Machine Learning Intro

CompSci 370
Ronald Parr
Department of Computer Science
Duke University

1

Why Study Learning?

- Considered a hallmark of intelligence
- Viewed as way to reduce programming burden
  - Not enough programmers in the world to produce custom solutions to all problems – even if we knew how
  - Programmers are expensive!
- Many algorithms assume parameters that are difficult to determine exactly a priori
  - What is the right formula to filter spam?
  - When should your smart thermostat turn on the heat?

2

Examples

- SPAM classification
- Computational Biology/medicine
  - Distinguish healthy/diseased tissue (e.g., skin/colon cancer)
  - Find structure in biological data (regulatory pathways)
- Financial events
  - Predict good/bad credit risks
  - Predict price changes
  - Response to marketing
- Object/person recognition
- Natural language processing
- Document categorization and user preferences
- Recommend products to users
- Learn to play games, e.g., go, chess, etc.
- Learn to control systems, e.g., robots or helicopters
- Public database of (old) benchmark learning problems:
  - http://www.ics.uci.edu/~mlearn/MLSummary.html

3

What is Machine Learning?

- Learning Element
  - The thing that learns
- Performance Element
  - Objective measure of progress
- Learning is simply an increase in the ability of the learning element over time (with data) to achieve the task specified by the performance element

7

ML vs. Statistics?

- Machine learning is:
  - Younger
  - More empirical
  - More algorithmic
  - (arguably) More practical
  - (arguably) More decision theoretic

Look at this cool result!
Maybe somebody can explain why it works later?

- Statistics is:
  - More mature
  - (arguably) More formal and rigorous

Let's model this situation and prove that we converge to a consistent answer!

8

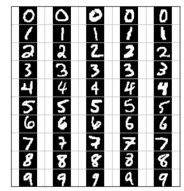
ML vs. Data Mining

- Machine Learning is:
  - (Arguably) more formal
  - (Arguably) more task driven/decision theoretic
- Data Mining is:
  - More constrained by size of data set
  - More closely tied to database techniques

9

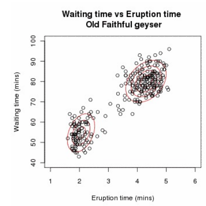
Feedback in Learning

- Supervised Learning
  - Given examples of correct behavior
  - Example input: Labeled x-rays
  - Example use: Cancer diagnosis



Recognizing handwritten digits

- Unsupervised Learning
  - No external notion of what is correct
  - Example: Unlabeled x-rays
  - Example use: Clustering based on appearance



- Reinforcement Learning
  - Indirect indication of effectiveness
  - Example use: PacMan, go, chess

11

Learning Methodology

- Distinction between training and testing is crucial
- Correct performance on training set is just memorization!
- Researcher should ***never*** look at the test data
  (but in practice always does)
- Raises issues for "benchmark" learning problems

12

Types of Supervised Learning

- Training input:
  - Feature vector for each datum: $x_1 \ldots x_n$
  - Target value: y

- Classification – assigning labels/classes
- Regression – assigning real numbers

24

Features and Targets

- Features can be anything
  - Images, sounds, text
  - Real values (height, weight)
  - Integers, or binaries
- Targets can be discrete classes:
  - Safe mushrooms vs. poisonous
  - Malignant vs. benign
  - Good credit risk vs. bad
  - Label of image
- Or numbers
  - Selling price of house
  - Life expectancy

25

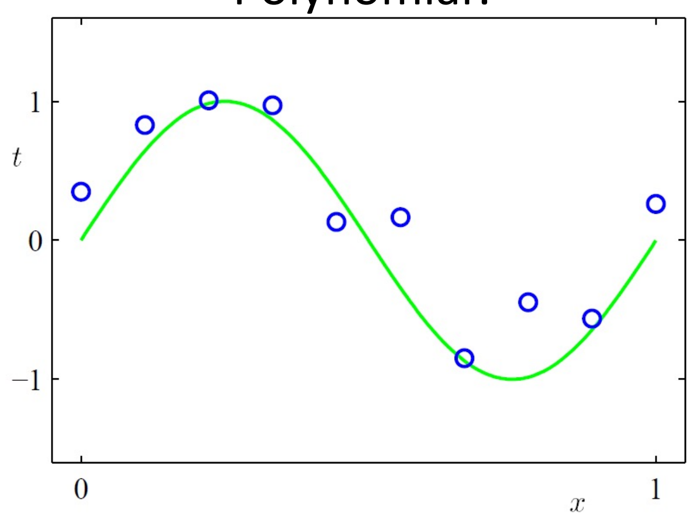
How Most Supervised Learning Algorithms Work

- Main idea: Minimize error on training set
- How this is done depends on:
  - Hypothesis space
  - Type of data

- Big Question: What is the “right” hypothesis space?

