CSC 561: Neural Networks and Deep Learning

Learning (part 2)

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Neural Networks
Learning the network: Backprop

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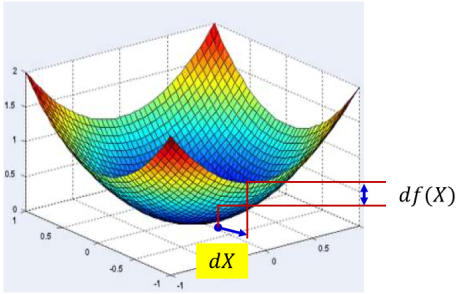
Lecture 4

Gradient of a scalar function of a vector

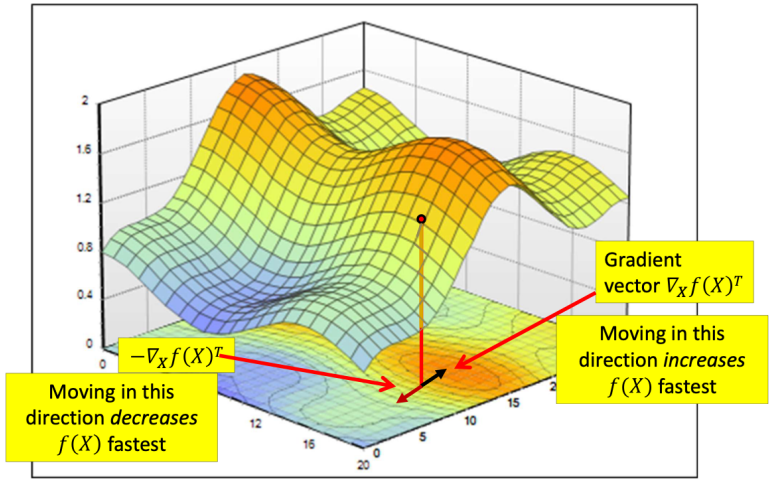


- The *derivative* $\nabla_X f(X)$ of a scalar function $f(X)$ of a multi-variate input X is a multiplicative factor that gives us the change in $f(X)$ for tiny variations in X

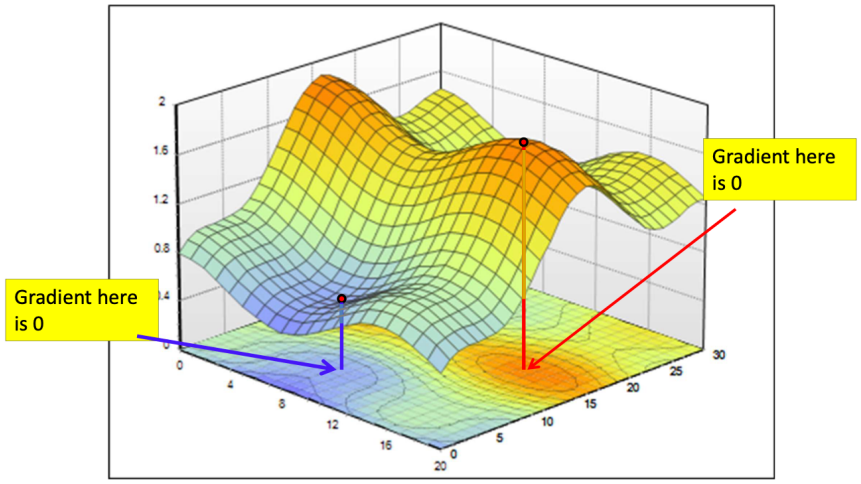
$$df(X) = \nabla_X f(X) dX$$

  - $\nabla_X f(X) = \left[\frac{\partial f(X)}{\partial x_1} \quad \frac{\partial f(X)}{\partial x_2} \quad \cdots \quad \frac{\partial f(X)}{\partial x_n}\right]$
- The ***gradient*** is the transpose of the derivative $\nabla_X f(X)^T$
  - A column vector of the same dimensionality as X

