Neural Networks
Learning the network: Part 1

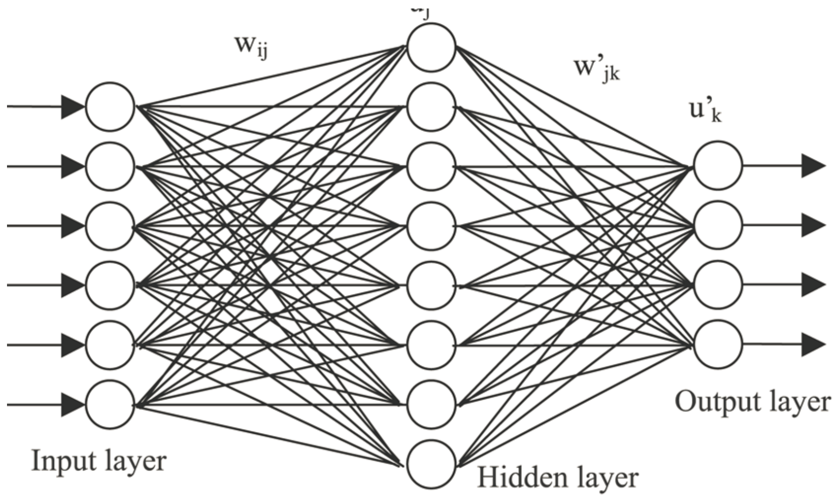
11-785, Spring 2021

Lecture 3

Topics for the day

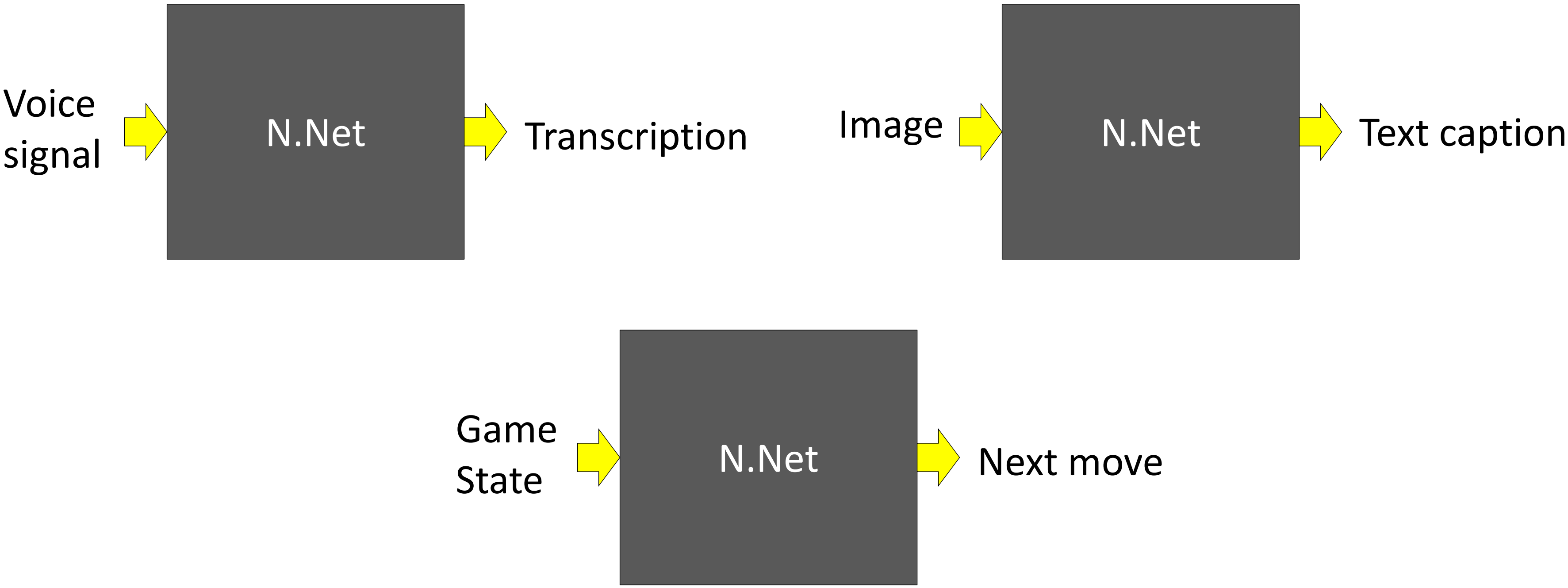
- The problem of learning
- The perceptron rule for perceptrons
  - And its inapplicability to multi-layer perceptrons
- Greedy solutions for classification networks: ADALINE and MADALINE
- Learning through Empirical Risk Minimization
- Intro to function optimization and gradient descent

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?

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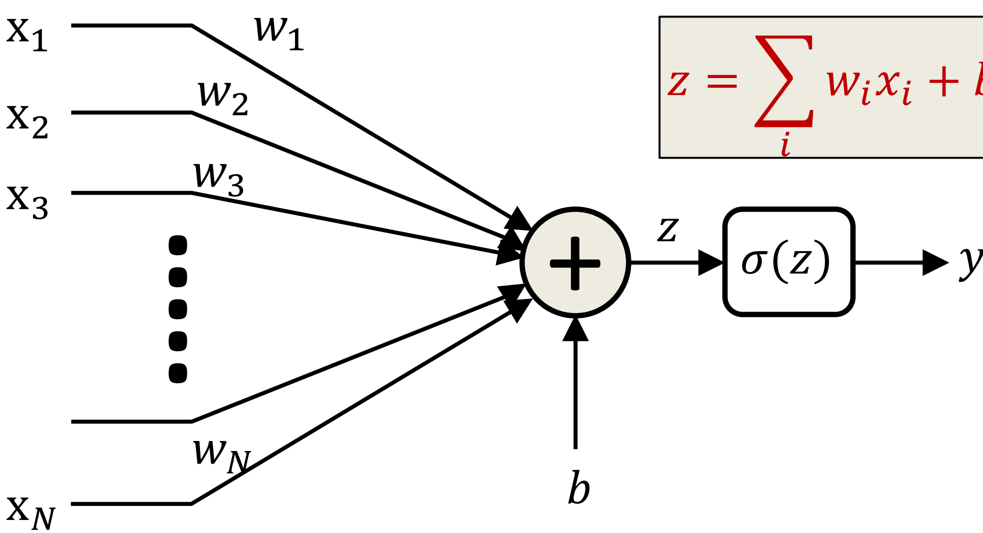
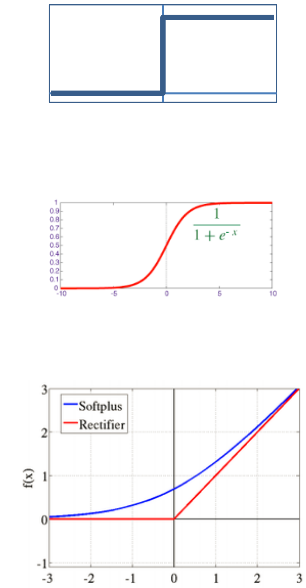
- Preliminaries:
  - How do we represent the input?
  - How do we represent the output?
- *How do we compose the network that performs the requisite function?*

A bit later in the program

Preliminaries: The units in the network – the perceptron



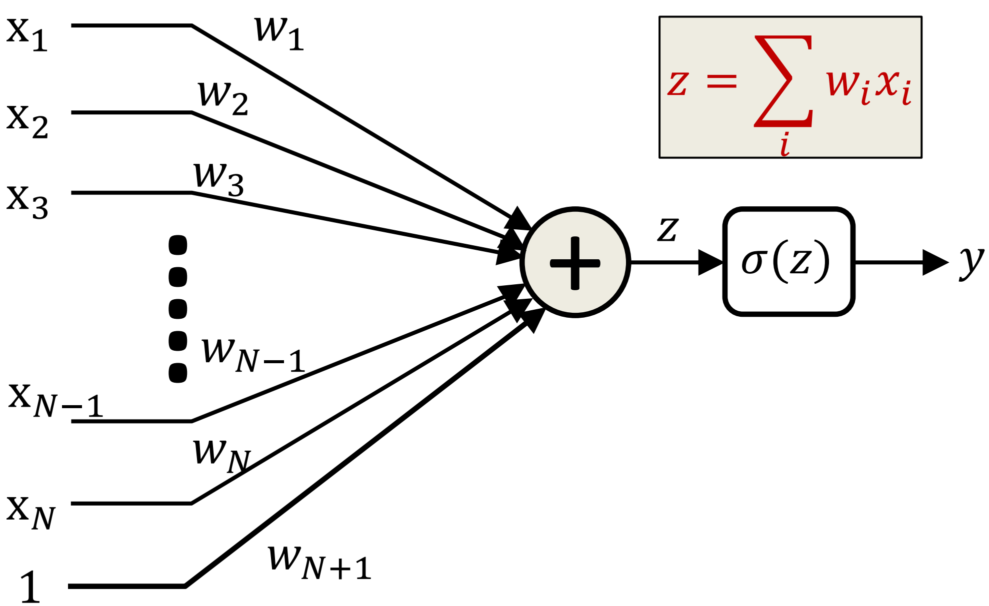
$$z = \sum_i w_i x_i + b$$

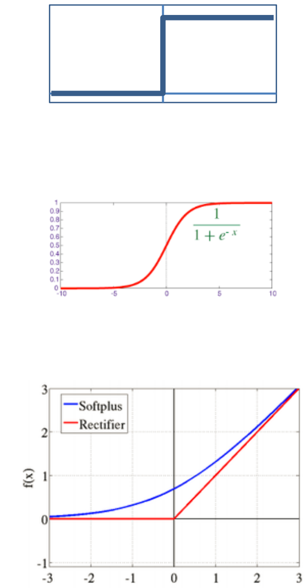


Activation functions $\sigma(z)$

- 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

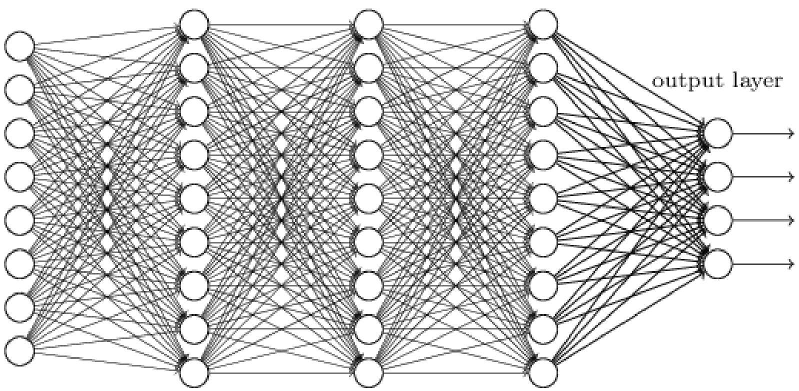


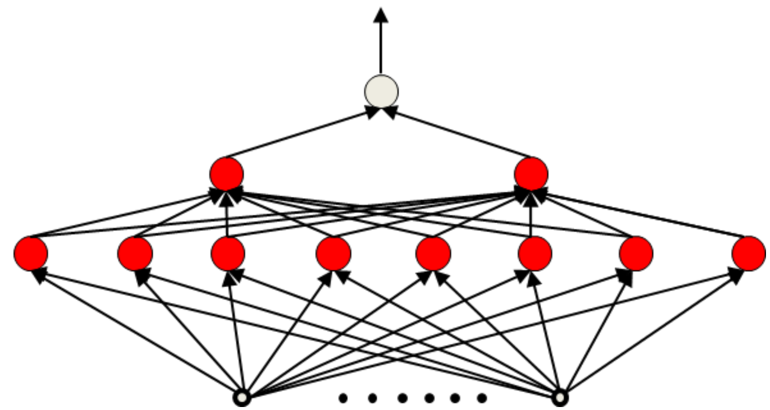


Activation functions $\sigma(z)$

- 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

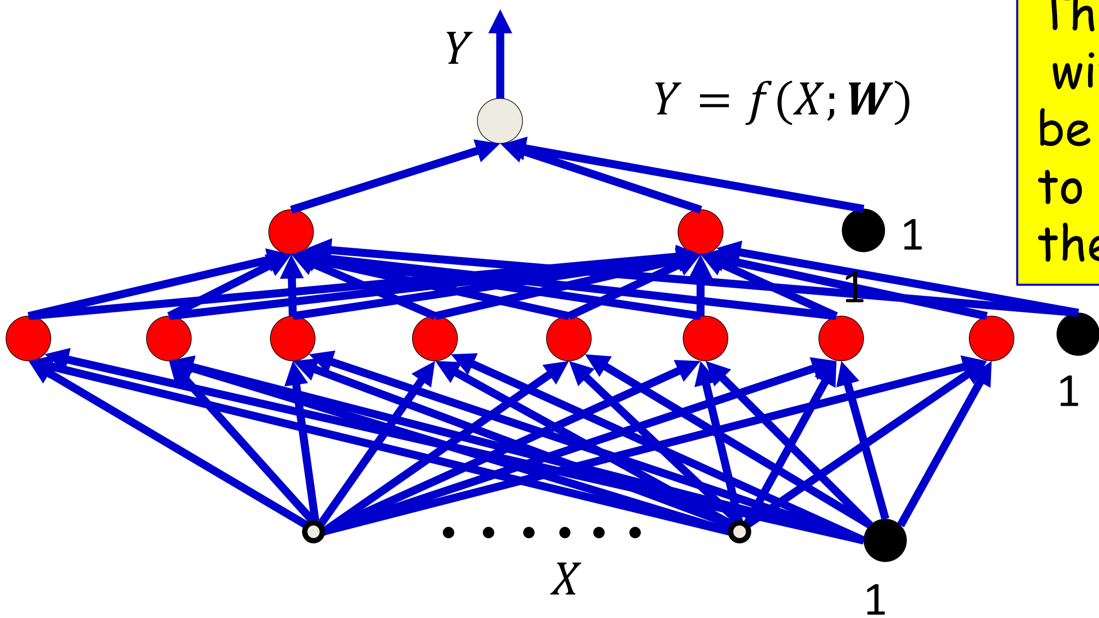
First: the structure of the network





- 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

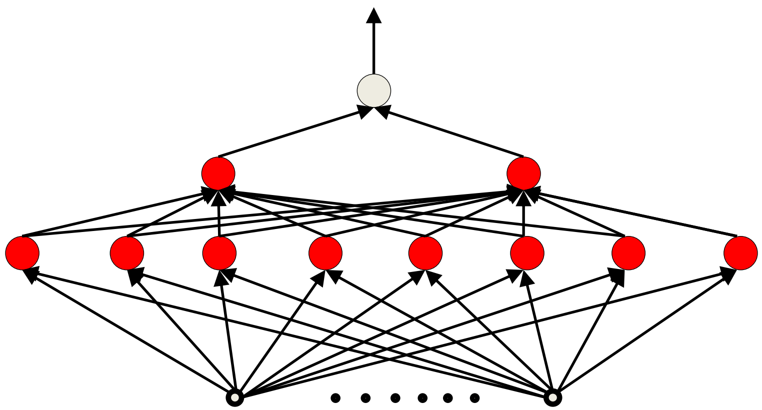


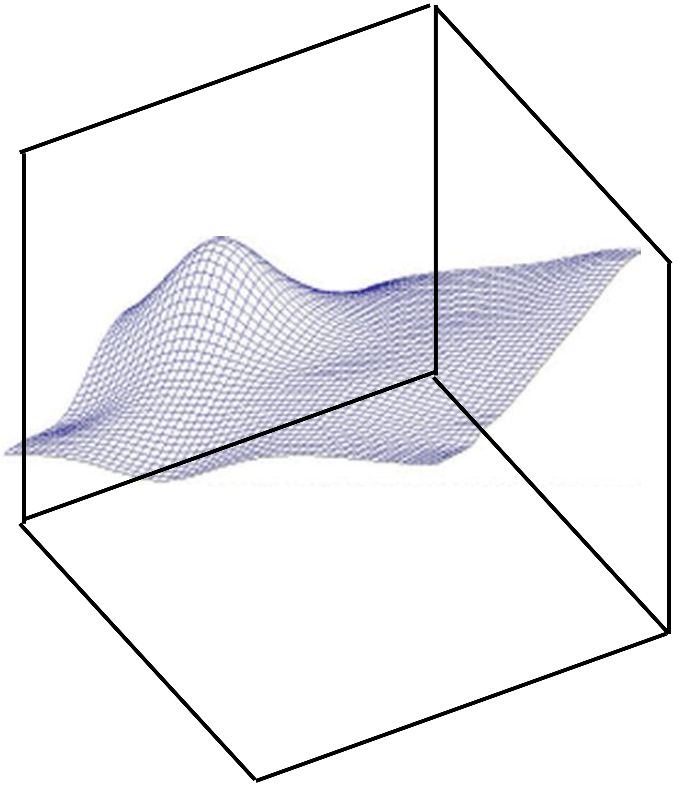
The network is a function f() with parameters W which must be set to the appropriate values to get the desired behavior from the net

- **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..

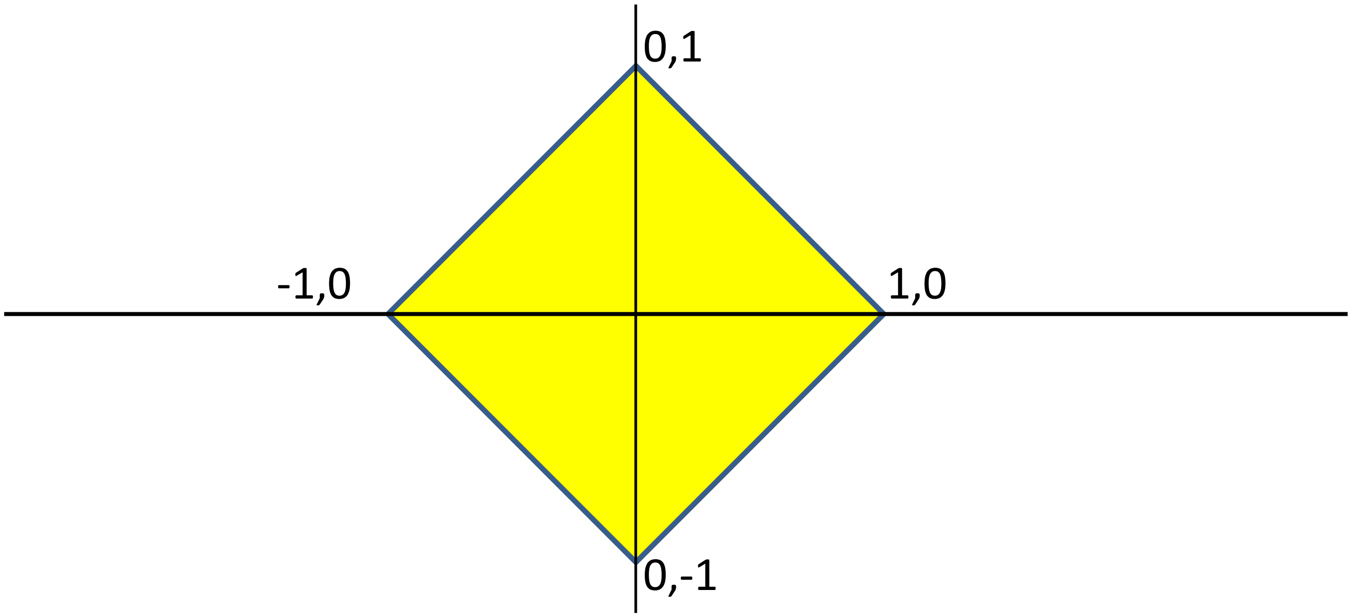
The MLP *can* represent anything





- 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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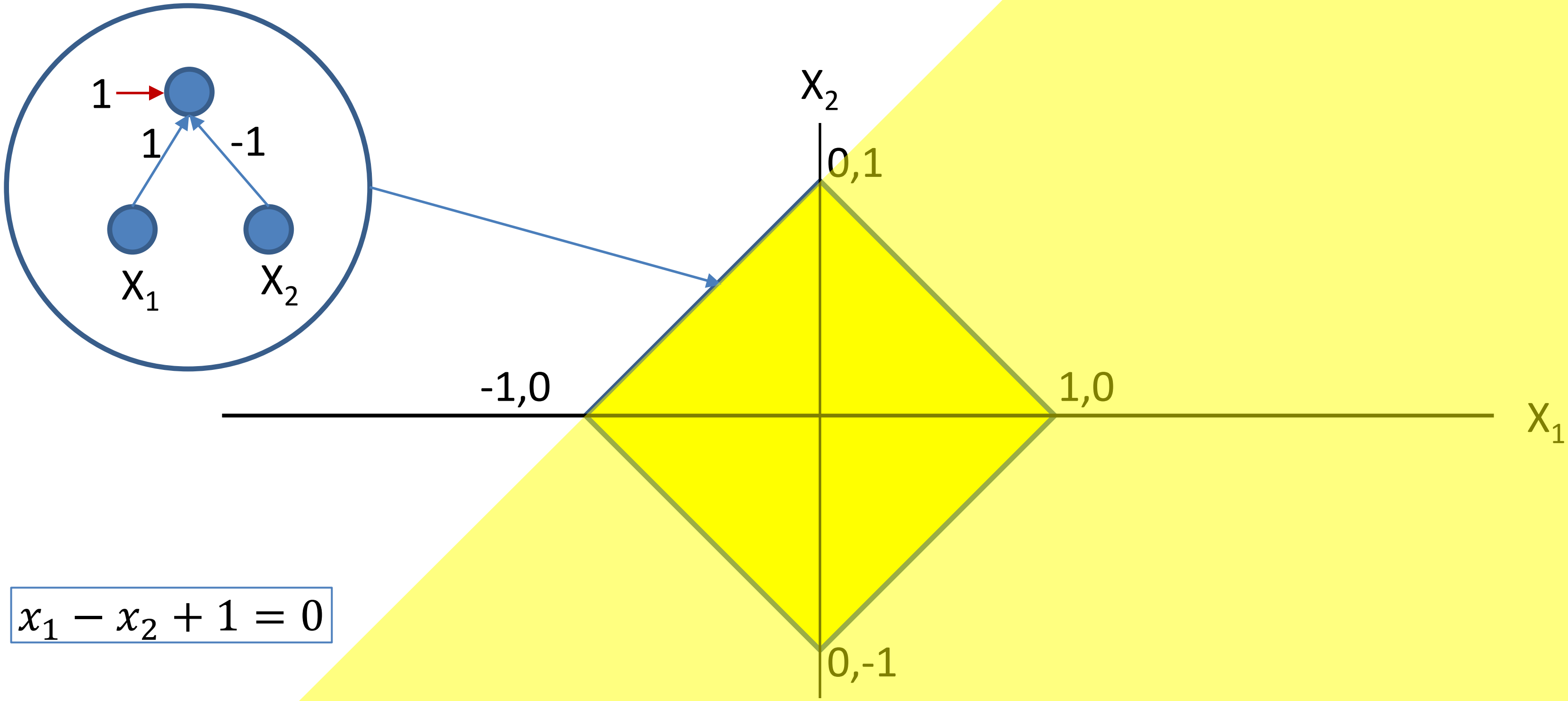
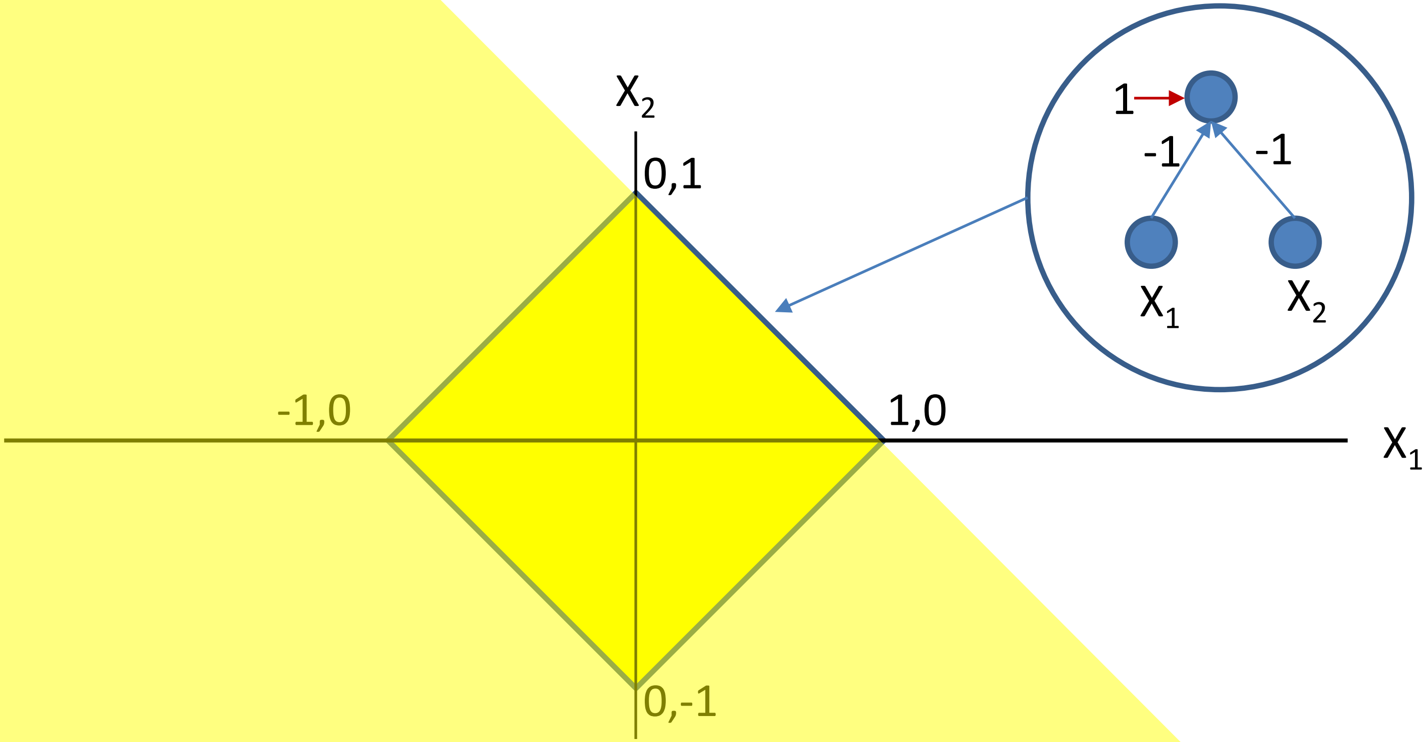


