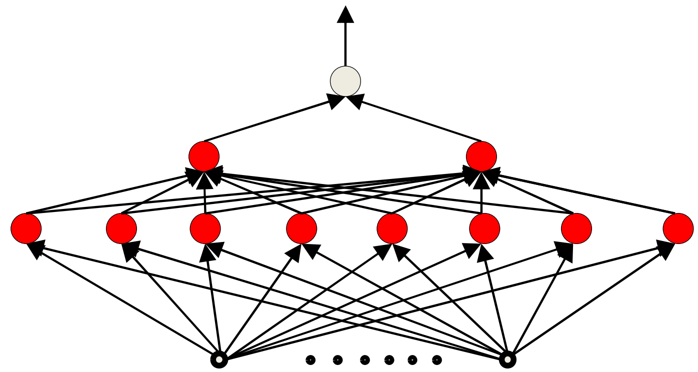
Neural Networks
Learning the network: Backprop

11-785, Fall 2022

Lecture 4

Recap: Empirical Risk Minimization

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



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

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

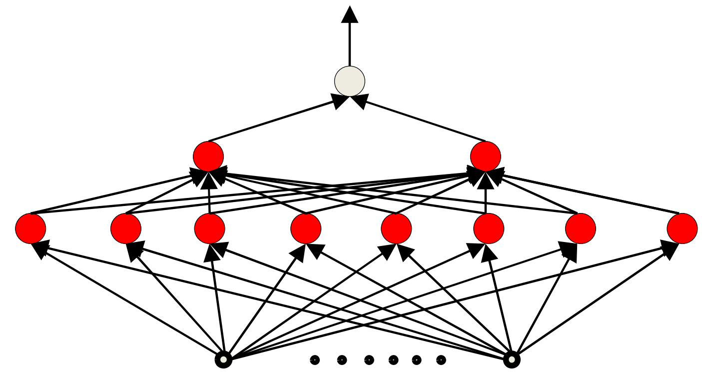
- Estimate the parameters to minimize the empirical estimate of expected divergence

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

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

Recap: Empirical Risk Minimization

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



This is an instance of function minimization (optimization)

- Given a training set of input-output pairs $(\boldsymbol{X}_1, \boldsymbol{d}_1), (\boldsymbol{X}_2, \boldsymbol{d}_2), \ldots, (\boldsymbol{X}_T, \boldsymbol{d}_T)$
  - Error on the i-th instance: $div(f(X_i; W), d_i)$
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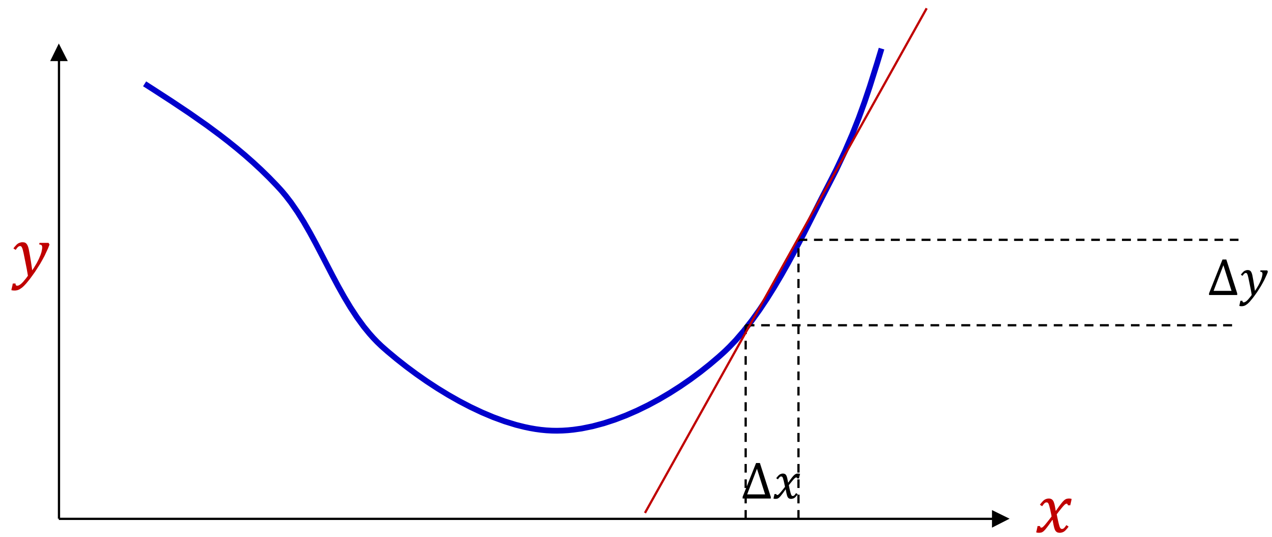
  - I.e. minimize the *empirical error* over the drawn samples

A quick intro to function optimization

with an initial discussion of derivatives

A brief note on derivatives..



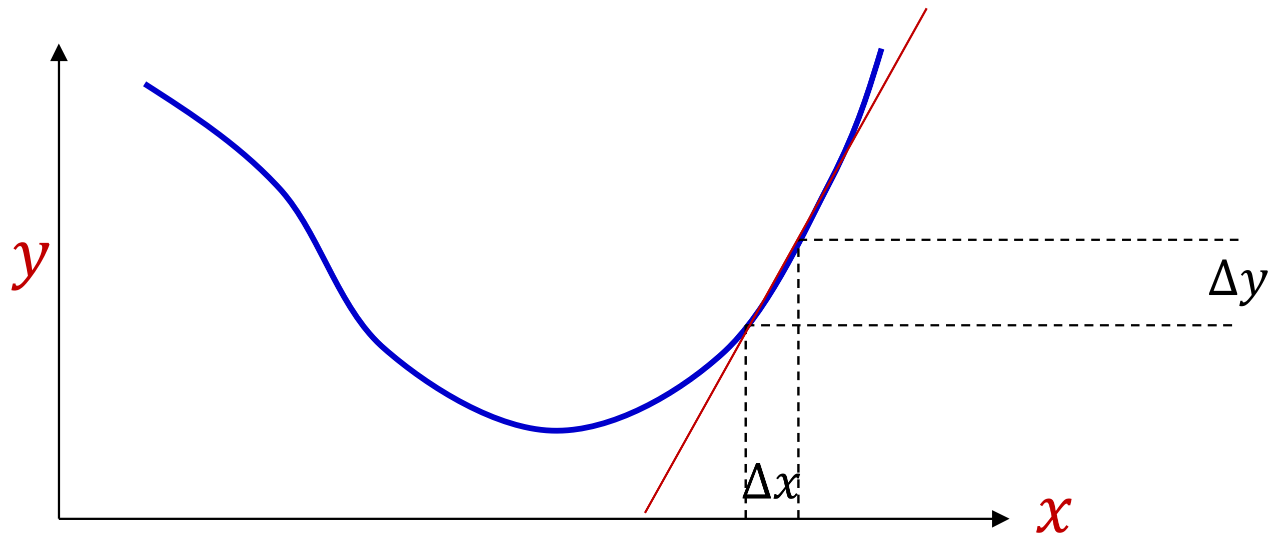
derivative

- 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

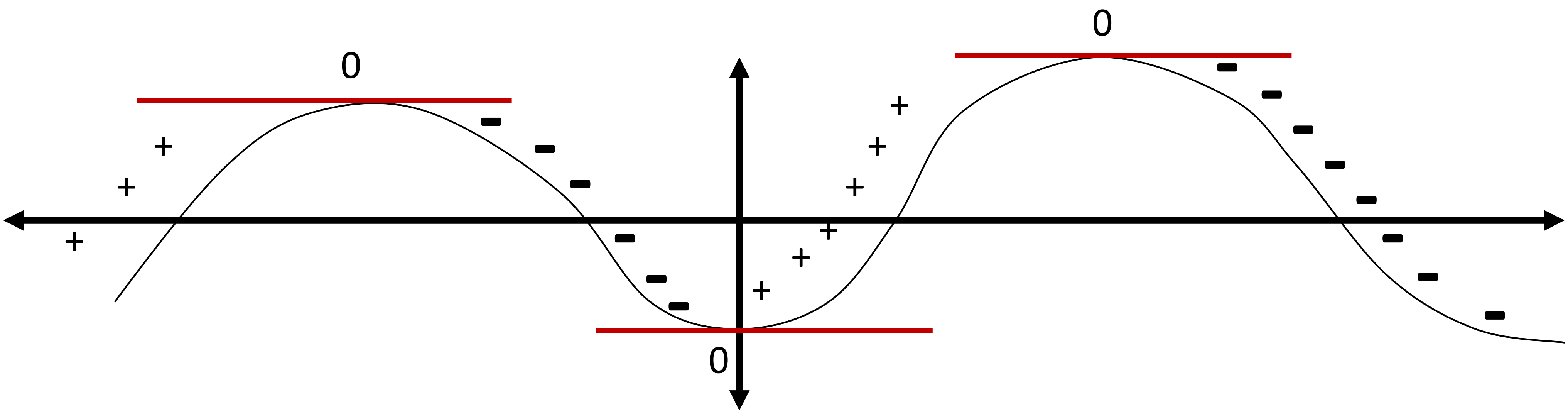
$$y = f(x)$$

  - 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

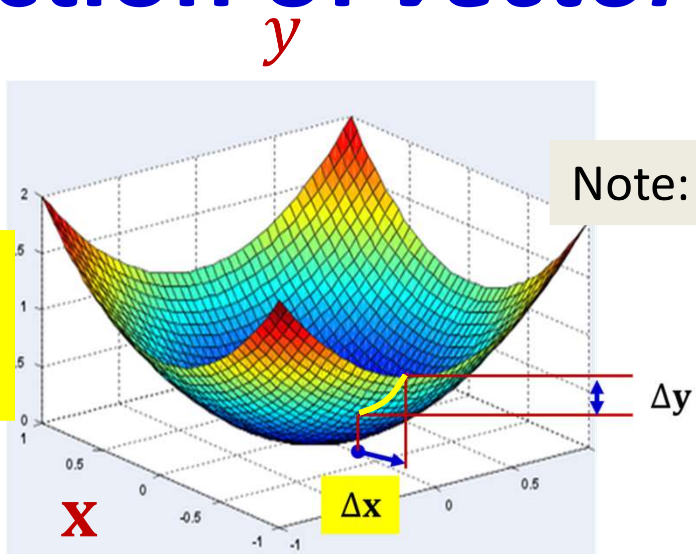
- It will be 0 where the function is locally flat (neither increasing nor decreasing)

Multivariate scalar function:

Scalar function of *vector* argument

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

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



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

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

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

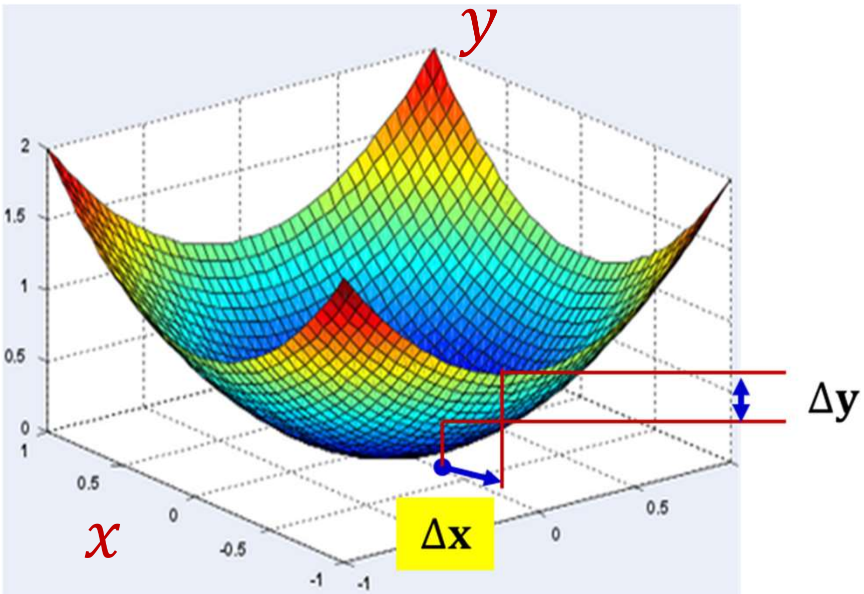
- Giving us that α is a row vector: $\alpha = [\alpha_1 \quad \cdots \quad \alpha_D]$

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

- 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

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

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

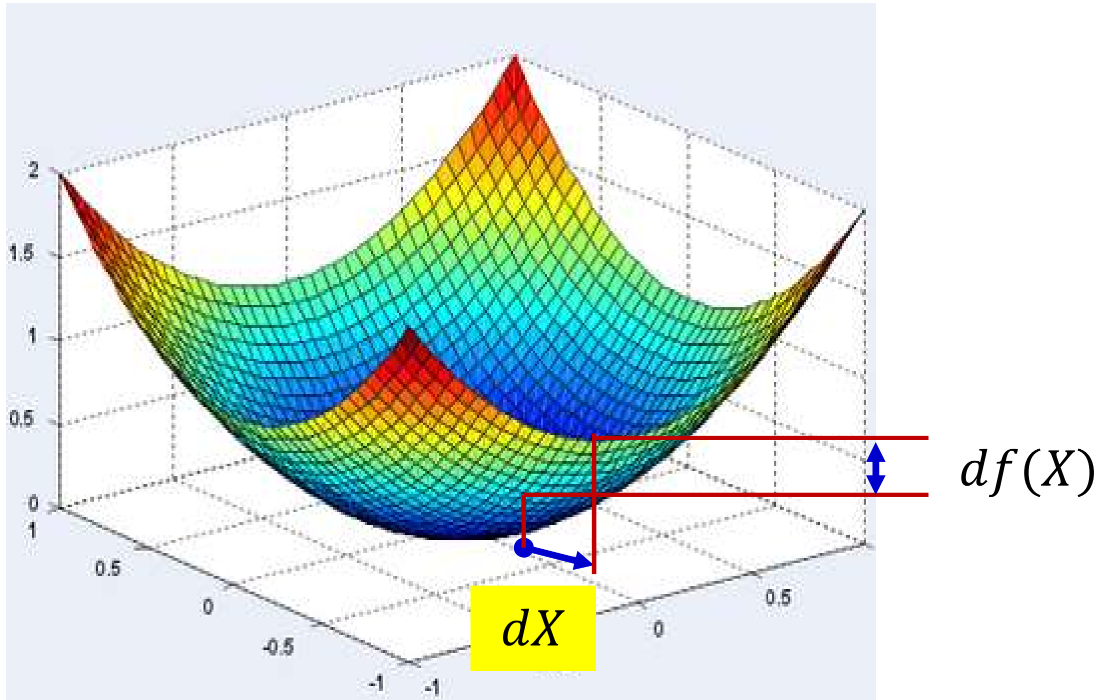
We will be using this symbol for vector and matrix derivatives

- 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

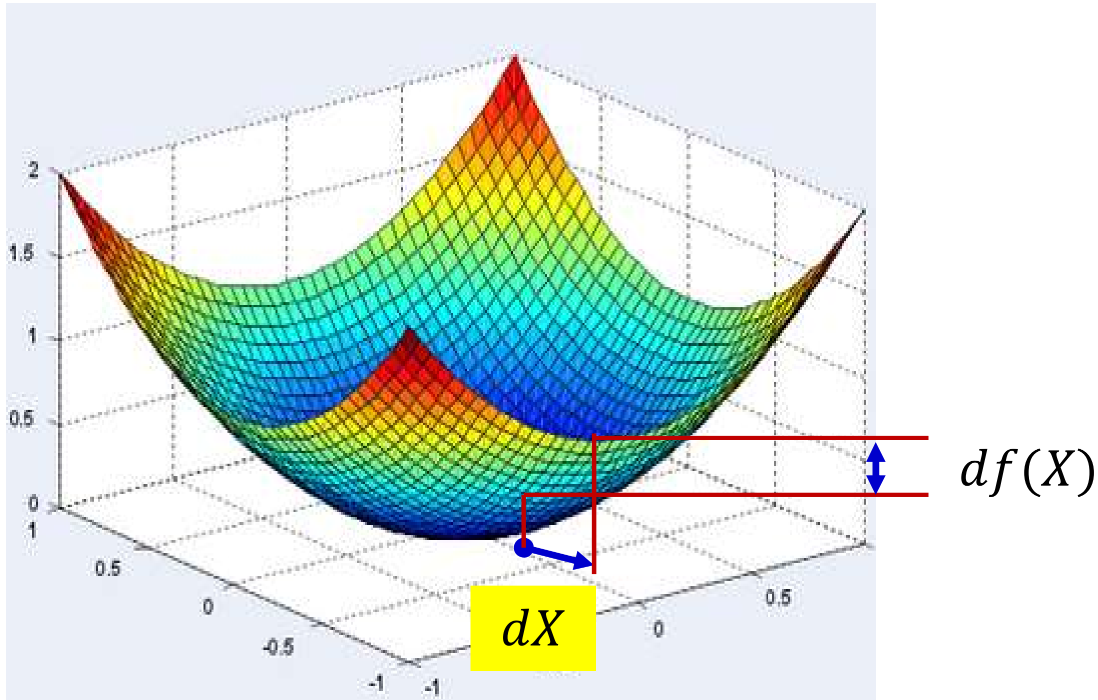


- The *derivative* $\nabla_X f(X)$ of a scalar function $f(X)$ of a multi-variate input X is a multiplicative factor that gives us the change in $f(X)$ for tiny variations in X

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

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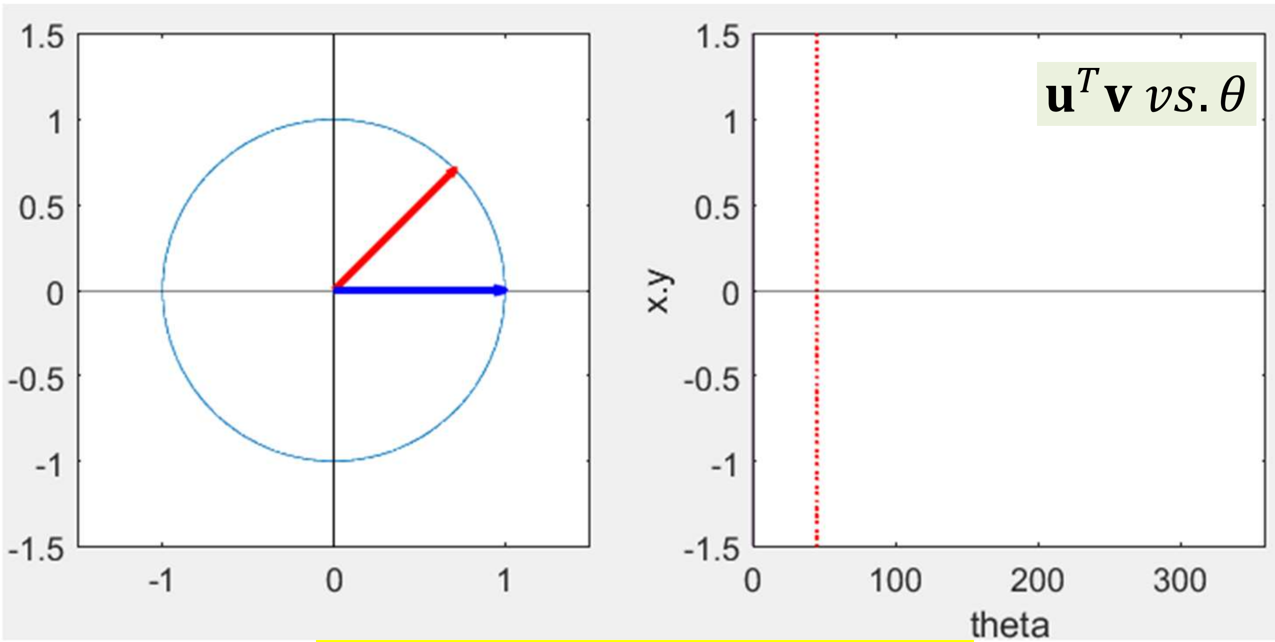
  - $\nabla_X f(X) = \left[\frac{\partial f(X)}{\partial x_1} \quad \frac{\partial f(X)}{\partial x_2} \quad \cdots \quad \frac{\partial f(X)}{\partial x_n} \right]$