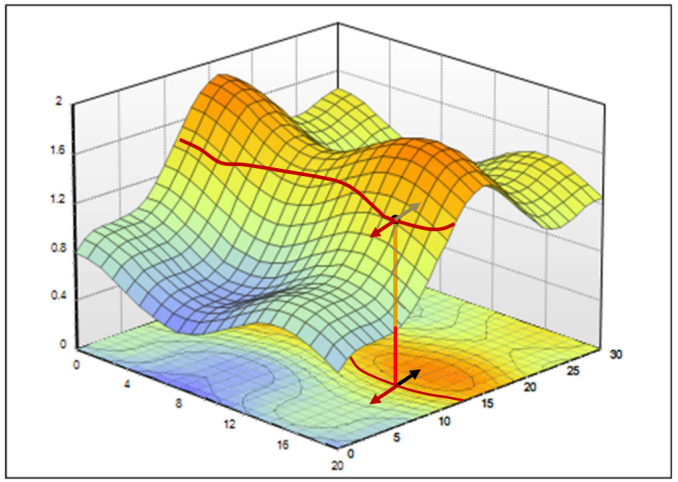
Gradient



Gradient



Properties of Gradient: 2



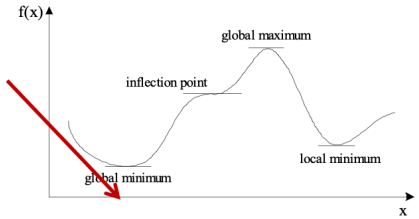
- The gradient vector $\nabla_X f(X)^T$ is perpendicular to the level curve

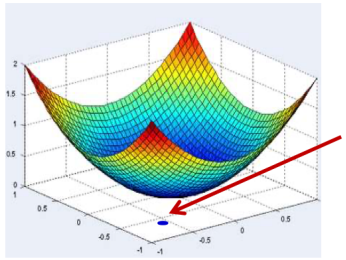
The Hessian

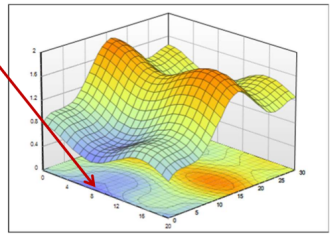
- The Hessian of a function $f(x_1, x_2, \ldots, x_n)$ is given by the second derivative

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

The problem of optimization

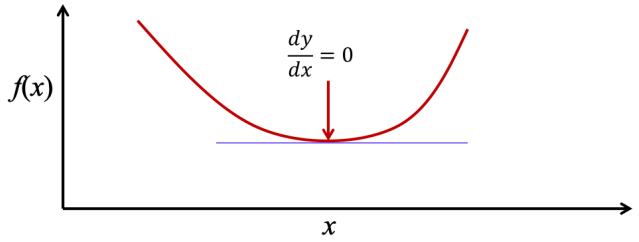






- General problem of optimization: Given a function $\mathbf{f}(\boldsymbol{x})$ of some variable $\boldsymbol{x}$ …
- Find the value of $\boldsymbol{x}$ where $\mathbf{f}(\boldsymbol{x})$ is minimum

Finding the minimum of a function

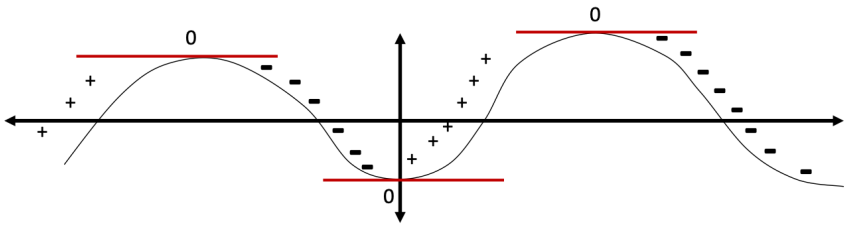


- Find the value x at which $f'(x) = 0$
  - Solve

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

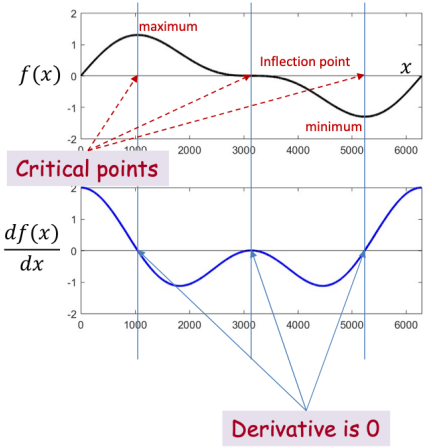
- The solution is a "turning point"
  - Derivatives go from positive to negative or vice versa at this point
- But is it a minimum?

