Neural Networks
Learning the network: Part 1

11-785, Fall 2017
Lecture 3
Designing a net..

• Binary addition:
  – Input: Two binary inputs
  – Output: The binary (bit-sequence) sum

• “Input units”? 
• Output units? 
• Architecture? 
• Output activation?
Designing a net..

• Clustering:
  – Input: Real-valued vector
  – Output: Cluster ID

• “Input units”?

• Output units?

• Architecture?

• Output activation?
Topics for the day

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

- **Neural networks are universal function approximators**
  - Can model any Boolean function
  - Can model any classification boundary
  - Can model any continuous valued function

- **Provided the network satisfies minimal architecture constraints**
  - Networks with fewer than required parameters can be very poor approximators
These boxes are functions

- Take an input
- Produce an output
- Can be modeled by a neural network!
Questions

• Preliminaries:
  – How do we represent the input?
  – How do we represent the output?

• How do we compose the network that performs the requisite function?
Questions

• Preliminaries:
  – How do we represent the input?
  – How do we represent the output?

• *How do we compose the network that performs the requisite function?*
The original perceptron

• Simple threshold unit
  – Unit comprises a set of weights and a threshold
Preliminaries: The units in the network

Perceptron

- General setting, inputs are real valued
- Activation functions are not necessarily threshold functions
- A \textit{bias} \( b \) representing a threshold to trigger the perceptron
The bias can also be viewed as the weight of another input component that is always set to 1

- If the bias is not explicitly mentioned, we will implicitly be assuming that every perceptron has an additional input that is always fixed at 1
First: the structure of the network

- We will assume a *feed-forward* network
  - No loops: Neuron outputs do not go feed back to their inputs directly or indirectly
  - Loopy networks are a future topic
- **Part of the design of a network: The architecture**
  - How many layers/neurons, which neuron connects to which and how, etc.
- **For now, assume the architecture of the network is capable of representing the needed function**
What we learn: The parameters of the network

Given:

- The architecture of the network

The parameters of the network:

- The weights and biases
  - The weights associated with the blue arrows in the picture

Learning the network:

- Determining the values of these parameters such that the network computes the desired function

The network is a function $f()$ with parameters $W$ which must be set to the appropriate values to get the desired behavior from the net.
• Moving on..
The MLP *can* represent anything

• The MLP *can be constructed* to represent anything
• But *how do we construct it?*
Option 1: Construct by hand

- Given a function, *handcraft* a network to satisfy it
- E.g.: Build an MLP to classify this decision boundary
- Not possible for all but the simplest problems..
Option 2: Automatic estimation of an MLP

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

When $f(X; W)$ has the capacity to exactly represent $g(X)$:

$$\hat{W} = \arg \min_W \int_X \text{div}(f(X; W), g(X))dX$$

- $\text{div}()$ is a divergence function that goes to zero when $f(X; W) = g(X)$
Problem $g(X)$ is unknown

- Function $g(X)$ must be fully specified
  - Known everywhere, i.e. for every input $X$
- In practice we will not have such specification
Sampling the function

- **Sample** $g(X)$
  - Basically, get input-output pairs for a number of samples of input $X_i$
    - Many samples $(X_i, d_i)$, where $d_i = g(X_i) + \text{noise}$
    - Good sampling: the samples of $X$ will be drawn from $P(X)$
  
- Very easy to do in most problems: just gather training data
  - E.g. set of images and their class labels
  - E.g. speech recordings and their transcription
• We must *learn* the *entire* function from these few examples
  – The “training” samples
Learning the function

\[ Y = f(X; W) \]

- Estimate the network parameters to “fit” the training points exactly
  - Assuming network architecture is sufficient for such a fit
  - Assuming unique output \( d \) at any \( X \)
    - And hopefully the function is also correct where we don’t have training samples
Let's begin with a simple task