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

A well-known vector property

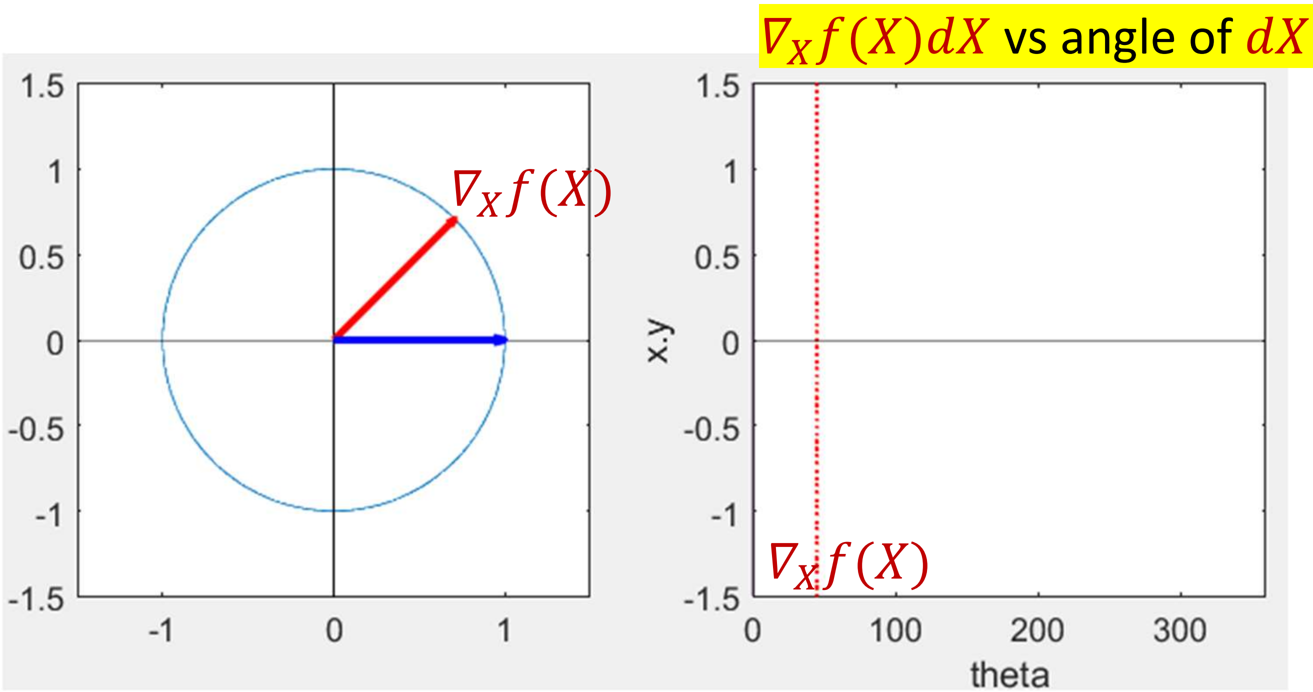


$$\mathbf{u}^T\mathbf{v} = |\mathbf{u}||\mathbf{v}|\cos\theta$$

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

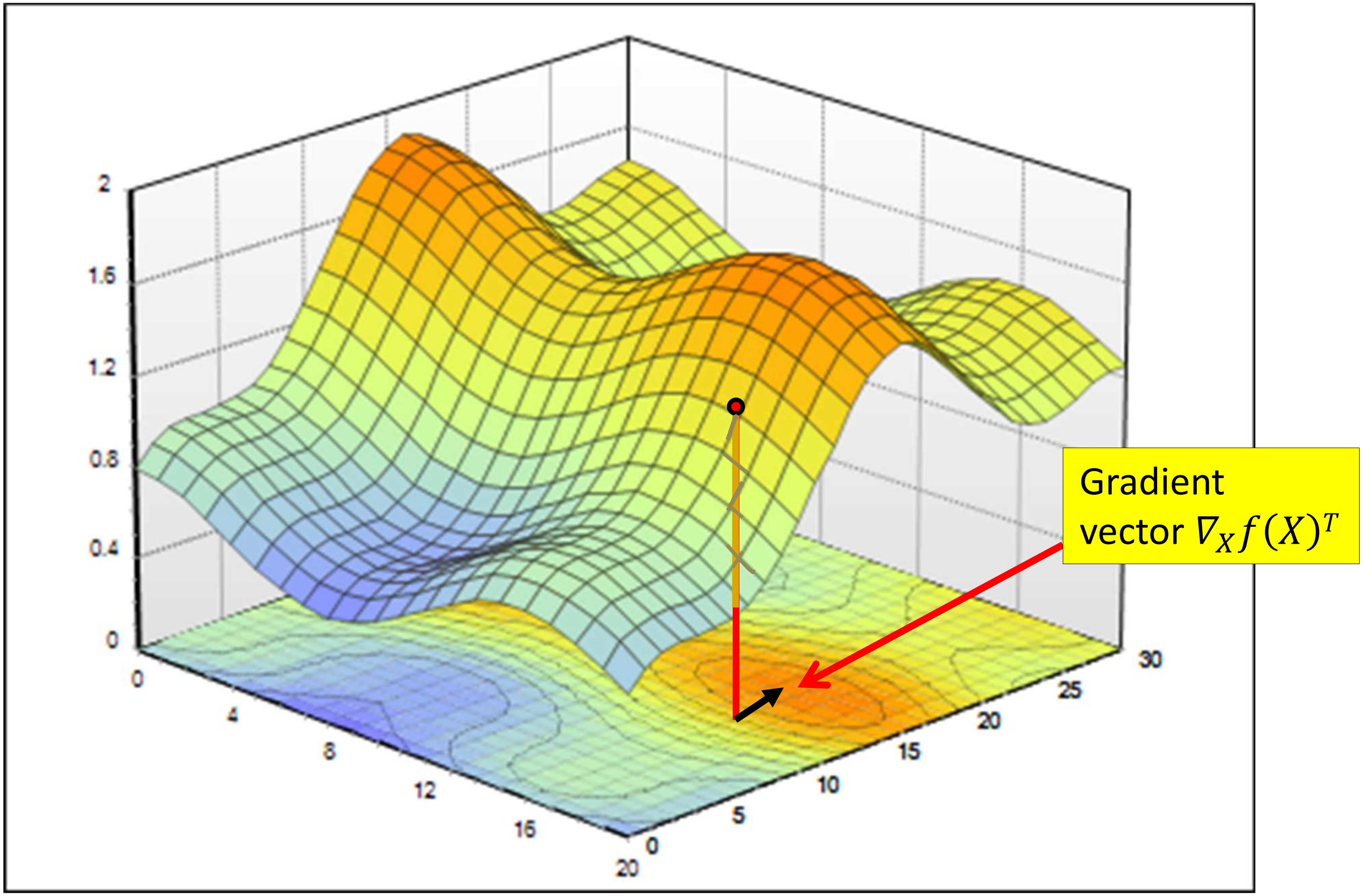
Properties of Gradient

Blue arrow is dX



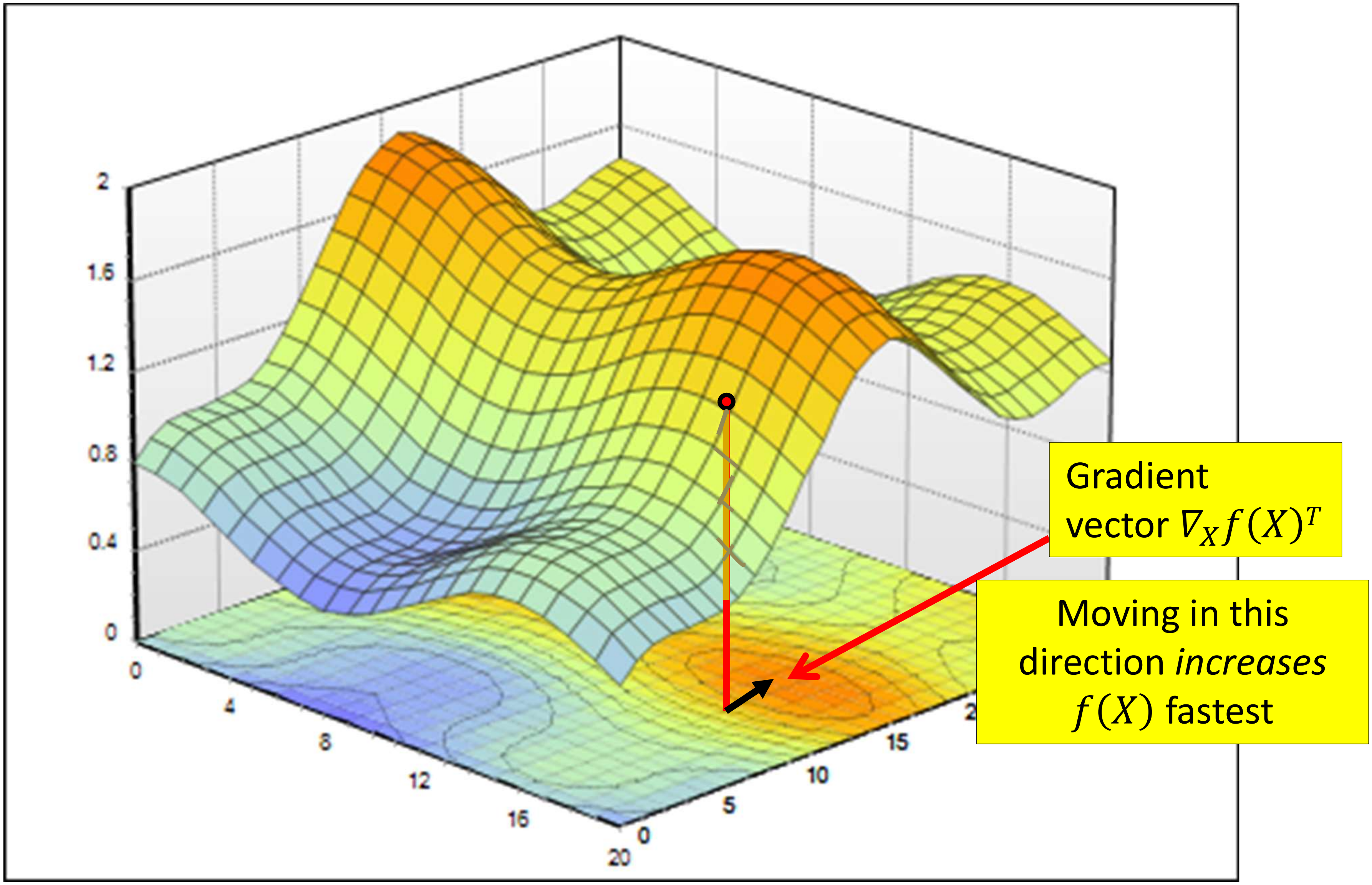
- $df(X) = \nabla_X f(X) dX$
- For an increment dX of any given length $df(X)$ is max if dX is aligned with $\nabla_X f(X)^{\mathrm{T}}$
  - The function $f(X)$ increases most rapidly if the input increment dX is exactly in the direction of $\nabla_X f(X)^{\mathrm{T}}$
- The gradient is the direction 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
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20
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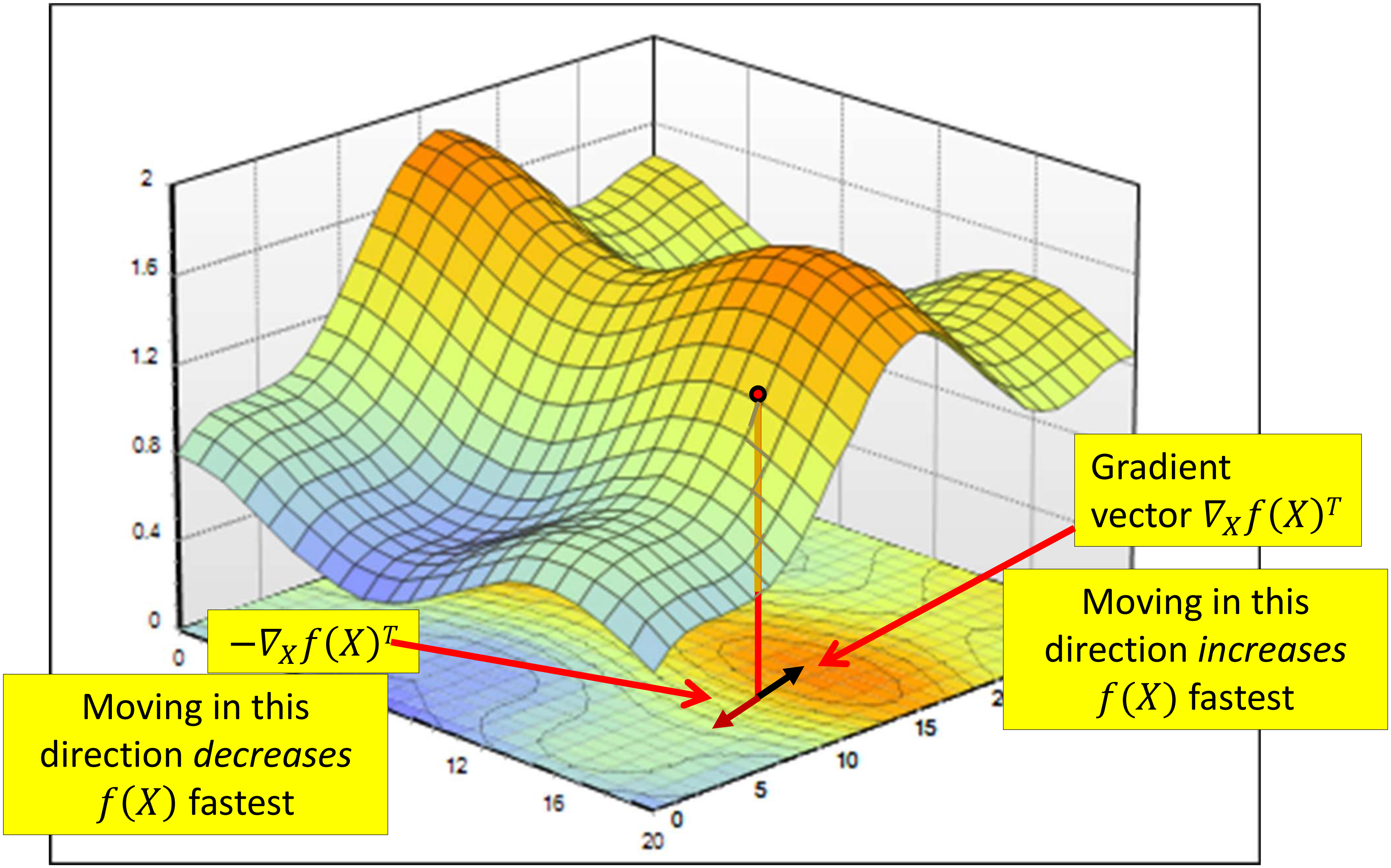
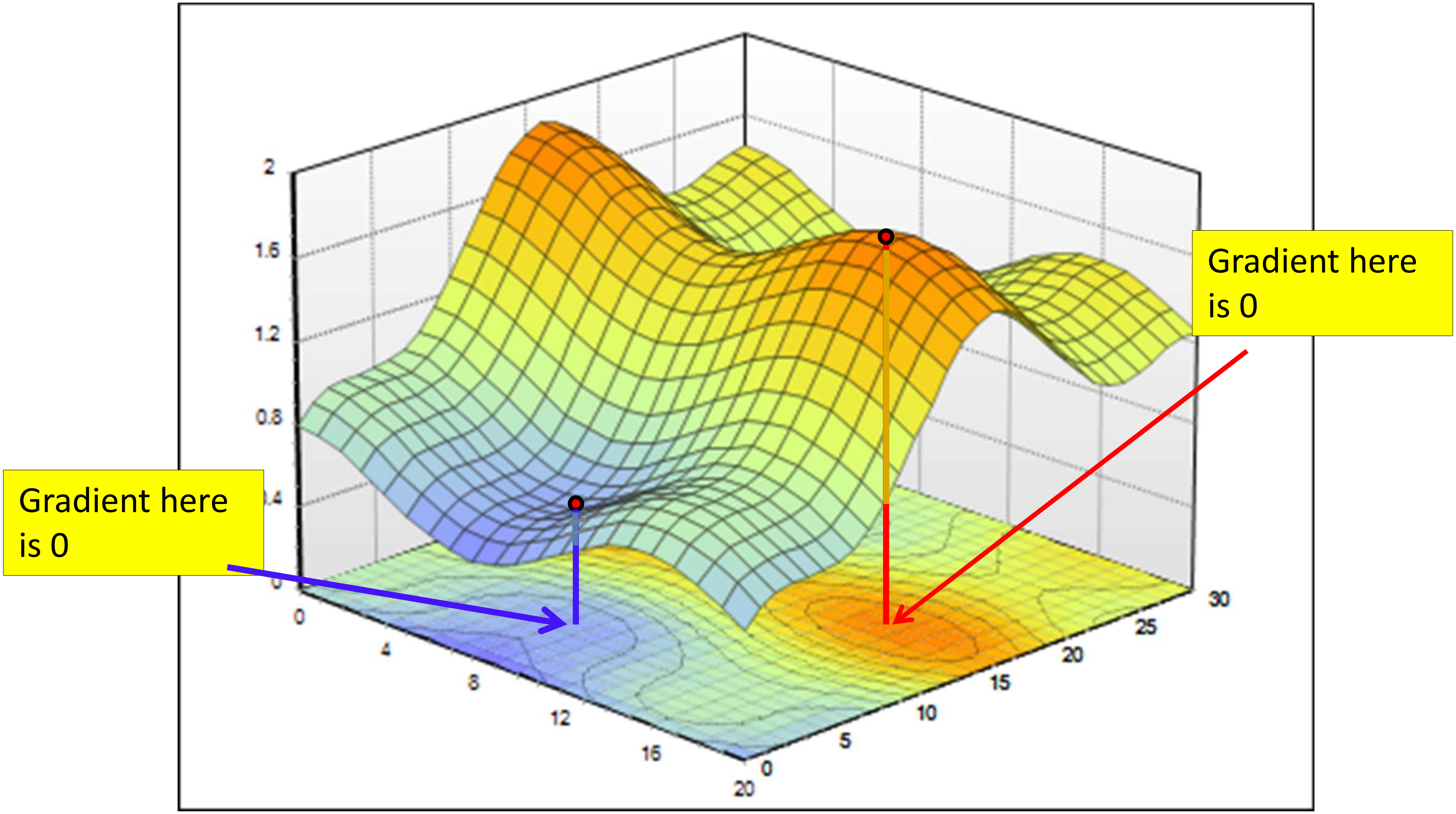
15
Gradient vector $\nabla_X f(X)^T$
Moving in this direction *increases* $f(X)$ fastest

Gradient



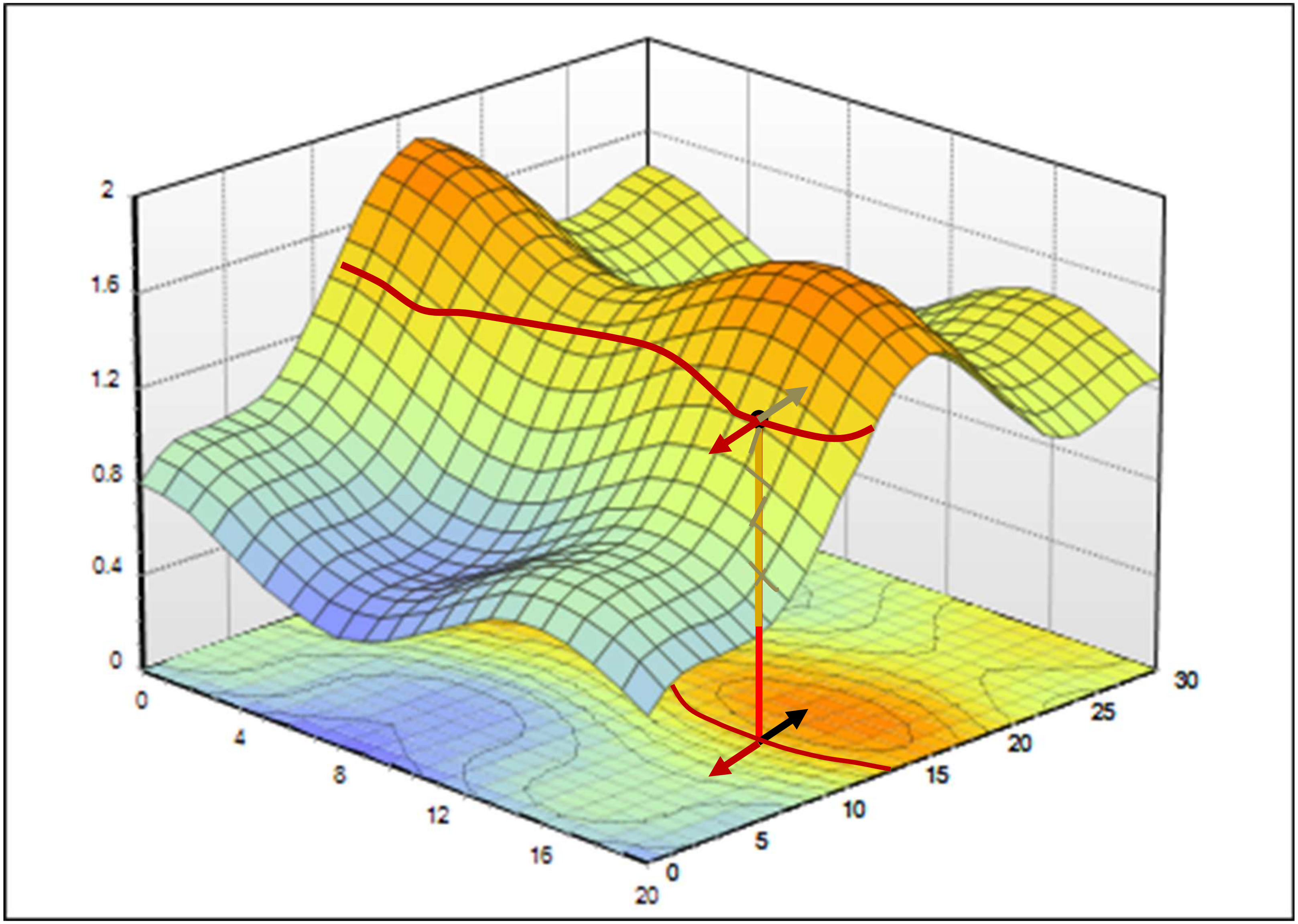
Gradient vector $\nabla_X f(X)^T$
Moving in this direction *increases* $f(X)$ fastest
$-\nabla_X f(X)^T$
Moving in this direction *decreases* $f(X)$ fastest
2
1.6
1.2
0.8
0.4
0
0
12
16
20
0
5
10
15