$x_1 - x_2 + 1 = 0$

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

Option 1: Construct by hand



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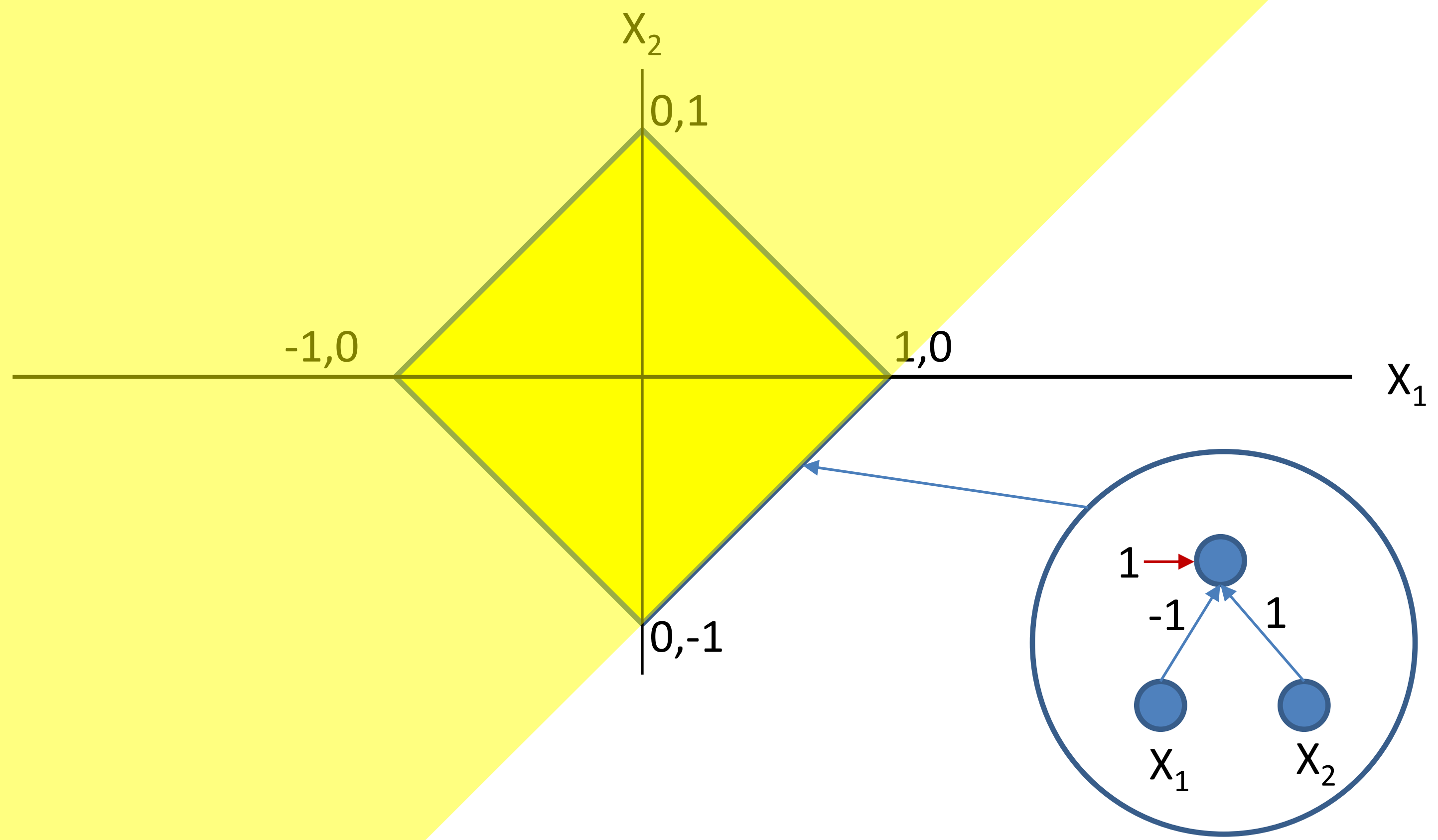

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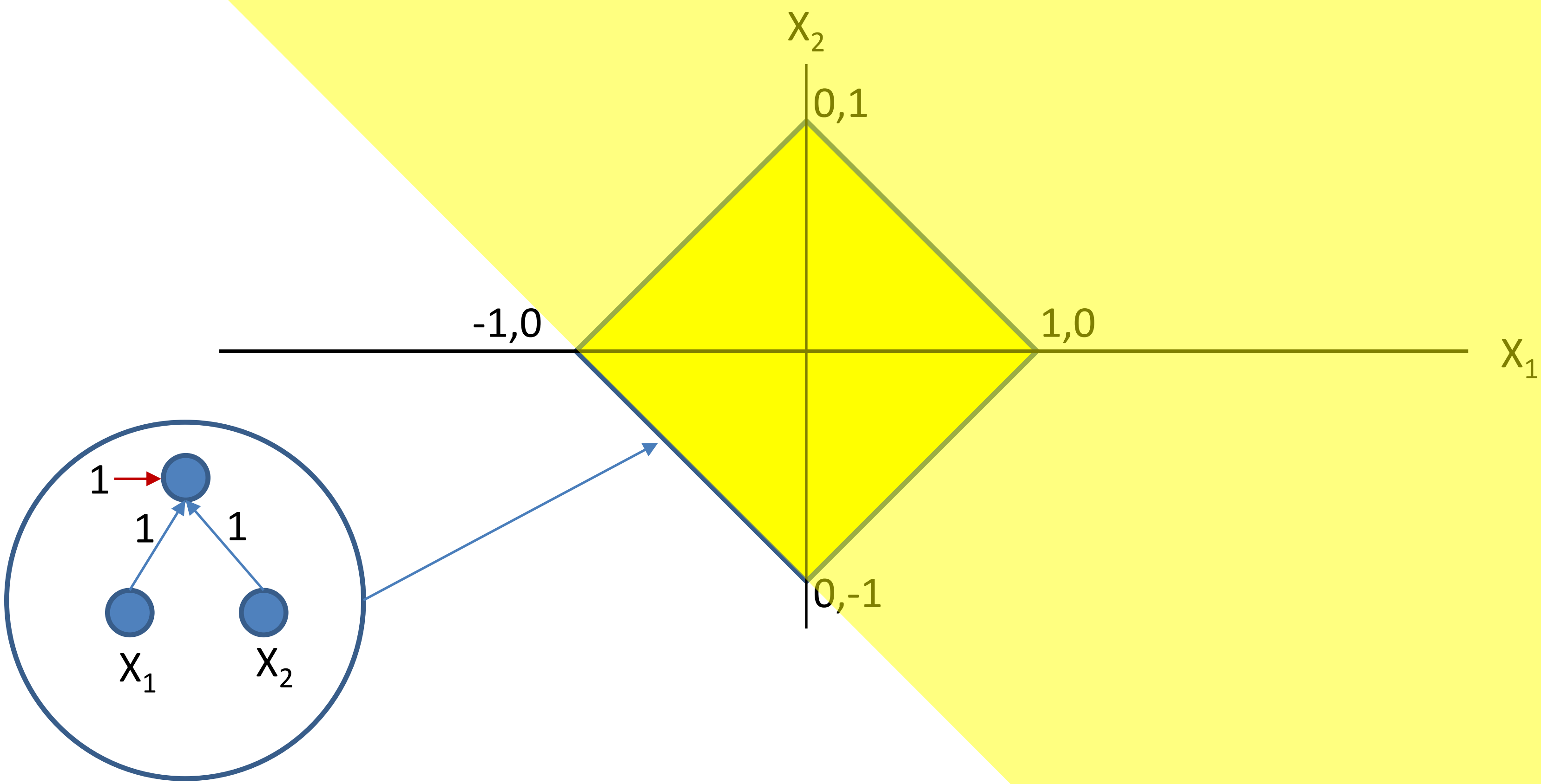

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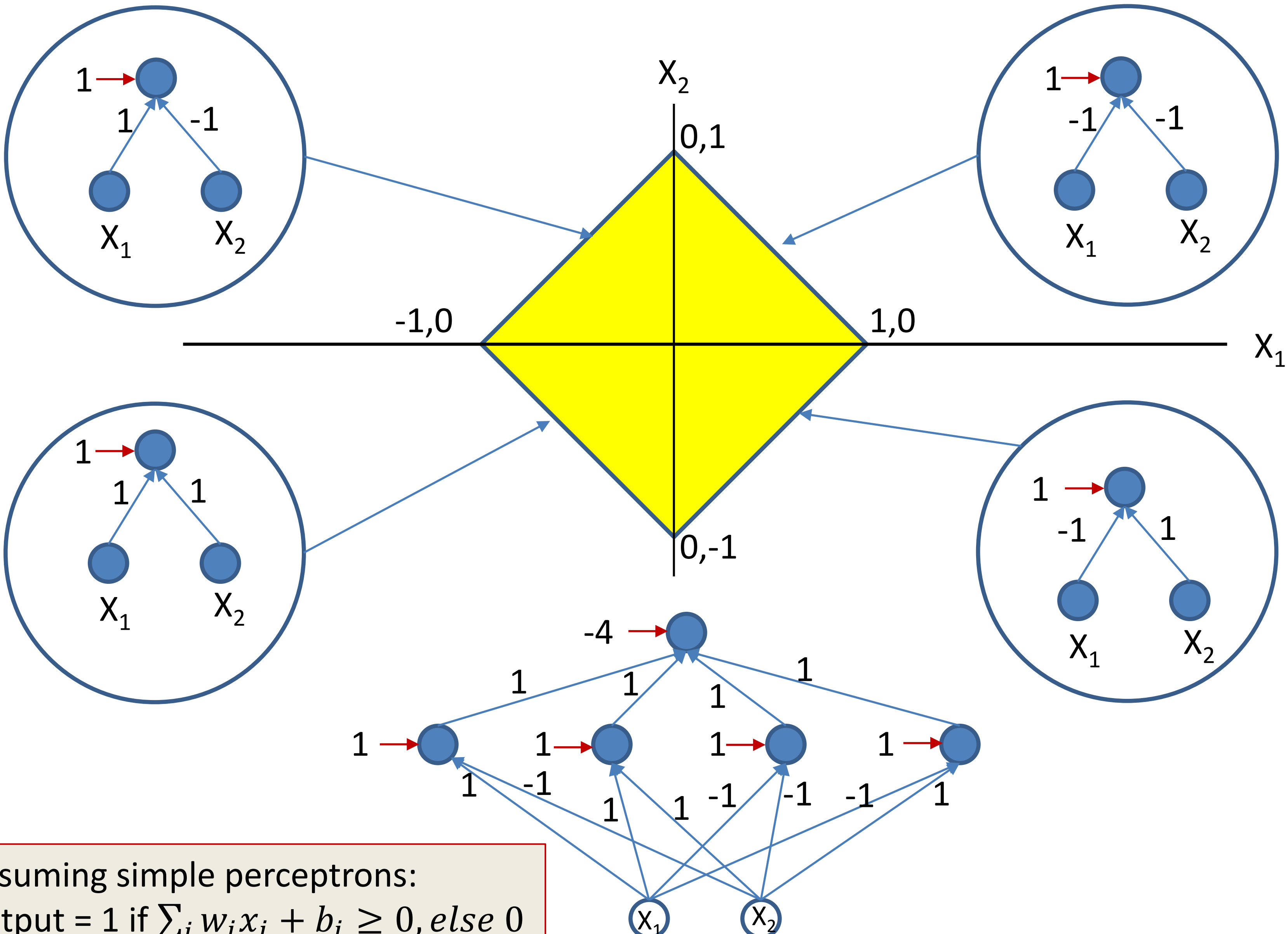

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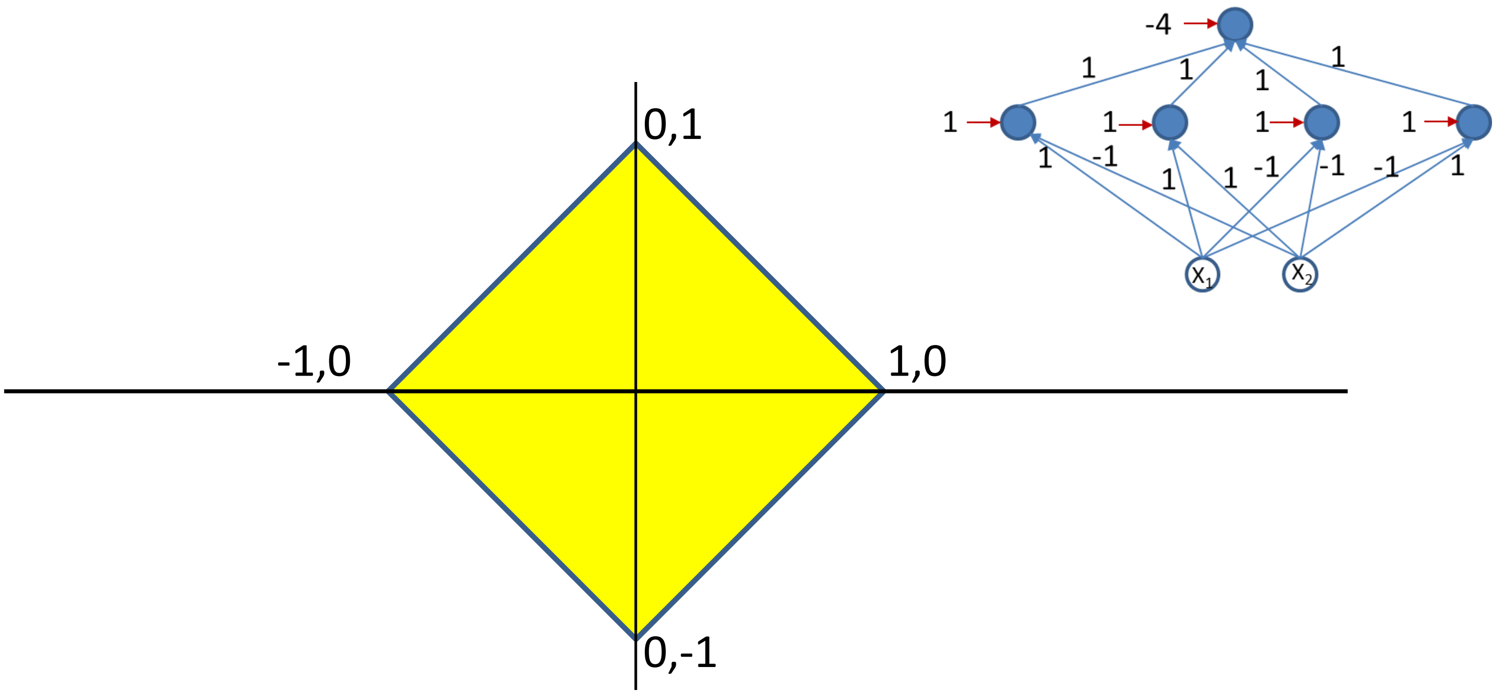
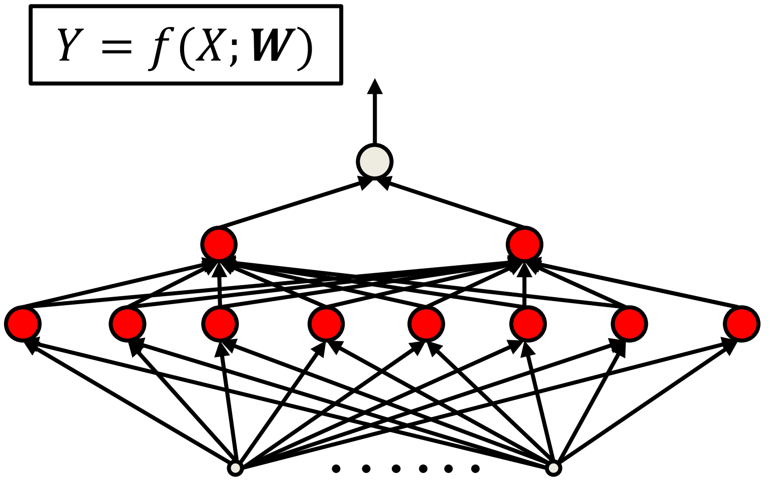
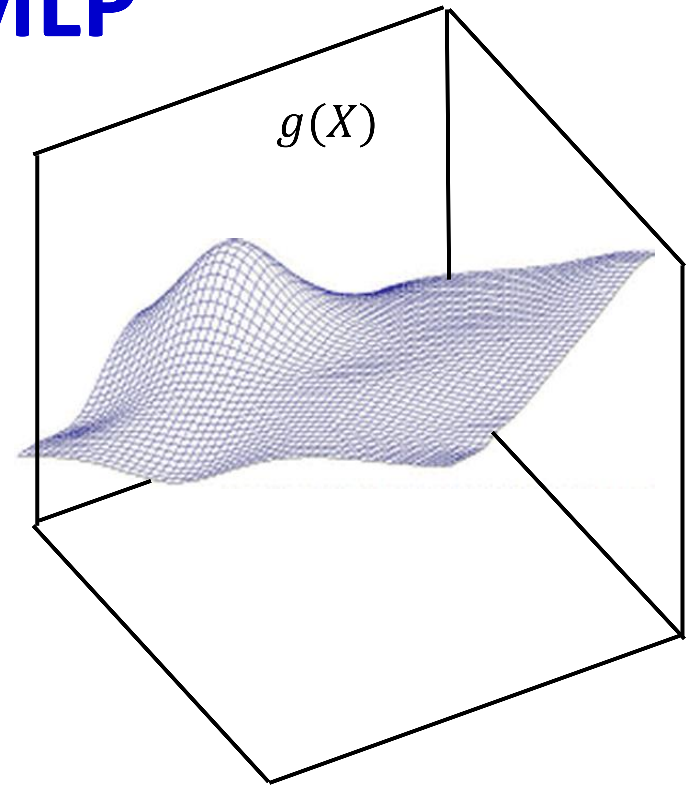


- Given a function, *handcraft* a network to satisfy it
- E.g.: Build an MLP to classify this decision boundary
- Not possible for all but the simplest problems..

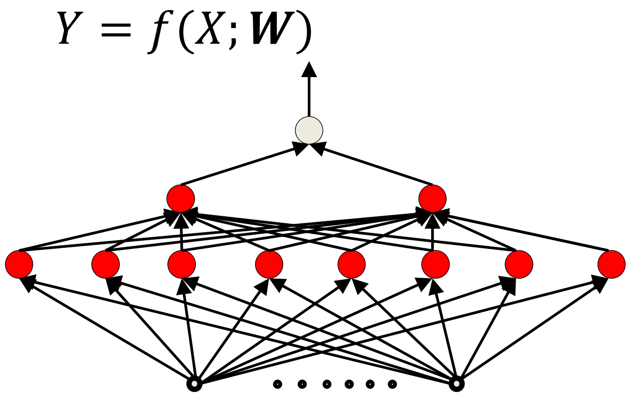
Option 2: Automatic estimation of an MLP

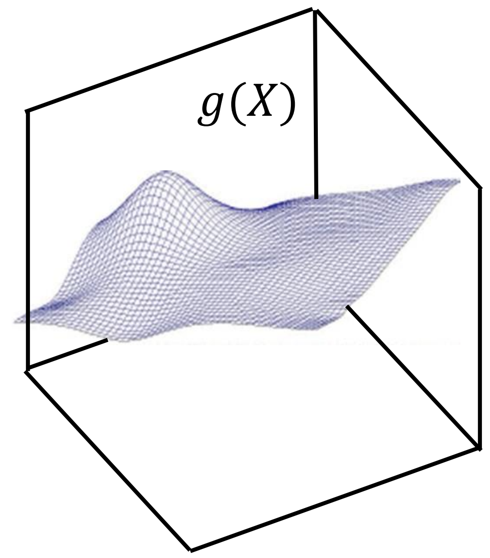




- More generally, *given* the function $g(X)$ to model, we can *derive* the parameters of the network to model it, through computation

How to learn a network?



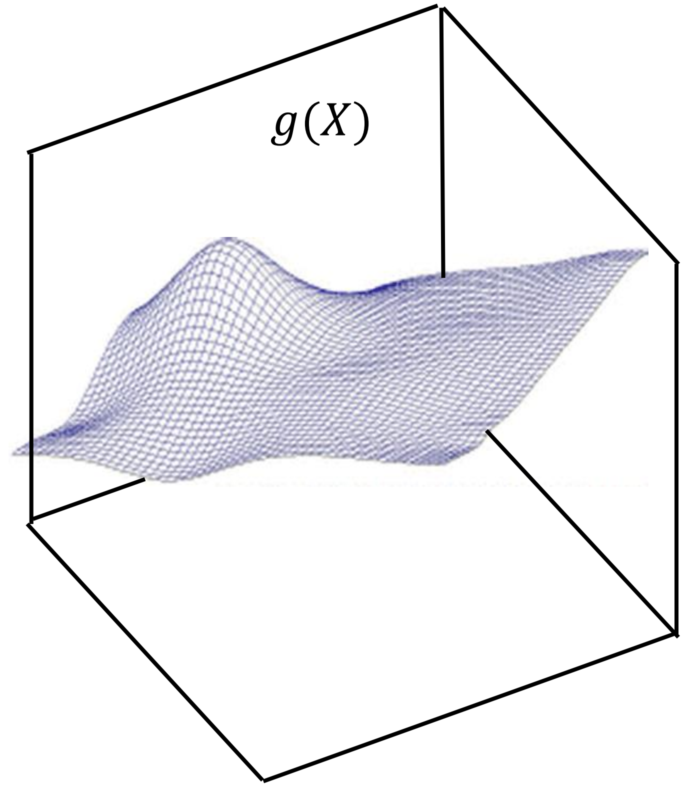


- When $f(X; \boldsymbol{W})$ has the capacity to exactly represent $g(X)$

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

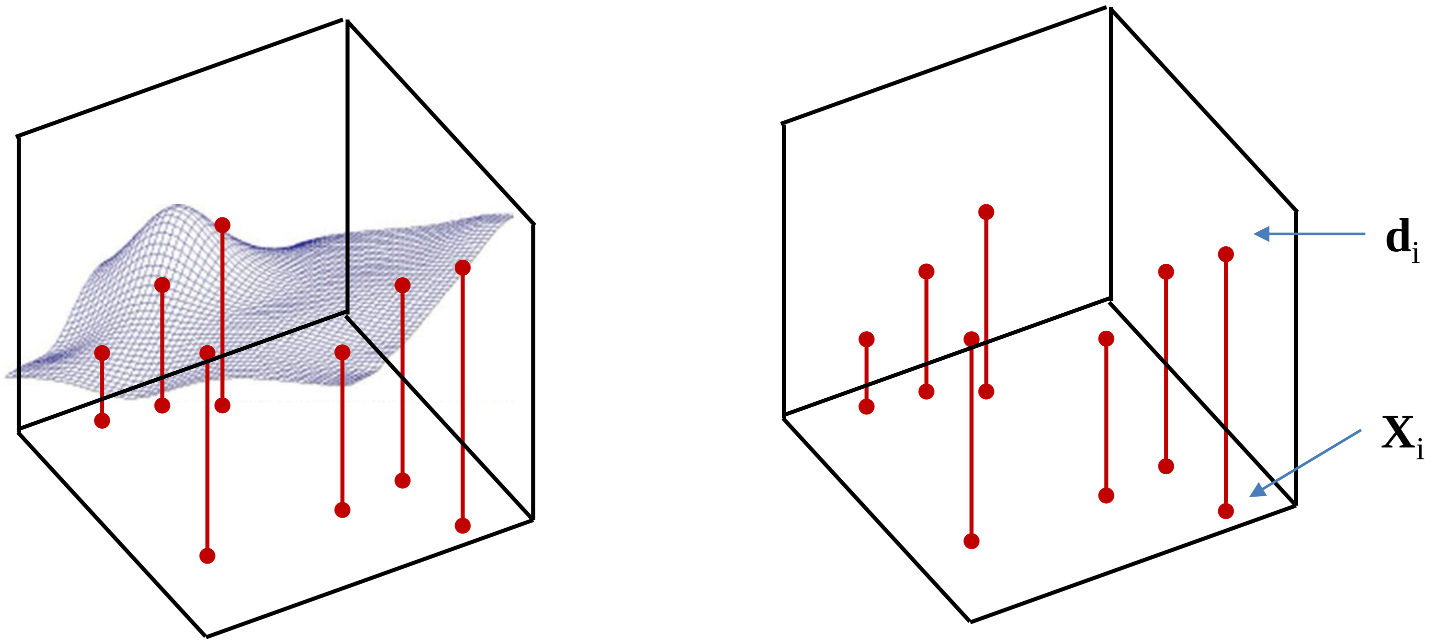
- $div()$ is a *divergence* function that goes to zero when $f(X; W) = g(X)$

