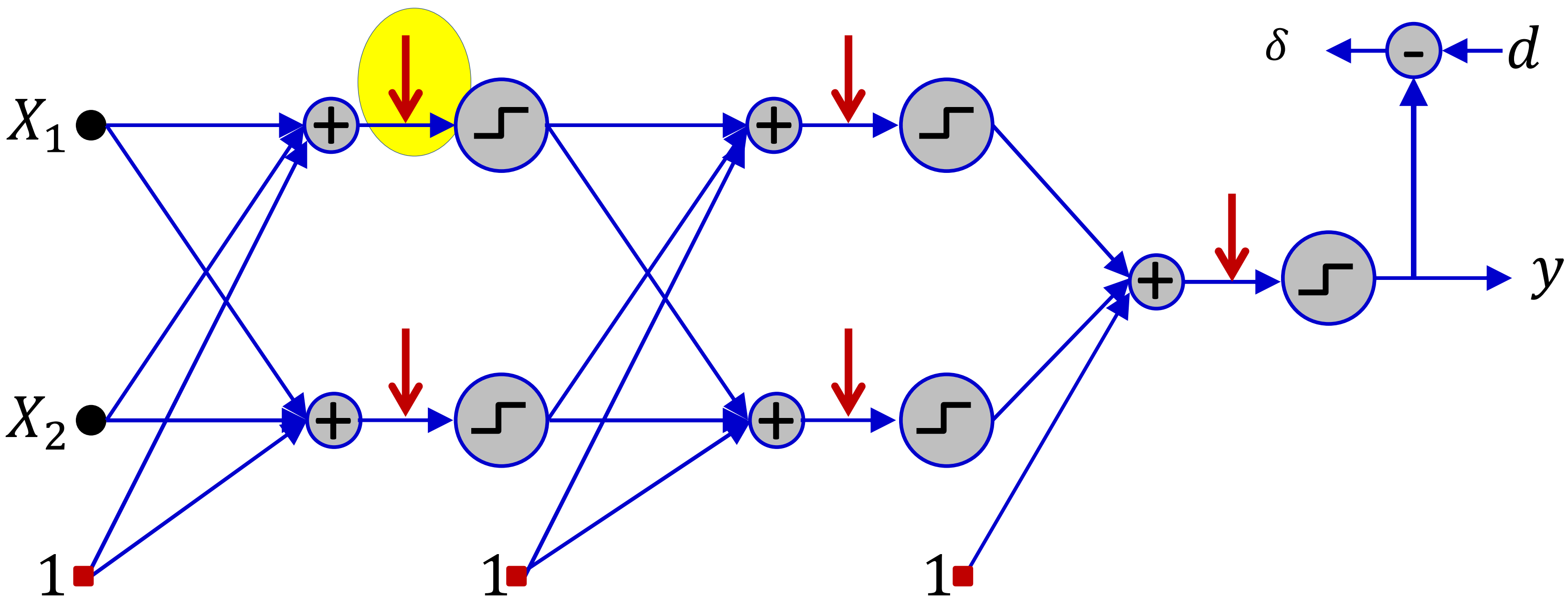
- *Update only on error*
  - $\delta \neq 0$
  - On inputs for which output and target values differ

MADALINE Training



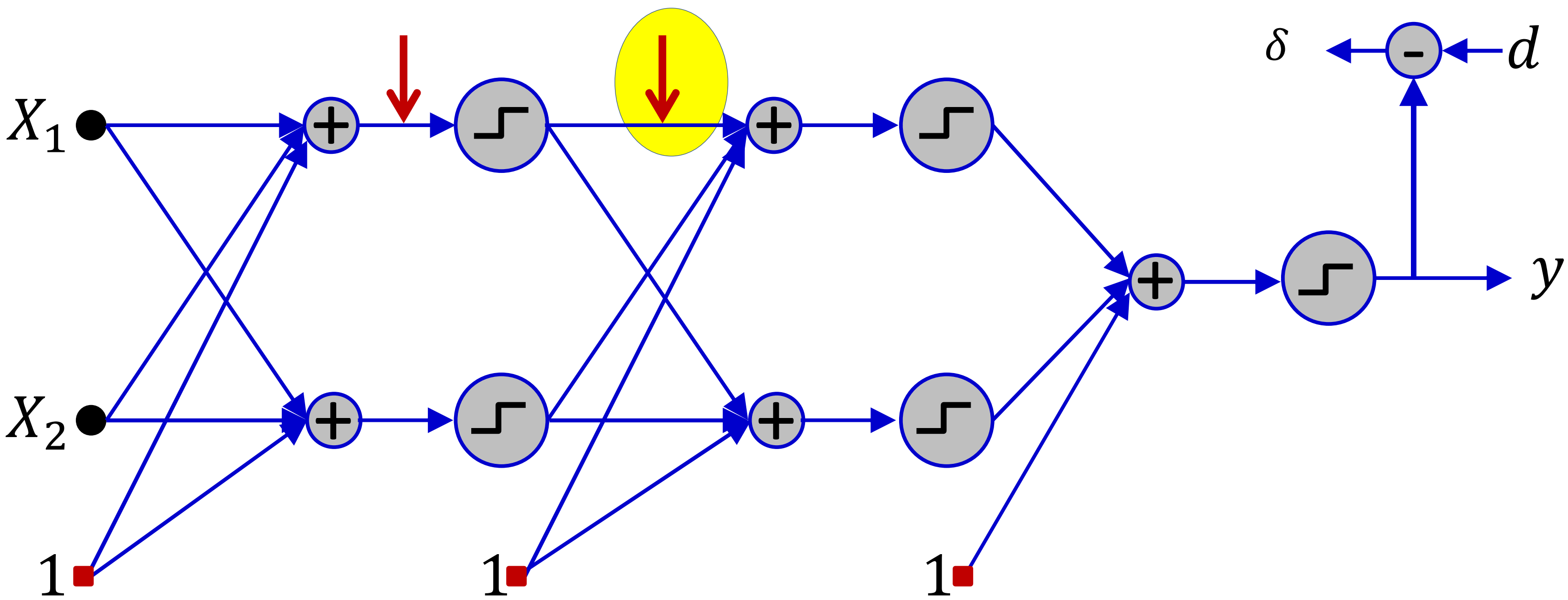
- While stopping criterion not met do:
  - Classify an input

MADALINE Training



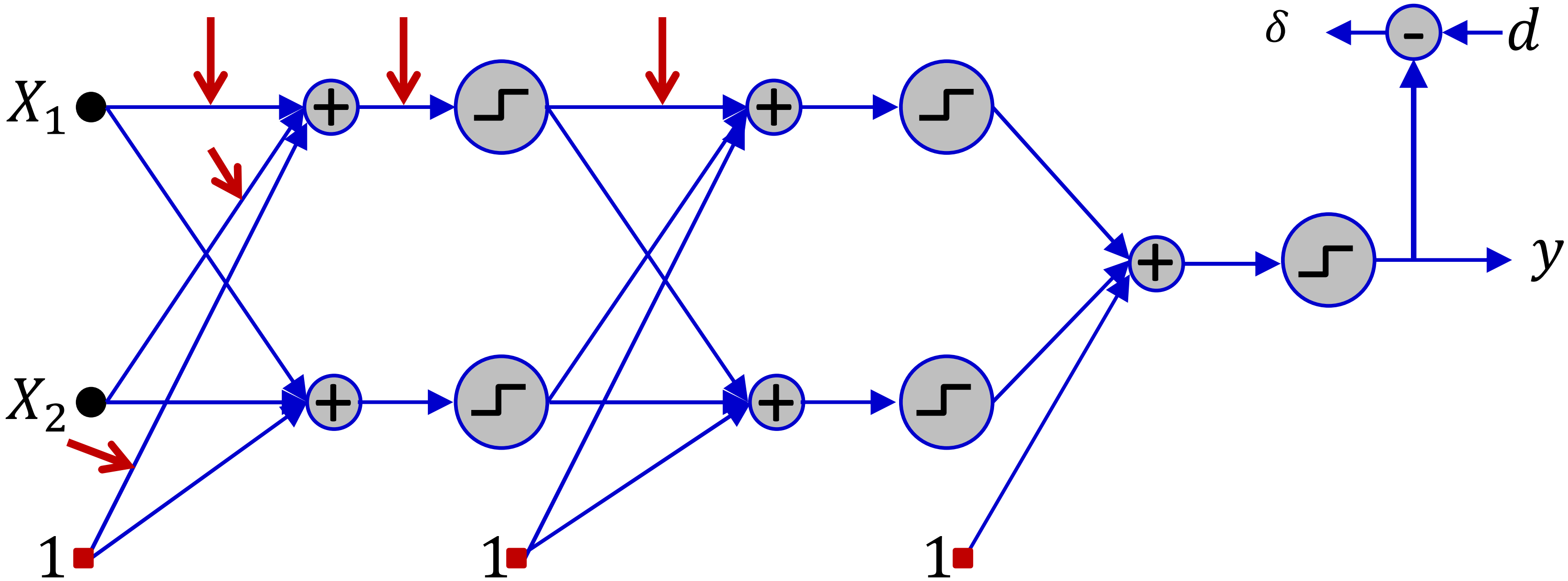
- While stopping criterion not met do:
  - Classify an input
  - If error, find the z that is closest to 0

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

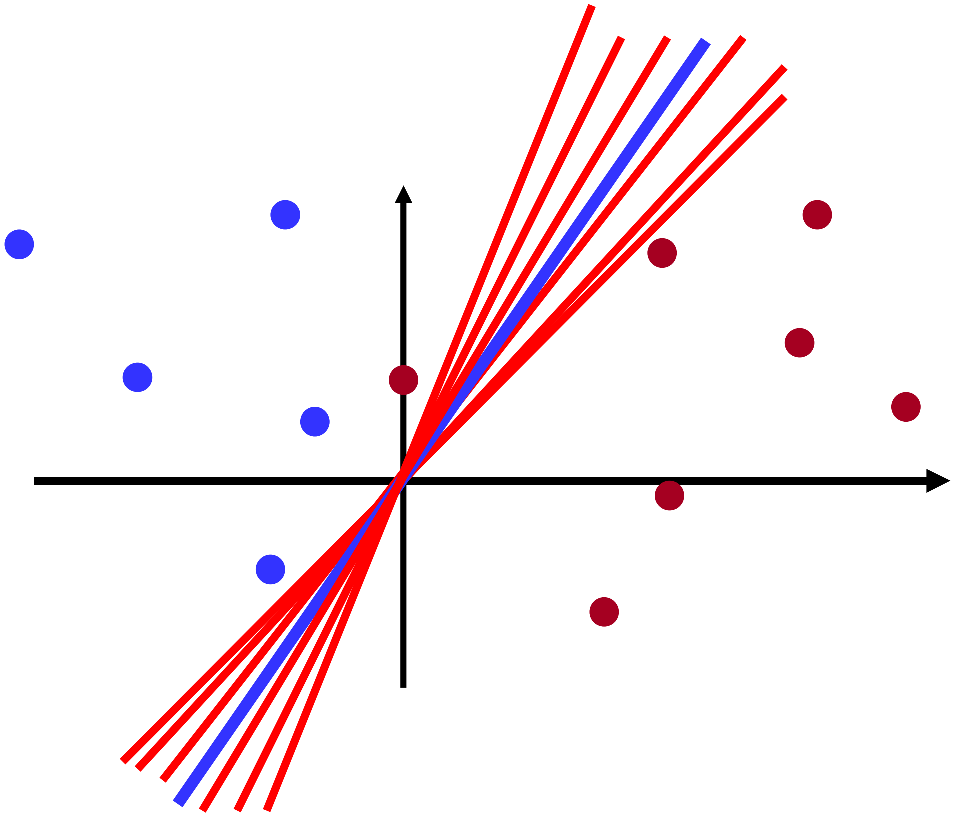
Story so far

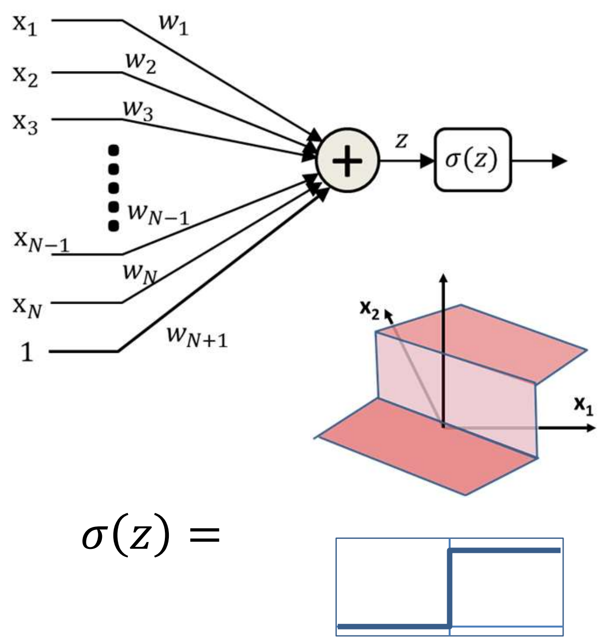
- "Learning" a network = learning the weights and biases to compute a target function
  - Will require a network with sufficient "capacity"
- In practice, we learn networks by "fitting" them to match the input-output relation of "training" instances drawn from the target function
- A linear decision boundary can be learned by a single perceptron (with a threshold-function activation) in linear time if classes are linearly separable
- Non-linear decision boundaries require networks of perceptrons
- Training an MLP with threshold-function activation perceptrons will require knowledge of the input-output relation for every training instance, for *every* perceptron in the network
  - These must be determined as part of training
  - For threshold activations, this is an NP-complete combinatorial optimization problem

History..

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

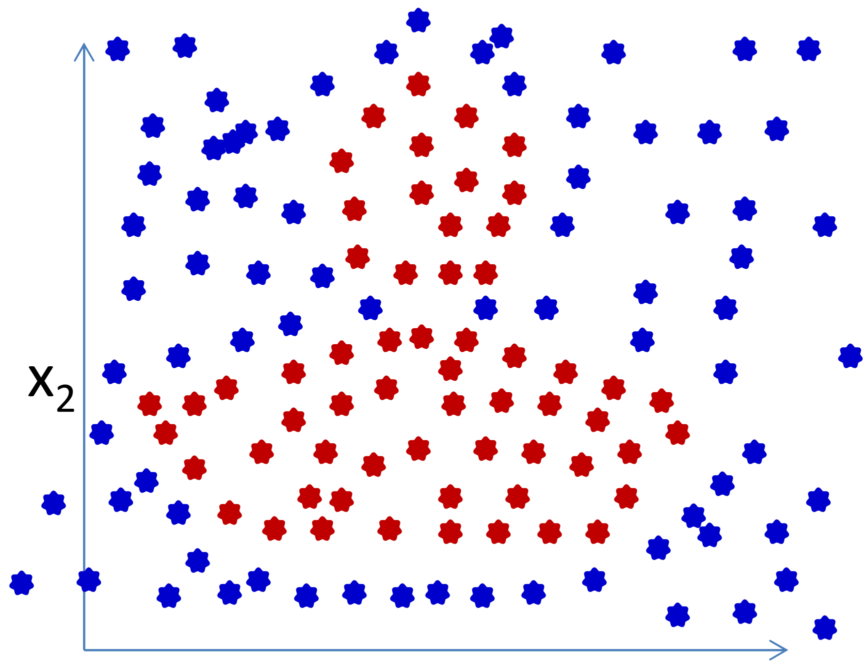
Why this problem?

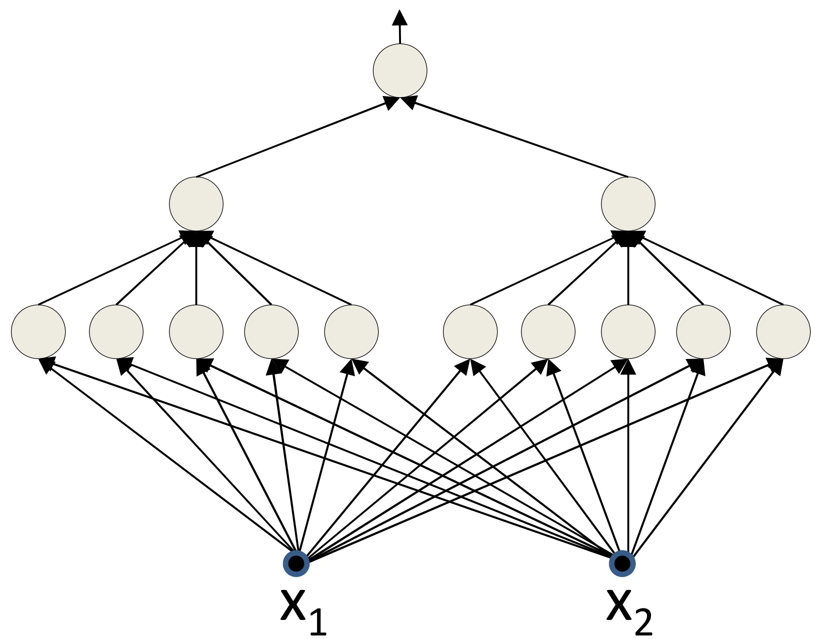




- The perceptron is a flat function with zero derivative everywhere, except at 0 where it is non-differentiable
  - You can vary the weights a *lot* without changing the error
  - There is no indication of which direction to change the weights to reduce error

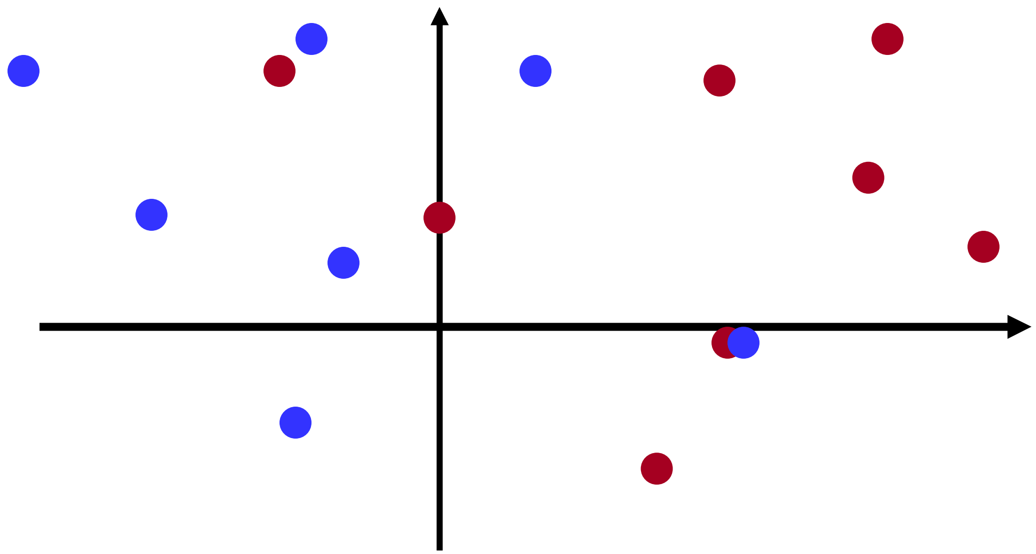
This only compounds on larger problems





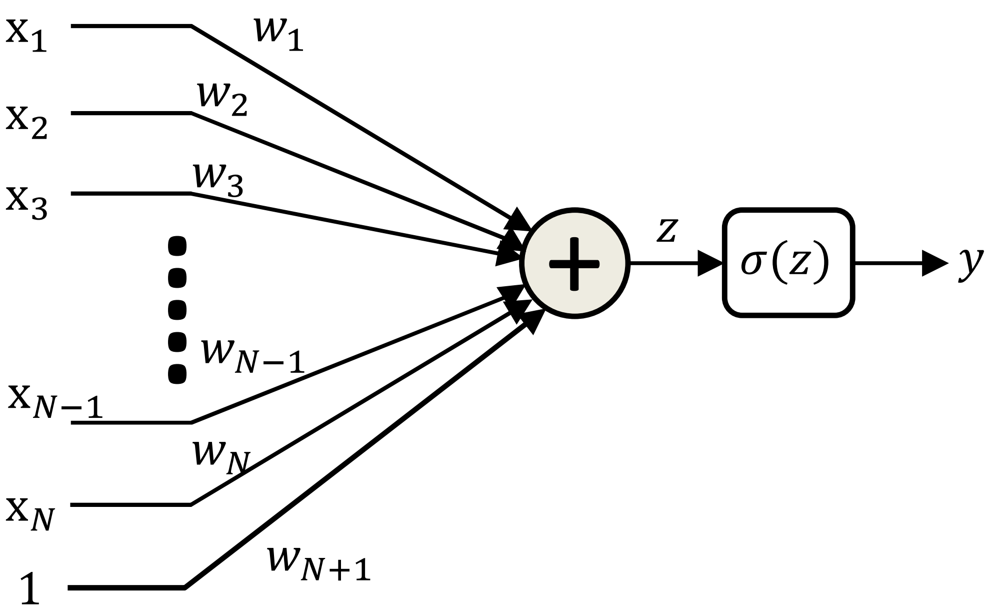
- Individual neurons' weights can change significantly without changing overall error
- The simple MLP is a flat, non-differentiable function
  - Actually a function with 0 derivative nearly everywhere, and no derivatives at the boundaries

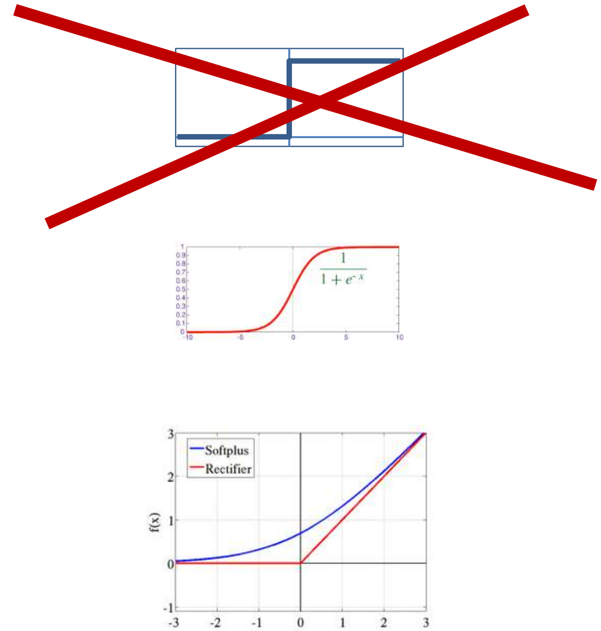
A second problem: What we *actually* model



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

Solution

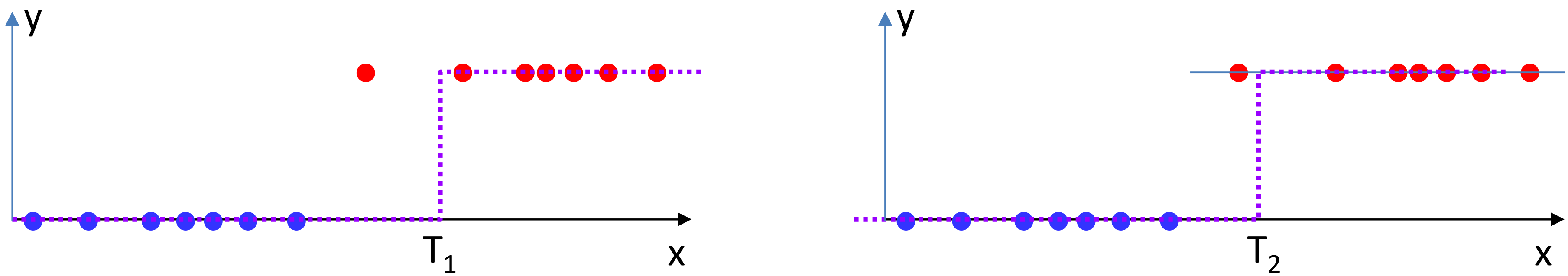




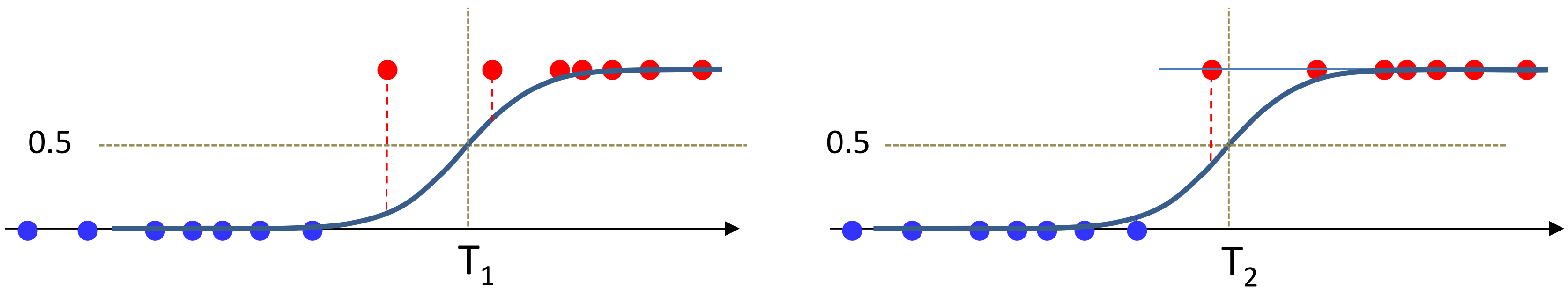
$Activation\ functions\ \sigma(z)$

- Lets make the neuron differentiable, *with non-zero derivatives over much of the input space*
  - Small changes in weight can result in non-negligible changes in output
  - This enables us to estimate the parameters using gradient descent techniques..