Gradient



Gradient here is 0
Gradient here is 0
2
1.6
1.2
0.8
0.4
0
0
4
8
12
16
20
0
5
10
15
20
25
30

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

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

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 Nx1 column vector variable x. What is the shape of the derivative of y with respect to x
  - Scalar
  - N x 1 column vector
  - 1 x N row vector
  - There is insufficient information to decide

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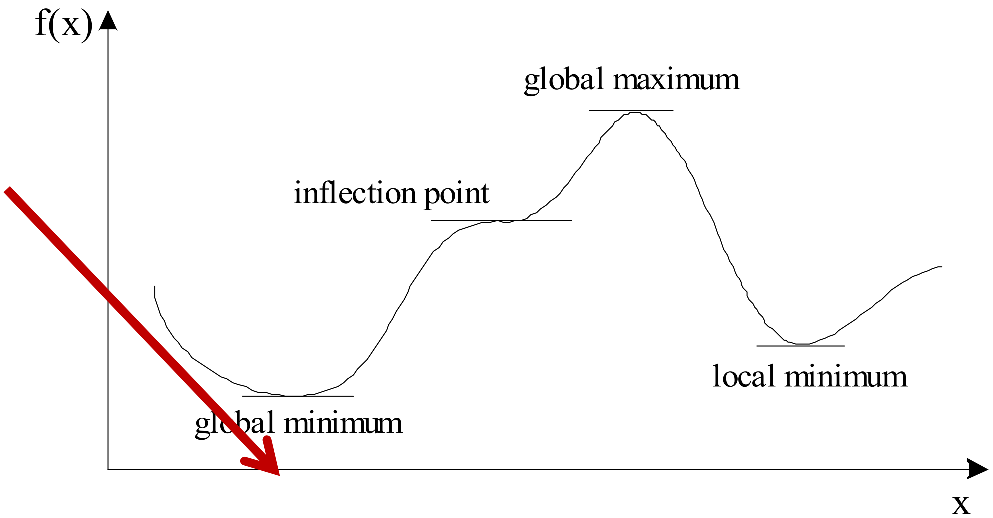
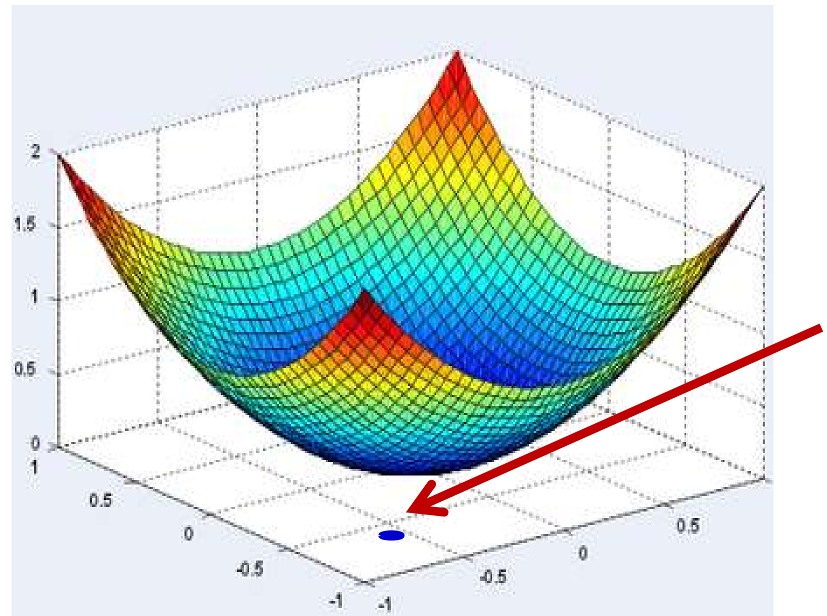
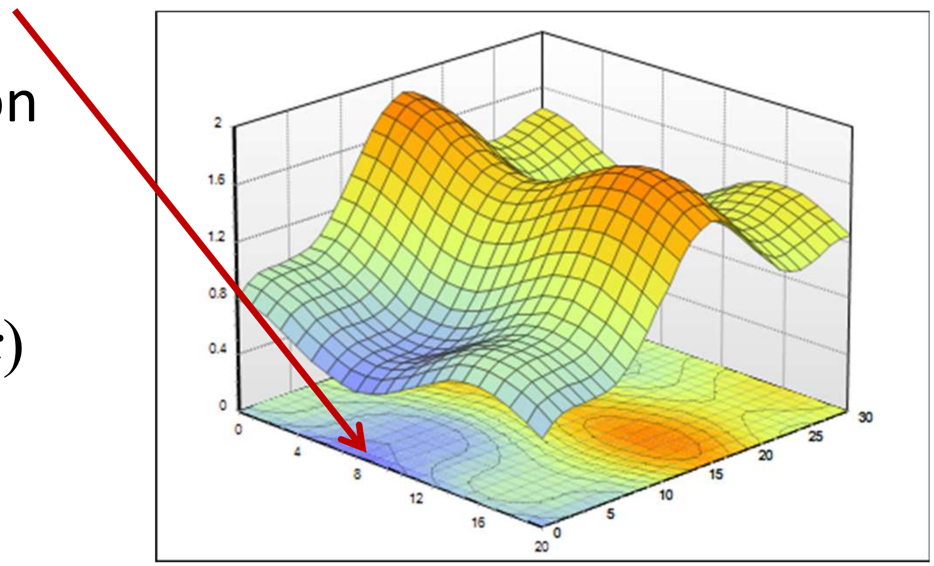
The problem of optimization



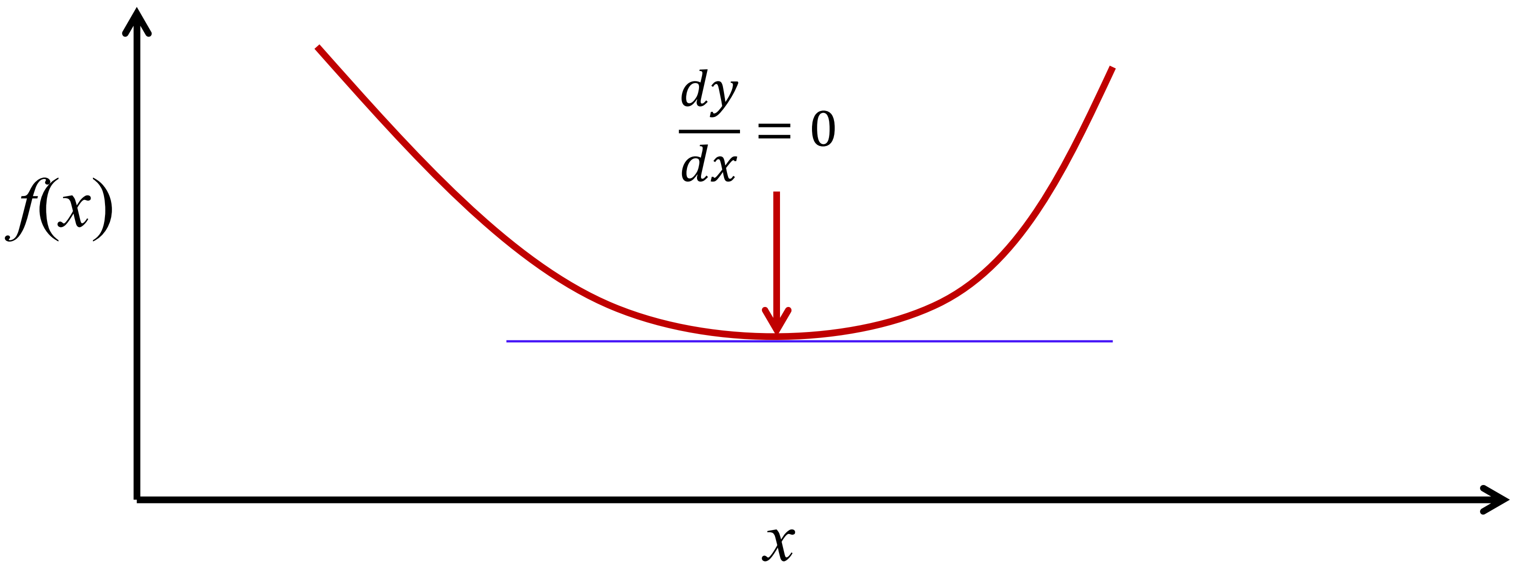




- General problem of optimization: Given a function $\mathbf{f}(x)$ of some variable x …

- Find the value of x where $\mathbf{f}(x)$ 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

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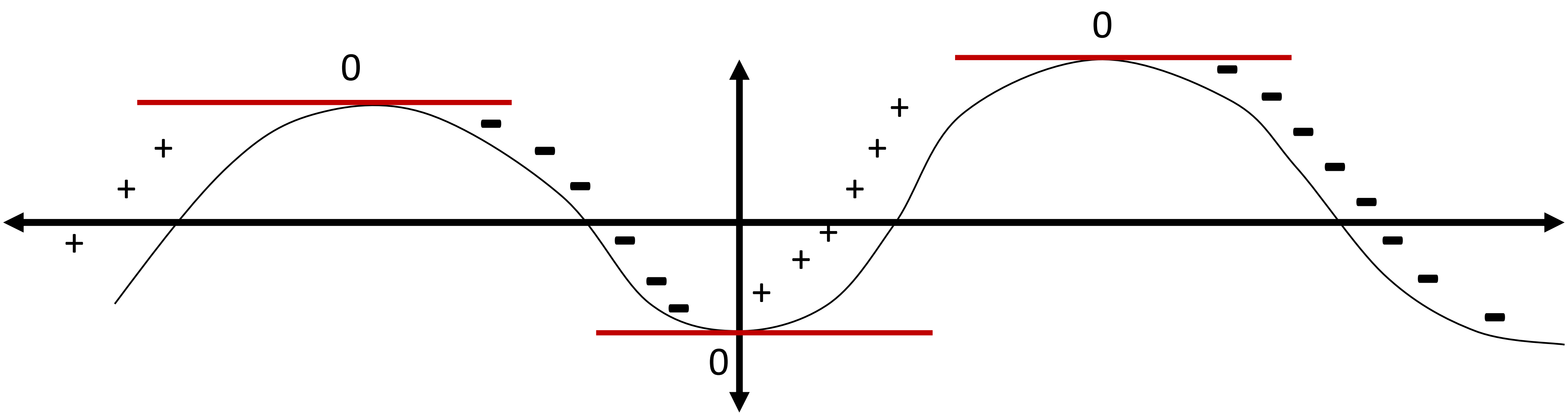
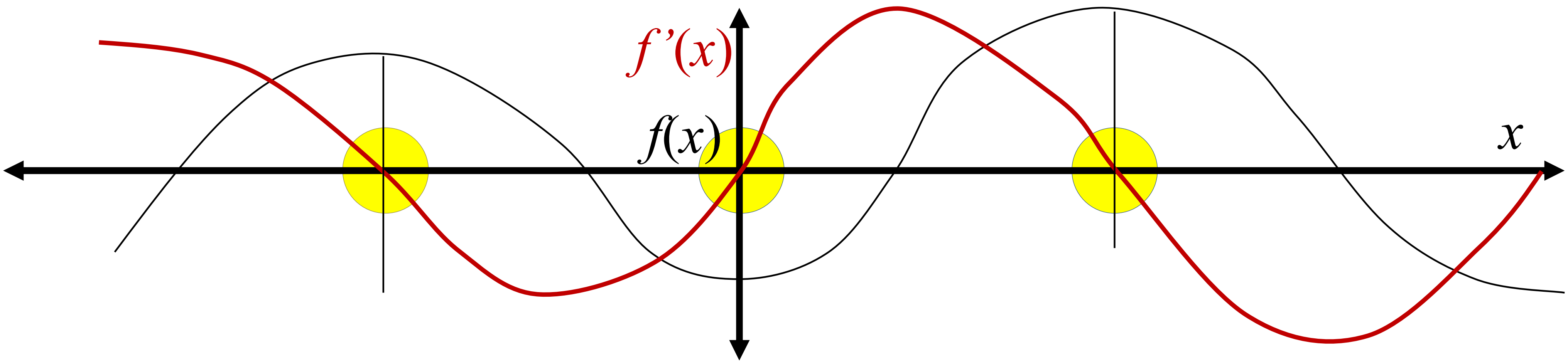
1. The derivative f'(x) = 0 at the minimum. This is the only condition to be satisfied
2. f'(x) = 0 and the second derivative f"(x) is negative
3. **f'(x) = 0 and the second derivative f"(x) is positive**

Turning Points



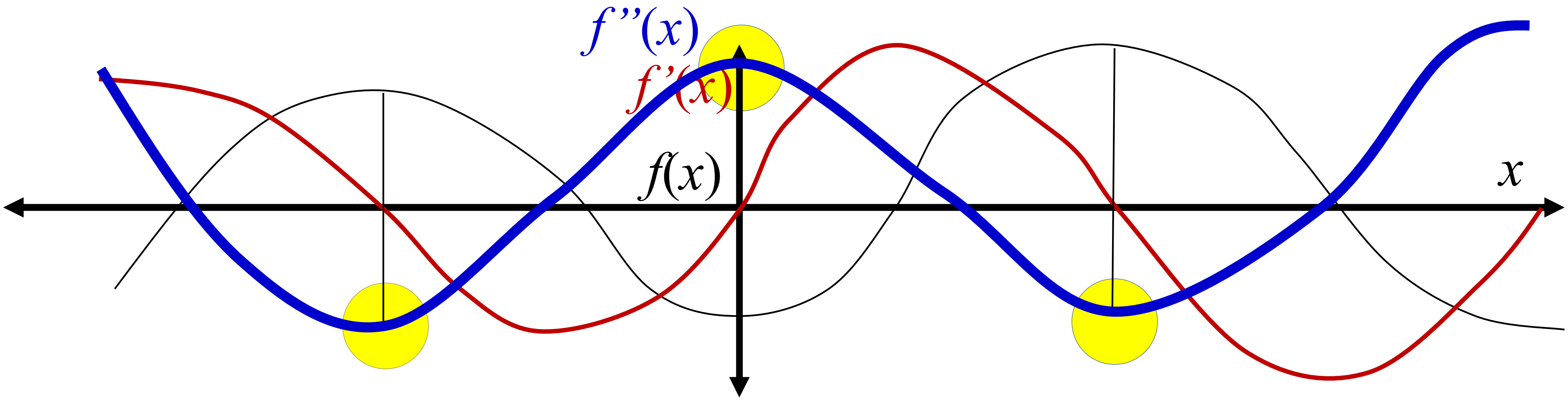
- Both *maxima* and *minima* have zero derivative
- Both are turning points

Derivatives of a curve



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

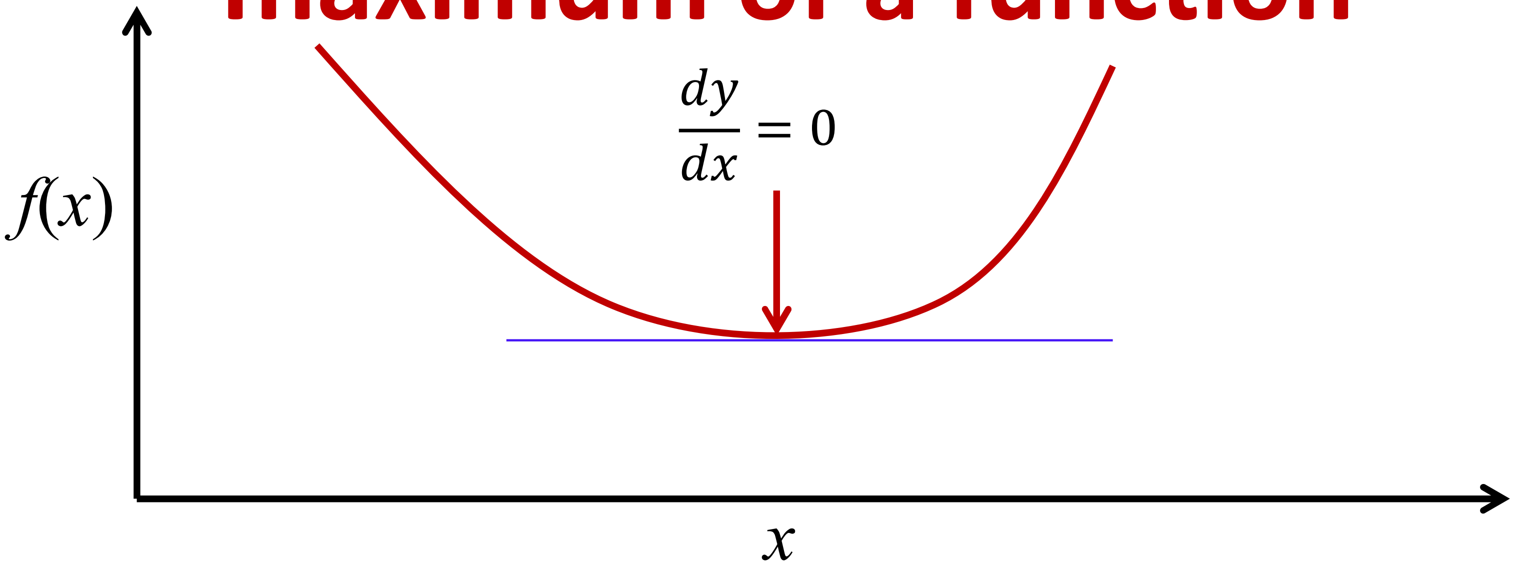
Derivative of the derivative of the curve



