

Gradient Descent

Problem Statement

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

- Minimize the following function

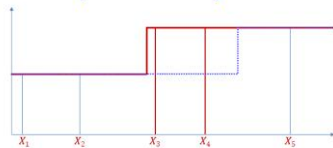
$$Loss(W) = \frac{1}{N} \sum_i \text{div}(f(X_i; W), d_i)$$

w.r.t W

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

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The Empirical Classification error



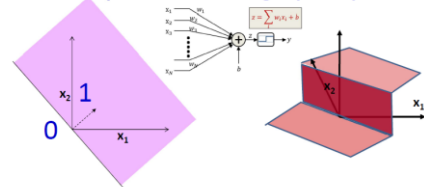
- The obvious error metric in a classifier is binary
 - The classifier is either right (error=0) or wrong (error=1)
 - Either $f(X; W) = d$, or $f(X; W) \neq d$

$$\text{EmpiricalError}(W) = \frac{1}{N} \sum_{i=1}^N \mathbb{1}(f(X_i; W) \neq d_i)$$

- Learning the classifier: Minimizing the count of misclassifications

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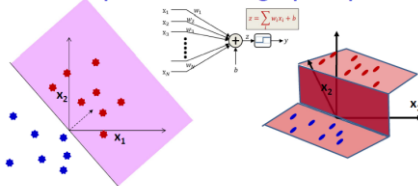
The simplest MLP: a single perceptron



- Learn this function
 - A step function across a hyperplane

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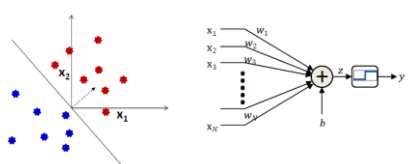
The simplest MLP: a single perceptron



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

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Learning the perceptron



- Given a number of input output pairs, learn the weights and bias

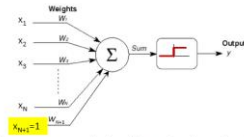
$$y = \begin{cases} 1 & \text{if } \sum_{i=1}^N w_i X_i + b \geq 0 \\ 0 & \text{otherwise} \end{cases}$$

Learn $W = [w_1, \dots, w_N]^T$ and b , given several (X, y) pairs

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

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Restating the perceptron



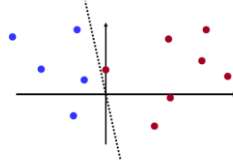
- Restating the perceptron equation by adding another dimension to X

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

where $X_{N+1} = 1$

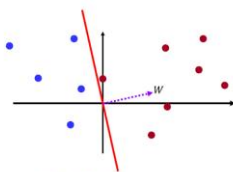
- Note that the boundary $\sum_{i=1}^{N+1} w_i X_i = 0$ is now a hyperplane through origin

The Perceptron Problem



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

The Perceptron Problem

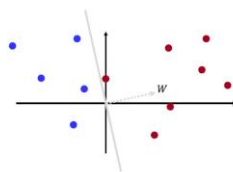


Key: Red 1, Blue -1

When the inner product of two vectors is zero, what would be the angle between two vectors?

- Find the hyperplane $\sum_{i=1}^{N+1} w_i X_i = 0$ that perfectly separates the two groups of points
 - Let vector $W = [w_1, w_2, \dots, w_{N+1}]^T$ and vector $X = [x_1, x_2, \dots, x_N, 1]^T$
 - $\sum_{i=1}^{N+1} w_i X_i = W^T X$ is an inner product
 - $W^T X = 0$ is the hyperplane comprising all X 's orthogonal to vector W
- Learning the perceptron = finding the weight vector W for the separating hyperplane
 - W points in the direction of the positive class

The Perceptron Problem



Key: Red 1, Blue -1

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

Perceptron Algorithm: Summary

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

$$W = W + X_i$$
 - If instance is negative class (negative misclassified as positive)

$$W = W - X_i$$

Perceptron Learning Algorithm

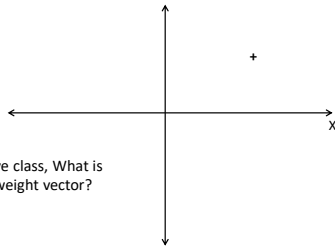
- Given N training instances $(X_1, y_1), (X_2, y_2), \dots, (X_N, y_N)$
 - $y_i = +1$ or -1

Using a $\pm 1/-1$ representation for classes to simplify notation

- Initialize W
- Cycle through the training instances:

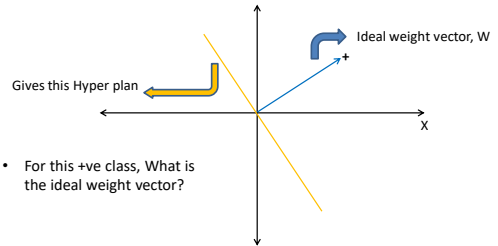
```
do
  For  $i = 1 \dots N_{\text{train}}$ 
     $O(X_i) = \text{sign}(W^T X_i)$ 
    if  $O(X_i) \neq y_i$ 
       $W = W + y_i X_i$ 
until no more classification errors
```

Ideal Weight vector



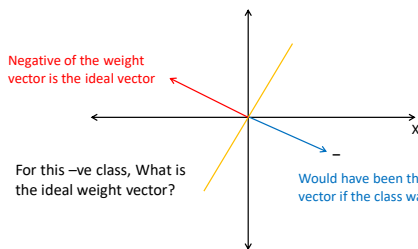
- For this +ve class, What is the ideal weight vector?

Ideal Weight vector



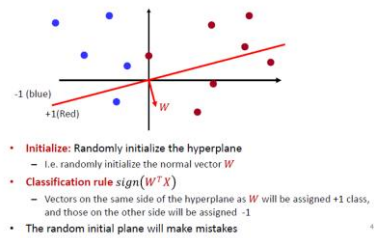
- For this +ve class, What is the ideal weight vector?

Ideal Weight vector



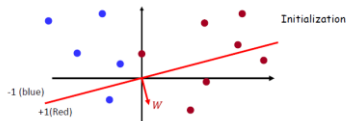
- For this -ve class, What is the ideal weight vector?
- Would have been the ideal weight vector if the class was +ve instance

A Simple Method: The Perceptron Algorithm



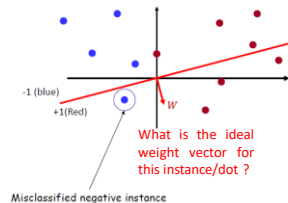
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Perceptron Algorithm



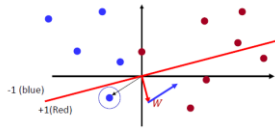
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Perceptron Algorithm



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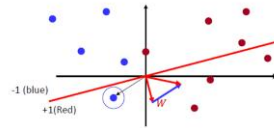
Perceptron Algorithm



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

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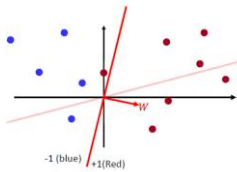
Perceptron Algorithm



The new weight

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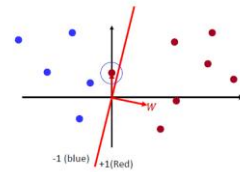
Perceptron Algorithm



The new weight (and boundary)

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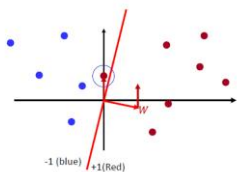
Perceptron Algorithm



Misclassified *positive* instance

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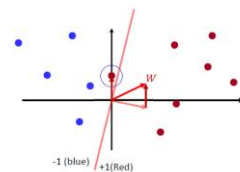
Perceptron Algorithm



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

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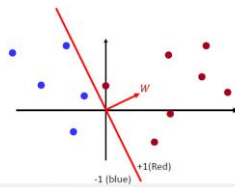
Perceptron Algorithm



The new weight vector

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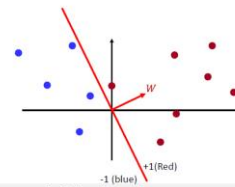
Perceptron Algorithm



The new decision boundary
Perfect classification, no more updates, we are done

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Perceptron Algorithm



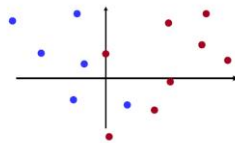
The new decision boundary
Perfect classification, no more updates, we are done

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

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The Perceptron Solution: when classes are not linearly separable

Key: Red 1, Blue = -1

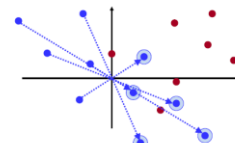


- When classes are not linearly separable, not possible to find a separating hyperplane
 - No "support" plane for reflected data
 - Some points will always lie on the other side
- Model does not support perfect classification of this data
- Perceptron algorithm will never converge