Differentiable activation function

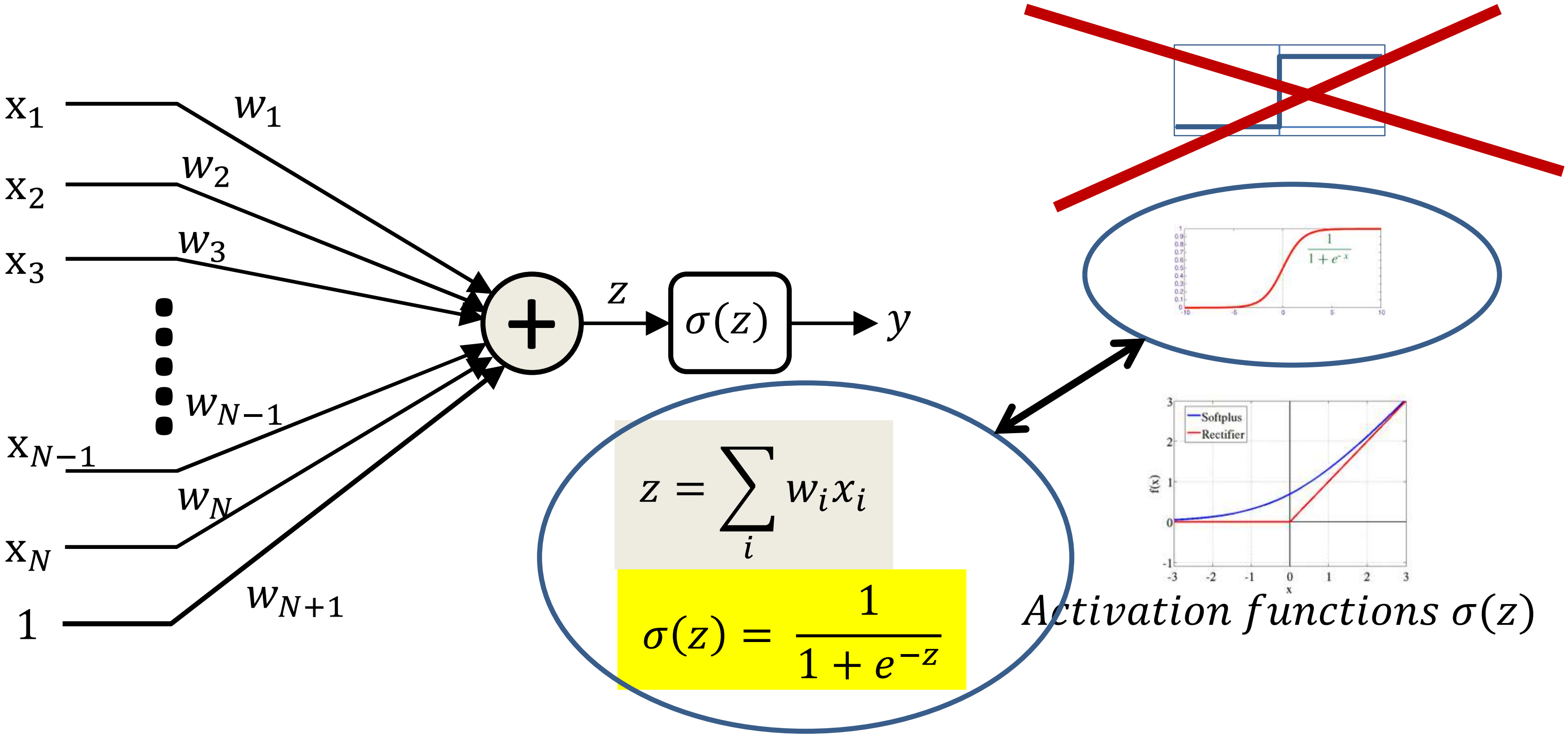


- Threshold activation: shifting the threshold from T_1 to T_2 does not change classification error
  - Does not indicate if moving the threshold left was good or not



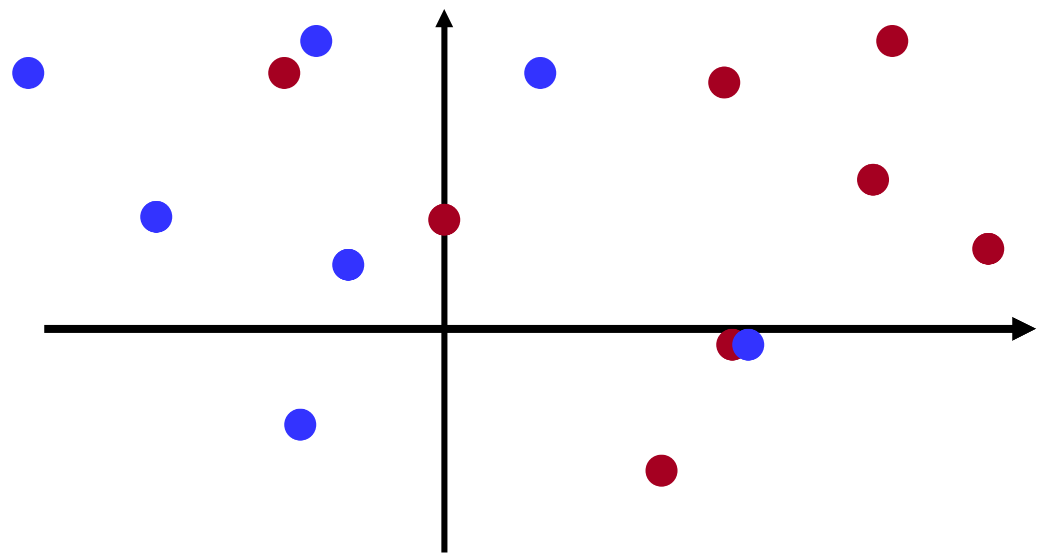
- Smooth, continuously varying activation: Classification based on whether the output is greater than 0.5 or less
  - Can now quantify *how much* the output differs from the desired target value (0 or 1)
  - Moving the function left or right changes this quantity, even if the classification error itself doesn't change

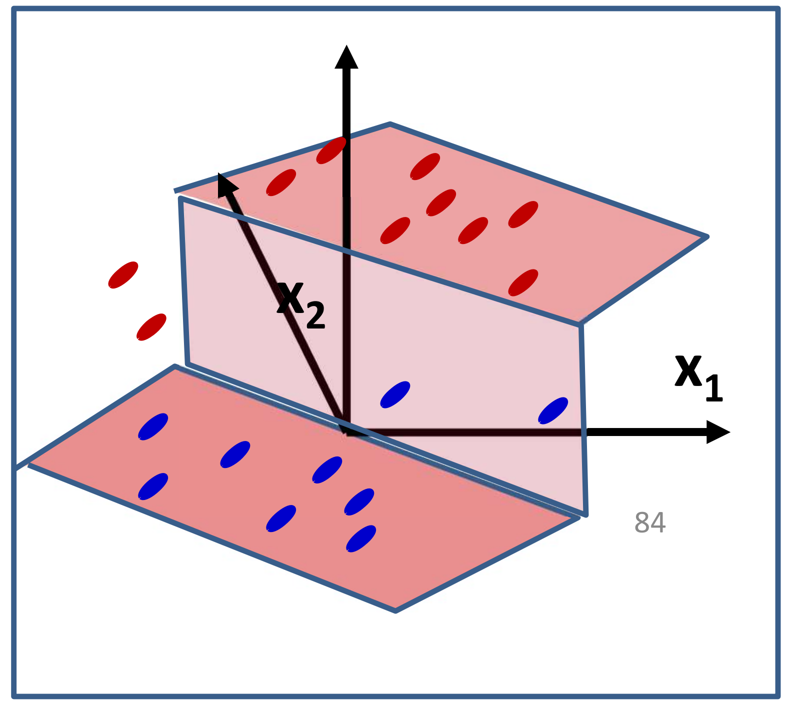
The sigmoid activation is special



- This particular one has a nice interpretation
- It can be interpreted as $P(y = 1|x)$

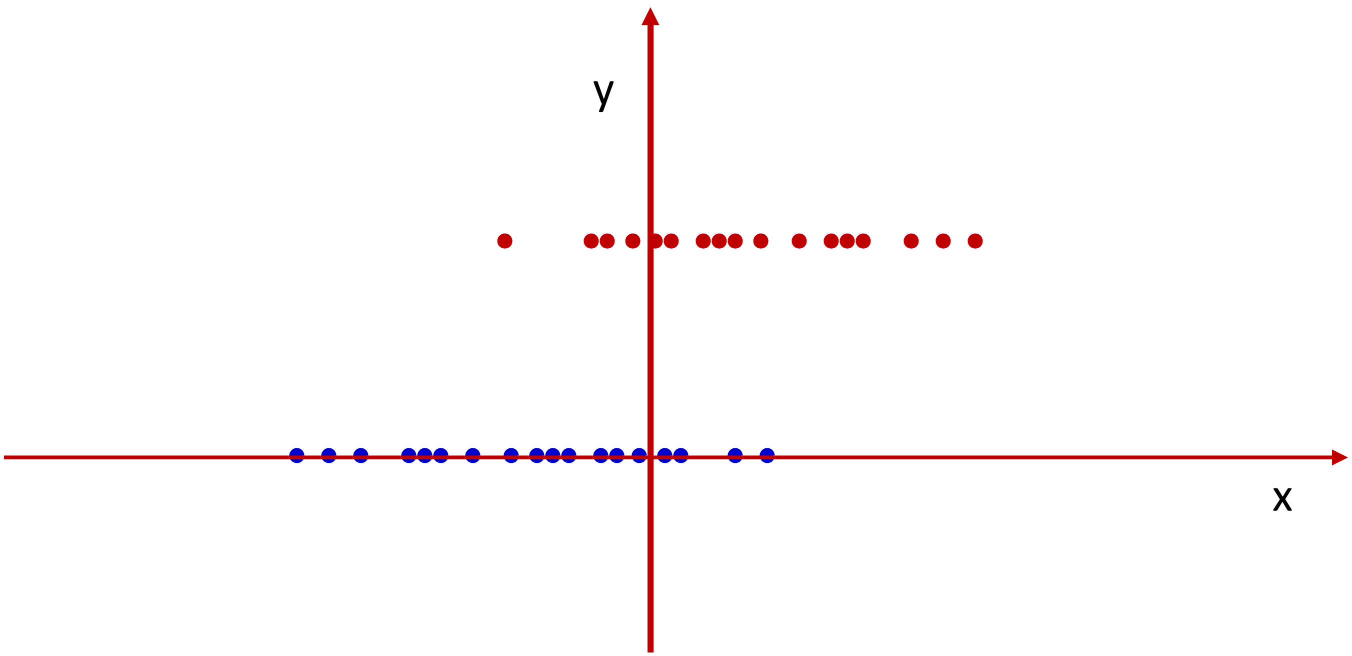
Non-linearly separable data





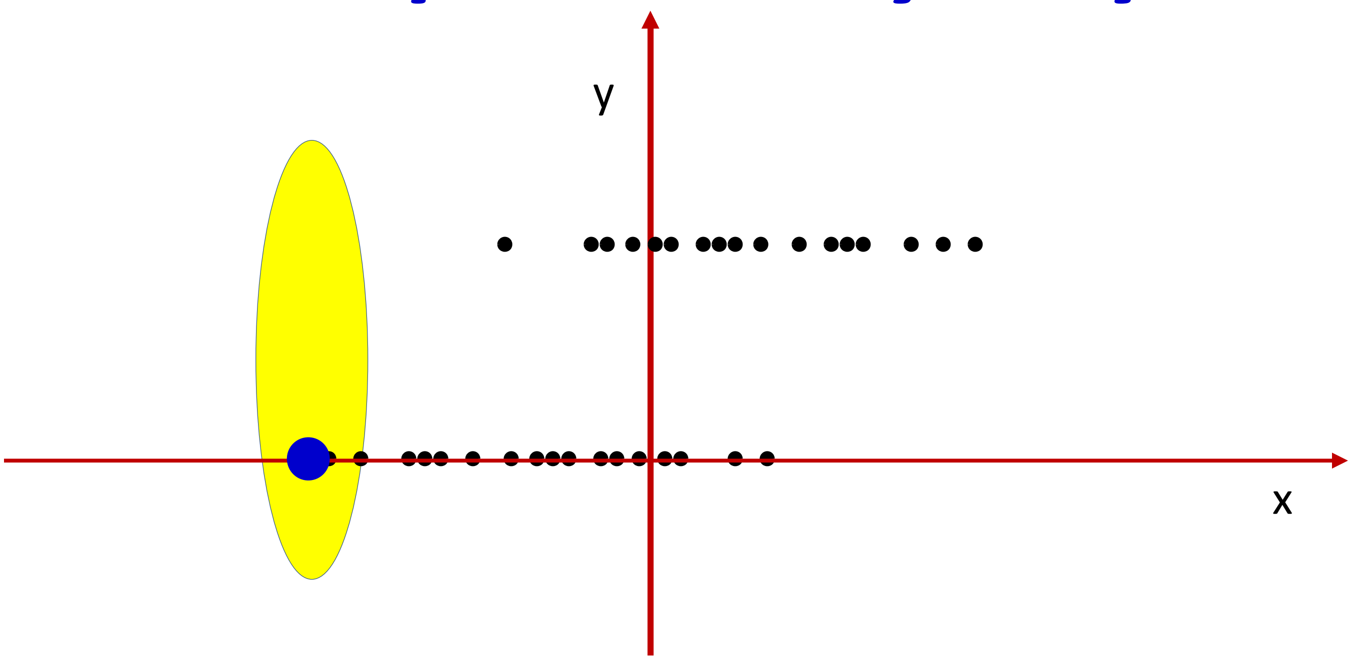
- Two-dimensional example
  - Blue dots (on the floor) on the “red” side
  - Red dots (suspended at Y=1) on the “blue” side
  - No line will cleanly separate the two colors

Non-linearly separable data: 1-D example



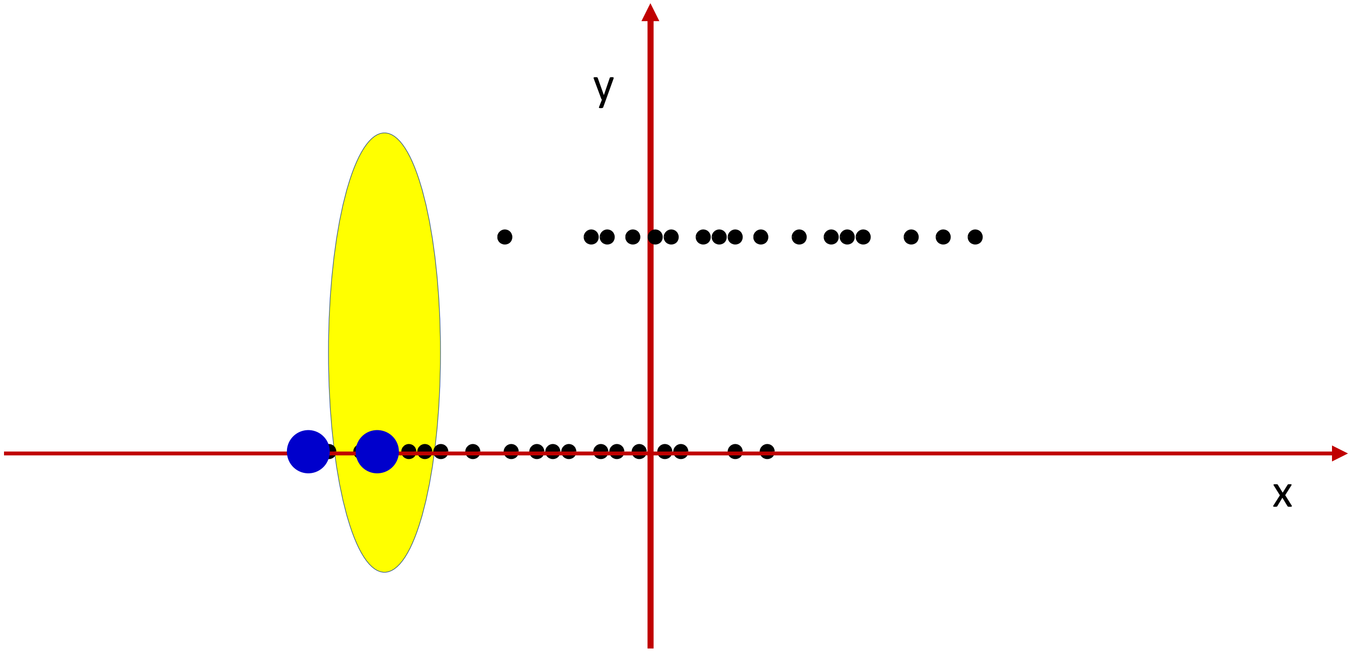
- One-dimensional example for visualization
  - All (red) dots at Y=1 represent instances of class Y=1
  - All (blue) dots at Y=0 are from class Y=0
  - The data are not linearly separable
    - In this 1-D example, a linear separator is a threshold
    - No threshold will cleanly separate red and blue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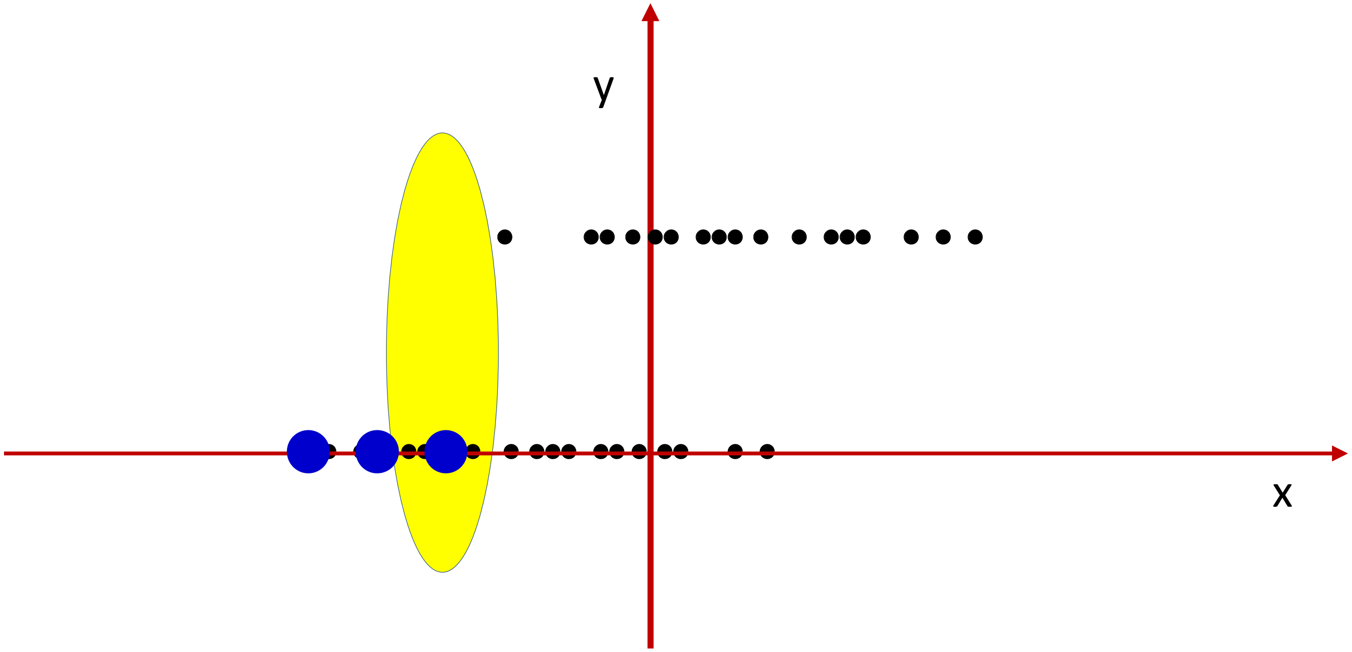
The *probability* of y=1



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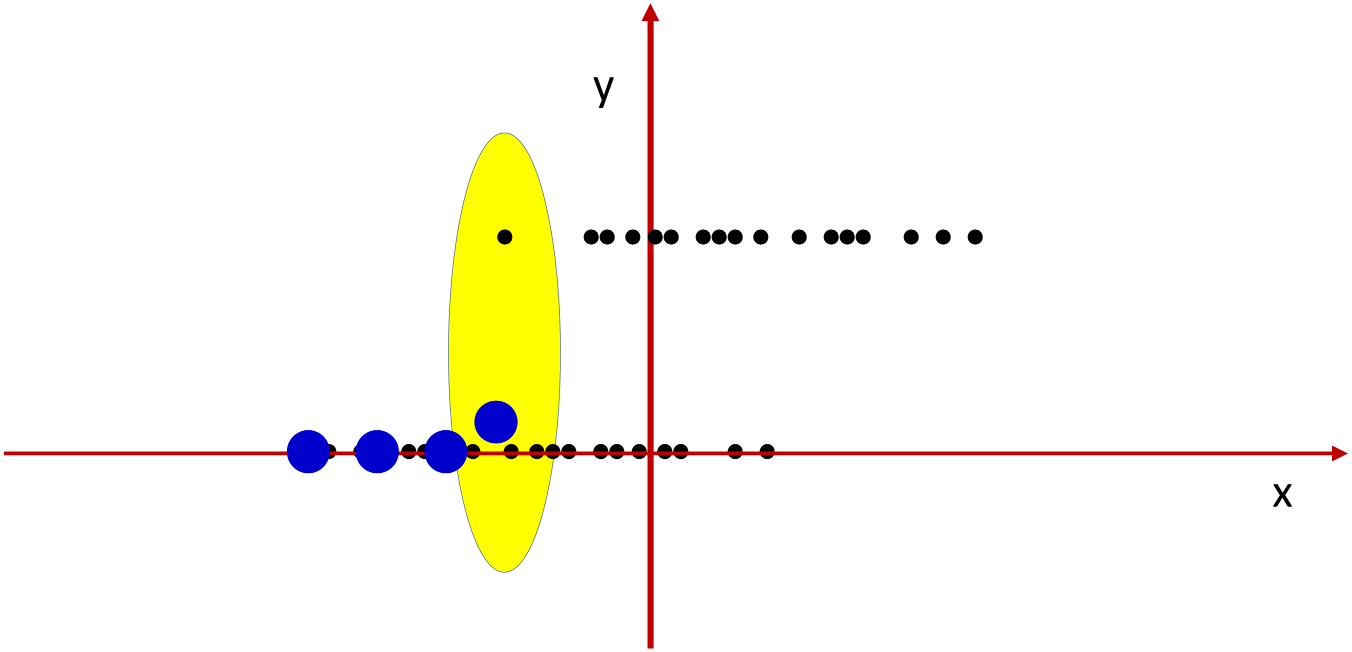