• Learning a classifier
  – Simpler than regressions

• This was among the earliest problems addressed using MLPs

• Specifically, consider binary classification
  – Generalizes to multi-class
History: The original MLP

- The original MLP as proposed by Minsky: a network of threshold units
  - But how do you train it?
The simplest MLP: a single perceptron

• Learn this function
  – A step function across a hyperplane
The simplest MLP: a single perceptron

- Learn this function
  - A step function across a hyperplane
  - Given only samples form it
Learning the perceptron

- Given a number of input output pairs, learn the weights and bias
  - \( y = \max(0, \sum_i w_i x_i + b) \)
  - Learn \( W = [w_1 \ldots w_N] \) and \( b \), given several \((X, y)\) pairs
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 $X_{N+1} = 1$
• Find the hyperplane $\sum_{i=1}^{N+1} w_i X_i = 0$ that perfectly separates the two groups of points.
Perceptron Learning Algorithm

• Given \( N \) training instances \((X_1, Y_1), (X_2, Y_2), \ldots, (X_N, Y_N)\)
  – \( Y_i = +1 \) or \(-1\)

• Initialize \( W \)

• Cycle through the training instances:
  • While more classification errors
    – For \( i = 1 \ldots N_{\text{train}} \)
      \[ O(X_i) = \text{sign}(W^T X_i) \]
    • If \( O(X_i) \neq Y_i \)
      \[ W = W + Y_i X_i \]
Perceptron Algorithm: Summary

• Cycle through the training instances
• Only update $W$ on misclassified instances
• If instance misclassified:
  – If instance is positive class
    \[ W = W + X_i \]
  – If instance is negative class
    \[ W = W - X_i \]
A Simple Method: The Perceptron Algorithm

- Initialize: Randomly initialize the hyperplane
  - I.e. randomly initialize the normal vector \( W \)
  - Classification rule \( \text{sign}(W^T X) \)
  - The random initial plane will make mistakes
Perceptron Algorithm

Initialization

$w$
Perceptron Algorithm

Misclassified positive instance
Perceptron Algorithm

\[ W \]

+1 (green)

-1 (Red)
Perceptron Algorithm

Misclassified positive instance, add it to W
Perceptron Algorithm
Perceptron Algorithm

Misclassified instance, negative class

+1 (green)  -1 (Red)
Perceptron Algorithm

+1 (green)  -1 (Red)
Perceptron Algorithm

Misclassified *negative* instance, *subtract* it from $W$
Perceptron Algorithm
Perfect classification, no more updates
Convergence of Perceptron Algorithm

• Guaranteed to converge if classes are linearly separable
  – After no more than \( \left( \frac{R}{\gamma} \right)^2 \) misclassifications
    • Specifically when \( W \) is initialized to 0
  – \( R \) is length of longest training point
  – \( \gamma \) is the best case closest distance of a training point from the classifier
    • Same as the margin in an SVM
  – Intuitively – takes many increments of size \( \gamma \) to undo an error resulting from a step of size \( R \)
Perceptron Algorithm

\[ g \] is the best-case margin
\[ R \] is the length of the longest vector

\( \gamma \) is the best-case margin
R is the length of the longest vector
History: A more complex problem

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

- Even using the perfect architecture
- Can we use the perceptron algorithm?
The pattern to be learned at the lower level

- The lower-level neurons are linear classifiers

- The actually provided labels are not linearly separated

Challenge: Must also learn the labels for the lowest units!
The pattern to be learned at the lower level

- The lower-level neurons are linear classifiers
  - They require linearly separated labels to be learned
The pattern to be learned at the lower level

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The pattern to be learned at the lower level

- The lower-level neurons are linear classifiers
  - They require linearly separated labels to be learned
  - The actually provided labels are not linearly separated
  - Challenge: Must also learn the labels for the lowest units!
Individual neurons represent one of the lines that compose the figure (linear classifiers)