- 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

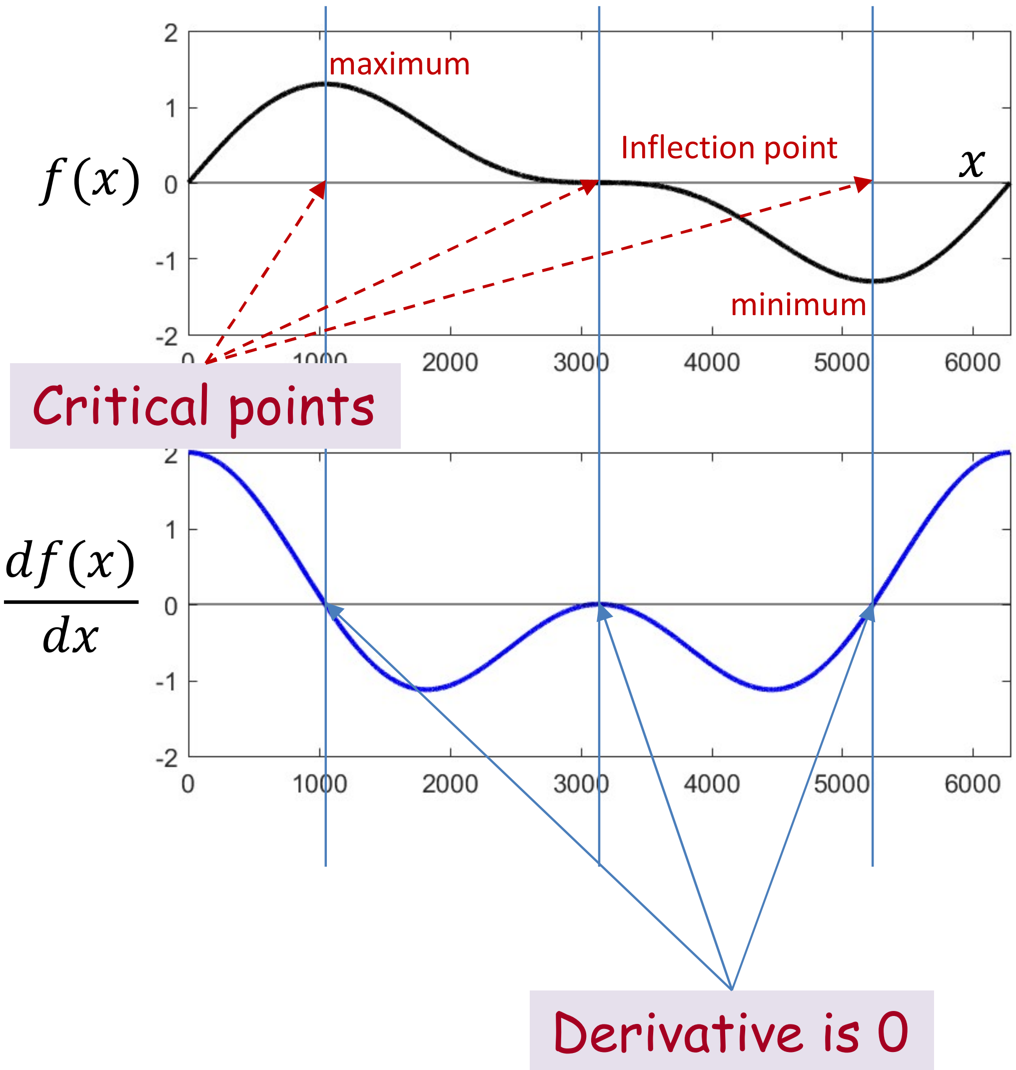
$$\frac{df(x)}{dx} = 0$$

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

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

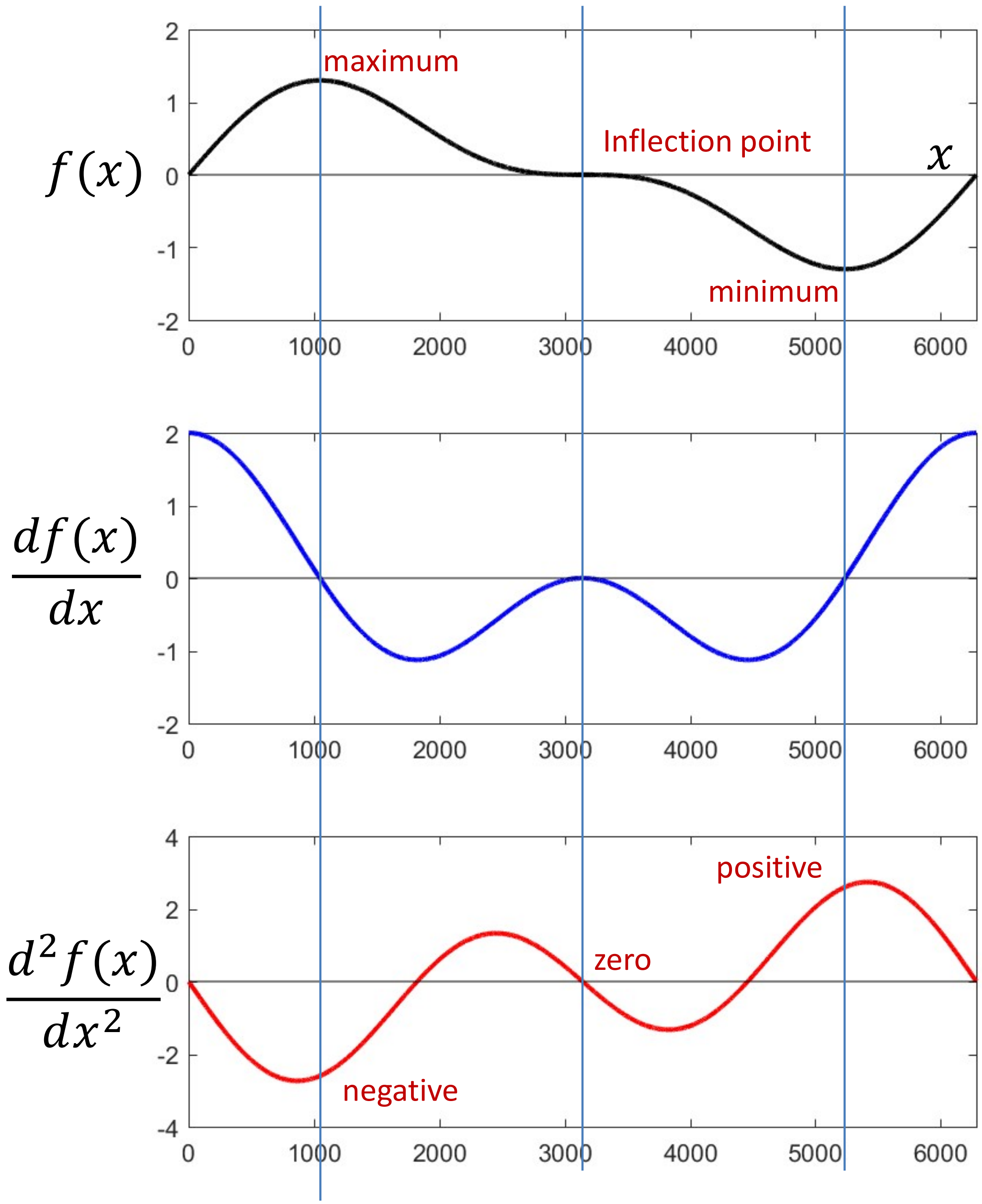
- If $f''(x_{soln})$ is positive x_{soln} is a minimum, otherwise it is a maximum

A note on derivatives of functions of single variable



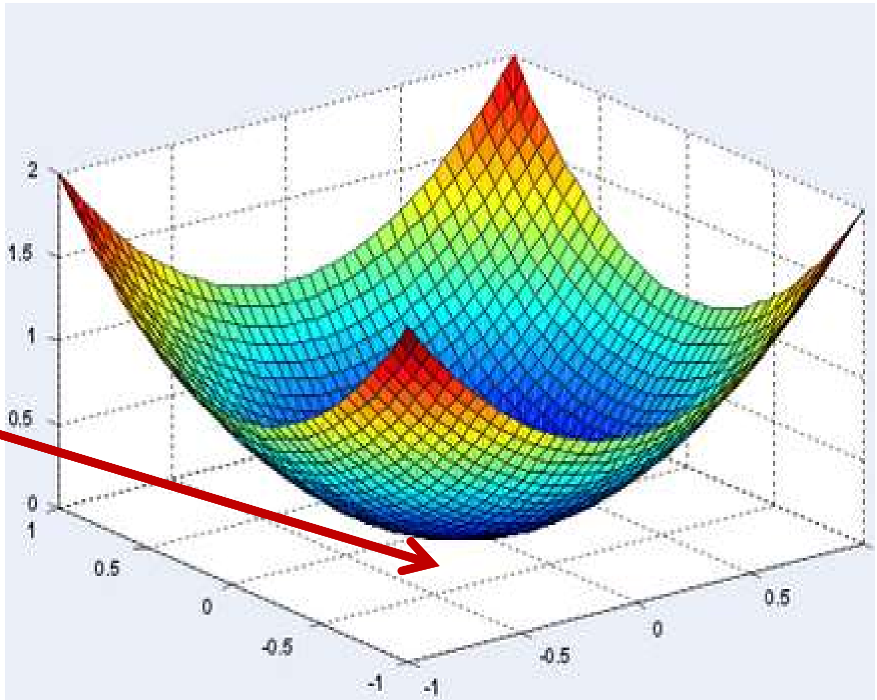
- All locations with zero derivative are *critical* points
  - These can be local maxima, local minima, or inflection points
- The *second* derivative is
  - Positive (or 0) at minima
  - Negative (or 0) at maxima
  - Zero at inflection points

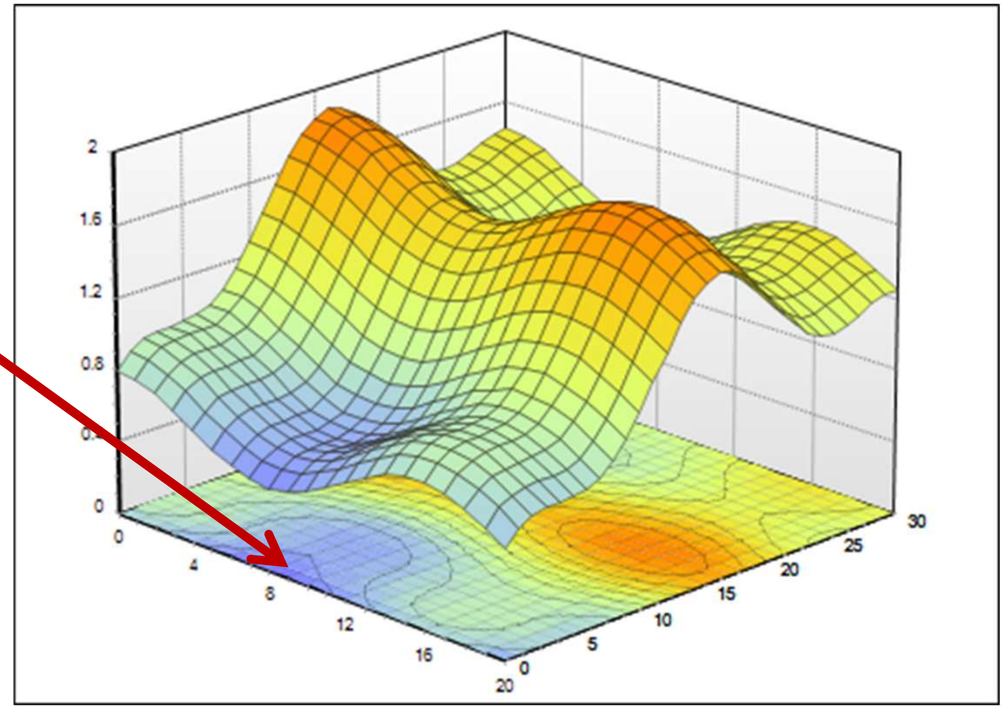
A note on derivatives of functions of single variable



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

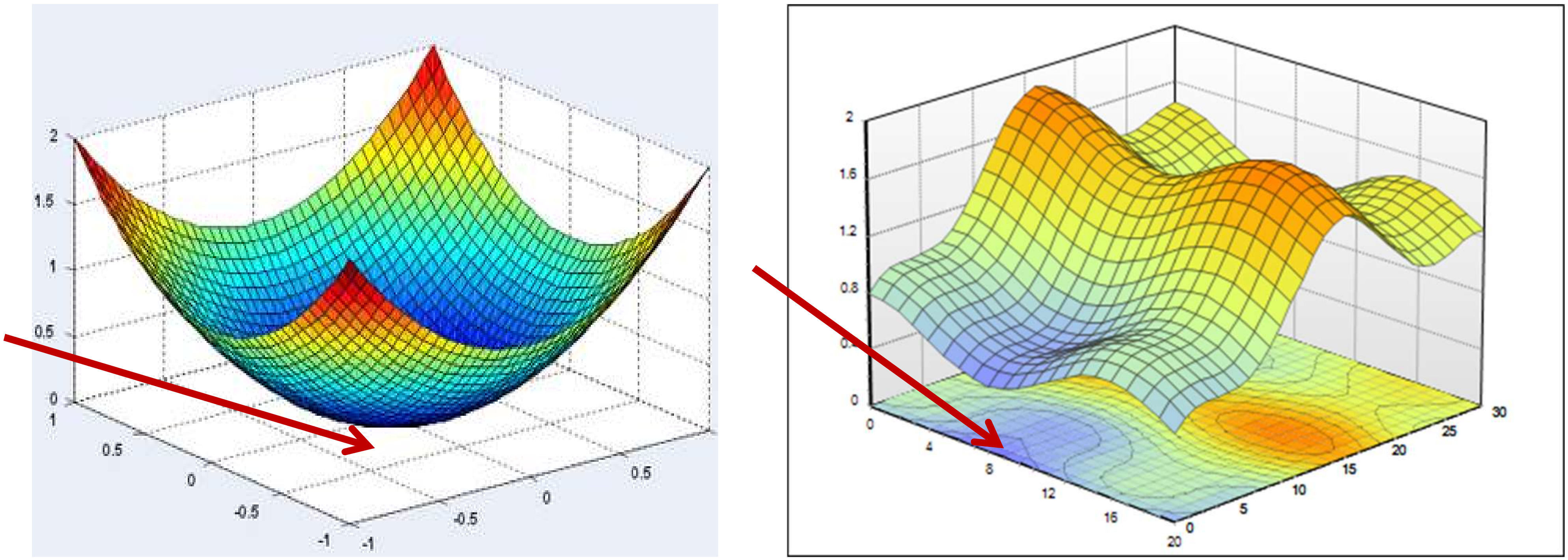
What about functions of multiple variables?





- The optimum point is still "turning" point
  - Shifting in any direction will increase the value
  - For smooth functions, 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

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

- Gradient

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

Unconstrained Minimization of function (Example)

- Set the gradient to null

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

- Solving the 3 equations system with 3 unknowns

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

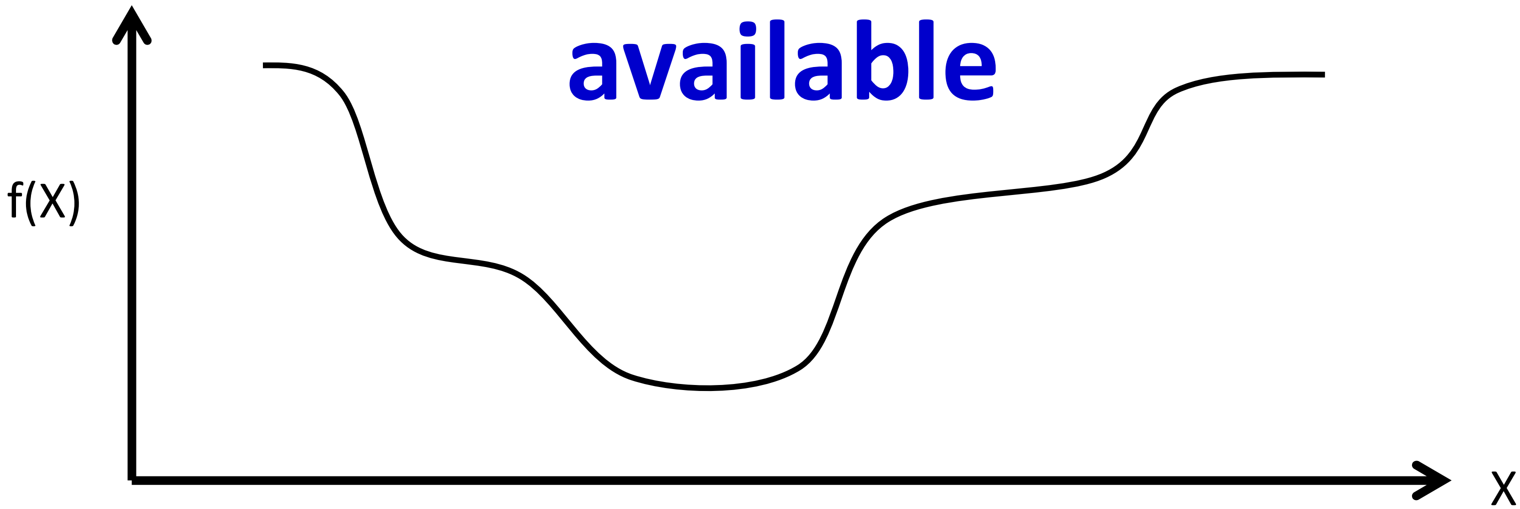
Unconstrained Minimization of function (Example)

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

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

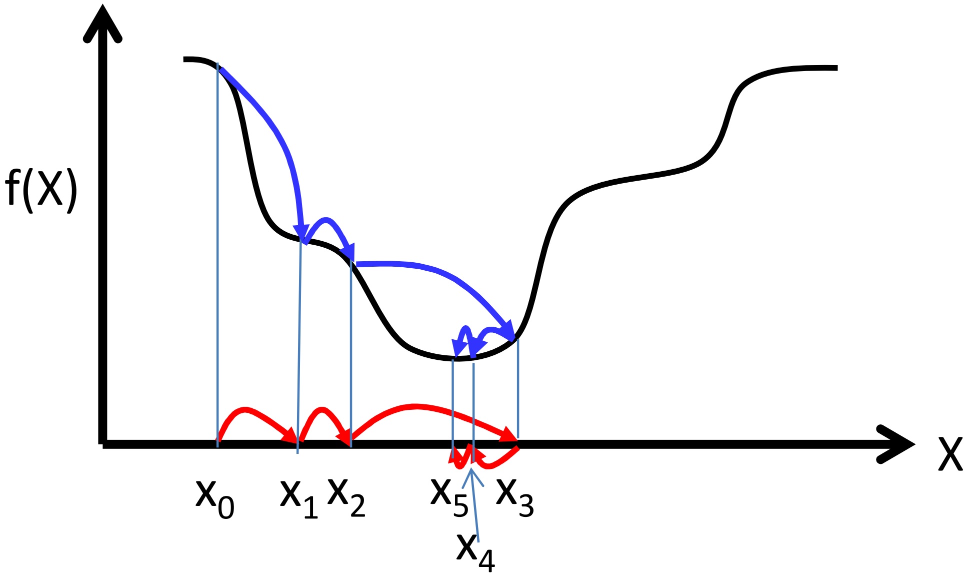
- All the eigenvalues are positives => the Hessian matrix is positive definite
- The point $x = \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} = \begin{bmatrix} -1 \\ -1 \\ -1 \end{bmatrix}$ is a minimum

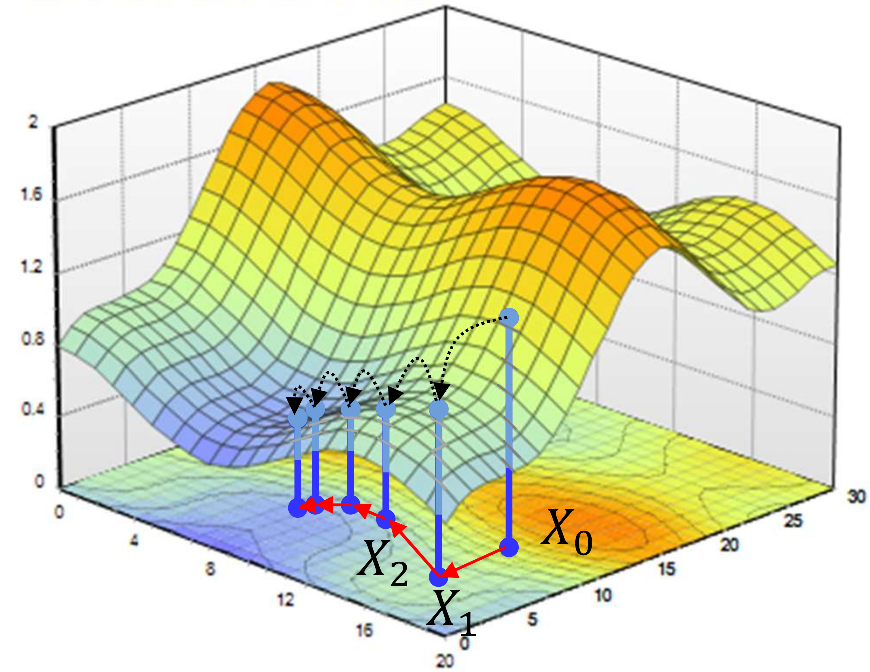
Closed Form Solutions are not always available