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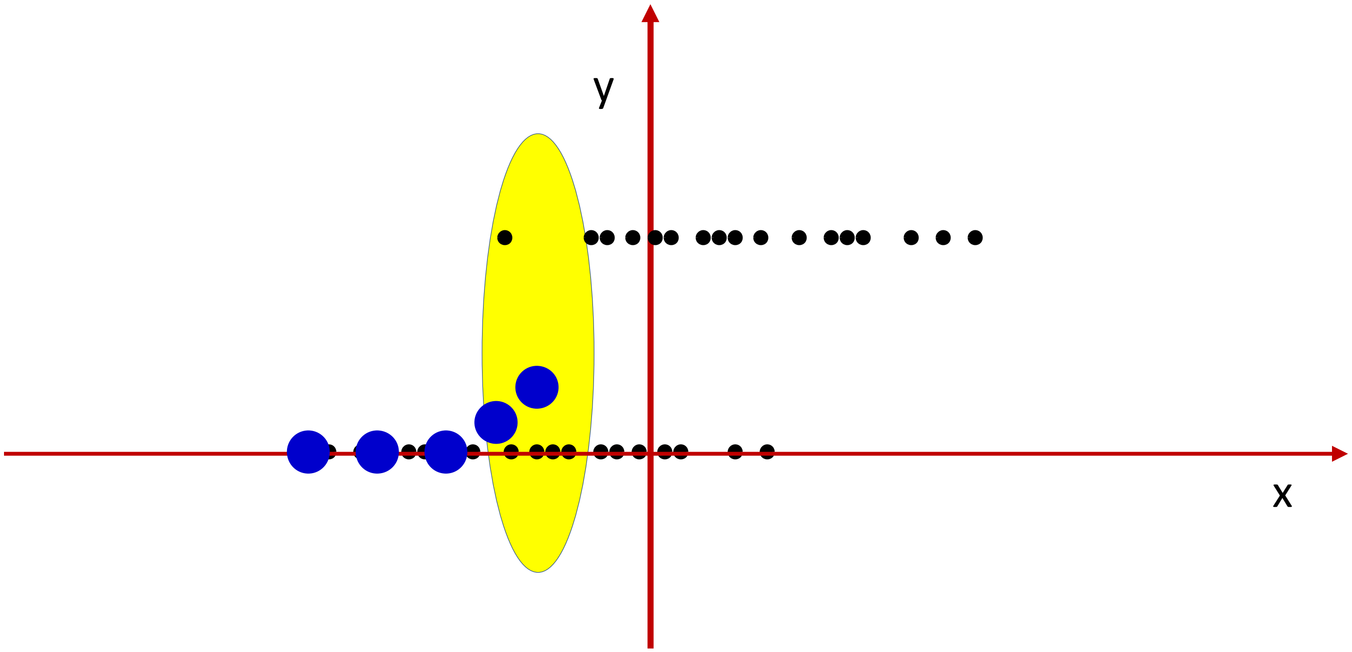

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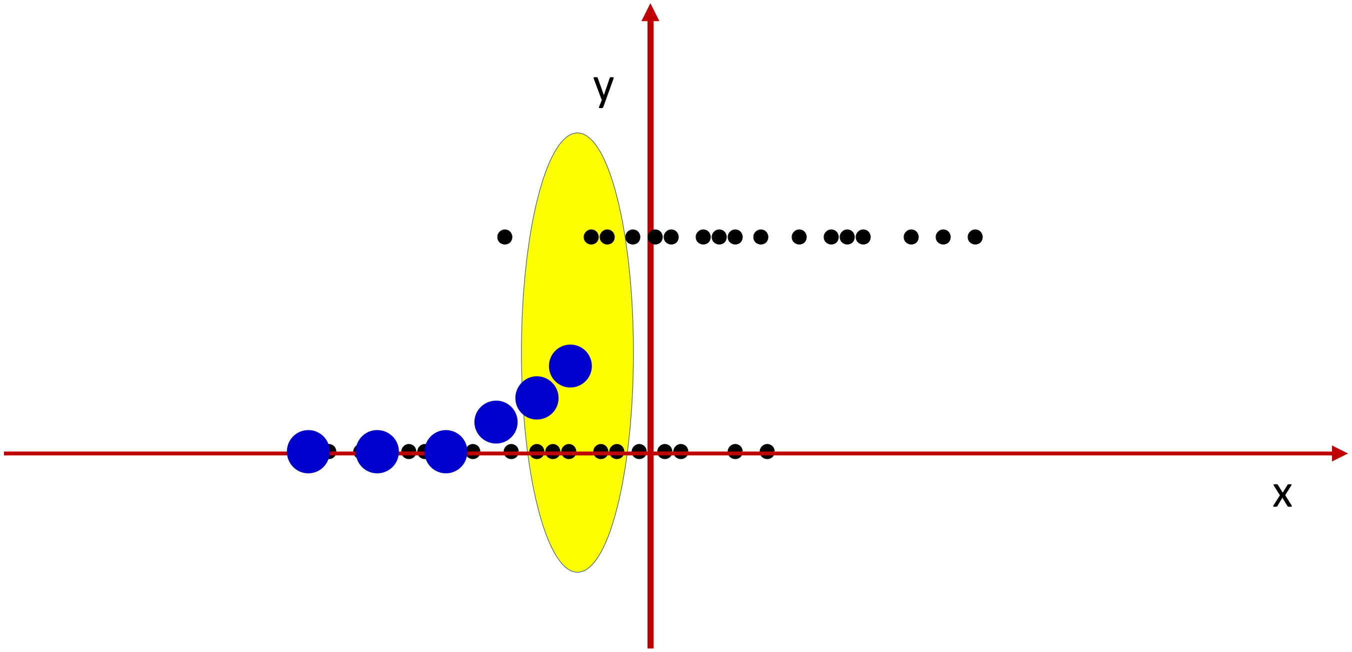

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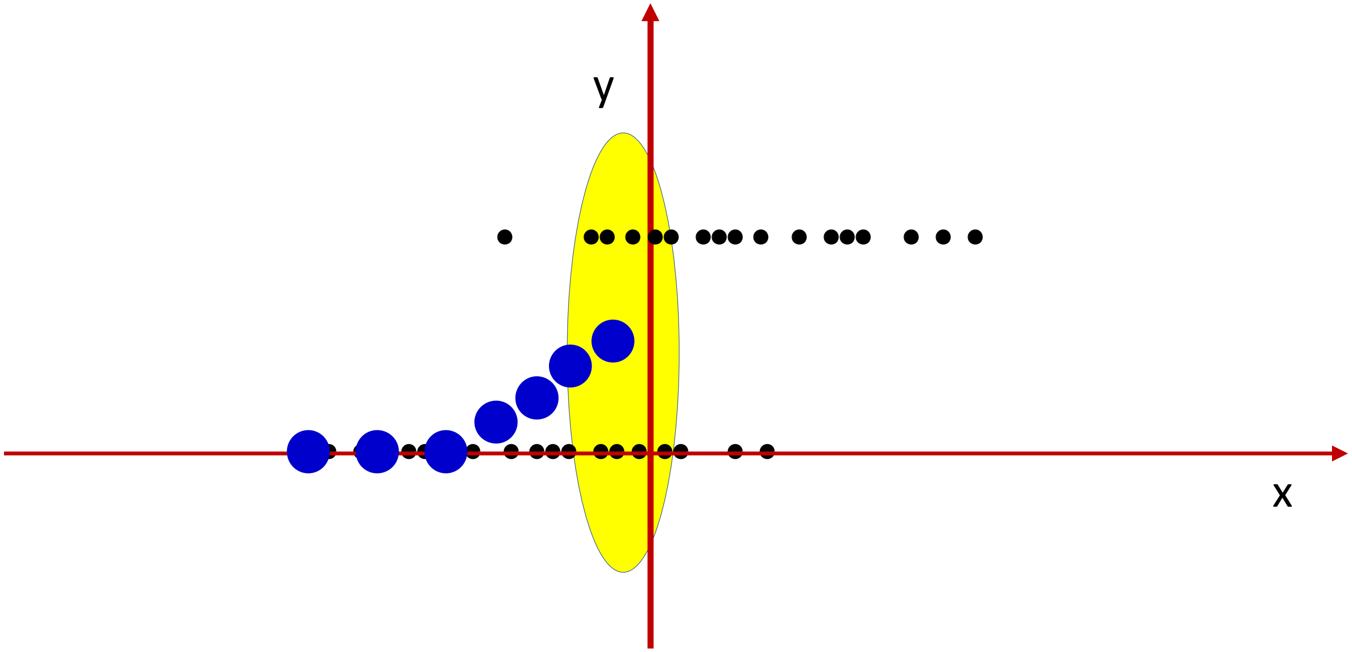
The *probability* of y=1



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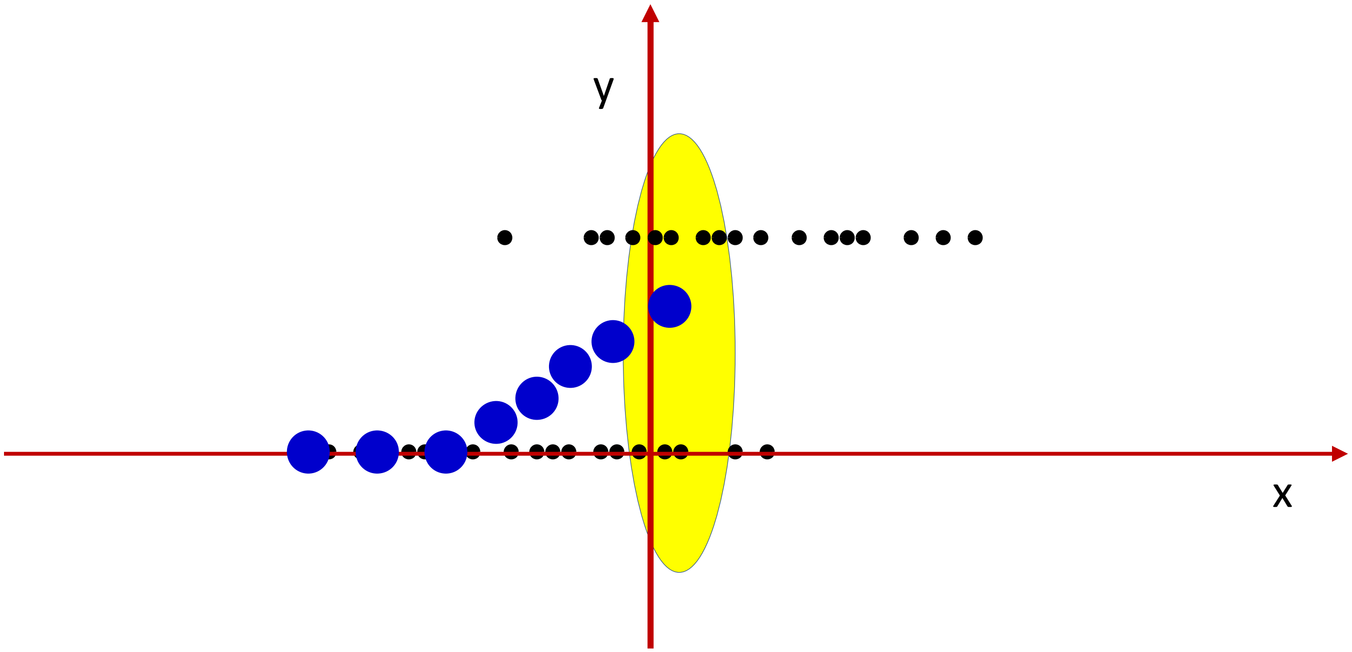
- Plot the average value within the window
  – This is an approximation of the *probability* of 1 at that point

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
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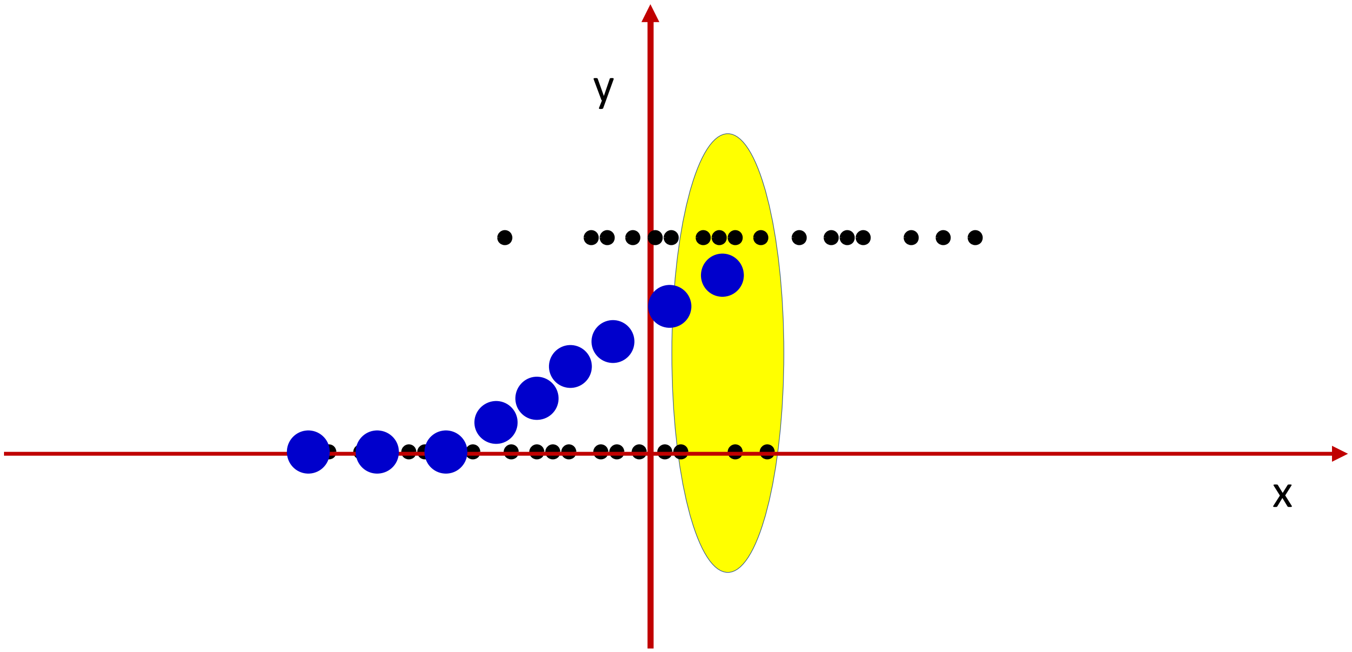
The *probability* of y=1



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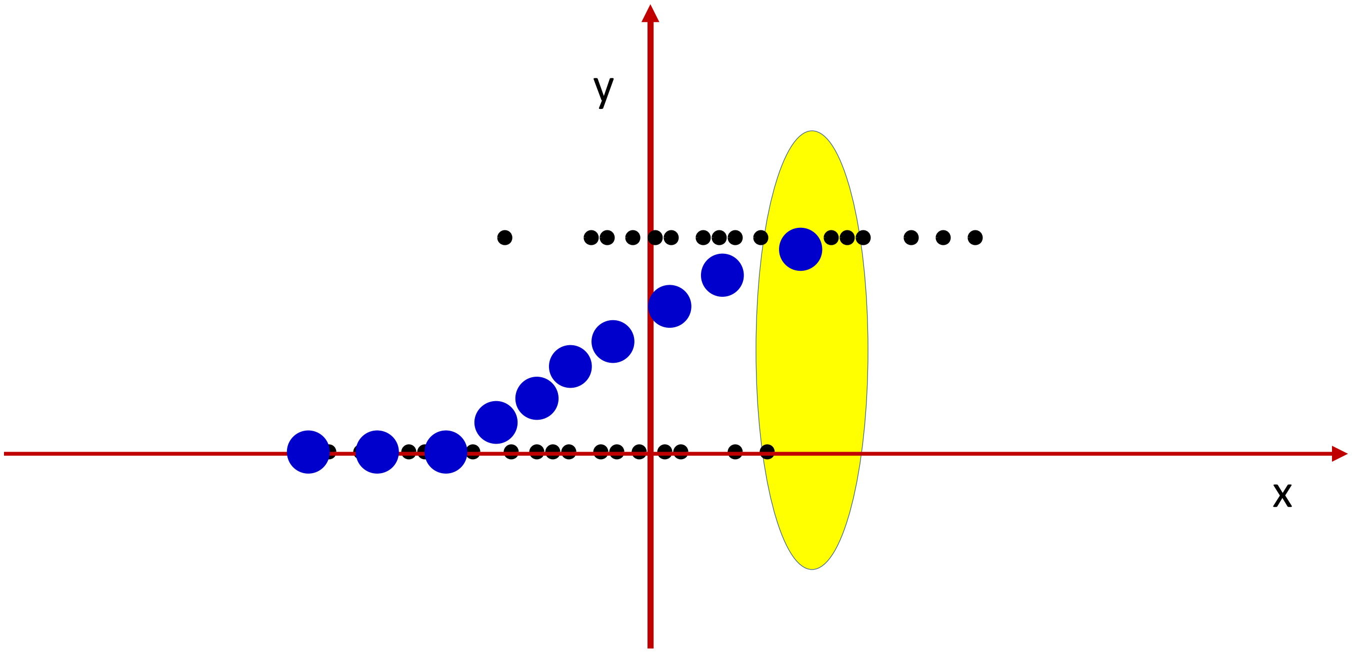
The *probability* of y=1



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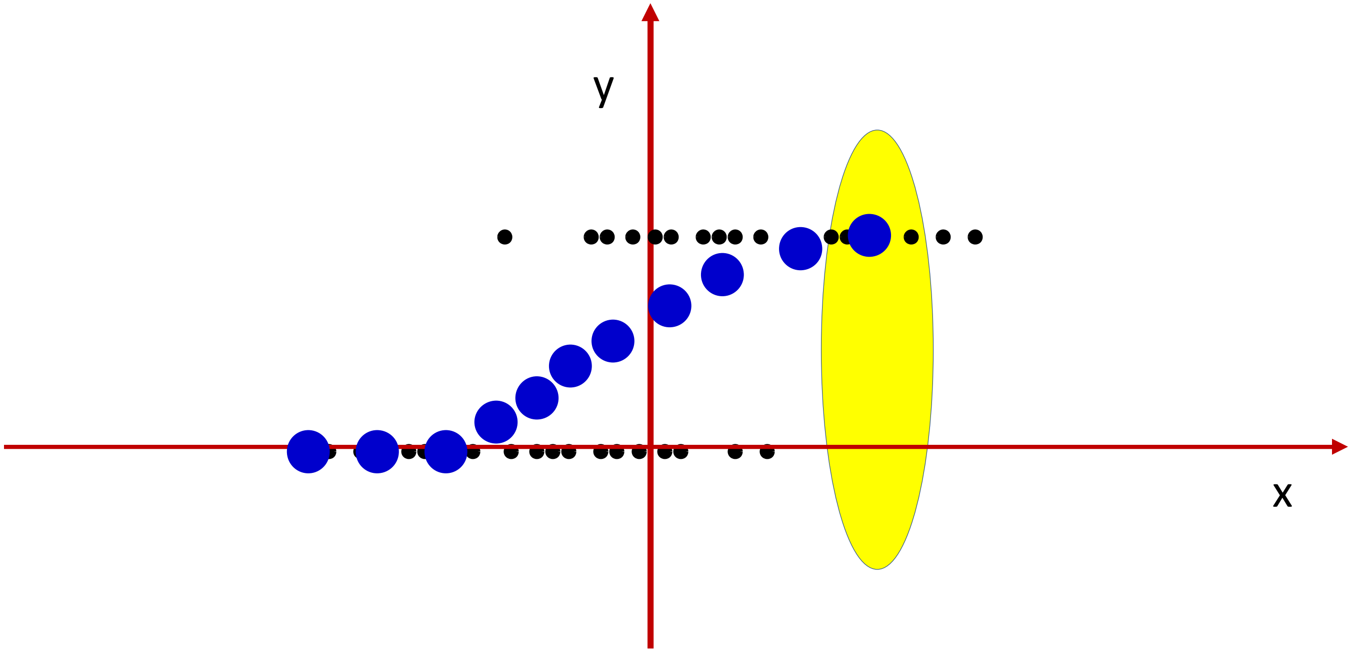

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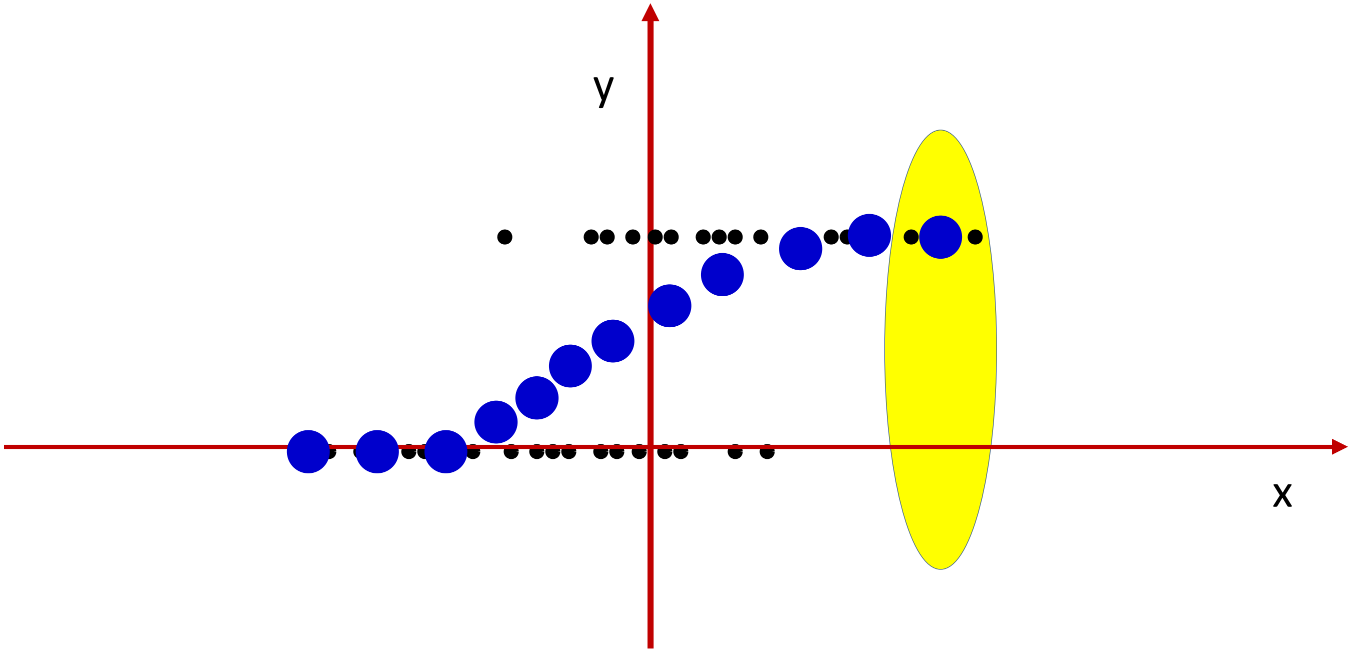