Turning Points



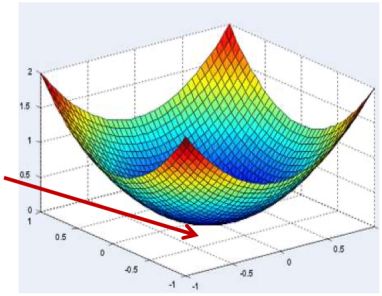
- Both *maxima* and *minima* have zero derivative
- Both are turning points

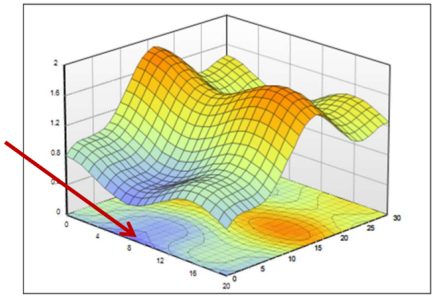
A note on derivatives of functions of single variable



- 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

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

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

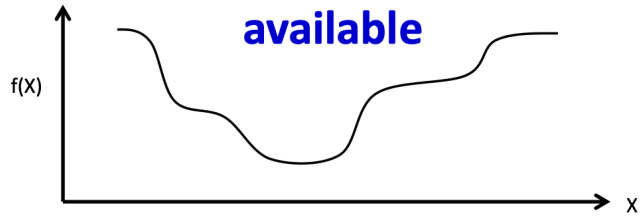
Unconstrained Minimization of function (Example)

- 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

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

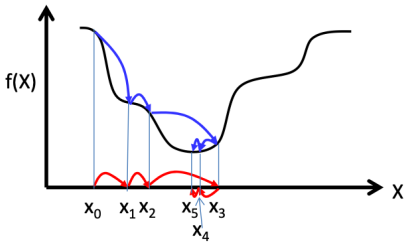
- All the eigenvalues are positives => the Hessian matrix is positive definite
- The point $x = \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} = \begin{bmatrix} -1 \\ -1 \\ -1 \end{bmatrix}$ is a minimum

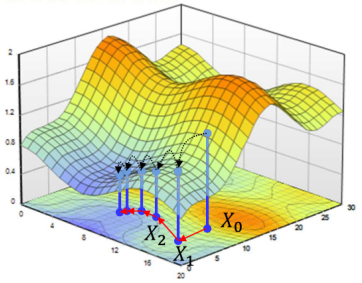
Closed Form Solutions are not always available



- 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

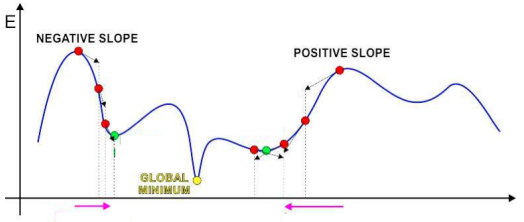
Iterative solutions





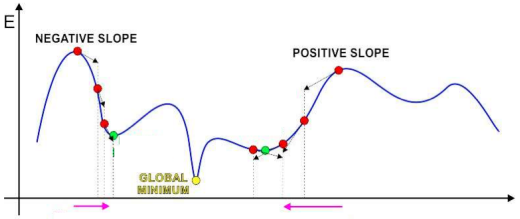
- Iterative solutions
  - Start from an initial guess X_0 for the optimal X
  - Update the guess towards a (hopefully) "better" value of $f(X)$
  - Stop when $f(X)$ no longer decreases
- Problems:
  - Which direction to step in
  - How big must the steps be

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 → moving right decreases error
      - A positive derivative → moving left decreases error
  - Shift point in this direction

The Approach of Gradient Descent



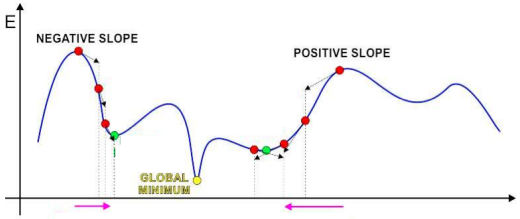
- Iterative solution: Trivial algorithm
  - Initialize x^0
  - While $f'(x^k) \neq 0$
    - If $sign\left(f'(x^k)\right)$ is positive:

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

    - Else

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

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

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 η^k

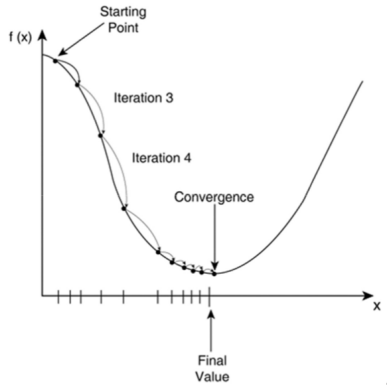
Gradient descent convergence criteria

- 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

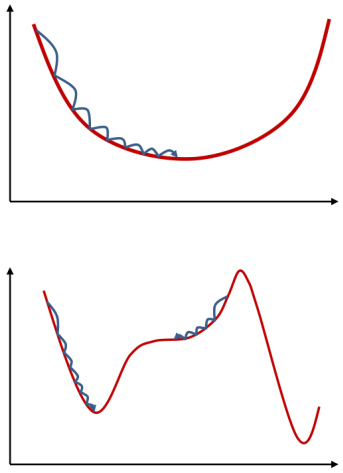
$$\left\|\nabla_x f(x^k)\right\| < \varepsilon_2$$



Overall Gradient Descent Algorithm

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

- Returning to our problem from our detour..

Problem Statement

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

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

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

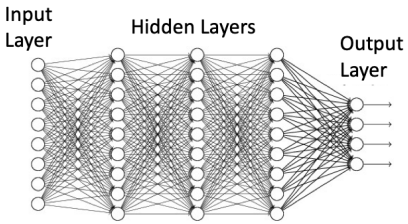
Problem Setup: Things to define

- 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

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

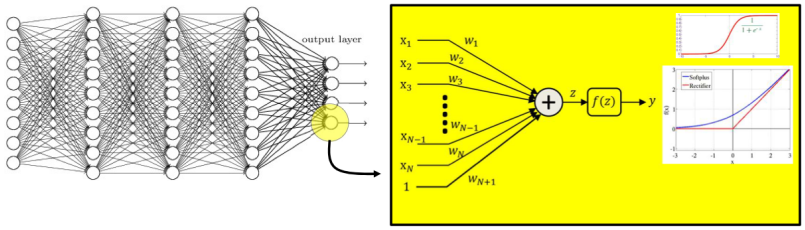
What is f() and what are its parameters W?

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

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

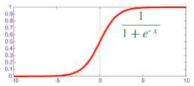
We will assume this unless otherwise specified

Parameters are weights w_i and bias b

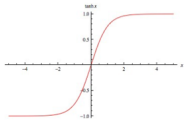
  - More generally: *any* differentiable function

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

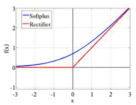
Activations and their derivatives



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



$f(z) = \tanh(z)$ | $f'(z) = (1-f^2(z))$

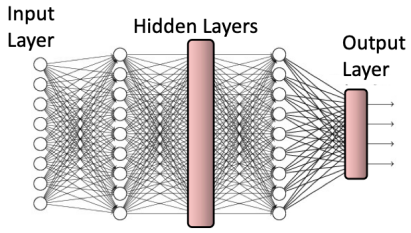


$f(z) = \begin{cases} z, & z \geq 0 \\ 0, & z < 0 \end{cases}$ [*] $f'(z) = \begin{cases} 1, z \geq 0 \\ 0, z < 0 \end{cases}$

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

- Some popular activation functions and their derivatives

Vector Activations

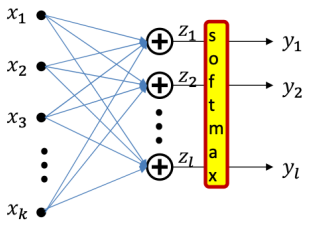


- We can also have neurons that have *multiple coupled* outputs

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

  - 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



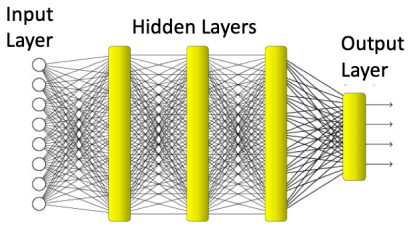
- Example: Softmax *vector* activation

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

Parameters are weights w_{ji} and bias b_i

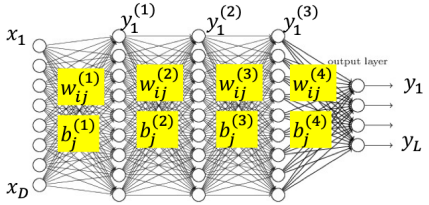
$$y = \frac{exp(z_i)}{\sum_j exp(z_j)}$$

