

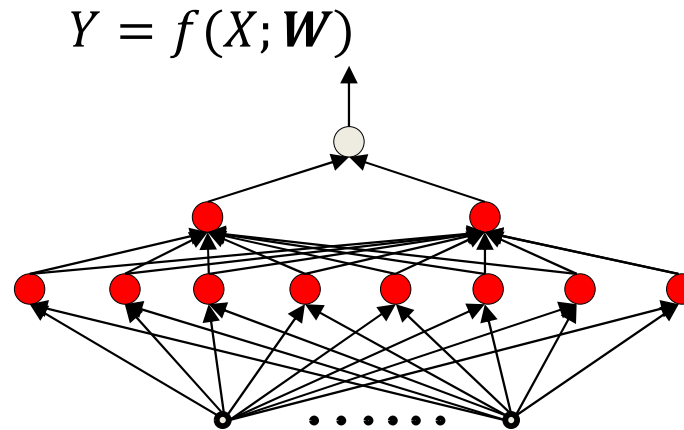
# **Neural Networks**

## **Learning the network: Backprop**

**11-785, Spring 2022**

**Lecture 4**

# Recap: Empirical Risk Minimization



- Given a training set of input-output pairs  $(X_1, d_1), (X_2, d_2), \dots, (X_T, d_T)$ 
  - Divergence on the  $i$ -th instance:  $\text{div}(f(X_i; W), d_i)$
  - Empirical average divergence on all training data:

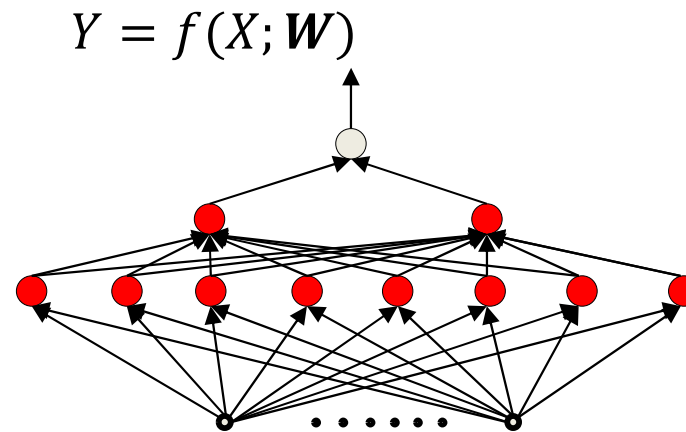
$$\text{Loss}(W) = \frac{1}{T} \sum_i \text{div}(f(X_i; W), d_i)$$

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

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

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

# Recap: Empirical Risk Minimization



This is an instance of function minimization (optimization)

- Given a training set of input-output pairs  $(X_1, d_1), (X_2, d_2), \dots, (X_T, d_T)$ 
  - Error on the  $i$ -th instance:  $div(f(X_i; W), d_i)$
  - Empirical average error on all training data:

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

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

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

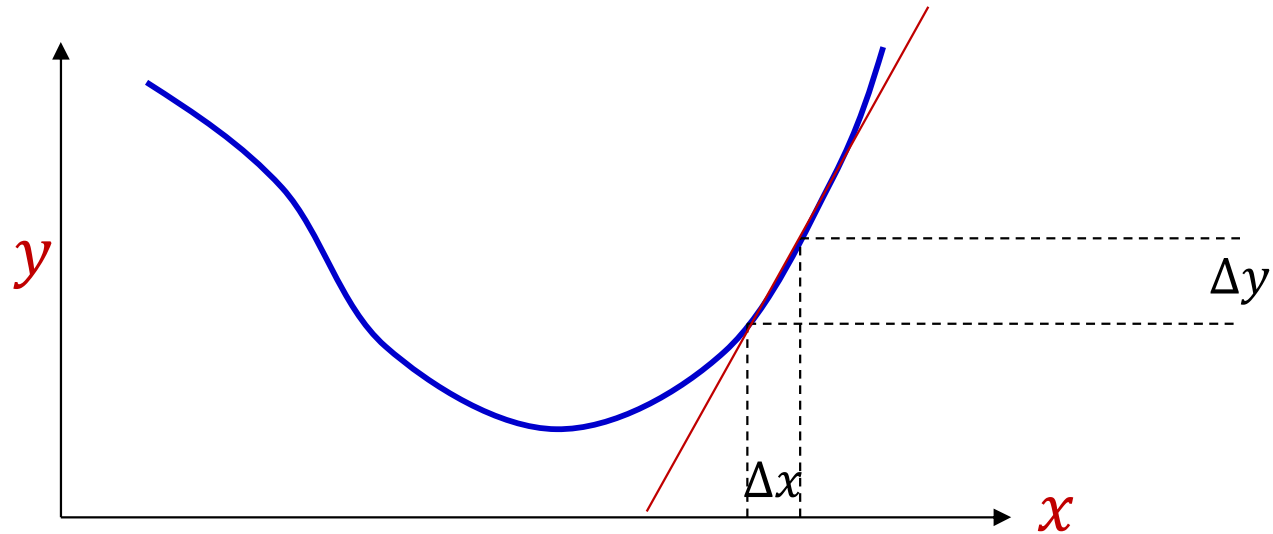
- I.e. minimize the *empirical error* over the drawn samples

# A quick intro to function optimization

with an initial discussion of  
derivatives

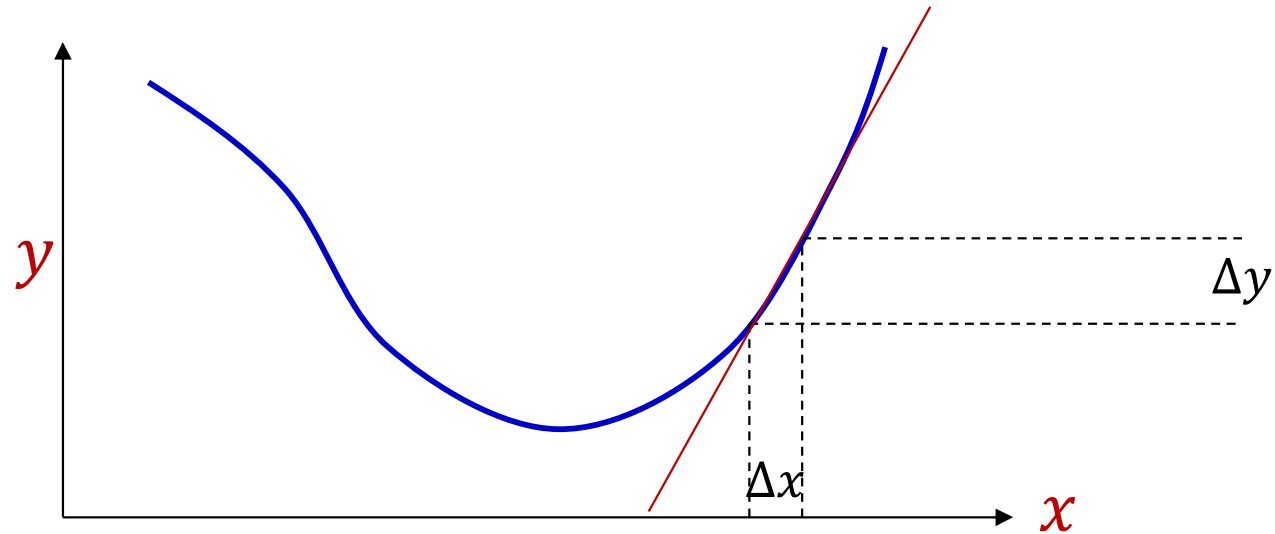


# A brief note on derivatives..



- A derivative of a function at any point tells us how much a minute increment to the *argument* of the function will increment the *value* of the function
  - For any  $y = f(x)$ , expressed as a multiplier  $\alpha$  to a tiny increment  $\Delta x$  to obtain the increments  $\Delta y$  to the output
$$\Delta y = \alpha \Delta x$$
  - Based on the fact that at a fine enough resolution, any smooth, continuous function is locally linear at any point

# Scalar function of scalar argument



- When  $x$  and  $y$  are scalar

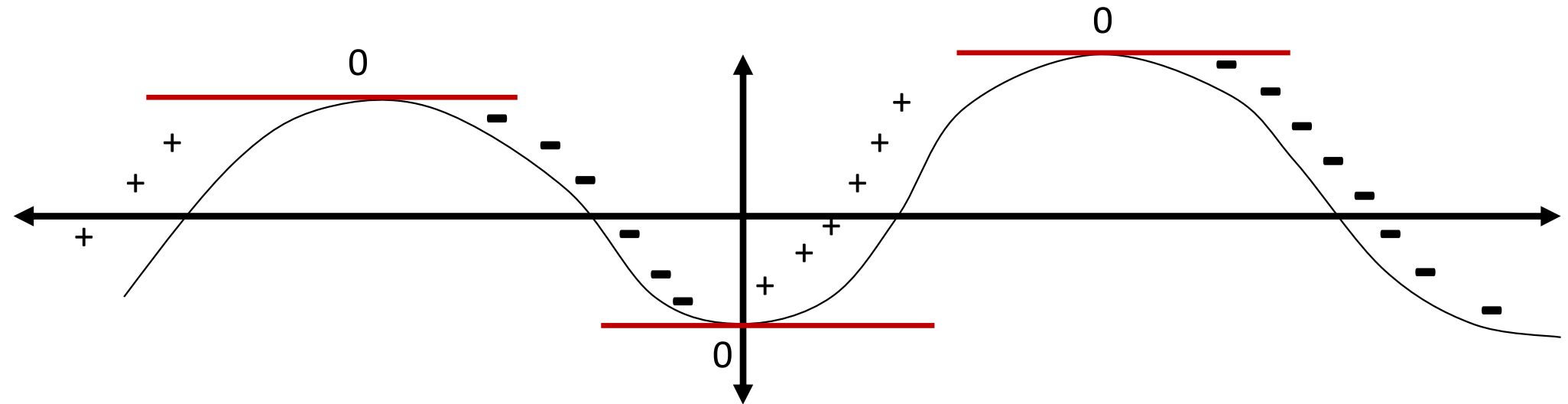
$$y = f(x)$$

- Derivative:

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

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

# Scalar function of scalar argument



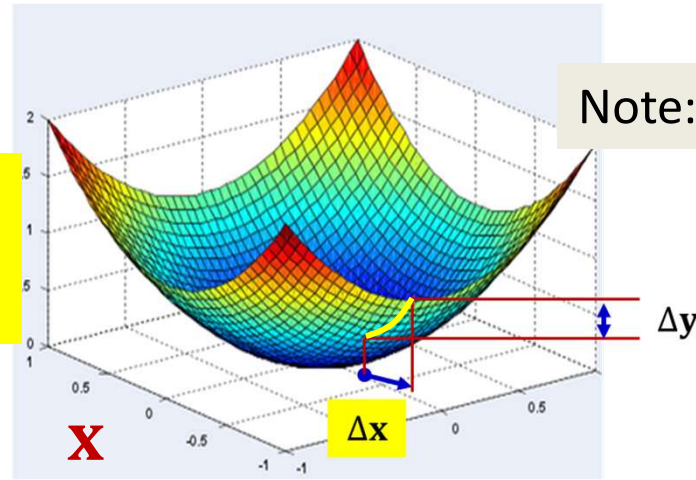
- Derivative  $f'(x)$  is the *rate of change* of the function at  $x$ 
  - How fast it increases with increasing  $x$
  - The magnitude of  $f'(x)$  gives you the steepness of the curve at  $x$ 
    - Larger  $|f'(x)| \rightarrow$  the function is increasing or decreasing more rapidly
- It will be positive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

$$y = f(\mathbf{x})$$

$\mathbf{x}$  is now a vector:  $\mathbf{x} = \begin{bmatrix} x_1 \\ \vdots \\ x_D \end{bmatrix}$



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

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

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

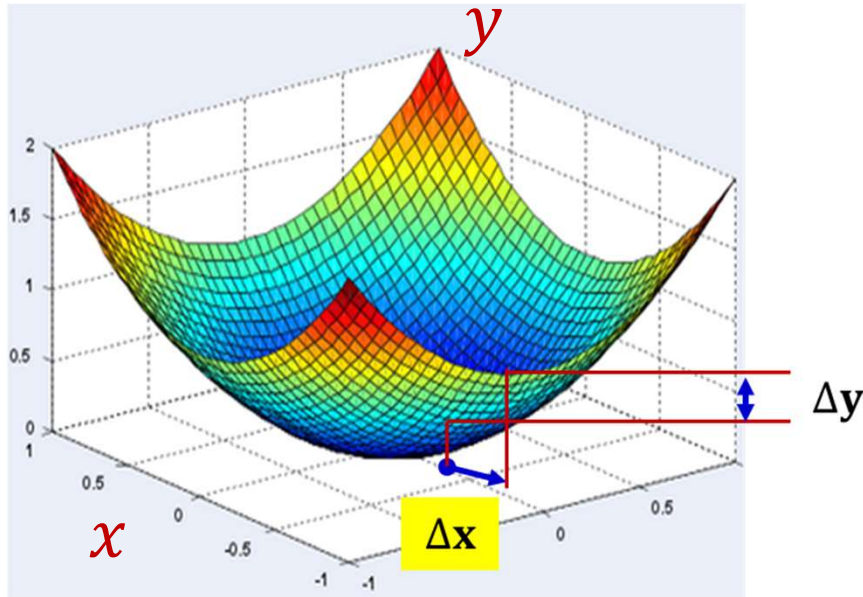
- Giving us that  $\alpha$  is a row vector:  $\alpha = [\alpha_1 \quad \cdots \quad \alpha_D]$ 
$$\Delta y = \alpha_1 \Delta x_1 + \alpha_2 \Delta x_2 + \cdots + \alpha_D \Delta x_D$$
- The *partial* derivative  $\alpha_i$  gives us how  $y$  increments when *only*  $x_i$  is incremented
- Often represented as  $\frac{\partial y}{\partial x_i}$

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



# Multivariate scalar function:

## Scalar function of *vector* argument



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

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

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

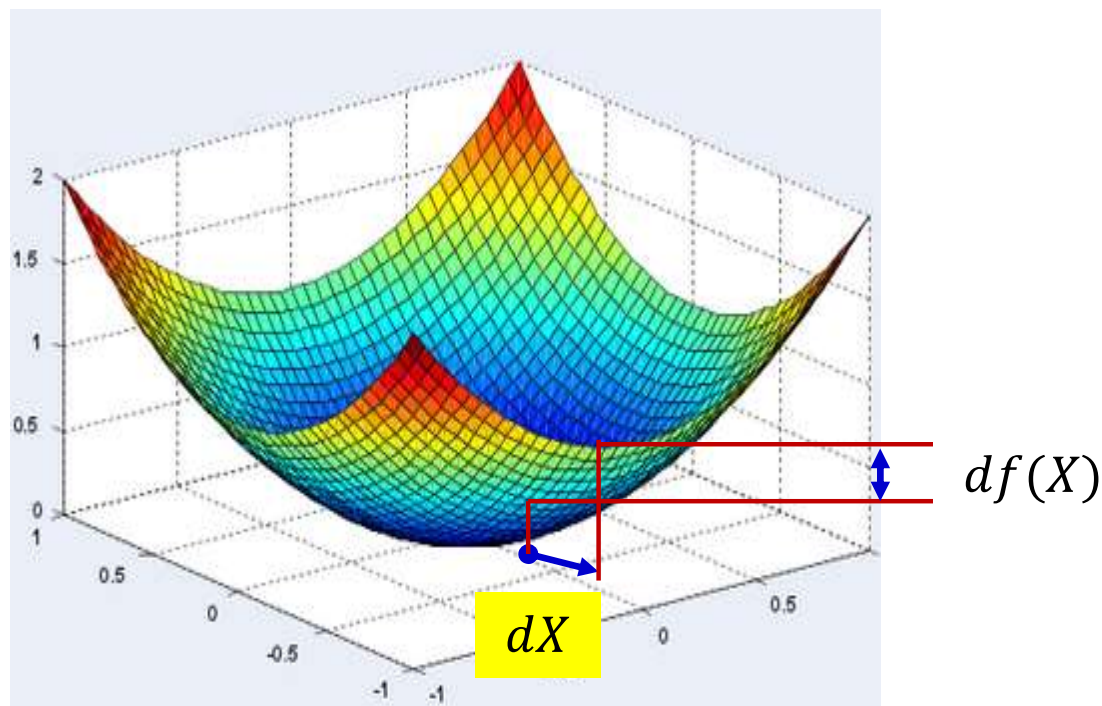
- Where

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

We will be using this symbol for vector and matrix derivatives

- 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

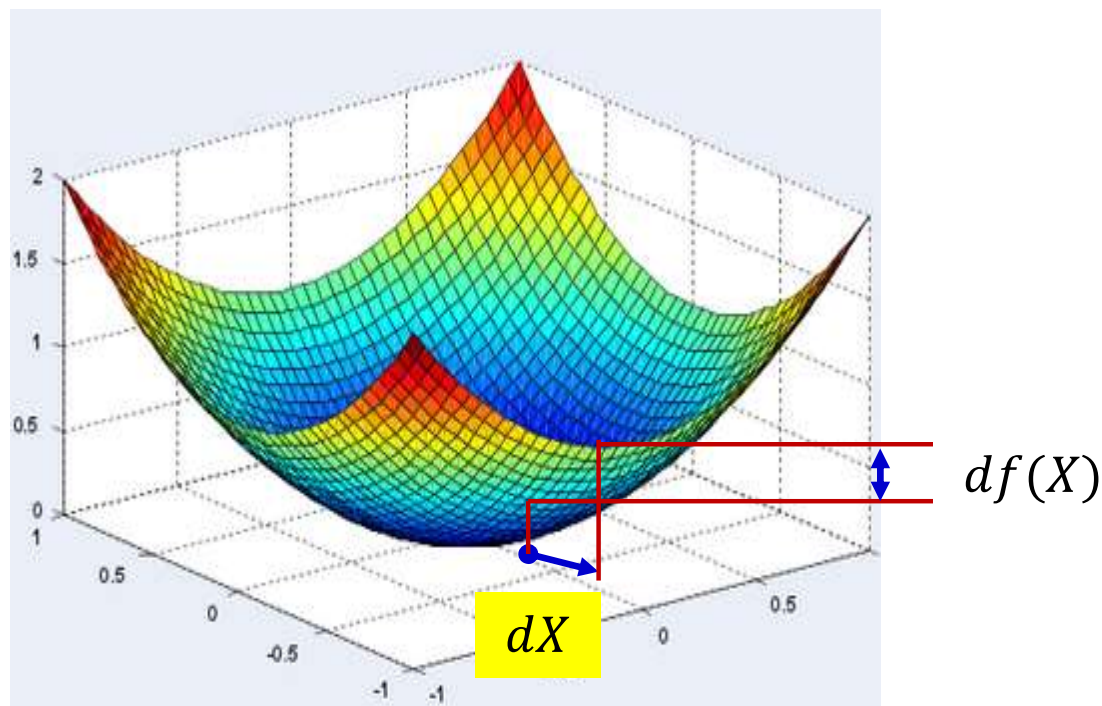


- The *derivative*  $\nabla_X f(X)$  of a scalar function  $f(X)$  of a multi-variate input  $X$  is a multiplicative factor that gives us the change in  $f(X)$  for tiny variations in  $X$

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

- $\nabla_X f(X) = \begin{bmatrix} \frac{\partial f(X)}{\partial x_1} & \frac{\partial f(X)}{\partial x_2} & \dots & \frac{\partial f(X)}{\partial x_n} \end{bmatrix}$
- 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



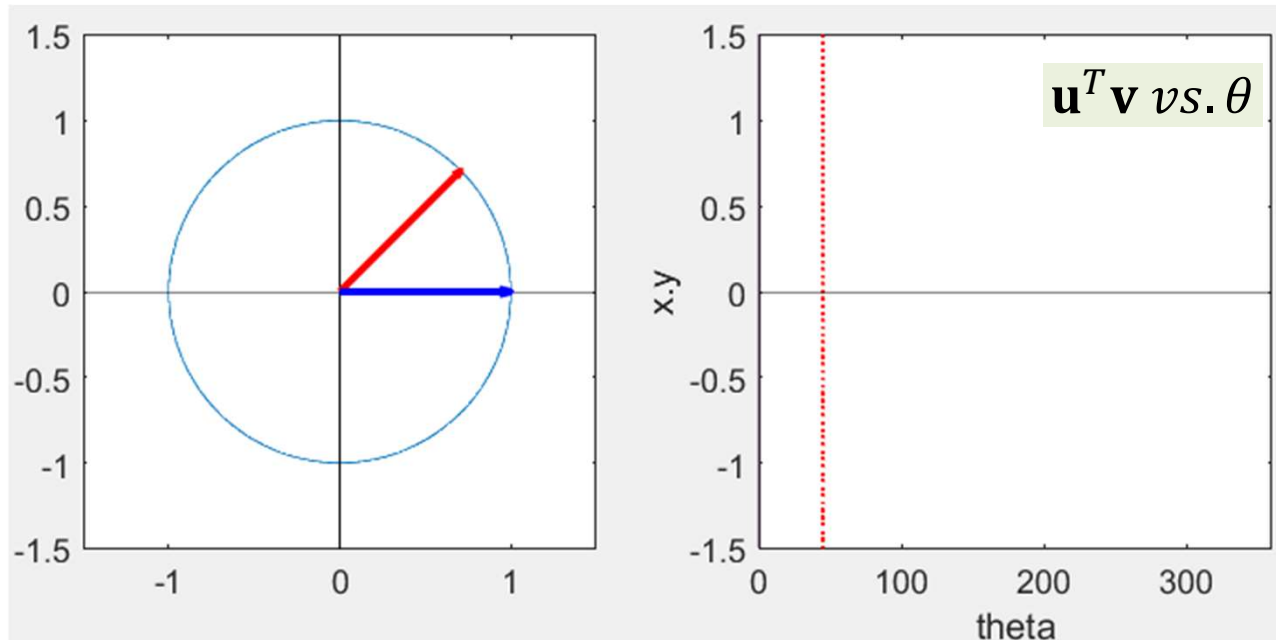
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$$df(X) = \nabla_X f(X) dX$$