26

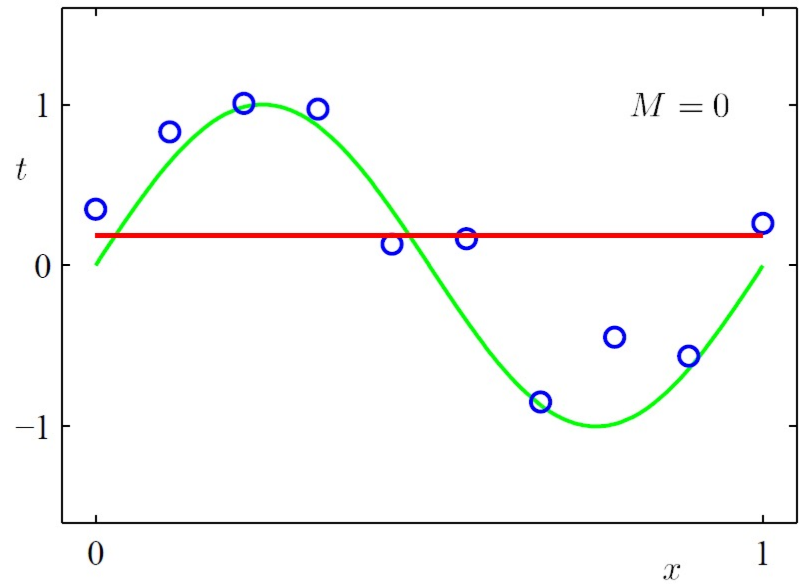
What is the Best Choice of Polynomial?