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**

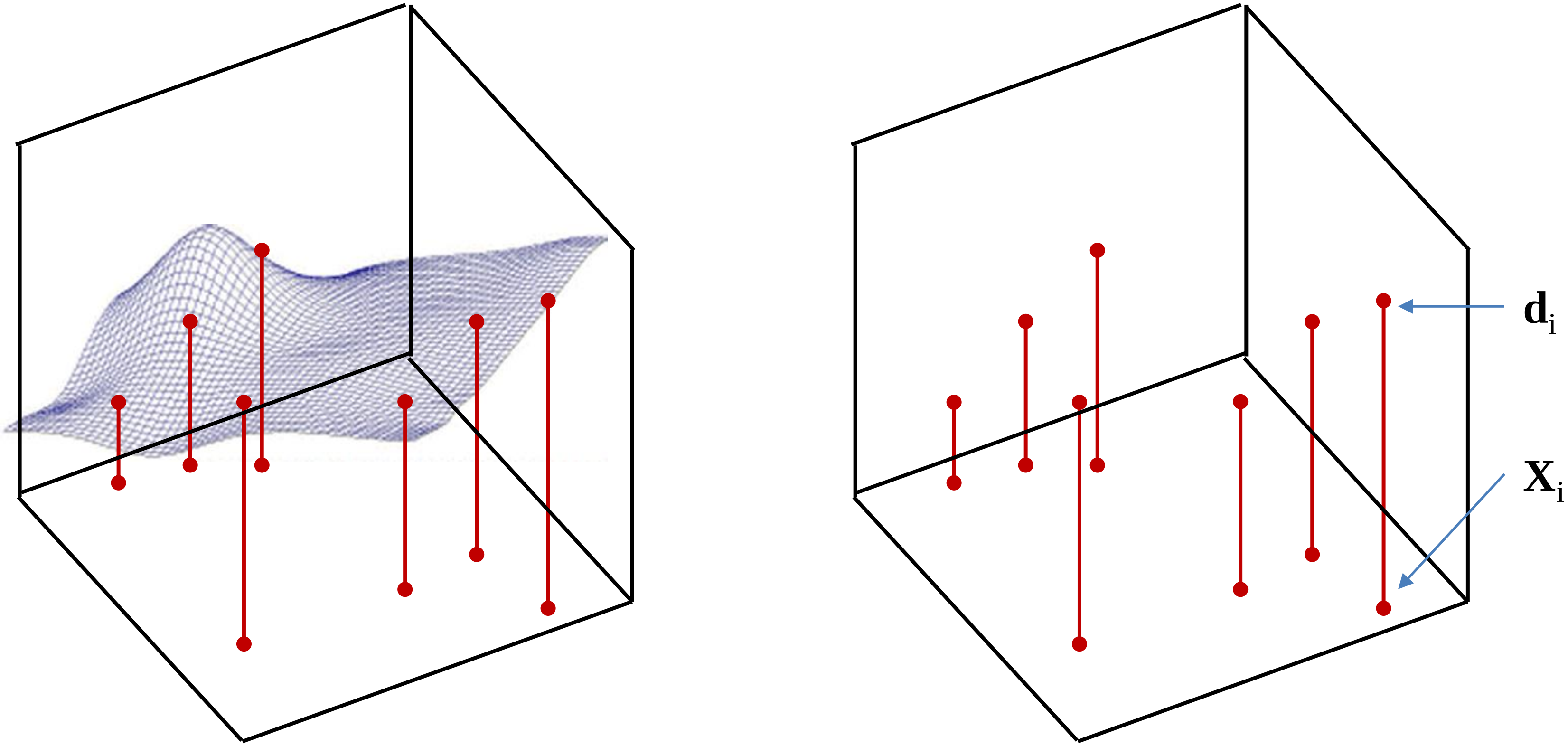
Sampling the function



- *Sample* $g(X)$
  - Basically, get input-output pairs for a number of samples of input X_i
    - Many samples (X_i, d_i), where $d_i = g(X_i) + noise$

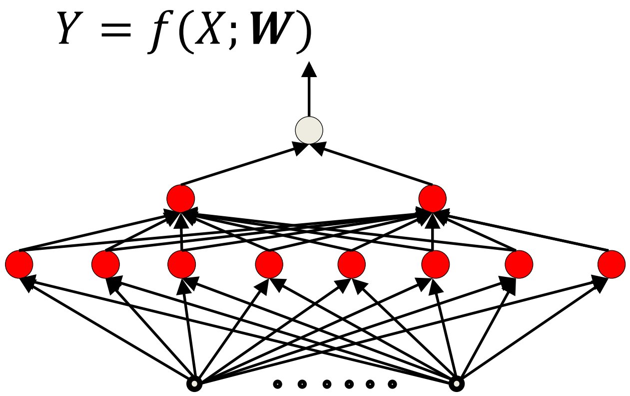
- Very easy to do in most problems: just gather training data
  - E.g. set of images and their class labels
  - E.g. speech recordings and their transcription

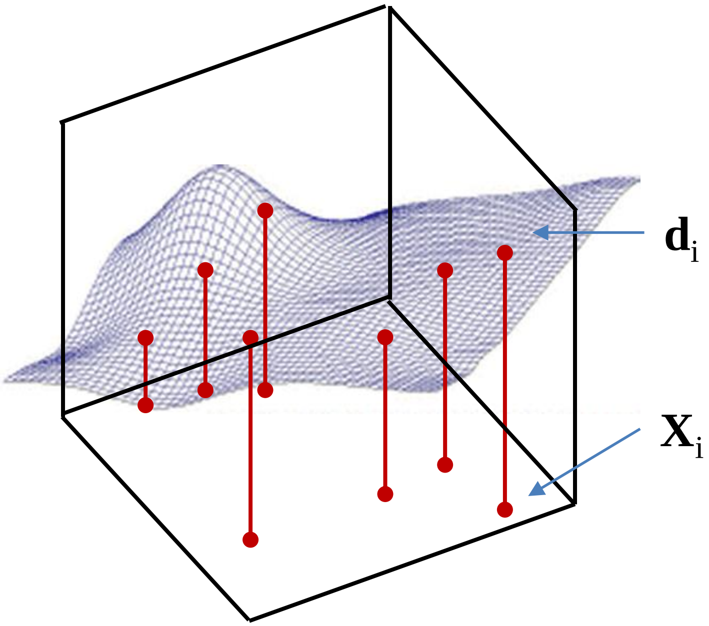
Drawing samples



- 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

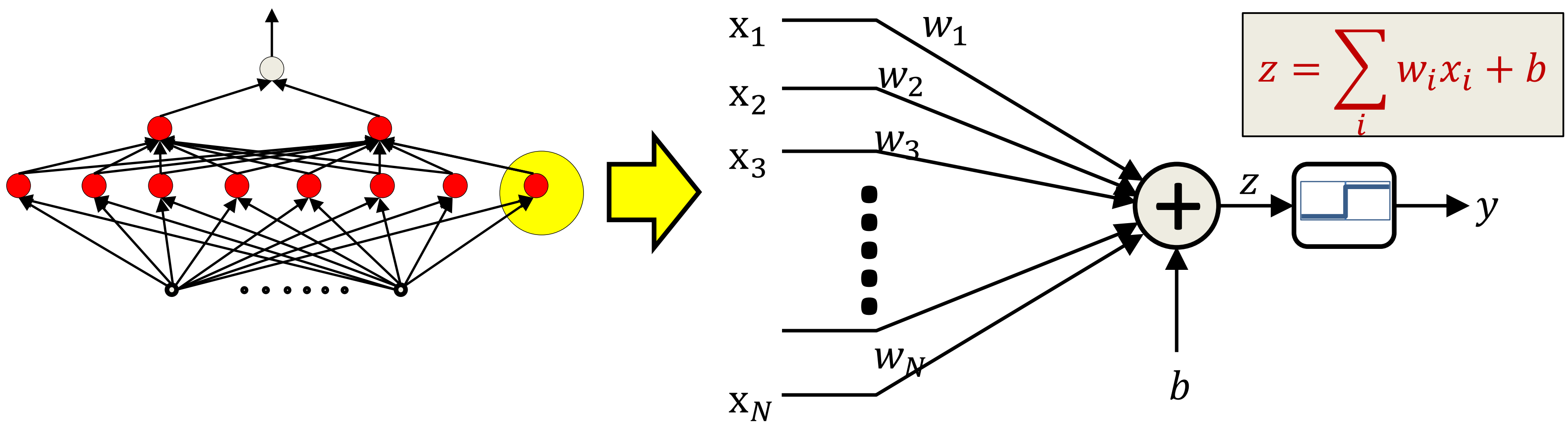
Let's begin with a simple task

- Learning a *classifier*
  - Simpler than regressions

- This was among the earliest problems addressed using MLPs

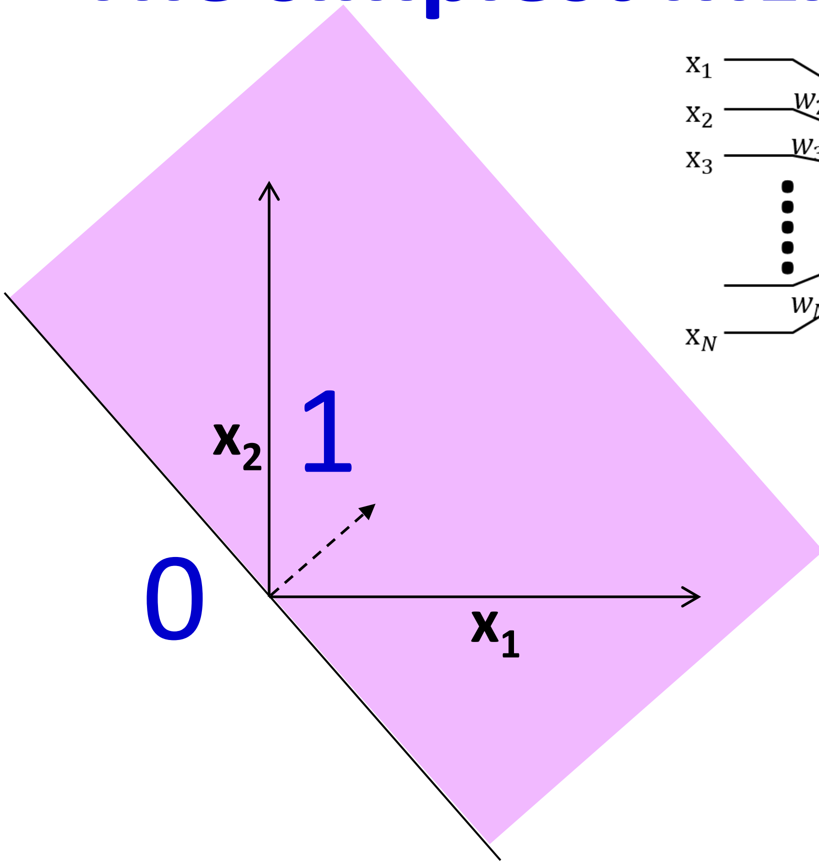
- Specifically, consider *binary* classification
  - Generalizes to multi-class

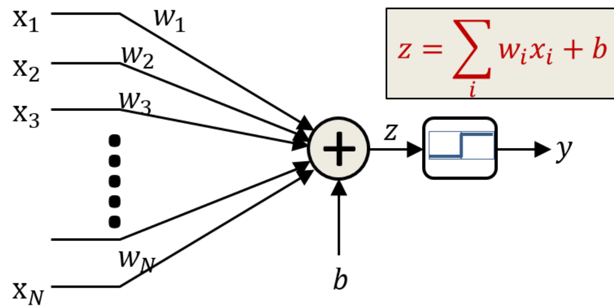
History: The original MLP

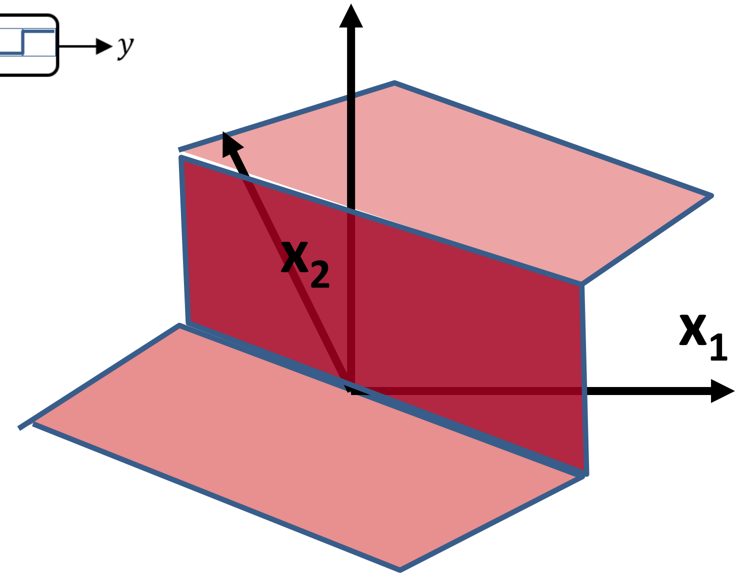


- The original MLP as proposed by Minsky: a network of threshold units
  - But how do you train it?
    - Given only “training” instances of input-output pairs

The simplest MLP: a single perceptron

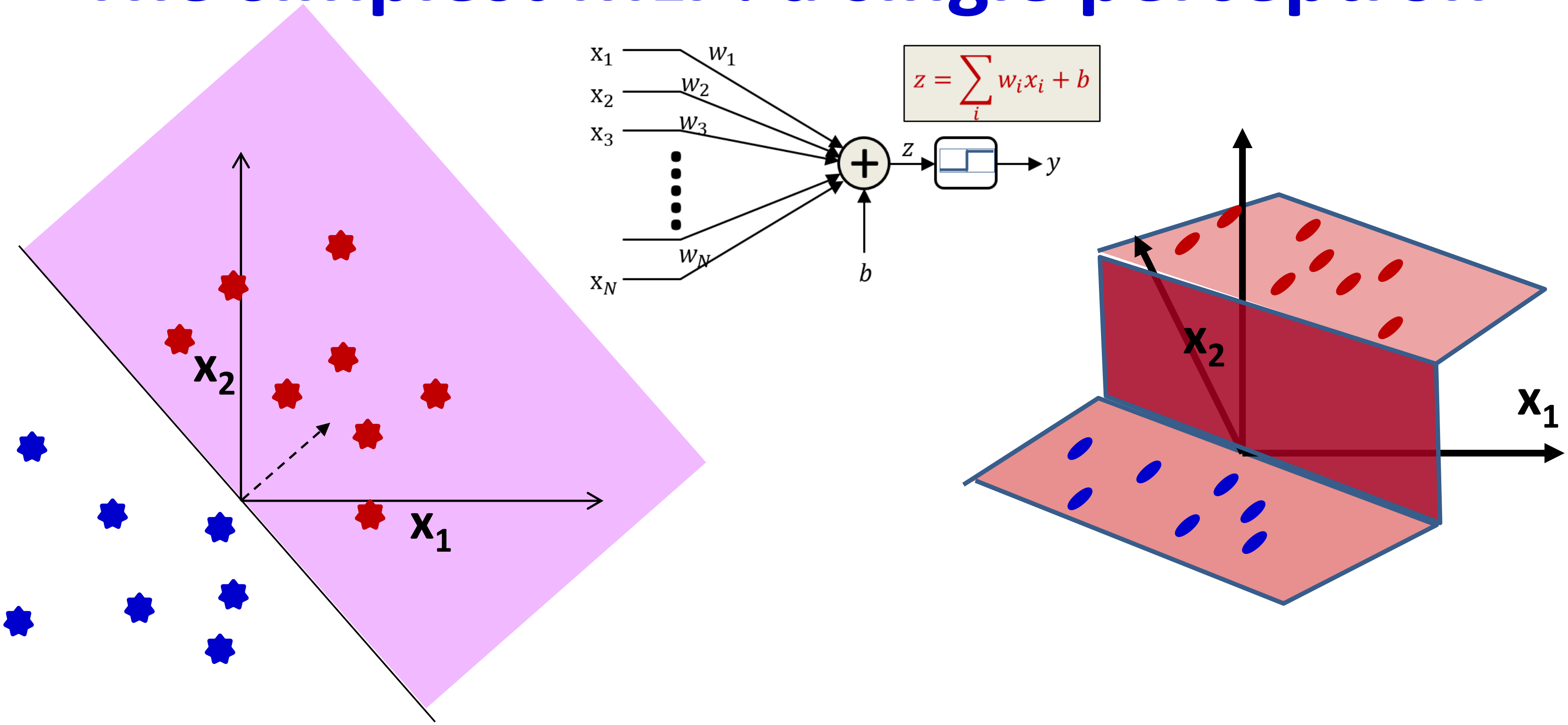






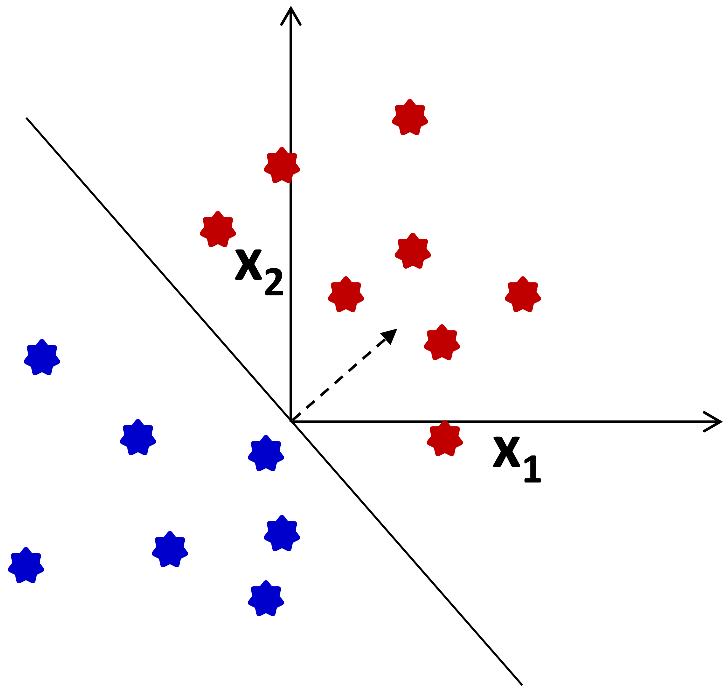
- Learn this function
  - **A step function across a hyperplane**

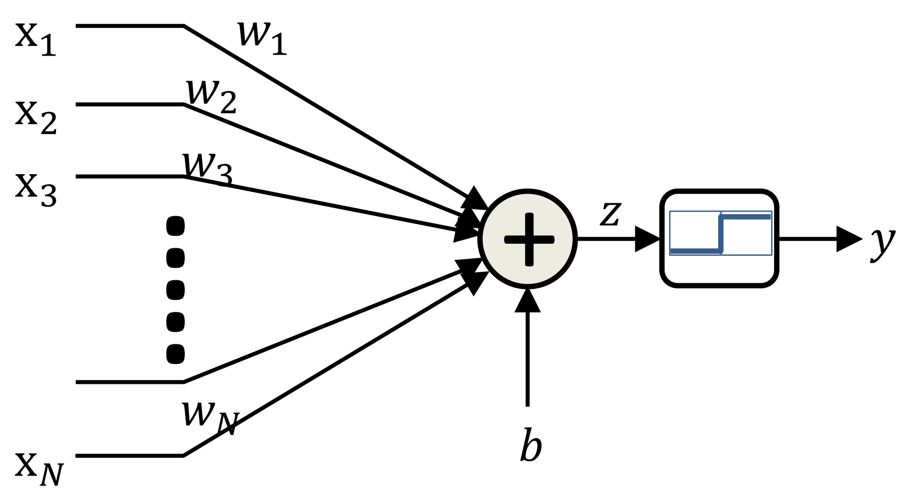
The simplest MLP: a single perceptron



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

Learning the perceptron

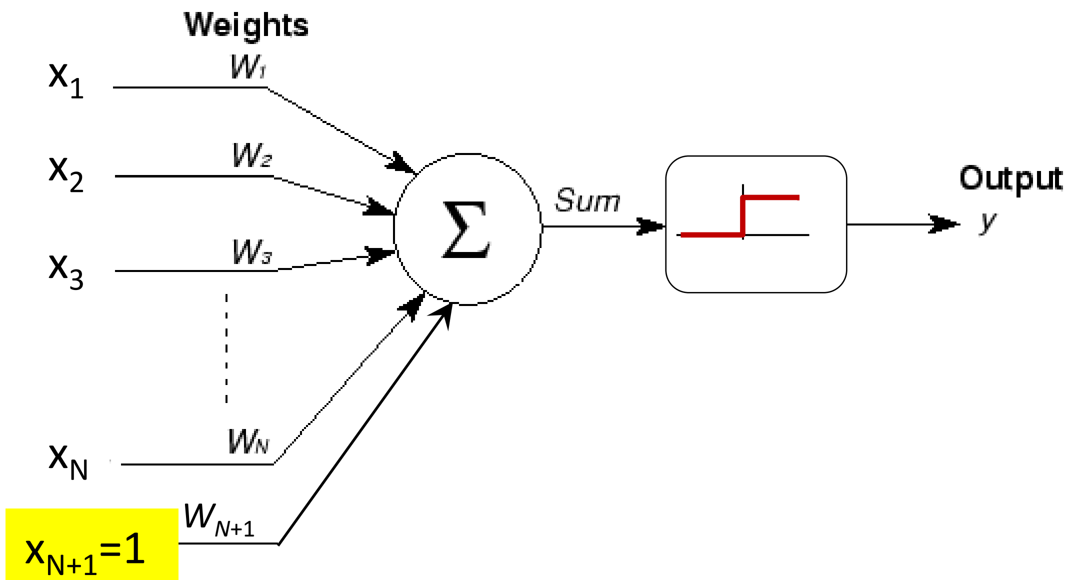




- Given a number of input output pairs, learn the weights and bias
  - $y = \begin{cases} 1 \;\; if \;\; \sum_{i=1}^{N} w_i X_i + b \geq 0 \\ 0 \qquad\qquad\qquad otherwise \end{cases}$
  - Learn $W = [w_1 .. w_N]^T$ and b, given several (X, y) pairs

Boundary: $\sum_{i=1}^{N} w_i X_i + b = 0$

Restating the perceptron



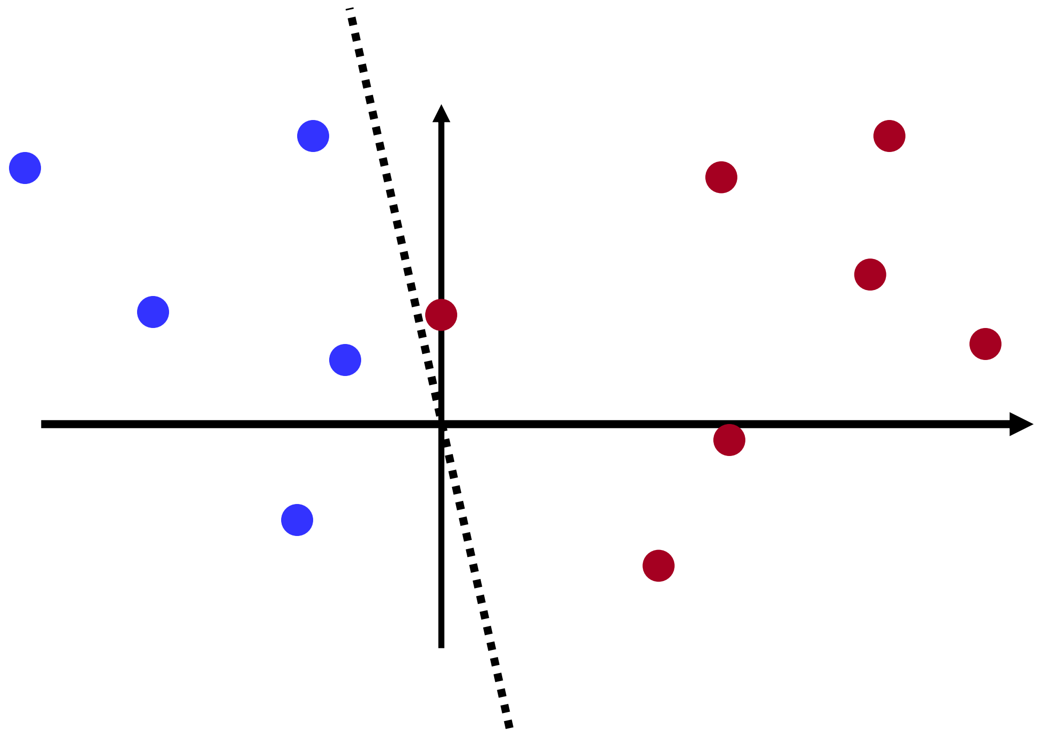
- Restating the perceptron equation by adding another dimension to X

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

where $X_{N+1} = 1$

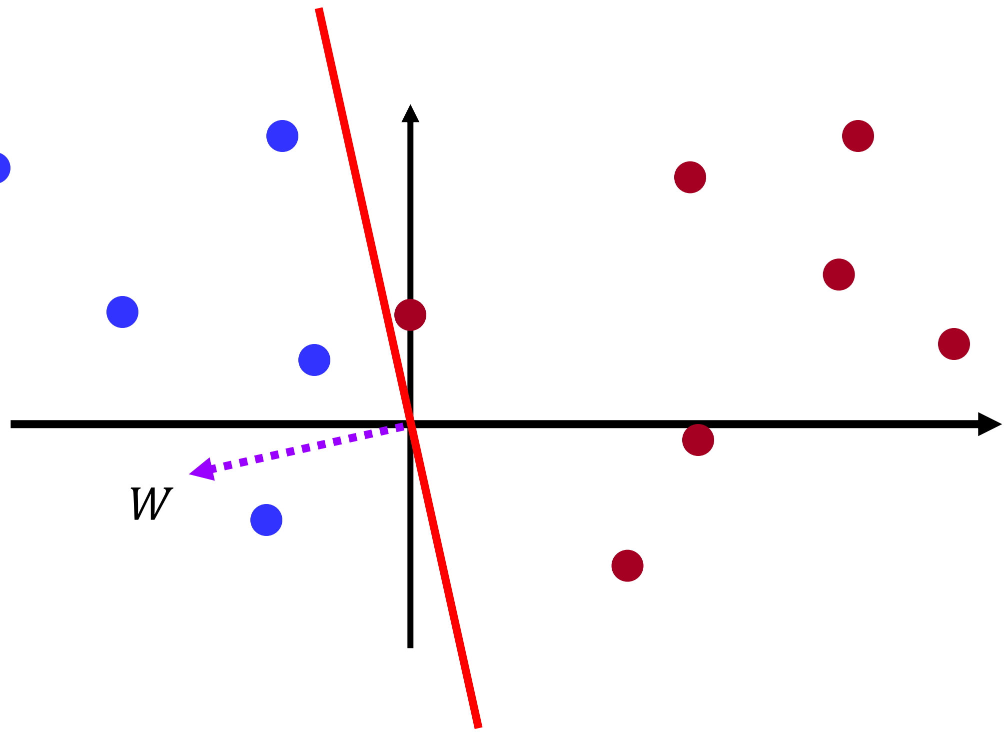
- Note that the boundary $\sum_{i=1}^{N+1} w_i X_i = 0$ is now a hyperplane through origin