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

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

# A well-known vector property

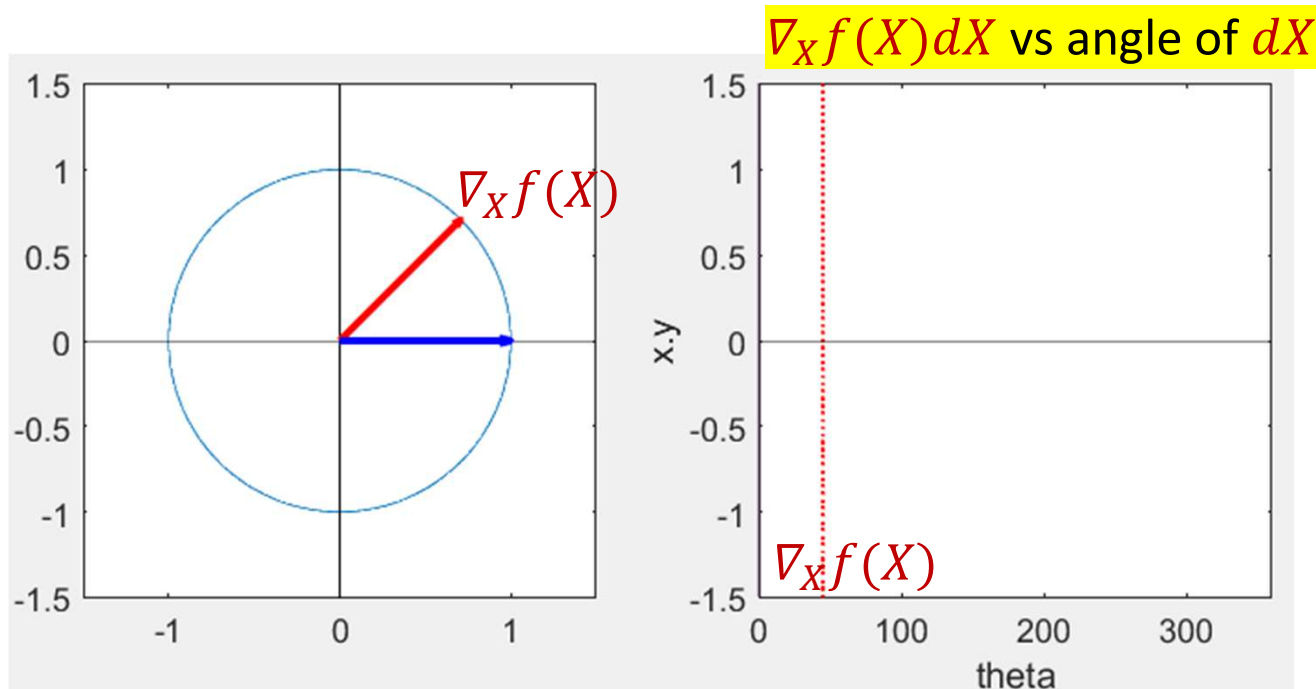


$$\mathbf{u}^T \mathbf{v} = |\mathbf{u}| |\mathbf{v}| \cos \theta$$

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

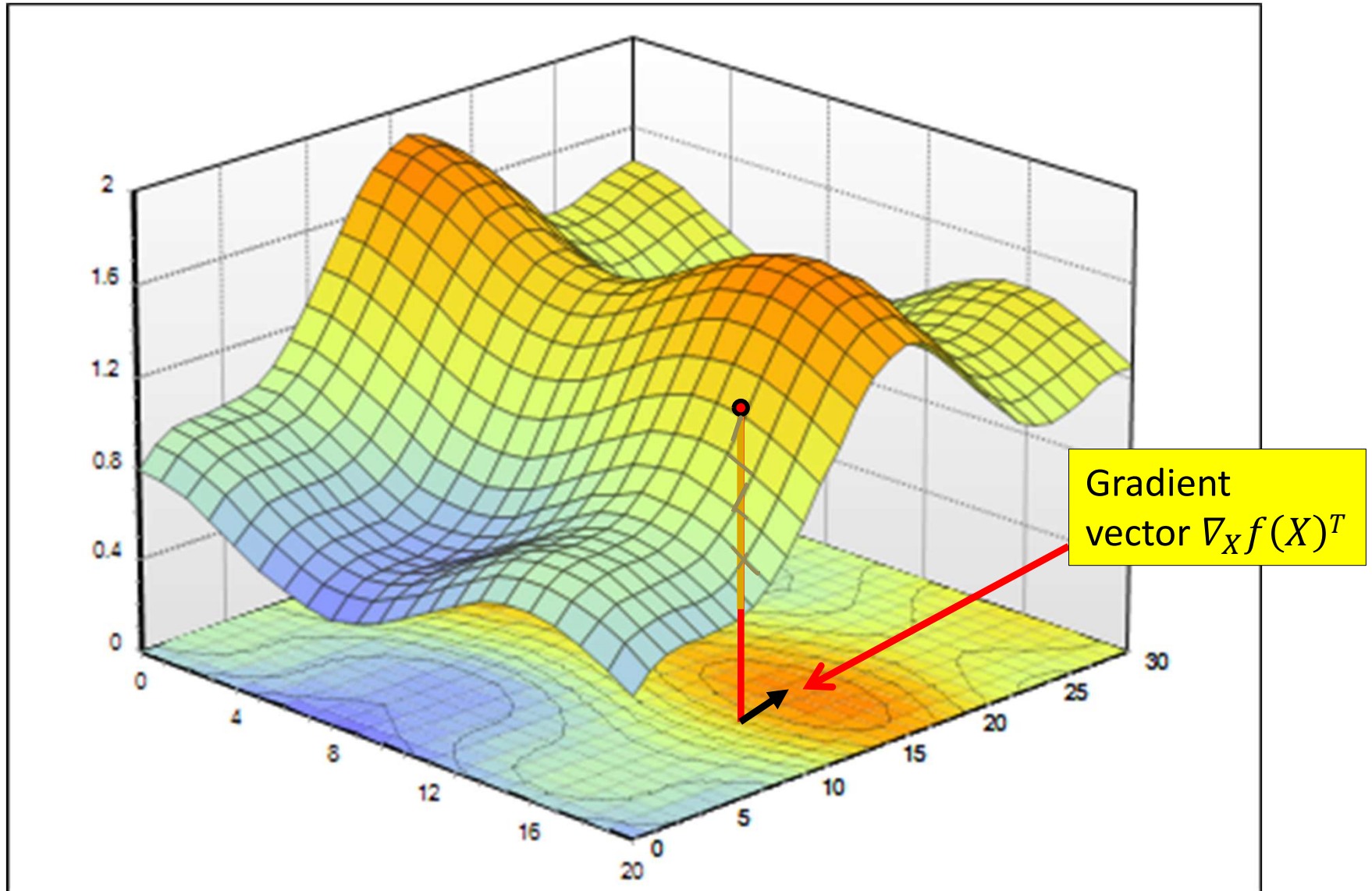
# Properties of Gradient

Blue arrow  
is  $dX$



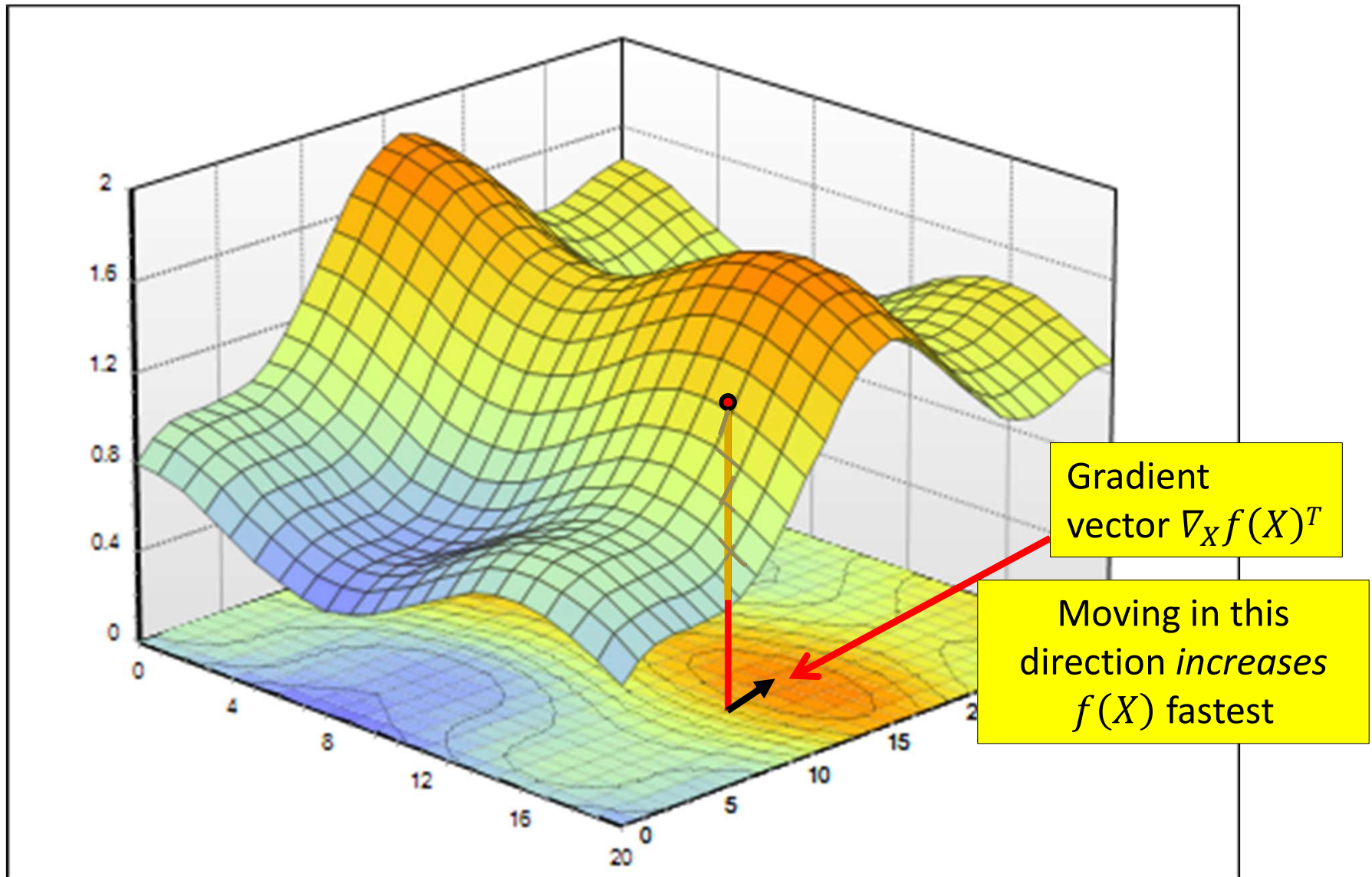
- $df(X) = \nabla_X f(X) dX$
- For an increment  $dX$  of any given length  $df(X)$  is max if  $dX$  is aligned with  $\nabla_X f(X)^T$ 
  - The function  $f(X)$  increases most rapidly if the input increment  $dX$  is exactly in the direction of  $\nabla_X f(X)^T$
- The gradient is the direction of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

# Gradient

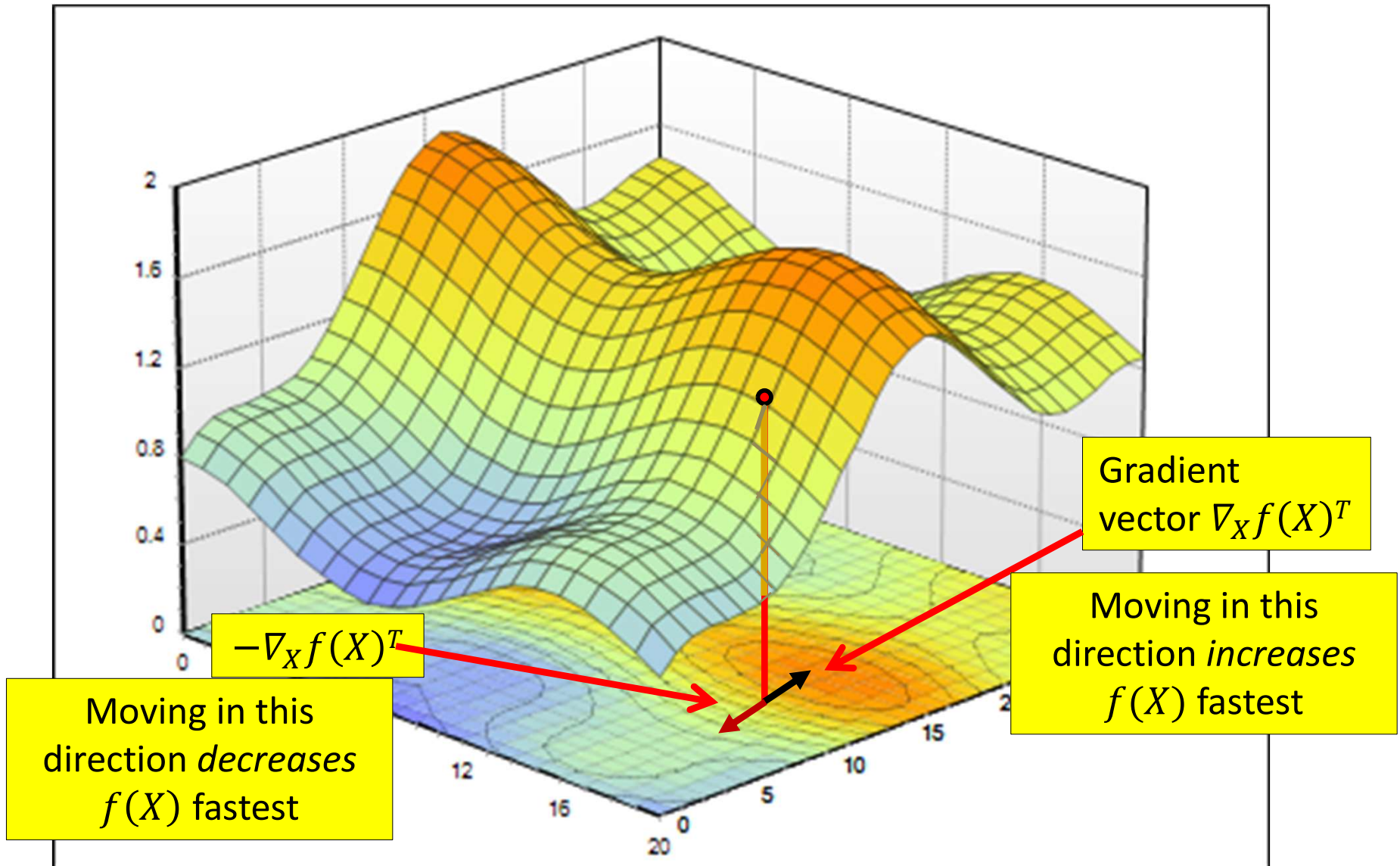




# Gradient

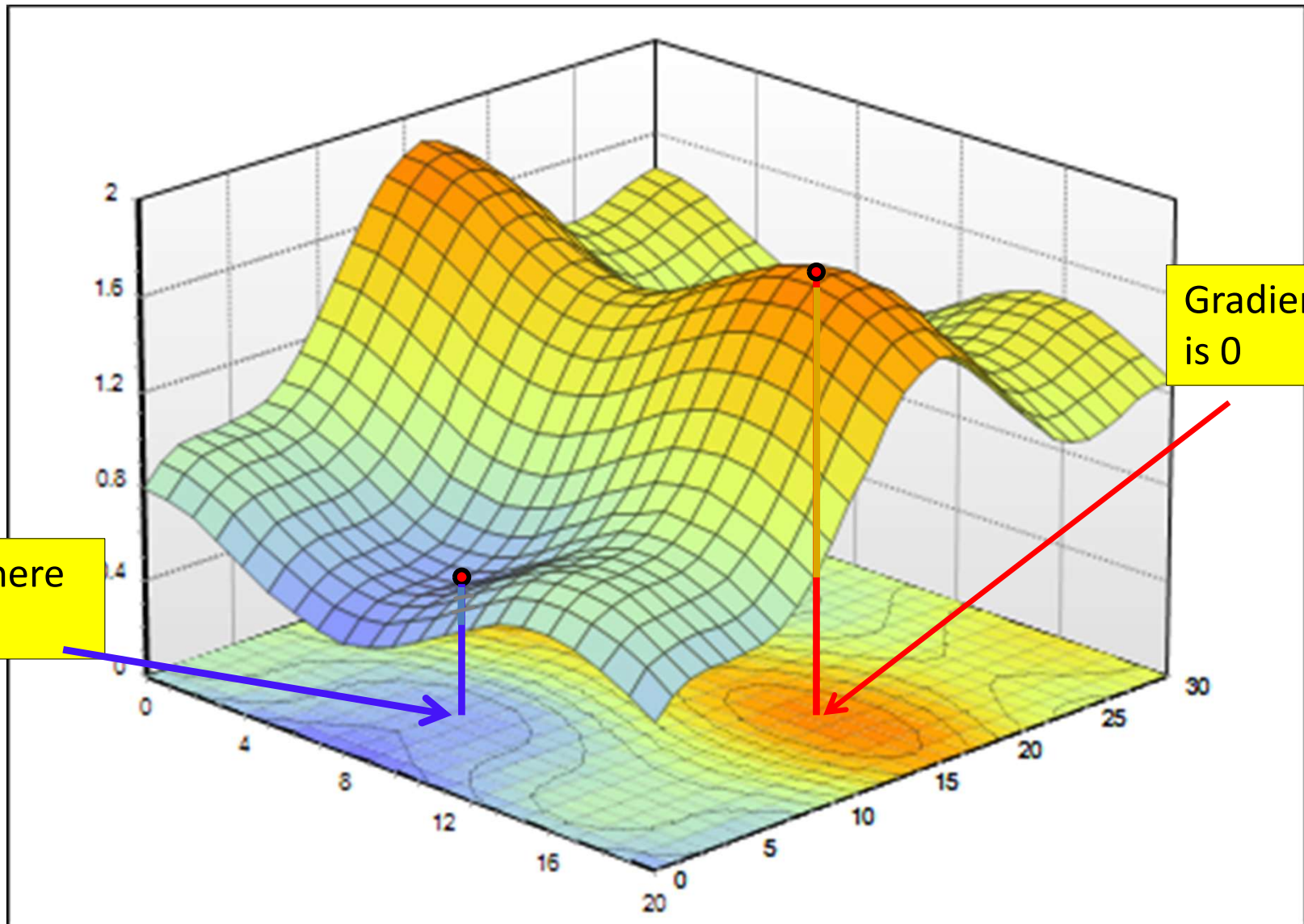


# Gradient

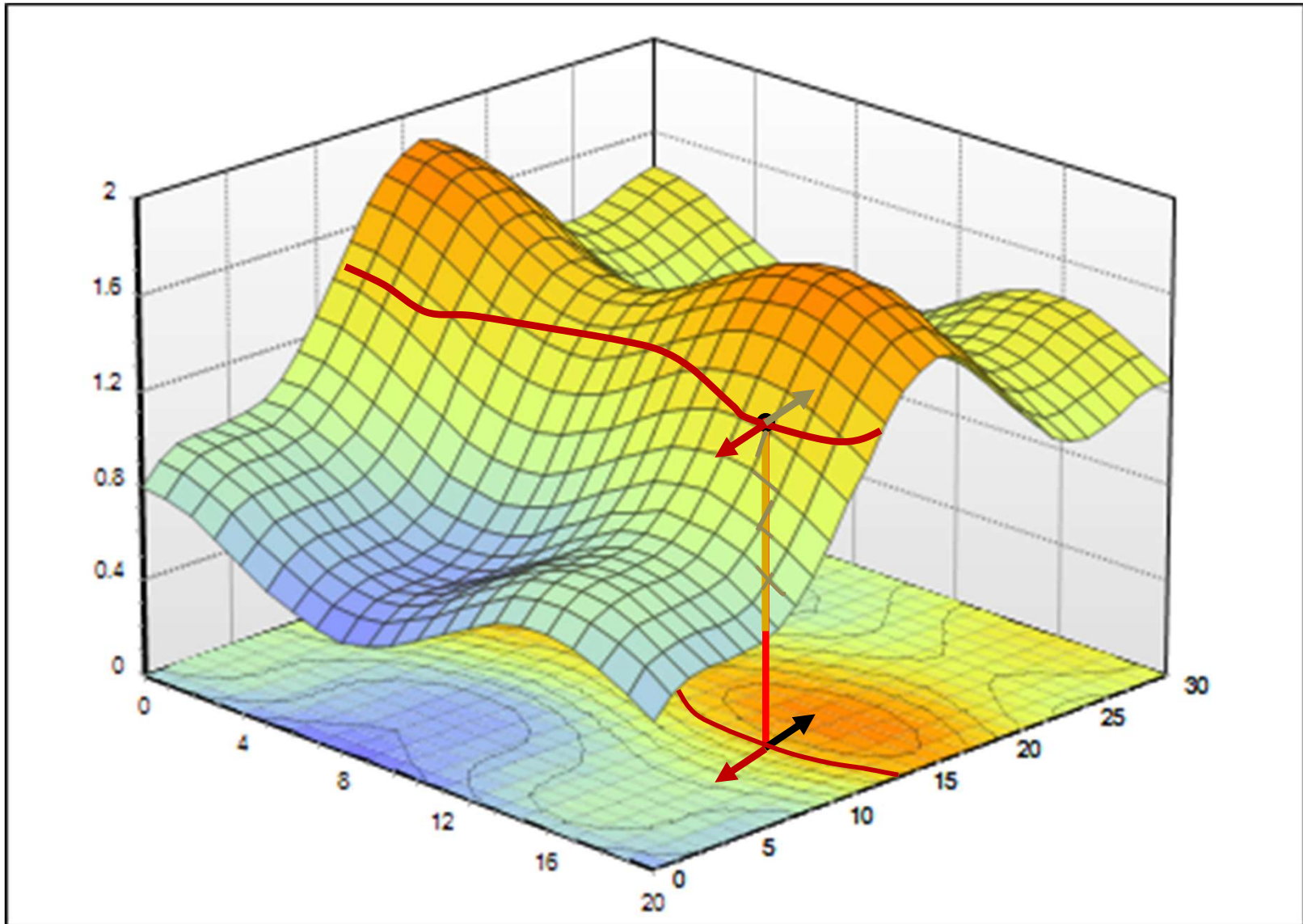




# Gradient



# 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

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

# Poll 1

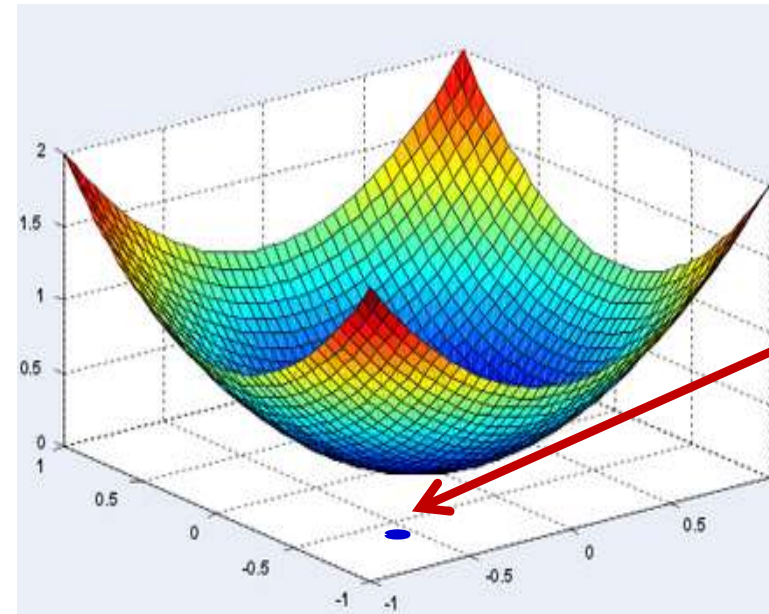
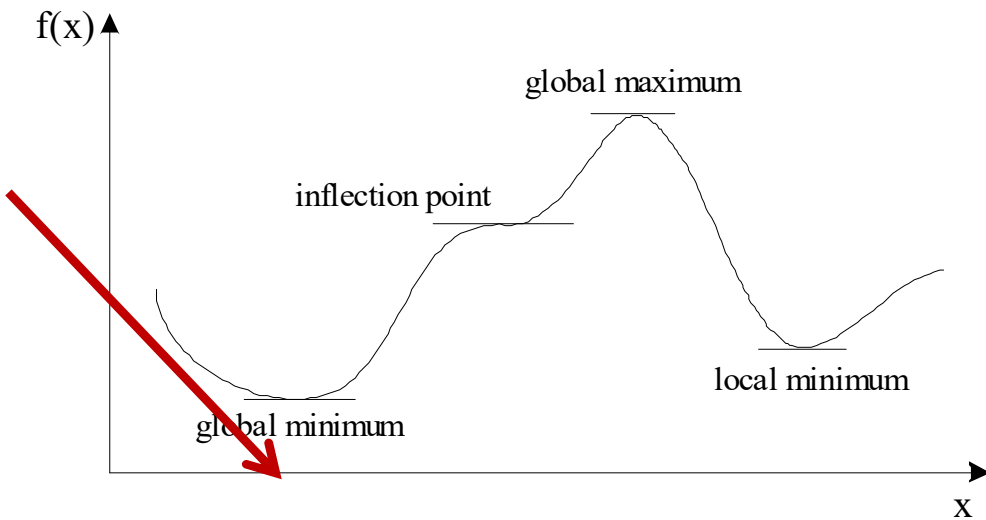
- Select all that are true about derivatives of a scalar function  $f(X)$  of multivariate inputs
  - At any location  $X$ , there may be many directions in which we can step, such that  $f(X)$  increases
  - The direction of the gradient is the direction in which the function increases fastest
  - The gradient is the derivative of  $f(X)$  w.r.t.  $X$
- $y = f(x)$  is a scalar function of an  $N \times 1$  column vector variable  $x$ . What is the shape of the derivative of  $y$  with respect to  $x$ 
  - Scalar
  - $N \times 1$  column vector
  - $1 \times N$  row vector
  - There is insufficient information to decide

