Machine Learning Neural Networks

Dr Ioannis Patras

Slide thanks: Tim Hospedales

Course Context

- Supervised Learning
 - (Linear) regression
 - (Linear) Classifiers and Logistic Regression
 - Neural Networks
- Unsupervised
 - Clustering
 - Density Estimation
 - HMMs

Overview

- Neural Nets Intro
- From Neurons to Neural Nets
- Multi-Layer Neural Nets for Non-Linear Functions
- Neural Net Prediction Details
- Training Neural Nets
- More considerations

Intro to Neural Nets

- The term 'neural network' has origins in attempts to find mathematical representations of information processing in biological systems.
 - (McCulloch and Pitts, 1943; Widrow and Hoff, 1960; Rosenblatt, 1962; Rumelhart et al., 1986).
- Neural Networks:
 - Inspired from algorithms that try to mimic the brain
 - Formalized as systems of interconnected "neurons"
 - Each neuron does a very simple calculation
 - Many layers of neurons put together.
 - The collective can do qualitatively more powerful computation than any individual unit.

Neural Nets in 2017!

- Until late 00's, they were largely shunned.
 - Now they are back!
- Superhuman performance at:
 - Character recognition
 - Face recognition
 - Object recognition
 - Atari video game playing
 - Go playing(!)
- Pervasive:
 - Run OCR in banks/mail.
 - Every facebook photo upload (millions per day) goes through a Deep CNN.
 - Run Cortana, Google's, Siri speech recognition.

In the Media

Facebook's DeepFace AI system is the scarily accurate future of facial recognition software

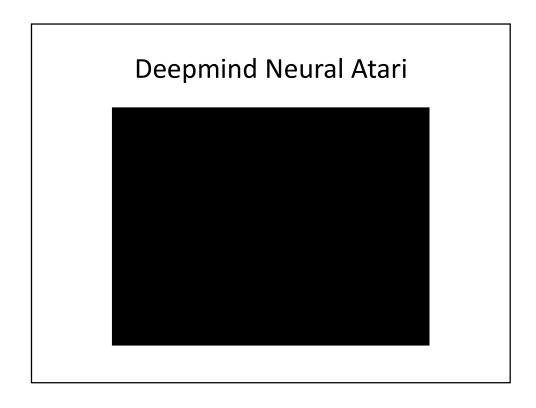


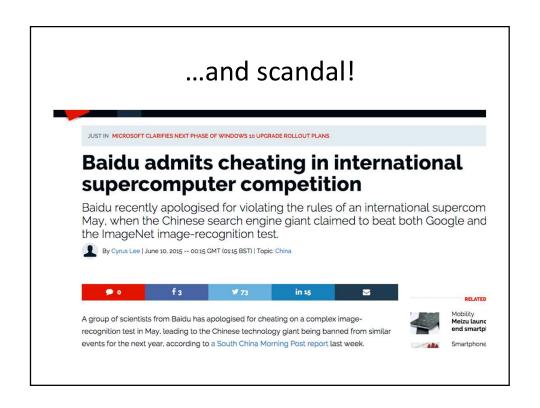
doi:10.1038/nature14236

Human-level control through deep reinforcement learning

Volodymyr Mnih¹*, Koray Kavukcuoglu¹*, David Silver¹*, Andrei A. Rusu¹, Joel Veness¹, Marc G. Bellemare¹, Alex Graves¹, Martin Riedmiller¹, Andreas K. Fidjeland¹, Georg Ostrovski¹, Stig Petersen¹, Charles Beattie¹, Amir Sadik¹, Ioannis Antonoglou Helen King¹, Dharshan Kumaran¹, Daan Wierstra¹, Shane Legg¹ & Demis Hassabis¹







Brain vs Computers

- Brain is massively parallel, but slow
 - 100 billion (10¹¹) neurons
 - 100 trillion (10¹⁴⁻¹⁵) connections (synapses)
 - -10^2 operations per second
- Contrast fast serial computers
 - 1-10³ processors
 - 1-10 billion operators per second