The Perceptron Problem



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

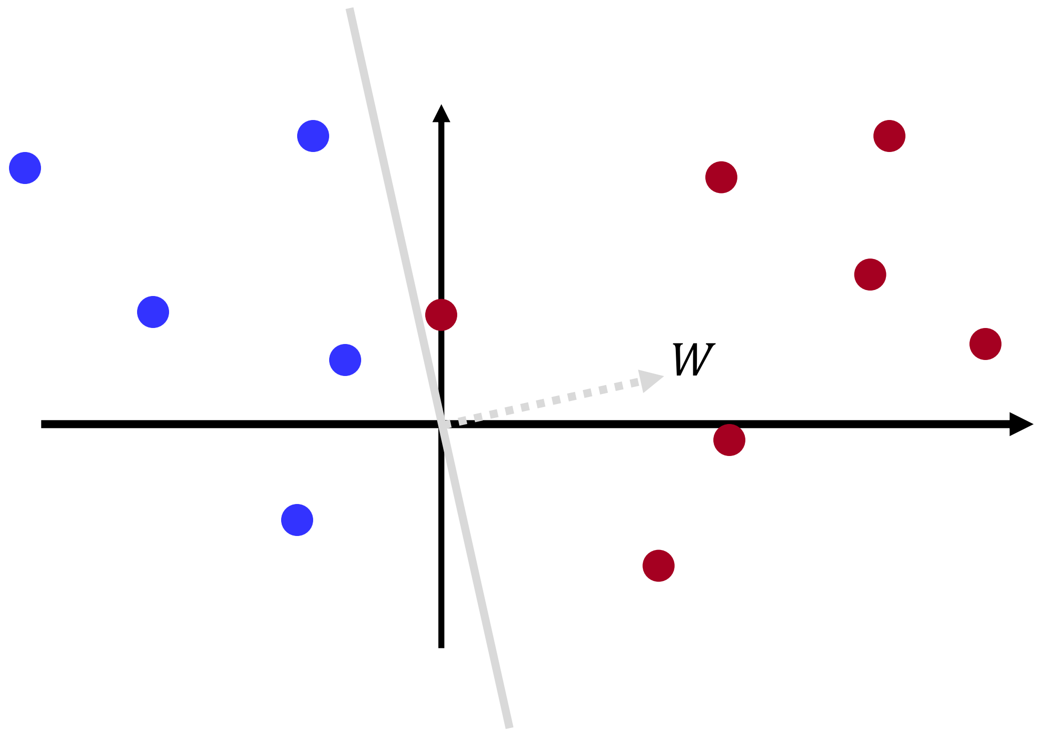
The Perceptron Problem



- Find the hyperplane $\sum_{i=1}^{N+1} w_i X_i = 0$ that perfectly separates the two groups of points
  - Let vector $W = [w_1, w_2, \dots, w_{N+1}]^T$ and vector $X = [x_1, x_2, \dots, x_N, 1]^T$
  - $\sum_{i=1}^{N+1} w_i X_i = W^T X$ is an inner product
  - $W^T X = 0$ is the hyperplane comprising all Xs orthogonal to vector W
    - Learning the perceptron = finding the weight vector W for the separating hyperplane
    - W points in the direction of the positive class

The Perceptron Problem

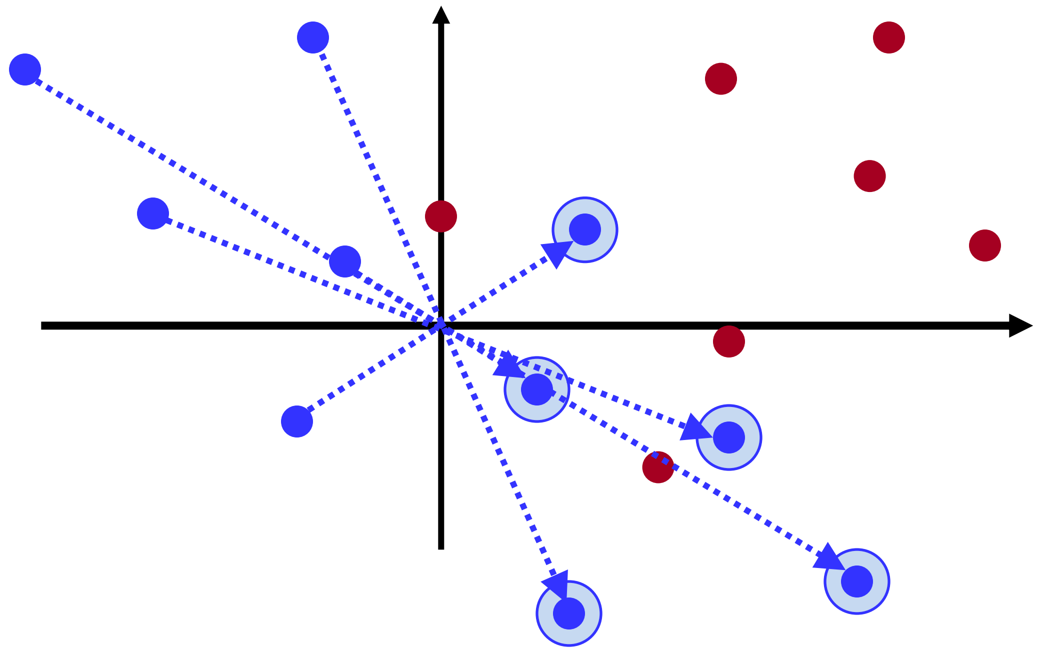
Key: Red 1, Blue = -1



- Learning the perceptron: Find the weights vector W such that the plane described by $W^T X = 0$ perfectly separates the classes
  - $W^T X$ is positive for all red dots and negative for all blue ones

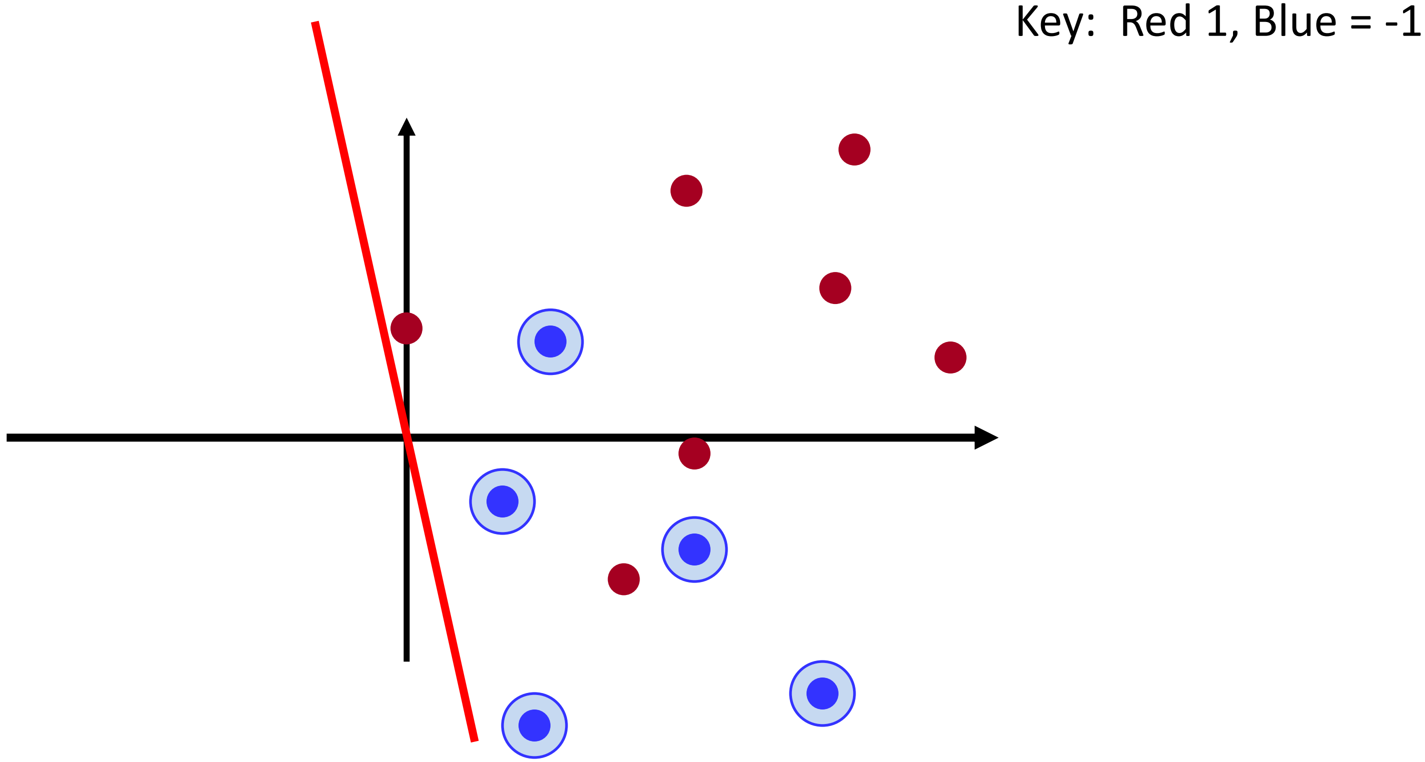
A simple solution

Key: Red 1, Blue = -1



- *Reflect* all the negative instances across the origin
  - Negate every component of vector X
- If we use class $y \in \{+1, -1\}$ notation for the labels (instead of $y \in \{0,1\}$), we can simply write the "reflected" values as $X' = yX$
  - Will retain the features X for the positive class, but reflect/negate them for the negative class

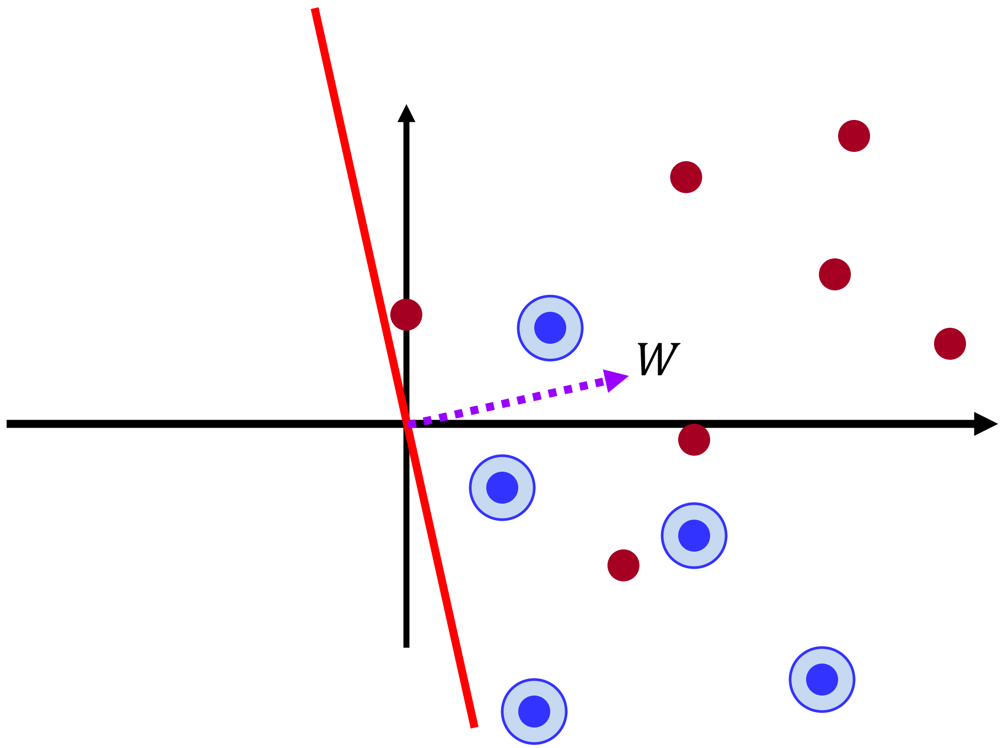
The Perceptron Solution



- Learning the perceptron: Find a plane such that all the modified (X') features lie on one side of the plane
  - Such a plane can always be found if the classes are linearly separable

The Perceptron Solution: Linearly separable case

Key: Red 1, Blue = -1



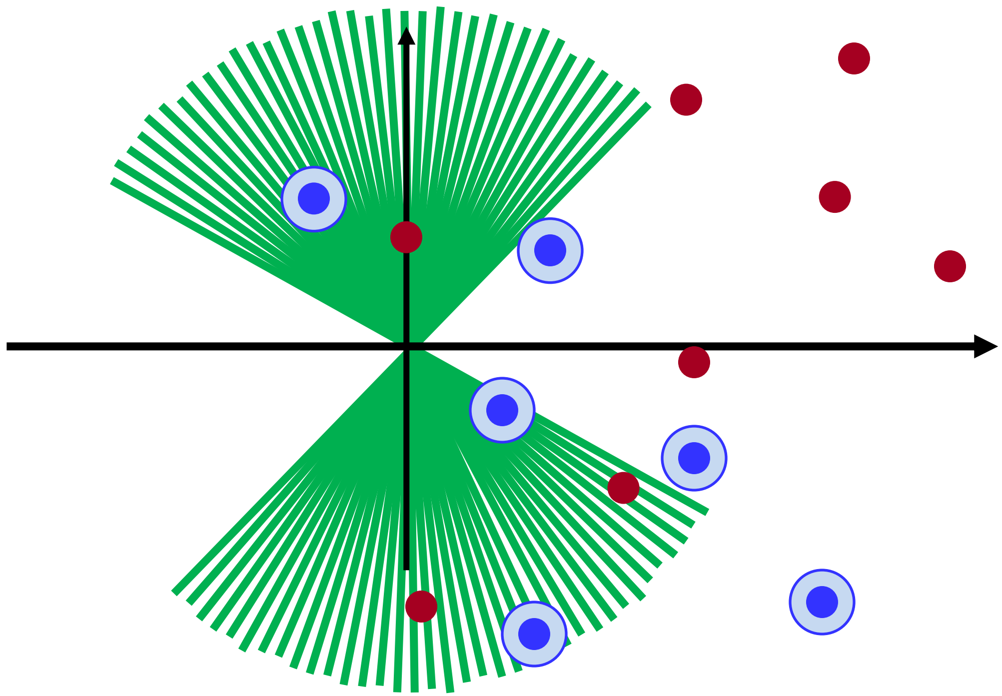
- When classes are linearly separable: a trivial solution

$$W = \frac{1}{N}\sum_i X_i' \qquad = \frac{1}{N}\sum_i y_i X_i$$

- Other solutions are also possible, e.g. max-margin solution

The Perceptron Solution: when classes are not linearly separable

Key: Red 1, Blue = -1



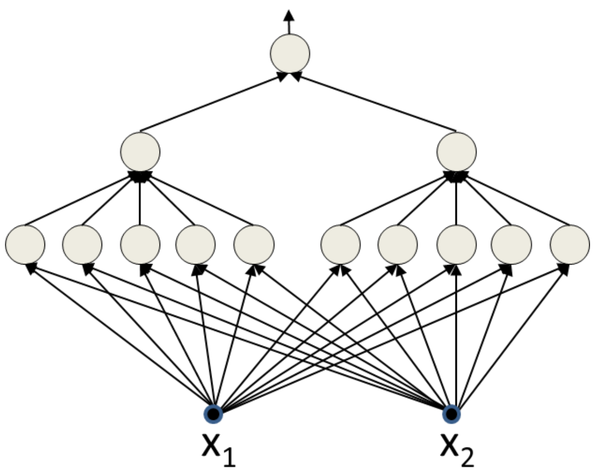
- When classes are not linearly separable, not possible to find a "support" plane
  - Some points will always lie on the other side
  - Model does not support perfect classification of this data

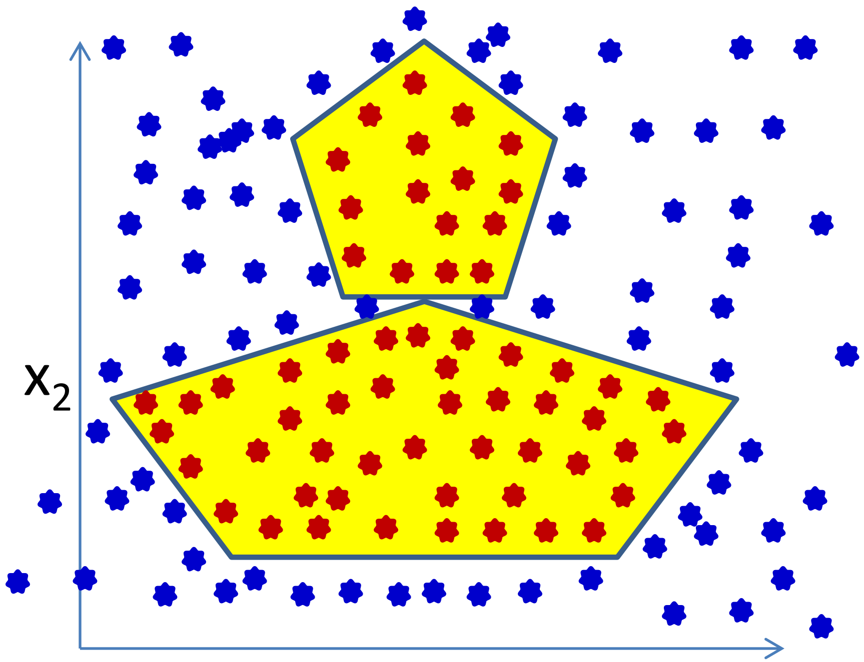
The *online* perceptron solution

- The more popular solution, originally proposed by Rosenblatt is an *online* algorithm
  - The famous “perceptron” algorithm

- Initializes W and incrementally updates it each time we encounter an instance that is incorrectly classified
  - Guaranteed to find the correct solution for linearly separable data
  - On following slides, but will not cover in class

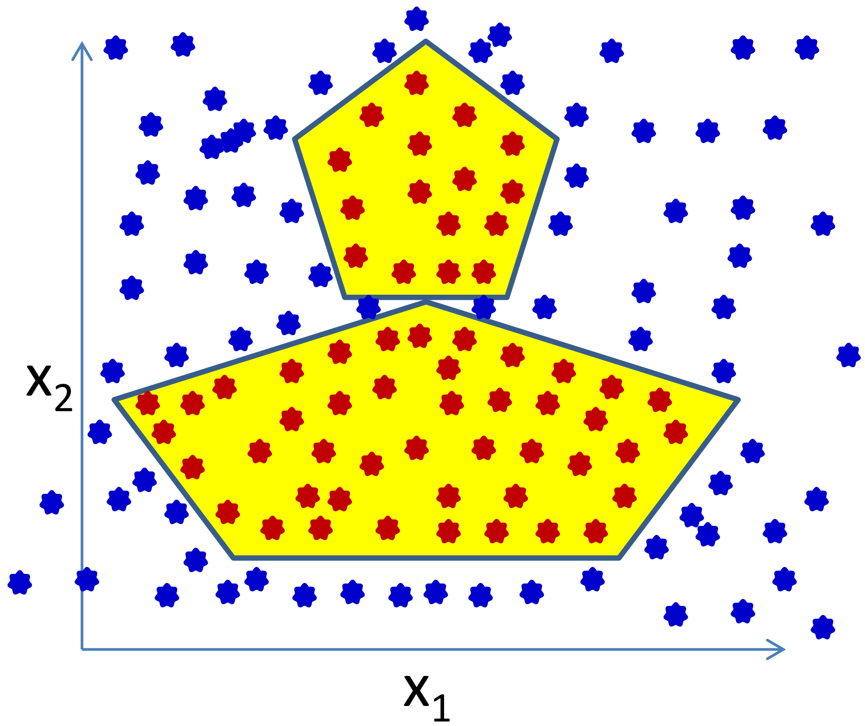
History: A more complex problem

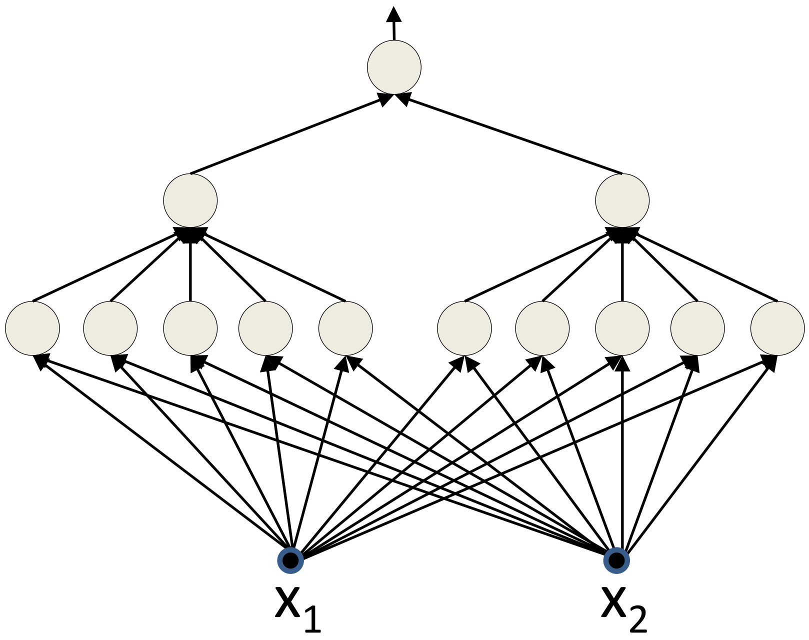




- Learn an *MLP* for this function
  - 1 in the yellow regions, 0 outside
- Using just the samples
- We know this can be perfectly represented using an MLP

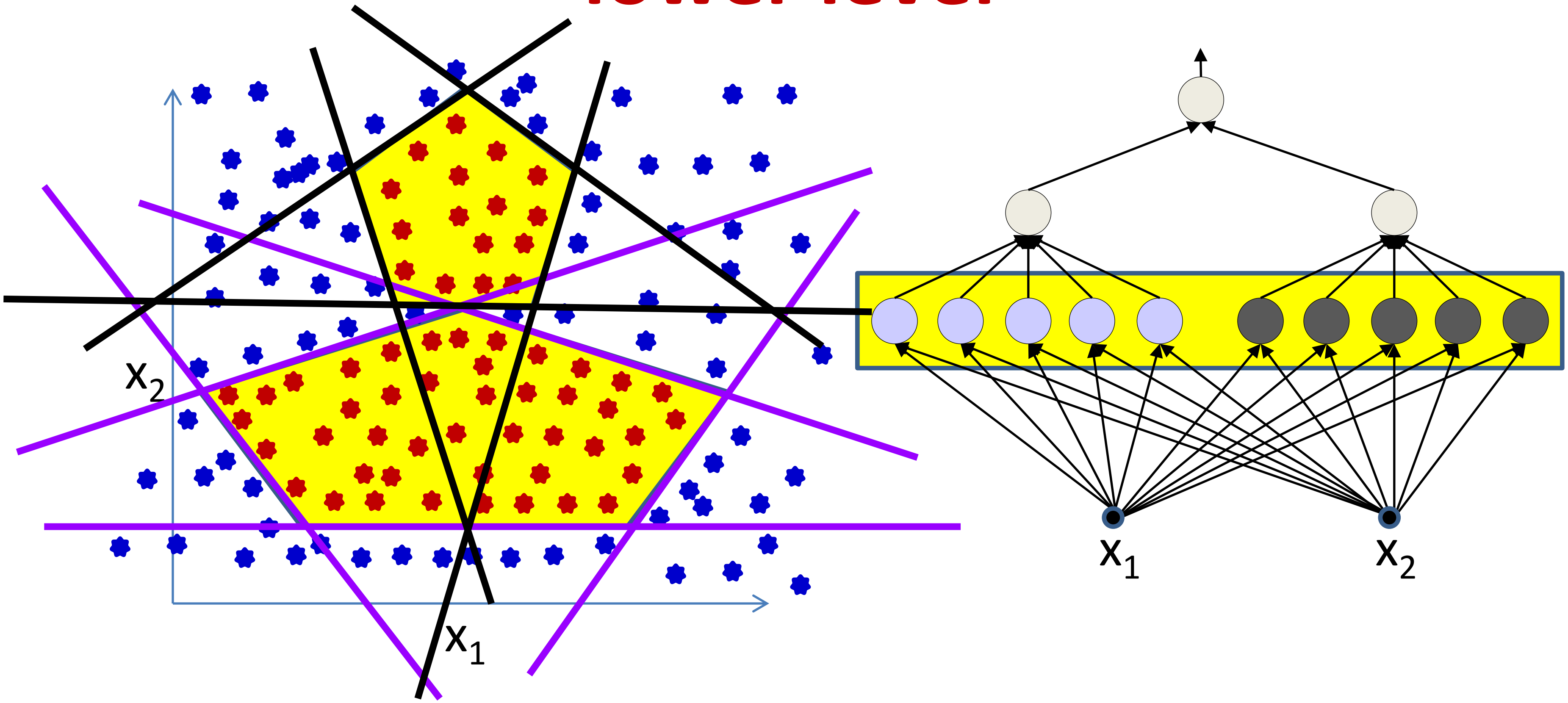
More complex decision boundaries





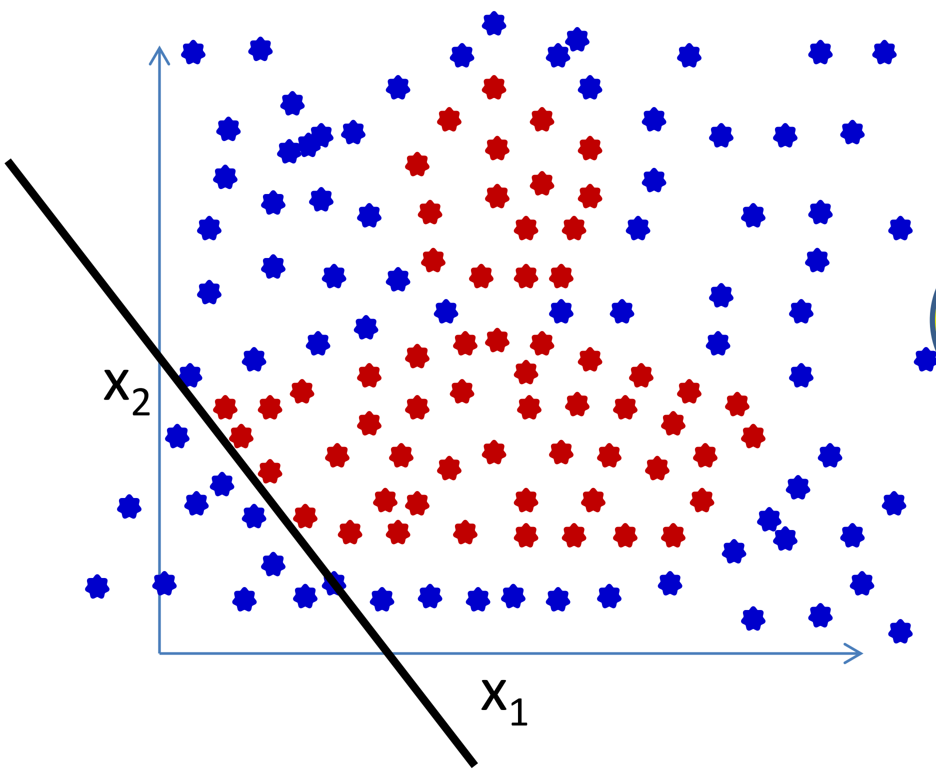
- Even using the perfect architecture…
- … can we use perceptron learning rules to learn this classification function?