# Poll 1

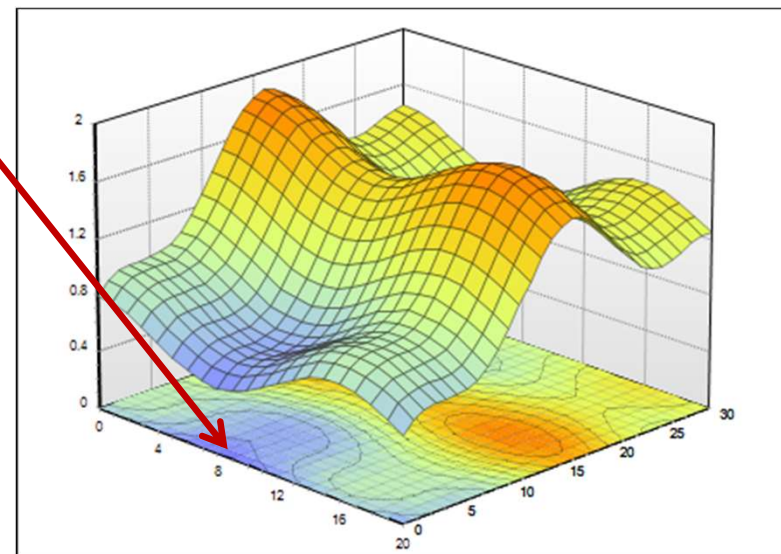
- Select all that are true about derivatives of a scalar function  $f(X)$  of multivariate inputs
  - **At any location  $X$ , there may be many directions in which we can step, such that  $f(X)$  increases**
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  - **$1 \times N$  row vector**
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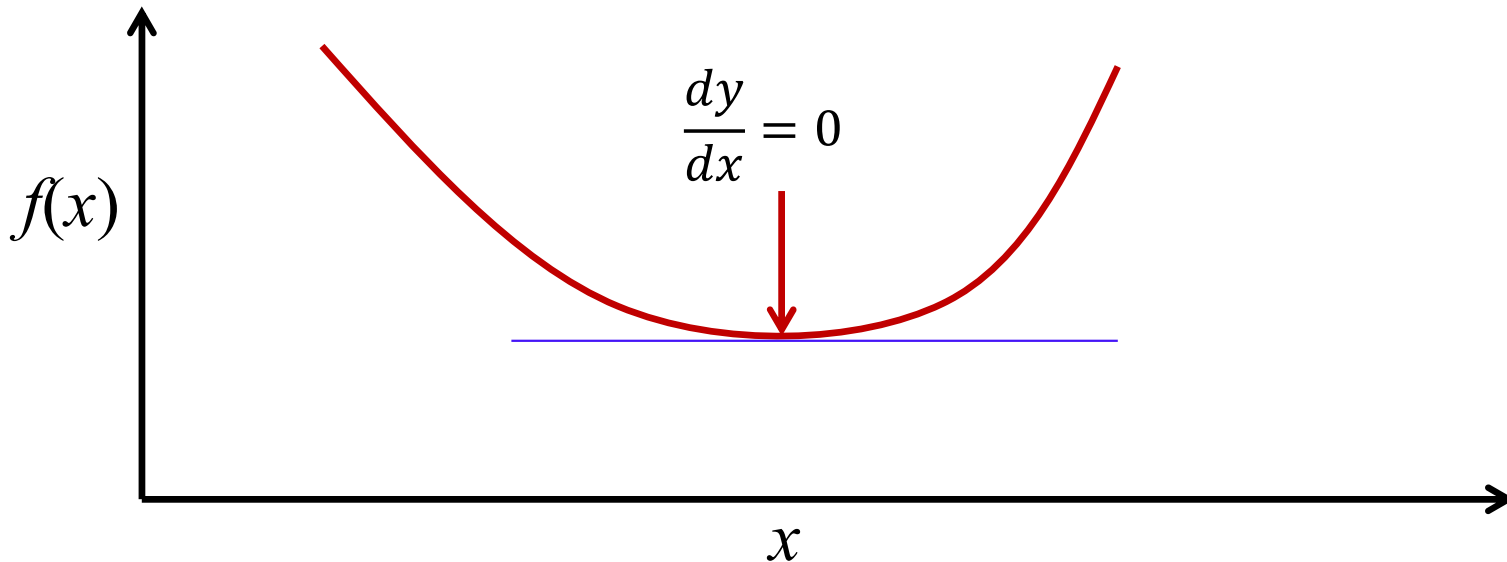
# The problem of optimization



- General problem of optimization: Given a function  $f(x)$  of some variable  $x$  ...
- Find the value of  $x$  where  $f(x)$  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?

## Poll 2

Which of the following is true (choose only one) about the minimum of a function  $f(x)$

1. The derivative  $f'(x) = 0$  at the minimum. This is the only condition to be satisfied
2.  $f'(x) = 0$  and the second derivative  $f''(x)$  is negative
3.  $f'(x) = 0$  and the second derivative  $f''(x)$  is positive

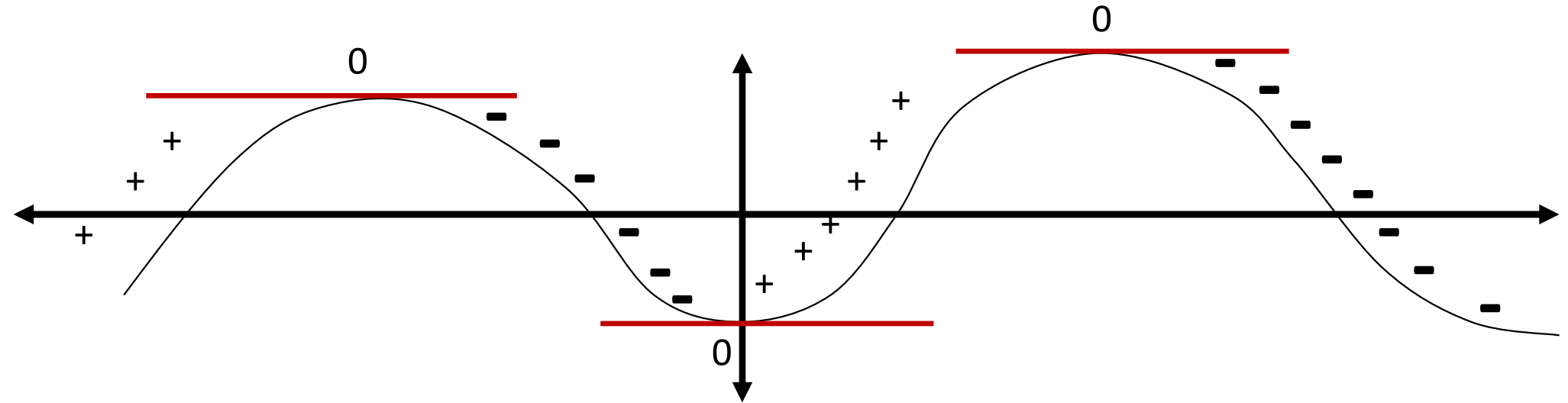


## Poll 2

Which of the following is true (choose only one) about the minimum of a function  $f(x)$

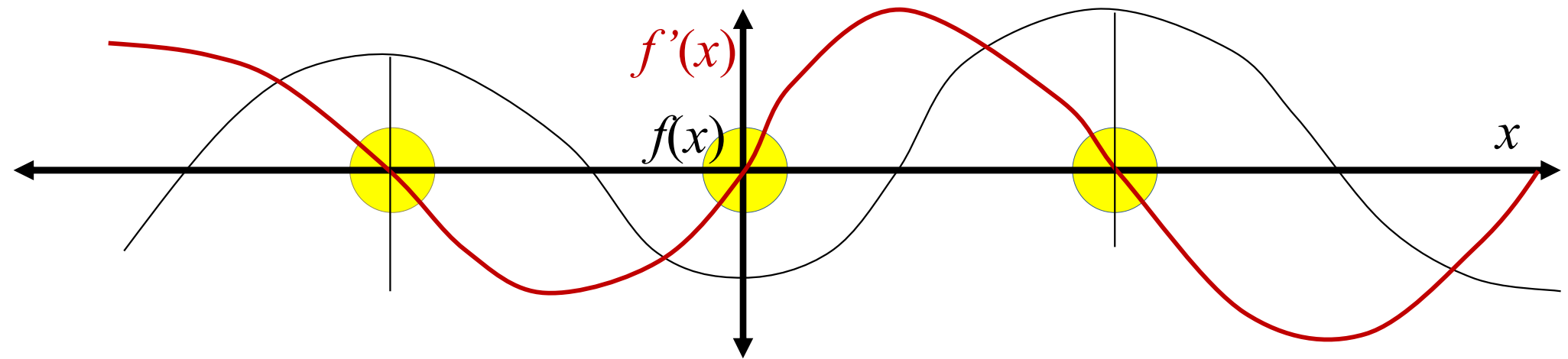
1. The derivative  $f'(x) = 0$  at the minimum. This is the only condition to be satisfied
2.  $f'(x) = 0$  and the second derivative  $f''(x)$  is negative
3.  **$f'(x) = 0$  and the second derivative  $f''(x)$  is positive**

# Turning Points



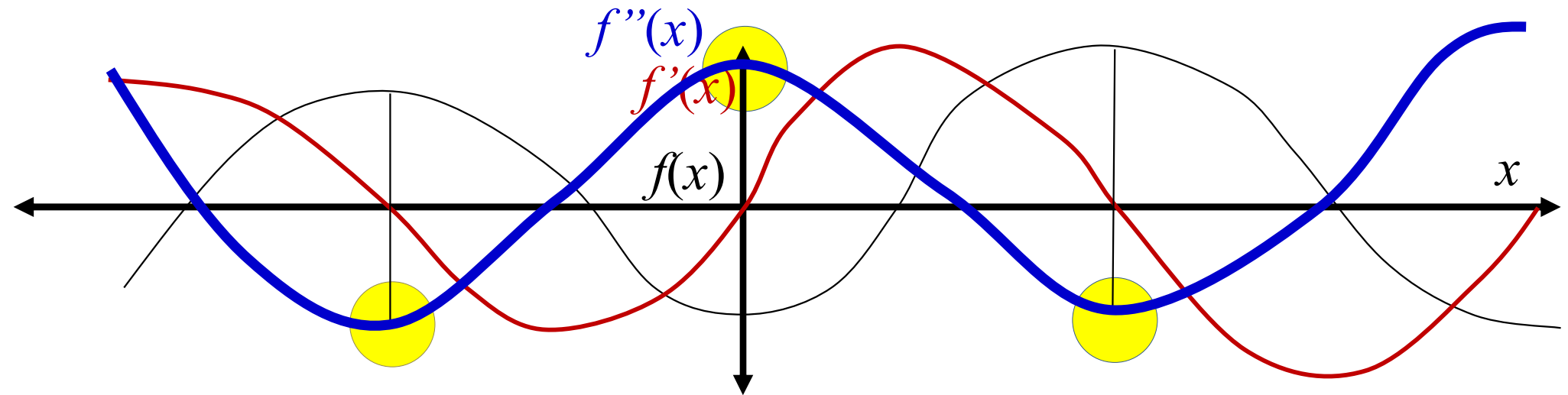
- Both *maxima* and *minima* have zero derivative
- Both are turning points

# Derivatives of a curve



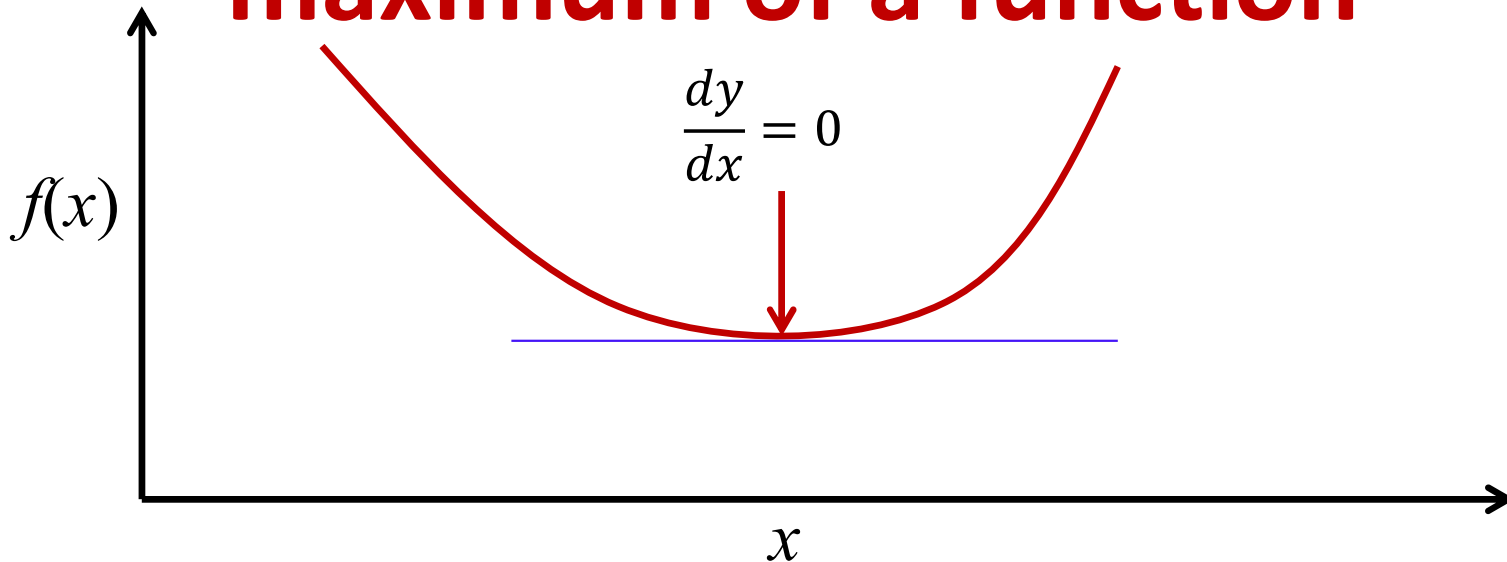
- Both *maxima* and *minima* are turning points
- Both *maxima* and *minima* have **zero derivative**

# 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

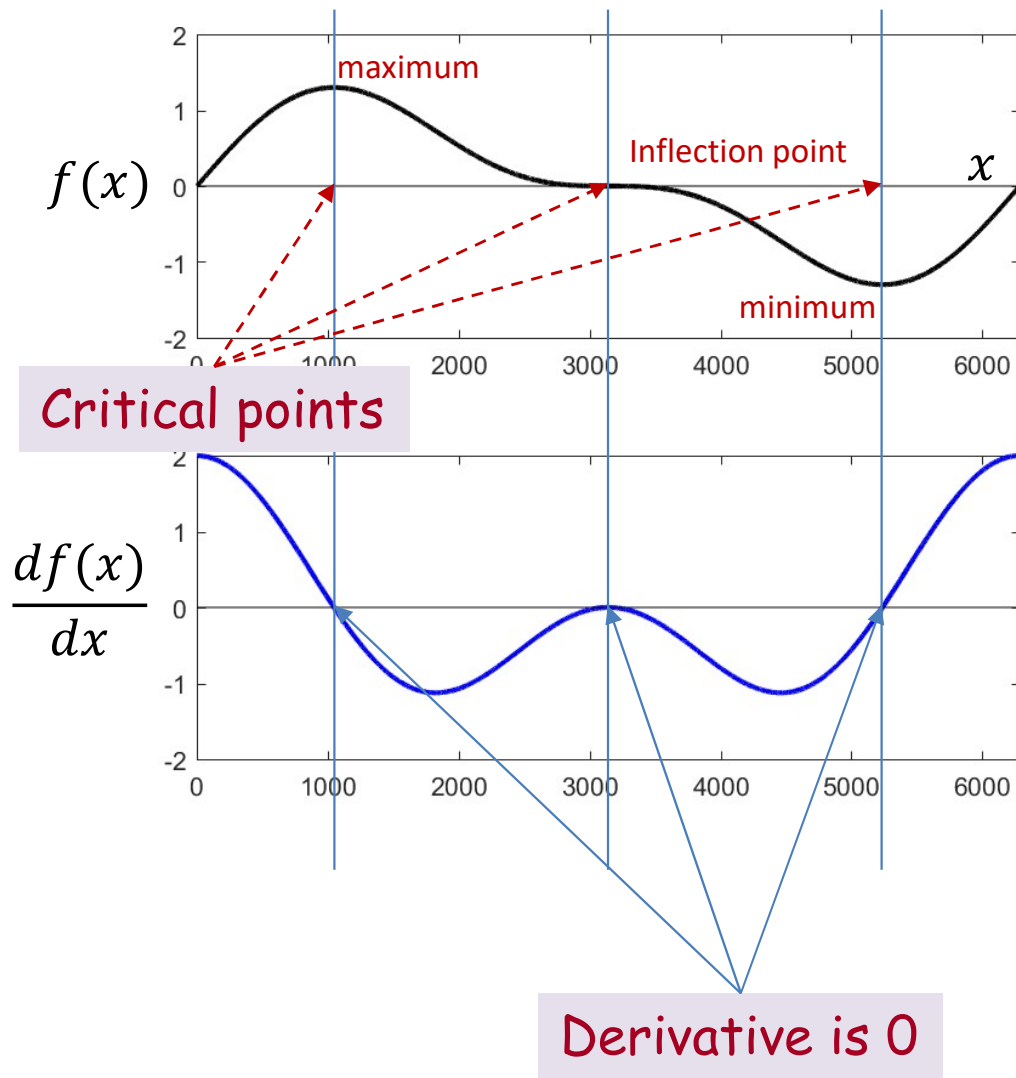
$$\frac{df(x)}{dx} = 0$$

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

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

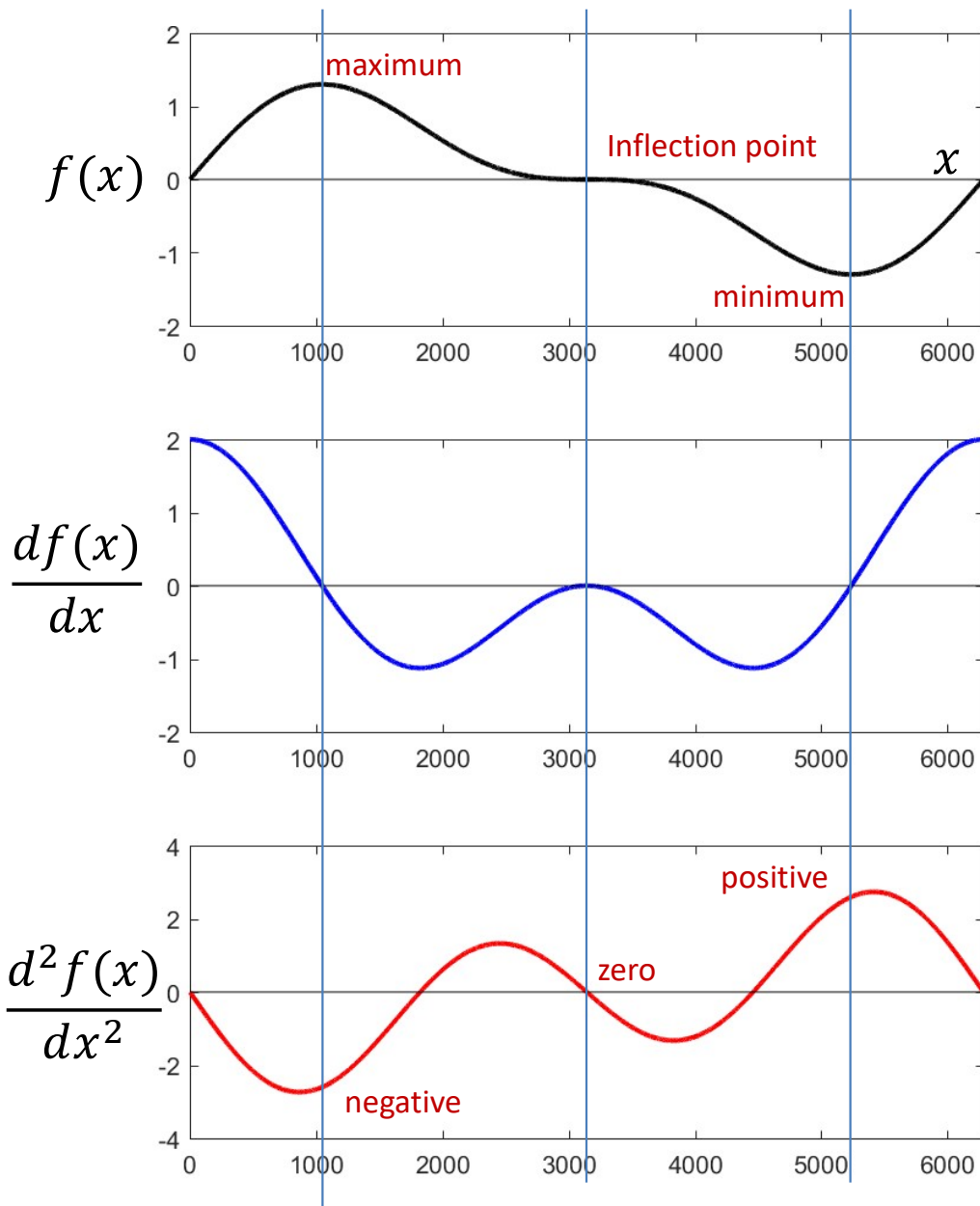
- If  $f''(x_{soln})$  is positive  $x_{soln}$  is a minimum, otherwise it is a maximum