Must know the output of every neuron for every training instance, in order to learn this neuron
The outputs should be such that the neuron individually has a linearly separable task
The linear separators must combine to form the desired boundary

This must be done for every neuron
Getting any of them wrong will result in incorrect output!
Learning a *multilayer* perceptron

Training data only specifies input and output of network

Intermediate outputs (outputs of individual neurons) are not specified

- Training this network using the perceptron rule is a combinatorial optimization problems
- We don’t know the outputs of the individual intermediate neurons in the network for any training input
- **Must also determine the correct output for each neuron for every training instance**
- **NP!** Exponential complexity
Greedy algorithms: Adaline and Madaline

• The perceptron learning algorithm cannot directly be used to learn an MLP
  – Exponential complexity of assigning intermediate labels
    • Even worse when classes are not actually separable

• Can we use a greedy algorithm instead?
  – Adaline / Madaline
  – On slides, will skip in class (check the quiz)
A little bit of History: Widrow

Bernie Widrow
- Scientist, Professor, Entrepreneur
- Inventor of most useful things in signal processing and machine learning!

- First known attempt at an analytical solution to training the perceptron and the MLP
- Now famous as the LMS algorithm
  - Used everywhere
  - Also known as the “delta rule”
History: ADALINE

\[ z = \sum_{t} w_i x_i \]

\[ y = \begin{cases} 
0, & z < 0 \\
1, & z \geq 0 
\end{cases} \]

- Adaptive linear element
  (Hopf and Widrow, 1960)

- Actually just a regular perceptron
  - Weighted sum on inputs and bias passed through a thresholding function

- ADALINE differs in the learning rule
History: Learning in ADALINE

\[ z = \sum_{i} w_i x_i \]

\[ \text{out} = \begin{cases} 
0, & z < 0 \\
1, & z \geq 0 
\end{cases} \]

- During learning, minimize the squared error assuming \( z \) to be real output
- The desired output is still binary!

\[ \text{Err}(x) = \frac{1}{2} (d - z)^2 \]

Error for a single input

\[ \frac{d\text{Err}(x)}{dw_i} = -(d - z)x_i \]
History: Learning in ADALINE

\[ z = \sum_{t} w_i x_i \]

\[ Err(x) = \frac{1}{2} (d - z)^2 \]  
\[ \text{Error for a single input} \]

\[ \frac{dErr(x)}{dw_i} = -(d - z)x_i \]

- If we just have a single training input, the gradient descent update rule is

\[ w_i = w_i + \eta (d - z)x_i \]
The ADALINE learning rule

• Online learning rule
• **After each input** \( x \), **that has** target (binary) output \( d \), compute and update:

\[
\delta = d - z
\]

\[
w_i = w_i + \eta \delta x_i
\]

• This is the famous *delta rule*
  – Also called the LMS update rule
The Delta Rule

- In fact both the Perceptron and ADALINE use variants of the delta rule!
  - Perceptron: Output used in delta rule is $y$
  - ADALINE: Output used to estimate weights is $z$

\[ \delta = d - y \]
\[ w_i = w_i + \eta \delta x_i \]
Aside: Generalized delta rule

• For any differentiable activation function the following update rule is used

\[ \delta = d - y \]

\[ w_i = w_i + \eta \delta f'(z)x_i \]

• This is the famous Widrow-Hoff update rule
  – Lookahead: Note that this is exactly backpropagation in multilayer nets if we let \( f(z) \) represent the entire network between \( z \) and \( y \)

• It is possibly the most-used update rule in machine learning and signal processing
  – Variants of it appear in almost every problem
**Multilayer perceptron:** MADALINE

- **Multiple Adaline**
  - A multilayer perceptron with threshold activations
  - The MADALINE
MADALINE Training