- 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

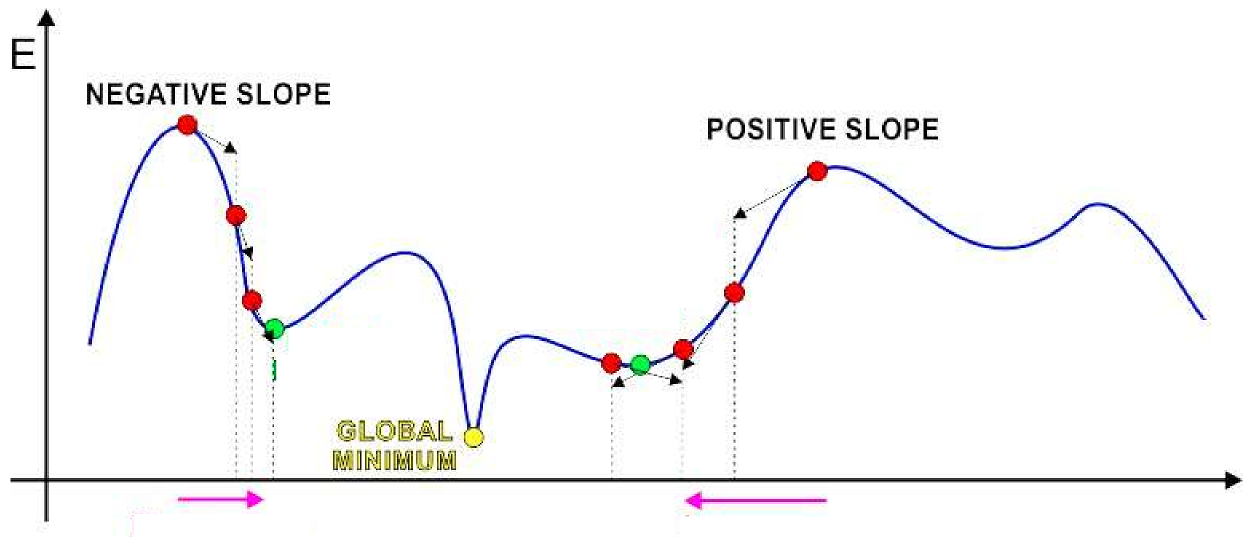
Iterative solutions





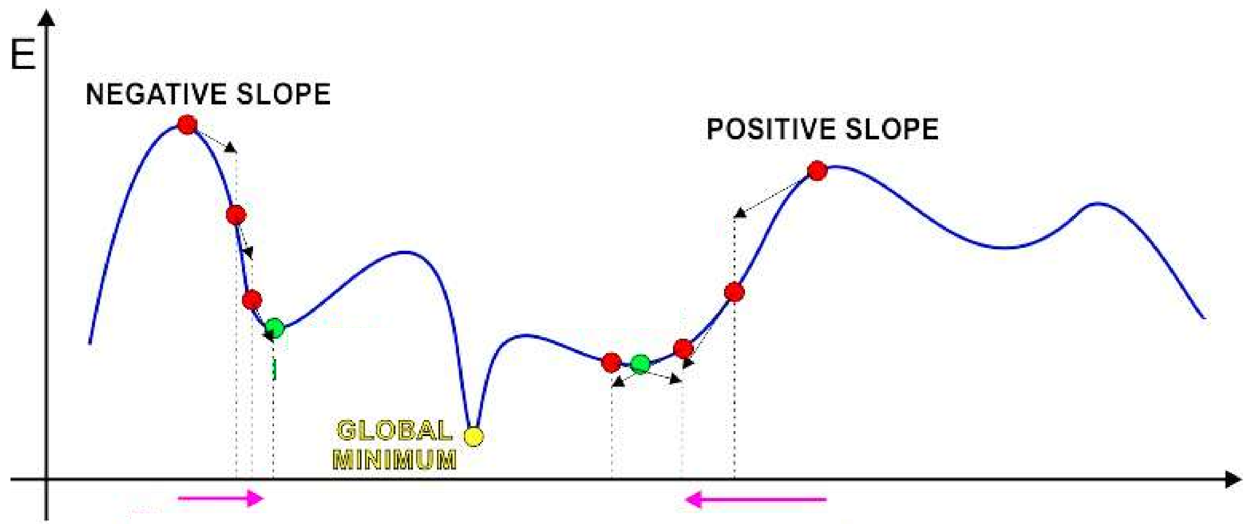
- Iterative solutions
  - Start from an initial guess X_0 for the optimal X
  - Update the guess towards a (hopefully) “better” value of $\mathrm{f}(X)$
  - Stop when $\mathrm{f}(X)$ no longer decreases
- Problems:
  - Which direction to step in
  - How big must the steps be

The Approach of Gradient Descent



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

The Approach of Gradient Descent



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

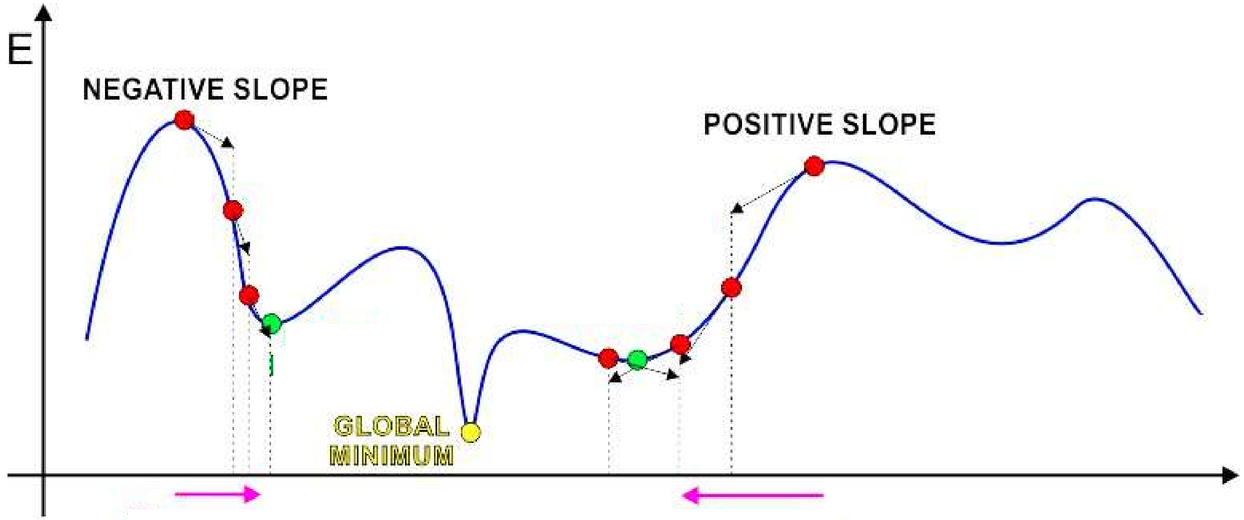
$$x^{k+1} = x^k - step$$

    - Else

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

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

The Approach of Gradient Descent

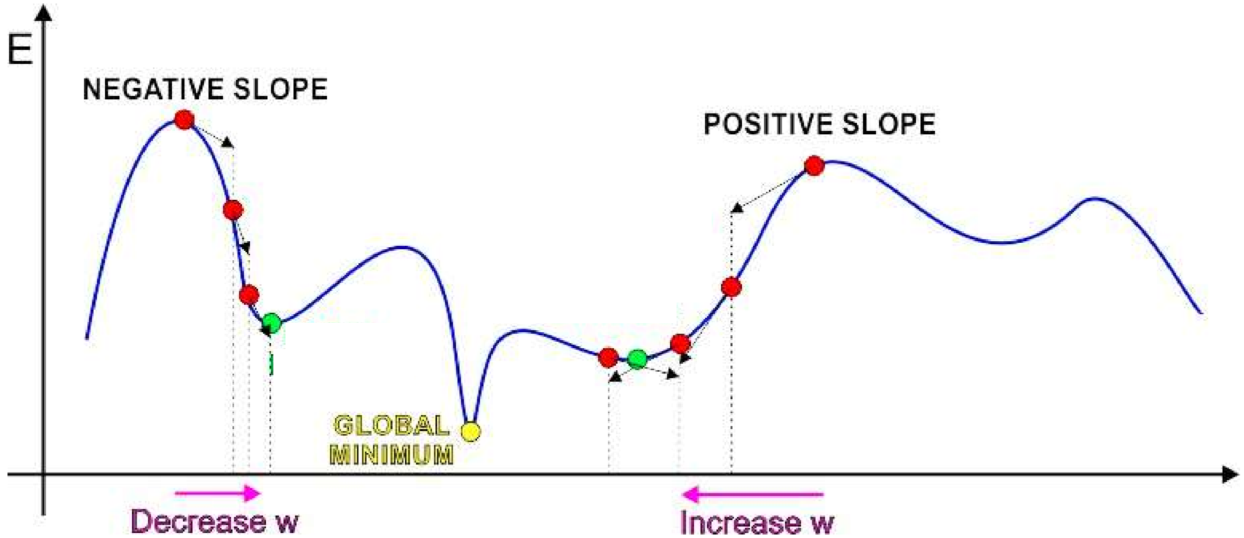


- Iterative solution: Trivial algorithm
  - Initialize x^0
  - While $f'(x^k) \neq 0$

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

- Identical to previous algorithm

The Approach of Gradient Descent



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

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

- η^k is the "step size"

Poll 3: Multivariate functions

- 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

Poll 3: Multivariate functions

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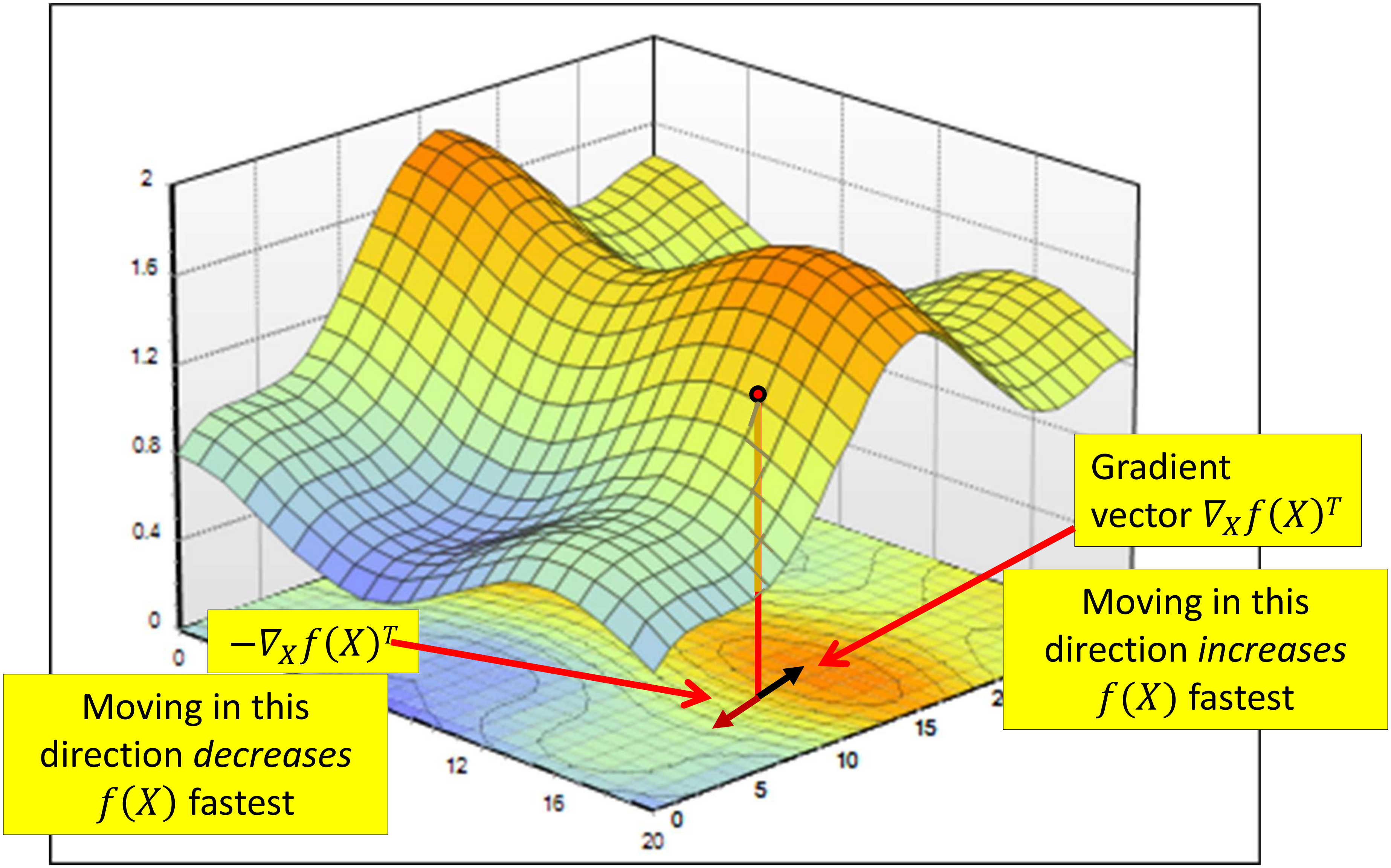
Gradients of multivariate functions



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*

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

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

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

- Many solutions to choosing step size η^k

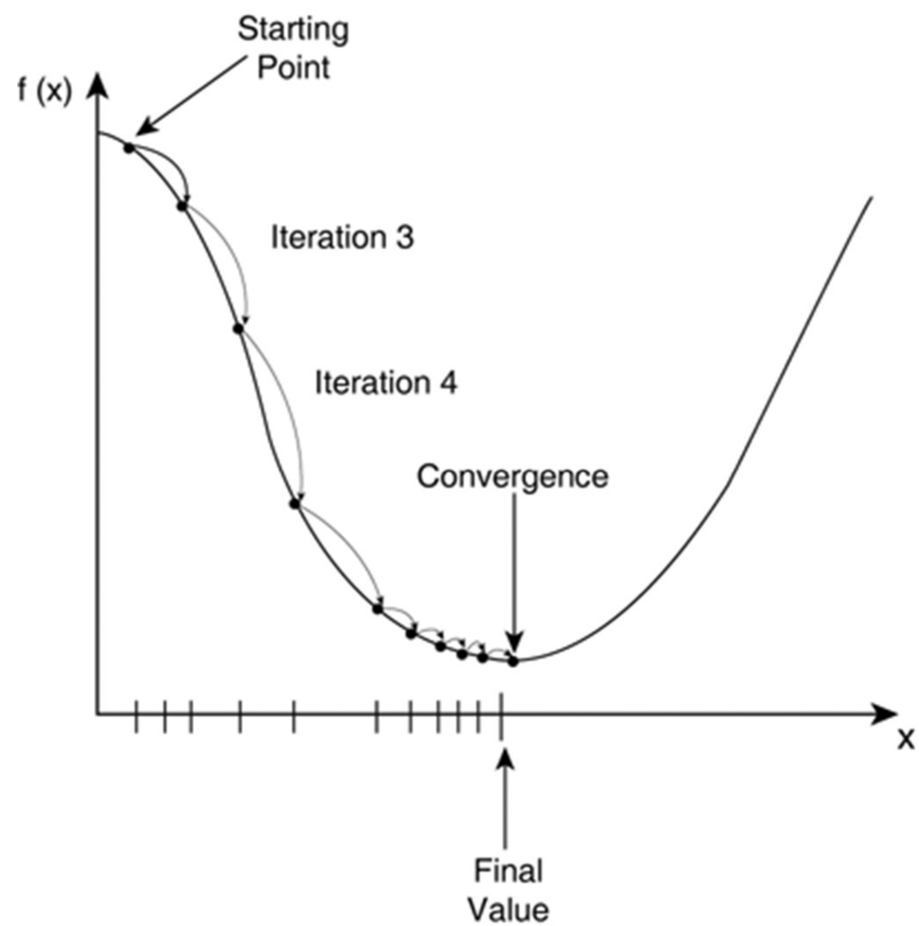
Gradient descent convergence criteria

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

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

- Or

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

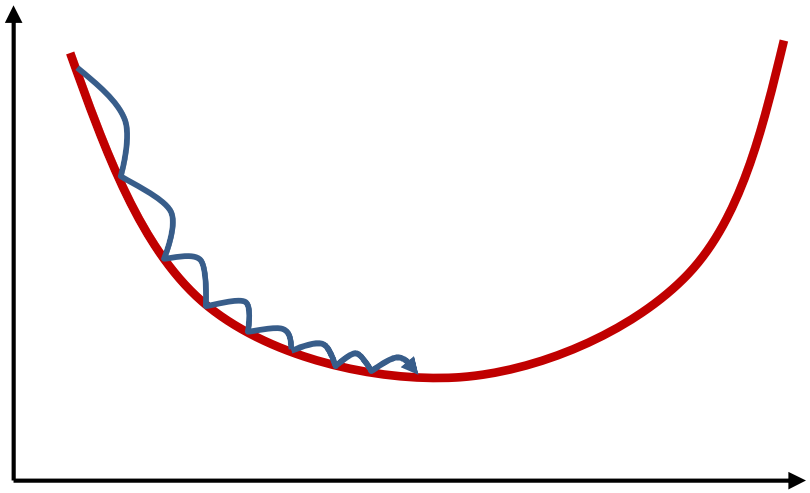


Overall Gradient Descent Algorithm

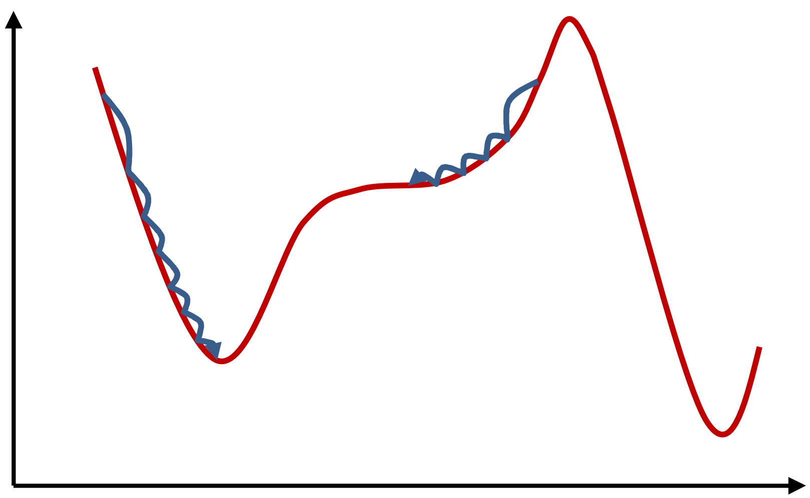
- Initialize:
  - x^0
  - $k = 0$

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

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 Nx1 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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Poll 4

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- Returning to our problem from our detour..

Problem Statement

- Given a training set of input-output pairs $(\boldsymbol{X}_1, \boldsymbol{d}_1), (\boldsymbol{X}_2, \boldsymbol{d}_2), \dots, (\boldsymbol{X}_T, \boldsymbol{d}_T)$

- 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

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

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

Preliminaries

- Before we proceed: the problem setup

Problem Setup: Things to define

- Given a training set of input-output pairs $(\boldsymbol{X}_1, \boldsymbol{d}_1), (\boldsymbol{X}_2, \boldsymbol{d}_2), \ldots, (\boldsymbol{X}_T, \boldsymbol{d}_T)$

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

Problem Setup: Things to define

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

What is the divergence div()?

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

Problem Setup: Things to define

- Given a training set of input-output pairs $(\boldsymbol{X}_1, \boldsymbol{d}_1), (\boldsymbol{X}_2, \boldsymbol{d}_2), \ldots, (\boldsymbol{X}_T, \boldsymbol{d}_T)$

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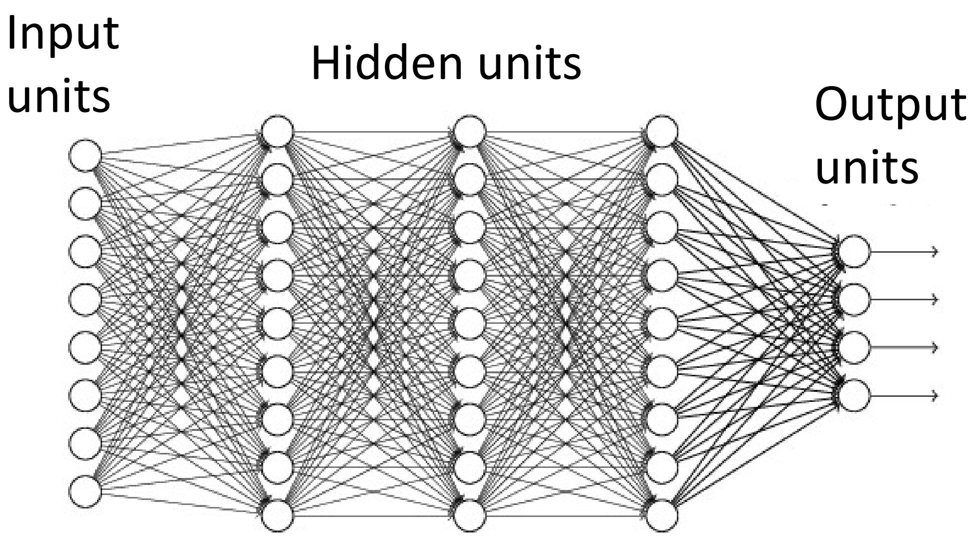
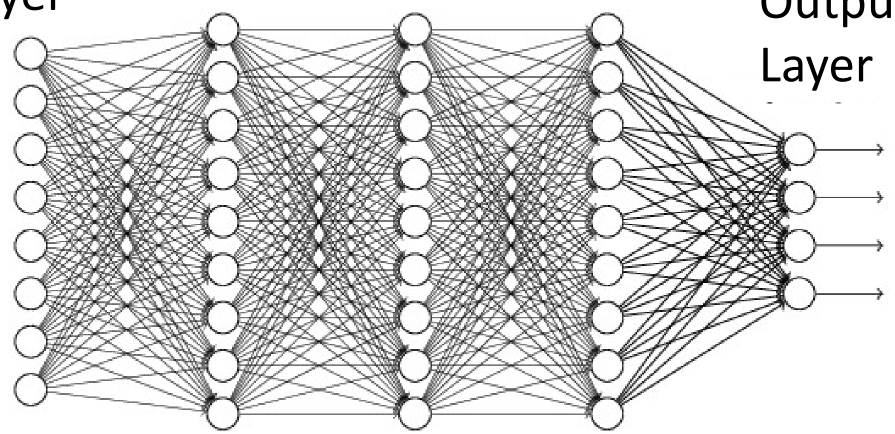
What is f() and what are its parameters W?