# A note on derivatives of functions of single variable



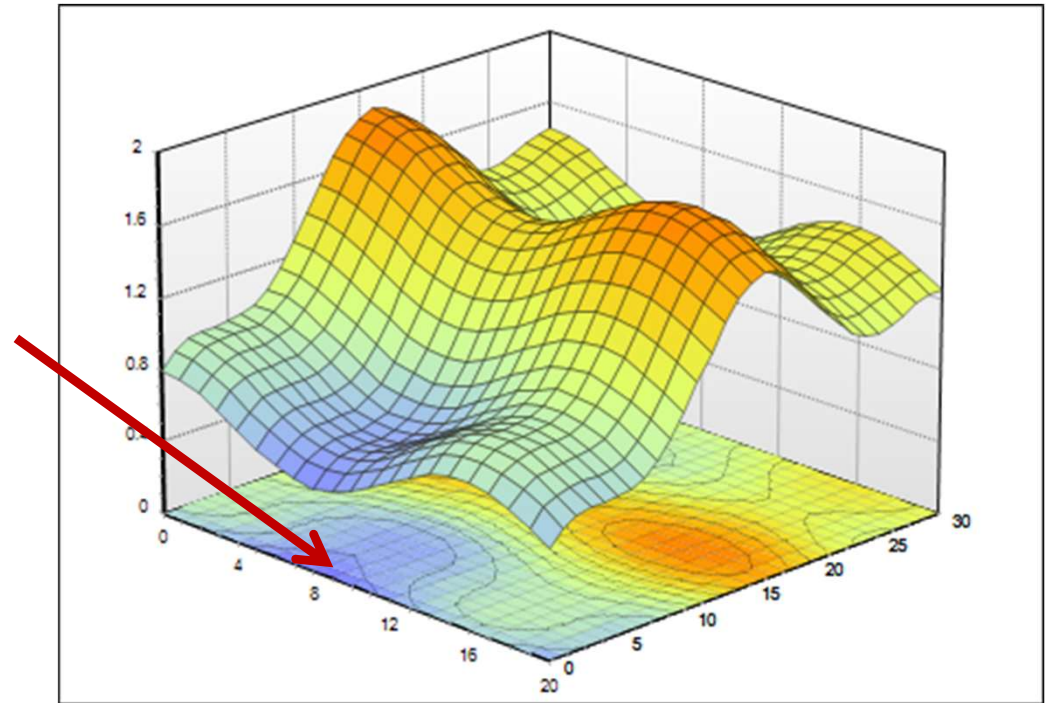
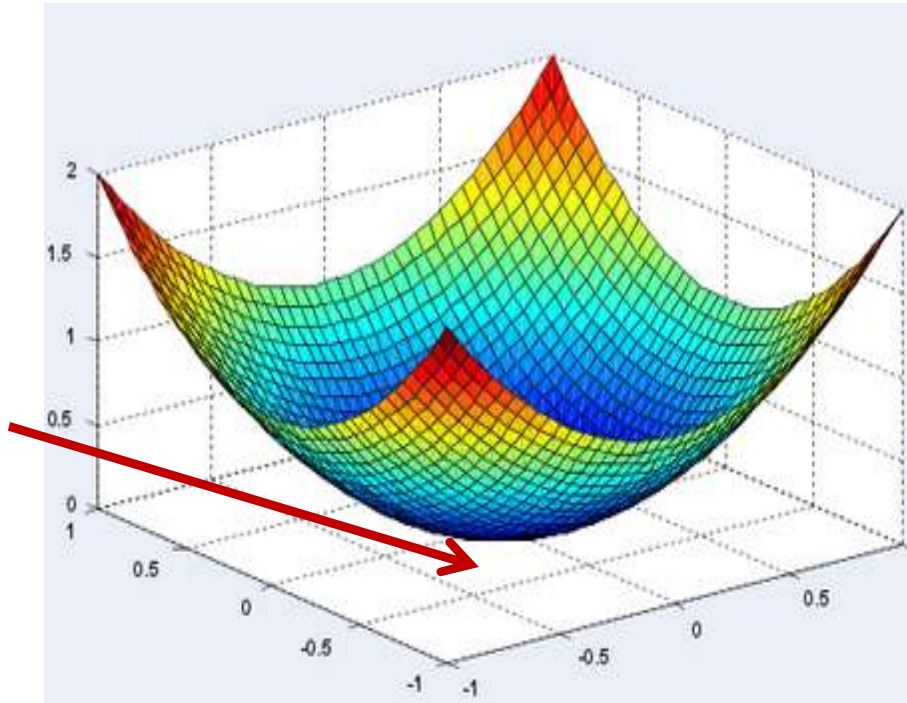
- All locations with zero derivative are *critical* points
  - These can be local maxima, local minima, or inflection points
- The *second* derivative is
  - Positive (or 0) at minima
  - Negative (or 0) at maxima
  - Zero at inflection points

# 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
  - $\geq 0$  at minima
  - $\leq 0$  at maxima
  - Zero at inflection points
- It's a little more complicated for functions of multiple variables..

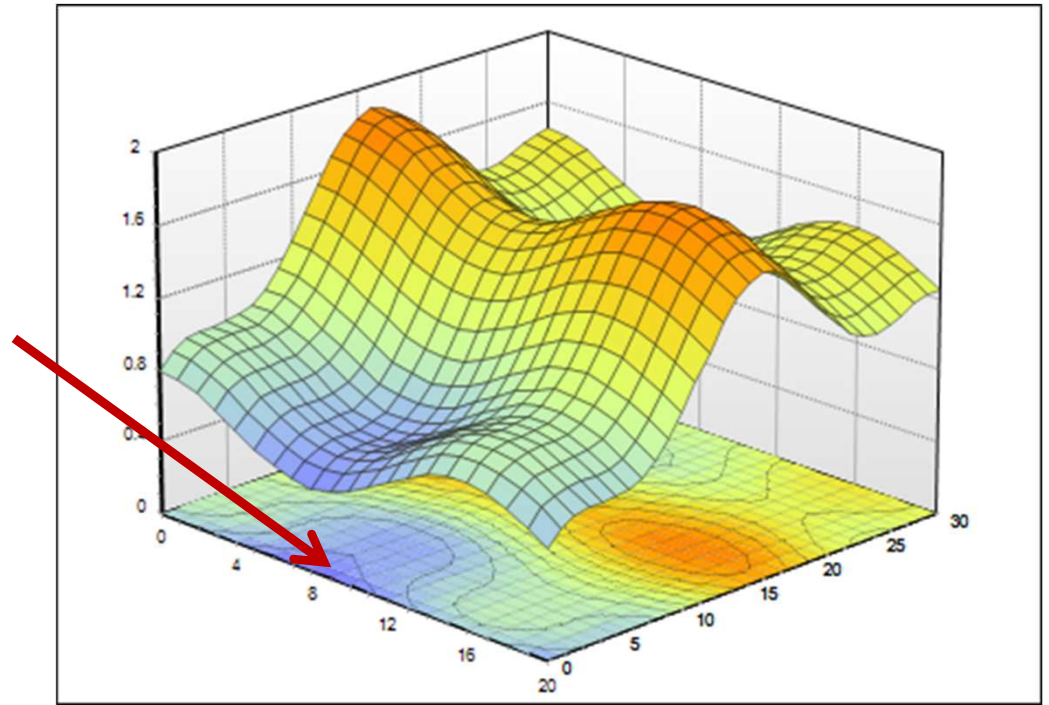
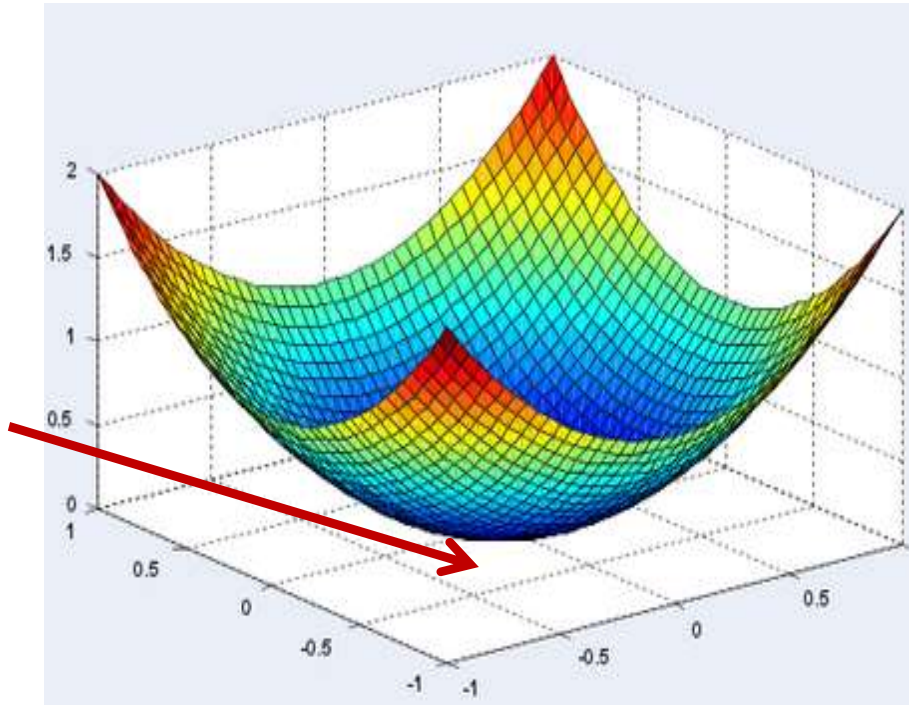
# What about functions of multiple variables?



- The optimum point is still “turning” point
  - Shifting in any direction will increase the value
  - For smooth functions, at the minimum/maximum, the gradient is 0
    - Really tiny shifts will not change the function value



# Finding the minimum of a scalar function of a multivariate input



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

$$f(x_1, x_2, x_3) = (x_1)^2 + x_1(1 - x_2) + (x_2)^2 - x_2x_3 + (x_3)^2 + x_3$$

- 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)

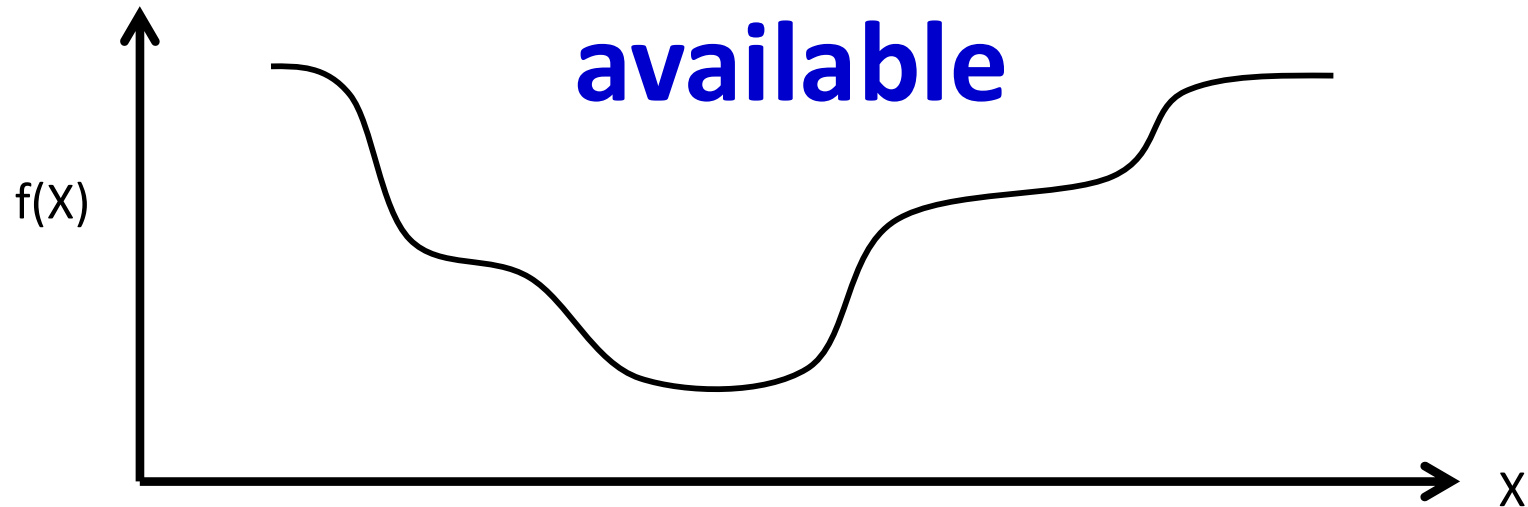
- Compute the Hessian matrix  $\nabla_x^2 f = \begin{bmatrix} 2 & -1 & 0 \\ -1 & 2 & -1 \\ 0 & -1 & 2 \end{bmatrix}$
- Evaluate the eigenvalues of the Hessian matrix

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

- All the eigenvalues are positives => the Hessian matrix is positive definite

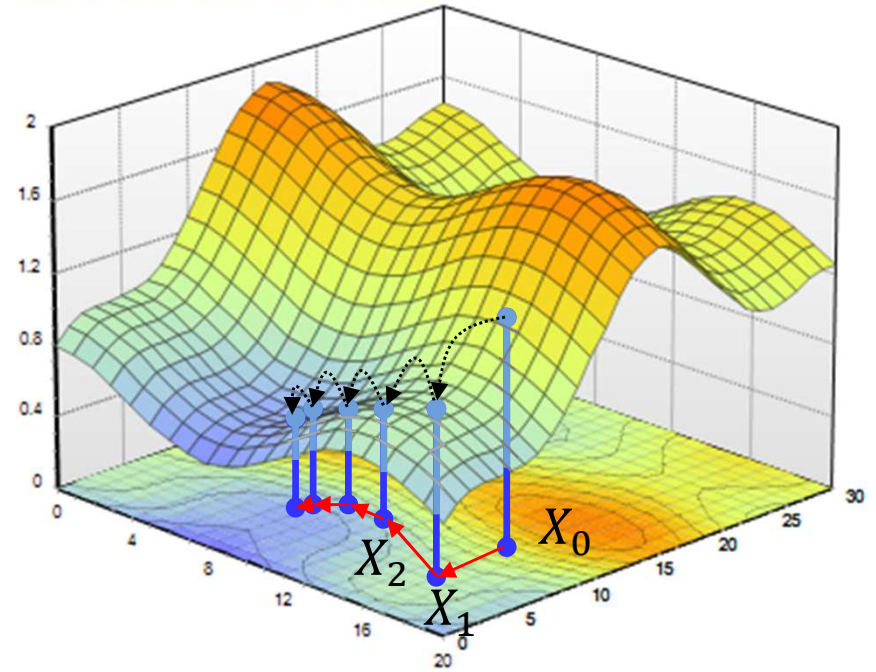
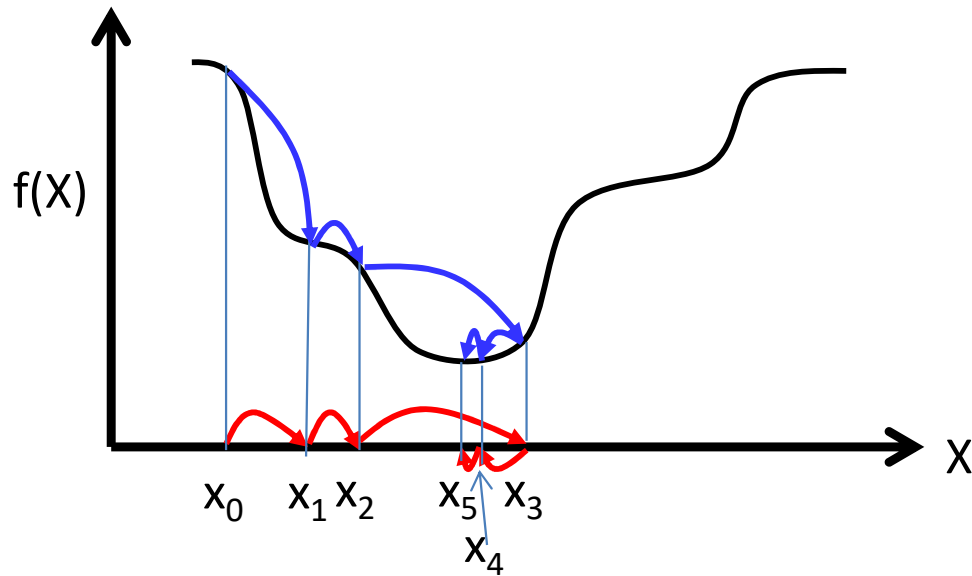
- The point  $x = \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} = \begin{bmatrix} -1 \\ -1 \\ -1 \end{bmatrix}$  is a minimum

# Closed Form Solutions are not always available



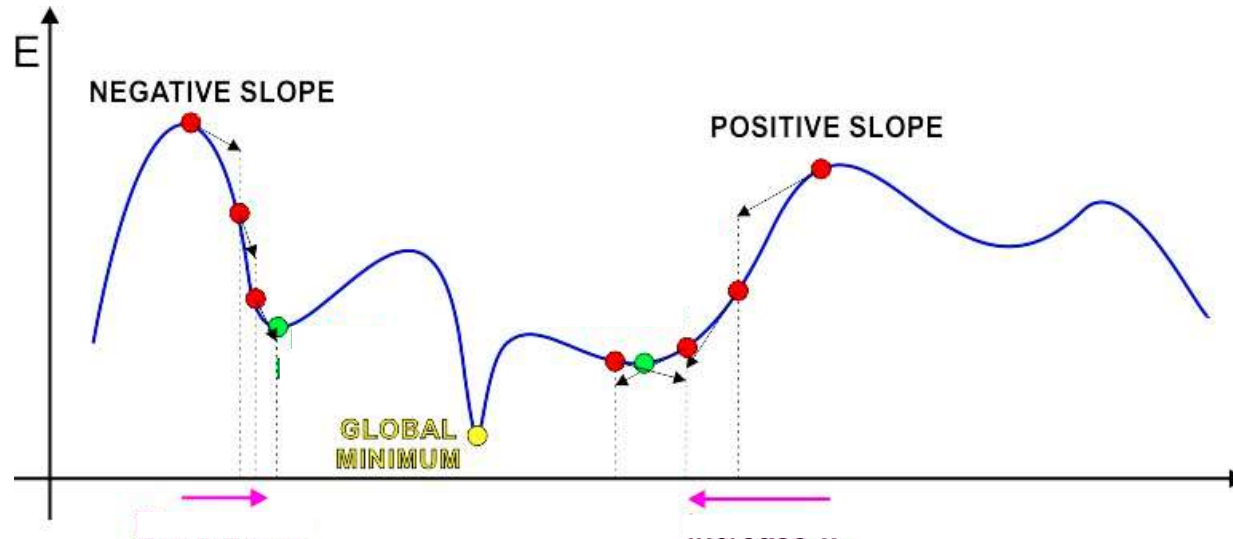
- Often it is not possible to simply solve  $\nabla_x f(X) = 0$ 
  - The function to minimize/maximize may have an intractable form
- In these situations, iterative solutions are used
  - Begin with a “guess” for the optimal  $X$  and refine it iteratively until the correct value is obtained

# Iterative solutions



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

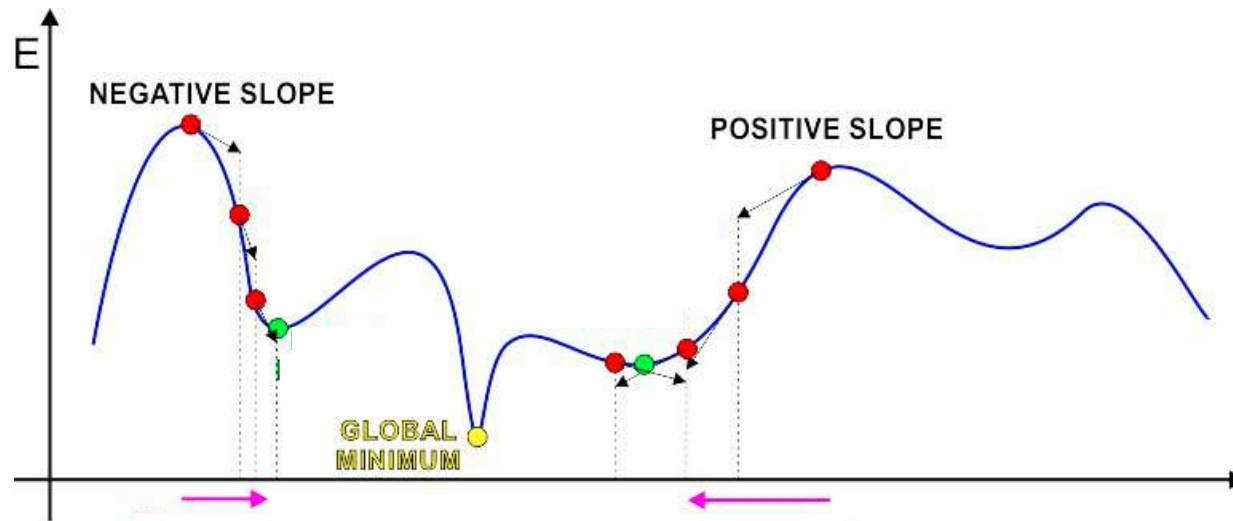
# The Approach of Gradient Descent



- 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  $\rightarrow$  moving right decreases error
      - A positive derivative  $\rightarrow$  moving left decreases error
  - Shift point in this direction

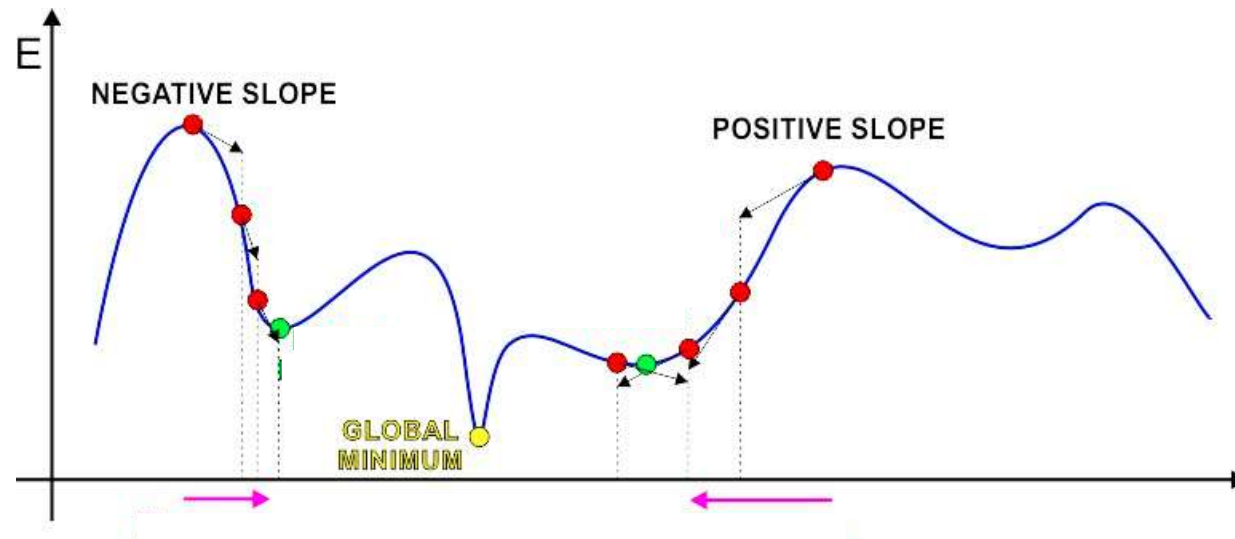


# The Approach of Gradient Descent



- Iterative solution: Trivial algorithm
  - Initialize  $x^0$
  - While  $f'(x^k) \neq 0$ 
    - If  $\text{sign}(f'(x^k))$  is positive:
$$x^{k+1} = x^k - \text{step}$$
    - Else
$$x^{k+1} = x^k + \text{step}$$
- What must step be to ensure we actually get to the optimum?