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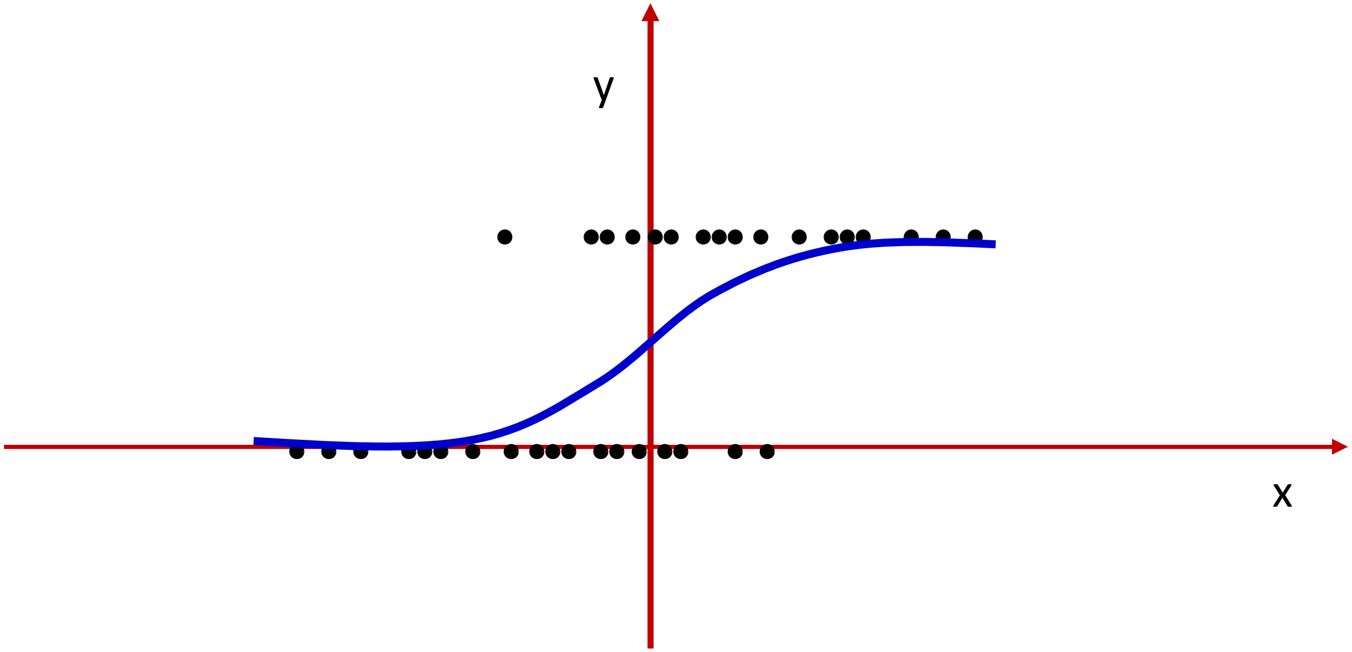
The *probability* of y=1



- Consider this differently: at each point look at a small window around that point
- Plot the average value within the window
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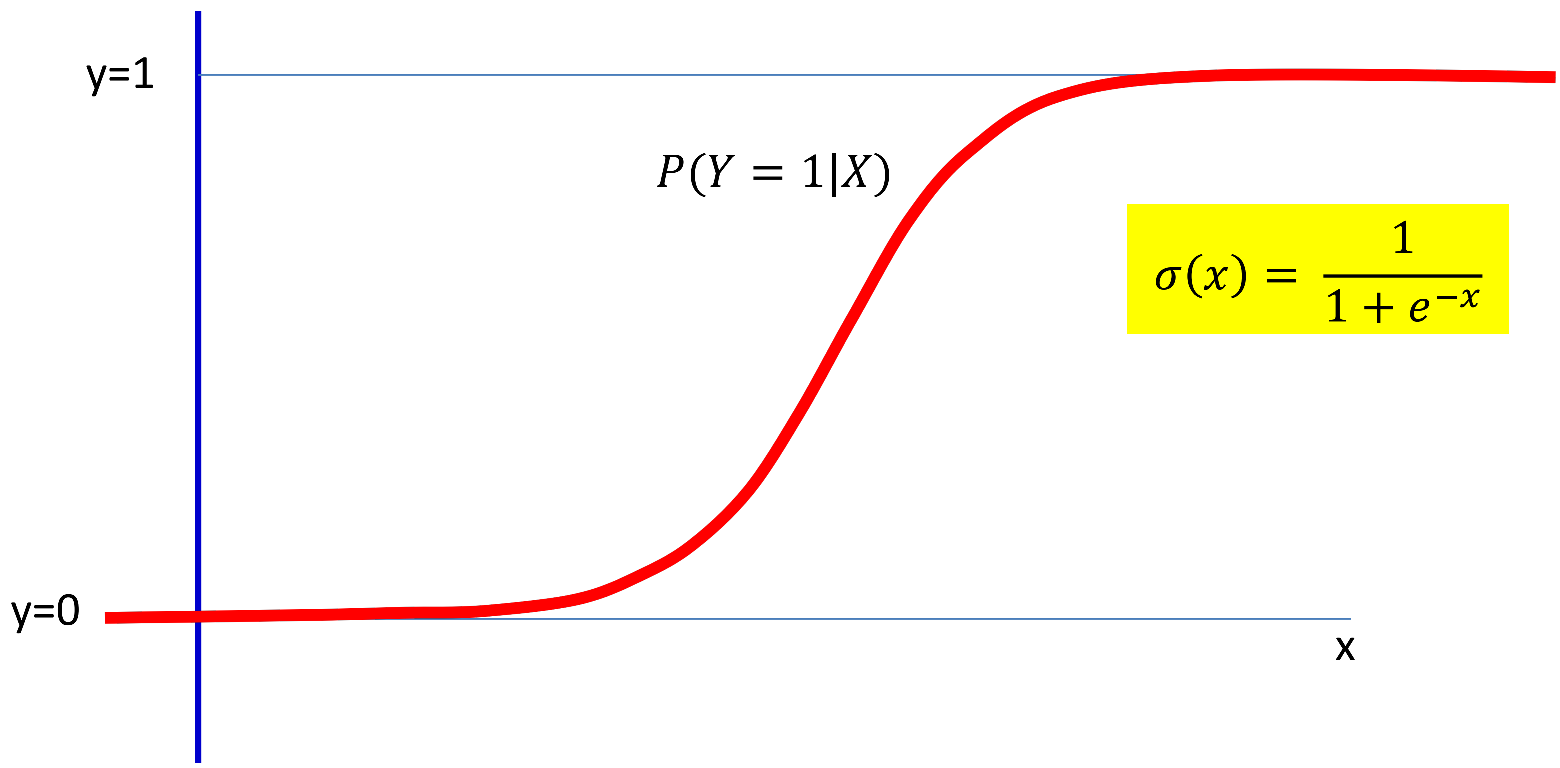
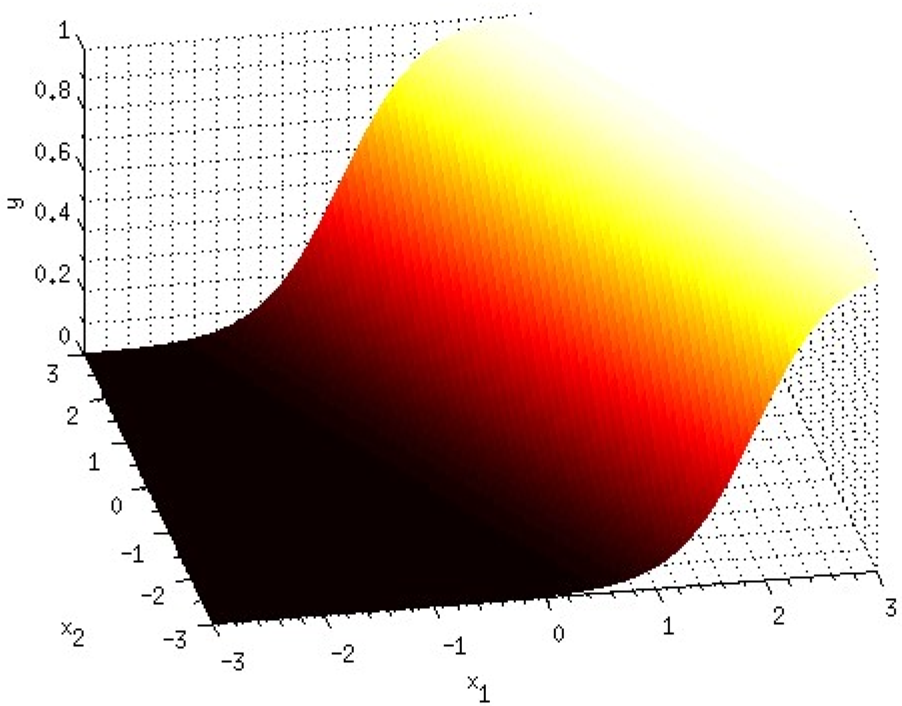
The logistic regression model

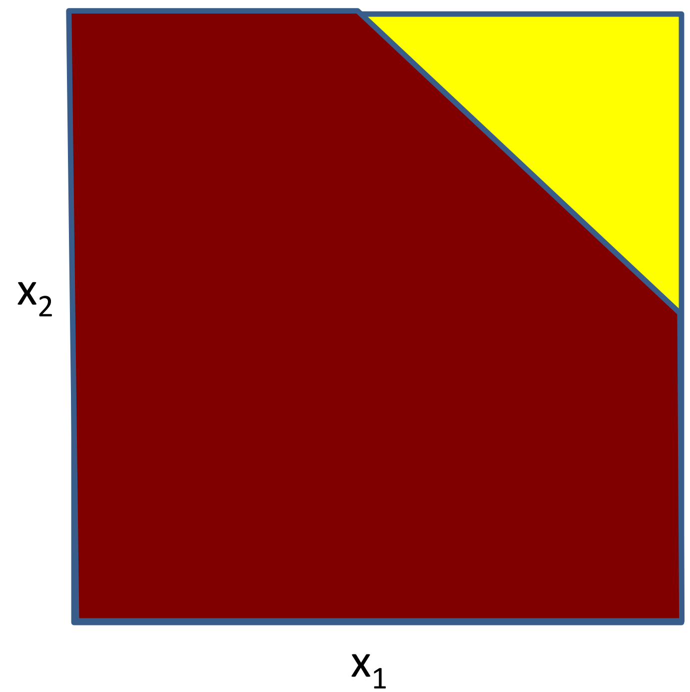


- Class 1 becomes increasingly probable going left to right
  - Very typical in many problems

Logistic regression

Decision: y > 0.5?





When X is a 2-D variable

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

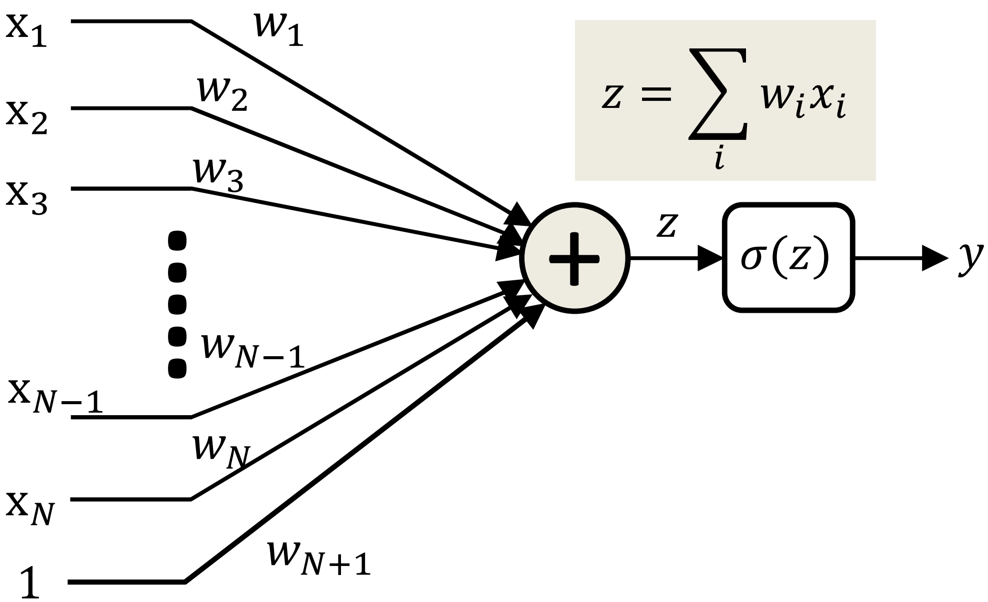
- This the perceptron with a sigmoid activation
  - It actually computes the *probability* that the input belongs to class 1

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



$$z = \sum_i w_i x_i$$

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

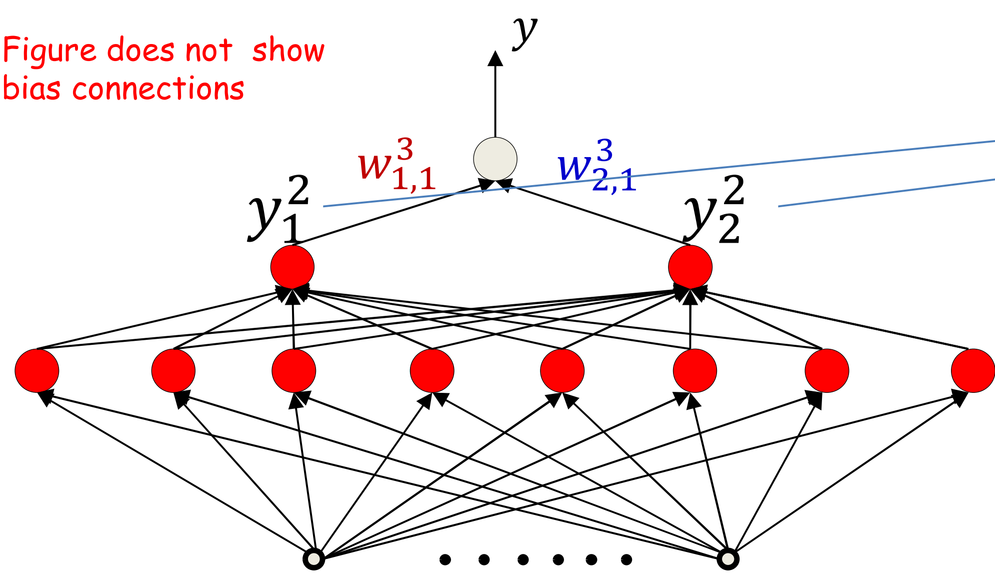
$$\frac{dy}{dw_i} = \frac{dy}{dz}\frac{dz}{dw_i} = \sigma'(z)x_i$$

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

- **$\boldsymbol{\sigma(z)}$is a differentiable function of $\boldsymbol{z}$**
  - $\frac{d\sigma(z)}{dz}$ is well-defined and finite for all z
- **Using the chain rule, $\boldsymbol{y}$ is a differentiable function of both inputs $\boldsymbol{x_i}$ and weights $\boldsymbol{w_i}$**
- **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

Figure does not show bias connections



$$y = \sigma(w_{1,1}^3 y_1^2 + w_{2,1}^3 y_2^2 + w_{3,1}^3)$$

y = output of overall network

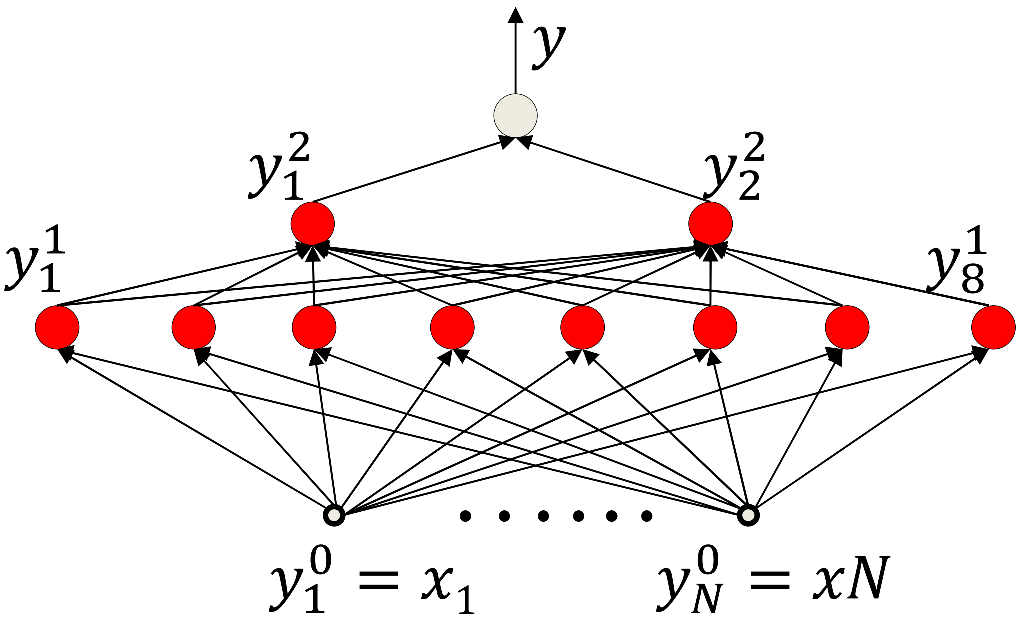
$w_{i,j}^k$ = weight connecting the ith unit of the (k-1)th layer to the jth unit of the k-th layer

y_i^k = output of the ith unit of the kth layer

$\sigma()$ is differentiable w.r.t both w and y_i^k

- 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

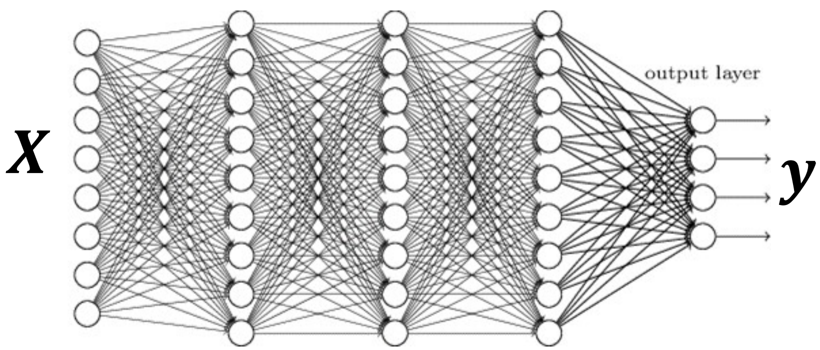
Overall function is differentiable

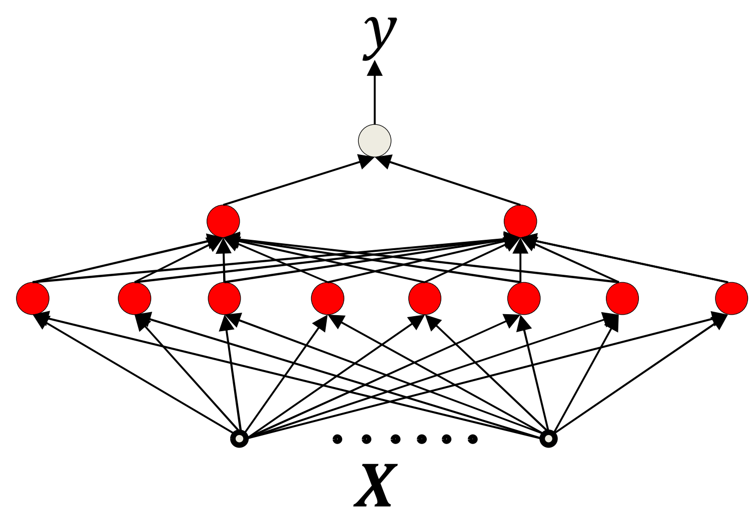


$$y_j^k = \sigma\left(\sum_i w_{i,j}^{k-1} y_i^{k-1}\right)$$

- The overall function is differentiable w.r.t every parameter
  - We can compute how small changes in the parameters change the output
    - For non-threshold activations the derivative are finite and generally non-zero
  - We will derive the actual derivatives using the chain rule later

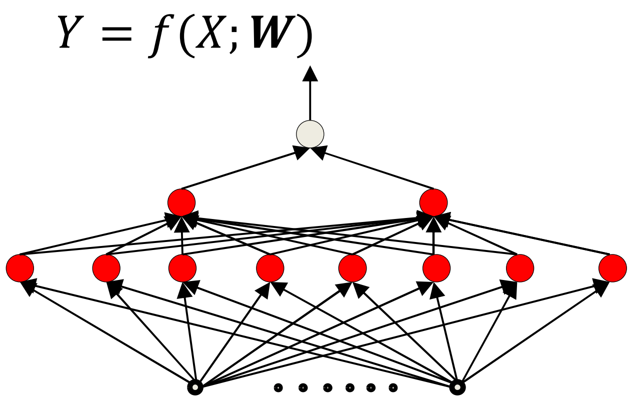
Overall setting for "Learning" the MLP

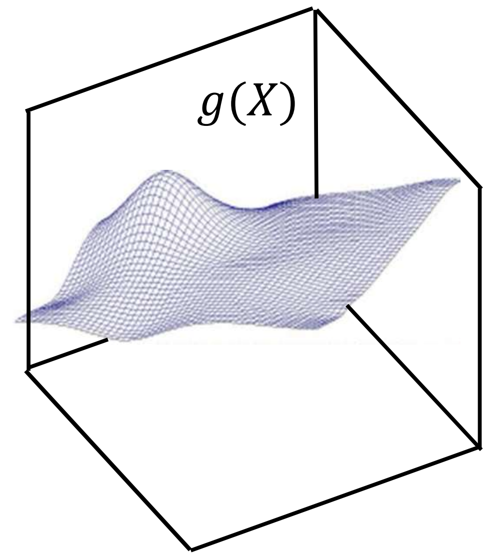




- Given a training set of input-output pairs $(\boldsymbol{X}_1, \boldsymbol{d}_1), (\boldsymbol{X}_2, \boldsymbol{d}_2), \ldots, (\boldsymbol{X}_N, \boldsymbol{d}_N)$ …
  - $\boldsymbol{d}$ is the *desired output* of the network in response to $\boldsymbol{X}$
  - $\boldsymbol{X}$ and $\boldsymbol{d}$ 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



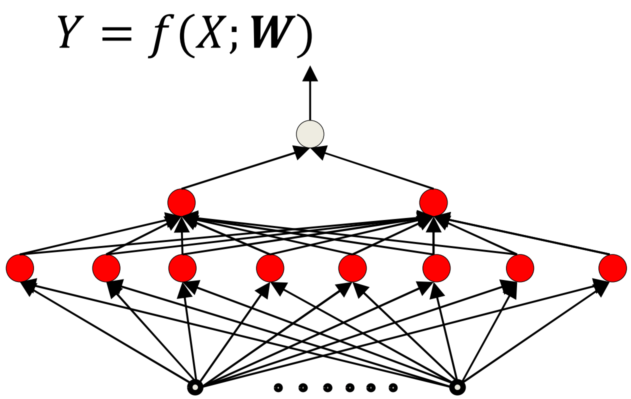


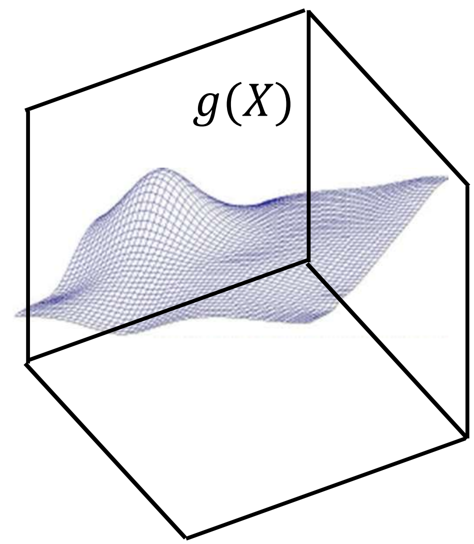
- When $f(X; \boldsymbol{W})$ has the capacity to exactly represent $g(X)$