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A simpler solution

Key: Red 1, Blue = -1

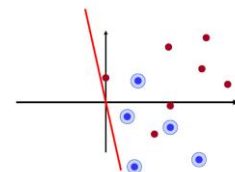


- Reflect all the negative instances across the origin
 - Negate every component of vector X
- If we use class $y \in \{-1, +1\}$ notation for the labels (instead of $y \in \{0, 1\}$), we can simply write the "reflected" values as $X' = yX$
 - Will retain the features X for the positive class, but reflect/negate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

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The Perceptron Solution

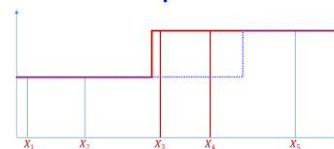
Key: Red 1, Blue = -1



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

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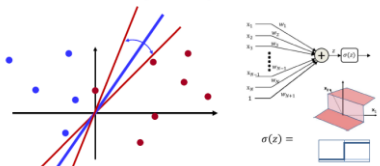
The problem



- Our binary error metric is not useful
 - To improve the classifier we must move the blue dotted line left
 - But if we move it only slightly, moving it either right or left results in no change in error

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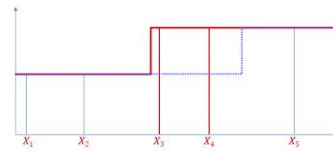
Why this problem?



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

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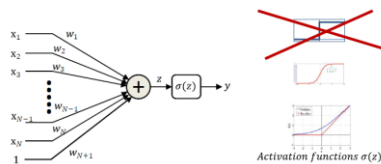
The solution



- Change our way of computing the mismatch such that modifying the classifier slightly lets us know if we are going the right way or not
 - This requires changing both, our activation functions, and the manner in which we evaluate the mismatch between the classifier output and the target output
 - Our mismatch function will now not actually count errors, but a proxy for it

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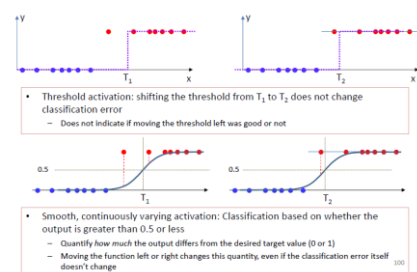
Solution: Differentiable activation



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

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Differentiable Mismatch function



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

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

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A brief note on derivatives..

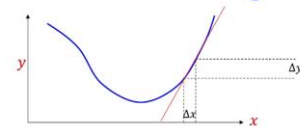


- A derivative of a function at any point tells us how much a minute increment to the *argument* of the function will increment the *value* of the function
 - For any $y = f(x)$, expressed as a multiplier α to a tiny increment Δx to obtain the increments Δy to the output

$$\Delta y = \alpha \Delta x$$
 - Based on the fact that at a fine enough resolution, any smooth, continuous function is locally linear at any point

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Scalar function of scalar argument



- When x and y are scalar

$$y = f(x)$$

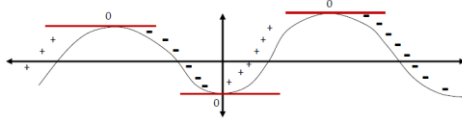
- Derivative:

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

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

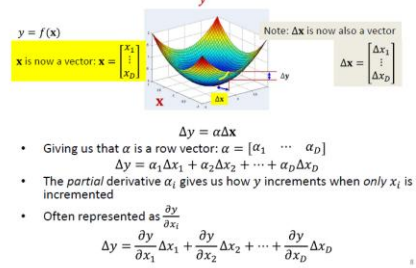
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Scalar function of scalar argument

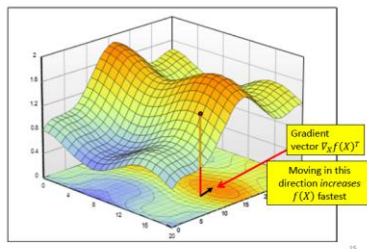


- Derivative $f'(x)$ is the *rate of change* of the function at x
 - How fast it increases with increasing x
 - The magnitude of $f'(x)$ gives you the steepness of the curve at x
 - Larger $|f'(x)| \rightarrow$ the function is increasing or decreasing more rapidly
- It will be positive where a small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