# The Approach of Gradient Descent



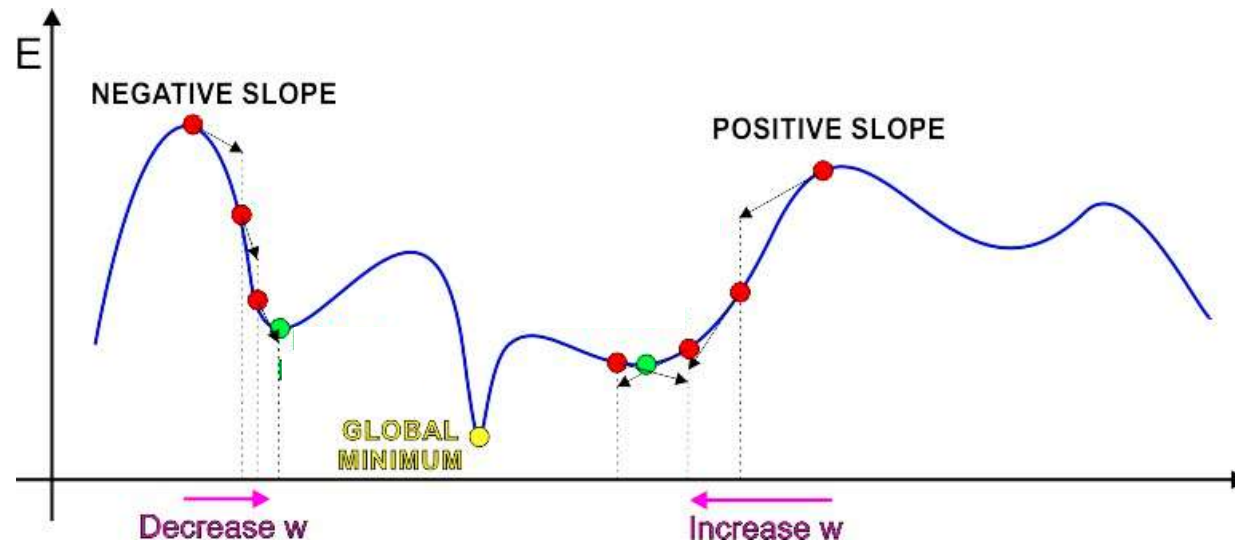
- Iterative solution: Trivial algorithm

- Initialize  $x^0$
- While  $f'(x^k) \neq 0$

$$x^{k+1} = x^k - \text{sign}(f'(x^k)) \cdot \text{step}$$

- Identical to previous algorithm

# The Approach of Gradient Descent



- Iterative solution: Trivial algorithm
  - Initialize  $x^0$
  - While  $f'(x^k) \neq 0$ 
$$x^{k+1} = x^k - \eta^k f'(x^k)$$
- $\eta^k$  is the “step size”

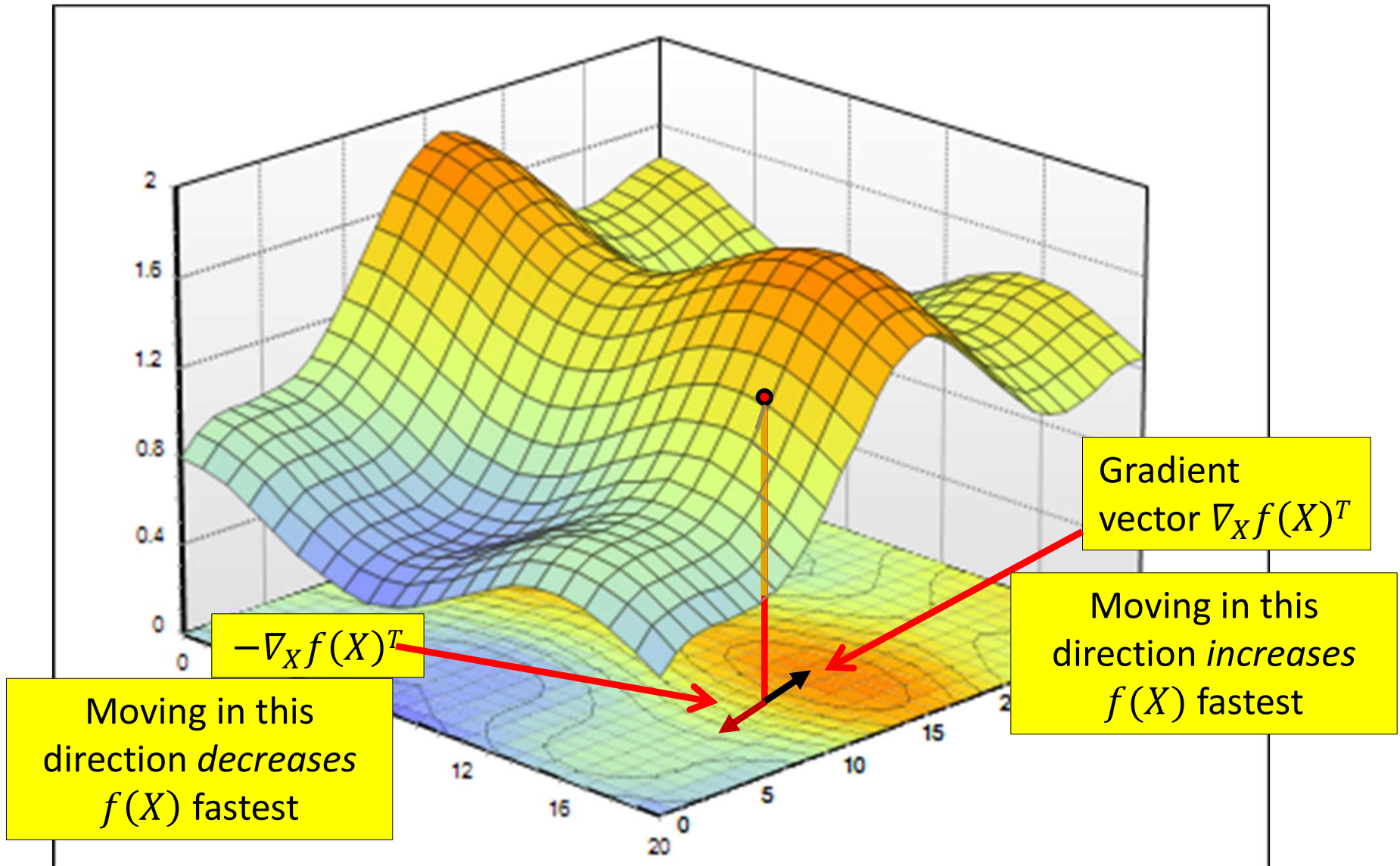
## Poll 3: Multivariate functions

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# Gradients of multivariate functions



# 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*

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

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

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

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

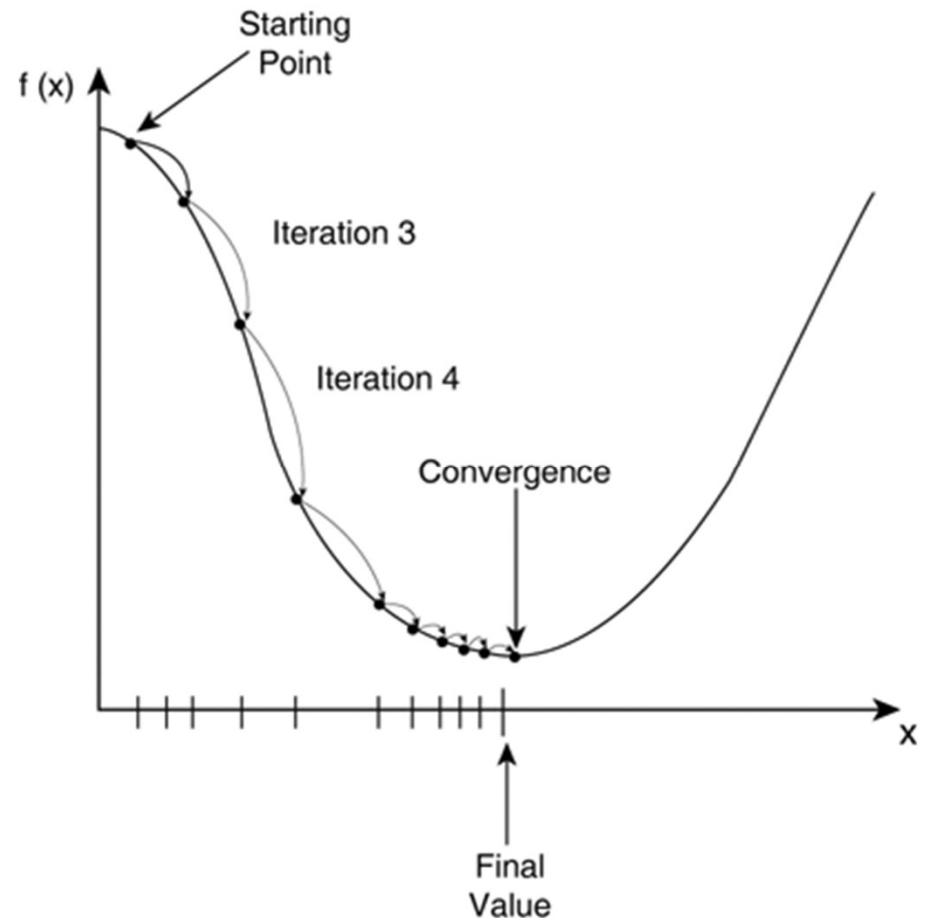
# Gradient descent convergence criteria

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

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

- Or

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

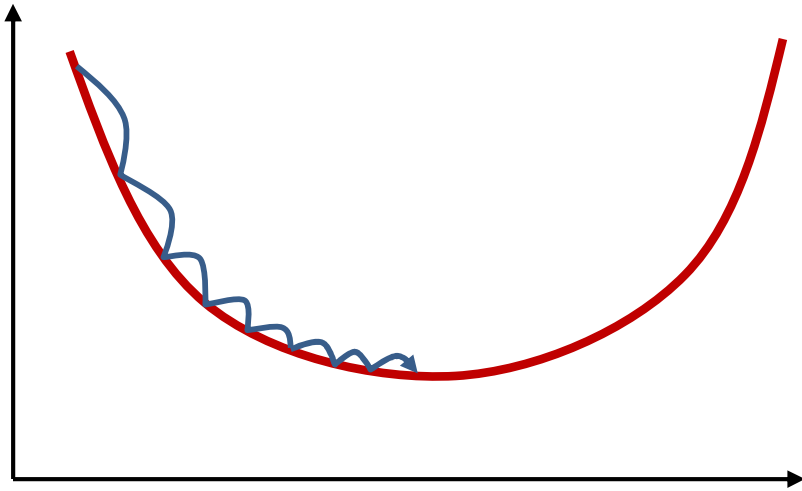




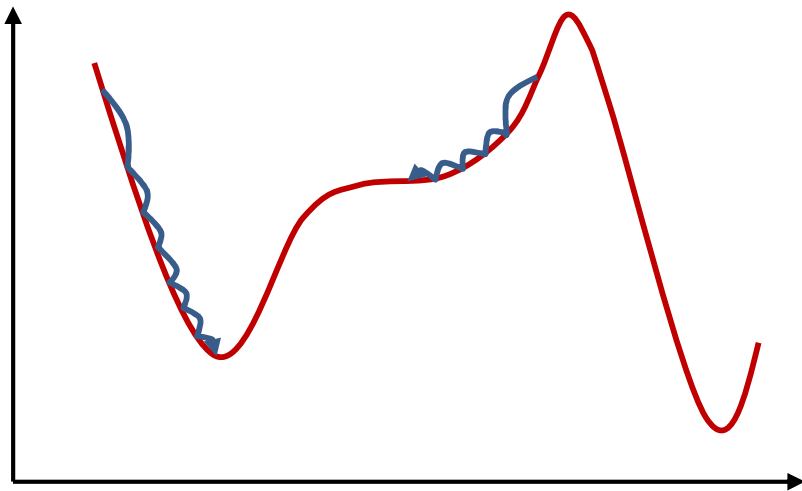
# Overall Gradient Descent Algorithm

- Initialize:
  - $x^0$
  - $k = 0$
- do
  - $x^{k+1} = x^k - \eta^k \nabla_x f(x^k)^T$
  - $k = k + 1$
- while  $|f(x^{k+1}) - f(x^k)| > \varepsilon$

# Convergence of Gradient Descent



- For appropriate step size, for convex (bowl-shaped) functions gradient descent will always find the minimum.



- For non-convex functions it will find a local minimum or an inflection point

## Poll 4

- $y = f(x)$  is a scalar function of an  $N \times 1$  column vector variable  $x$ . Starting from  $x = x_0$ , in which direction must we move in the space of  $x$ , to achieve the maximum decrease in  $f()$ ?
  - Exactly in the direction of the gradient of  $f(x)$  at  $x_0$
  - Exactly perpendicular to the direction of the gradient of  $f(x)$  at  $x_0$
  - Exactly opposite to the direction of the gradient of  $f(x)$  at  $x_0$
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  - **Exactly opposite to the direction of the gradient of  $f(x)$  at  $x_0$**
  - Exactly perpendicular to the direction of the gradient of  $f(x)$  at  $x_0$ .

- Returning to our problem from our detour..

# Problem Statement

- Given a training set of input-output pairs  $(X_1, d_1), (X_2, d_2), \dots, (X_T, d_T)$

- Minimize the following function

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

w.r.t  $W$

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

# Gradient Descent to train a network

- Initialize:

- $W^0$

- $k = 0$

do

- $W^{k+1} = W^k - \eta^k \nabla \text{Loss}(W^k)^T$

- $k = k + 1$

while  $|\text{Loss}(W^k) - \text{Loss}(W^{k-1})| > \varepsilon$

# Preliminaries

- Before we proceed: the problem setup



# Problem Setup: Things to define

- Given a training set of input-output pairs  $(X_1, d_1), (X_2, d_2), \dots, (X_T, d_T)$
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- Given a training set of input-output pairs  $(X_1, d_1), (X_2, d_2), \dots, (X_T, d_T)$

- What are these input-output pairs?

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What is  $f()$  and what are its parameters  $W$ ?

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What is the divergence  $div()$ ?

What is  $f()$  and what are its parameters  $W$ ?

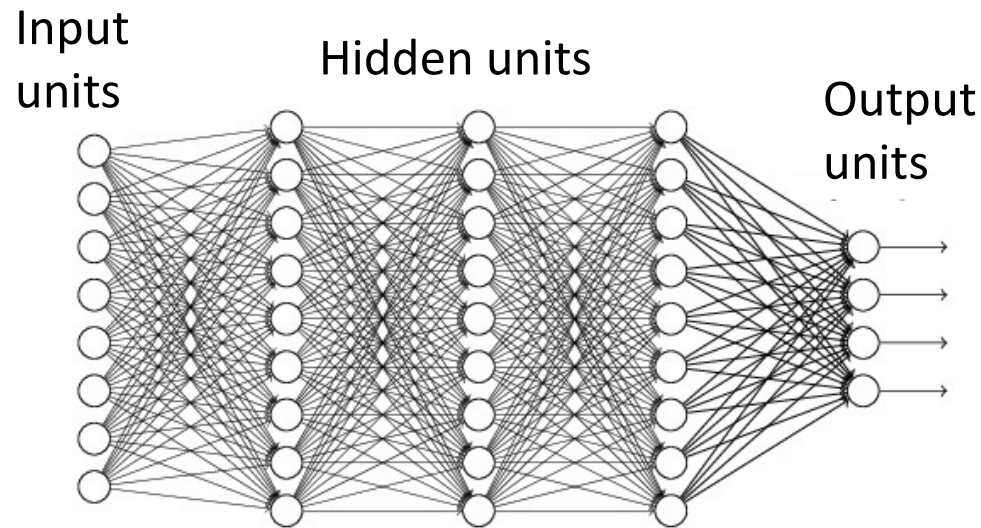
# Problem Setup: Things to define

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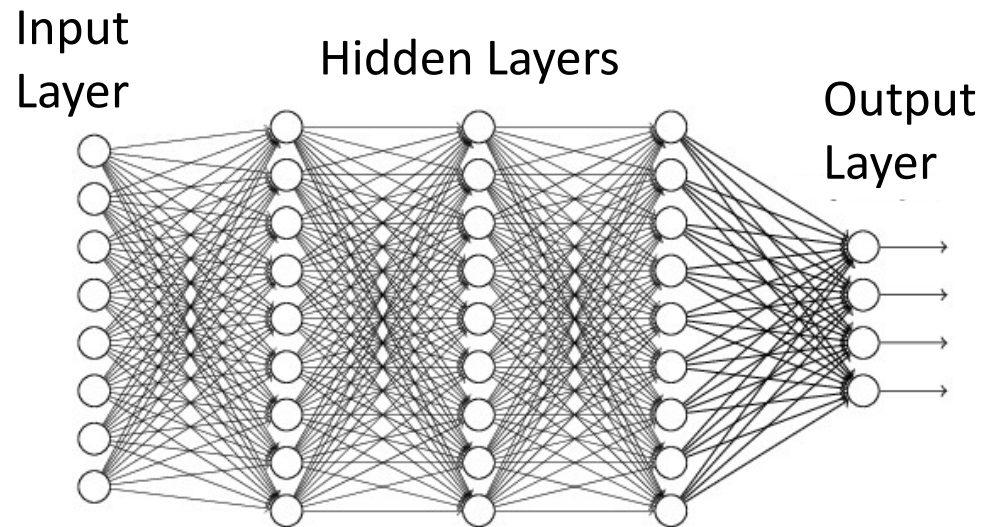
What is  $f()$  and what are its parameters  $W$ ?