Noisy Source Data

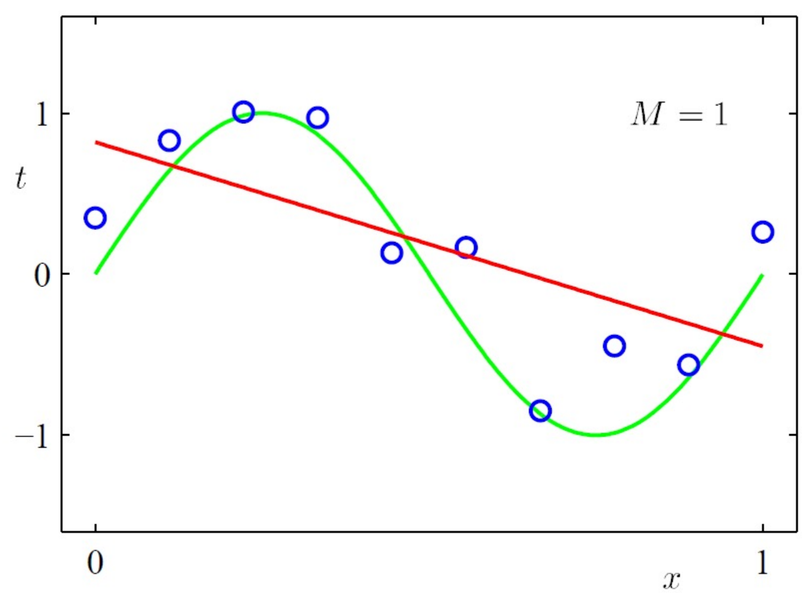
27

Degree 0 Fit



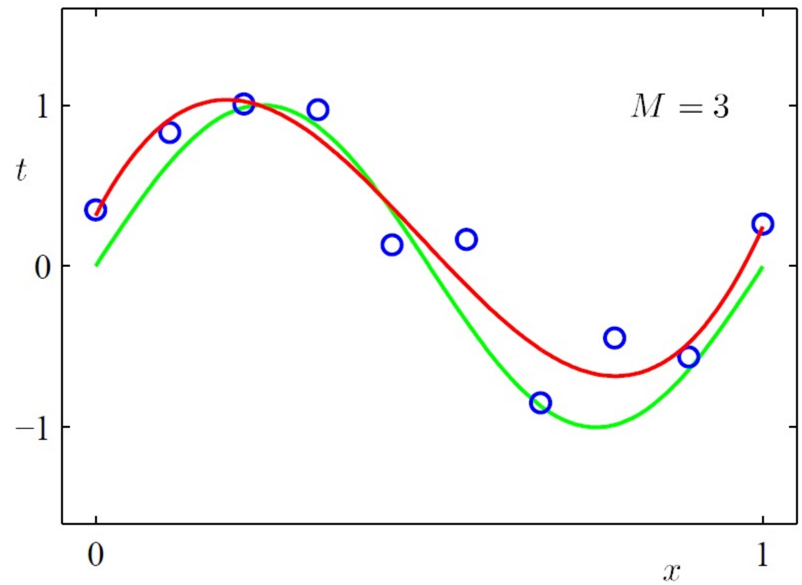
28

Degree 1 Fit



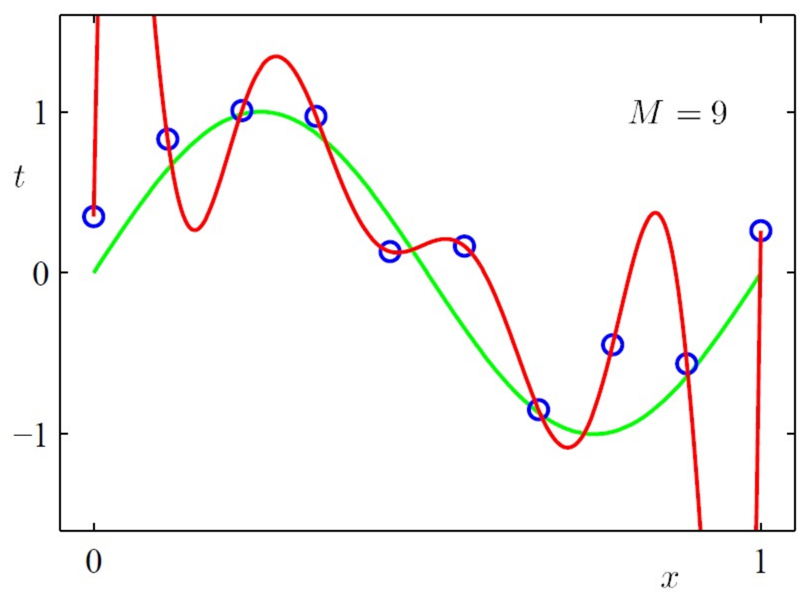
29

Degree 3 Fit



30

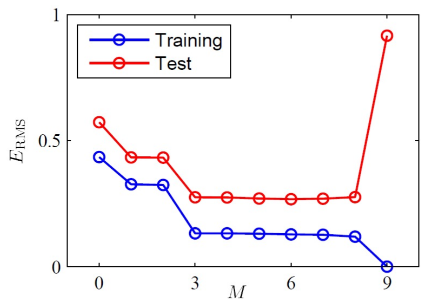
Degree 9 Fit



31

Observations

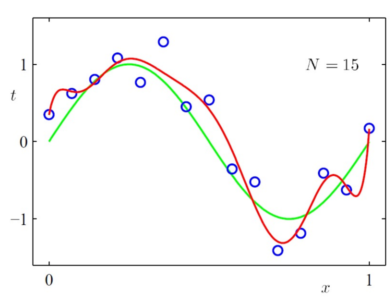
- Degree 3 is the best match to the source
- Degree 9 is the best match to the samples
- We call this **over-fitting**
- Performance on test data:

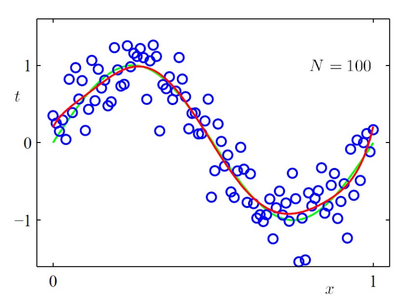


32

What went wrong?

- Is the problem a bad choice of polynomial?
- Is the problem that we don't have enough data?
- Answer: Yes





33

How to pick our hypothesis space?

- Learning theory (a rich subarea) gives some guidance on this, though it is often more abstract than directly applicable to real world applications

- Practical approaches:
  - Regularizer or prior to trade off training set error vs. hypothesis space complexity
  - Cross validation uses one or more mini test sets to help inform hypothesis space selection

34

Classification vs. Regression

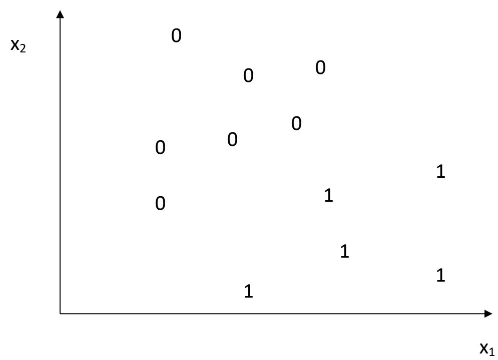
- Regression tries to hit the target values with the function we are fitting

- Classification tries to find a function that separates the classes

35

Decision Boundaries

- A classifier can be viewed as partitioning the input space or feature space X into decision regions



- A linear threshold unit always produces a linear decision boundary. A set of points that can be separated by a linear decision boundary is **linearly separable**.

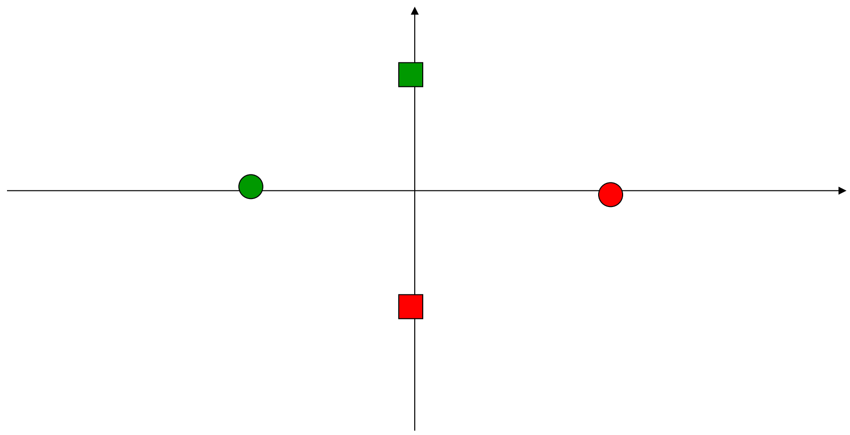
36

What can be expressed?