• Update only on error
  – \( \delta \neq 0 \)
  – On inputs for which output and target values differ
• While stopping criterion not met do:
  – Classify an input
• While stopping criterion not met do:
  – Classify an input
  – If error, find the z that is closest to 0
While stopping criterion not met do:
  – Classify an input
  – If error, find the $z$ that is closest to 0
  – Flip the output of corresponding unit and compute new output
MADALINE Training

While stopping criterion not met do:
  – Classify an input
  – If error, find the z that is closest to 0
  – Flip the output of corresponding unit and compute new output
  – If error reduces:
    • Set the desired output of the unit to the flipped value
    • Apply ADALINE rule to update weights of the unit
MADALINE

• Greedy algorithm, effective for small networks
• Not very useful for large nets
  – Too expensive
  – Too greedy
History..

• The realization that training an entire MLP was a combinatorial optimization problem stalled development of neural networks for well over a decade!
Why this problem?

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

- Individual neurons’ weights can change significantly without changing overall error
- The simple MLP is a flat, non-differentiable function
A second problem: What we *actually* model

- Real-life data are rarely clean
  - Not linearly separable
  - Rosenblatt’s perceptron wouldn’t work in the first place
• Lets make the neuron differentiable
  – Small changes in weight can result in non-negligible changes in output
  – This enables us to estimate the parameters using gradient descent techniques.
Differentiable Activations: An aside

This particular one has a nice interpretation

\[ z = \sum_{i} w_{i} x_{i} + w_{N+1} \]

\[ \sigma(z) = \frac{1}{1 + e^{-z}} \]
Non-linearly separable data

- Two-dimensional example
  - Blue dots (on the floor) on the “red” side
  - Red dots (suspended at Y=1) on the “blue” side
  - No line will cleanly separate the two colors
Non-linearly separable data: 1-D example

- One-dimensional example for visualization
  - All (red) dots at $Y=1$ represent instances of class $Y=1$
  - All (blue) dots at $Y=0$ are from class $Y=0$
  - The data are not linearly separable
    - In this 1-D example, a linear separator is a threshold
    - No threshold will cleanly separate red and blue dots
The *probability* of $y=1$

- Consider this differently: at each point look at a small window around that point
- Plot the average value within the window
  - This is an approximation of the *probability* of $Y=1$ at that point
The *probability* of $y=1$

- Consider this differently: at each point look at a small window around that point
- Plot the average value within the window
  - This is an approximation of the *probability* of 1 at that point
The probability of $y=1$

- Consider this differently: at each point look at a small window around that point
- Plot the average value within the window
  - This is an approximation of the probability of 1 at that point
The *probability* of $y=1$

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The probability of \( y=1 \)

- Consider this differently: at each point look at a small window around that point.
- Plot the average value within the window.
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The *probability* of $y=1$

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Plot the average value within the window.

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The probability of $y=1$

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The probability of $y=1$

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The *probability* of $y=1$

- Consider this differently: at each point look at a small window around that point
- Plot the average value within the window
  - This is an approximation of the *probability* of 1 at that point
The logistic regression model

- Class 1 becomes increasingly probable going left to right
  - Very typical in many problems
Logistic regression

When $X$ is a 2-D variable

- This the perceptron with a sigmoid activation
  - It actually computes the *probability* that the input belongs to class 1

\[
P(Y = 1|X) = \frac{1}{1 + \exp(-\sum_i w_i x_i - b)}
\]
Perceptrons and probabilities

• We will return to the fact that perceptrons with sigmoidal activations actually model class probabilities later

• But for now moving on..
Perceptrons with differentiable activation functions

\[ z = \sum_{i} w_i x_i \]

- \( \sigma(z) \) is a differentiable function of \( z \)
  - \( \frac{d\sigma(z)}{dz} \) is well-defined and finite for all \( z \)
- Using the chain rule, \( y \) is a differentiable function of both inputs \( x_i \) and weights \( w_i \)
- This means that we can compute the change in the output for small changes in either the input or the weights

\[
\frac{dy}{dw_i} = \frac{dy}{dz} \frac{dz}{dw_i} = \sigma'(z) x_i \\
\frac{dy}{dx_i} = \frac{dy}{dz} \frac{dz}{dx_i} = \sigma'(z) w_i
\]
Overall network is differentiable