What is f()? Typical network



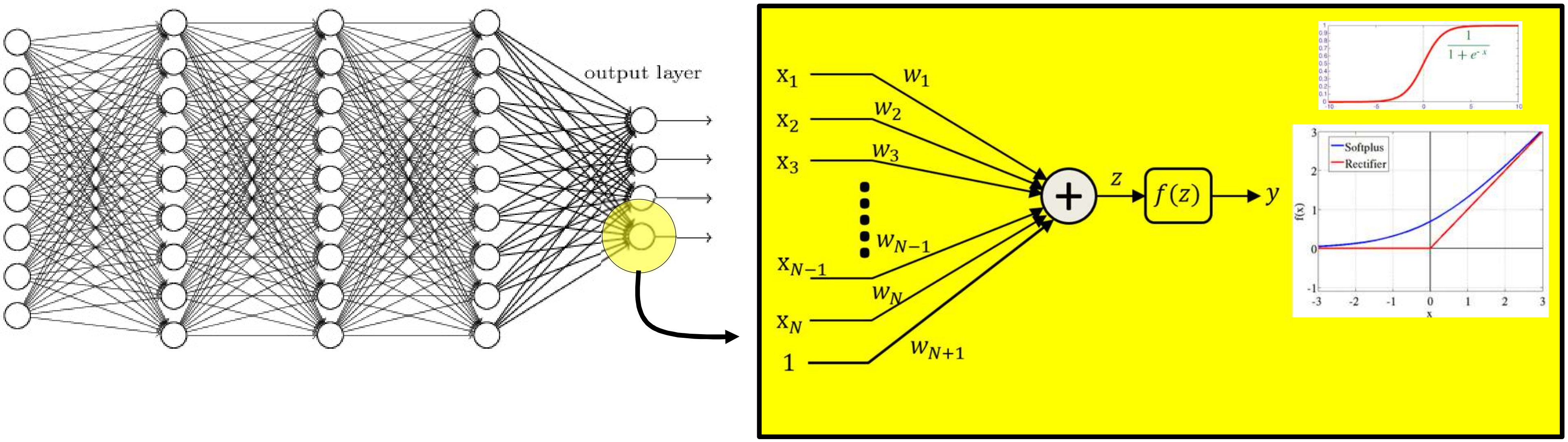
- Multi-layer perceptron
- A *directed* network with a set of inputs and outputs
  – No loops

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



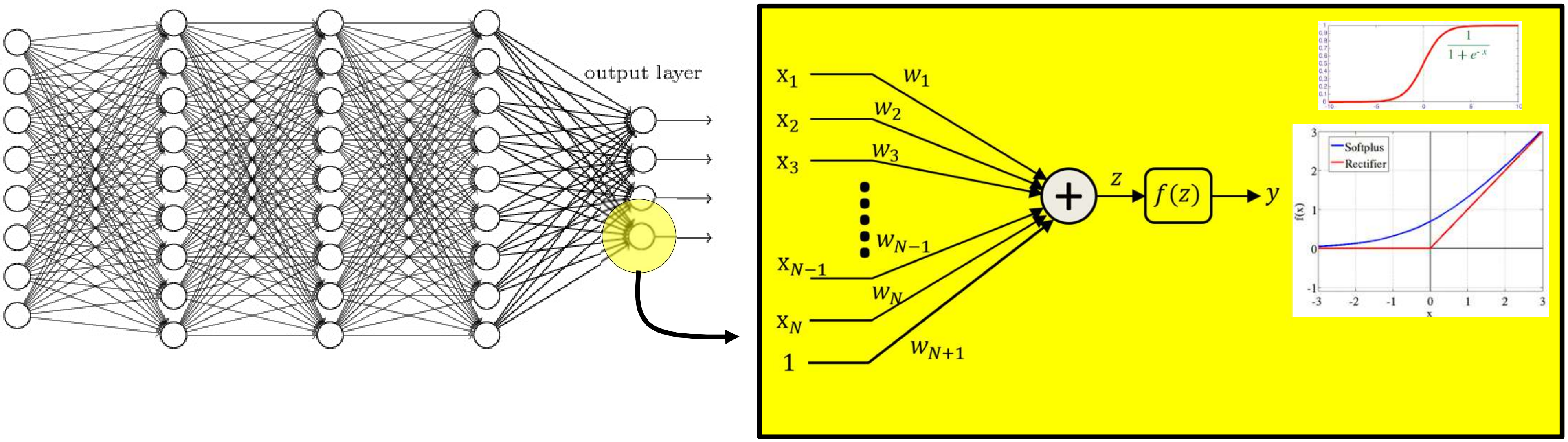
- Individual neurons operate on a set of inputs and produce a single output
  - **Standard setup:** A continuous activation function applied to an affine function of the inputs

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

  - More generally: *any* differentiable function

$$y = f(x_1, x_2, \ldots, x_N; W)$$

The individual neurons



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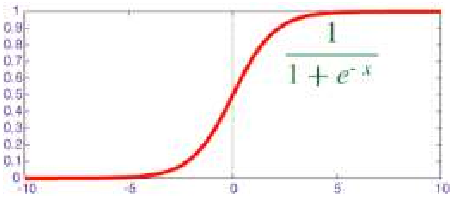
  - More generally: *any* differentiable function

$$y = f(x_1, x_2, \ldots, x_N; W)$$

We will assume this unless otherwise specified

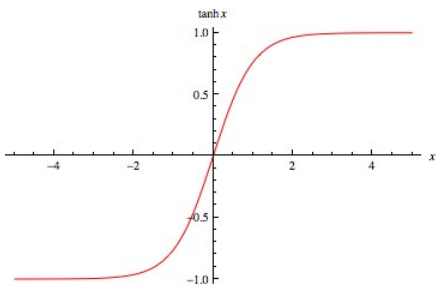
Parameters are weights w_i and bias b

Activations and their derivatives



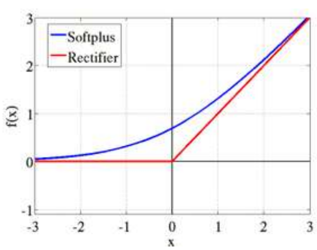
$$f(z) = \frac{1}{1+\exp(-z)}$$

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



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

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



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

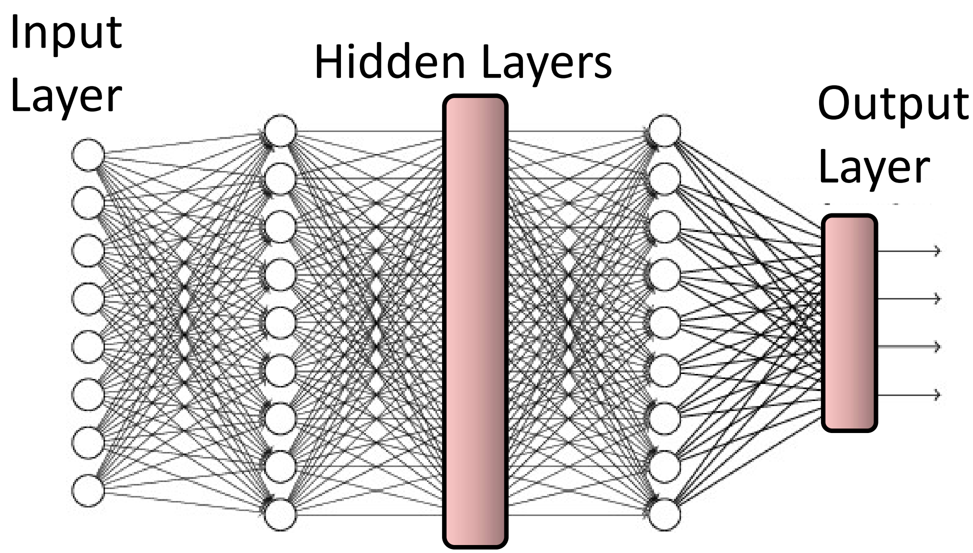
[*] $$f'(z) = \begin{cases} 1, z \geq 0 \\ 0, z < 0 \end{cases}$$

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

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

- Some popular activation functions and their derivatives

Vector Activations

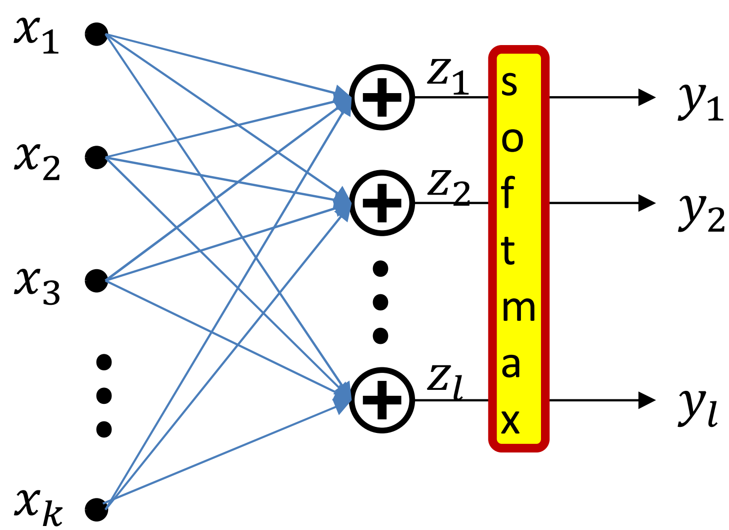


- We can also have neurons that have *multiple coupled* outputs

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

  - 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



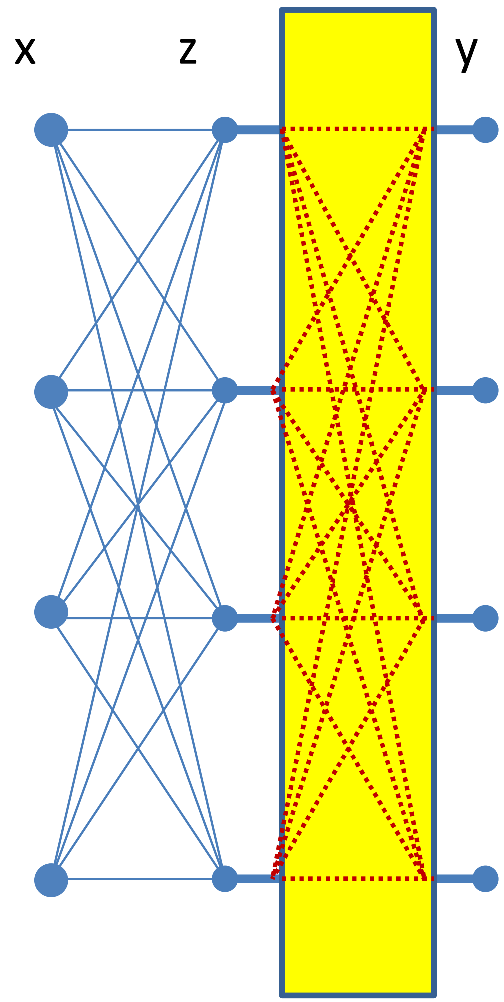
- Example: Softmax *vector* activation

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

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

Parameters are weights w_{ji} and bias b_i

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



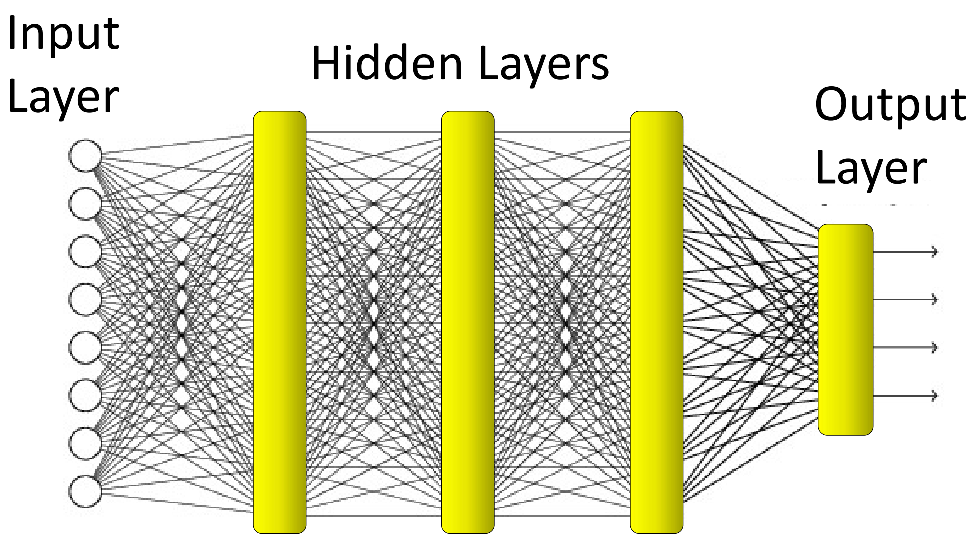
$$z_i = \sum_j w_{ji} x_j + b_i$$

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

Parameters are weights w_{ji} and bias b_i

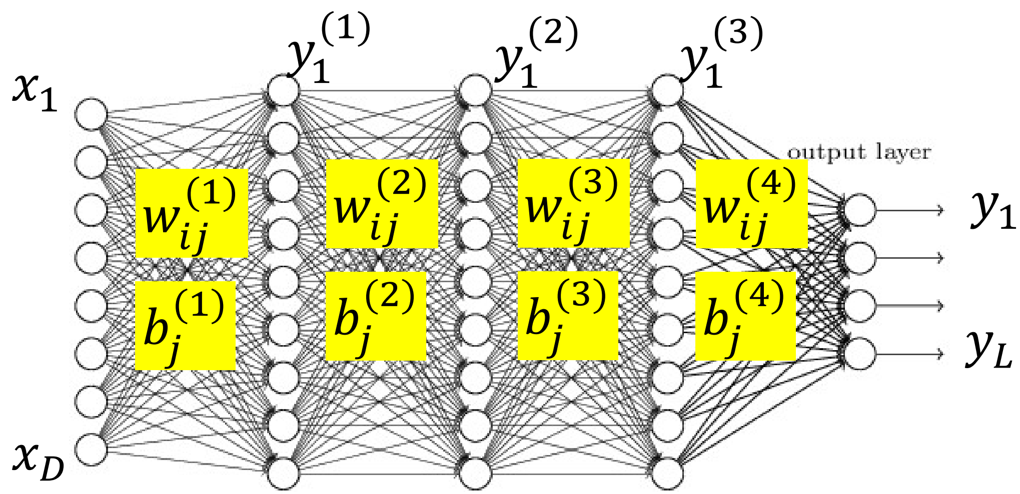
- A layer of multiplicative combination is a special case of vector activation

Typical network



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

Notation



- The input layer is the 0th layer
- We will represent the output of the i-th perceptron of the kth 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 jth unit of the k-th layer as $w_{ij}^{(k)}$
  - The bias to the jth unit of the k-th layer is $b_j^{(k)}$

Problem Setup: Things to define

- Given a training set of input-output pairs $(\boldsymbol{X}_1, \boldsymbol{d}_1), (\boldsymbol{X}_2, \boldsymbol{d}_2), \ldots, (\boldsymbol{X}_T, \boldsymbol{d}_T)$

- Minimize the following function

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

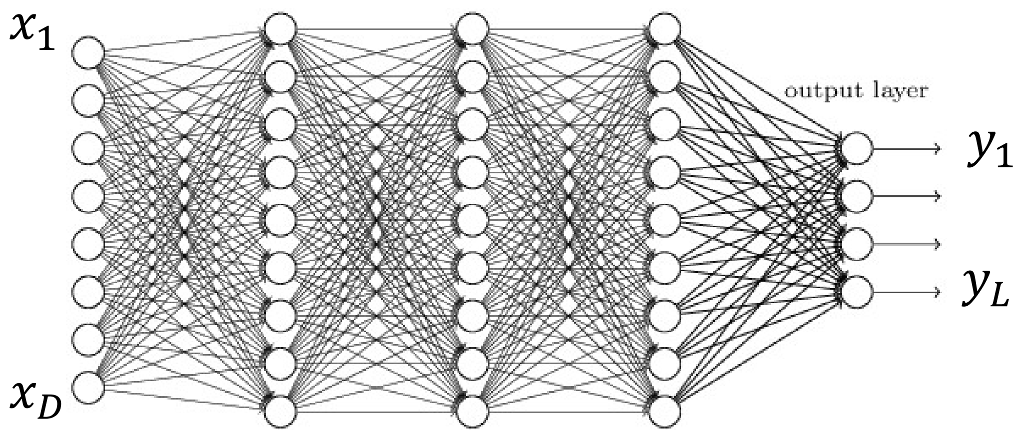
What is f() and what are its parameters W?

Problem Setup: Things to define

- Given a training set of input-output pairs $(\boldsymbol{X}_1, \boldsymbol{d}_1), (\boldsymbol{X}_2, \boldsymbol{d}_2), \ldots, (\boldsymbol{X}_T, \boldsymbol{d}_T)$
- What are these input-output pairs?