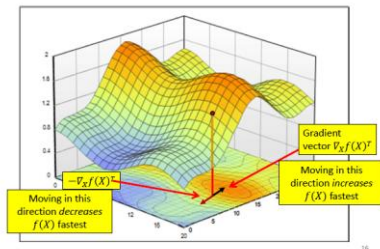
Multivariate scalar function: Scalar function of vector argument



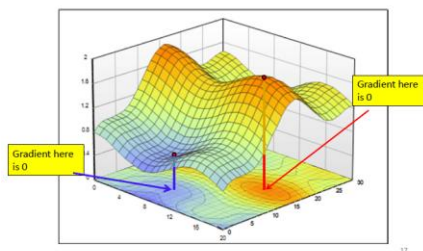
Gradient



Gradient



Gradient



Gradient

- At any location \mathbf{x} , there may be many directions in which we can step, such that $f(\mathbf{x})$ increases
- The direction of the gradient is the direction in which the function increases fastest

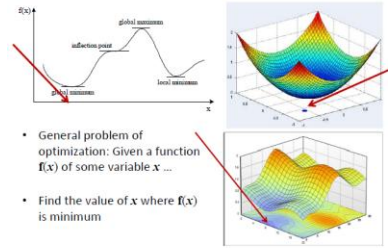
The Hessian

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

$$\nabla^2_z f(x_1, \dots, x_n) := \begin{bmatrix} \frac{\partial^2 f}{\partial x_1^2} & \frac{\partial^2 f}{\partial x_1 \partial x_2} & \dots & \frac{\partial^2 f}{\partial x_1 \partial x_n} \\ \frac{\partial^2 f}{\partial x_2 \partial x_1} & \frac{\partial^2 f}{\partial x_2^2} & \dots & \frac{\partial^2 f}{\partial x_2 \partial x_n} \\ \vdots & \vdots & \ddots & \vdots \\ \frac{\partial^2 f}{\partial x_n \partial x_1} & \frac{\partial^2 f}{\partial x_n \partial x_2} & \dots & \frac{\partial^2 f}{\partial x_n^2} \end{bmatrix}$$

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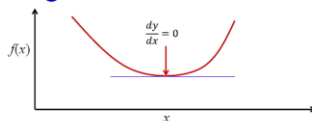
The problem of optimization



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

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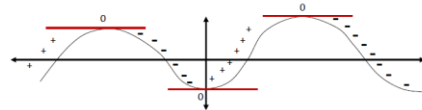
Finding the minimum of a function



- 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?

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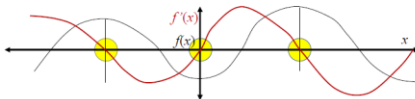
Turning Points



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

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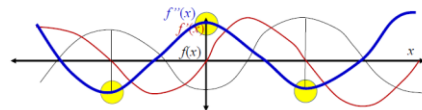
Derivatives of a curve



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

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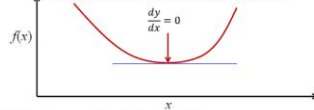
Derivative of the derivative of the curve



- 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!

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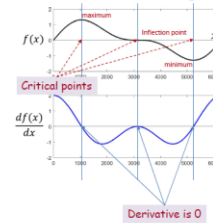
Solution: Finding the minimum or maximum of a function



- 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 $f''(x_{\text{soln}}) = \frac{d^2f(x_{\text{soln}})}{dx^2}$
- If $f''(x_{\text{soln}})$ is positive x_{soln} is a minimum, otherwise it is a maximum

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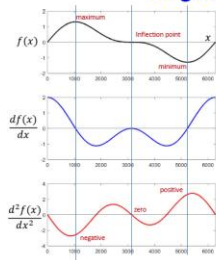
A note on derivatives of functions of single variable



- 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

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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..