- Every individual perceptron is differentiable w.r.t its inputs and its weights (including “bias” weight)
- By the chain rule, the overall function is differentiable w.r.t every parameter (weight or bias)
  - Small changes in the parameters result in measurable changes in output

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

\( y \) = output of overall network
\( w_{i,j}^k \) = weight connecting the ith unit of the kth layer to the jth unit of the k+1-th layer
\( y_i^k \) = output of the ith unit of the kth layer

\( \sigma() \) is differentiable w.r.t both \( w \) and \( y_i^k \)
The overall function is differentiable w.r.t every parameter
  – Small changes in the parameters result in measurable changes in the output
  – We will derive the actual derivatives using the chain rule later
Overall setting for “Learning” the MLP

- Given a training set of input-output pairs \((X_1, d_1), (X_2, d_2), \ldots, (X_N, d_N)\) ...
  - \(d\) is the desired output of the network in response to \(X\)
  - \(X\) and \(d\) may both be vectors
- ...we must find the network parameters such that the network produces the desired output for each training input
  - Or a close approximation of it
  - The architecture of the network must be specified by us
Recap: Learning the function

When $f(X; W)$ has the capacity to exactly represent $g(X)$

$$\bar{W} = \arg\min_W \int_X \text{div}(f(X; W), g(X)) dX$$

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

- More generally, assuming $X$ is a random variable

$$
\hat{W} = \arg\min_W \int_X div(f(X; W), g(X)) P(X) dX
= \arg\min_W E[div(f(X; W), g(X))]
$$
Recap: Sampling the function

• **Sample** $g(X)$
  - Basically, get input-output pairs for a number of samples of input $X_i$
    • Many samples $(X_i, d_i)$, where $d_i = g(X_i) + \text{noise}$
  - Good sampling: the samples of $X$ will be drawn from $P(X)$

• Estimate function from the samples
The *Empirical risk*

- The *expected* error is the average error over the entire input space

\[
E[\text{div}(f(X; W), g(X))] = \int_X \text{div}(f(X; W), g(X))P(X)dx
\]

- The *empirical estimate* of the expected error is the *average* error over the samples

\[
E[\text{div}(f(X; W), g(X))] \approx \frac{1}{N} \sum_{i=1}^{N} \text{div}(f(X_i; W), d_i)
\]
Empirical Risk Minimization

\[ Y = f(X; W) \]

- Given a training set of input-output pairs \((X_1, d_1), (X_2, d_2), \ldots, (X_N, d_N)\)
  - Error on the \(i\)th instance: \(\text{div}(f(X_i; W), d_i)\)
  - Empirical average error on all training data:
    \[
    \text{Err}(W) = \frac{1}{N} \sum_i \text{div}(f(X_i; W), d_i)
    \]
- Estimate the parameters to minimize the empirical estimate of expected error
  \[
  \hat{W} = \arg\min_W \text{Err}(W)
  \]
  - I.e. minimize the empirical error over the drawn samples
ERM for neural networks

Actual output of network:
\[ Y_i = \text{net}(X_i; \{w_{i,j}^k \forall i, j, k\}) \]
\[ = \text{net}(X_i; W^1, W^2, \ldots, W^K) \]

Desired output of network: \( d_i \)

Error on i-th training input: \( \text{Div}(Y_i, d_i; W^1, W^2, \ldots, W^K) \)

Total training error:
\[ Err(W^1, W^2, \ldots, W^K) = \frac{1}{N} \sum_{i=1}^{N} \text{Div}(Y_i, d_i; W^1, W^2, \ldots, W^K) \]

- What is the exact form of Div()? More on this later

- Optimize network parameters to minimize the total error over all training inputs
Problem Statement