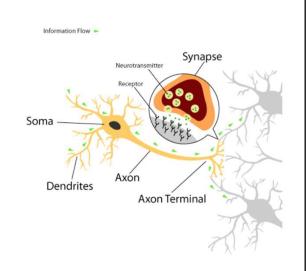
Von Neuman computer versus biological neural system

Artificial neural networks have an architecture roughly similar to the biological neural system

	Von Neumann computer	Biological neural system
Processor	Complex	Simple
	High speed	·Low speed
	One or a few	A large number
Memory	Separate from a processor Localized	Integrated into
	Noncontent addressable	processor Distributed
	Noncontent addressable	
		Content addressable
Computing	Centralized	Distributed
	Sequential	Parallel
	Stored programs	Self-learning
Reliability	Very vulnerable	Robust
Expertise	Numerical and symbolic	Perceptual
	manipulations	problems
Operating	Well-defined,	Poorly defined,
environment	t well-constrained	unconstrained

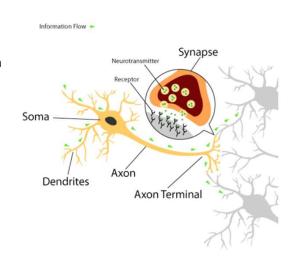
Real Neurons in Real Brains

- The Brain inspires NNs.
- In turn NNs and ML could (??) help us understand how the brain works
- Brains do massively parallel computation.
- Synapses change strength (cf weight change in ML model)
- Local signals used to change the strength



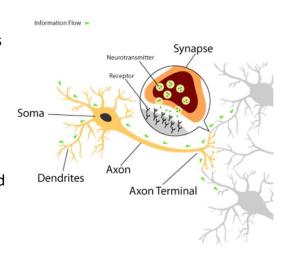
Real Neurons in Real Brains

- Dendrites collect incoming signals
- Polarization builds up in cell...
- After reaching a charge threshold, neuron fires
- Impluse travels down Axon
- And into other neurons via synapses
- ...and repeat



Real Neurons in Real Brains

- Real neurons use spikes not continuous outputs
- However, they have a minimum (0) and maximum firing rate
- Artificial neurons can roughly be considered to simulate natural neurons at firing rate level



Artificial Neural Networks

- Nodes (cf neurons)
- Adaptive Weights (cf synaptic strength)
- Defined by:
 - Interconnection pattern between layers of neurons
 - The activation function that converts a neuron's weighted input to its output activation.
 - The learning process for updating the interconnection weights
- Can model arbitrarily complex non-linear functions of inputs.

Fixed Versus Adaptive Basis Functions

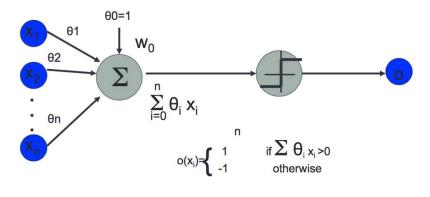
- Previously we used fixed linear combinations of features.
- Limited by the curse of dimensionality
- In contrast, Neural Nets adapt the parameters of the basis functions during training.

Overview

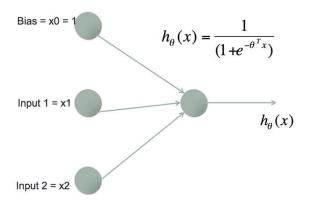
- Neural Nets Intro
- From Neurons to Neural Nets
- Multi-Layer Neural Nets for Non-Linear Functions
- Neural Net Prediction Details
- Training Neural Nets
- More considerations

Perceptron: A Simple Model Neuron

- Uses the step function as activation
 - Linear Threshold Unit (LTU)