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Unconstrained Minimization of function (Multivariate)

- Solve for the X where the derivative (or gradient) equals to zero $\nabla_X f(X) = 0$
- 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

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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

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

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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

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

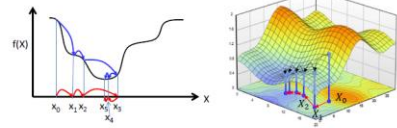
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Unconstrained Minimization of function (Example)

- Compute the Hessian matrix $\nabla_{xx}^2 f = \begin{bmatrix} 2 & -1 & 0 \\ -1 & 2 & -1 \\ 0 & -1 & 2 \end{bmatrix}$
- Evaluate the eigenvalues of the Hessian matrix
 $\lambda_1 = 3.414, \lambda_2 = 0.586, \lambda_3 = 2$
- All the eigenvalues are positives => the Hessian matrix is positive definite
- The point $x = \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} = \begin{bmatrix} -1 \\ -1 \\ -1 \end{bmatrix}$ is a minimum

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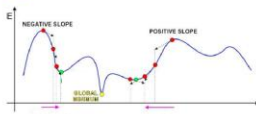
Iterative solutions



- 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

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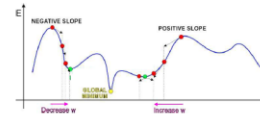
The Approach of Gradient Descent



- 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

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The Approach of Gradient Descent



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

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So far...

- Minimum of a function $f(x)$ is when : $f'(x) = 0$ and the second derivative $f''(x)$ is positive
- 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

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

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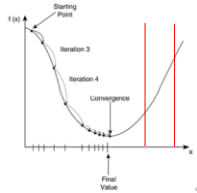
Gradient descent convergence criteria

- 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 $|f(x^{k+1}) - f(x^k)| > \varepsilon$

Preliminaries

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

$$Loss(W) = \frac{1}{T} \sum_i \text{div}(f(X_i; W), d_i)$$
 w.r.t W
- This is problem of function minimization
 - An instance of optimization

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

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

w.r.t W

Problem Setup: Things to define

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

- What are these input-output pairs?

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

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

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

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Problem Setup: Things to define

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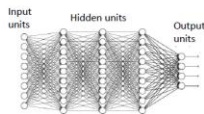
$$Loss(W) = \frac{1}{T} \sum_i \text{div}(f(X_i; W), d_i)$$

What is the divergence $\text{div}()$?

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

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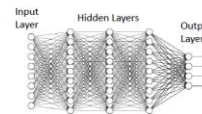
What is $f()$? Typical network



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

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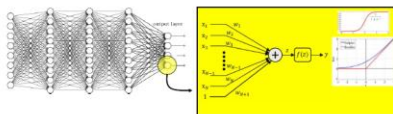
Typical network



- 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

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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

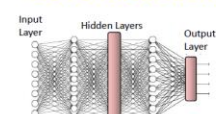
$$y = f\left(\sum_i w_i x_i + b\right)$$

- More generally: any differentiable function

$$y = f(x_1, x_2, \dots, x_n; W)$$

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Vector Activations



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

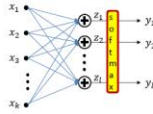
$$[y_1, y_2, \dots, y_l] = f(x_1, x_2, \dots, x_k; W)$$

- Function $f()$ operates on set of inputs to produce set of outputs

- Modifying a single parameter in W will affect *all* outputs

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Vector activation example: Softmax



- Example: Softmax **vector** activation

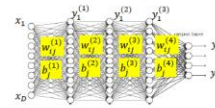
$$z_i = \sum_j w_{ji} x_j + b_i$$

Parameters are weights w_{ji} and bias b_i

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

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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 $b_j^{(k)}$

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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

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



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

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Problem Setup: Things to define

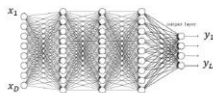
- Given a training set of input-output pairs $(X_1, d_1), (X_2, d_2), \dots, (X_T, d_T)$

- What are these input-output pairs?

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

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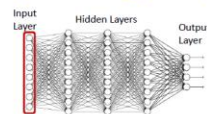
Input, target output, and actual output: Vector notation



- 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 nth input vector
- $d_n = [d_{n1}, d_{n2}, \dots, d_{nI}]^T$ is the nth desired output
- $Y_n = [y_{n1}, y_{n2}, \dots, y_{nI}]^T$ 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

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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
- Other real valued vectors

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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*

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Problem Setup: Things to define

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

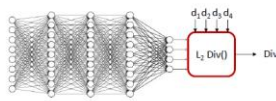
- Minimize the following function

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

What is the divergence $\text{div}()$?

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

Examples of divergence functions



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

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

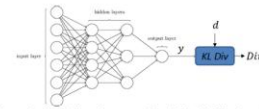
- Squared Euclidean distance between true and desired output
- Note: this is differentiable

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

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

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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

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

- Minimum when $d = Y$

- Derivative

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

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Summary

- 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
 - L_2 divergence for real-valued predictions
 - KL divergence for classifiers