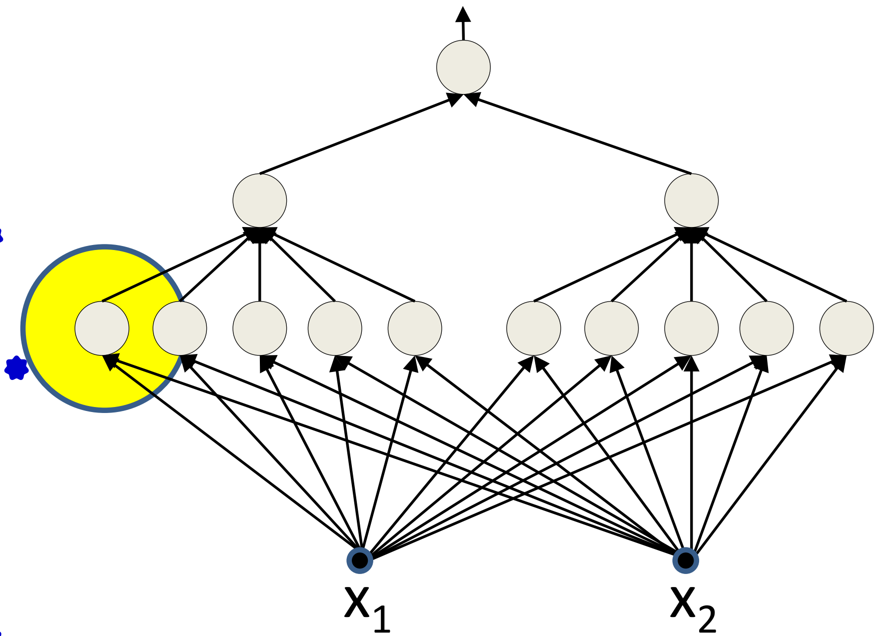
The pattern to be learned at the lower level



- 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!*

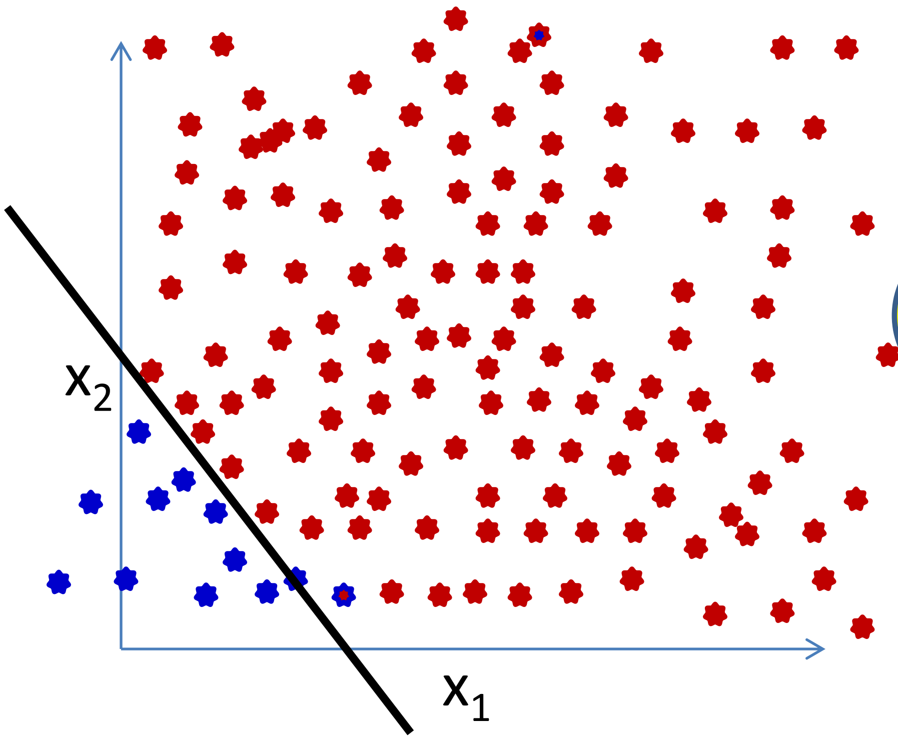
The pattern to be learned at the lower level

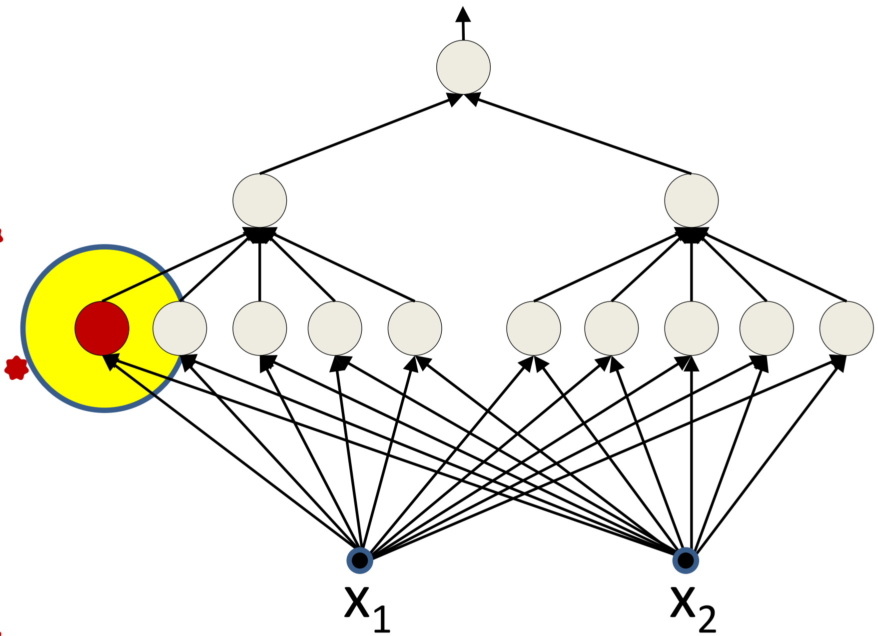




- Consider a single linear classifier that must be learned from the training data
  - Can it be learned from this data?

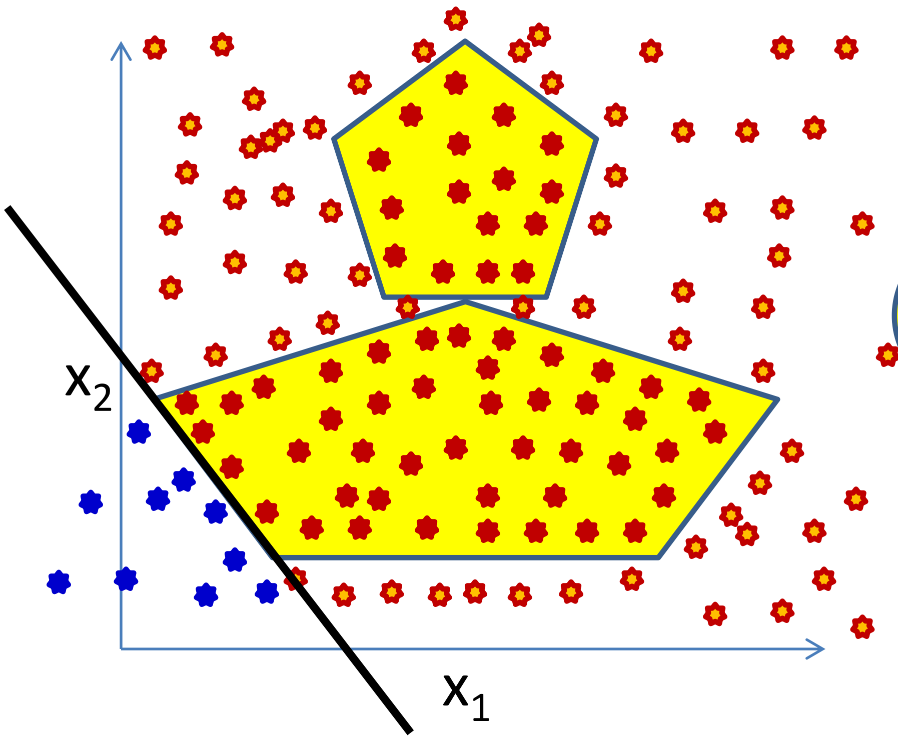
The pattern to be learned at the lower level

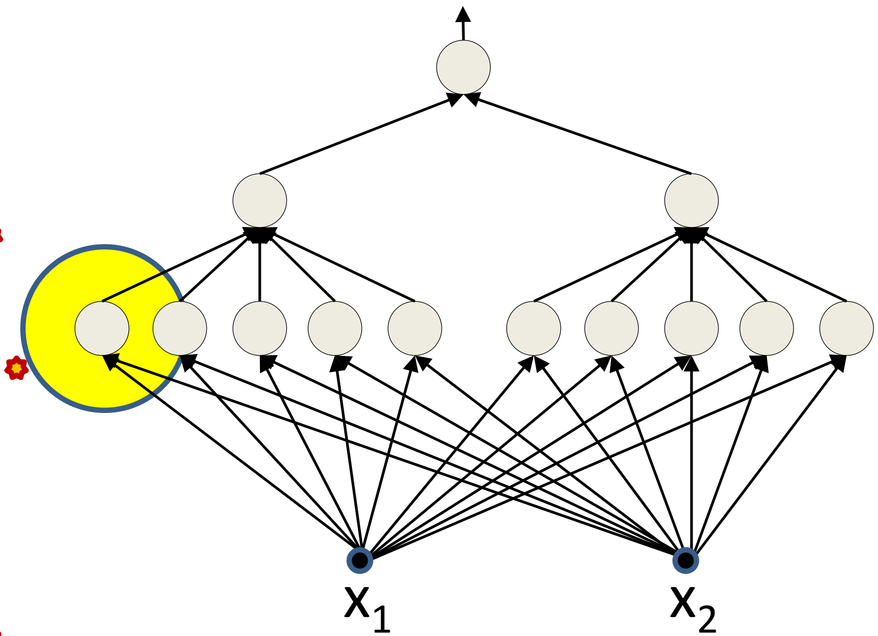




- Consider a single linear classifier that must be learned from the training data
  - Can it be learned from this data?
  - The individual classifier actually requires the kind of labelling shown here
    - Which is *not* given!!

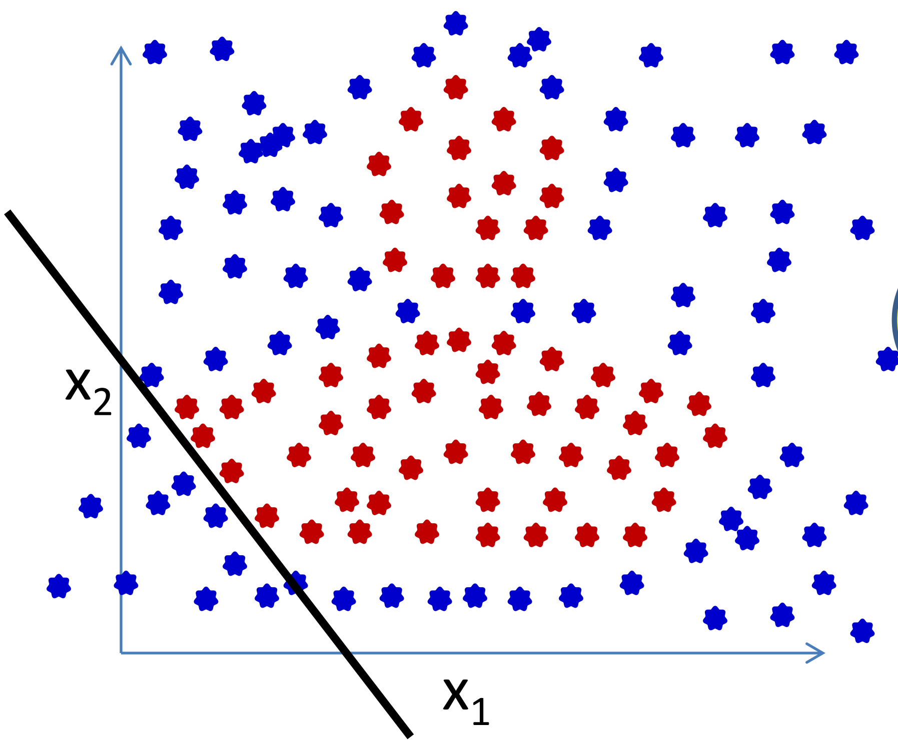
The pattern to be learned at the lower level

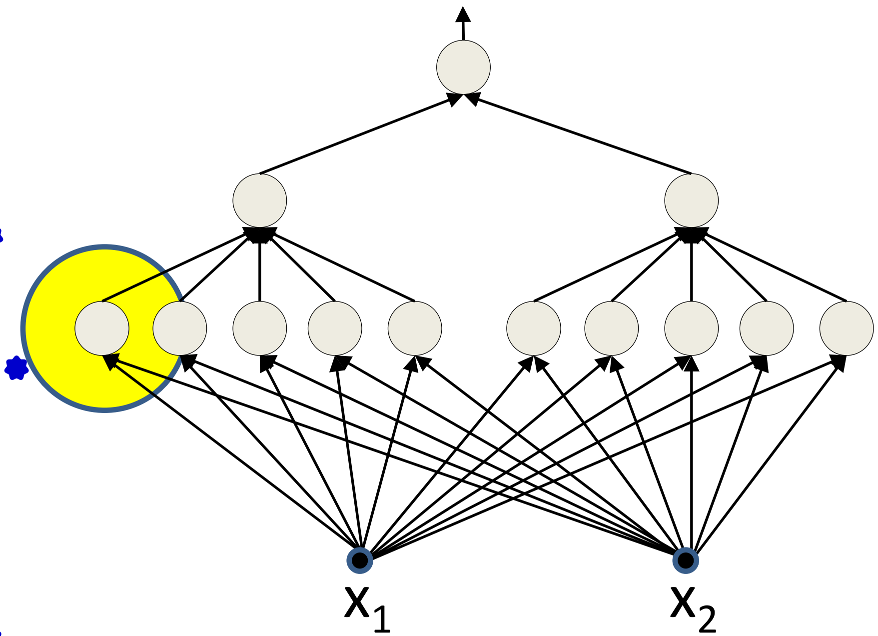




- The lower-level neurons are linear classifiers
  - They require linearly separated labels to be learned
  - The actually provided labels are not linearly separated
  - Challenge: *Must also learn the labels for the lowest units!*

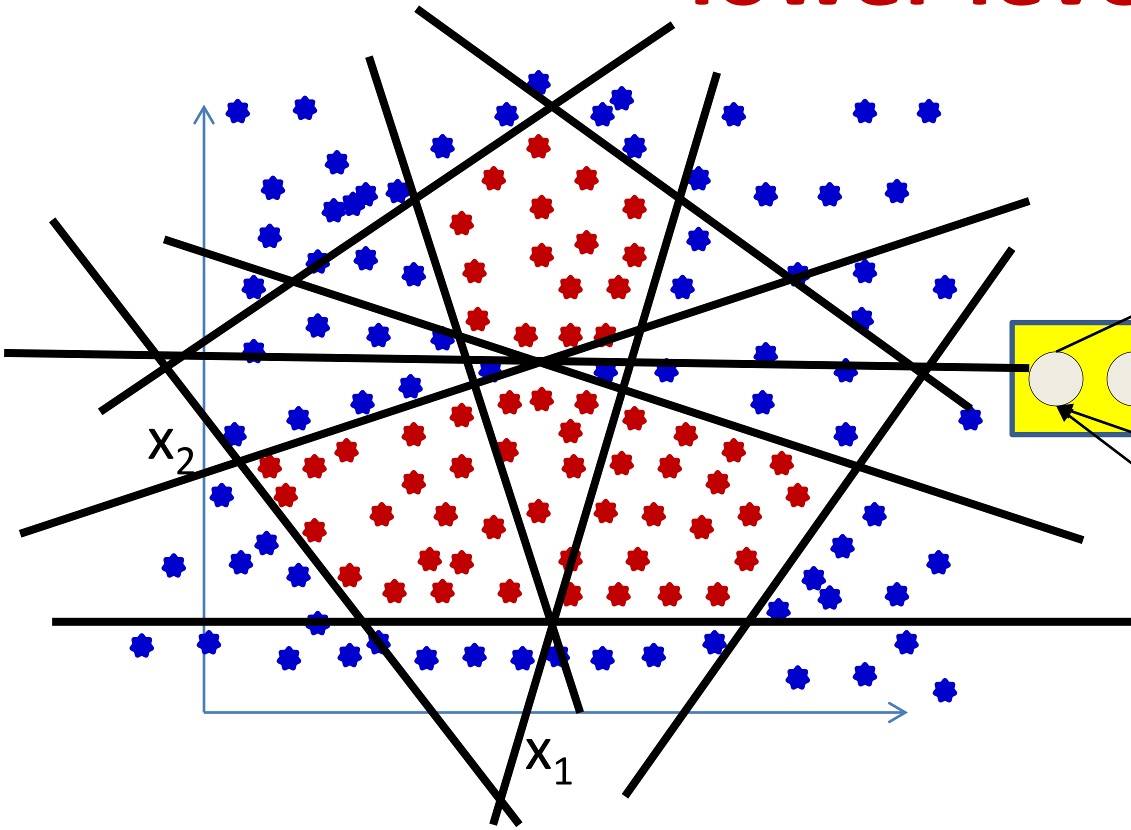
The pattern to be learned at the lower level

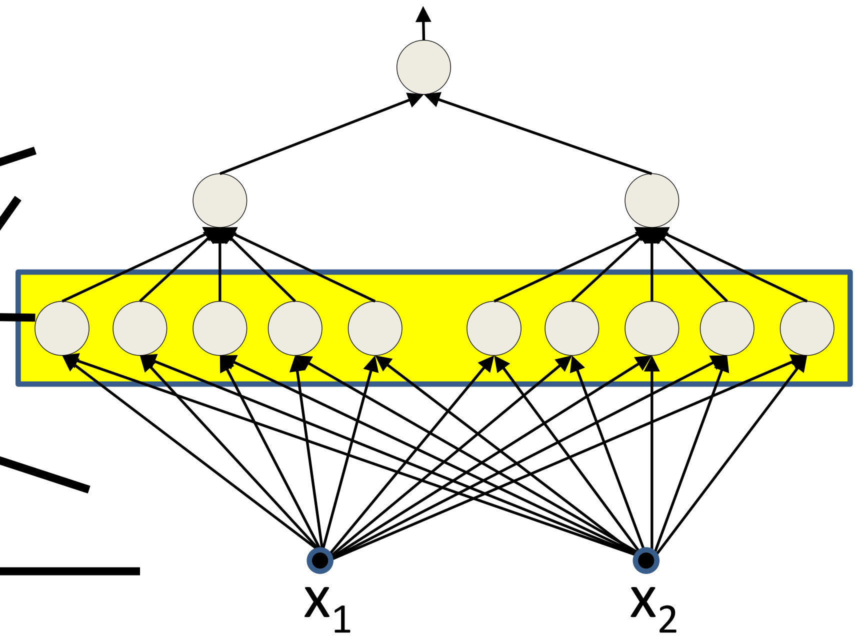




- For a single line:
  - Try out *every possible way of relabeling the blue dots such that we can learn a line that keeps all the red dots on one side!*

The pattern to be learned at the lower level





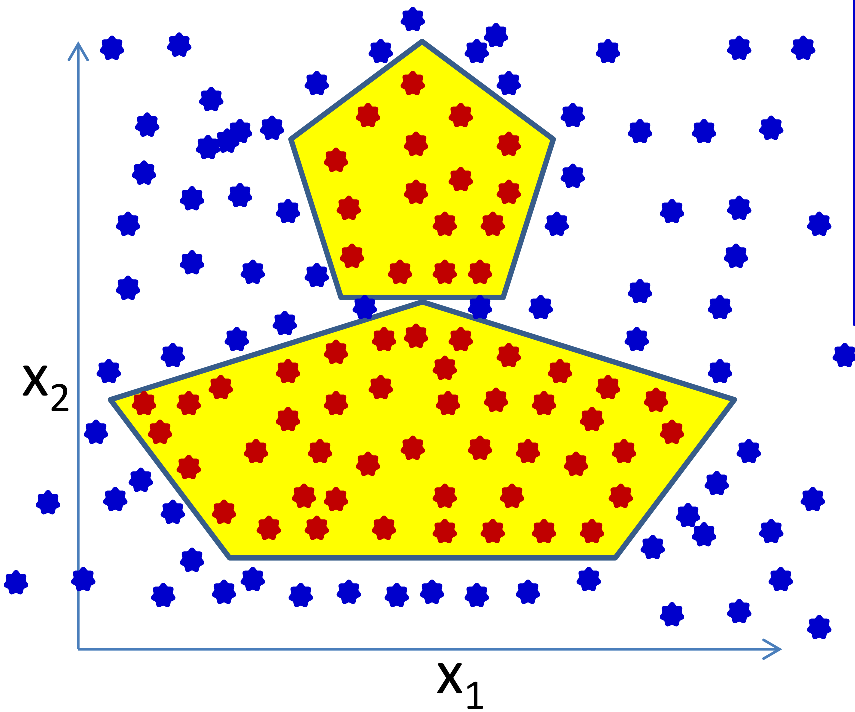
- This must be done for *each* of the lines (perceptrons)
- Such that, when all of them are combined by the higher-level perceptrons we get the desired pattern
  - Basically an exponential search over inputs

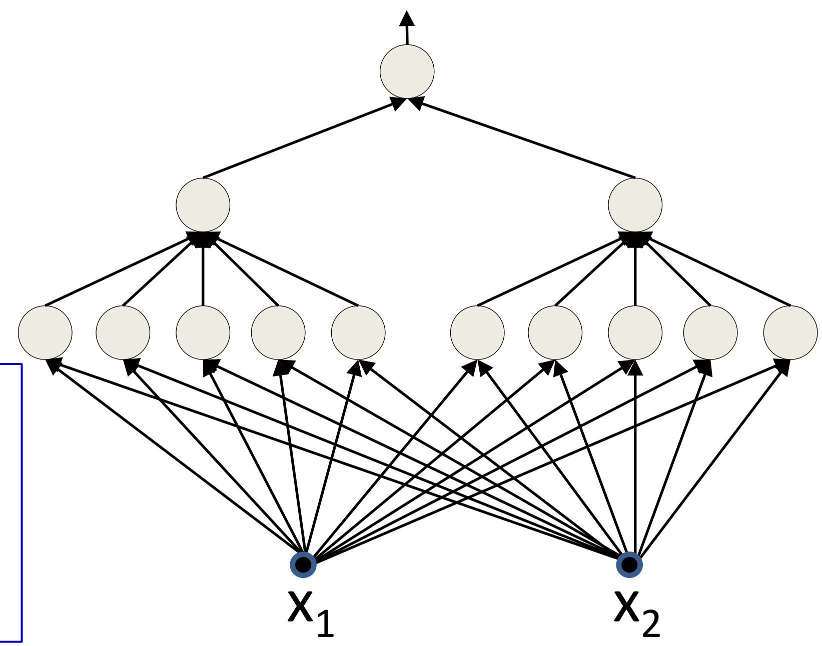
Individual neurons represent one of the lines that compose the figure (linear classifiers)

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

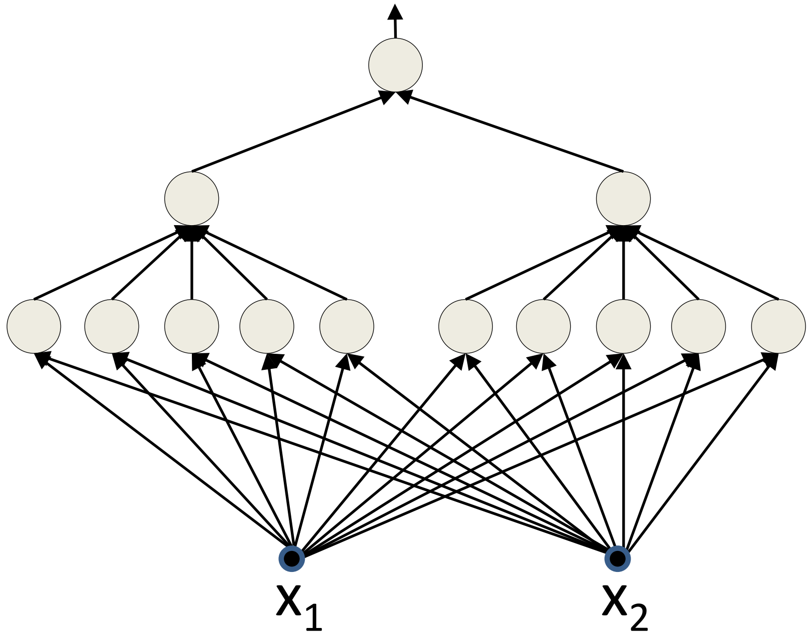




This must be done for *every* neuron

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**
- **At least exponential (in inputs) time complexity!!!!!!**