Neuron as a Logistic Regression Unit

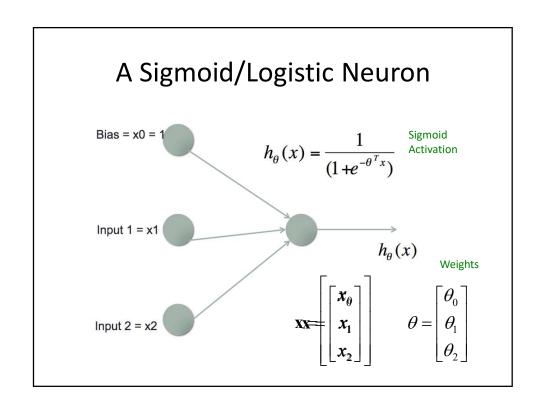


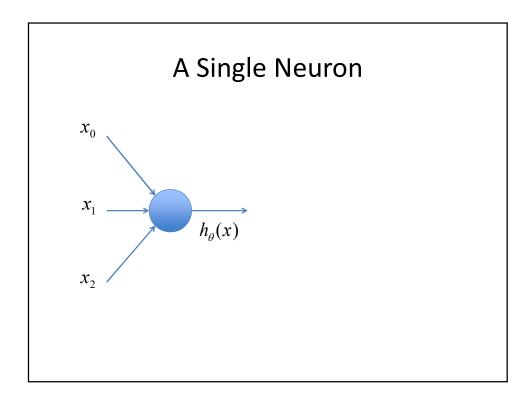
Can think of a logistic regression unit as a neuron (function) that multiplies the input by the parameters (weights) and squashes the resulting sum through the sigmoid.

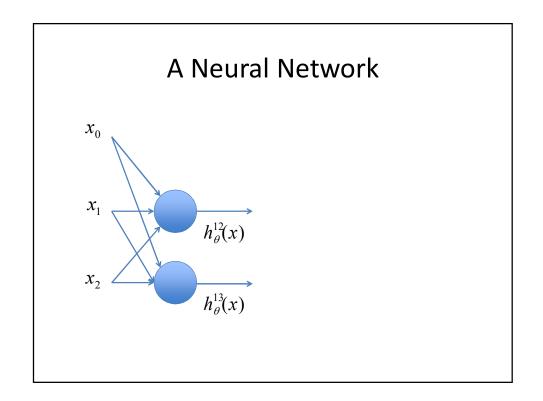
 Logistic Regression Unit => Perception if weight strength goes to infinity, so sigmoid => step.

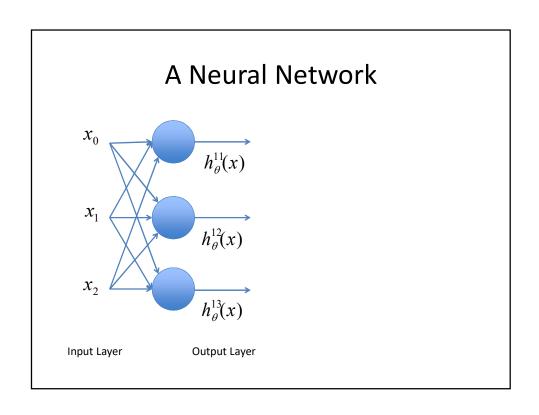
Feed Forward Neural Net

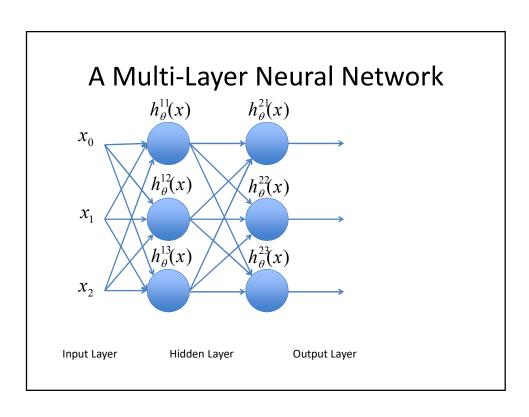
- · Connected set of logistic regression units
 - Arranged in layers.
 - Each unit's output is a non-linear function (e.g., sigmoid, step function) of a linear combination of its inputs.
- Input layer size:
 - Size of input to classify/regress
- Output layer size
 - Size of target for classification/regression
- Any number of hidden neurons
- Any number of hidden layers