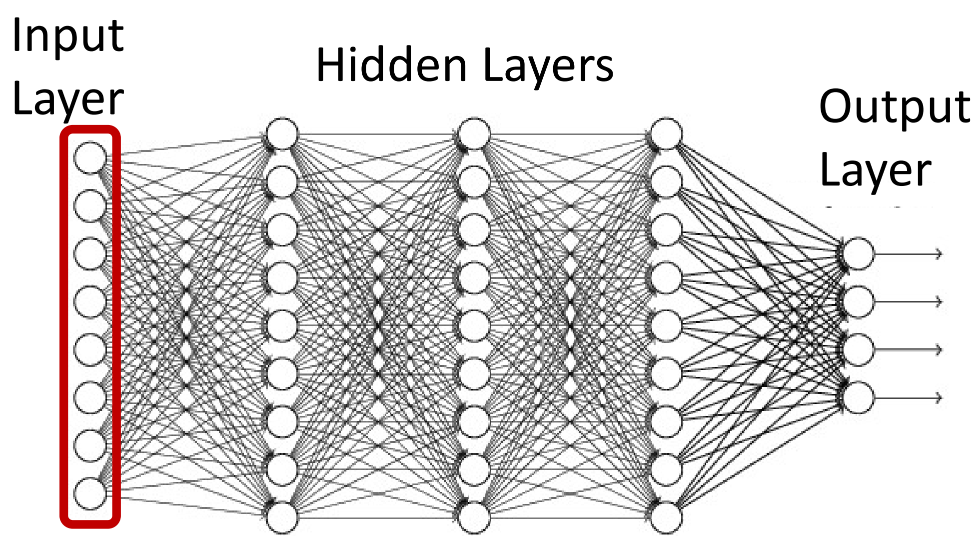
$$Loss(W) = \frac{1}{T}\sum_i div(f(X_i; W), d_i)$$

Input, target output, and actual output: Vector notation



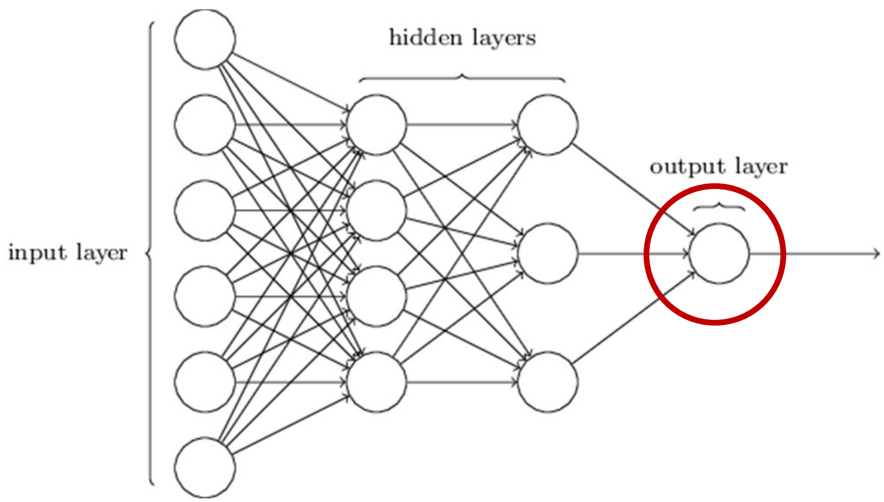
- Given a training set of input-output pairs $(X_1, d_1), (X_2, d_2), \ldots, (X_T, d_T)$
- $X_n = [x_{n1}, x_{n2}, \ldots, x_{nD}]^\top$ is the nth input vector
- $d_n = [d_{n1}, d_{n2}, \ldots, d_{nL}]^\top$ is the nth desired output
- $Y_n = [y_{n1}, y_{n2}, \ldots, y_{nL}]^\top$ is the nth vector 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

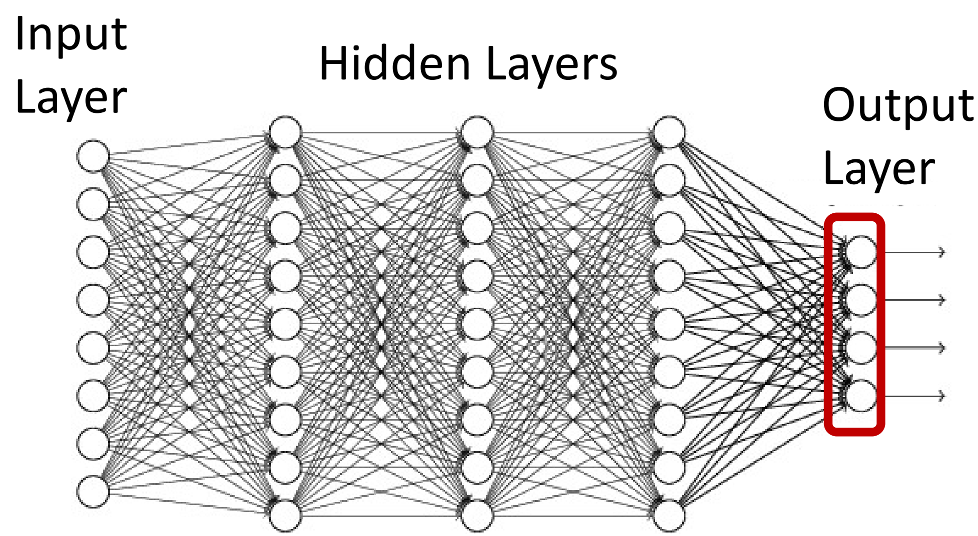
Representing the input



- 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

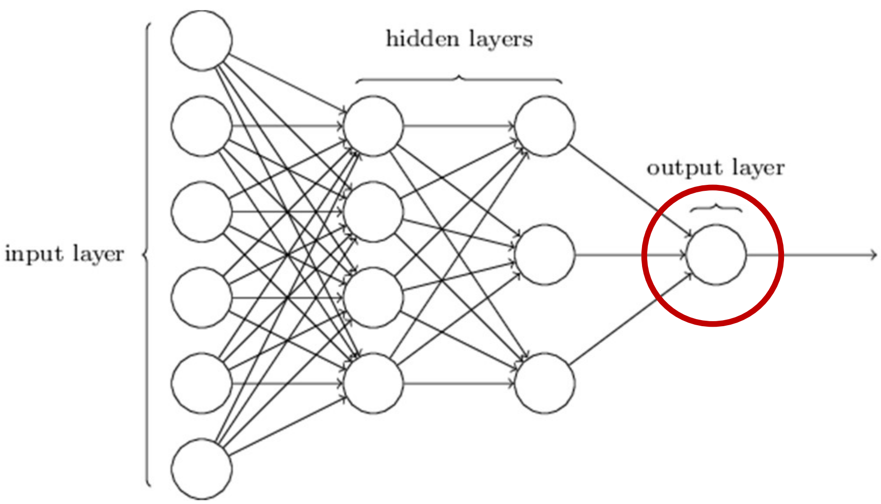
Representing the output





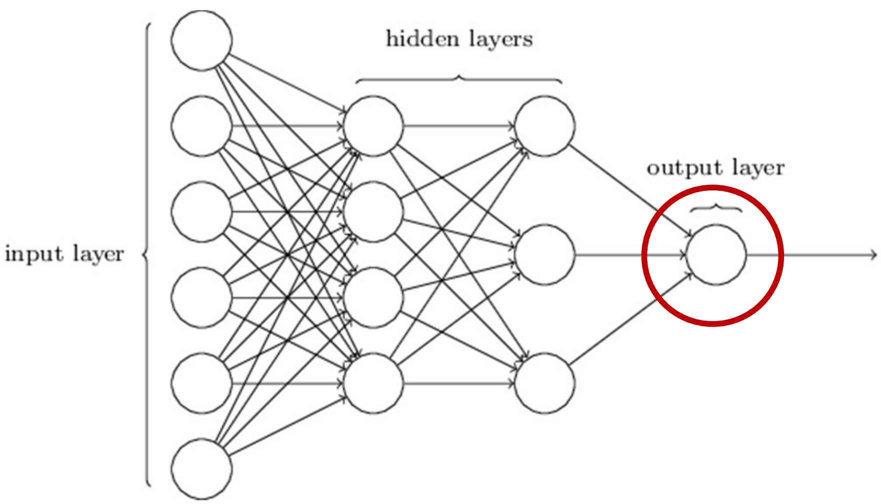
- If the desired *output* is real-valued, no special tricks are necessary
  - Scalar Output : single output neuron
    - d = scalar (real value)
  - Vector Output : as many output neurons as the dimension of the desired output
    - d = [d_1 d_2 .. d_L] (vector of real values)

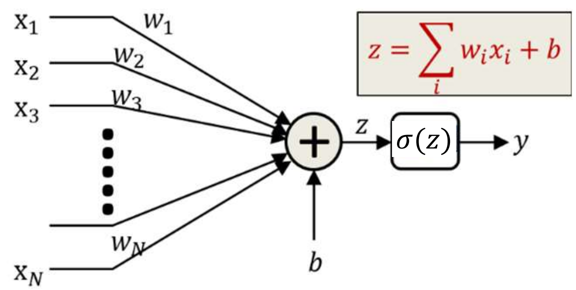
Representing the output

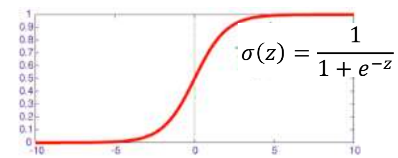


- If the desired output is binary (is this a cat or not), use a simple 1/0 representation of the desired output
  - 1 = Yes it's a cat
  - 0 = No it's not a cat.

Representing the output

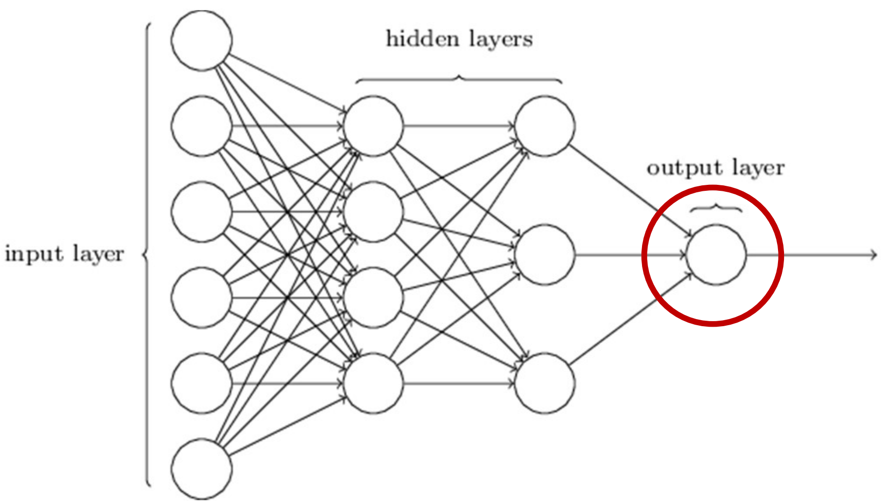


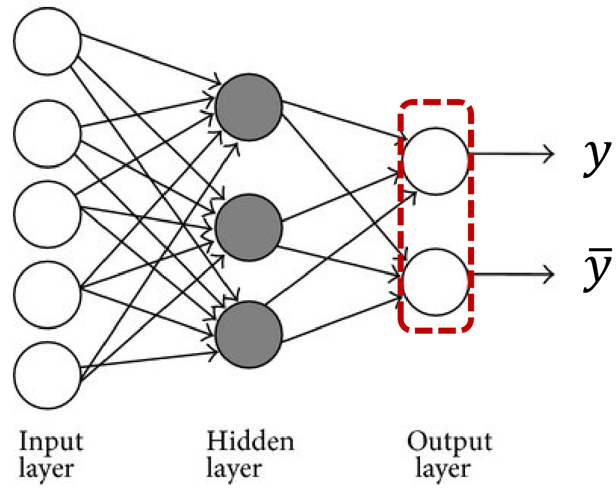




- If the desired output is binary (is this a cat or not), use a simple 1/0 representation of the desired output
- Output activation: Typically a sigmoid
  - Viewed as the *probability* $P(Y = 1|X)$ of class value 1
    - Indicating the fact that for actual data, in general a feature value X may occur 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: → [1 0]
  - No: → [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:

  $[\text{cat} \;\; \text{dog} \;\; \text{camel} \;\; \text{hat} \;\; \text{flower}]^T$

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

  cat: $[1\ 0\ 0\ 0\ 0]^T$

  dog: $[0\ 1\ 0\ 0\ 0]^T$

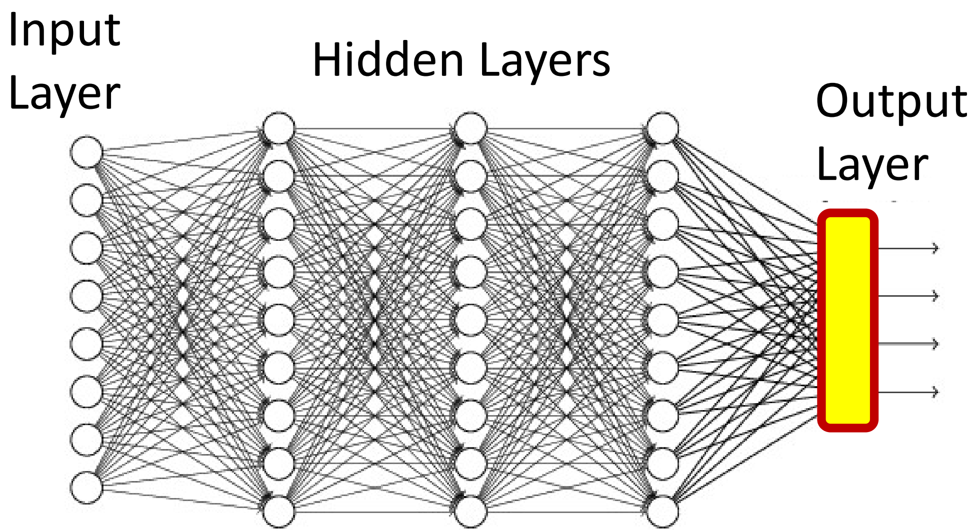
  camel: $[0\ 0\ 1\ 0\ 0]^T$

  hat: $[0\ 0\ 0\ 1\ 0]^T$

  flower: $[0\ 0\ 0\ 0\ 1]^T$

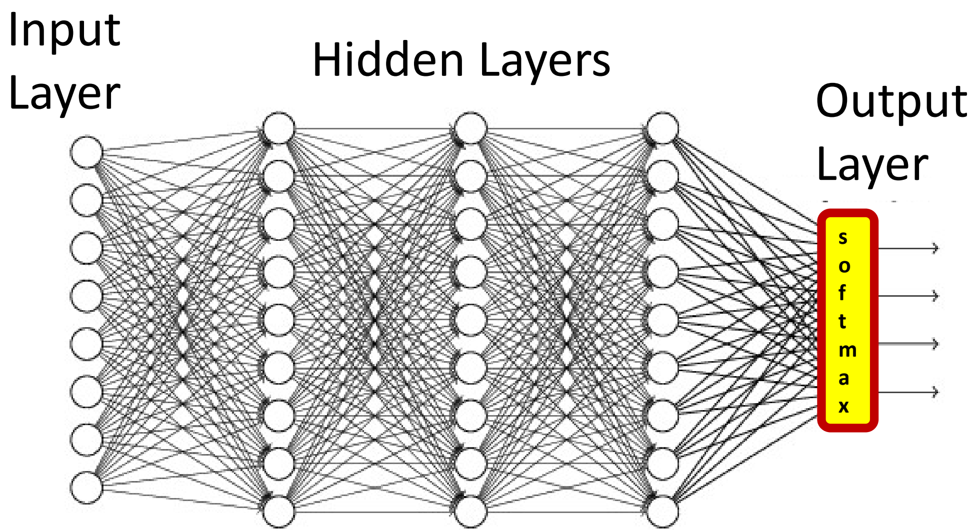
- For an input of any class, we will have a five-dimensional vector output with four zeros and a single 1 at the position of that class
- This is a *one hot vector*

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

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

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

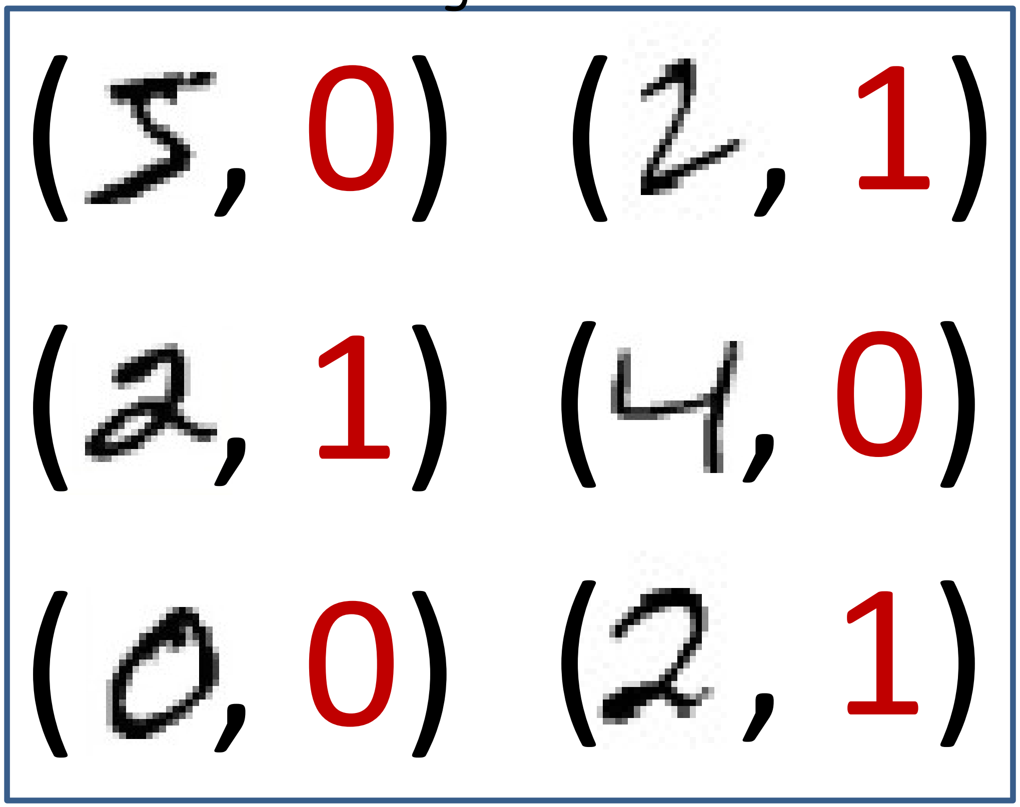
- This can be viewed as the probability $y_i = P(class = i|X)$

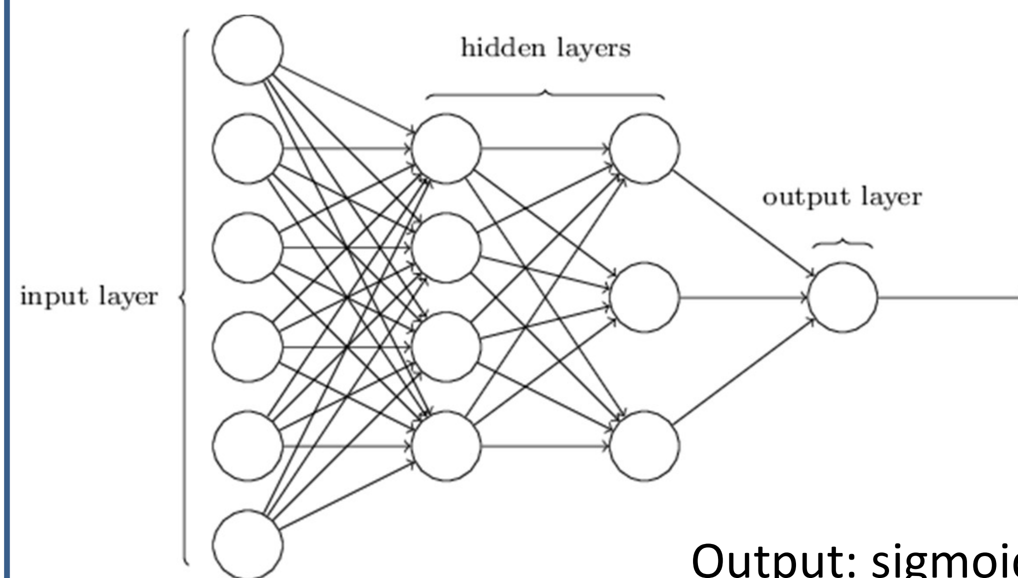
Inputs and outputs: Typical Problem Statement

- 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





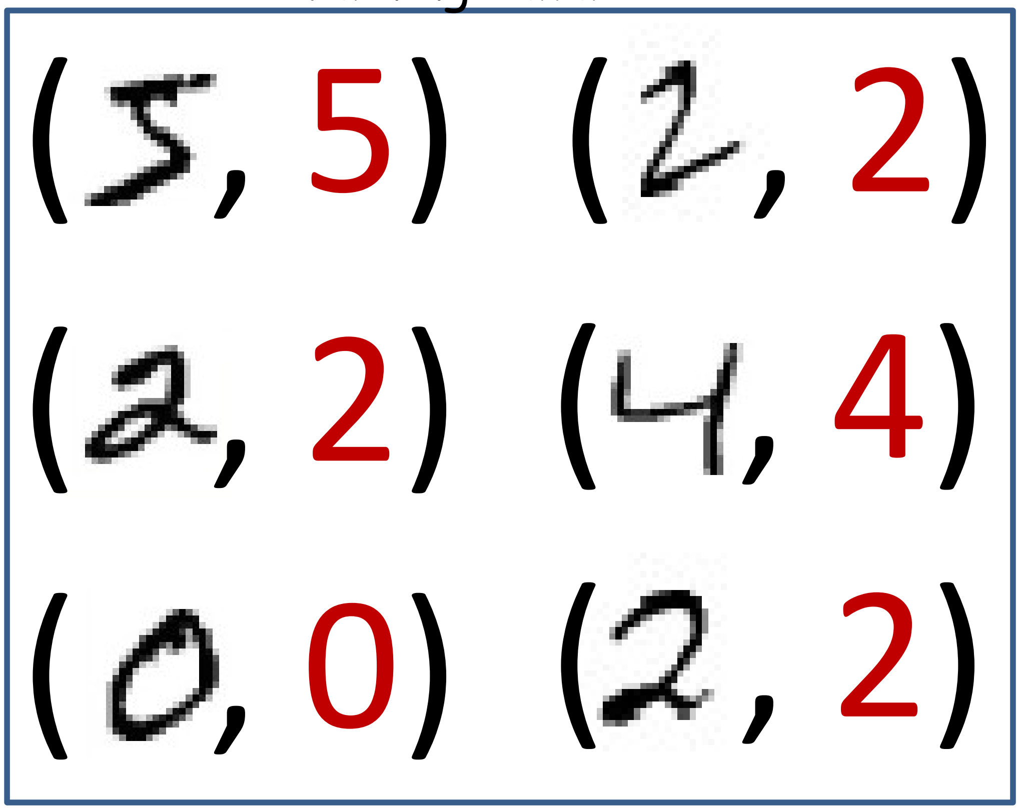
Output: sigmoid

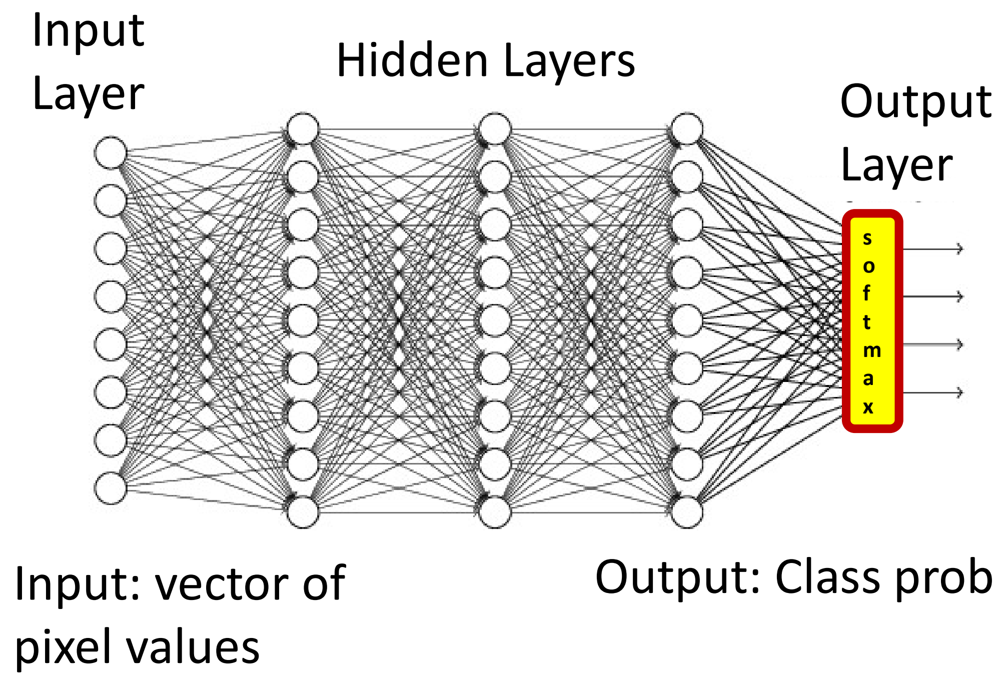
Input: vector of pixel values

- 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





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What is the divergence div()?