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

• Minimize the following function

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

w.r.t $W$

• This is problem of function minimization
  – An instance of optimization
• A CRASH COURSE ON FUNCTION OPTIMIZATION
Caveat about following slides

• The following slides speak of optimizing a function w.r.t a variable “x”

• This is only mathematical notation. In our actual network optimization problem we would be optimizing w.r.t. network weights “w”

• To reiterate – “x” in the slides represents the variable that we’re optimizing a function over and not the input to a neural network

• **Do not get confused!**
The problem of optimization

- General problem of optimization: find the value of $x$ where $f(x)$ is minimum
Finding the minimum of a function

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

\[ \frac{df(x)}{dx} = 0 \]

• The solution is a “turning point”
  – Derivatives go from positive to negative or vice versa at this point

• But is it a minimum?
- 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!
Find 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
What about functions of multiple variables?

- The optimum point is still “turning” point
  - Shifting in any direction will increase the value
  - For smooth functions, miniscule shifts will not result in any change at all
- We must find a point where shifting in any direction by a microscopic amount will not change the value of the function
A brief note on derivatives of multivariate functions
The *Gradient* 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 $X$.

$$df(X) = \nabla f(X)dX$$
Gradients of scalar functions with multi-variate inputs

- Consider $f(X) = f(x_1, x_2, \ldots, x_n)$

\[
\nabla f(X) = \begin{bmatrix}
\frac{\partial f(X)}{\partial x_1} & \frac{\partial f(X)}{\partial x_2} & \cdots & \frac{\partial f(X)}{\partial x_n}
\end{bmatrix}
\]

- Check:

\[
df(X) = \nabla f(X) dX = \frac{\partial f(X)}{\partial x_1} dx_1 + \frac{\partial f(X)}{\partial x_2} dx_2 + \cdots + \frac{\partial f(X)}{\partial x_n} dx_n
\]
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

- $df(X) = \nabla f(X) dX$
  - The inner product between $\nabla f(X)$ and $dX$

- Fixing the length of $dX$
  - E.g. $|dX| = 1$

- $df(X)$ is max if $dX$ is aligned with $\nabla f(X)$
  - $\angle \nabla f(X), dX = 0$
  - The function $f(X)$ increases most rapidly if the input increment $dX$ is perfectly aligned to $\nabla f(X)$

- The gradient is the direction of fastest increase in $f(X)$

Some sloppy maths here, with apology - comparing row and column vectors
Gradient

Gradient vector $\nabla f(X)$
Gradient

Gradient vector $\nabla f(X)$

Moving in this direction *increases* $f(X)$ fastest
Gradient

Moving in this direction increases $f(X)$ fastest.

$-\nabla f(X)$

Moving in this direction decreases $f(X)$ fastest.

Gradient vector $\nabla f(X)$
Gradient

Gradient here is 0

Gradient here is 0
Properties of Gradient: 2

- The gradient vector $\nabla f(X)$ 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

\[
\nabla^2 f(x_1, \ldots, x_n) := \begin{bmatrix}
\frac{\partial^2 f}{\partial x_1^2} & \frac{\partial^2 f}{\partial x_1 \partial x_2} & \cdots & \frac{\partial^2 f}{\partial x_1 \partial x_n} \\
\frac{\partial^2 f}{\partial x_2 \partial x_1} & \frac{\partial^2 f}{\partial x_2^2} & \cdots & \frac{\partial^2 f}{\partial x_2 \partial x_n} \\
\vdots & \vdots & \ddots & \vdots \\
\frac{\partial^2 f}{\partial x_n \partial x_1} & \frac{\partial^2 f}{\partial x_n \partial x_2} & \cdots & \frac{\partial^2 f}{\partial x_n^2}
\end{bmatrix}
\]
Returning to direct optimization...
Finding the minimum of a scalar function of a multi-variate input