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

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

Minimizing *expected* error

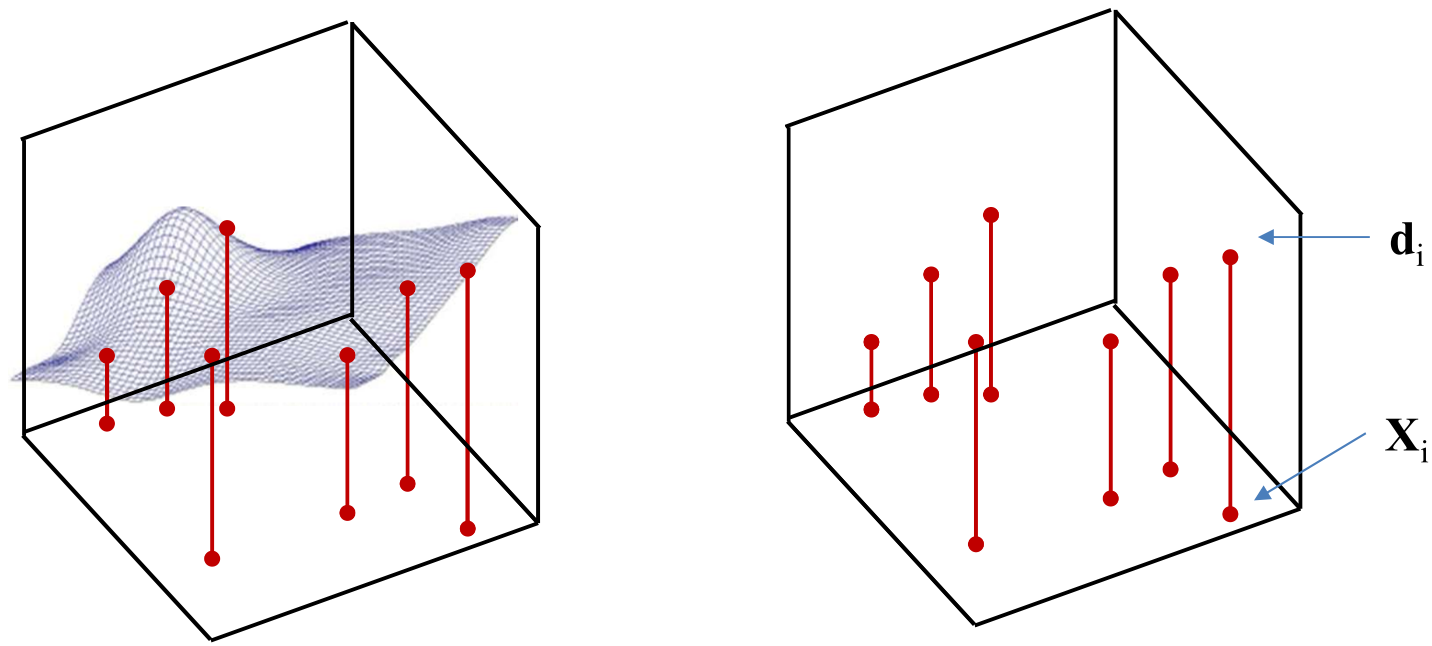




- More generally, assuming X is a random variable

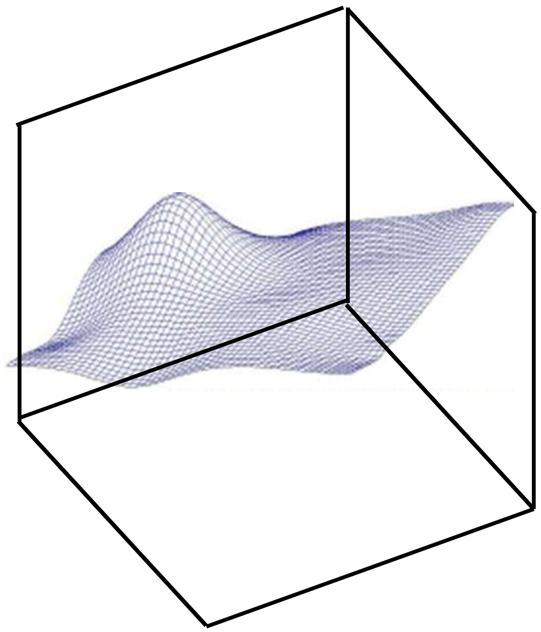
$$\widehat{\boldsymbol{W}} = \underset{W}{\operatorname{argmin}} \int_X div\big(f(X;W), g(X)\big) P(X) dX$$
$$= \underset{W}{\operatorname{argmin}}\, E\big[div\big(f(X;W), g(X)\big)\big]$$

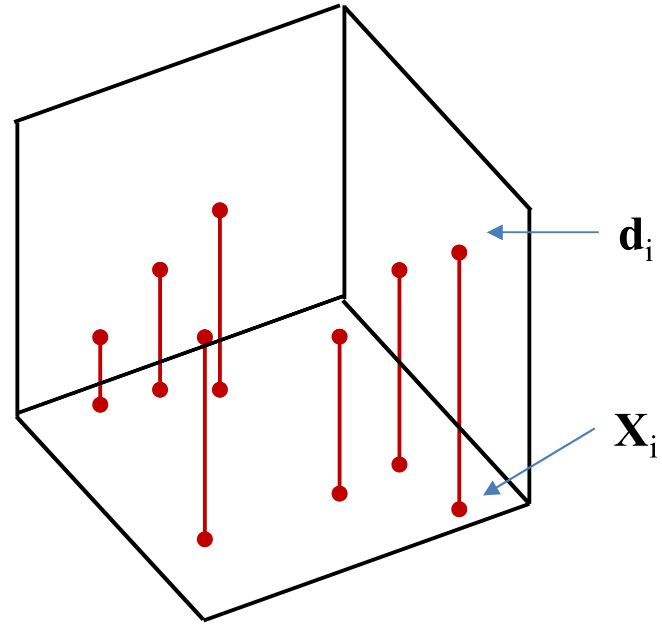
Recap: Sampling the function



- *Sample* $g(X)$
  - Obtain 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





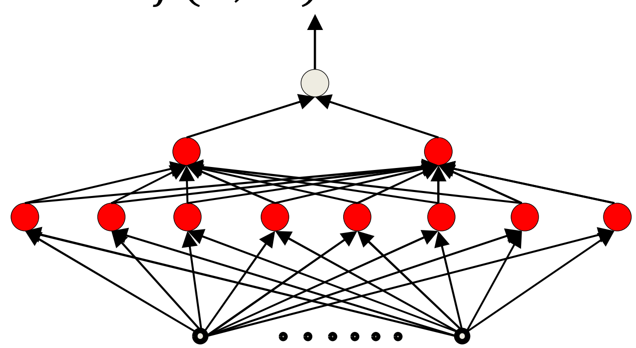
- The *expected* divergence (or risk) is the average divergence over the entire input space

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

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

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

Empirical Risk Minimization



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

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

- Estimate the parameters to minimize the empirical estimate of expected divergence (empiricial risk)

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

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

Empirical Risk Minimization

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

Note : Its really a measure of error, but using standard terminology, we will call it a "Loss"

Note 2: The empirical risk $Loss(W)$ 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

Note 3: For a *given training set* the loss is only a function of W

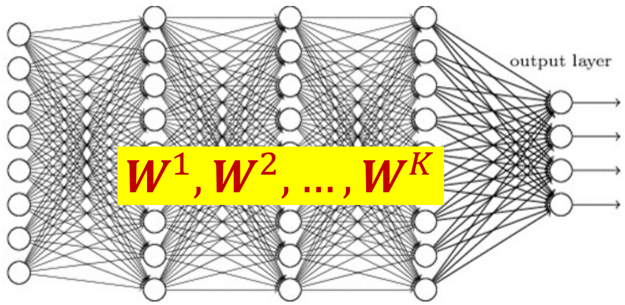
$$Loss(W) = \frac{1}{N}\sum_i div(f(X_i; W), d_i)$$

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

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

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

ERM for neural networks



Actual output of network:

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

Desired output of network: d_i

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

Average training error(loss):

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

– 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

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

w.r.t W

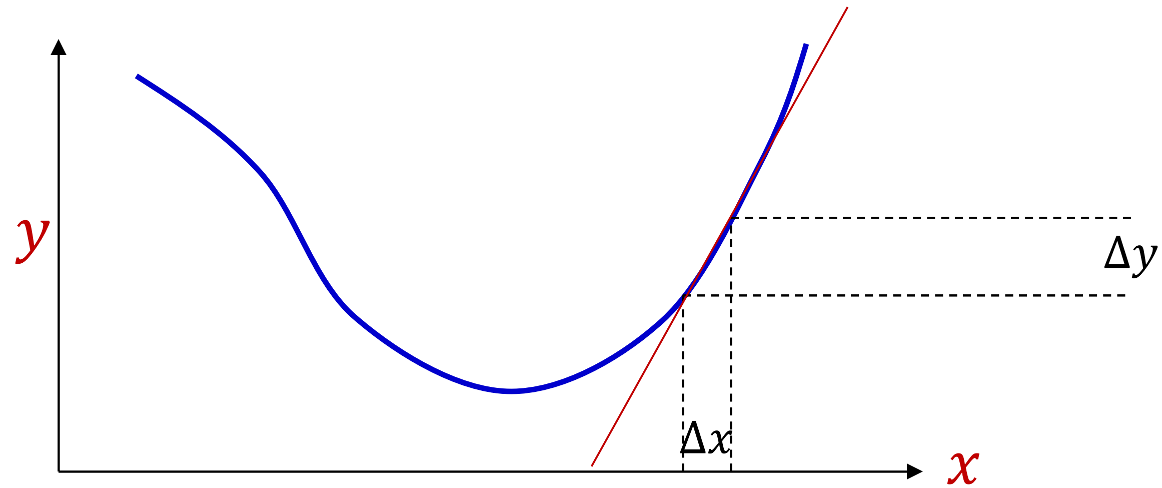
- This is problem of function minimization
  – An instance of optimization

Story so far

- We learn networks by "fitting" them to training instances drawn from a target function
- Learning networks of threshold-activation perceptrons requires solving a hard combinatorial-optimization problem
  - Because we cannot compute the influence of small changes to the parameters on the overall error
- Instead we use continuous activation functions with non-zero derivatives to enables us to estimate network parameters
  - This makes the output of the network differentiable w.r.t every parameter in the network
  - The *logistic* activation perceptron actually computes the *a posteriori* probability of the output given the input
- We define differentiable *divergence* between the output of the network and the desired output for the training instances
  - And a total error, which is the average divergence over all training instances
- We optimize network parameters to minimize this error
  - Empirical risk minimization
- This is an instance of function minimization

- **A CRASH COURSE ON FUNCTION OPTIMIZATION**

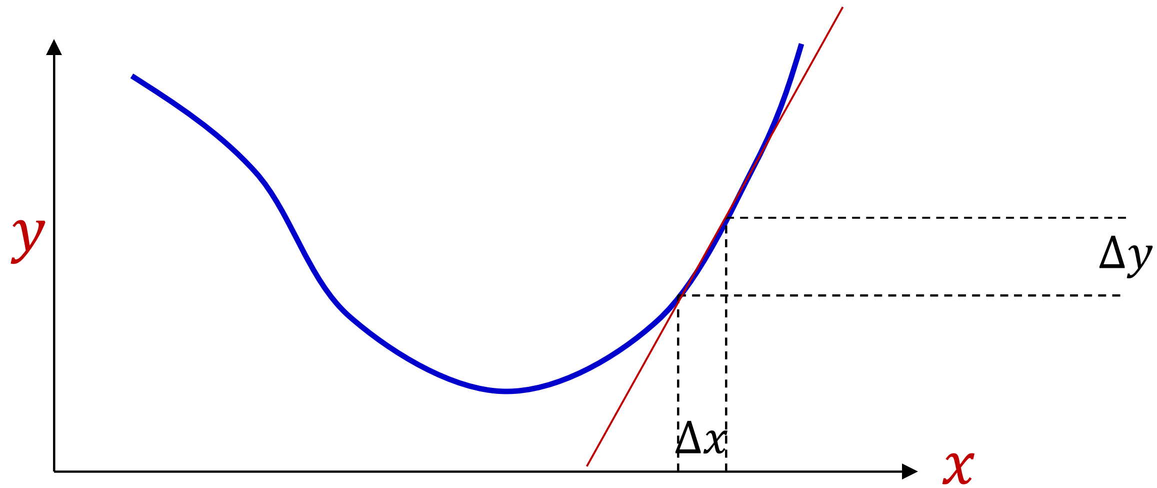
A brief note on derivatives..



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 α to a tiny increment Δx to obtain the increments Δy 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

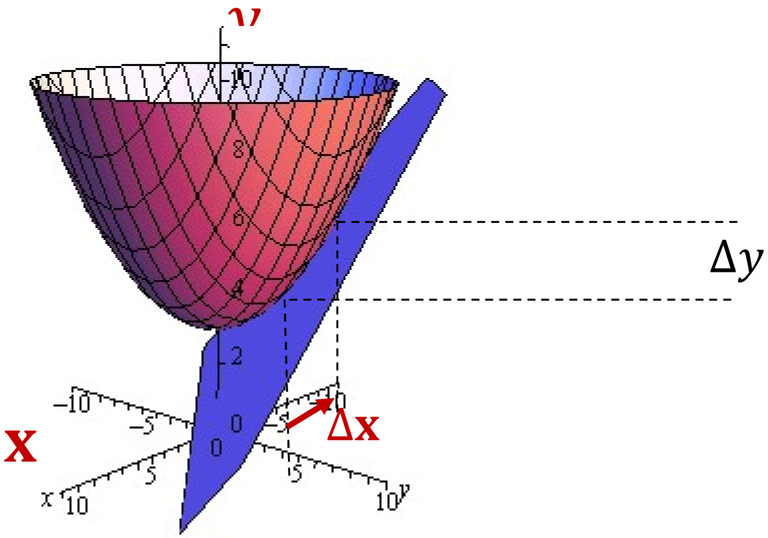
$$y = f(x)$$

  - 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

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

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

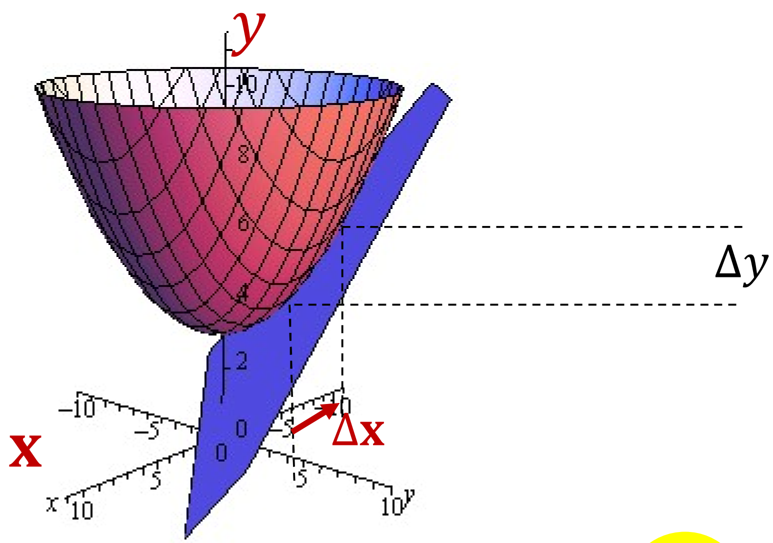
- Giving us that α is a row vector: $\alpha = [\alpha_1 \quad \cdots \quad \alpha_D]$

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

- The *partial* derivative α_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

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

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

We will be using this symbol for vector and matrix derivatives

- Where

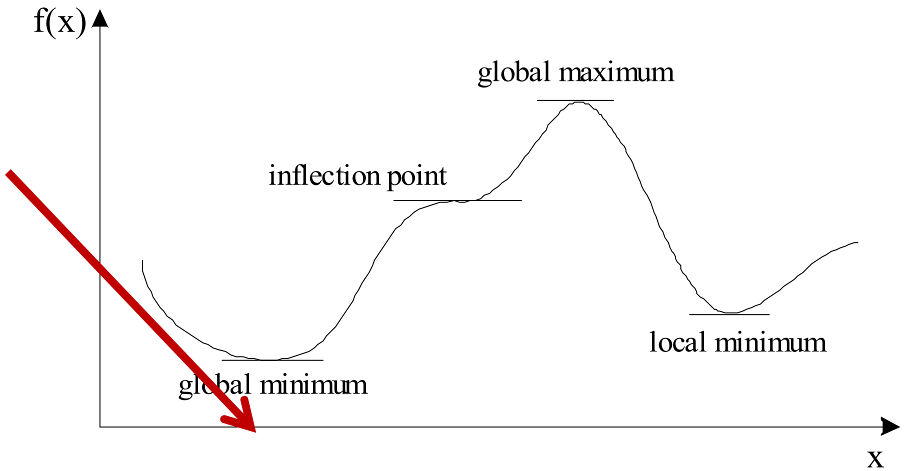
$$\nabla_{\mathbf{x}} y = \begin{bmatrix} \frac{\partial y}{\partial x_1} & \cdots & \frac{\partial y}{\partial x_D} \end{bmatrix}$$

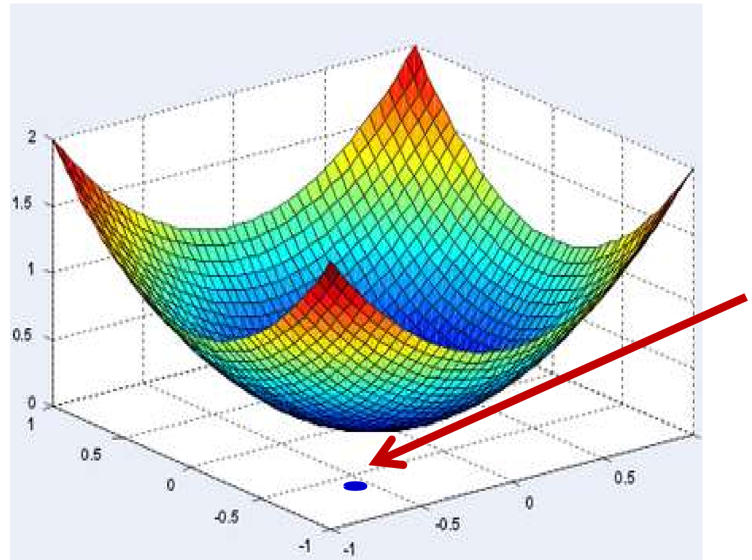
  - You may be more familiar with the term “gradient” which is actually defined as the transpose of the derivative

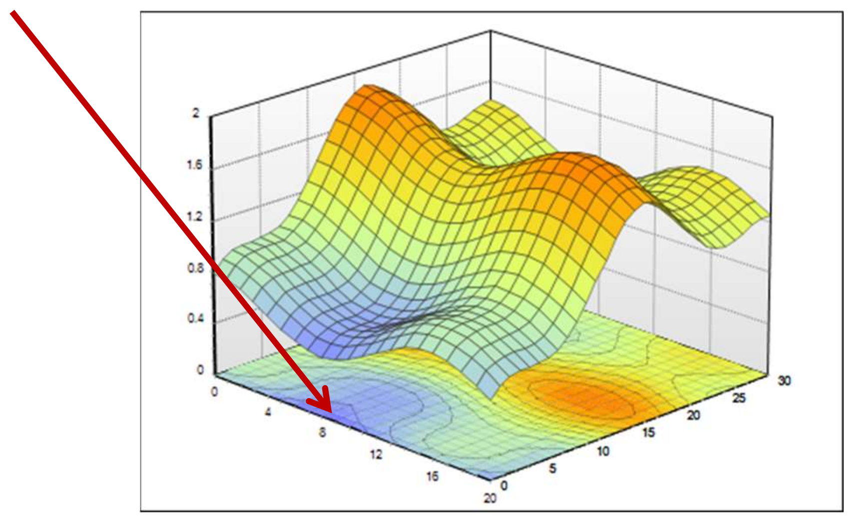
Caveat about following slides

- 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

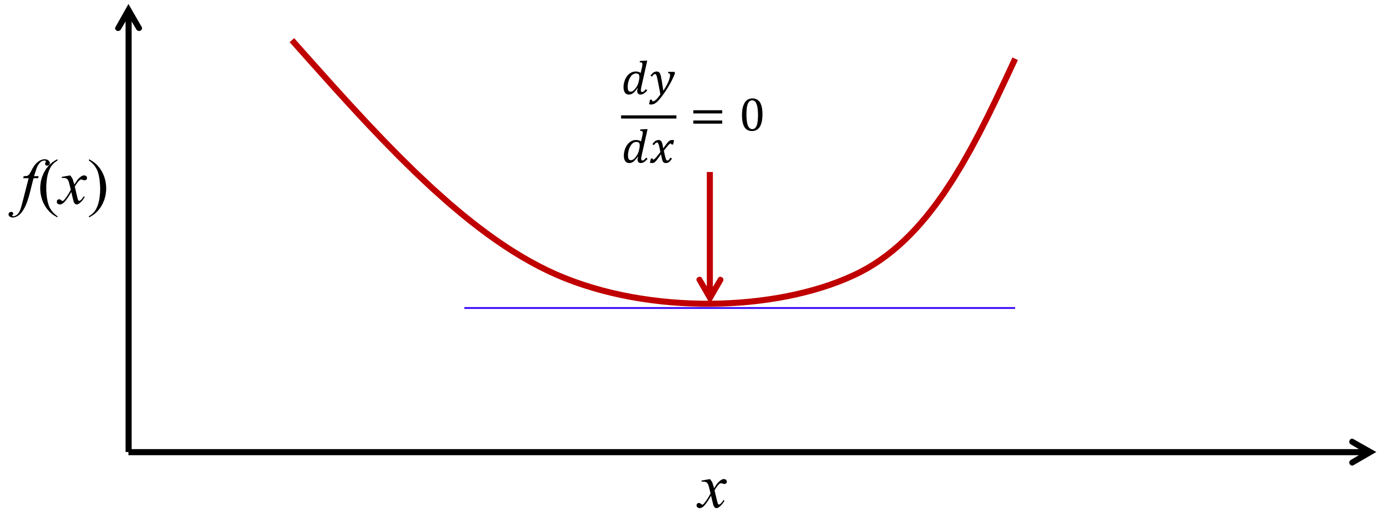






- General problem of optimization: find the value of $\boldsymbol{x}$ where $\mathbf{f}(\boldsymbol{x})$ is minimum

Finding the minimum of a function

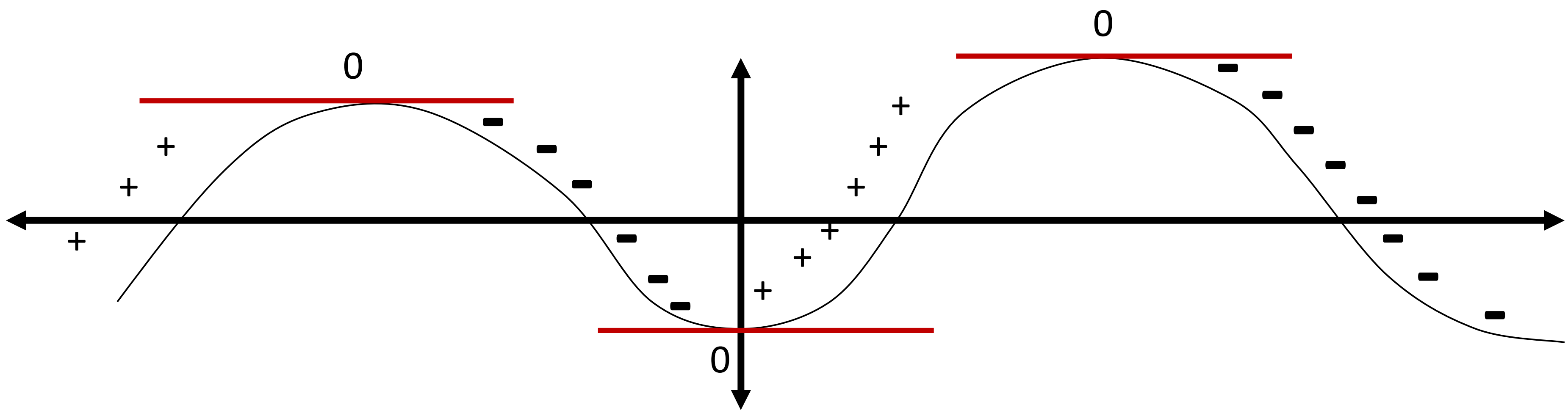


- Find the value x at which $f'(x) = 0$
  - Solve

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

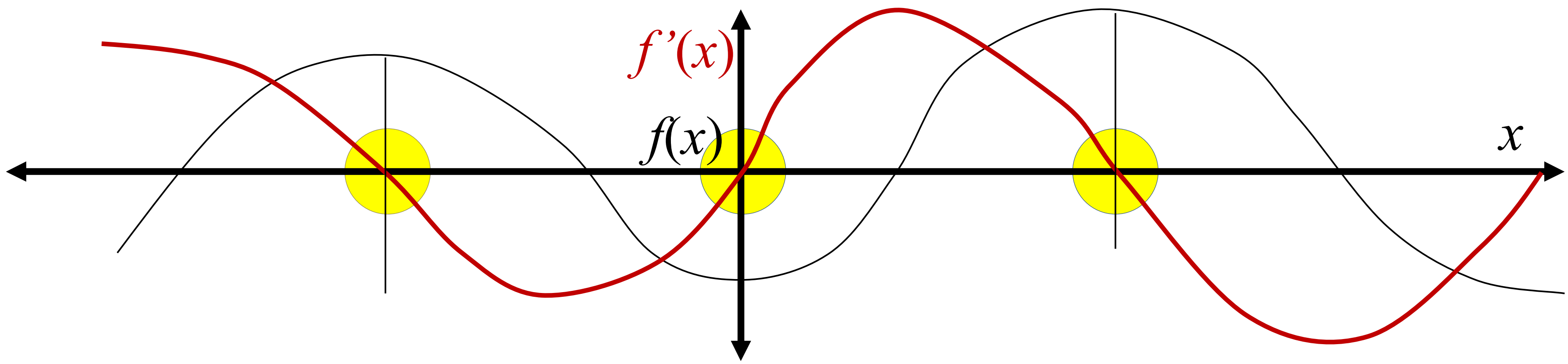
- The solution is a "turning point"
  - Derivatives go from positive to negative or vice versa at this point
- But is it a minimum?