- Examples of things that can be expressed
  (Assume n Boolean (0/1 features)
  - Conjunctions:
    - $x_1 \wedge x_3 \wedge x_4$: $1 \cdot x_1 + 0 \cdot x_2 + 1 \cdot x_3 + 1 \cdot x_4 \geq 3$
    - $x_1 \wedge \neg x_3 \wedge x_4$: $1 \cdot x_1 + 0 \cdot x_2 + -1 \cdot x_3 + 1 \cdot x_4 \geq 2$
  - at-least-m-of-n
    - at-least-2-of(x_1,x_2,x_4)
    - $1 \cdot x_1 + 1 \cdot x_2 + 0 \cdot x_3 + 1 \cdot x_4 \geq 2$
- Examples of things that cannot be expressed:
  - Non-trivial disjunctions:
    - $(x_1 \wedge x_3) + (x_3 \wedge x_4)$
  - Exclusive-Or
    - $(x_1 \wedge \neg x_2) + (\neg x_1 \wedge x_2)$

37

Limitations of Linearly Separable Functions



Is red linearly separable from green?
Are the circles linearly separable from the squares?

38

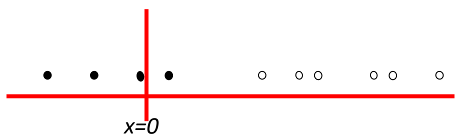
Feature Engineering

- All data are represented in "feature space"- the space spanned by all possible values of all features
- Feature space is largely a choice, like the degree of your polynomial, i.e., feature space engineering = hypothesis space engineering
- If you don't like your performance, you can change your feature space – but don't forget peril of overfitting

39

Suppose we're in 1-dimension

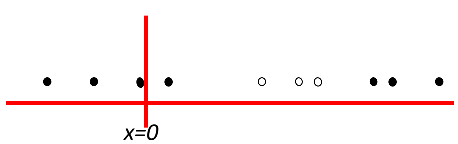
Easy to find a
linear separator



40

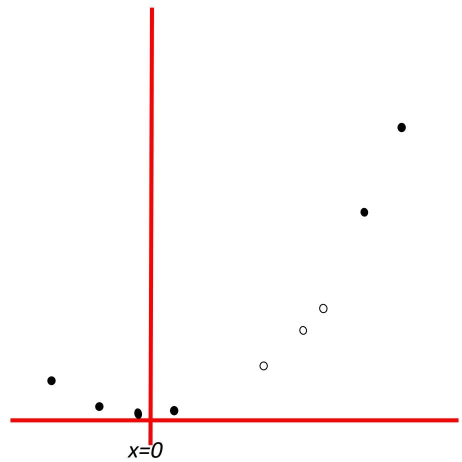
Harder 1-dimensional dataset

What can be done
about this?



41

Harder 1-dimensional dataset



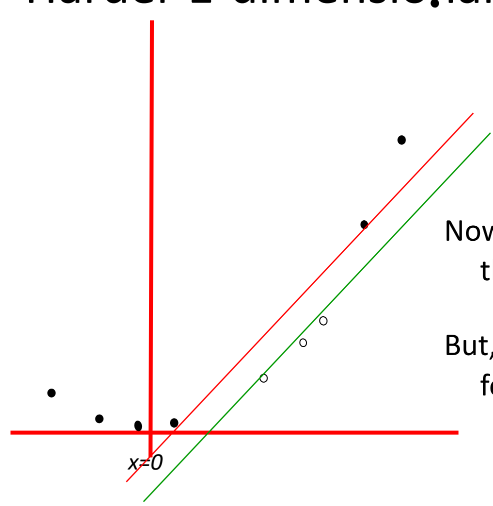
Remember how permitting non-linear features (higher degree polynomials) made linear regression so much more powerful?

Let's permit them here too

$$\Phi = (x, x^2)$$

42

Harder 1-dimensional dataset



Now **linearly separable** in the new feature space

But, what if the right feature set isn't obvious

$$\Phi = (x, x^2)$$

43

Motivation for non-linear Classifiers

- Linear methods are "weak"
  - Make strong assumptions
  - Can only express relatively simple functions of inputs
- Coming up with good features can be hard
  - Requires human input
  - Knowledge of the domain
- Role of neural networks
  - Neural networks started as linear models of single neurons
  - Combining ultimately led to non-linear functions that don't necessarily need careful feature engineering

44

Neural Network Motivation

- Human brains are only known example of actual intelligence
- Individual neurons are slow, boring
- Brains succeed by using massive parallelism
- Idea: Copy what works

- Raises many issues:
  - Is the computational metaphor suited to the computational hardware?
  - How do we know if we are copying the important part?
  - Are we aiming too low?

45

Why Neural Networks?

Maybe computers should be more brain-like:

	Computers	Brains
Computational Units	10^{10} transistors/CPU	10^{11} neurons/brain
Storage Units	10^{11} bits RAM 10^{13} bits HD	10^{11} neurons 10^{14} synapses
Cycle Time	10^{-9} S	10^{-3} S
Bandwidth	10^{10} bits/s*	10^{14} bits/s
Compute Power	10^{10} Ops/s	10^{14} Ops/s

46

Comments on Summit

(world's fastest supercomputer as of 10/19)

- 149 Petaflops
- ~10^{18} Ops/s (Summit) vs. 10^{14} Ops/s (brain)
- 2.4M cores (conflicting reports)
- 2.8 PB RAM (10^{17} bits)
- 10 Megawatts power(~$10M/year in electricity [my estimate])
- ~$200M cost

Note: recently surpassed by Fugaku – 3x more cores, 3x more energy, 3x performance, 5x cost
Fugaku expected to replaced by Frontier this year, 2x Fugaku performance, same energy, 60% cost

47

More Comments on Summit

- What is wrong with this picture?
  - Weight
  - Size
  - Power Consumption
- What is missing?
  - Still can't replicate human abilities
    (though vastly exceeds human abilities in many areas)
  - Are we running the wrong programs?
  - Is the architecture well suited to the programs we might need to run?