- The optimum point is a turning point – the gradient will be 0
Unconstrained Minimization of function (Multivariate)

1. Solve for the $X$ where the gradient equation equals to zero

$$\nabla f(X) = 0$$

2. Compute the Hessian Matrix $\nabla^2 f(X)$ at the candidate solution and verify that
   - Hessian is positive definite (eigenvalues positive) $->$ to identify local minima
   - Hessian is negative definite (eigenvalues negative) $->$ to identify local maxima
Unconstrained Minimization of function (Example)

• Minimize

\[ f(x_1, x_2, x_3) = (x_1)^2 + x_1(1-x_2) - (x_2)^2 - x_2x_3 + (x_3)^2 + x_3 \]

• Gradient

\[ \nabla f = \begin{bmatrix} 2x_1 + 1 - x_2 \\ -x_1 + 2x_2 - x_3 \\ -x_2 + 2x_3 + 1 \end{bmatrix}^T \]
Unconstrained Minimization of function (Example)

• Set the gradient to null

\[
\nabla f = 0 \implies \begin{bmatrix}
2x_1 + 1 - x_2 \\
-x_1 + 2x_2 - x_3 \\
-x_2 + 2x_3 + 1
\end{bmatrix} = \begin{bmatrix}
0 \\
0 \\
0
\end{bmatrix}
\]

• 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 $\nabla^2 f = \begin{bmatrix} 2 & -1 & 0 \\ -1 & 2 & -1 \\ 0 & -1 & 2 \end{bmatrix}$

• 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 $\Rightarrow$ the Hessian matrix is positive definite

\[ \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} = \begin{bmatrix} -1 \\ -1 \\ -1 \end{bmatrix} \]

• The point $x = \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix}$ is a minimum
Closed Form Solutions are not always available

- Often it is not possible to simply solve $\nabla f(X) = 0$
  - 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

- 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 positive derivative $\rightarrow$ moving left decreases error
      – A negative derivative $\rightarrow$ moving right decreases error
  – Shift point in this direction
The Approach of Gradient Descent

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

• Iterative solution: Trivial algorithm
  – Initialize $x^0$
  – While $f'(x^k) \neq 0$
    • $x^{k+1} = x^k - \text{sign}(f'(x^k)) \cdot \text{step}$
  – Identical to previous algorithm
The Approach of Gradient Descent

• Iterative solution: Trivial algorithm
  – Initialize $x_0$
  – While $f'(x^k) \neq 0$
    • $x^{k+1} = x^k - \eta^k f'(x^k)$
  – $\eta^k$ is the “step size”
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
    \[ x^{k+1} = x^k + \eta^k \nabla f(x^k)^T \]
  – To find a minimum move exactly opposite the direction of the gradient
    \[ x^{k+1} = x^k - \eta^k \nabla f(x^k)^T \]

• Many solutions to choosing step size $\eta^k$
1. Fixed step size

- Fixed step size
  - Use fixed value for $\eta^k$
Influence of step size example (constant step size)

\[ f(x_1, x_2) = (x_1)^2 + x_1 x_2 + 4(x_2)^2 \]

\[ x^{\text{initial}} = \begin{bmatrix} 3 \\ 3 \end{bmatrix} \]

\( \eta = 0.1 \)

\( \eta = 0.2 \)
What is the optimal step size?

• Step size is critical for fast optimization
• Will revisit this topic later
• For now, simply assume a potentially-iteration-dependent step size
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 \[ \|\nabla f(x^k)\| < \varepsilon_2 \]
Overall Gradient Descent Algorithm

• Initialize:
  – $x^0$
  – $k = 0$

• While $|f(x^{k+1}) - f(x^k)| > \varepsilon$
  – $x^{k+1} = x^k - \eta^k \nabla f(x^k)^T$
  – $k = k + 1$
Next up

• Gradient descent to train neural networks

• A.K.A. Back propagation