Greedy algorithms: Adaline and Madaline

- Perceptron learning rules 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)

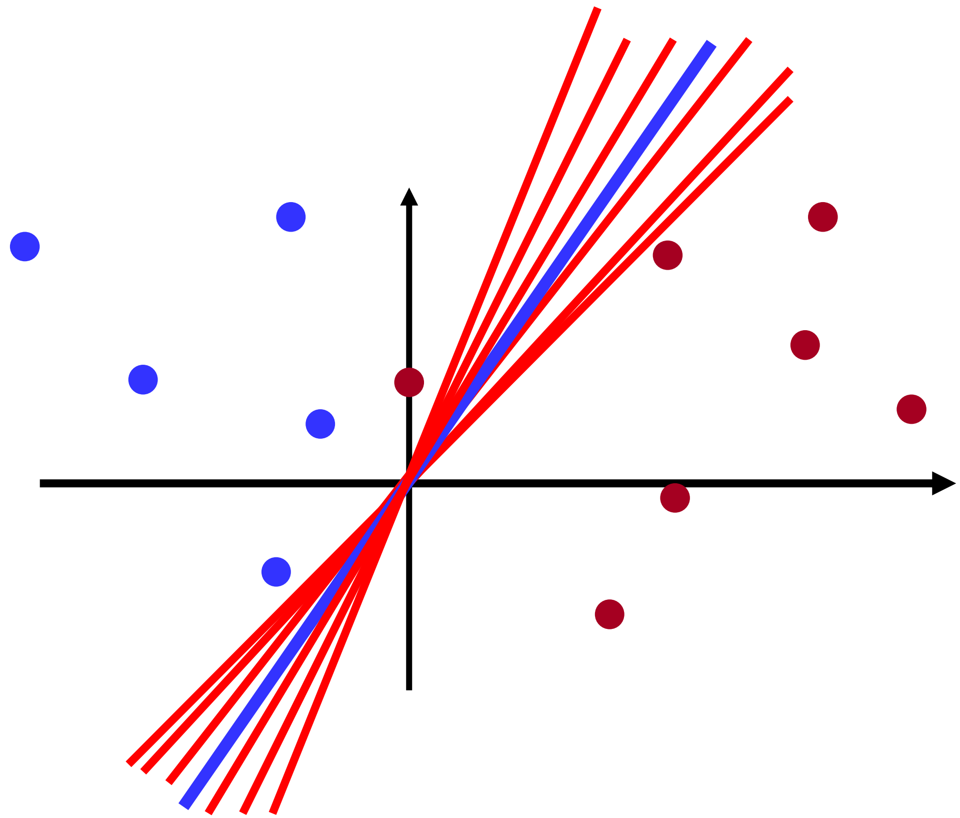
Story so far

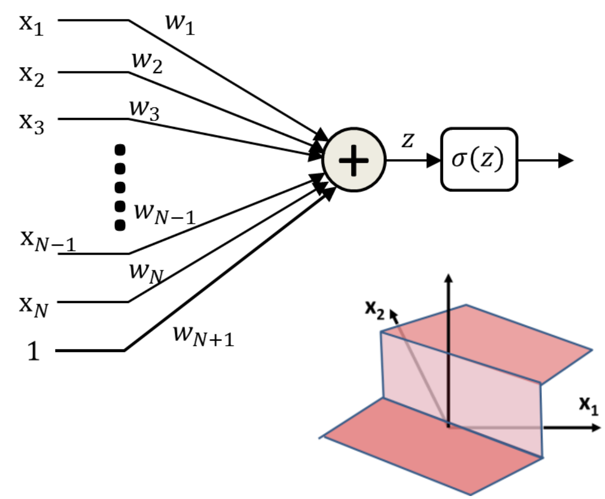
- "Learning" a network = learning the weights and biases to compute a target function
  - Will require a network with sufficient "capacity"
- In practice, we learn networks by "fitting" them to match the input-output relation of "training" instances drawn from the target function
- A linear decision 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

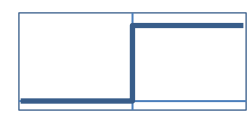
History..

- 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?

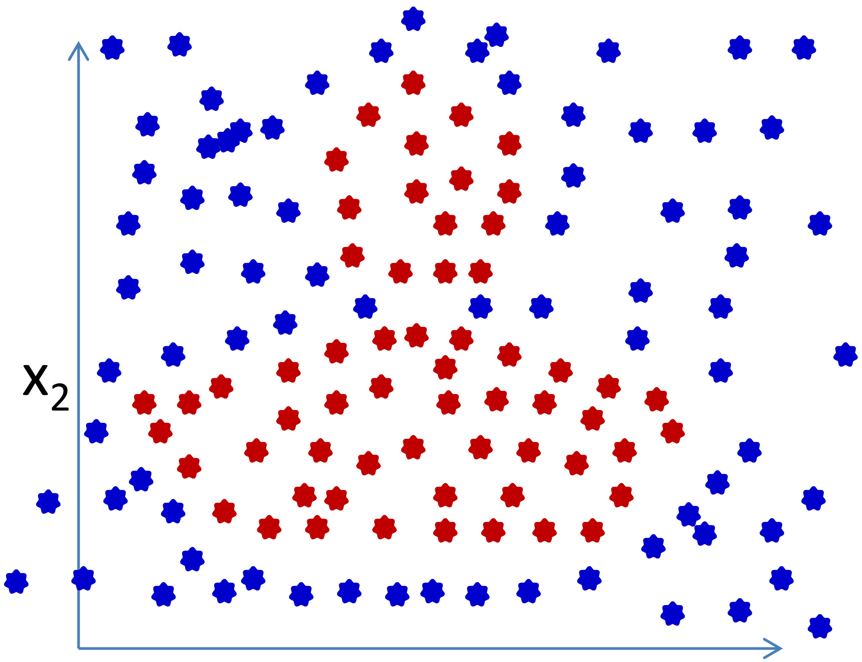


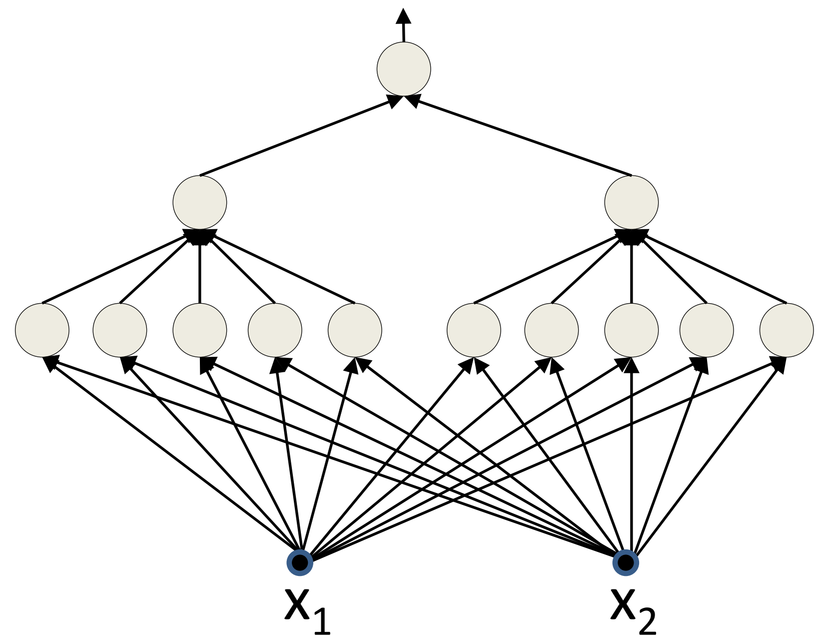


$\sigma(z) =$ 

- 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

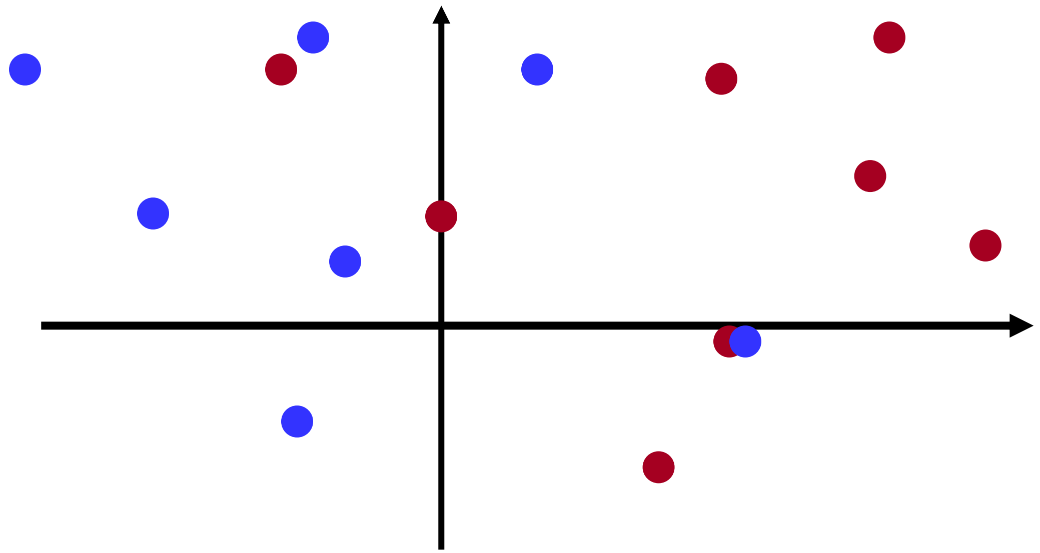
This only compounds on larger problems





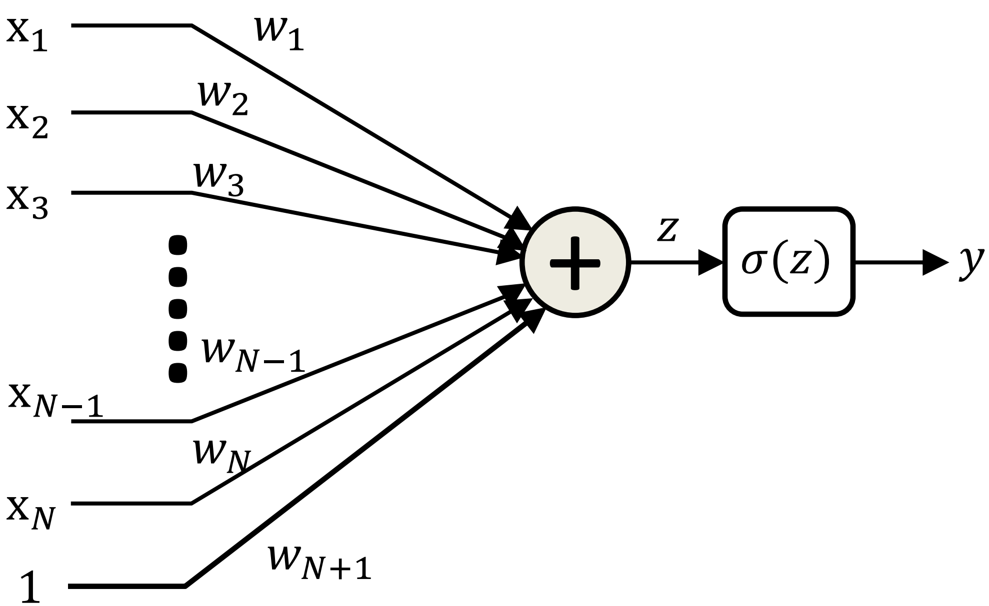
- Individual neurons' weights can change significantly without changing overall error
- The simple MLP is a flat, non-differentiable function
  - Actually a function with 0 derivative nearly everywhere, and no derivatives at the boundaries

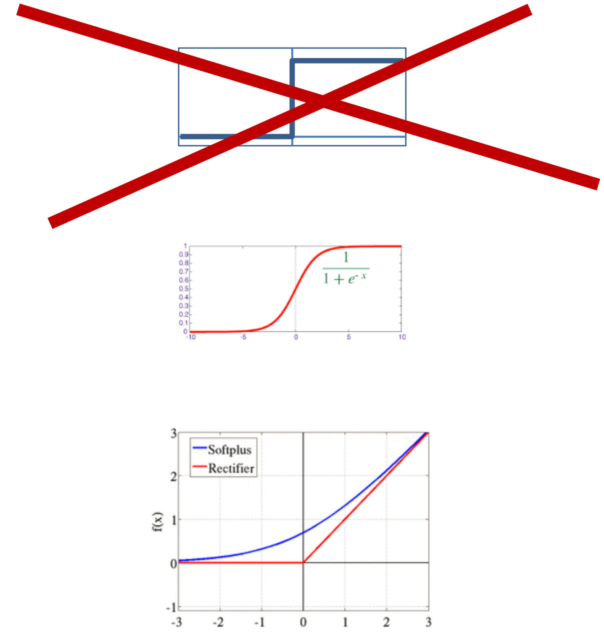
A second problem: What we *actually* model



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

Solution

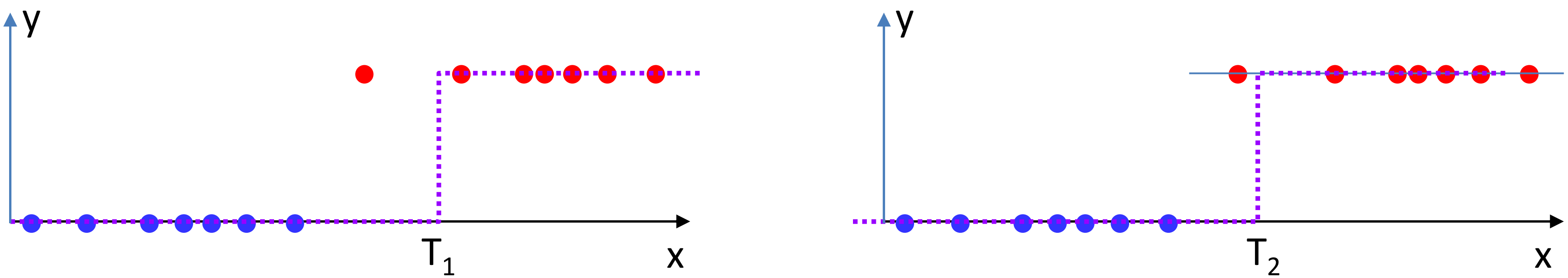




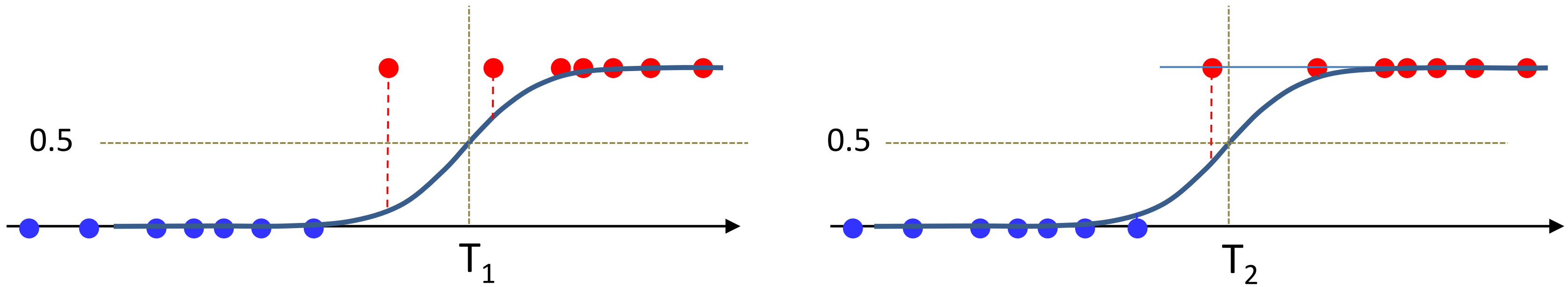
$Activation\ functions\ \sigma(z)$

- 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

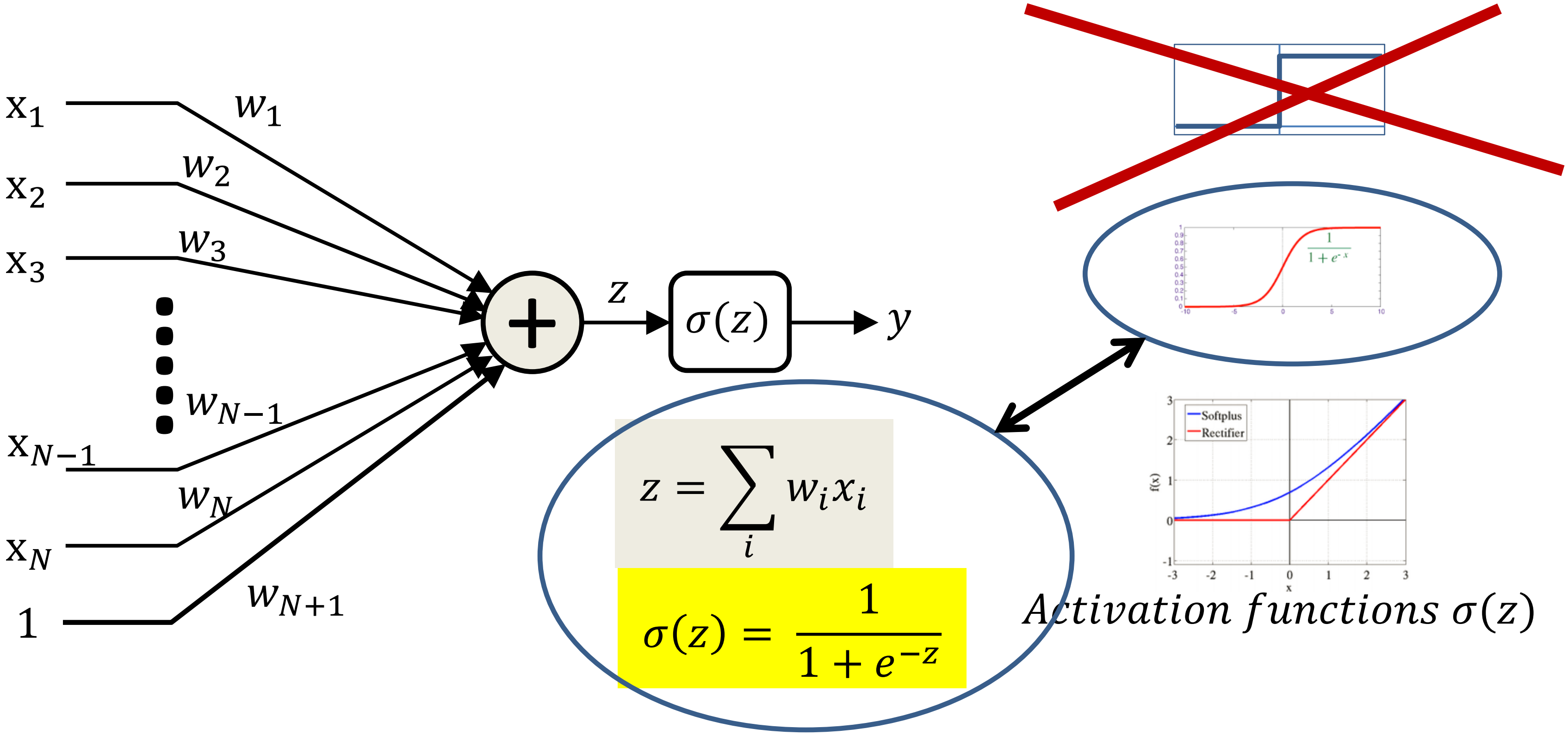


- Threshold activation: shifting the threshold from T_1 to T_2 does not change classification error
  - Does not indicate if moving the threshold left was good or not



- 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



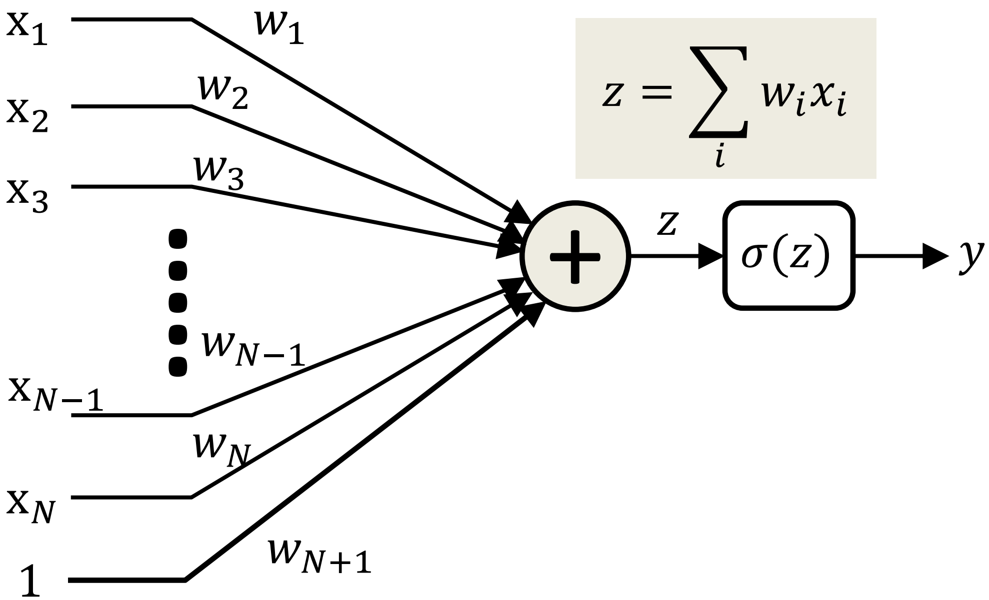
- This particular one has a nice interpretation
- It can be interpreted as $P(y = 1|x)$

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



$$z = \sum_i w_i x_i$$

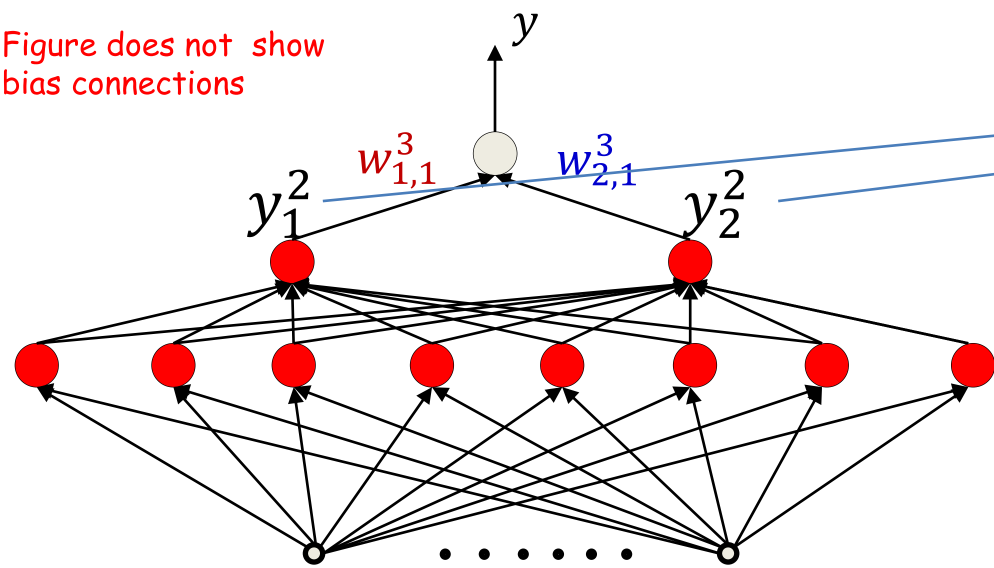
$$\frac{dy}{dz} = \sigma'(z)$$

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

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

- **$\sigma(z)$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



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

y = output of overall network

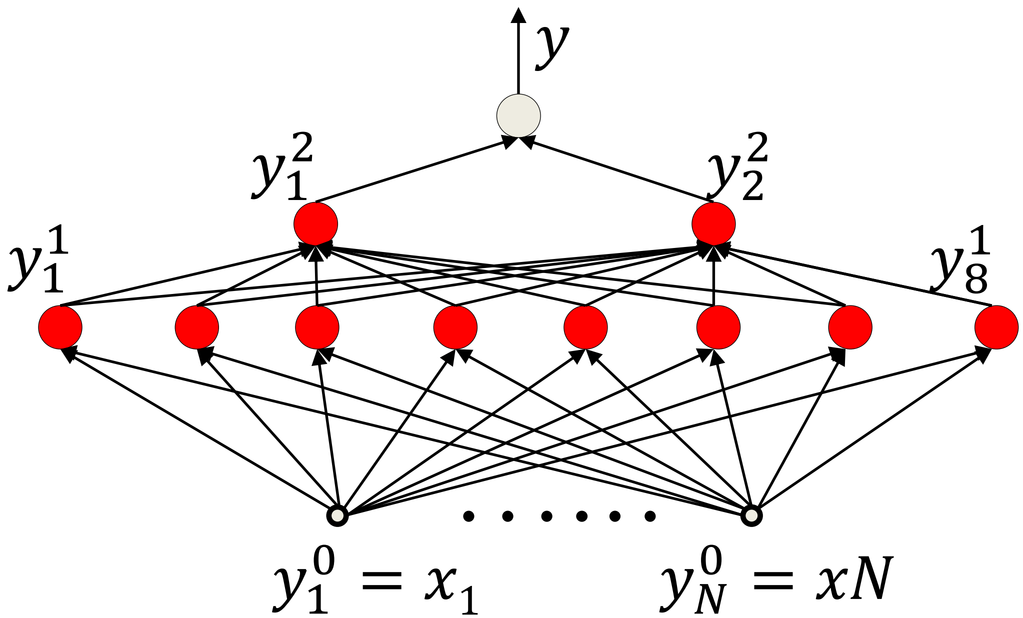
$w_{i,j}^k$ = weight connecting the ith unit of the (k-1)th layer to the jth unit of the k-th layer