Typical network



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

Notation



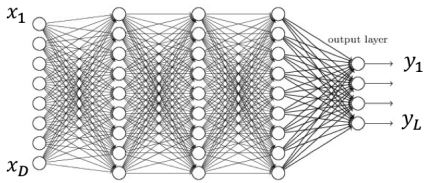
- The input layer is the 0th layer
- We will represent the output of the i-th perceptron of the kth layer as $y_i^{(k)}$
  - **Input to network:** $y_i^{(0)} = x_i$
  - **Output of network:** $y_i = y_i^{(N)}$
- We will represent the weight of the connection between the i-th unit of the k-1th layer and 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 $(\boldsymbol{X}_1, \boldsymbol{d}_1), (\boldsymbol{X}_2, \boldsymbol{d}_2), \ldots, (\boldsymbol{X}_T, \boldsymbol{d}_T)$
- What are these input-output pairs?

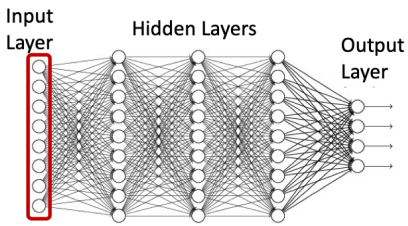
$$Loss(W) = \frac{1}{T}\sum_i div(f(X_i; W), d_i)$$

Input, target output, and actual output: Vector notation



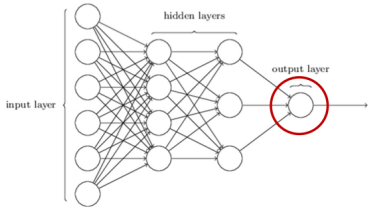
- Given a training set of input-output pairs $(X_1, d_1), (X_2, d_2), \ldots, (X_T, d_T)$
- $X_n = [x_{n1}, x_{n2}, \ldots, x_{nD}]^\top$ is the nth input vector
- $d_n = [d_{n1}, d_{n2}, \ldots, d_{nL}]^\top$ is the nth desired output
- $Y_n = [y_{n1}, y_{n2}, \ldots, y_{nL}]^\top$ is the nth vector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

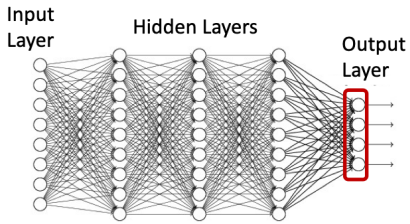
Representing the input



- 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

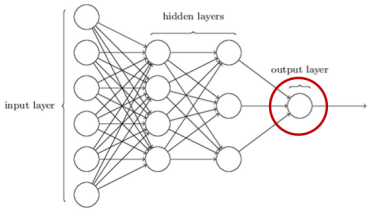
Representing the output





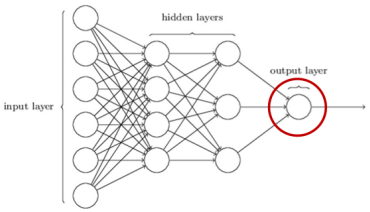
- If the desired *output* is real-valued, no special tricks are necessary
  - Scalar Output : single output neuron
    - d = scalar (real value)
  - Vector Output : as many output neurons as the dimension of the desired output
    - d = [d_1 d_2 .. d_L] (vector of real values)

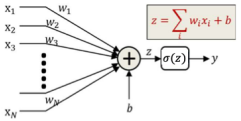
Representing the output

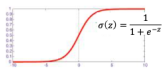


- If the desired output is binary (is this a cat or not), use a simple 1/0 representation of the desired output
  - 1 = Yes, it's a cat
  - 0 = No, it's not a cat.

Representing the output

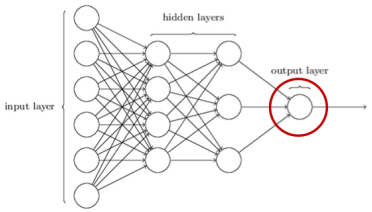


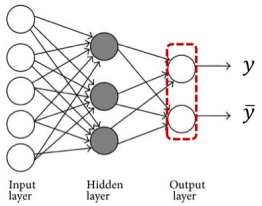




- If the desired output is binary (is this a cat or not), use a simple 1/0 representation of the desired output
- Output activation: Typically, a sigmoid
  - Viewed as the *probability* $P(Y = 1|X)$ of class value 1
    - Indicating the fact that for actual data, in general a feature value X may occur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