# What is $f()$ ? Typical network



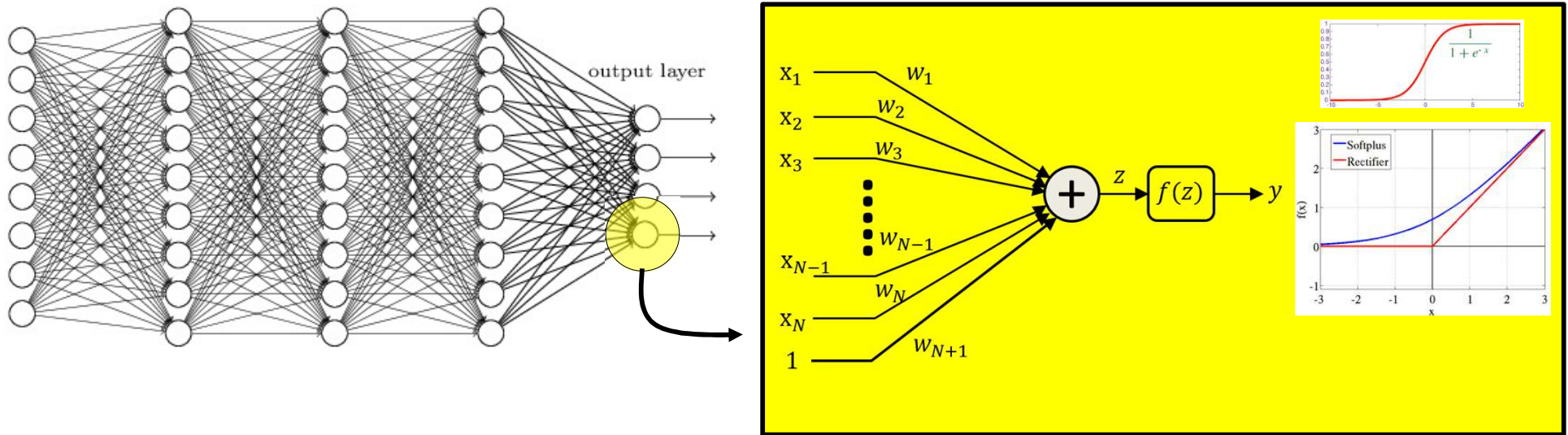
- Multi-layer perceptron
- A *directed* network with a set of inputs and outputs
  - No loops

# Typical network



- We assume a “layered” network for simplicity
  - Each “layer” of neurons only gets inputs from the earlier layer(s) and outputs signals only to later layer(s)
  - We will refer to the inputs as the **input layer**
    - No neurons here – the “layer” simply refers to inputs
  - We refer to the outputs as the **output layer**
  - Intermediate layers are **“hidden” layers**

# The individual neurons



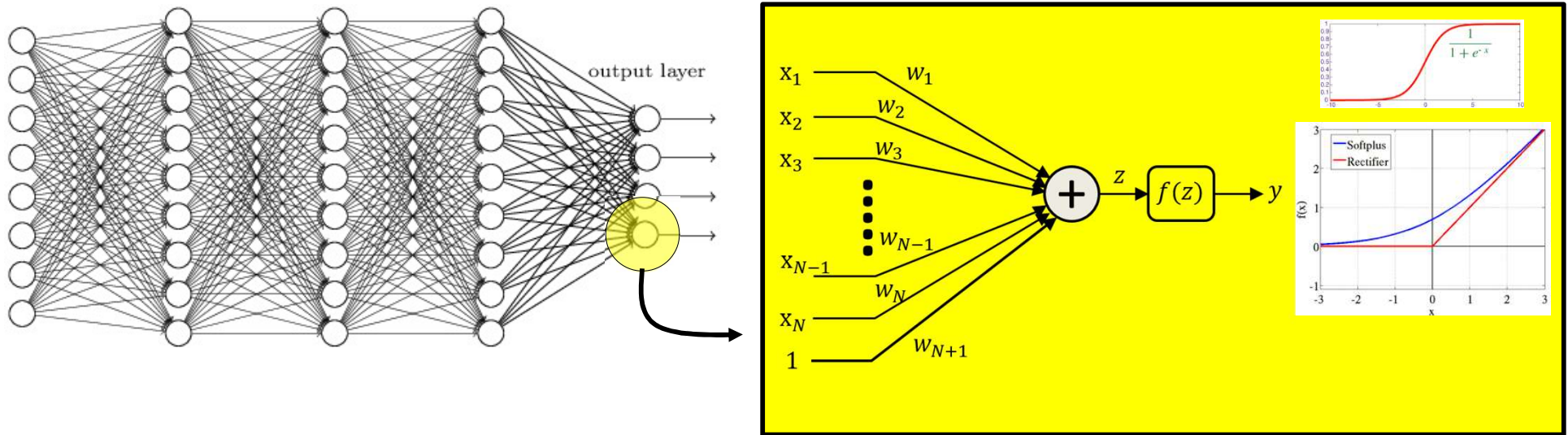
- Individual neurons operate on a set of inputs and produce a single output
  - **Standard setup:** A continuous activation function applied to an affine function of the inputs

$$y = f\left(\sum_i w_i x_i + b\right)$$

- More generally: *any* differentiable function
$$y = f(x_1, x_2, \dots, x_N; W)$$



# The individual neurons



- Individual neurons operate on a set of inputs and produce a single output
  - **Standard setup:** A continuous activation function applied to an affine function of the inputs

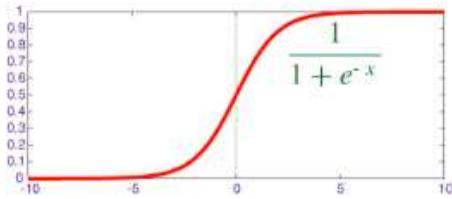
$$y = f\left(\sum_i w_i x_i + b\right)$$

- More generally: *any* differentiable function
$$y = f(x_1, x_2, \dots, x_N; W)$$

We will assume this unless otherwise specified

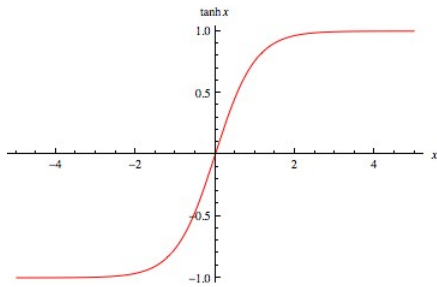
Parameters are weights  $w_i$  and bias  $b$

# Activations and their derivatives



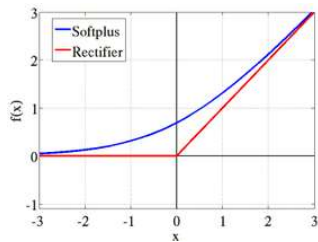
$$f(z) = \frac{1}{1 + \exp(-z)}$$

$$f'(z) = f(z)(1 - f(z))$$



$$f(z) = \tanh(z)$$

$$f'(z) = (1 - f^2(z))$$



$$f(z) = \begin{cases} z, & z \geq 0 \\ 0, & z < 0 \end{cases}$$

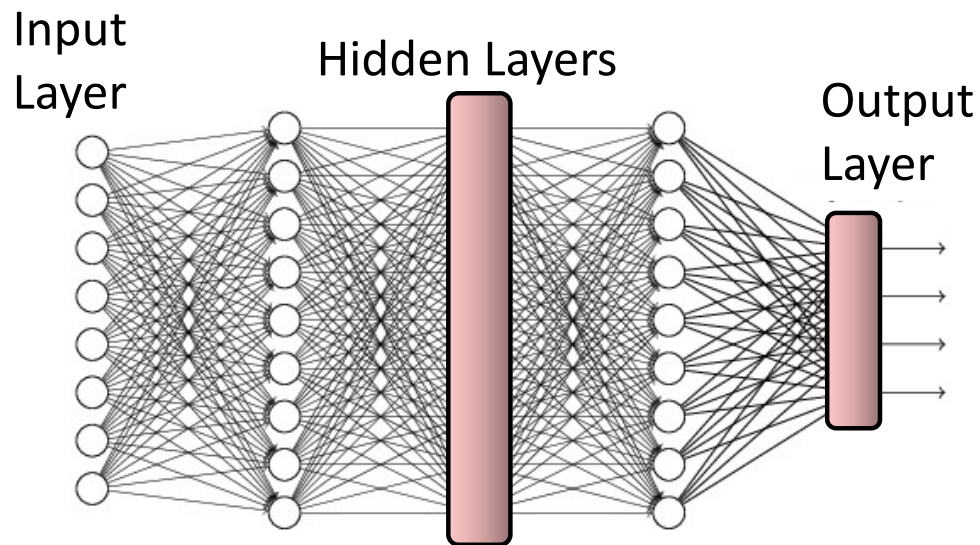
$$[*] \quad f'(z) = \begin{cases} 1, & z \geq 0 \\ 0, & z < 0 \end{cases}$$

$$f(z) = \log(1 + \exp(z))$$

$$f'(z) = \frac{1}{1 + \exp(-z)}$$

- Some popular activation functions and their derivatives

# Vector Activations

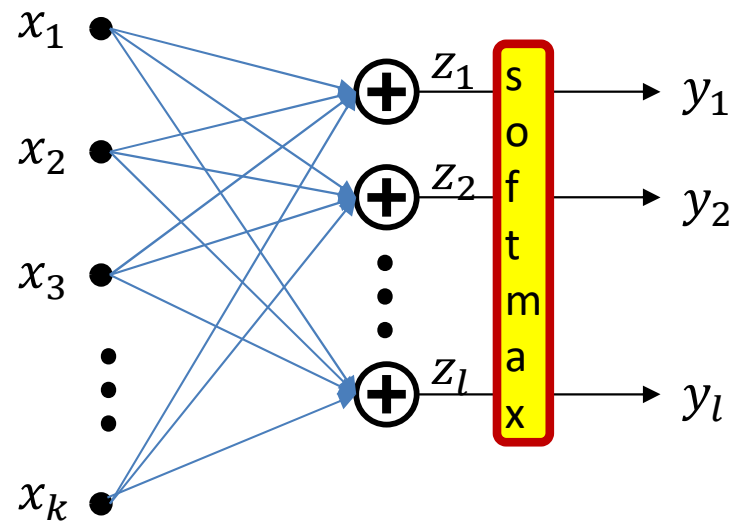


- We can also have neurons that have *multiple coupled* outputs

$$[y_1, y_2, \dots, y_l] = f(x_1, x_2, \dots, x_k; W)$$

- Function  $f()$  operates on set of inputs to produce set of outputs
- Modifying a single parameter in  $W$  will affect *all* outputs

# Vector activation example: Softmax



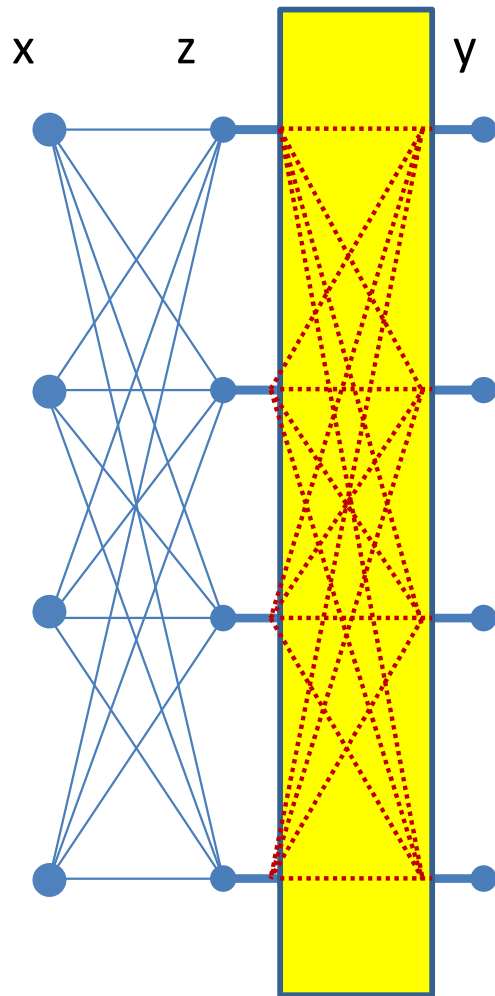
- Example: Softmax *vector* activation

$$z_i = \sum_j w_{ji} x_j + b_i$$

$$y = \frac{\exp(z_i)}{\sum_j \exp(z_j)}$$

Parameters are weights  $w_{ji}$  and bias  $b_i$

# Multiplicative combination: Can be viewed as a case of vector activations



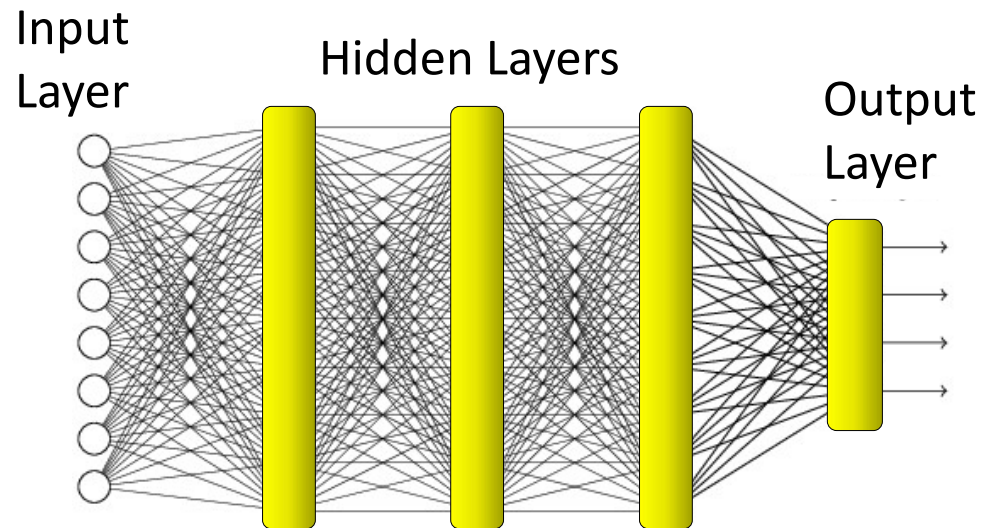
$$z_i = \sum_j w_{ji} x_j + b_i$$

$$y_i = \prod_l (z_l)^{\alpha_{li}}$$

Parameters are  
weights  $w_{ji}$   
and bias  $b_i$

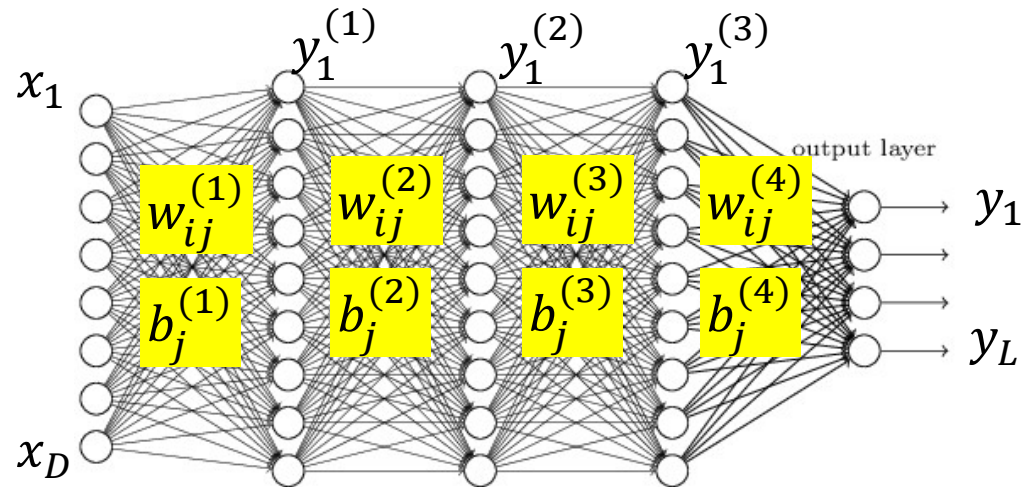
- A layer of multiplicative combination is a special case of vector activation

# Typical network



- In a layered network, each layer of perceptrons can be viewed as a single vector activation

# Notation



- The input layer is the 0<sup>th</sup> layer
- We will represent the output of the  $i$ -th perceptron of the  $k$ <sup>th</sup> layer as  $y_i^{(k)}$ 
  - **Input to network:**  $y_i^{(0)} = x_i$
  - **Output of network:**  $y_i = y_i^{(N)}$
- We will represent the weight of the connection between the  $i$ -th unit of the  $k$ -1th layer and the  $j$ th unit of the  $k$ -th layer as  $w_{ij}^{(k)}$ 
  - The bias to the  $j$ th unit of the  $k$ -th layer is  $b_j^{(k)}$

# Problem Setup: Things to define

- Given a training set of input-output pairs  $(X_1, d_1), (X_2, d_2), \dots, (X_T, d_T)$
- Minimize the following function

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



What is  $f()$  and what are its parameters  $W$ ?



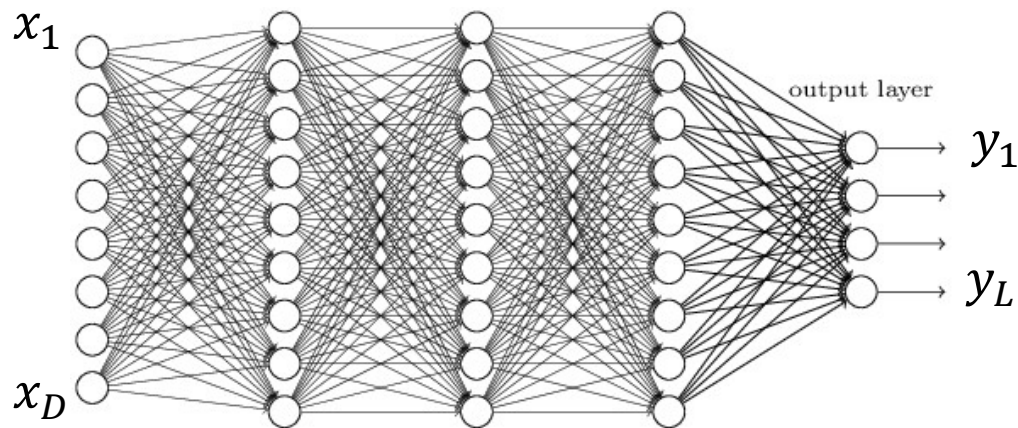
# Problem Setup: Things to define

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- What are these input-output pairs?

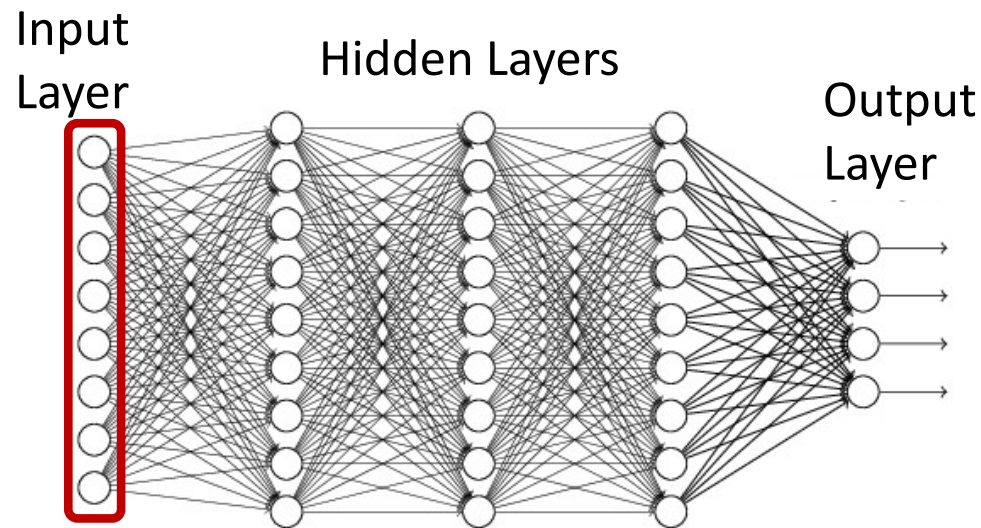
$$Loss(W) = \frac{1}{T} \sum_i div(f(X_i; W), d_i)$$

# Input, target output, and actual output: Vector notation



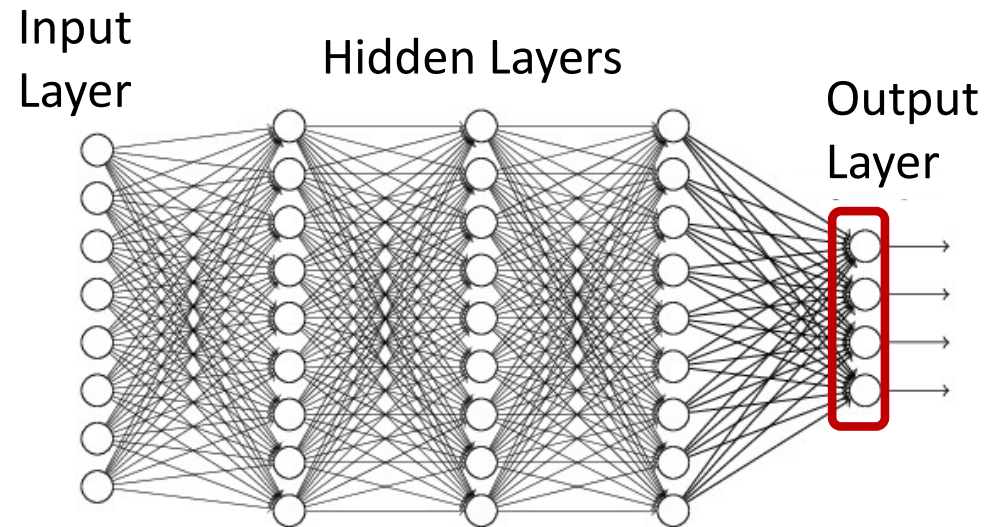
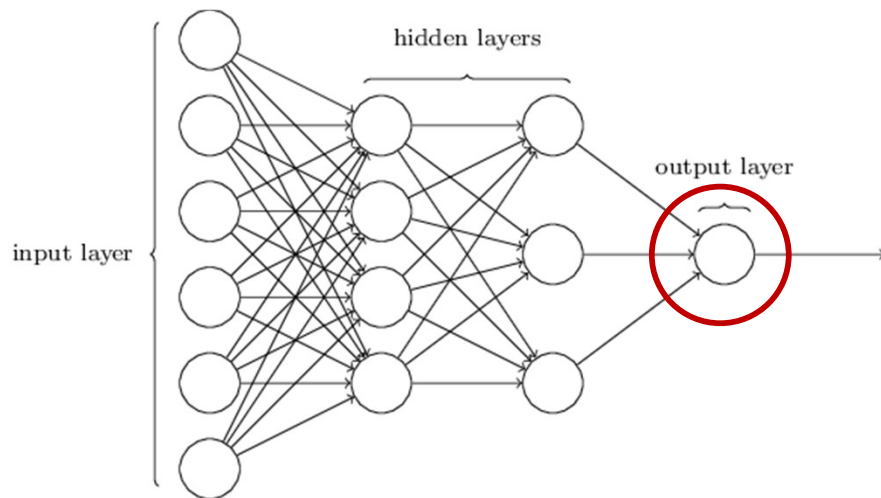
- Given a training set of input-output pairs  $(X_1, d_1), (X_2, d_2), \dots, (X_T, d_T)$
- $X_n = [x_{n1}, x_{n2}, \dots, x_{nD}]^T$  is the  $n$ th input vector
- $d_n = [d_{n1}, d_{n2}, \dots, d_{nL}]^T$  is the  $n$ th desired output
- $Y_n = [y_{n1}, y_{n2}, \dots, y_{nL}]^T$  is the  $n$ th vector of *actual* outputs of the network
  - Function of input  $X_n$  and network parameters
- We will sometimes drop the first subscript when referring to a *specific* instance

# Representing the input



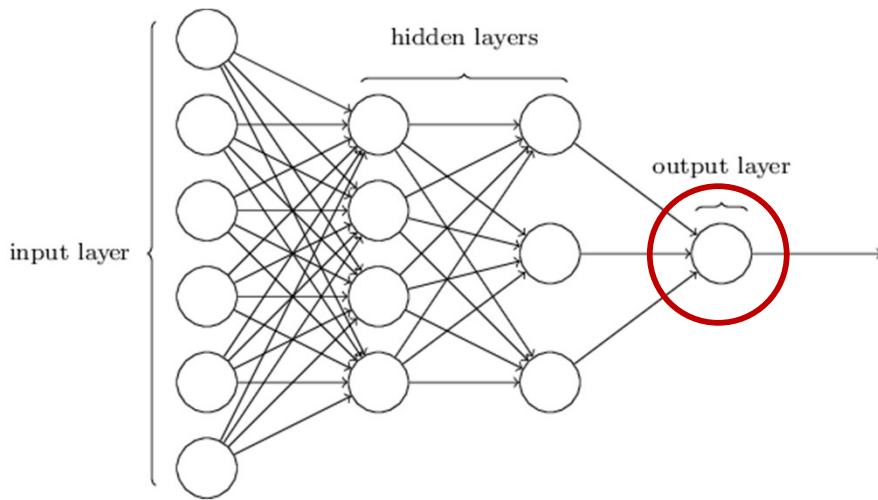
- Vectors of numbers
  - (or may even be just a scalar, if input layer is of size 1)
  - E.g. vector of pixel values
  - E.g. vector of speech features
  - E.g. real-valued vector representing text
    - We will see how this happens later in the course
  - Other real valued vectors