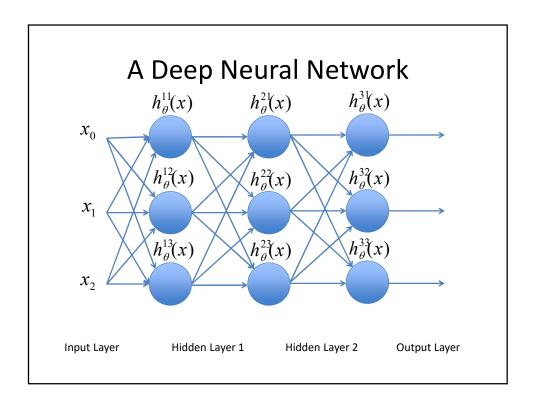










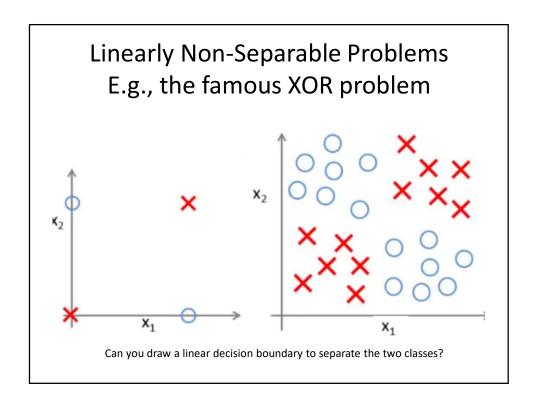


Summary:

- Neural nets as interconnected layers of (e.g., sigmoid / logistic regression) neurons/units.
- Layer l+1's inputs are layer l's outputs.
- Can have any number of layers.

Overview

- Neural Nets Intro
- From Neurons to Neural Nets
- Multi-Layer Neural Nets for Non-Linear Functions
- Neural Net Prediction Details
- Training Neural Nets
- More considerations



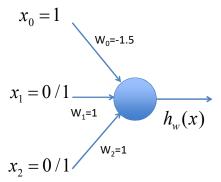
How can a NN help?

- It can combine decision boundaries at each level of the network.
 - The decision of one layer can become the input of the next
- This can make more complex boundaries overall.
- Lets look at some examples...

Logical Functions

- Neural AND?
- Neural OR?
- Neural XOR?

Logistic Unit AND



A B AANDB

0 0 <0

0 1 <0

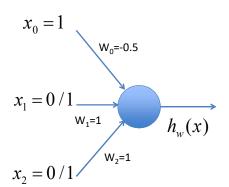
1 0 <0

1 1 >0 (class 1)

What weights will give AND?