  [cat dog camel hat flower]^T
- For inputs of each of the five classes the desired output is:

  cat: [1 0 0 0 0]^T

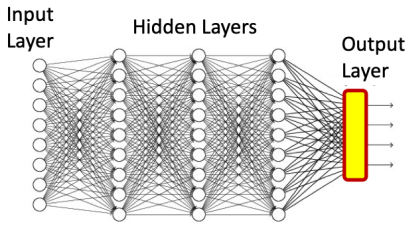
  dog: [0 1 0 0 0]^T

  camel: [0 0 1 0 0]^T

  hat: [0 0 0 1 0]^T

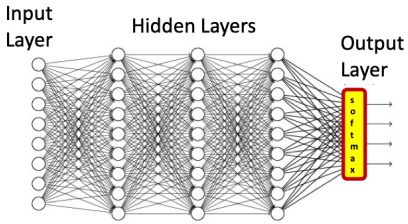
  flower: [0 0 0 0 1]^T
- For an input of any class, we will have a five-dimensional vector output with four zeros and a single 1 at the position of that class
- This is a *one hot vector*

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 $y_i = P(class = i|X)$

Problem Setup: Things to define

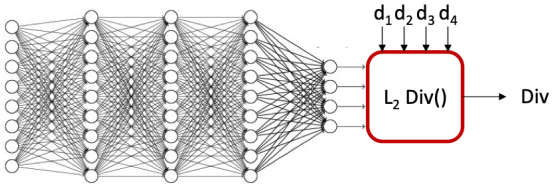
- Given a training set of input-output pairs $(\boldsymbol{X}_1, \boldsymbol{d}_1), (\boldsymbol{X}_2, \boldsymbol{d}_2), \ldots, (\boldsymbol{X}_T, \boldsymbol{d}_T)$
- Minimize the following function

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

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

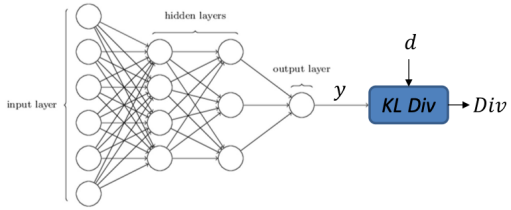
$$Div(Y,d) = \frac{1}{2}\|Y-d\|^2 = \frac{1}{2}\sum_i (y_i - d_i)^2$$

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

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

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

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

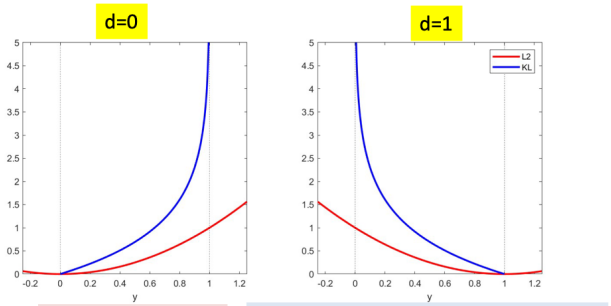
$$Div(Y,d) = -dlogY - (1-d)\log(1-Y)$$

  - Minimum when $d = Y$
- Derivative

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

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

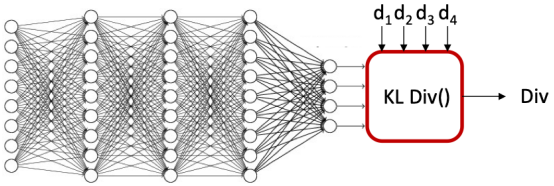
KL vs L2



$L2(Y,d) = (y-d)^2$ $\quad$ $KL(Y,d) = -dlogY - (1-d)\log(1-Y)$

- 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 multi-class classification



- Desired output d is a one hot vector [0 0 … 1 … 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

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:

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

- When the desired target d_i is one-hot, $\sum_i d_i \log d_i = 0$
  - KL and cross-entropy are identical
  - $Xent(Y,d) = -\log y_i$
  - Minimizing cross-entropy simply maximizes the probability of the target class
- We will continue discussing in terms of KL, but the discussion applies directly to Cross-entropy as well

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:

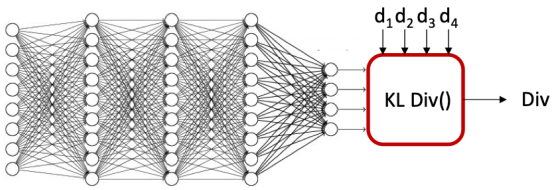
$$Xent(Y,d) = -\sum_i d_i \log y_i$$

- More generally, 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

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