# Representing the **output**



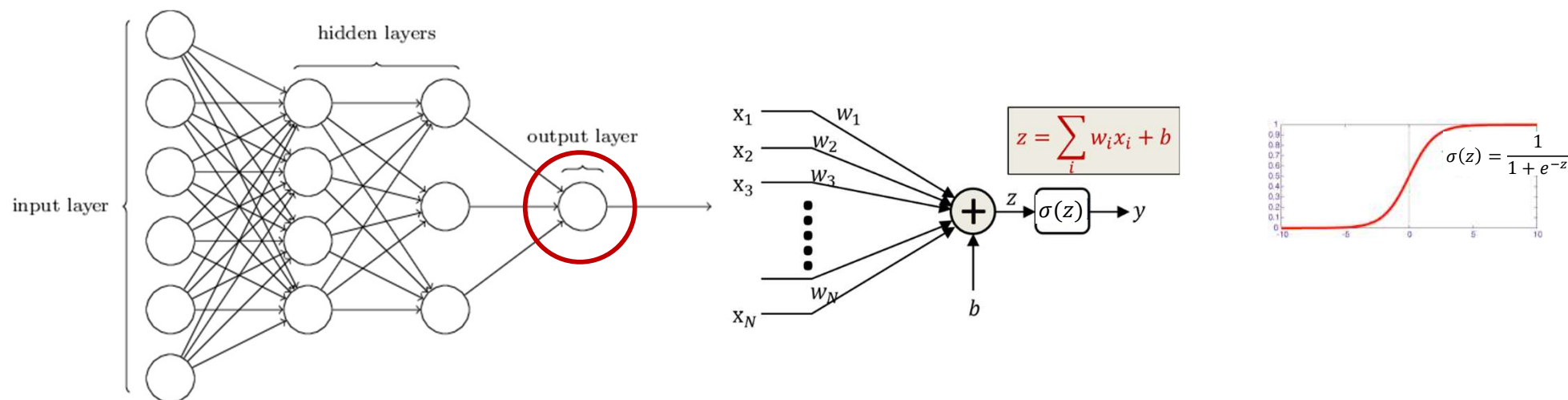
- If the desired *output* is **real-valued**, no special tricks are necessary
  - Scalar Output : single output neuron
    - $d = \text{scalar (real value)}$
  - Vector Output : as many output neurons as the dimension of the desired output
    - $d = [d_1 \ d_2 \ .. \ d_L]$  (vector of real values)

# Representing the output



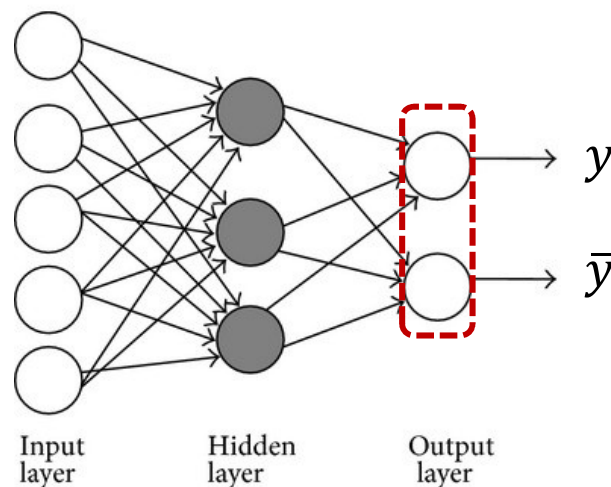
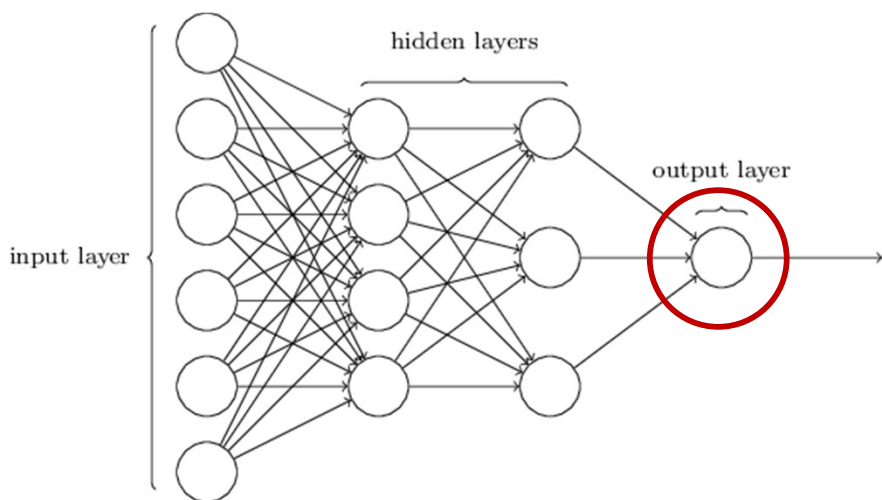
- If the desired output is **binary** (is this a cat or not), use a simple 1/0 representation of the desired output
  - 1 = Yes it's a cat
  - 0 = No it's not a cat.

# Representing the output



- If the desired output is binary (is this a cat or not), use a simple 1/0 representation of the desired output
- Output activation: Typically a sigmoid
  - Viewed as the *probability*  $P(Y = 1|X)$  of class value 1
    - Indicating the fact that for actual data, in general a feature value  $X$  may occur for both classes, but with different probabilities
    - Is differentiable

# Representing the output



- If the desired output is binary (is this a cat or not), use a simple 1/0 representation of the desired output
  - 1 = Yes it's a cat
  - 0 = No it's not a cat.
- Sometimes represented by *two* outputs, one representing the desired output, the other representing the *negation* of the desired output
  - Yes:  $\rightarrow [1 \ 0]$
  - No:  $\rightarrow [0 \ 1]$
- The output explicitly becomes a 2-output softmax



# Multi-class output: One-hot representations

- Consider a network that must distinguish if an input is a cat, a dog, a camel, a hat, or a flower
- We can represent this set as the following vector, with the classes arranged in a chosen order:

[cat dog camel hat flower]<sup>T</sup>

- For inputs of each of the five classes the desired output is:

cat: [1 0 0 0 0]<sup>T</sup>

dog: [0 1 0 0 0]<sup>T</sup>

camel: [0 0 1 0 0]<sup>T</sup>

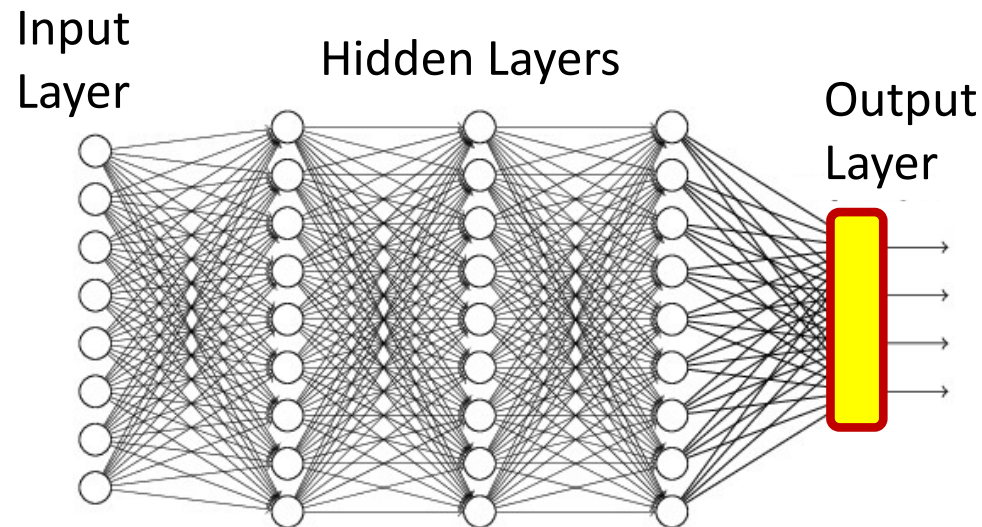
hat: [0 0 0 1 0]<sup>T</sup>

flower: [0 0 0 0 1]<sup>T</sup>

- For an input of any class, we will have a five-dimensional vector output with four zeros and a single 1 at the position of that class
- This is a *one hot vector*

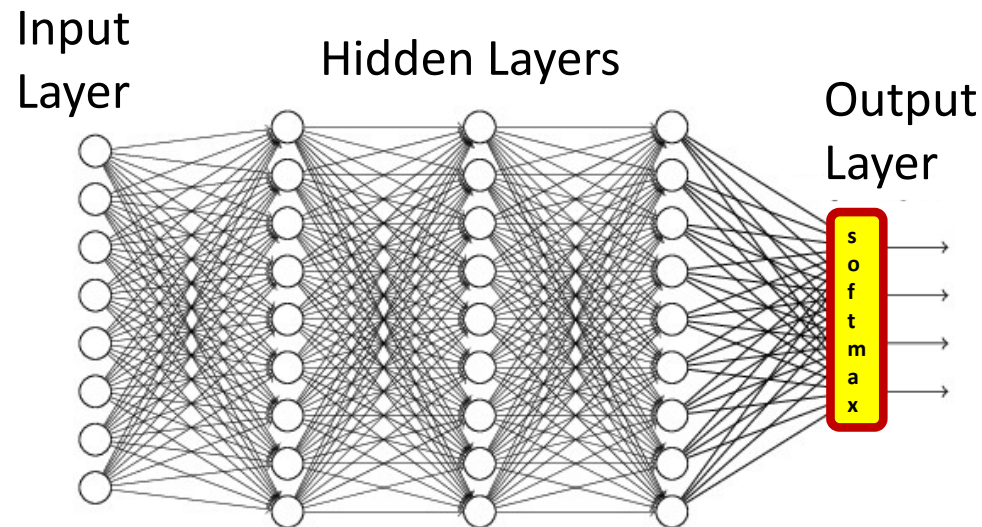


# Multi-class networks



- For a multi-class classifier with  $N$  classes, the one-hot representation will have  $N$  binary target outputs
  - The **desired** output  $d$  is an  $N$ -dimensional binary vector
- The neural network's **actual** output too must ideally be binary ( $N-1$  zeros and a single 1 in the right place)
- More realistically, it will be a probability vector
  - $N$  probability values that sum to 1.

# Multi-class classification: Output



- Softmax *vector* activation is often used at the output of multi-class classifier nets

$$z_i = \sum_j w_{ji}^{(n)} y_j^{(n-1)}$$

$$y_i = \frac{\exp(z_i)}{\sum_j \exp(z_j)}$$

- This can be viewed as the probability  $y_i = P(\text{class} = i|X)$

# Inputs and outputs:

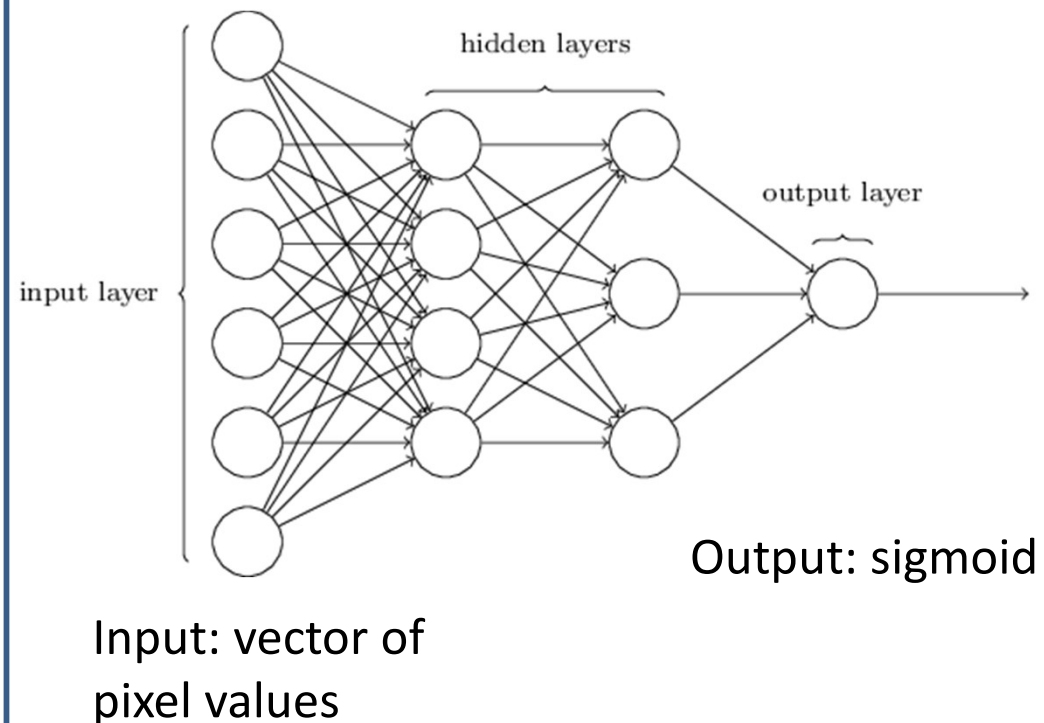
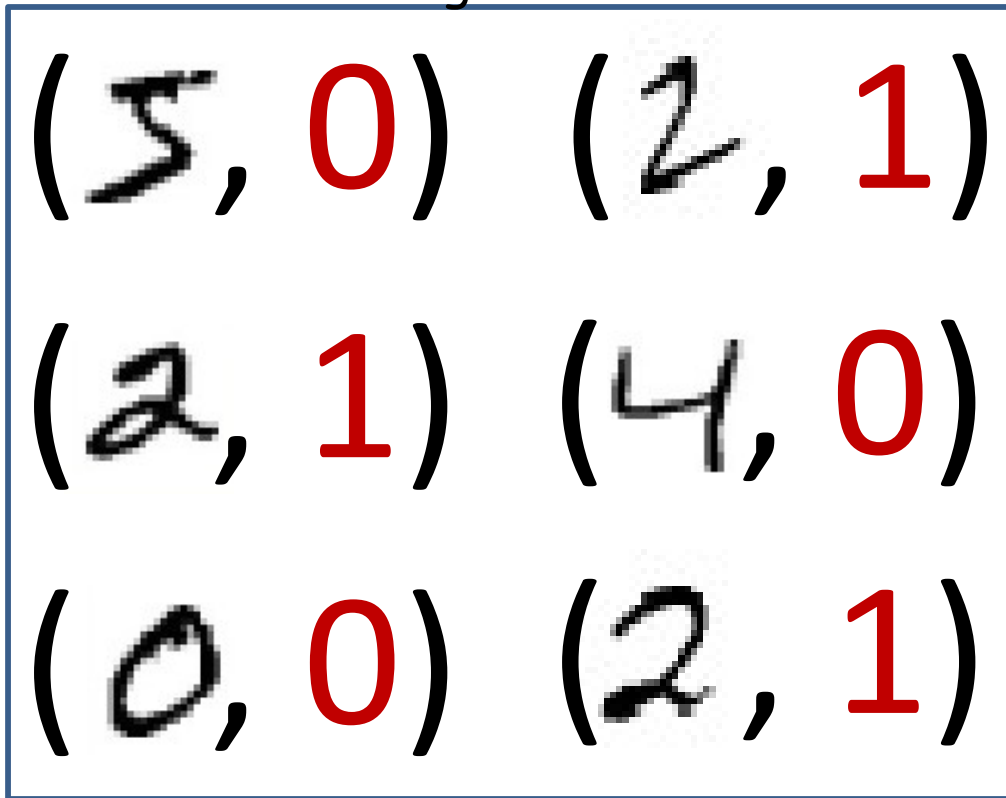
## Typical Problem Statement



- We are given a number of “training” data instances
- E.g. images of digits, along with information about which digit the image represents
- Tasks:
  - Binary recognition: Is this a “2” or not
  - Multi-class recognition: Which digit is this?

# Typical Problem statement: binary classification

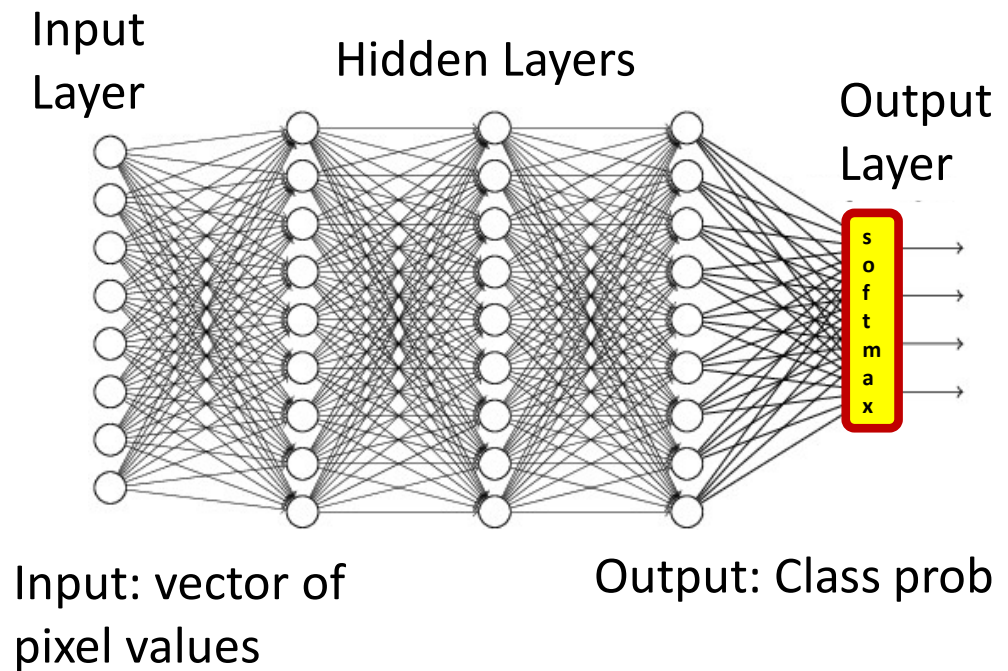
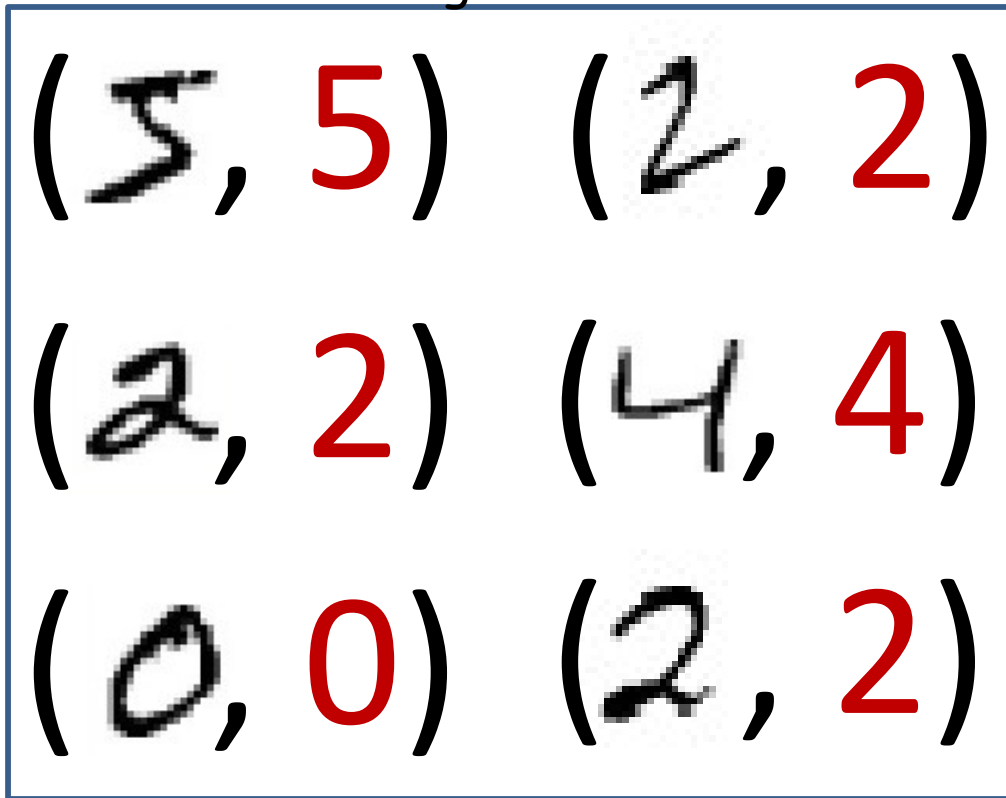
Training data



- Given, many positive and negative examples (training data),
  - learn all weights such that the network does the desired job

# Typical Problem statement: multiclass classification

Training data



- Given, many positive and negative examples (training data),
  - learn all weights such that the network does the desired job

# Problem Setup: Things to define

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- Minimize the following function

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

What is the  
divergence  $div()$ ?

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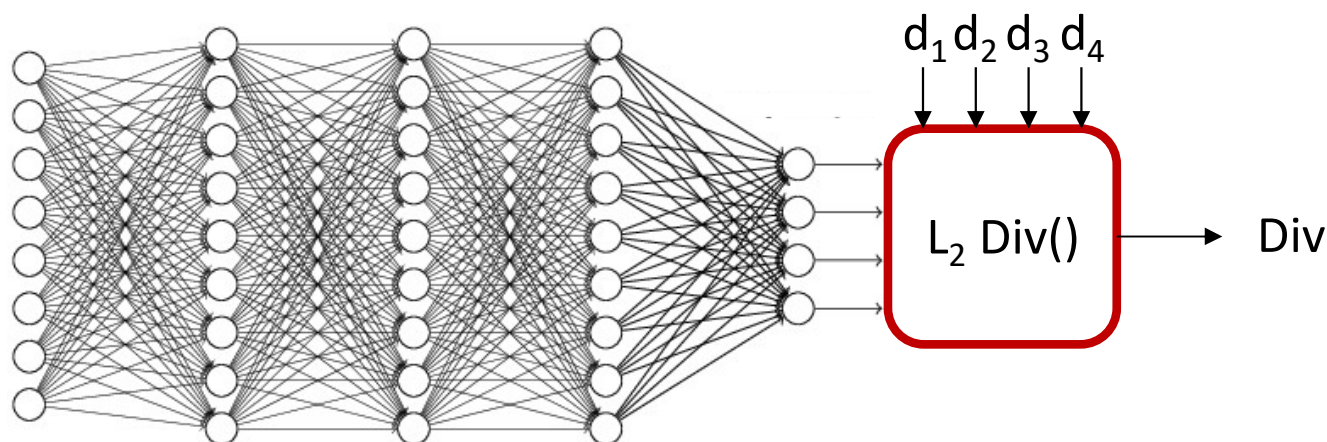
$$Loss(W) = \frac{1}{T} \sum_i div(f(X_i; W), d_i)$$

What is the divergence  $div()$ ?