48

Artificial Neural Networks

- Develop *abstraction* of function of actual neurons
- Simulate large, massively parallel artificial neural networks on conventional computers – note that even supercomputers have very low connectivity compared to a brain
- Some have tried to build the hardware too
- Try to approximate human learning, robustness to noise, robustness to damage, etc.

49

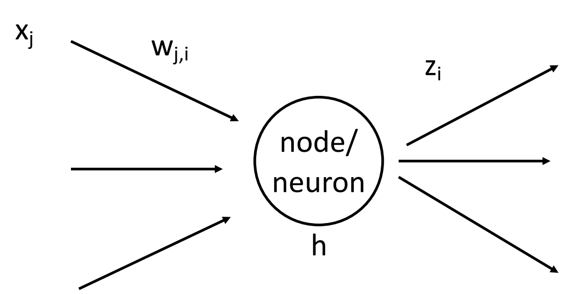
Neural Network Lore

- Neural nets have been adopted with an almost religious fervor within the AI community – several times
  - First coming: Perceptron
  - Second coming: Multilayer networks
  - Third coming (present): Deep networks

- Sound science behind neural networks: gradient descent
- Unsound social phenomenon behind neural networks: **HYPE!**

50

Artificial Neurons

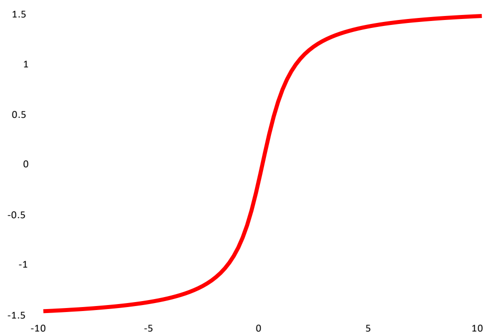


$$a_i = h(\sum_j w_{j,i} x_j)$$

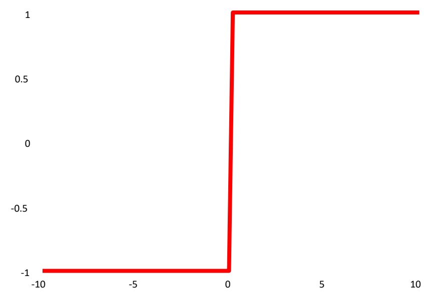
h can be any function, but usually a smoothed step function

51

Threshold Functions



h(x)=sgn(x)
(perceptron)



h(x)=tanh(x) or 1/(1+exp(-x))
(logistic sigmoid)

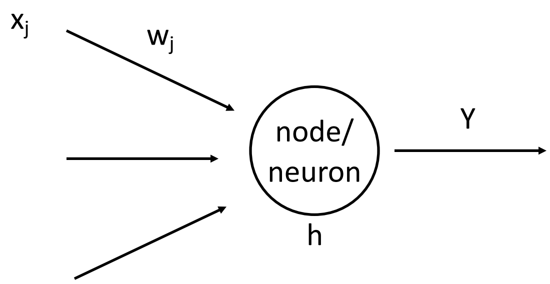
52

Feedforward Networks

- We consider acyclic networks
- One or more computational layers
- Entire network can be viewed as computing a complicated non-linear function
- Typical uses in learning:
  - Classification (usually involving complex patterns)
  - General continuous function approximation
- Many other variations possible

54

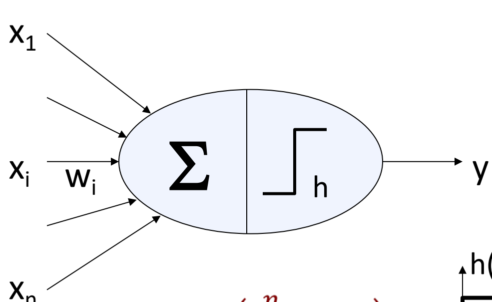
Special Case: Perceptron

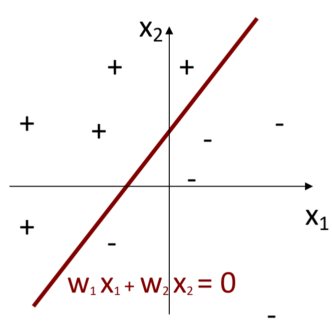


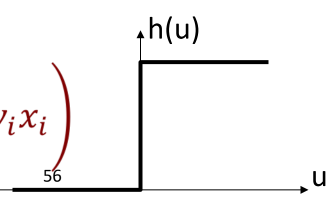
h is a simple step function (sgn)