Problem Setup: Things to define

- Given a training set of input-output pairs $(\boldsymbol{X}_1, \boldsymbol{d}_1), (\boldsymbol{X}_2, \boldsymbol{d}_2), \ldots, (\boldsymbol{X}_T, \boldsymbol{d}_T)$

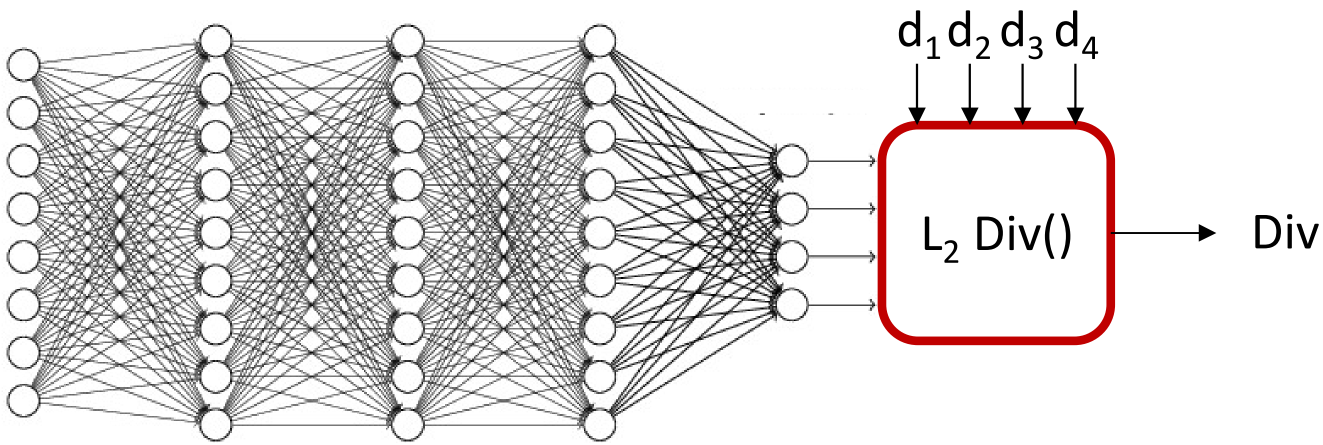
- Minimize the following function

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

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

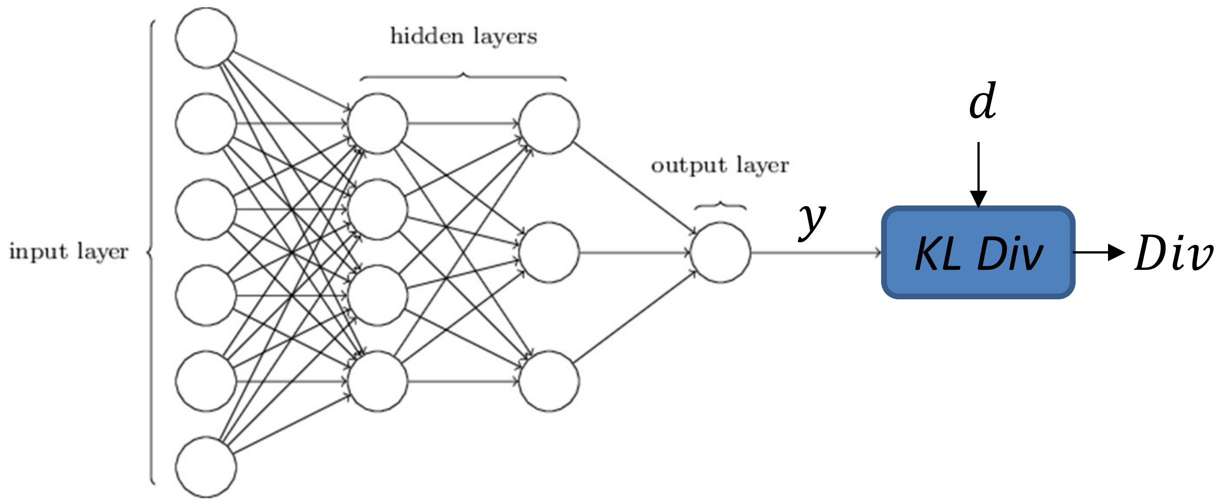
$$Div(Y,d) = \frac{1}{2}\|Y-d\|^2 = \frac{1}{2}\sum_i (y_i - d_i)^2$$

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

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

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

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

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

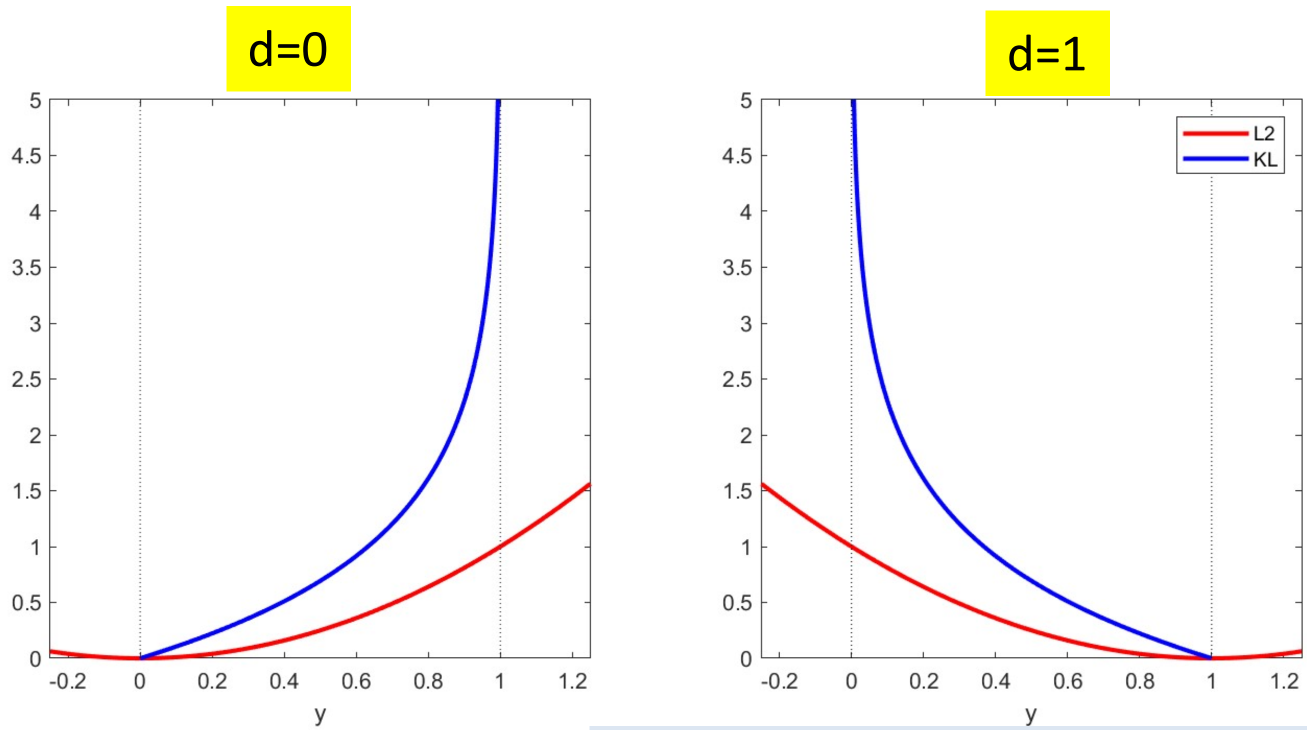
  - Minimum when $d = Y$

- Derivative

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

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

KL vs L2

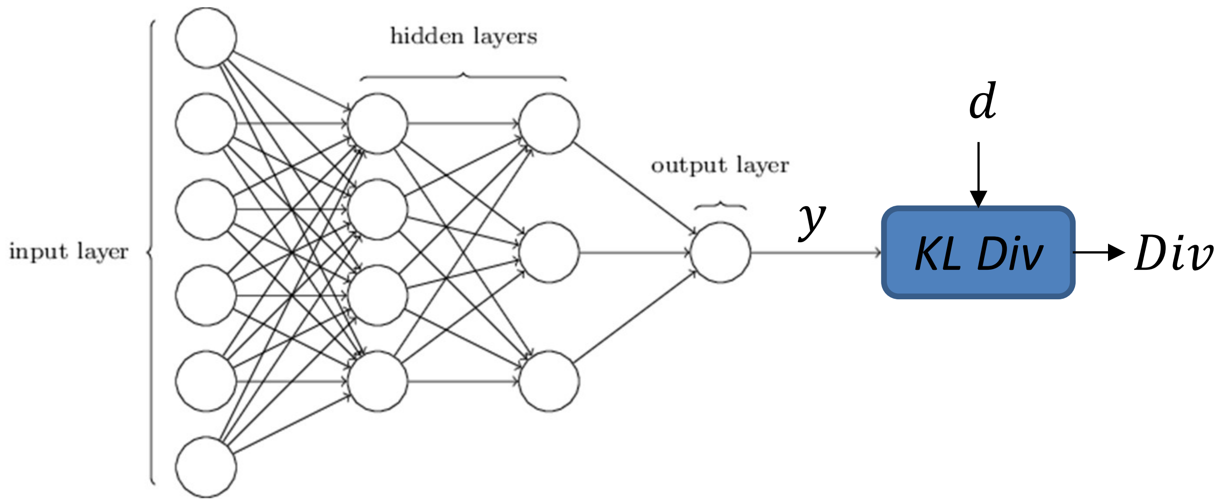


$$L2(Y,d) = (y-d)^2$$

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

- 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



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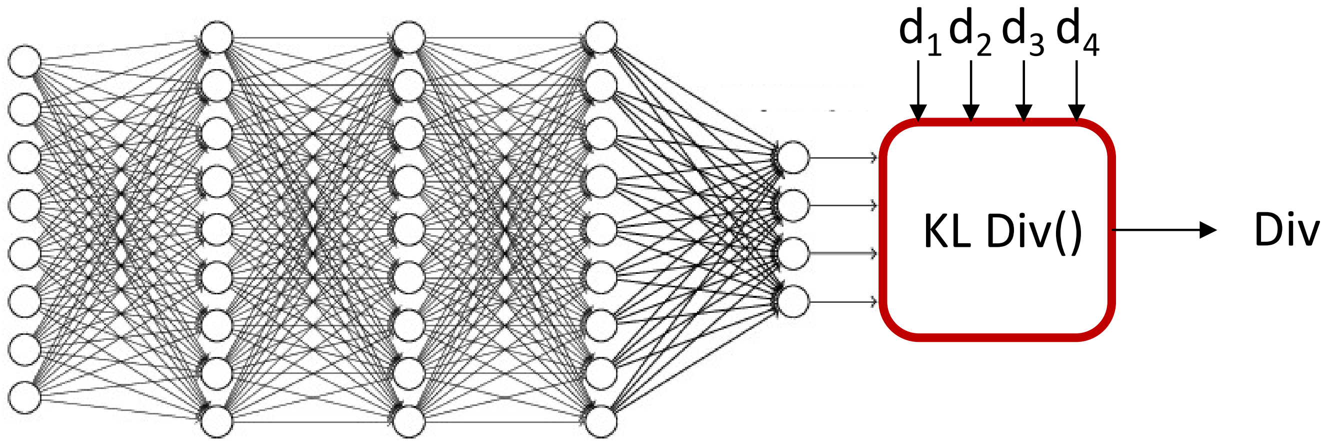
Note: when $y = d$ the derivative is *not* 0

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

For multi-class classification



- Desired output d is a one hot vector $[0\ 0\ \ldots\ 1\ \ \ldots\ 0\ 0\ 0\ ]$ with the 1 in the c-th position (for class c)
- Actual output will be probability distribution $[y_1, y_2, \ldots\ ]$
- 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

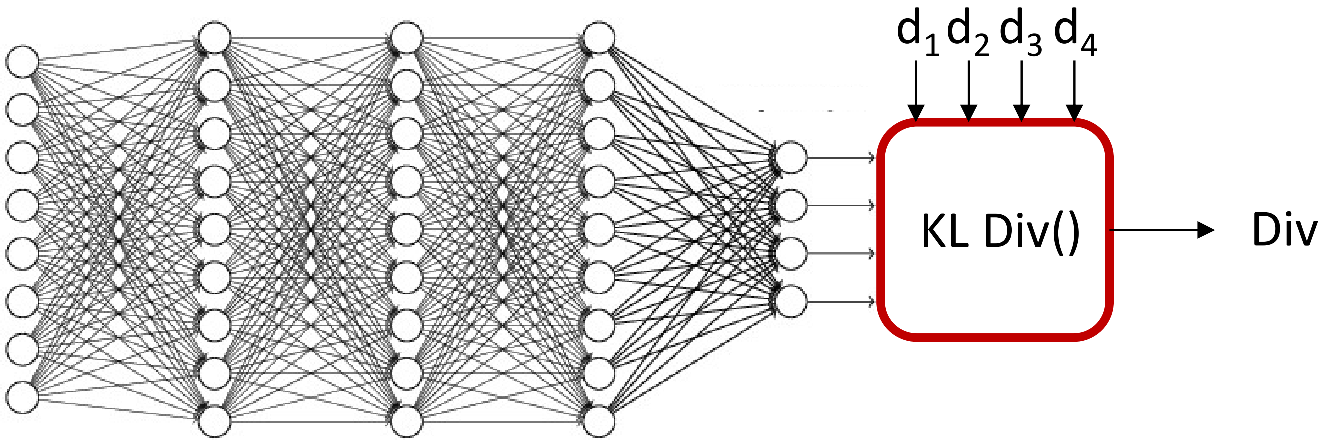
$$\frac{dDiv(Y,d)}{dY_i} = \begin{cases} -\frac{1}{y_c} & for\ the\ c-th\ component \\ 0 & for\ remaining\ component \end{cases}$$

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

The slope is negative w.r.t. y_c

Indicates *increasing* y_c will *reduce* divergence

For multi-class classification



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

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

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

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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:

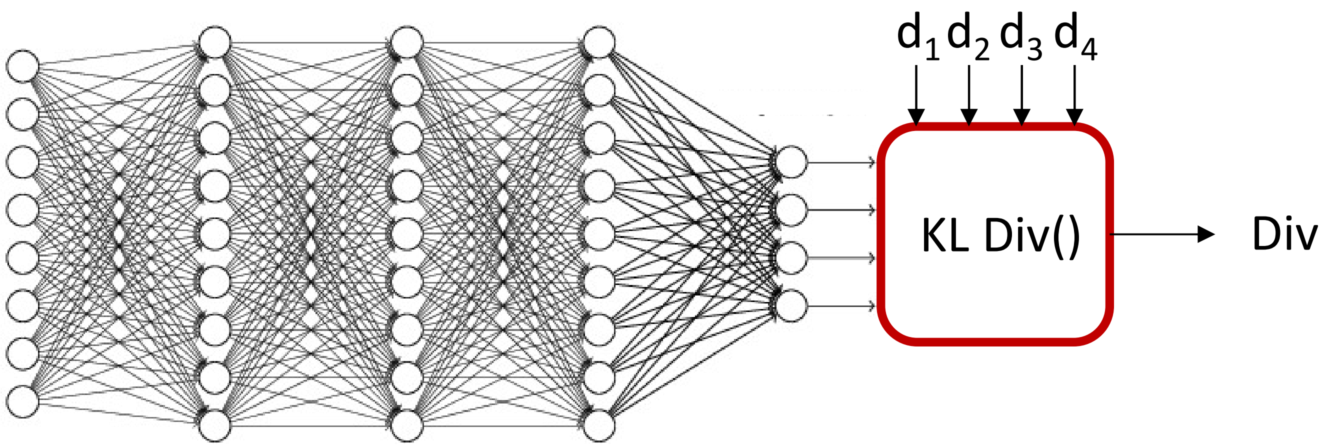
$$Xent(Y,d) = -\sum_i d_i \log y_i$$

- 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 $[\epsilon \;\; \epsilon \ldots (1-(K-1)\epsilon) \ldots \epsilon \;\; \epsilon \;\; \epsilon]$ with the value $1-(\mathrm{K}-1)\epsilon$ in the c-th position (for class c) and ϵ elsewhere for some small ϵ
  - "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

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

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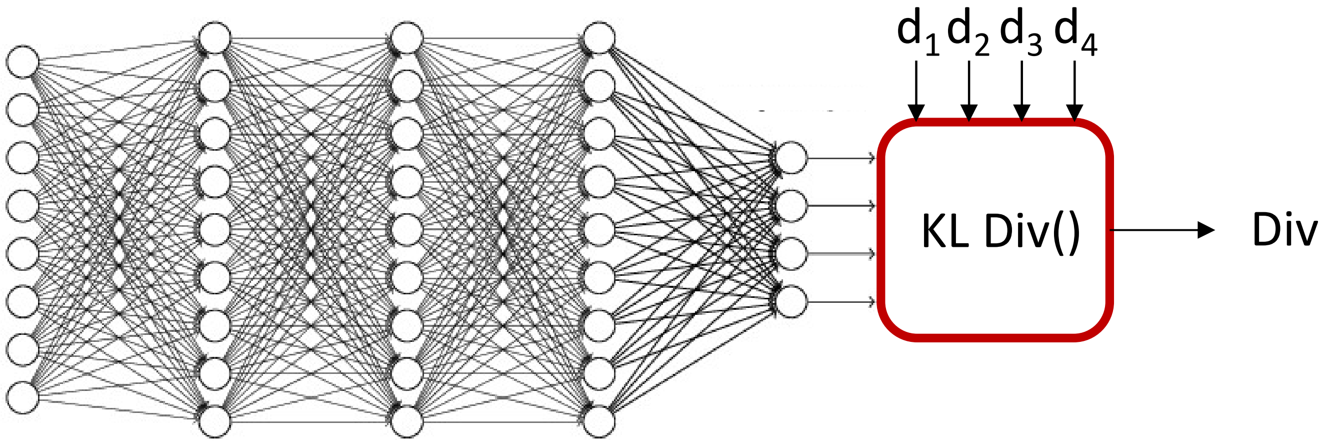

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Negative derivatives encourage *increasing* the probabilities of *all* classes, including *incorrect* classes! (Seems wrong, no?)

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- Minimize the following function

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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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  - If the gradient is not 0 at a minimum, it must be a local minimum

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