Recall $H_w(x)=1$ if $w_1x_1+w_2x_2+w_0>0$ Otherwise $H_w(x)=0$

Logistic Unit OR



A B AORB

0 0

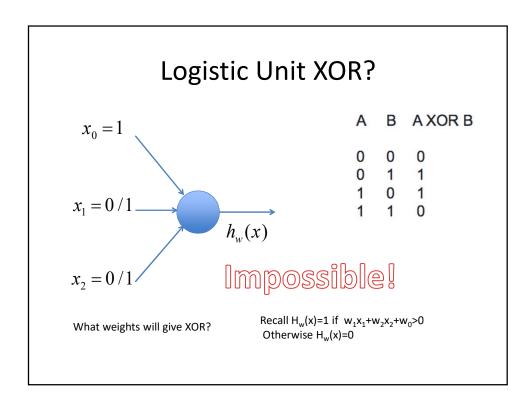
0 1 1

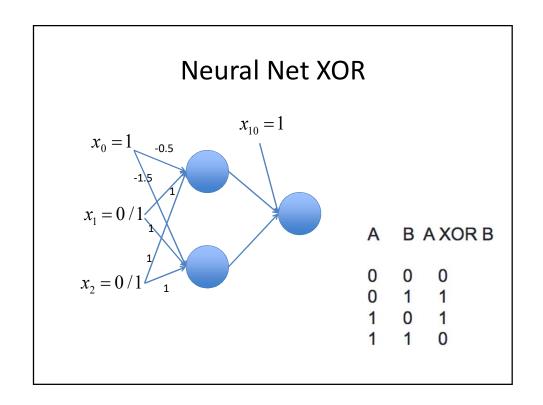
1 0 1

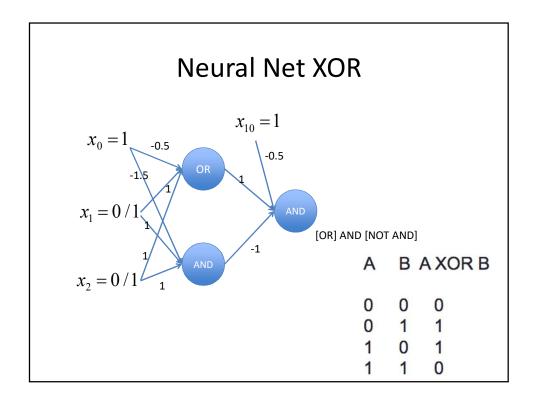
What weights will give OR?

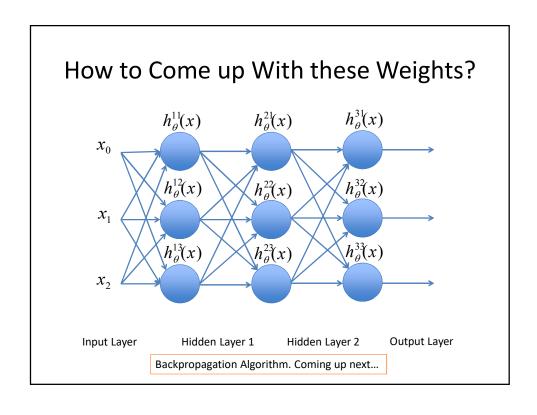
Recall $H_w(x)=1$ if $w_1x_1+w_2x_2+w_0>0$

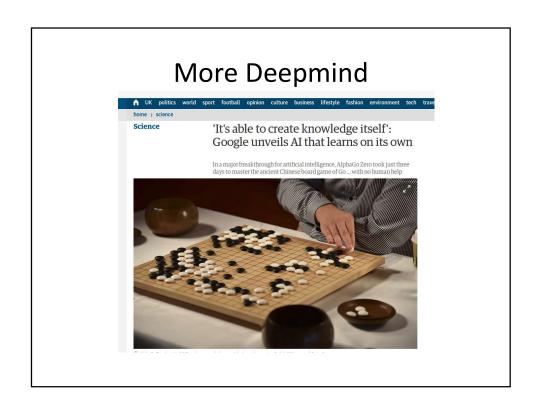
Otherwise $H_w(x)=0$

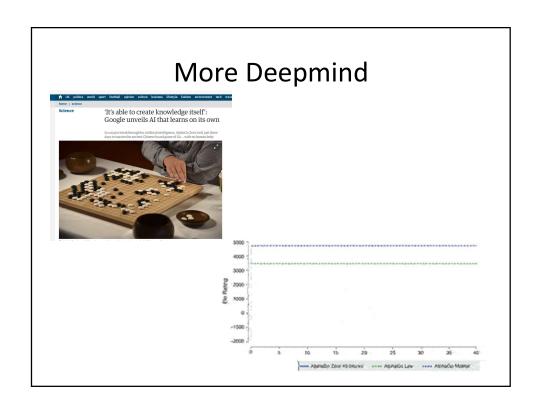












Summary:

- Single neurons can only do linear decision boundaries.
- Networks of neurons can do (arbitrarily) complicated non-linear decisions.

Overview

- Neural Nets Intro
- From Neurons to Neural Nets
- Multi-Layer Neural Nets for Non-Linear Functions
- Neural Net Prediction Details
- Training Neural Nets
- More considerations

Typical Activations

- Each neuron computes $h(\mathbf{w}^T\mathbf{x}) = h(\sum_{i=1}^n w_i x_i + w_0)$
- Activation functions h(a)
 - Perception (step-function activation)
 - Issue: Not differentiable wrt weights.

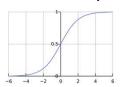
 $h(a) = \begin{cases} 1 & if & a > 0 \\ -1 & if & a < 0 \end{cases}$

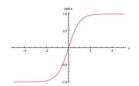
- Sigmoid

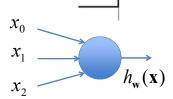
– tanh

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

- Identity...