55

Perceptron is a Linear Classifier







$$y = f(\boldsymbol{x}, \boldsymbol{w}) = h\left(\sum_{i=1}^{n} w_i x_i\right)$$

56

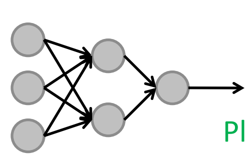
Good News/Bad News

- Good news
  - *Perceptron learning rule* can learn to distinguish any two classes that are linearly separable
  - ***If*** classes are separable, perceptron learning rule will converge for any learning rate
- Bad news
  - Linear separability is a strong assumption
  - Failure to appreciate this led to excessive optimism and first neural network crash

57

Multilayer Networks

- Once people realized how simple perceptrons were, they lost interest in neural networks for a while
- Multilayer networks turn out to be much more expressive (with a smoothed step function)
  - Use sigmoid, e.g., $h=\tanh(w^T x)$ or logistic sigmoid
  - With 2 layers, can represent any continuous function
  - With 3 layers, can represent many discontinuous functions
- Tricky part: How to adjust the weights



Play with it at: http://playground.tensorflow.org

59

Smoothing Things Out

- Idea: Do gradient descent on a smooth error function
- Error function is sum of squared errors
- Consider a single training example first

$$E = 0.5 error(X^{(i)}, w)^2$$

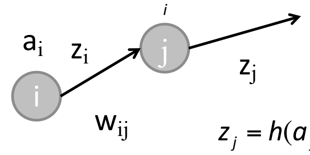
$$\frac{\partial E}{\partial w_{ij}} = \frac{\partial E}{\partial a_j}\frac{\partial a_j}{\partial w_{ij}}$$

$$\frac{\partial E}{\partial a_j} = \delta_j$$ ← Notation

$$\frac{\partial a_j}{\partial w_{ij}} = z_i$$ ← Calculus

$$\frac{\partial E}{\partial w_{ij}} = \delta_j z_i$$

$$a_j = \sum_i w_{ij} z_i$$



$$z_j = h(a_j)$$

60

Calculus Reminder

- Chain rule for one variable: $\frac{\partial f \circ g}{\partial x} = \frac{\partial f}{\partial g}\frac{\partial g}{\partial x}$
- Chain rule for: $f: \Re^n \rightarrow \Re^k, g: \Re^m \rightarrow \Re^n$

$$J_x(f \circ g) = J_{g(x)}(f) J_x(g) = \left(k \times n\right)\left(n \times m\right)$$

- For k=1, m=1

$$J_x(f \circ g) = \sum_{i=1}^{n} \frac{\partial f}{\partial g(x)_i}\frac{\partial g(x)_i}{\partial x}$$

61

Propagating Errors

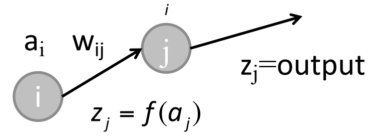
$$\frac{\partial E}{\partial w_{ij}} = \frac{\partial E}{\partial a_j}\frac{\partial a_j}{\partial w_{ij}} = \delta_j z_i$$

$$\frac{\partial E}{\partial a_j} = \delta_j, \quad \frac{\partial a_j}{\partial w_{ij}} = z_i,$$

- For output units (assuming no weights on outputs)

$$\frac{\partial E}{\partial a_j} = \delta_j = y - t$$

$$a_j = \sum_i w_{ij} z_i$$



$$z_j = f(a_j)$$

- For hidden units

Chain rule

$$\frac{\partial E}{\partial a_i} = \delta_i = \sum_k \frac{\partial E}{\partial a_k}\frac{\partial a_k}{\partial a_i} = \sum_k \frac{\partial E}{\partial a_k} w_{ik} \frac{\partial h_i}{\partial a_i} = h'(a_i)\sum_k w_{ik}\delta_k$$

All upstream nodes from i

Error gradient of upstream nodes

62

Differentiating h

- Recall the logistic sigmoid:

$$h(x) = \frac{e^x}{1+e^x} = \frac{1}{1+e^{-x}}$$

$$1 - h(x) = \frac{e^{-x}}{1+e^{-x}} = \frac{1}{1+e^x}$$

- Differentiating:

$$h'(x) = \frac{e^{-x}}{(1+e^{-x})^2} = \frac{1}{(1+e^{-x})}\frac{e^{-x}}{(1+e^{-x})} = h(x)(1-h(x))$$

63

Putting it together

- Apply input **x** to network (sum for multiple inputs)
  - Compute all activation levels
  - Compute final output (forward pass)
- Compute δ for output units

$$\delta = y - t$$

- Backpropagate δs to hidden units

$$\delta_j = \sum_k \frac{\partial E}{\partial a_k}\frac{\partial a_k}{\partial a_j} = h'(a_j)\sum_k w_{kj}\delta_k$$