Turning Points



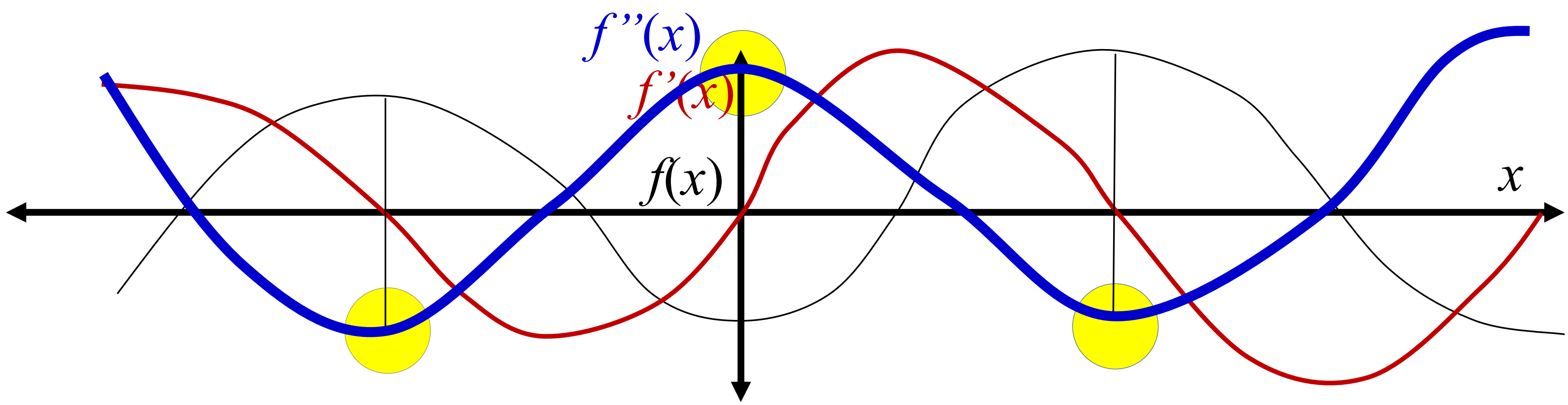
- Both *maxima* and *minima* have zero derivative
- Both are turning points

Derivatives of a curve



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

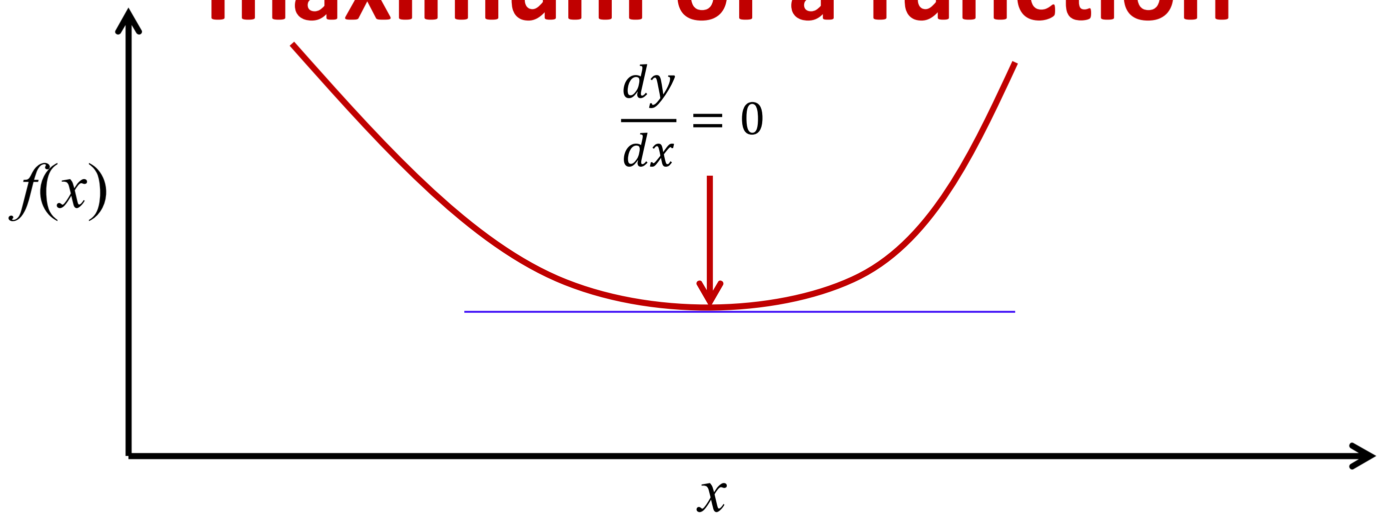
Derivative of the derivative of the curve



- 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!

Solution: Finding the minimum or maximum of a function



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

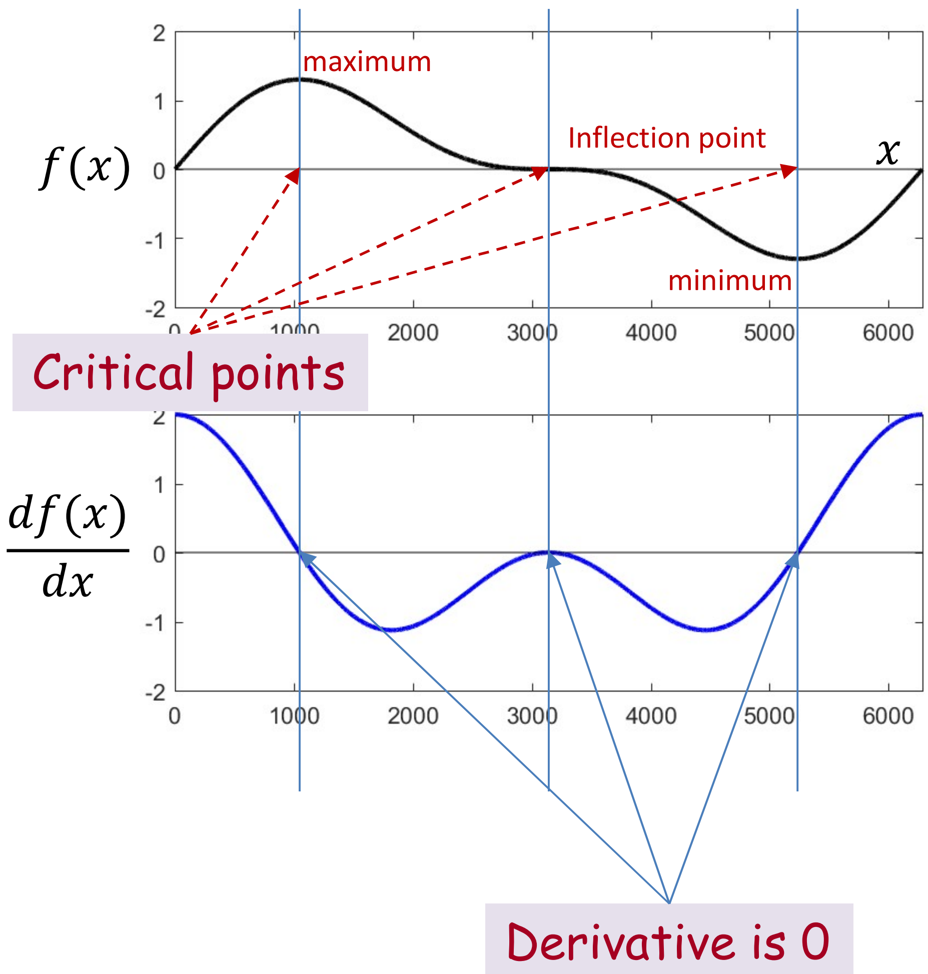
$$\frac{df(x)}{dx} = 0$$

- 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

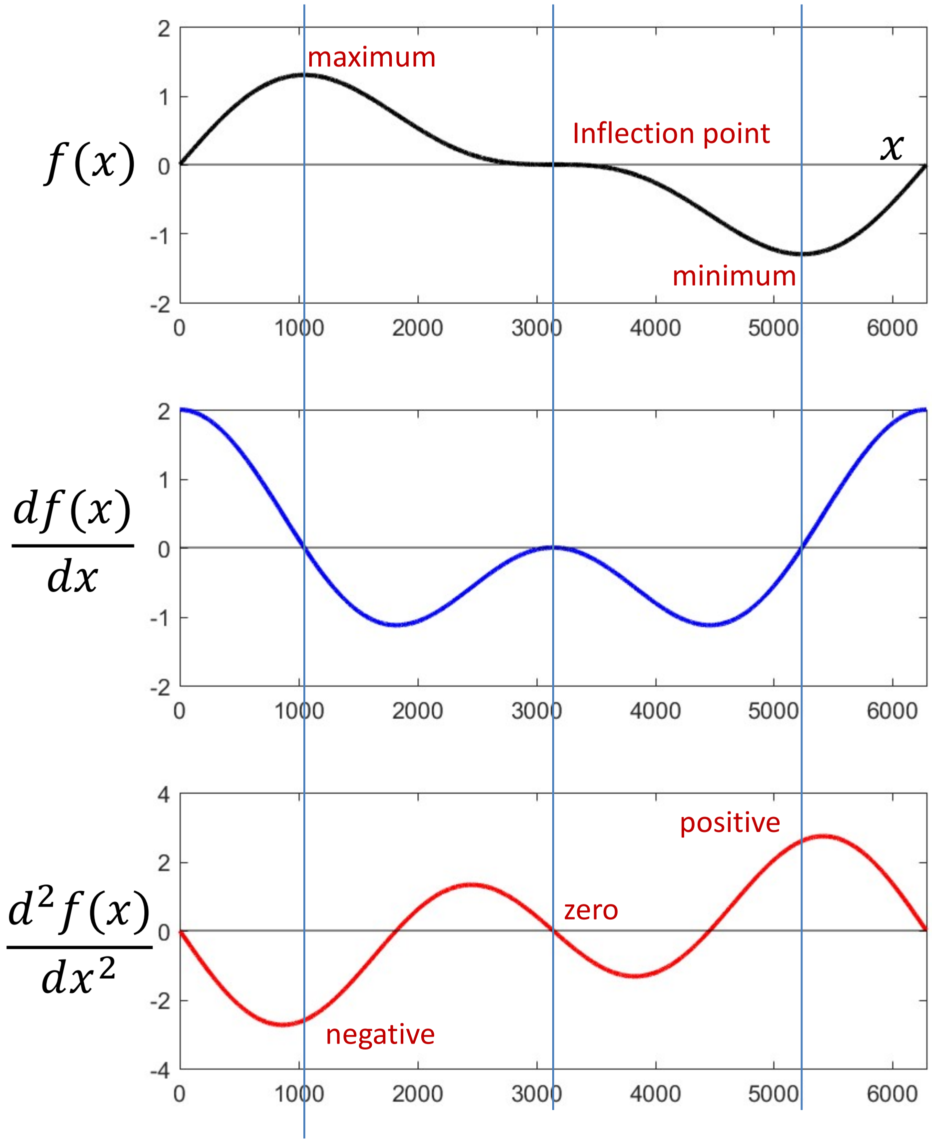
A note on derivatives of functions of single variable



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

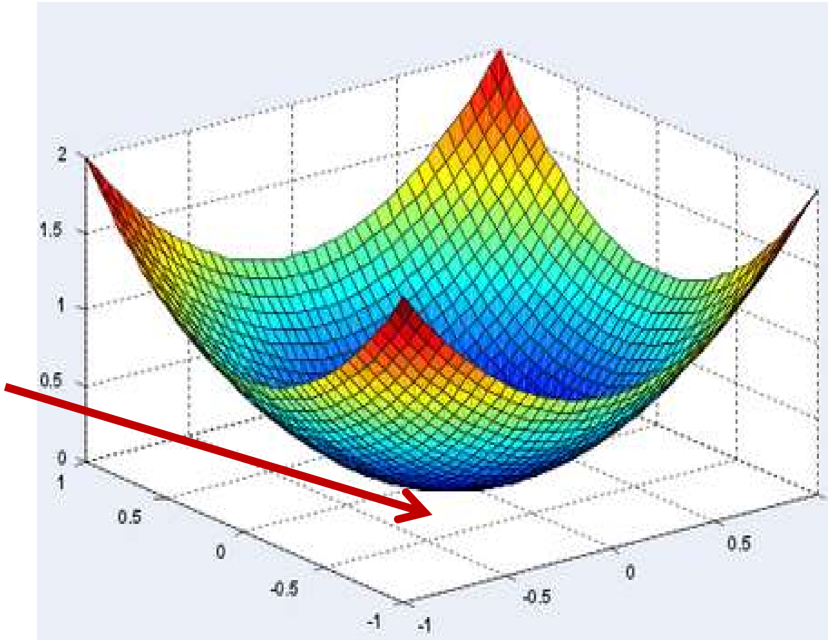
- The *second* derivative is
  - Positive (or 0) at minima
  - Negative (or 0) at maxima
  - Zero at inflection points

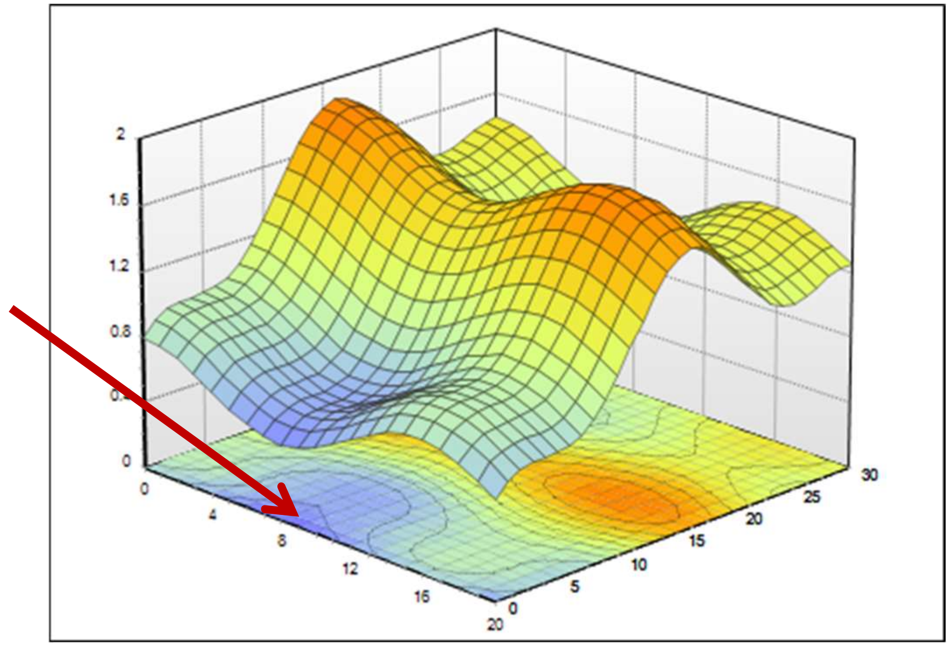
A note on derivatives of functions of single variable



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

What about functions of multiple variables?

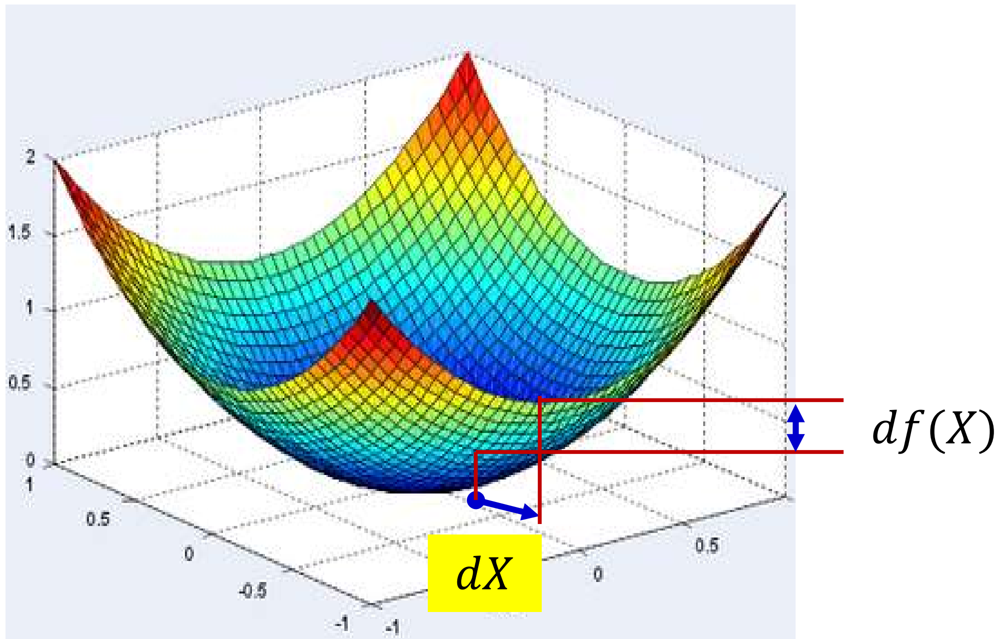




- The optimum point is still "turning" point
  - Shifting in any direction will increase the value
  - For smooth functions, miniscule shifts will not result in any change at all
- We must find a point where shifting in any direction by a microscopic amount will not change the value of the function

A brief note on derivatives of multivariate functions

The *Gradient* of a scalar function



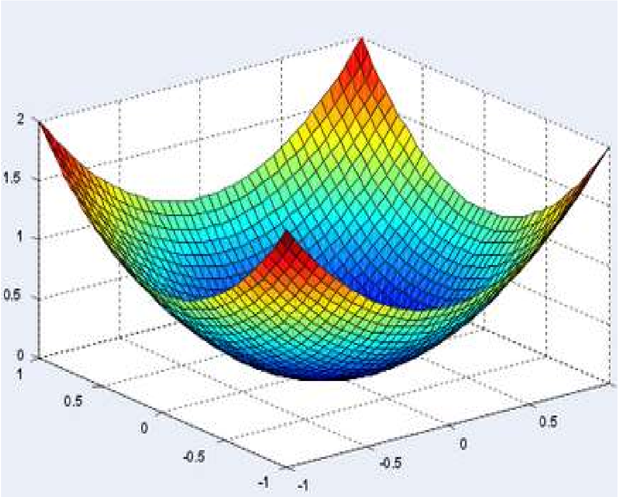
- The *derivative* $\nabla_X f(X)$ of a scalar function $f(X)$ of a multi-variate input X is a multiplicative factor that gives us the change in $f(X)$ for tiny variations in X

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

  – The ***gradient*** is the transpose of the derivative $\nabla_X f(X)^T$

Gradients of scalar functions with multi-variate inputs

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



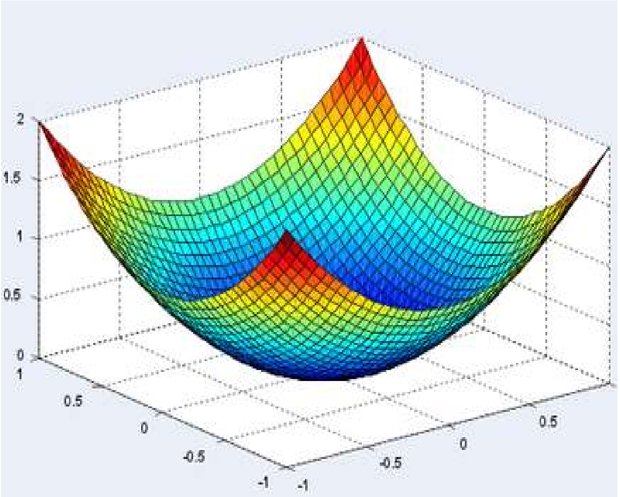
$$\nabla_X f(X) = \left[\frac{\partial f(X)}{\partial x_1} \quad \frac{\partial f(X)}{\partial x_2} \quad \cdots \quad \frac{\partial f(X)}{\partial x_n}\right]$$

- Relation:

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

Gradients of scalar functions with multivariate inputs

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



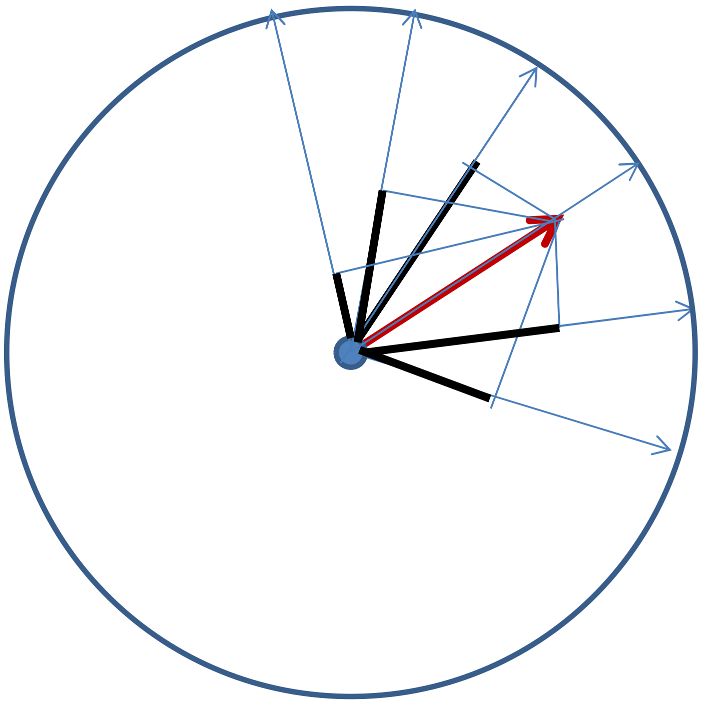
$$\nabla_X f(X) = \left[\frac{\partial f(X)}{\partial x_1} \quad \frac{\partial f(X)}{\partial x_2} \quad \cdots \quad \frac{\partial f(X)}{\partial x_n}\right]$$