Unpacking the Prediction Made

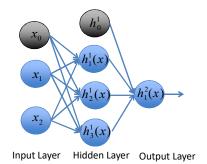
• What's the prediction made?

$$h_1^1(\mathbf{x}) = h(w_{10}^1 + w_{11}^1 x_1 + w_{21}^1 x_2)$$

$$h_2^1(\mathbf{x}) = h(w_{20}^1 + w_{21}^1 x_1 + w_{22}^1 x_2)$$

$$h_3^1(\mathbf{x}) = h(w_{30}^1 + w_{31}^1 x_1 + w_{32}^1 x_2)$$

$$h_1^2(\mathbf{x}) = h(w_{10}^2 + w_{11}^2 h_1^1 + w_{12}^2 h_2^1 + w_{13}^2 h_3^1)$$



Unpacking the Prediction Made

• What's the prediction made?

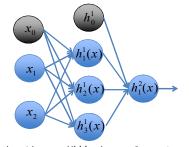
$$h_1^1(\mathbf{x}) = h(w_{10}^1 + w_{11}^1 x_1 + w_{21}^1 x_2)$$

$$h_2^1(\mathbf{x}) = h(w_{20}^1 + w_{21}^1 x_1 + w_{22}^1 x_2)$$

$$h_3^1(\mathbf{x}) = h(w_{30}^1 + w_{31}^1 x_1 + w_{32}^1 x_2)$$

$$h_1^2(\mathbf{x}) = h(w_{10}^2 + w_{11}^1 h_1^1 + w_{12}^2 h_2^1 + w_{13}^2 h_3^1)$$

$$h^{2}_{k}(\mathbf{x}) = h_{k} \left(\sum_{j=1}^{M} w^{(2)}_{kj} \cdot h_{j} \left(\sum_{i=1}^{D} w^{(1)}_{ji} x_{i} \right) \right)$$



nput Layer Hidden Layer Output Layer

Unpacking the Prediction Made

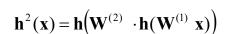
• What's the prediction made?

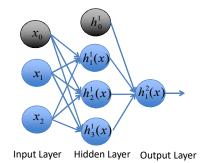
$$h_1^1(\mathbf{x}) = h(w_{10}^1 + w_{11}^1 x_1 + w_{21}^1 x_2)$$

$$h_2^1(\mathbf{x}) = h(w_{20}^1 + w_{21}^1 x_1 + w_{22}^1 x_2)$$

$$h_3^1(\mathbf{x}) = h(w_{30}^1 + w_{31}^1 x_1 + w_{32}^1 x_2)$$

$$h_1^2(\mathbf{x}) = h(w_{10}^2 + w_{11}^2 h_1^1 + w_{12}^2 h_2^1 + w_{13}^2 h_3^1)$$





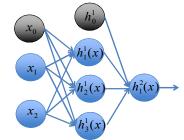
Aside: Non-linearities are important.

- What's the prediction made?
 - Suppose we used linear activation h. h(a) = a
 - What happens to the prediction?

$$\mathbf{h}^{2}(\mathbf{x}) = \mathbf{h} \big(\mathbf{W}^{(2)} \cdot \mathbf{h} (\mathbf{W}^{(1)} \mathbf{x}) \big)$$

$$\mathbf{h}^{2}(\mathbf{x}) = \mathbf{W}^{(2)}\mathbf{W}^{(1)} \mathbf{x}$$

- $\mathbf{h}^2(\mathbf{x}) = \mathbf{W}'\mathbf{x}$
- No matter how many layers....
 - Still a simple linear model



Input Layer Hidden Layer Output Layer

Neural Nets can do many tasks

- Single output regression
- Multiple output regression
- Binary classification.
- Multiclass classification.
- Binary multi-label classification.
- ... by changing the activation function of output layer.