- Compute gradient update: $\frac{\partial E}{\partial w_{ij}} = \delta_j a_i$

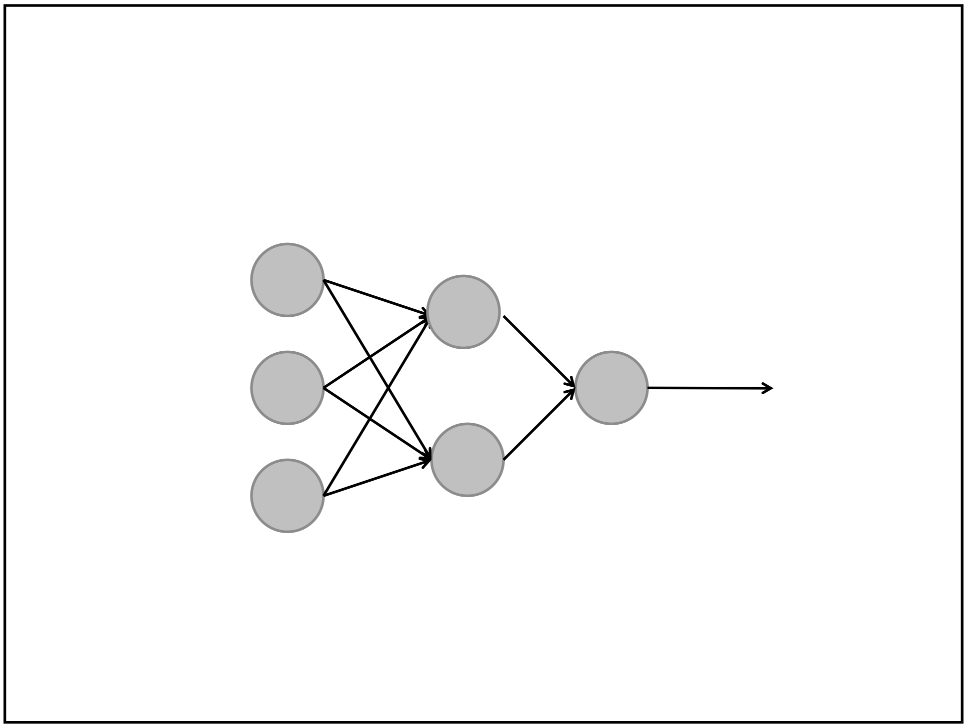
64

Summary of Gradient Update

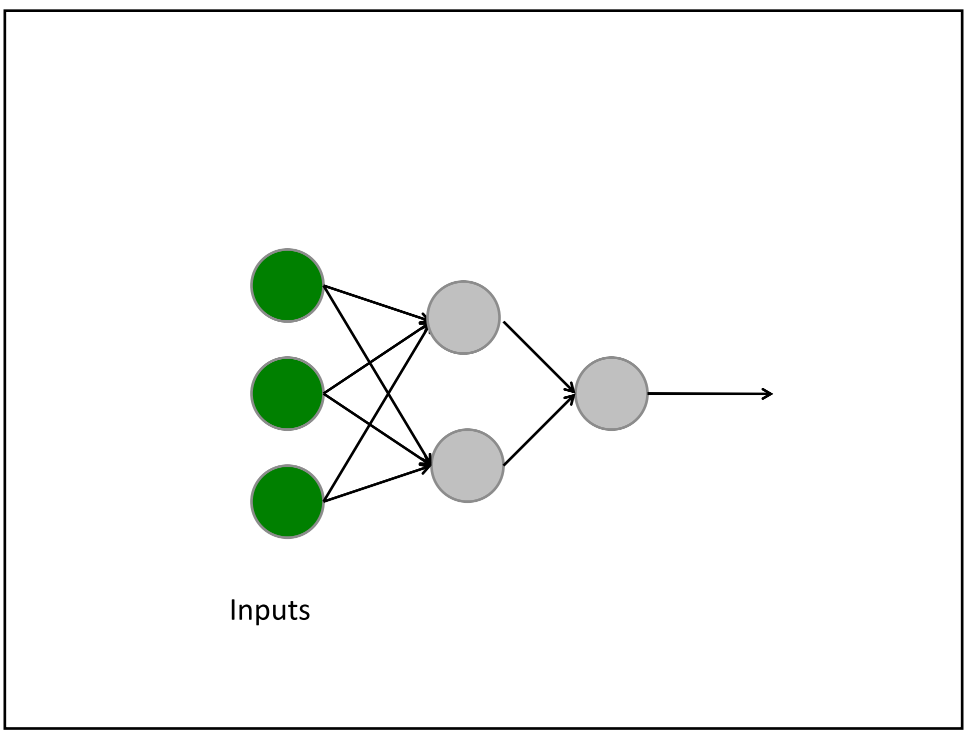
- Gradient calculation, parameter updates have recursive formulation
- Decomposes into:
  - Local message passing
  - No transcendentals:
    - h'(x)=1-h(x)^2 for tanh(x)
    - H'(x)=h(x)(1-h(x)) for logistic sigmoid
- Highly parallelizable
- Biologically plausible(?)