- Relation:

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

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

A well-known vector property



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

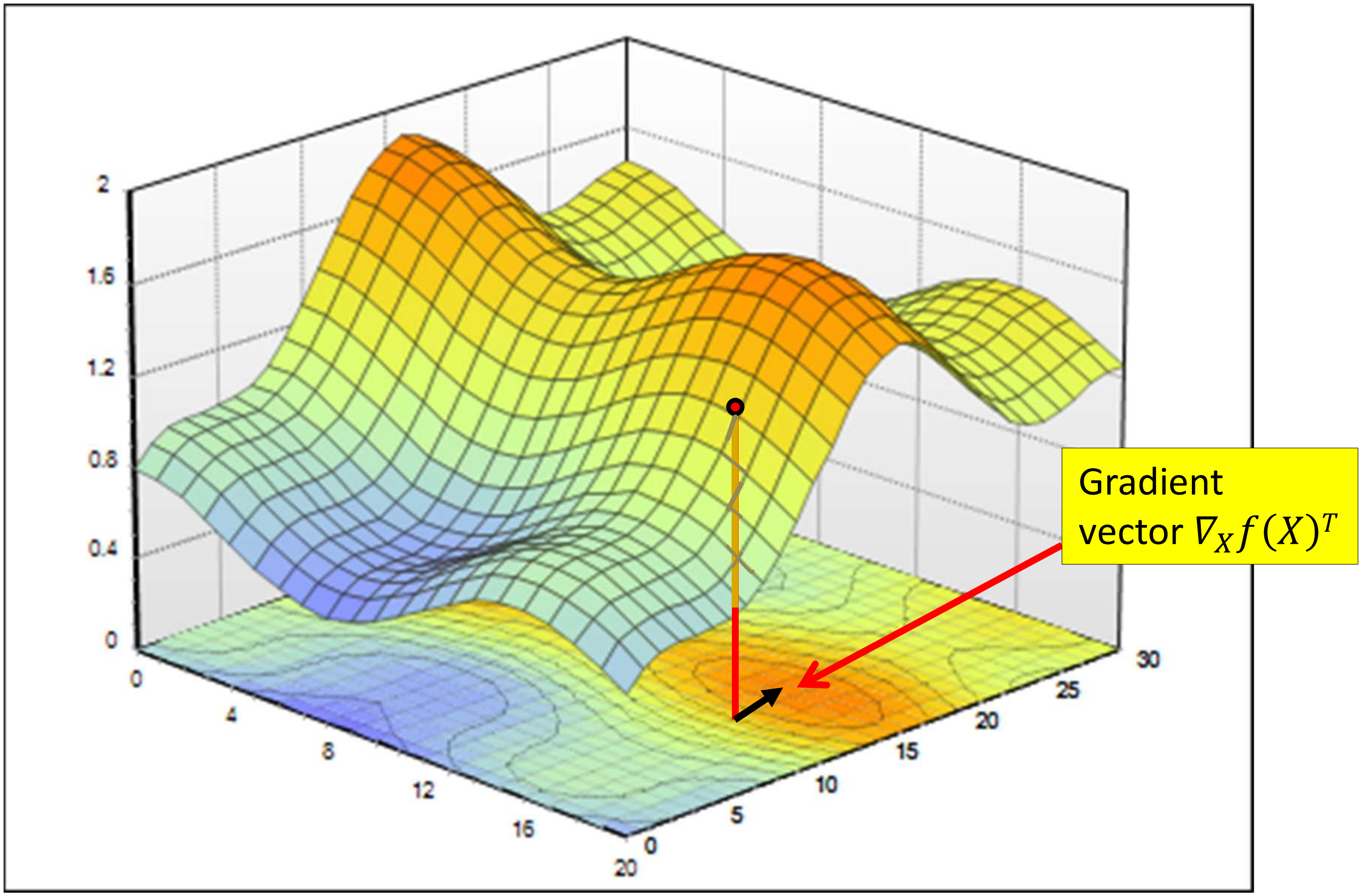
- The inner product between two vectors of fixed lengths is maximum when the two vectors are aligned
  - i.e. when $\theta = 0$

Properties of Gradient

- $df(X) = \nabla_X f(X) dX$
  - The inner product between $\nabla_X f(X)^{\mathrm{T}}$ and dX

- Fixing the length of dX
  - E.g. $|dX| = 1$
- $df(X)$ is max if dX is aligned with $\nabla_X f(X)^{\mathrm{T}}$
  - $\angle(\nabla_X f(X)^{\mathrm{T}}, dX) = 0$
  - The function $f(X)$ increases most rapidly if the input increment dX is perfectly aligned to $\nabla_X f(X)^{\mathrm{T}}$
- The gradient is the direction of fastest increase in $f(X)$

Gradient



2
1.6
1.2
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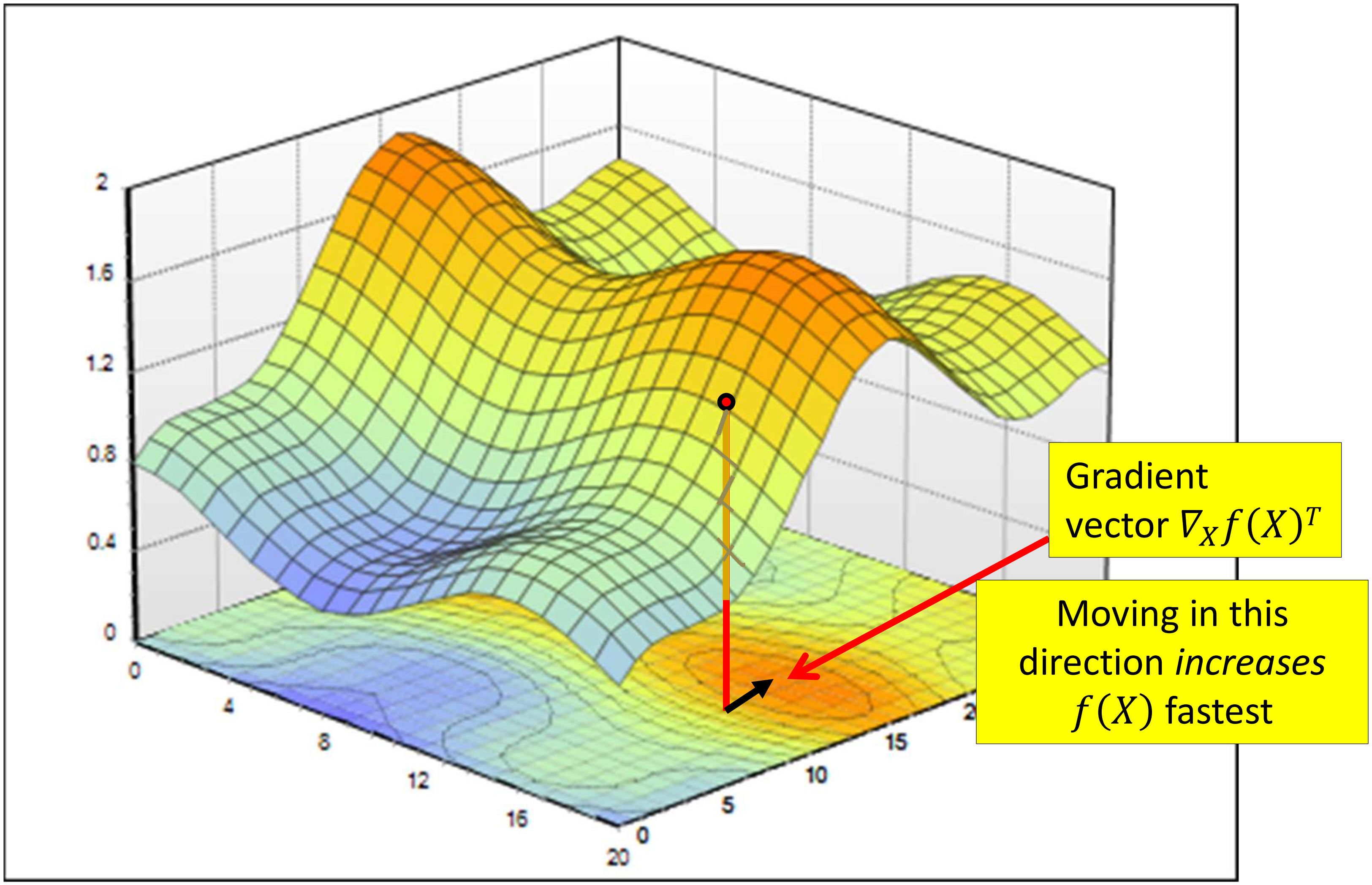
Gradient vector $\nabla_X f(X)^T$

Gradient


Gradient vector $\nabla_X f(X)^T$
Moving in this direction *increases* $f(X)$ fastest
2
1.6
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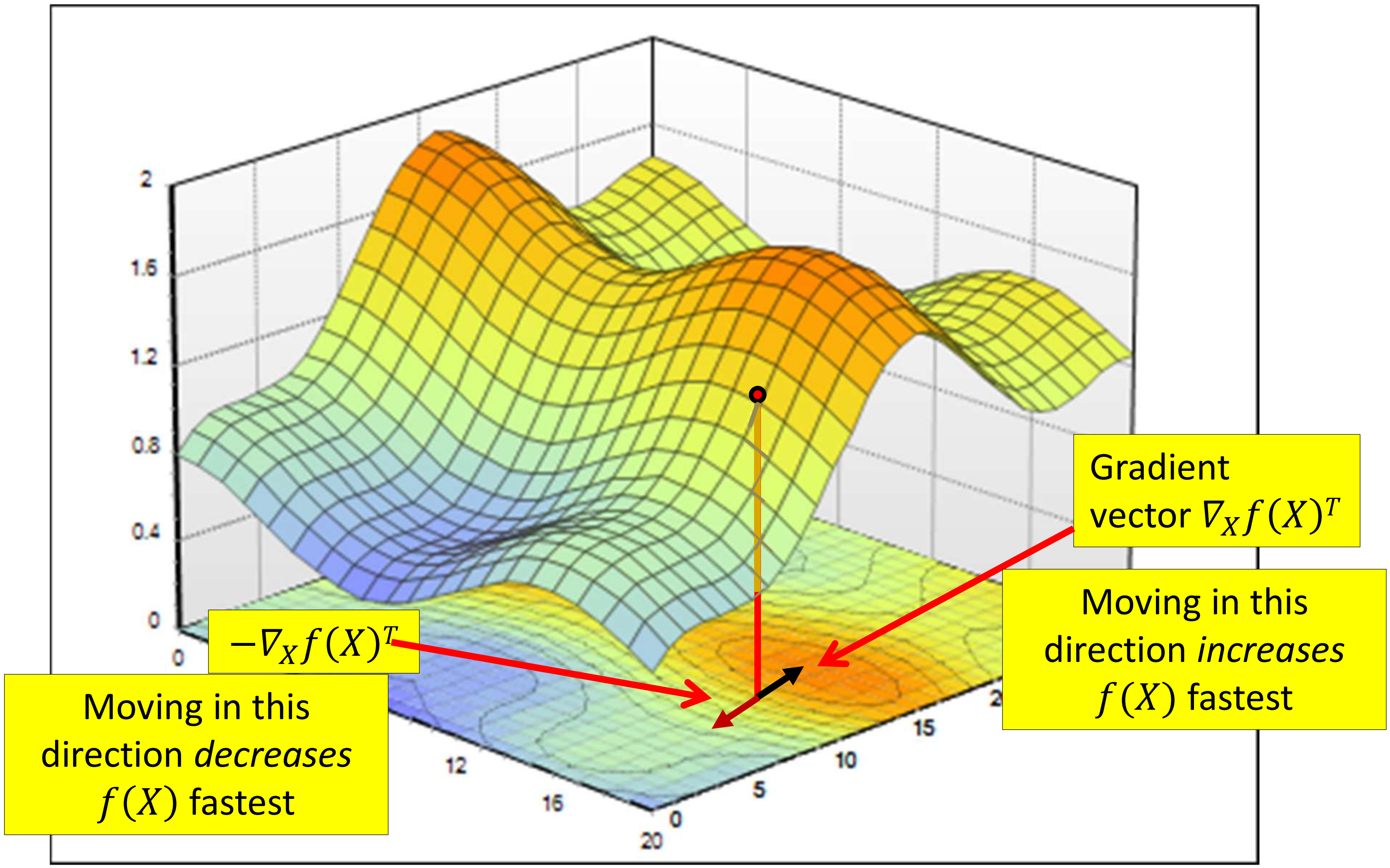
Gradient



2
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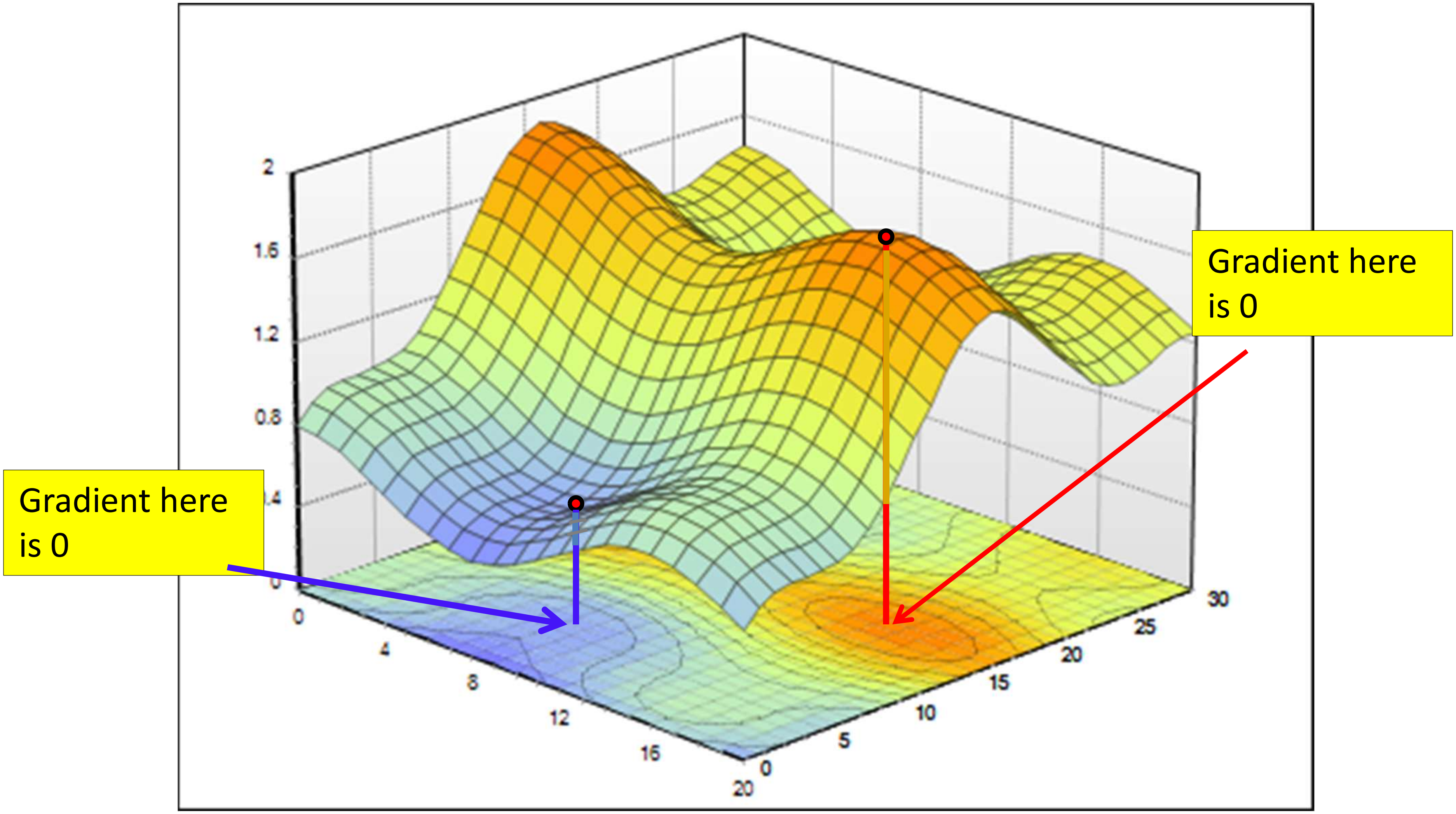
Gradient vector $\nabla_X f(X)^T$
Moving in this direction *increases* $f(X)$ fastest
$-\nabla_X f(X)^T$
Moving in this direction *decreases* $f(X)$ fastest

Gradient



2
1.6
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25
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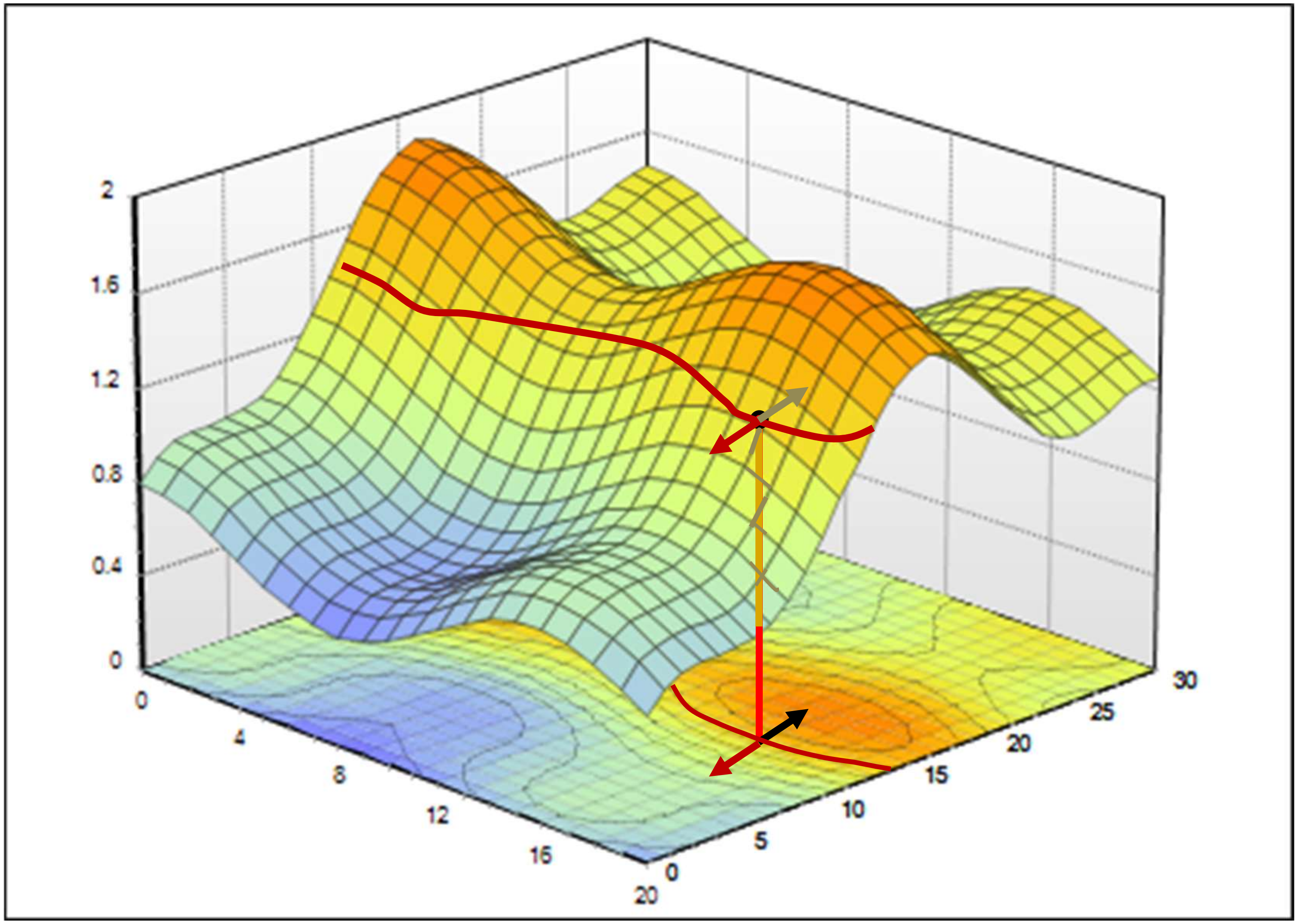
Gradient here is 0
Gradient here is 0

Properties of Gradient: 2



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

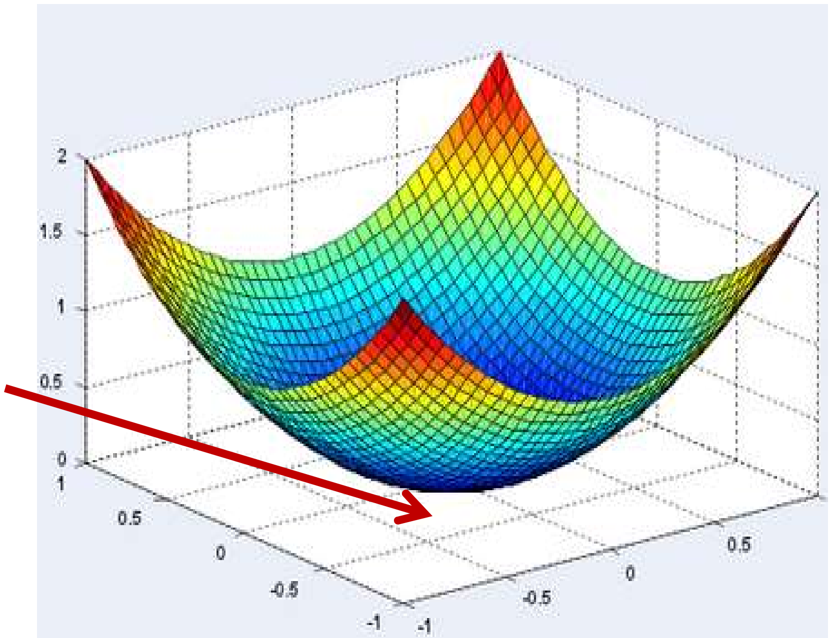
The Hessian

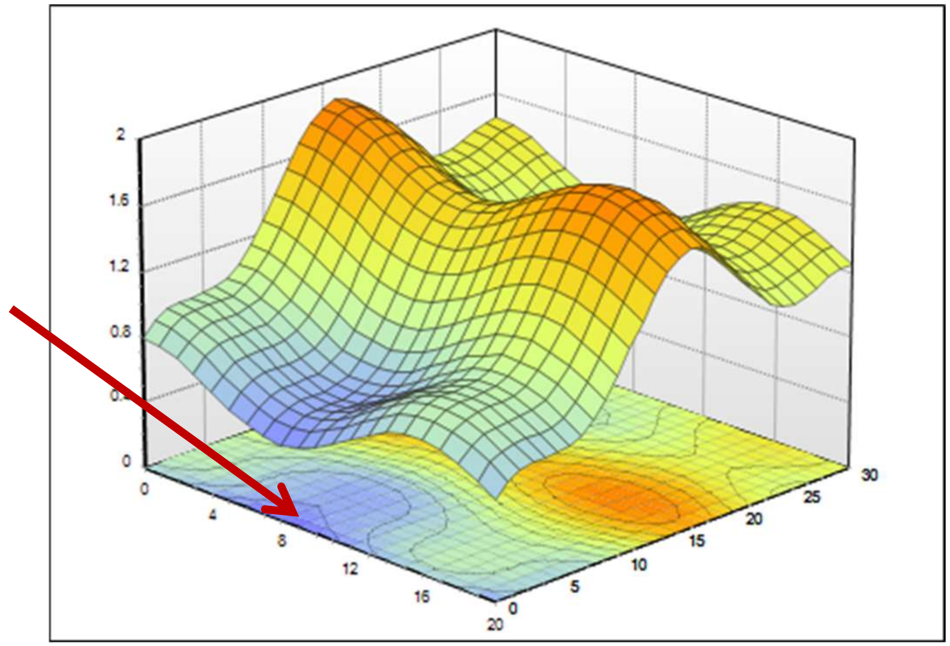
- The Hessian of a function $f(x_1, x_2, \dots, x_n)$ is given by the second derivative

$$\nabla_X^2 f(x_1,\dots,x_n) := \begin{bmatrix} \dfrac{\partial^2 f}{\partial x_1{}^2} & \dfrac{\partial^2 f}{\partial x_1 \partial x_2} & \cdot & \cdot & \dfrac{\partial^2 f}{\partial x_1 \partial x_n} \\ \dfrac{\partial^2 f}{\partial x_2 \partial x_1} & \dfrac{\partial^2 f}{\partial x_2{}^2} & \cdot & \cdot & \dfrac{\partial^2 f}{\partial x_2 \partial x_n} \\ \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot \\ \dfrac{\partial^2 f}{\partial x_n \partial x_1} & \dfrac{\partial^2 f}{\partial x_n \partial x_2} & \cdot & \cdot & \dfrac{\partial^2 f}{\partial x_n{}^2} \end{bmatrix}$$