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

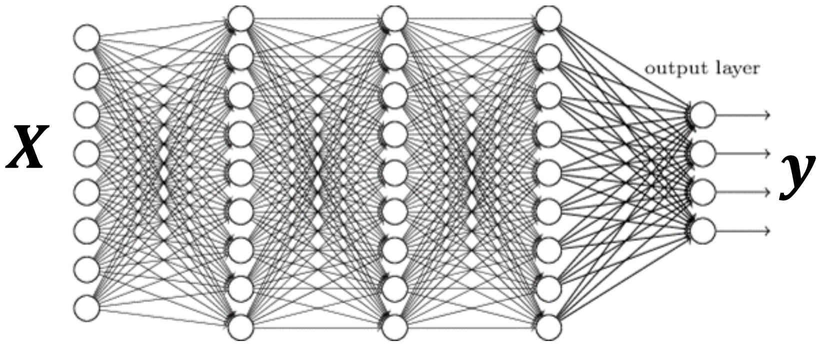
Overall function is differentiable

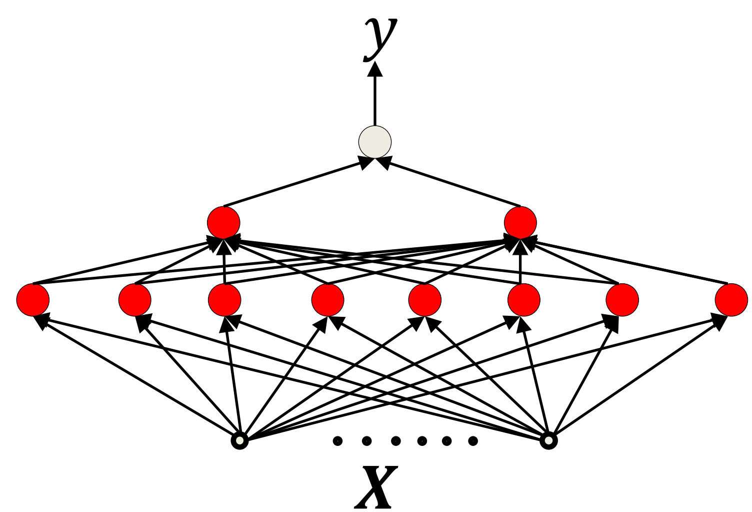


$$y_j^k = \sigma\left(\sum_i w_{i,j}^{k-1} y_i^{k-1}\right)$$

- 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

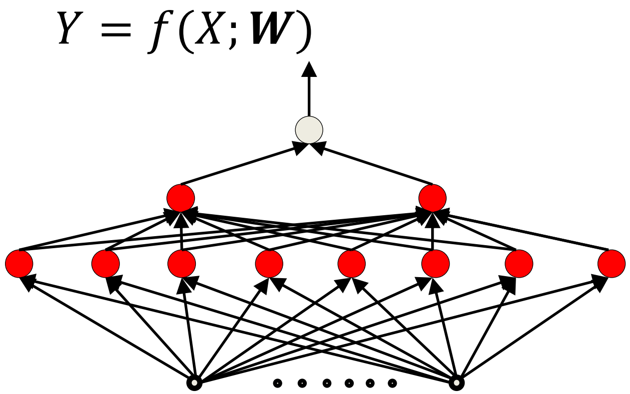
Overall setting for "Learning" the MLP

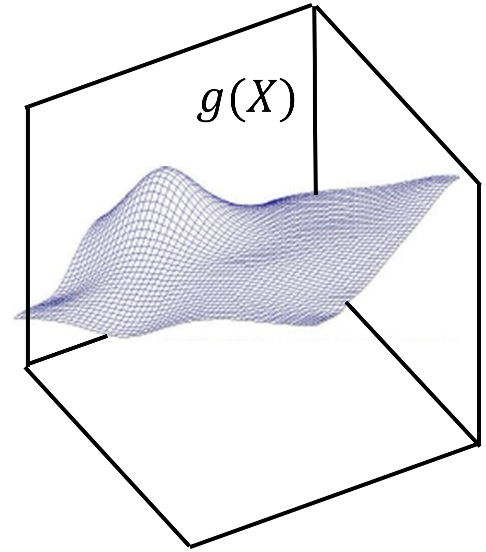




- Given a training set of input-output pairs $(\boldsymbol{X}_1, \boldsymbol{d}_1), (\boldsymbol{X}_2, \boldsymbol{d}_2), \ldots, (\boldsymbol{X}_N, \boldsymbol{d}_N)$ …
  - $\boldsymbol{d}$ is the *desired output* of the network in response to $\boldsymbol{X}$
  - $\boldsymbol{X}$ and $\boldsymbol{d}$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



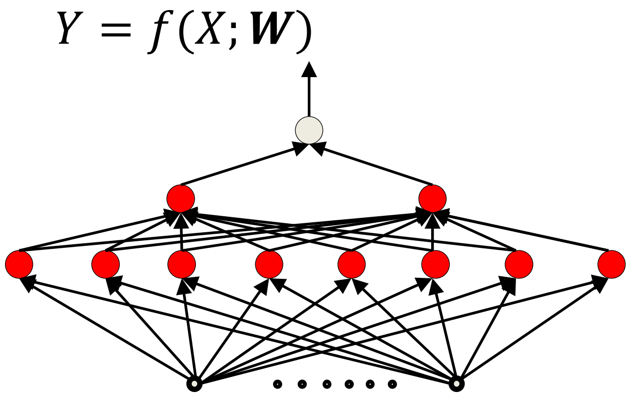


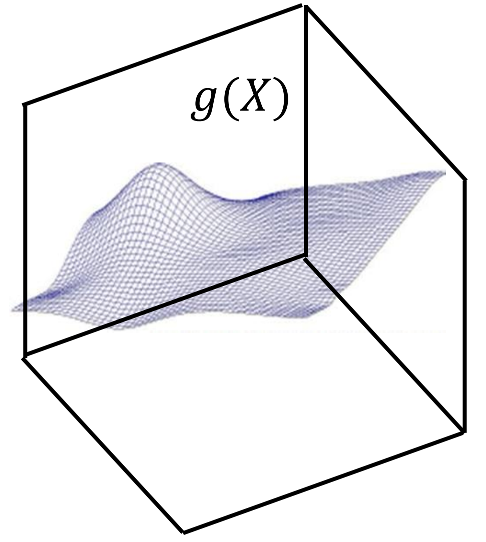
- When $f(X; \boldsymbol{W})$ has the capacity to exactly represent $g(X)$

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

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

Minimizing *expected* error



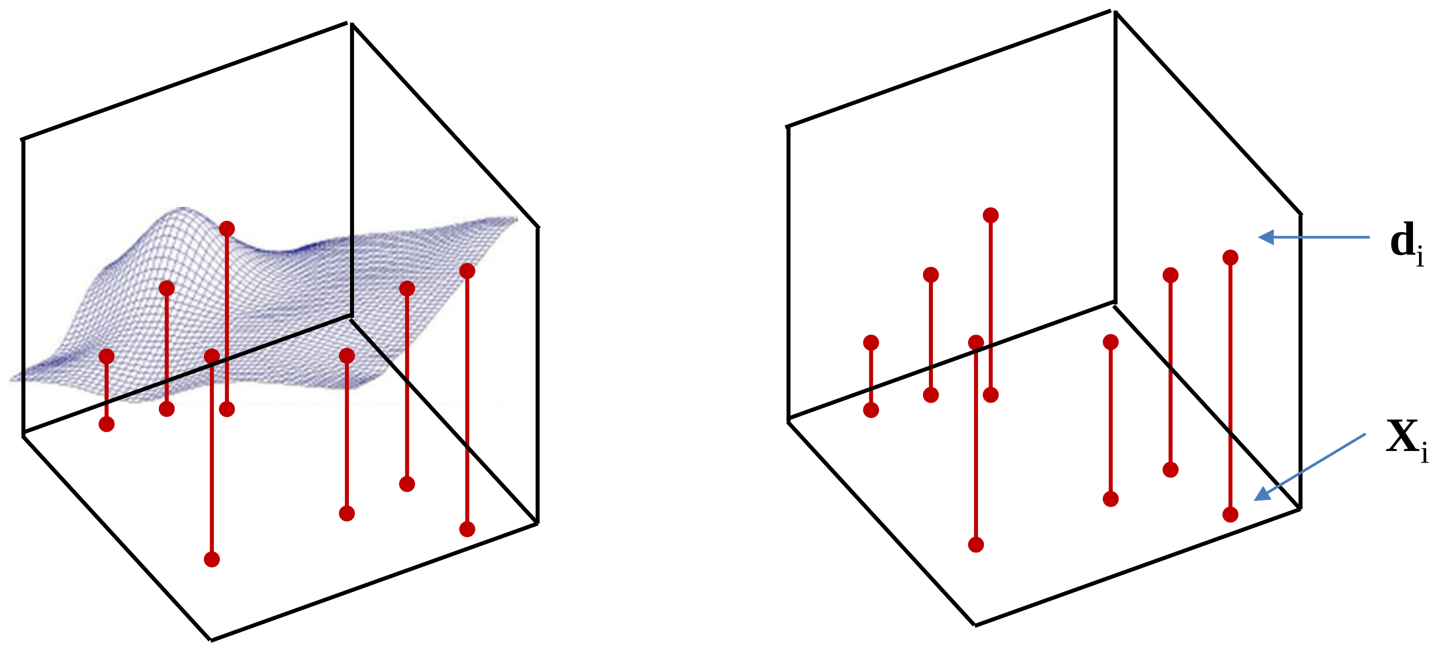


- More generally, assuming X is a random variable

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

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

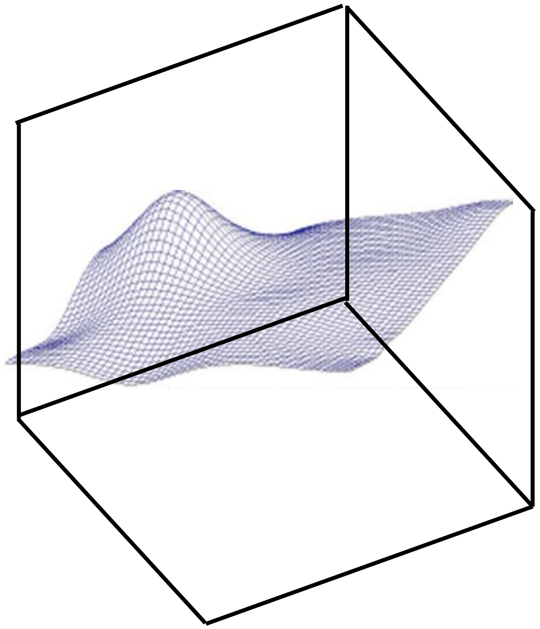
Recap: Sampling the function

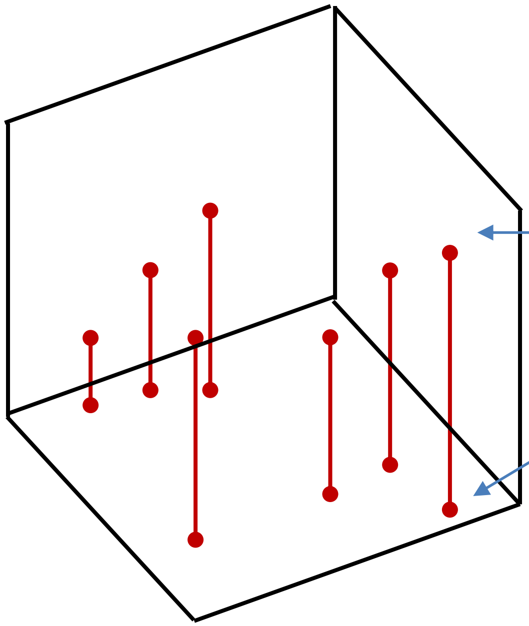


- *We don't have g(X) so sample* $g(X)$
  - Obtain input-output pairs for a number of samples of input X_i
  - Good sampling: the samples of X will be drawn from $P(X)$

- Estimate function from the samples

The *Empirical* risk





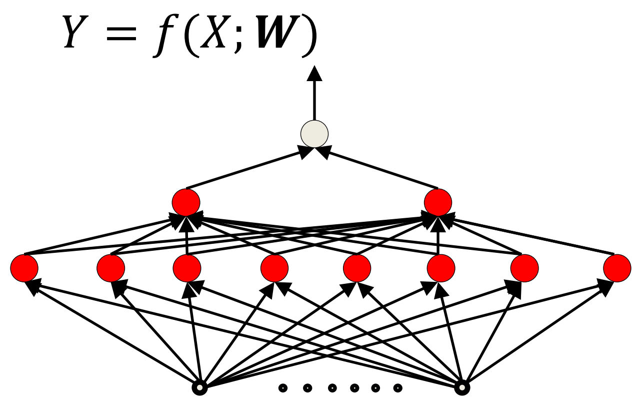
- The *expected* divergence (or risk) is the average divergence over the entire input space

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

- 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 $(\boldsymbol{X}_1, \boldsymbol{d}_1), (\boldsymbol{X}_2, \boldsymbol{d}_2), \dots, (\boldsymbol{X}_N, \boldsymbol{d}_N)$
  - Quantification of error on the ith instance: $div(f(X_i; W), d_i)$
  - Empirical average divergence (Empirical Risk) on all training data:

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

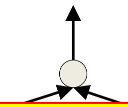
- Estimate the parameters to minimize the empirical estimate of expected divergence (empiricial risk)

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

  - 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

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

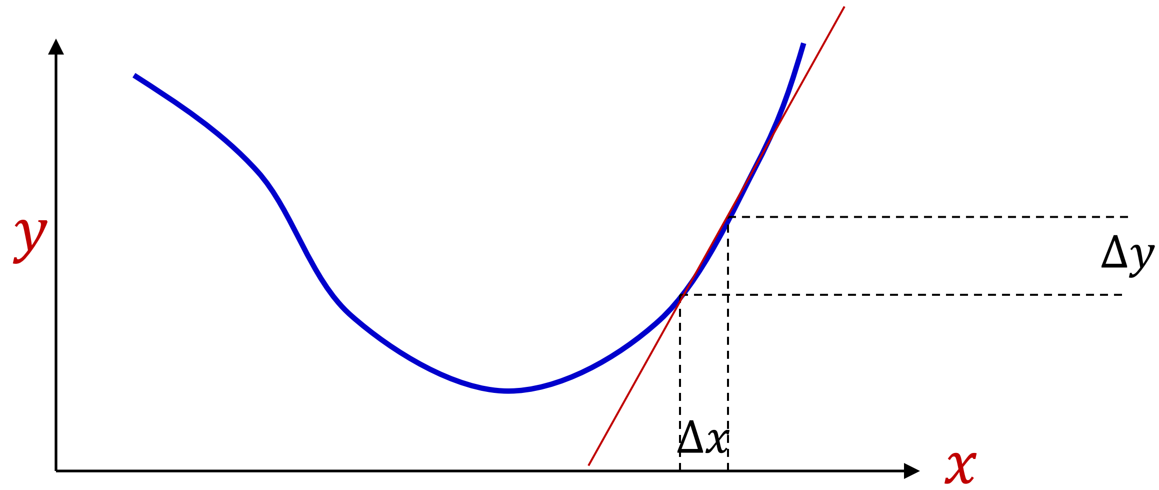
- This is problem of function minimization
  - An instance of optimization

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**
  - **With an initial discussion of derivatives**

A brief note on derivatives..



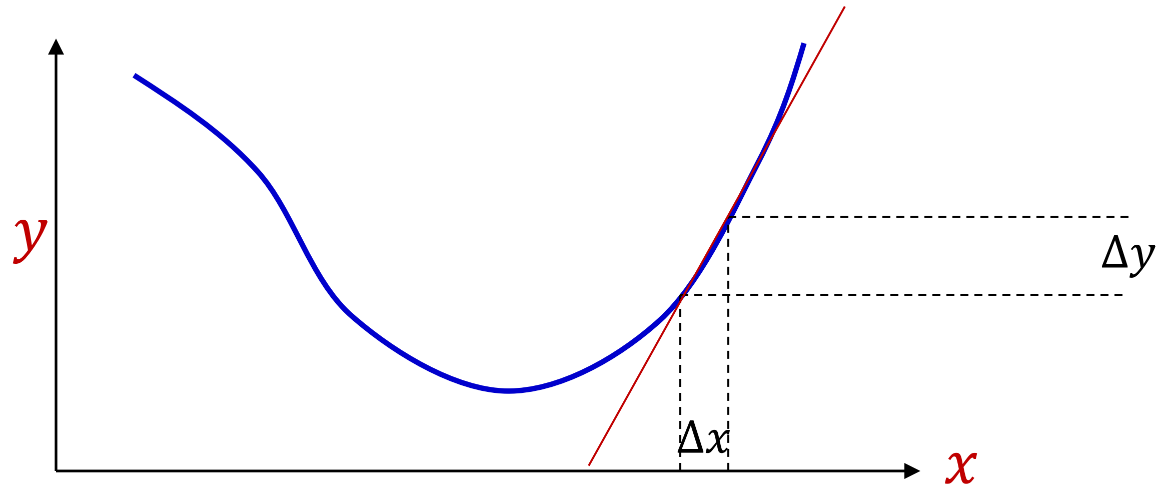
derivative

- 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

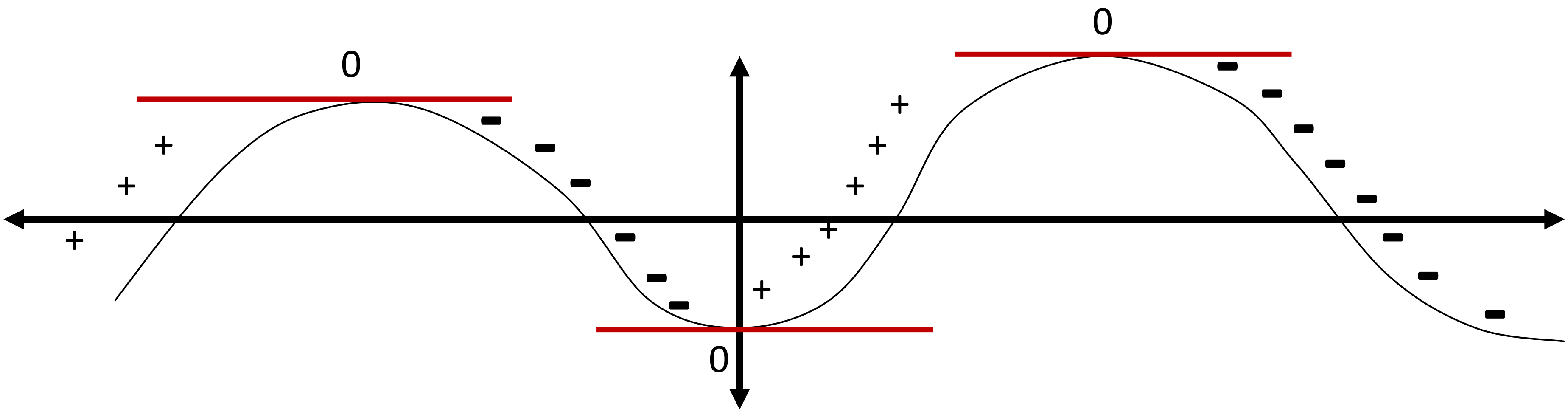
$$y = f(x)$$

  - Derivative:

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

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

Scalar function of scalar argument

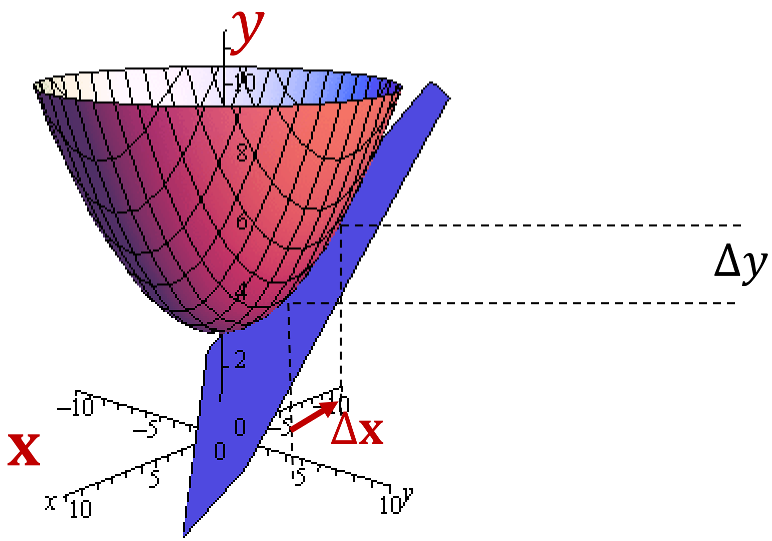


- Derivative $f'(x)$ is the *rate of change* of the function at x
  - How fast it increases with increasing x
  - The magnitude of f'(x) gives you the steepness of the curve at x
    - Larger |f'(x)| → the function is increasing or decreasing more rapidly

- It will be positive where a small increase in x results in an *increase* of f(x)
  - Regions of positive slope
- It will be negative where a small increase in x results in a *decrease* of f(x)
  - Regions of negative slope

- It will be 0 where the function is locally flat (neither increasing nor decreasing)

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: $\alpha = [\alpha_1 \quad \cdots \quad \alpha_D]$

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

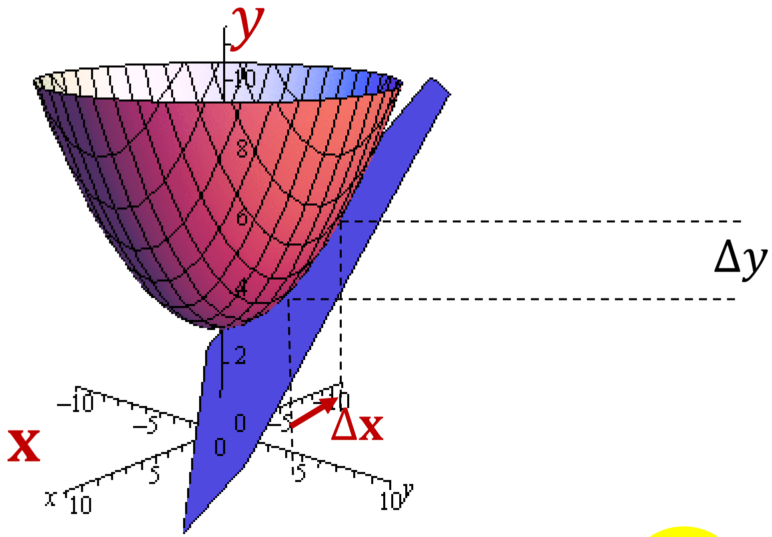
- The *partial* derivative α_i gives us how y increments when *only* x_i is incremented

- 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

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

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

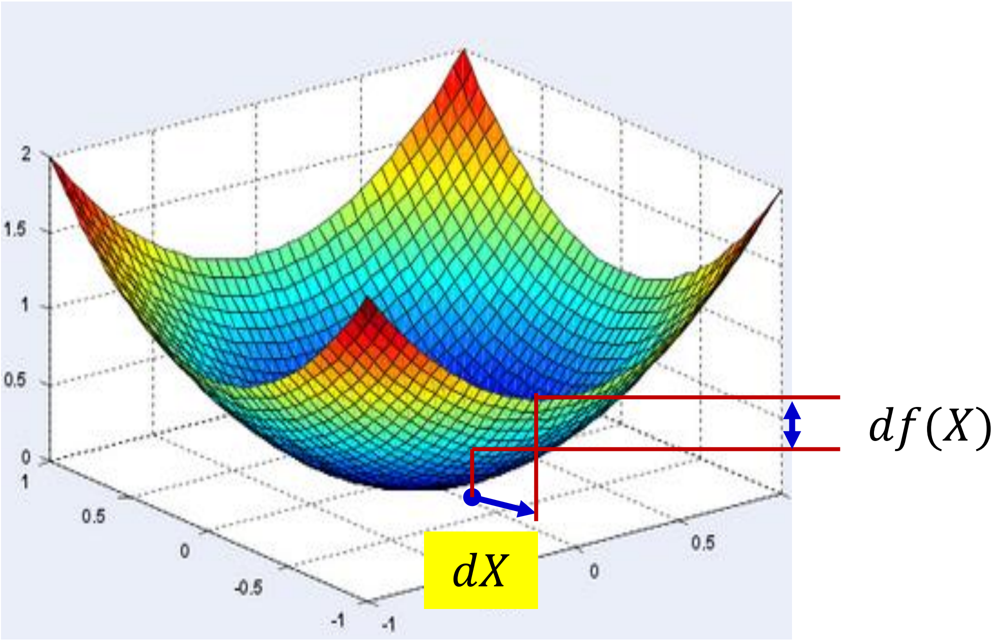
We will be using this symbol for vector and matrix derivatives