Note: For  $Loss(W)$  to be differentiable w.r.t  $W$ ,  $div()$  must be differentiable



# Examples of divergence functions



- For real-valued output vectors, the (scaled)  $L_2$  divergence is popular

$$\text{Div}(Y, d) = \frac{1}{2} \|Y - d\|^2 = \frac{1}{2} \sum_i (y_i - d_i)^2$$

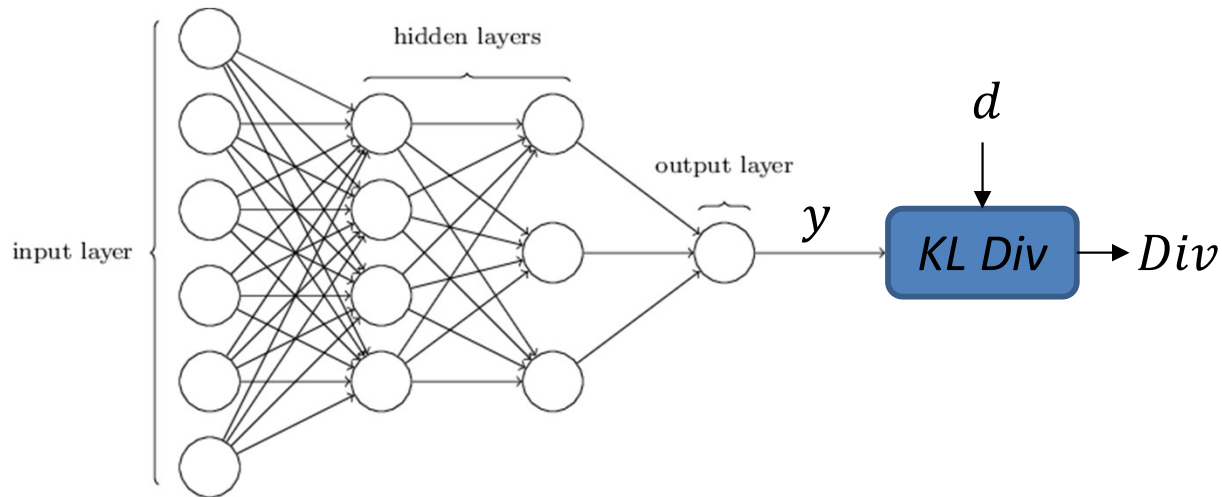
- Squared Euclidean distance between true and desired output
- Note: this is differentiable

$$\frac{d\text{Div}(Y, d)}{dy_i} = (y_i - d_i)$$

$$\nabla_Y \text{Div}(Y, d) = [y_1 - d_1, y_2 - d_2, \dots]$$



# For binary classifier



- For binary classifier with scalar output,  $Y \in (0,1)$ ,  $d$  is 0/1, the Kullback Leibler (KL) divergence between the probability distribution  $[Y, 1 - Y]$  and the ideal output probability  $[d, 1 - d]$  is popular

$$Div(Y, d) = -d \log Y - (1 - d) \log(1 - Y)$$

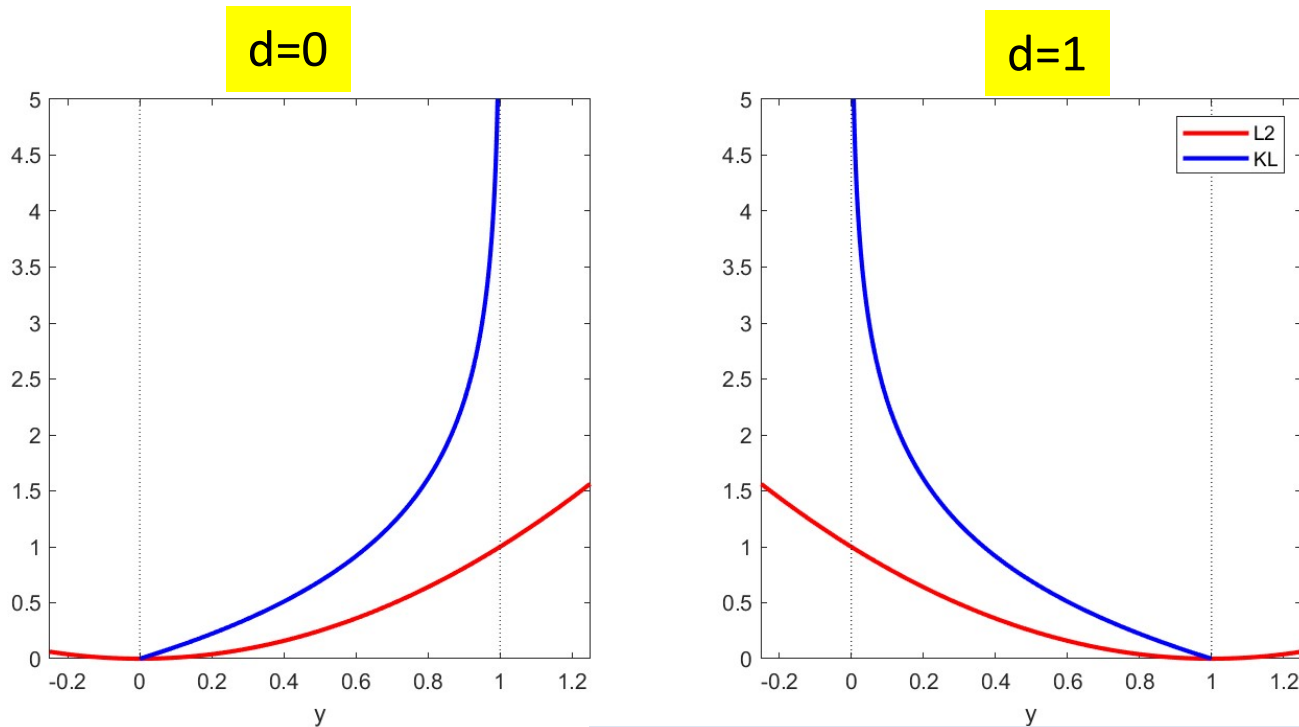
– Minimum when  $d = Y$

- Derivative

$$\frac{dDiv(Y, d)}{dY} = \begin{cases} -\frac{1}{Y} & \text{if } d = 1 \\ \frac{1}{1 - Y} & \text{if } d = 0 \end{cases}$$

$$\frac{dKLDiv(Y, d)}{dY} = \begin{cases} -\frac{1}{Y} & \text{if } d = 1 \\ \frac{1}{1-Y} & \text{if } d = 0 \end{cases}$$

# KL vs L2

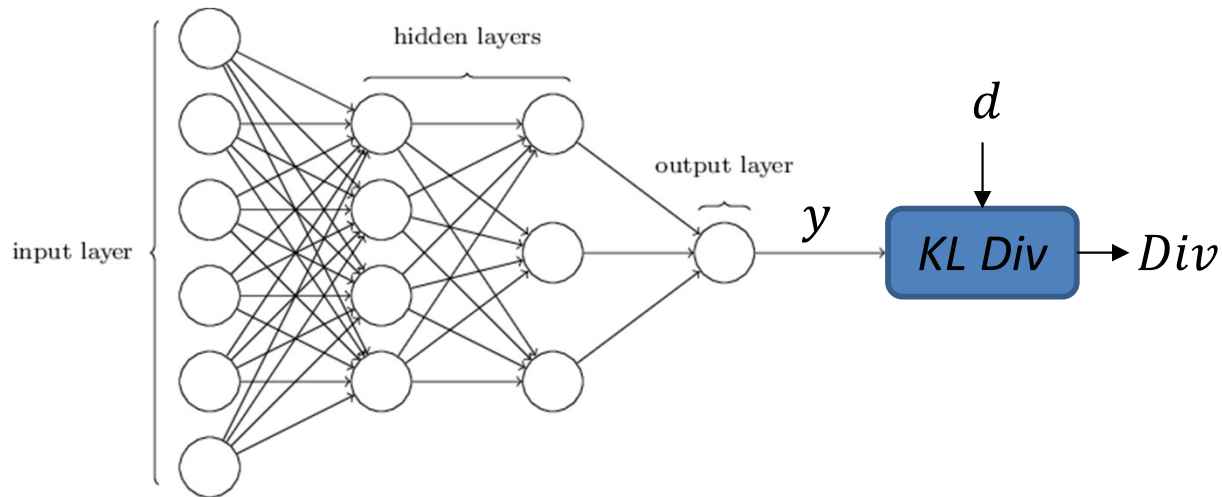


$$L2(Y, d) = (y - d)^2$$

$$KL(Y, d) = -d \log Y - (1 - d) \log(1 - Y)$$

- Both KL and L2 have a minimum when  $y$  is the target value of  $d$
- KL rises much more steeply away from  $d$ 
  - Encouraging faster convergence of gradient descent
- The derivative of KL is *not* equal to 0 at the minimum
  - It is 0 for L2, though

# For binary classifier



- For binary classifier with scalar output,  $Y \in (0,1)$ ,  $d$  is 0/1, the Kullback Leibler (KL) divergence between the probability distribution  $[Y, 1 - Y]$  and the ideal output probability  $[d, 1 - d]$  is popular

$$Div(Y, d) = -d \log Y - (1 - d) \log(1 - Y)$$

– Minimum when  $d = Y$

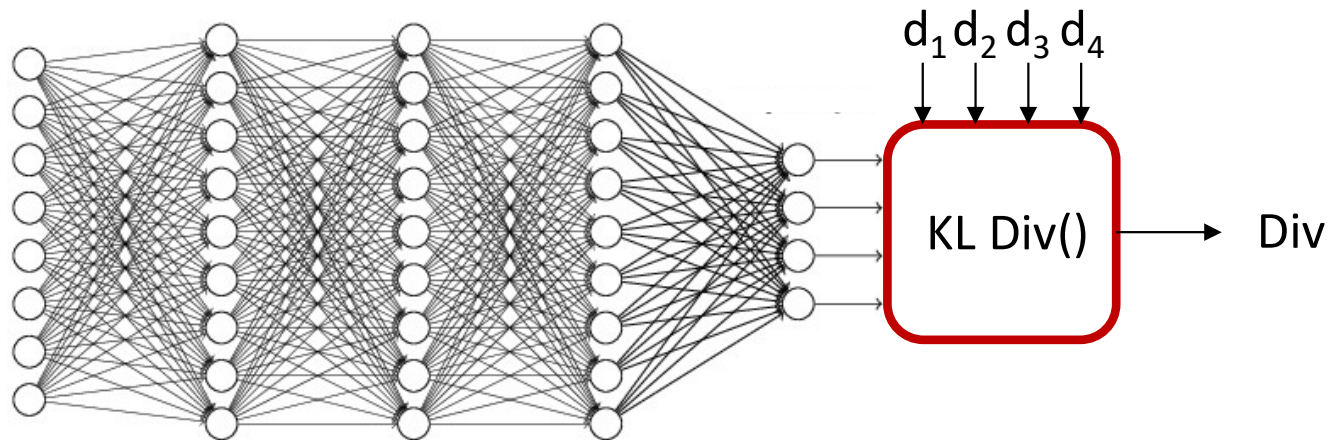
- Derivative

$$\frac{dDiv(Y, d)}{dY} = \begin{cases} -\frac{1}{Y} & \text{if } d = 1 \\ \frac{1}{1 - Y} & \text{if } d = 0 \end{cases}$$

Note: when  $y = d$  the derivative is *not* 0

*Even though  $div() = 0$  (minimum) when  $y = d$*

# For multi-class classification



- Desired output  $d$  is a one hot vector  $[0 \ 0 \ \dots \ 1 \ \dots \ 0 \ 0 \ 0]$  with the 1 in the  $c$ -th position (for class  $c$ )
- Actual output will be probability distribution  $[y_1, y_2, \dots]$
- The KL divergence between the desired one-hot output and actual output:

$$Div(Y, d) = \sum_i d_i \log \frac{d_i}{y_i} = \sum_i d_i \log d_i - \sum_i d_i \log y_i = -\log y_c$$

- Derivative

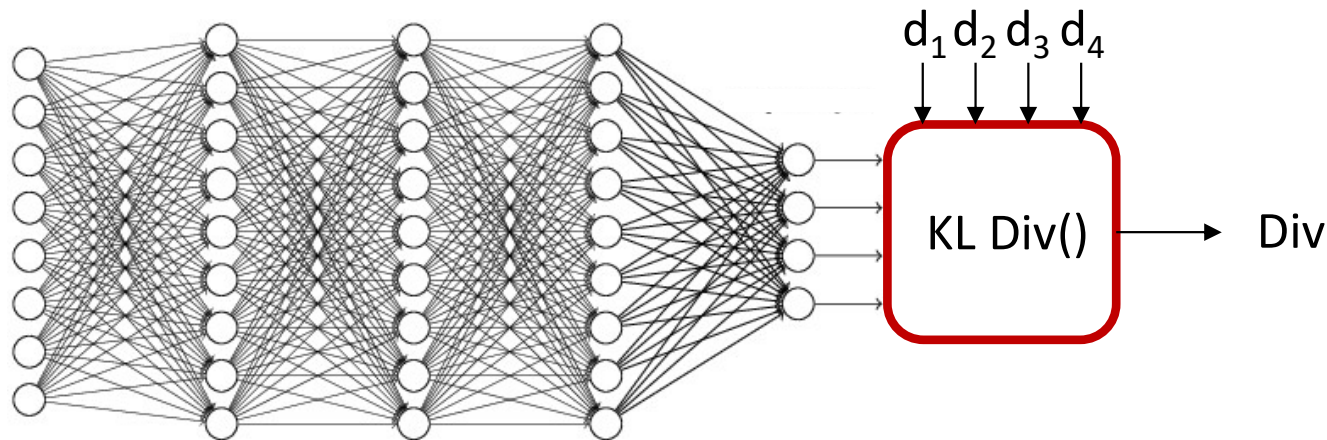
$$\frac{dDiv(Y, d)}{dY_i} = \begin{cases} -\frac{1}{y_c} & \text{for the } c\text{-th component} \\ 0 & \text{for remaining component} \end{cases}$$

$$\nabla_Y Div(Y, d) = \begin{bmatrix} 0 & 0 & \dots & -\frac{1}{y_c} & \dots & 0 & 0 \end{bmatrix}$$

The slope is negative  
w.r.t.  $y_c$

Indicates *increasing*  $y_c$   
will *reduce* divergence

# For multi-class classification



- Desired output  $d$  is a one hot vector  $[0 \ 0 \ \dots \ 1 \ \dots \ 0 \ 0 \ 0]$  with the 1 in the  $c$ -th position (for class  $c$ )
- Actual output will be probability distribution  $[y_1, y_2, \dots]$
- The KL divergence between the desired one-hot output and actual output:

$$Div(Y, d) = \sum_i d_i \log d_i - \sum_i d_i \log y_i = 0 - \log y_c = -\log y_c$$

Note: when  $y = d$  the derivative is *not* 0

*Even though  $div() = 0$  (minimum) when  $y = d$*

$$\frac{dDiv(Y, d)}{dY_i} = \begin{cases} -\frac{1}{y_c} & \text{for the } c\text{-th component} \\ 0 & \text{for remaining component} \end{cases}$$

$$\nabla_Y Div(Y, d) = \left[ 0 \ 0 \ \dots \ -\frac{1}{y_c} \ \dots \ 0 \ 0 \right]$$

The slope is negative w.r.t.  $y_c$

Indicates *increasing*  $y_c$  will *reduce* divergence

# KL divergence vs cross entropy

- KL divergence between  $d$  and  $y$ :

$$KL(Y, d) = \sum_i d_i \log d_i - \sum_i d_i \log y_i$$

- *Cross-entropy* between  $d$  and  $y$ :

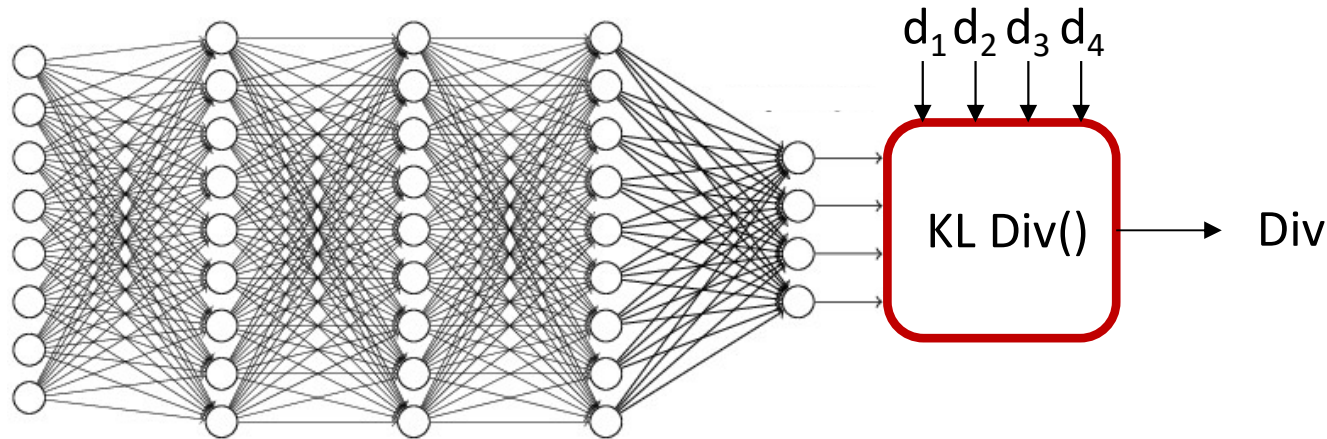
$$Xent(Y, d) = - \sum_i d_i \log y_i$$

- The cross entropy is merely the KL - entropy of  $d$

$$Xent(Y, d) = KL(Y, d) - \sum_i d_i \log d_i = KL(Y, d) - H(d)$$

- The  $W$  that minimizes cross-entropy will minimize the KL divergence
  - since  $d$  is the desired output and does not depend on the network,  $H(d)$  does not depend on the net
  - In fact, for one-hot  $d$ ,  $H(d) = 0$  (and  $KL = Xent$ )
- We will generally minimize to the *cross-entropy* loss rather than the KL divergence
  - The  $Xent$  is *not* a divergence, and although it attains its minimum when  $y = d$ , its minimum value is not 0

# “Label smoothing”



- It is sometimes useful to set the target output to  $[\epsilon \ \epsilon \ \dots (1 - (K - 1)\epsilon) \ \dots \epsilon \ \epsilon \ \epsilon]$  with the value  $1 - (K - 1)\epsilon$  in the  $c$ -th position (for class  $c$ ) and  $\epsilon$  elsewhere for some small  $\epsilon$ 
  - “Label smoothing” -- aids gradient descent
- The KL divergence remains:

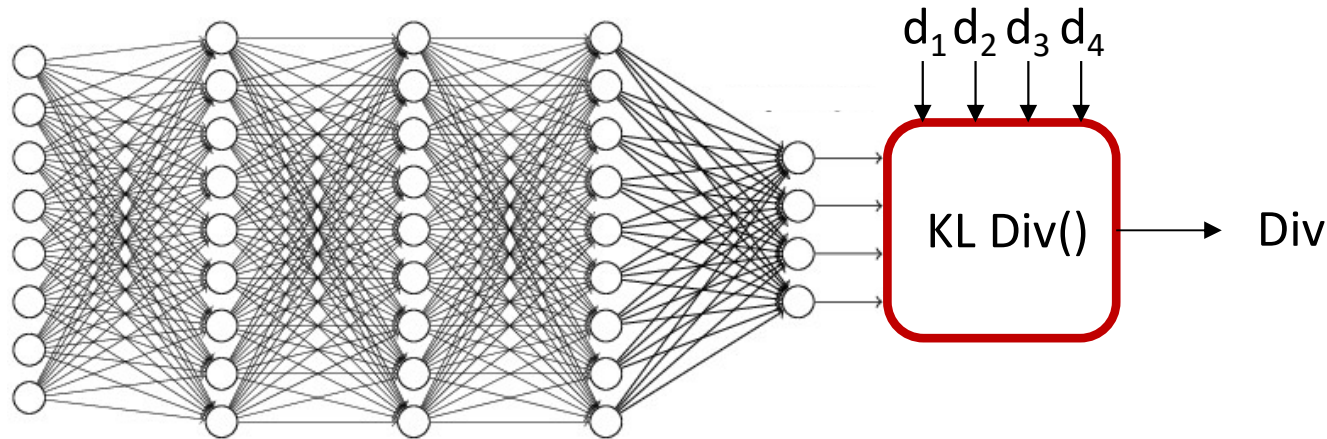
$$Div(Y, d) = \sum_i d_i \log d_i - \sum_i d_i \log y_i$$

- Derivative

$$\frac{dDiv(Y, d)}{dY_i} = \begin{cases} -\frac{1 - (K - 1)\epsilon}{y_c} & \text{for the } c - \text{th component} \\ -\frac{\epsilon}{y_i} & \text{for remaining components} \end{cases}$$



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- Derivative

$$\frac{dDiv(Y, d)}{dY_i} = \begin{cases} -\frac{1 - (K - 1)\epsilon}{y_c} & \text{for the } c - \text{th component} \\ -\frac{\epsilon}{y_i} & \text{for remaining components} \end{cases}$$

Negative derivatives encourage *increasing* the probabilities of *all* classes, including *incorrect* classes! (Seems wrong, no?)



# Problem Setup: Things to define

- Given a training set of input-output pairs  $(X_1, d_1), (X_2, d_2), \dots, (X_T, d_T)$
- Minimize the following function

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

ALL TERMS HAVE BEEN DEFINED

## Poll 5

- Select all that are correct
  - The gradient of the loss will always be 0 or close to 0 at a minimum
  - The gradient of the loss may be 0 or close to 0 at a minimum
  - The gradient of the loss may have large magnitude at a minimum
  - If the gradient is not 0 at a minimum, it must be a local minimum

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# Story so far

- Neural nets are universal approximators
- Neural networks are trained to approximate functions by adjusting their parameters to minimize the average divergence between their actual output and the desired output at a set of “training instances”
  - Input-output samples from the function to be learned
  - The average divergence is the “Loss” to be minimized
- To train them, several terms must be defined
  - The network itself
  - The manner in which inputs are represented as numbers
  - The manner in which outputs are represented as numbers
    - As numeric vectors for real predictions
    - As one-hot vectors for classification functions
  - The divergence function that computes the error between actual and desired outputs
    - L2 divergence for real-valued predictions
    - KL divergence for classifiers

# Next Class

- Backpropagation