Returning to direct optimization…

Finding the minimum of a scalar function of a multivariate 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 derivative (or gradient) equals to zero

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

2. Compute the Hessian Matrix $\nabla_X^2 f(X)$ 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

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

Unconstrained Minimization of function (Example)

- Set the gradient to null

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

- Solving the 3 equations system with 3 unknowns

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

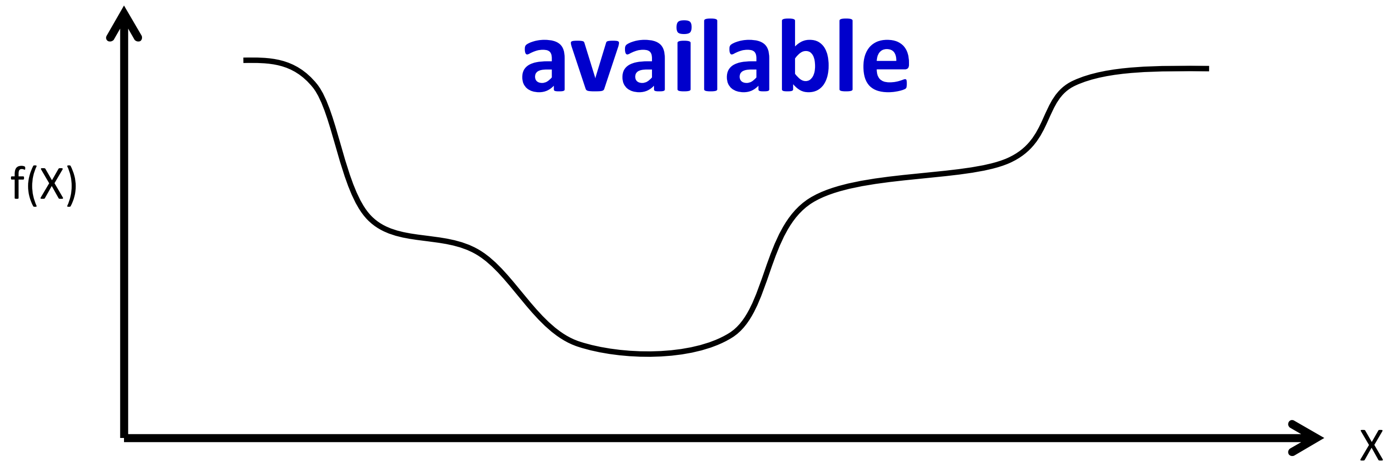
Unconstrained Minimization of function (Example)

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

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

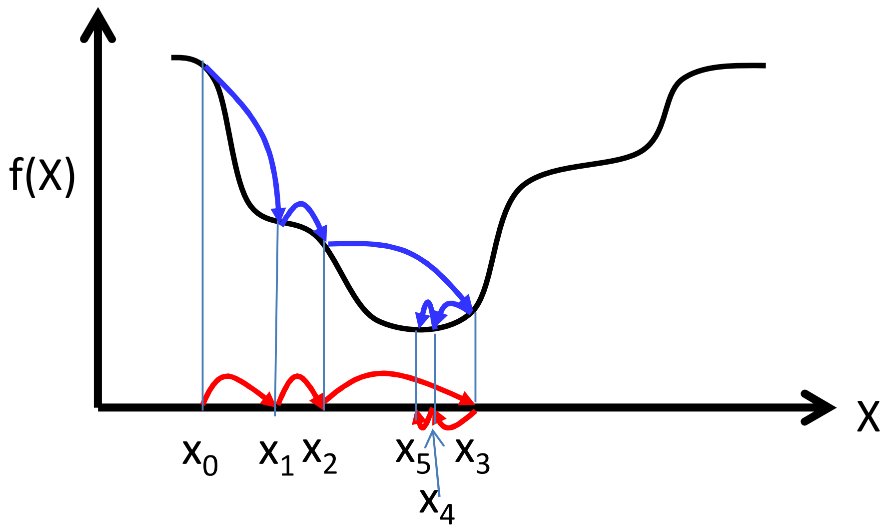
- All the eigenvalues are positives => the Hessian matrix is positive definite
- The point $x = \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} = \begin{bmatrix} -1 \\ -1 \\ -1 \end{bmatrix}$ is a minimum

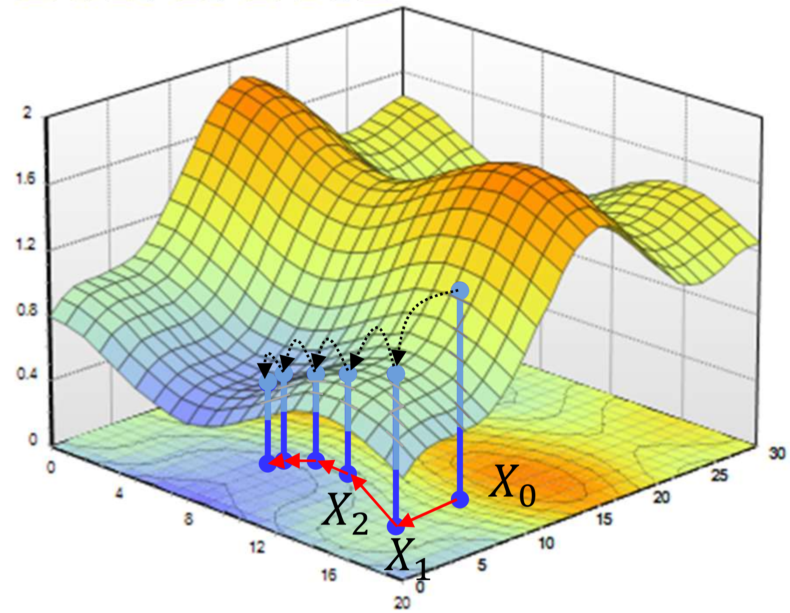
Closed Form Solutions are not always available



- Often it is not possible to simply solve $\nabla_X f(X) = 0$
  - 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

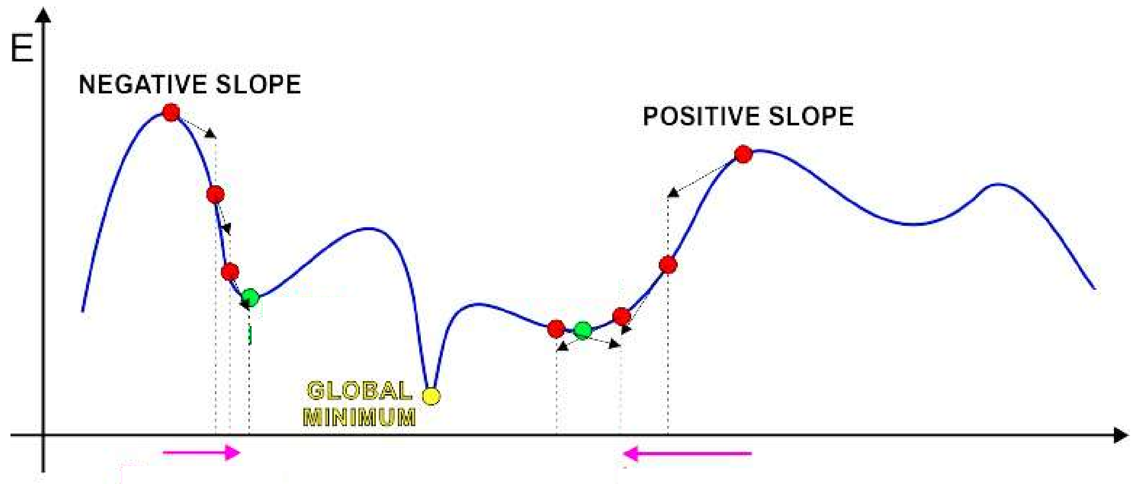
Iterative solutions





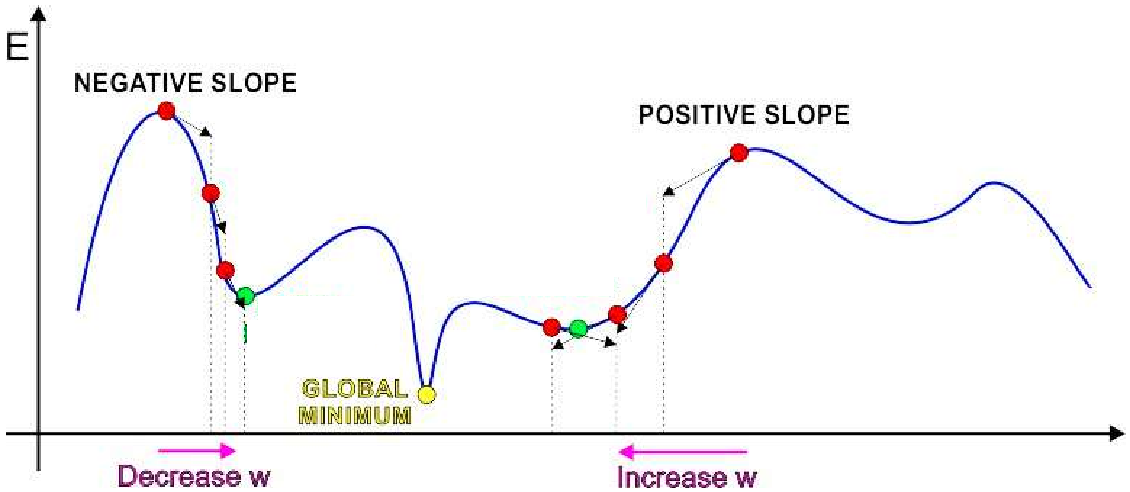
- Iterative solutions
  - Start from an initial guess X_0 for the optimal X
  - Update the guess towards a (hopefully) "better" value of $\mathrm{f}(X)$
  - Stop when $\mathrm{f}(X)$ no longer decreases
- Problems:
  - Which direction to step in
  - How big must the steps be

The Approach of Gradient Descent



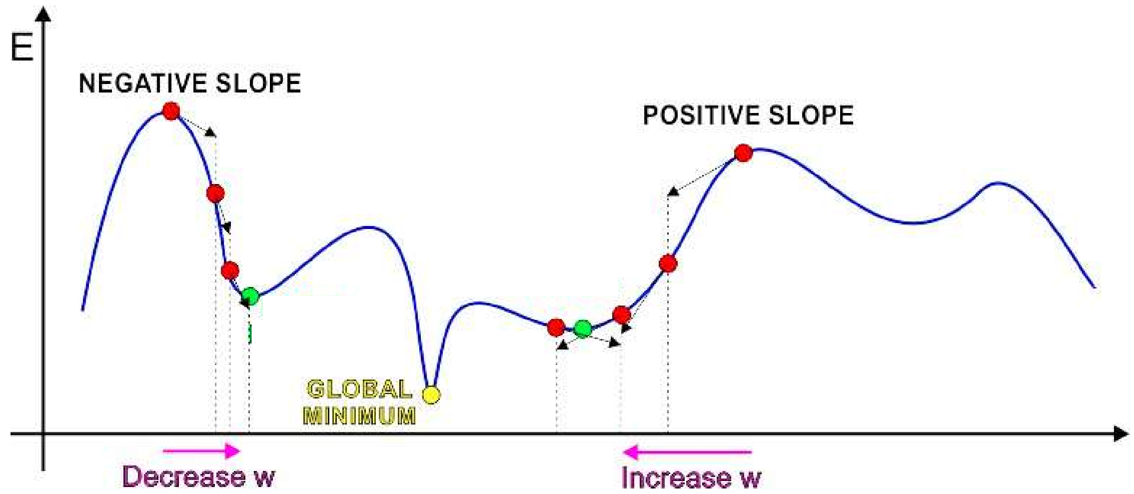
- Iterative solution:
  - Start at some point
  - Find direction in which to shift this point to decrease error
    - This can be found from the derivative of the function
      - A negative derivative → moving right decreases error
      - A positive derivative → moving left decreases error
  - Shift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

The Approach of Gradient Descent



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

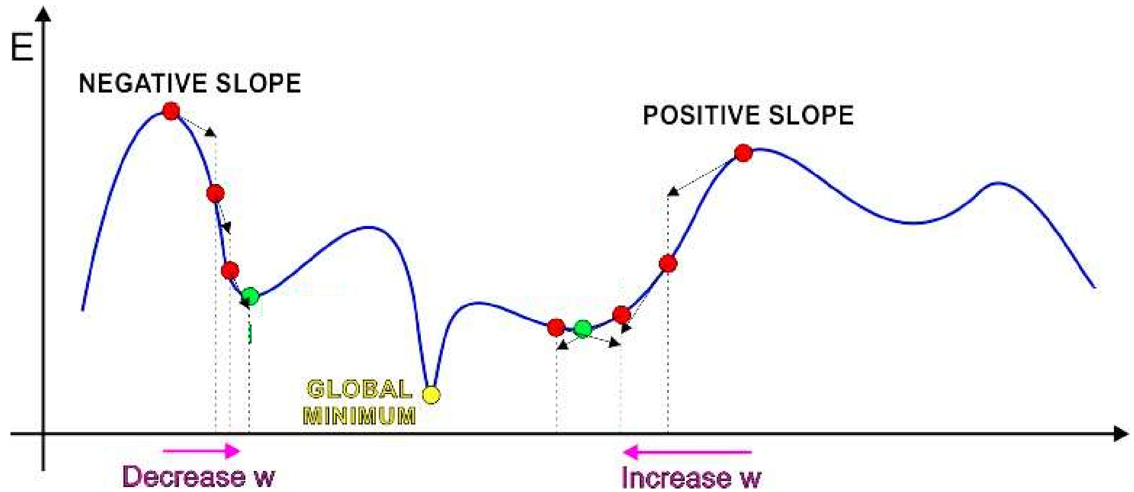


- Iterative solution: Trivial algorithm
  - Initialize x^0
  - While $f'\left(x^k\right) \neq 0$

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

- Identical to previous algorithm

The Approach of Gradient Descent



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

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

- η^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*

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

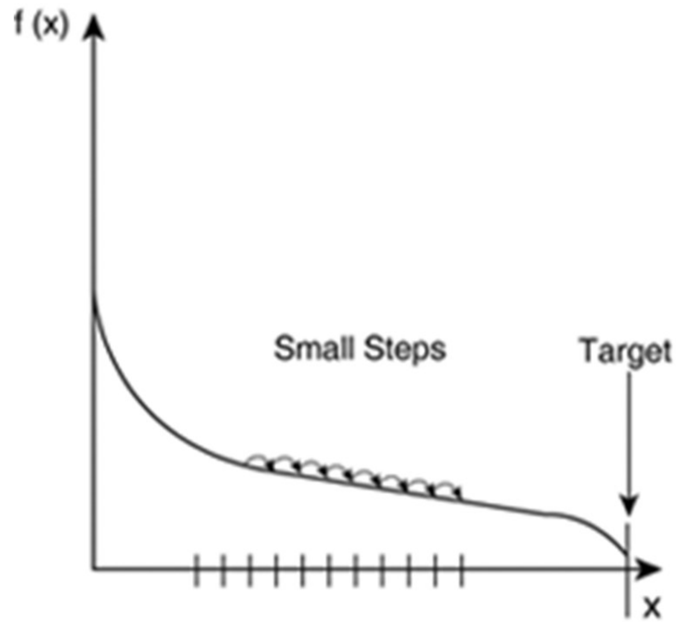
  - To find a *minimum* move *exactly opposite the direction of the gradient*

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

- Many solutions to choosing step size η^k

1. Fixed step size

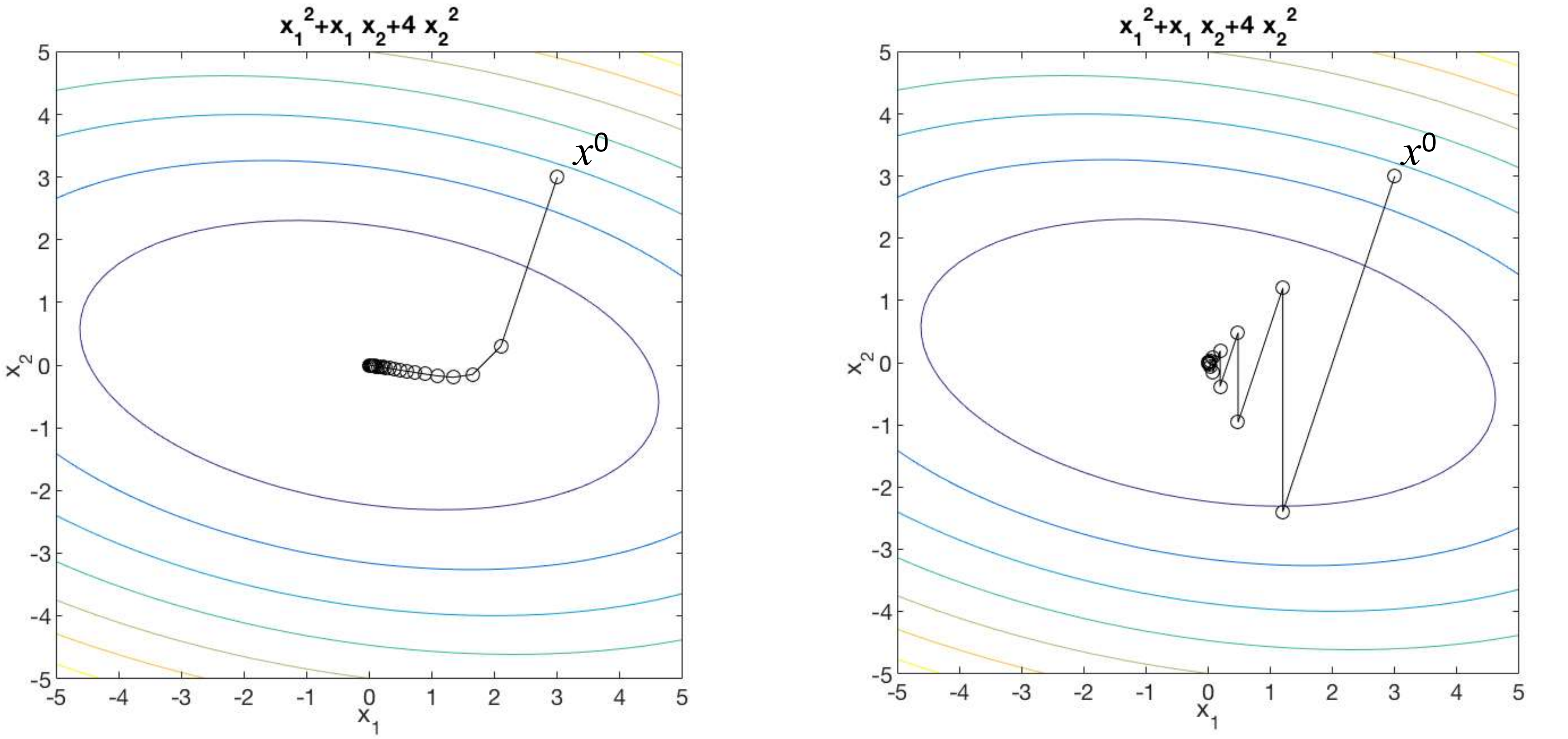
- Fixed step size
  - Use fixed value for η^k



Influence of step size example (constant step size)

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

$\eta = 0.1$ $\qquad$ $\eta = 0.2$



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

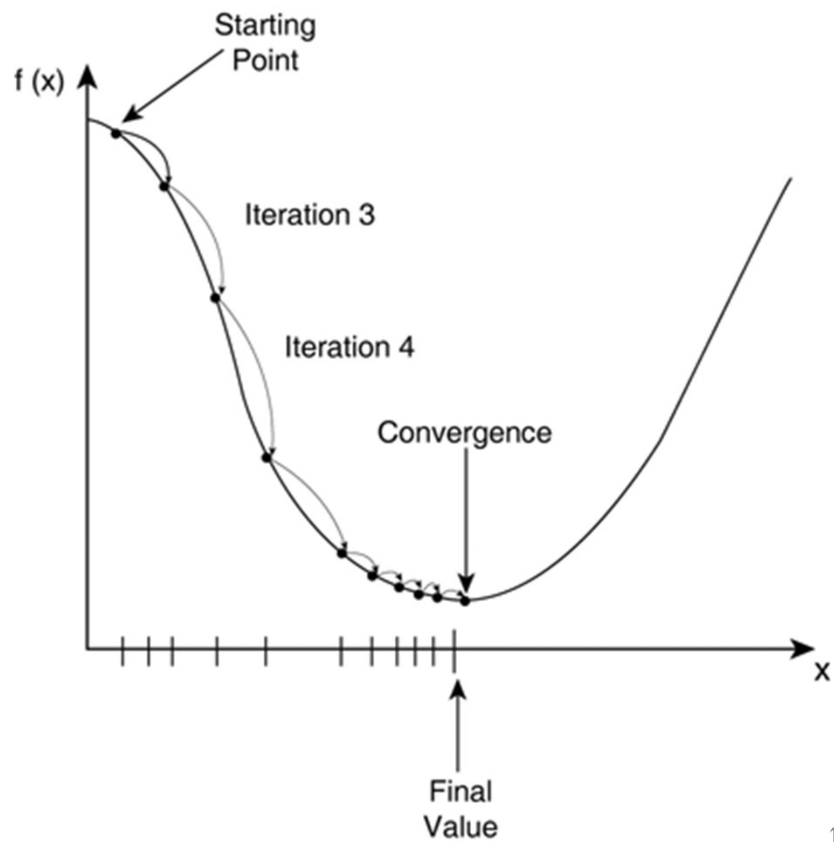
Gradient descent convergence criteria

- 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

$$\left\| \nabla_x f(x^k) \right\| < \varepsilon_2$$



Overall Gradient Descent Algorithm

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

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

Next up

- Gradient descent to train neural networks

- A.K.A. Back propagation