- 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

Gradient of a scalar function of a vector



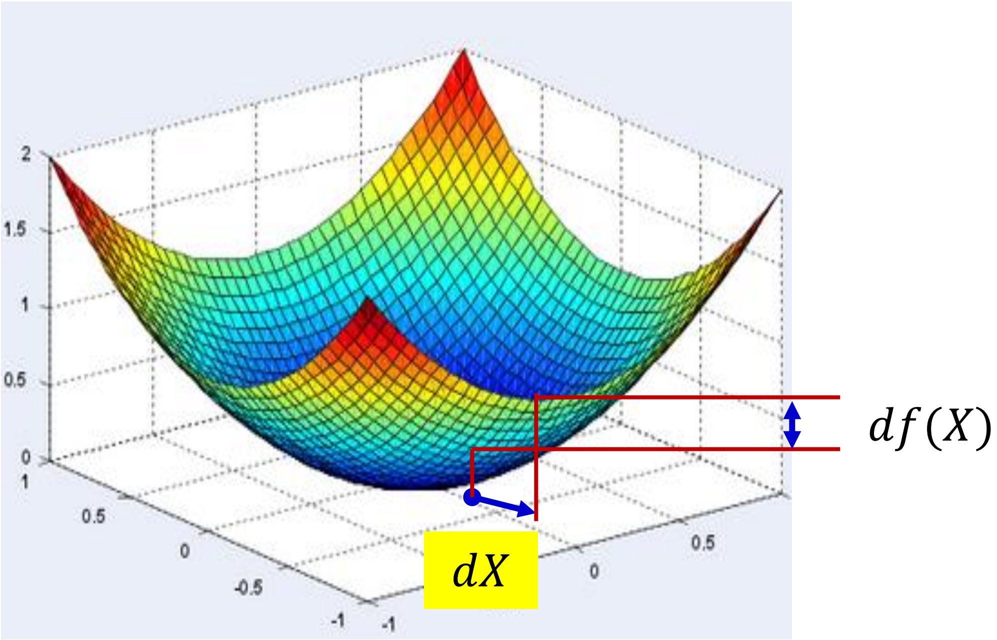
- The *derivative* $\nabla_X f(X)$ of a scalar function $f(X)$ of a multi-variate input X is a multiplicative factor that gives us the change in $f(X)$ for tiny variations in X

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

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

- The ***gradient*** is the transpose of the derivative $\nabla_X f(X)^T$
  – A column vector of the same dimensionality as X

Gradient of a scalar function of a vector



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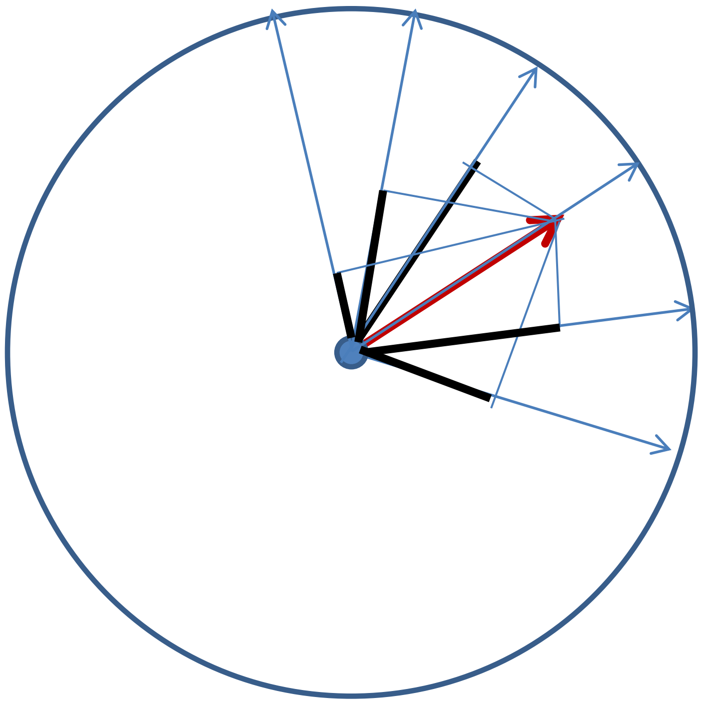
This is a vector inner product. To understand its behavior lets consider a well-known property of inner products

A well-known vector property

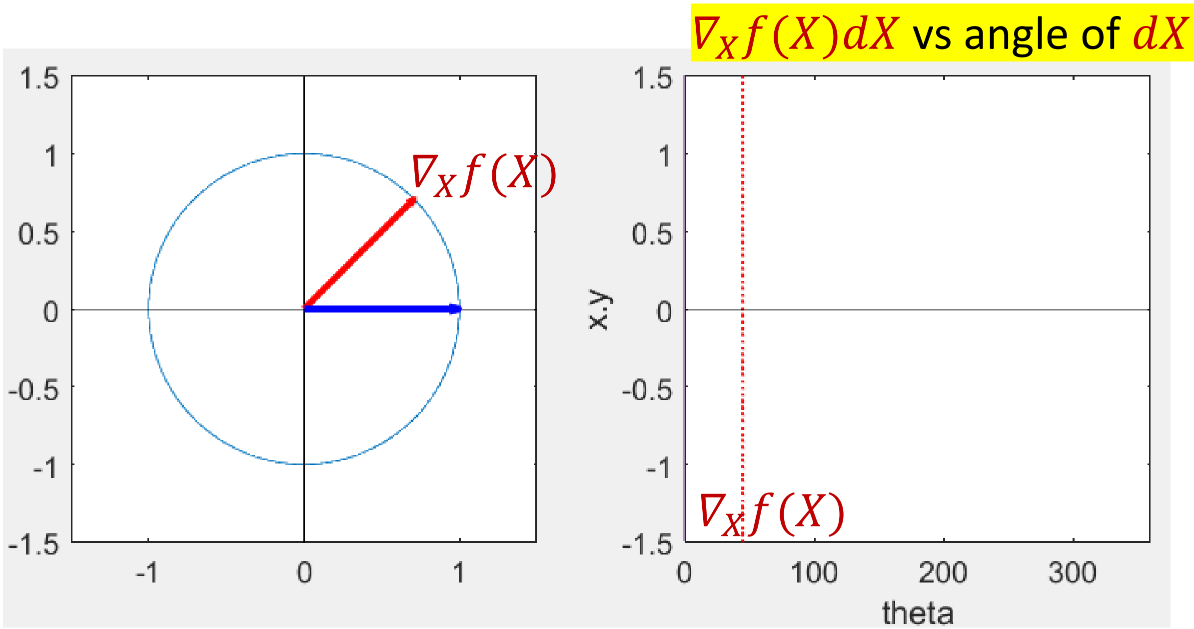


$$\mathbf{u}^{\mathrm{T}}\mathbf{v} = |\mathbf{u}||\mathbf{v}|cos\theta$$

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

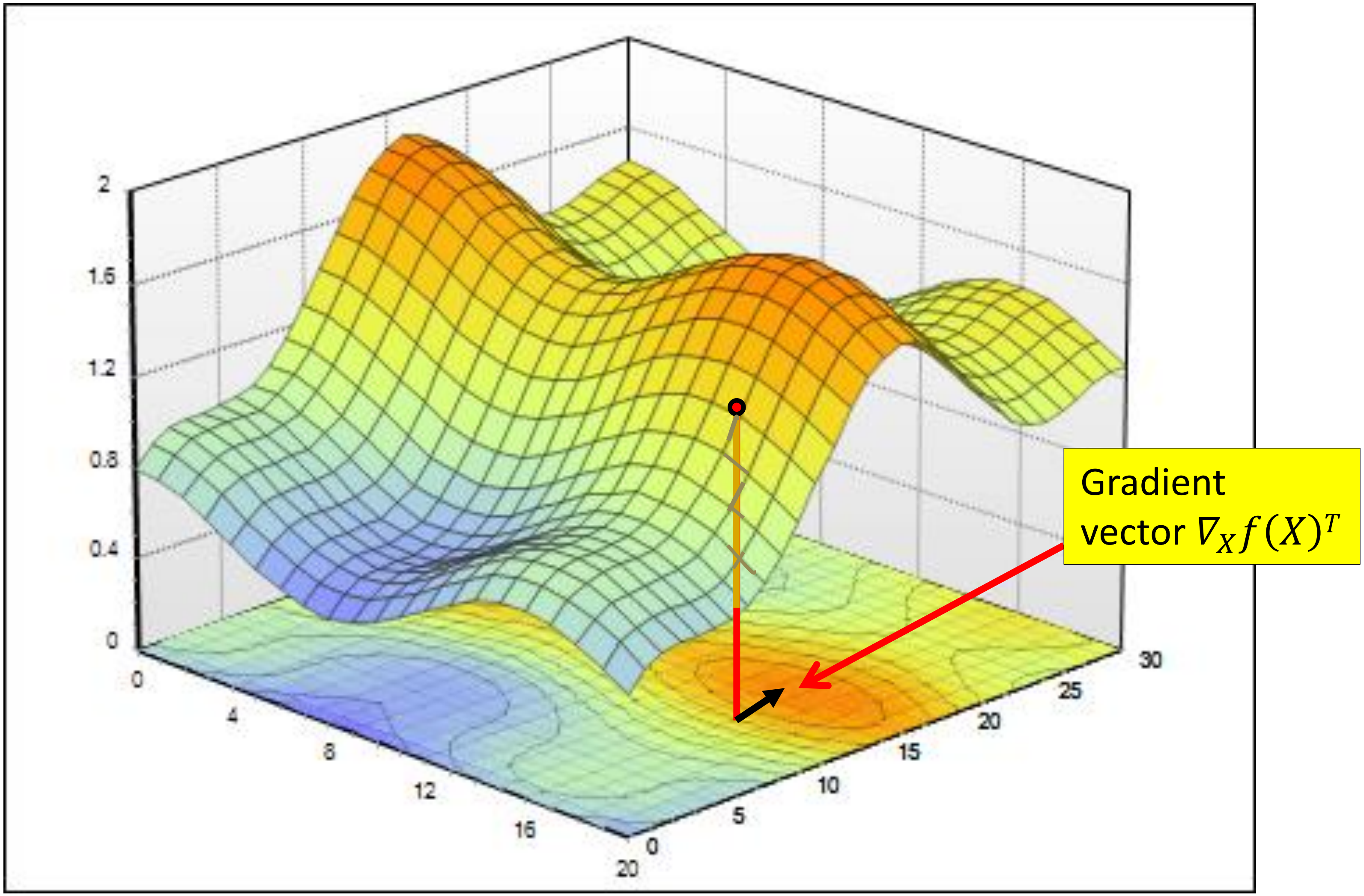
Properties of Gradient

Blue arrow is dX



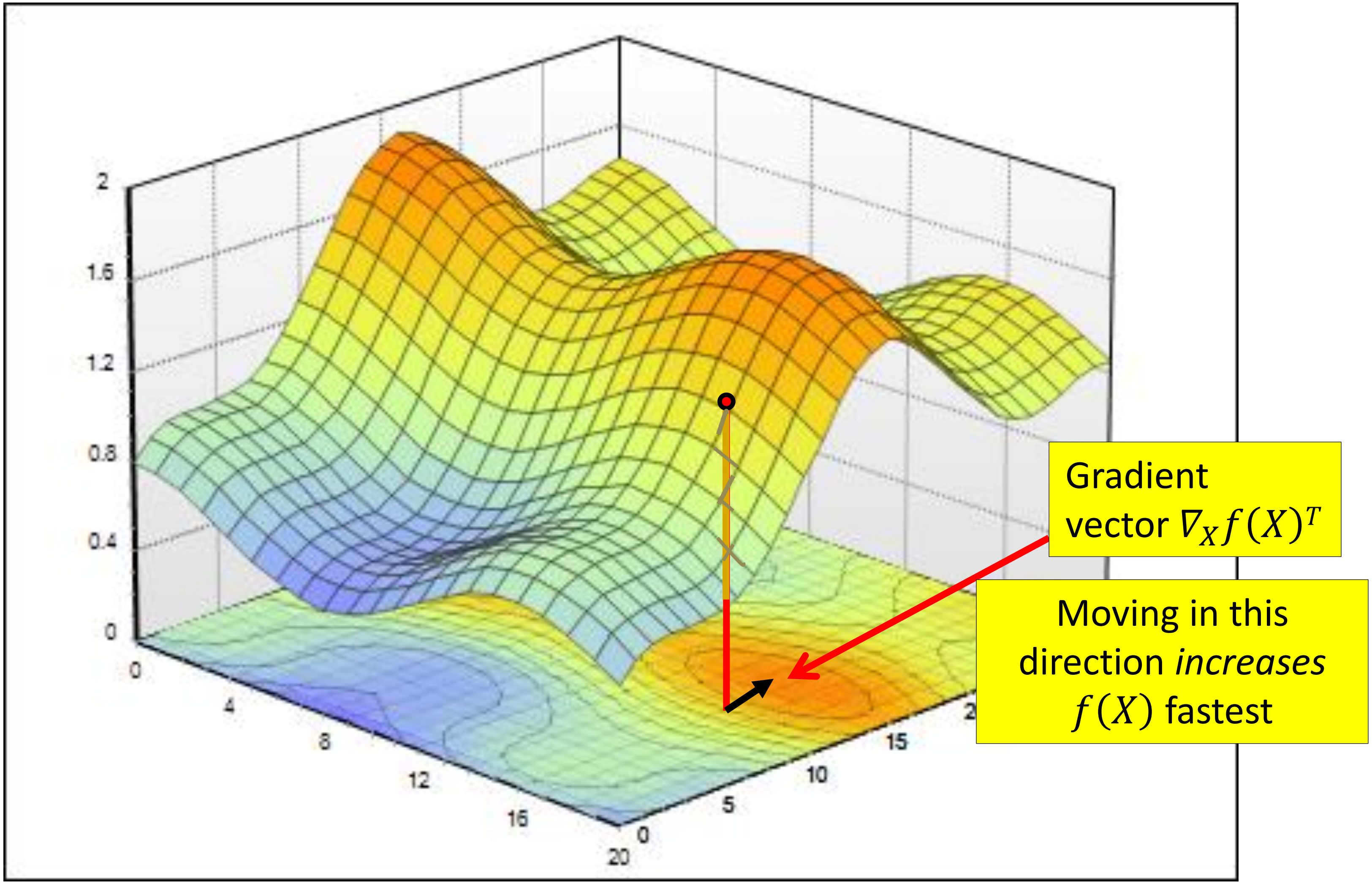
- $df(X) = \nabla_X f(X) dX$
- For an increment dX of any given length $df(X)$ is max if dX is aligned with $\nabla_X f(X)^{\mathrm{T}}$
  - The function $f(X)$ increases most rapidly if the input increment dX is exactly in the direction of $\nabla_X f(X)^{\mathrm{T}}$
- The gradient is the direction of fastest increase in $f(X)$

Gradient



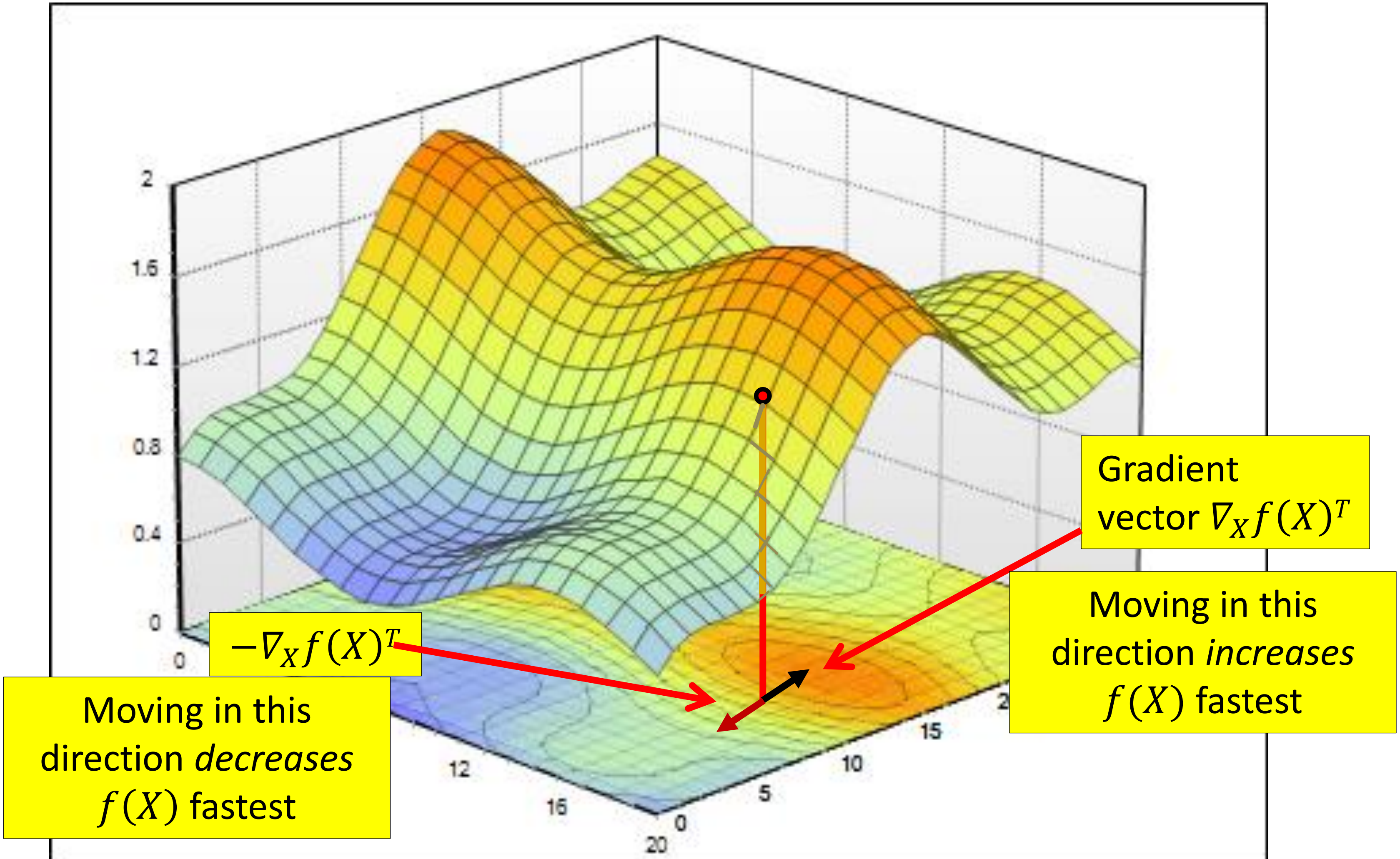
2
1.6
1.2
0.8
0.4
0
0
4
8
12
16
20
0
5
10
15
20
25
30
Gradient vector $\nabla_X f(X)^T$

Gradient



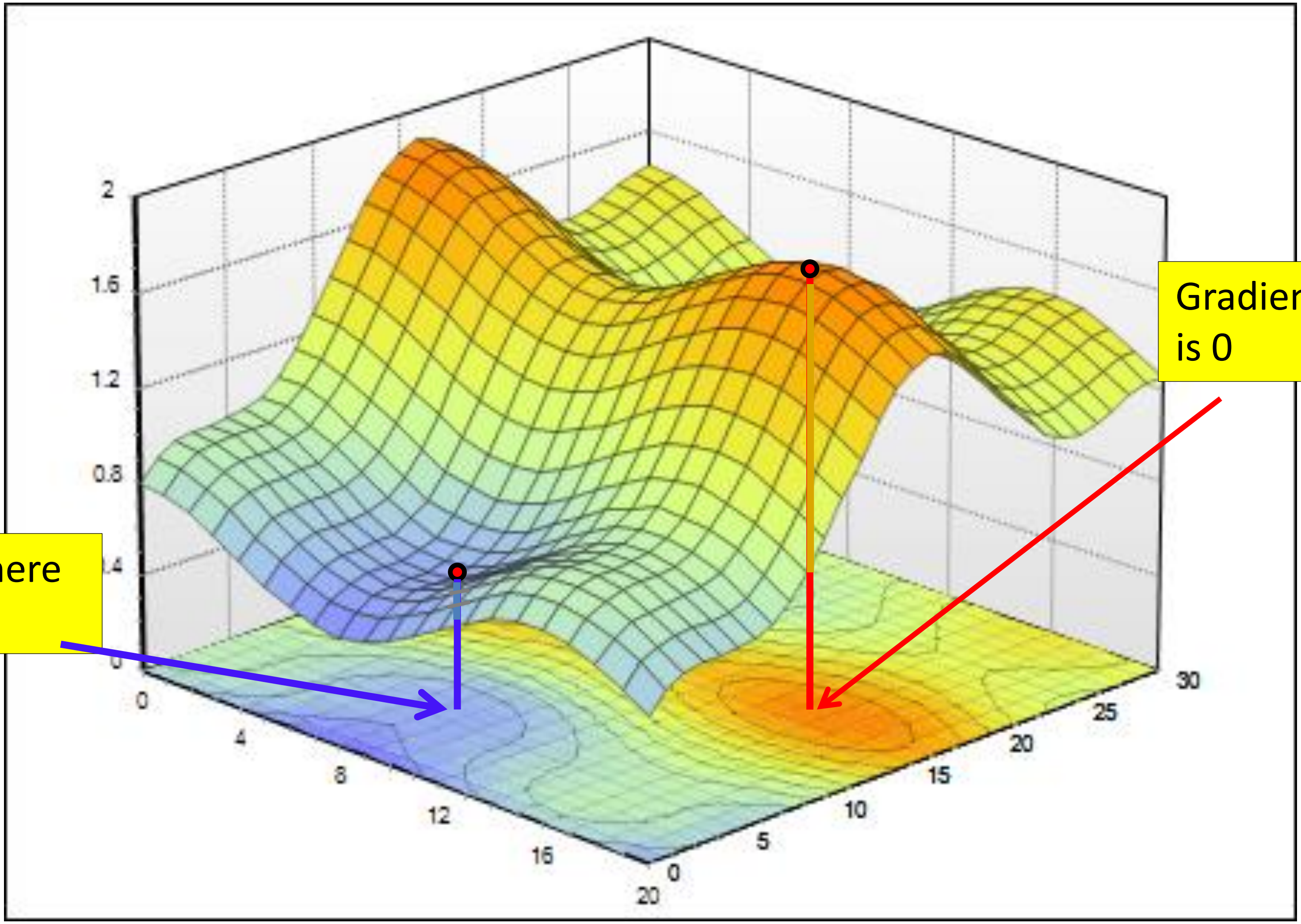
2
1.6
1.2
0.8
0.4
0
0
4
8
12
16
20
0
5
10
15
Gradient vector $\nabla_X f(X)^T$
Moving in this direction *increases* $f(X)$ fastest

Gradient



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

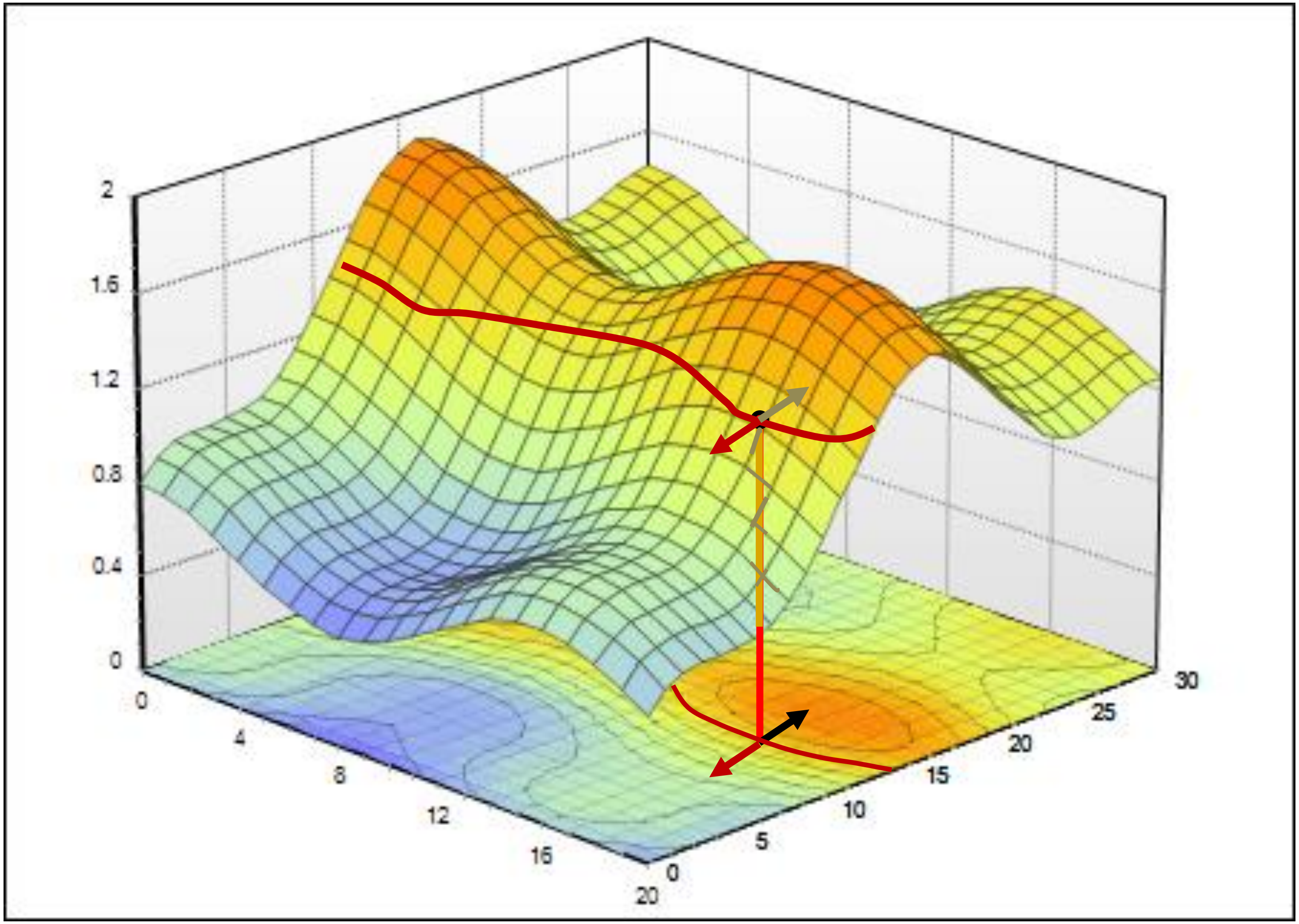
Gradient



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 $f(x_1, x_2, \ldots, x_n)$ is given by the second derivative

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

Next up

- Continuing on function optimization

- Gradient descent to train neural networks

- A.K.A. Back propagation