- Celebrated *backpropagation* algorithm

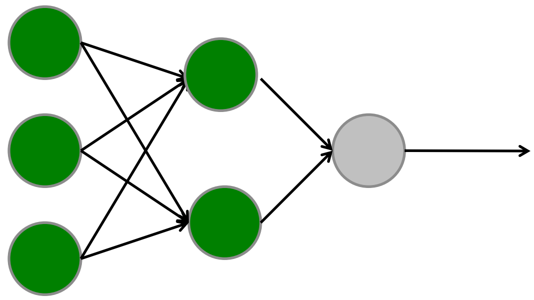
65



66

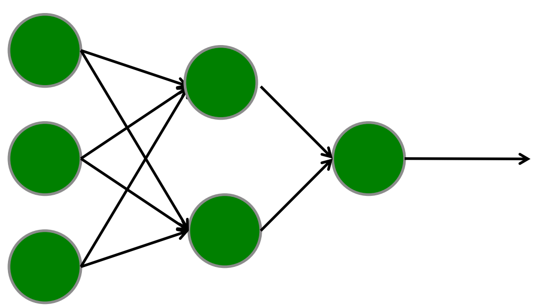


67



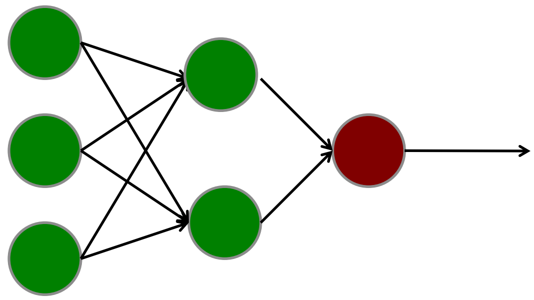
Propagate forward, computing activation levels,
outputs to next layer

68



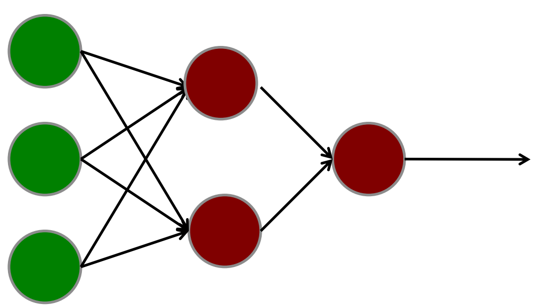
Compute the output of the final layer

69



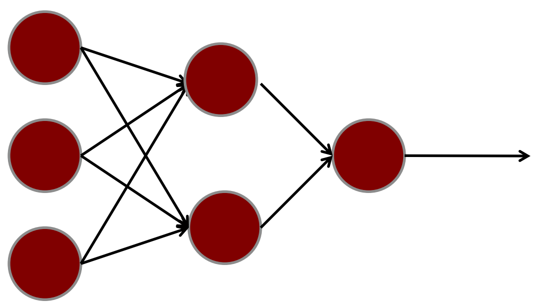
Compute the error (δ) for the final layer

70



Compute the error δ's and gradient updates for earlier layers: $\frac{\partial E}{\partial w_{ij}} = \delta_j a_i$

71



Complete training for one datum – now repeat for entire training set

72

Good News

- Can represent any continuous function with two layers (1 hidden)
- Can represent essentially any function with 3 layers
- (But how many hidden nodes?)

- Multilayer nets are a universal approximation architecture with a highly parallelizable training algorithm

73

Early Successes of Multilayer Nets

- Trained to pronounce English
  - Training set: Sliding window over text, sounds
  - 95% accuracy on training set
  - 78% accuracy on test set
- Trained to recognize handwritten digits
  - >99% accuracy
- Trained to drive (Pomerleau et al. no-hands across America 1995)

https://www.cs.cmu.edu/~tjochem/nhaa/navlab5_details.html

74

Backprop Issues

- Backprop = gradient descent on an error function
- Function is nonlinear (= powerful)
- Function is nonlinear (= local minima)
- Big nets:
  - Many parameters
    - Many optima
    - Slow gradient descent
    - Risk of overfitting
  - Biological plausibility ≠ Electronic plausibility
- Many NN experts became experts in numerical analysis (by necessity)

75

NN History Through the Second Coming

- Second wave of interest in neural networks lost research momentum in the 1990s – though still continued to enjoy many practical applications
- Neural network tricks were not sufficient to overcome competing methods:
  - Support vector machines
  - Clever feature selection methods wrapped around simple or linear methods
- 2000-2010 was an era of linear + special sauce
- What changed?

76

Deep Networks

- Not a learning algorithm, but a family of techniques
  - Improved training techniques (though still essentially gradient descent)
  - Clever crafting of network structure – convolutional nets
  - Some new activation functions
- Exploit massive computational power
  - Parallel computing
  - GPU computing
  - Very large data sets (can reduce overfitting)

77

Deep Networks Today

- Still on the upward swing of the hype pendulum
- State of the art performance for many tasks:
  - Speech recognition
  - Object recognition
  - Playing video games
- Controversial but increasingly accepted in practice:
  - Hype, hype, hype! (but it really does work well in many cases!)
  - Theory lags practice
  - Collection of tricks, not an entirely a science yet
  - Results are not human-interpretable

78

Conclusions

- Supervised learning = successful way to take training (input, output pairs) and induce functions that generalize to test data drawn from the same distribution as the training data.
- Methods for learning linear functions are well understood and perform well with good features
- Non-linear methods, such as neural networks are more powerful and require less feature engineering but are more computationally expensive and less predictable in practice
  - Historically wild swings in popularity
  - Currently on upswing due to clever changes in training methods, use of parallel computation, and large data sets

79