Neural Nets can do many tasks: Single output regression

- Single output regression
 - Identity activation

$$h^2(a) = a$$

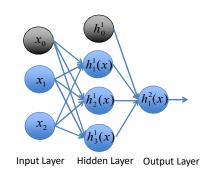
• Linear combination of previous layer is range +/- inf.

$$h_1^1(\mathbf{x}) = h(w_{10}^1 + w_{11}^1 x_1 + w_{21}^1 x_2)$$

$$h_2^1(\mathbf{x}) = h(w_{20}^1 + w_{21}^1 x_1 + w_{22}^1 x_2)$$

$$h_3^1(\mathbf{x}) = h(w_{30}^1 + w_{31}^1 x_1 + w_{32}^1 x_2)$$

$$h_1^2(\mathbf{x}) = w_{10}^2 + w_{11}^2 h_1^1 + w_{12}^2 h_2^1 + w_{13}^2 h_3^1$$



Neural Nets can do many tasks: Multiple output regression

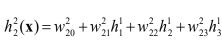
- Multiple output regression
 - Identity activation

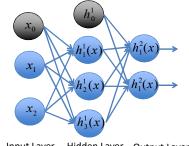
$$h^2(a) = a$$

- Linear combination of previous layer is range +/- inf.
- Use multiple output units.

$$h_1^2(\mathbf{x}) = w_{10}^2 + w_{11}^2 h_1^1 + w_{12}^2 h_2^1 + w_{13}^2 h_3^1$$

$$h_1^2(\mathbf{x}) = w_1^2 + w_1^2 h_1^1 + w_2^2 h_1^1 + w_2^2 h_1^1$$





Input Layer Hidden Layer Output Layer

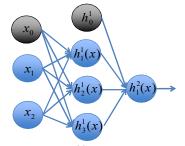
Neural Nets can do many tasks: Binary classification

- Binary classification
 - Sigmoid activation

$$h^2(a) = 1/(1+e^{-a})$$

• Linear combination of previous layer squashed into range [0,1].

$$h_1^2(\mathbf{x}) = \sigma(w_{10}^2 + w_{11}^2 h_1^1 + w_{12}^2 h_2^1 + w_{13}^2 h_3^1)$$



Input Layer Hidden Layer Output Layer

Neural Nets can do many tasks: Multiclass/Multi-label classification

- Multiclass classification
 - Sigmoid activation

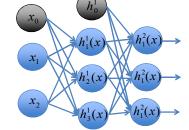
$$h^2(a) = 1/(1+e^{-a})$$

- Linear combination of previous layer squashed into range [0,1]
- Use multiple output units in 1-of-K encoding.

$$h_1^2(\mathbf{x}) = \sigma(w_{10}^2 + w_{11}^2 h_1^1 + w_{12}^2 h_2^1 + w_{13}^2 h_3^1)$$

$$h_2^2(\mathbf{x}) = \sigma(w_{20}^2 + w_{21}^2 h_1^1 + w_{22}^2 h_2^1 + w_{23}^2 h_3^1)$$

$$h_3^2(\mathbf{x}) = \sigma(w_{30}^2 + w_{31}^2 h_1^1 + w_{32}^2 h_2^1 + w_{33}^2 h_3^1)$$



Input Layer Hidden Layer Output Layer

Neural Nets can do many tasks: Multiclass/Multi-label classification

- Multiclass classification
 - Sigmoid activation

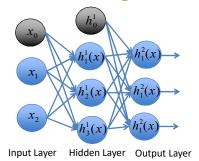
$$h^2(a) = 1/(1+e^{-a})$$

- Linear combination of previous layer squashed into range [0,1]
- Use multiple output units in 1-of-K encoding.
- I.e., Train set would be

-y=[1,0,0]: person

-y=[0,1,0]: car

-y=[0,0,1]: truck

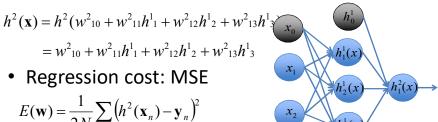


Overview

- Neural Nets Intro
- From Neurons to Neural Nets
- Multi-Layer Neural Nets for Non-Linear Functions
- Neural Net Prediction Details
- Training Neural Nets
- More considerations

Cost Functions: Regression

- As with linear & logistic regression, to train a Neural Net we'll need a cost function.
 - And training data $D=\{x,y\}$ pairs....
- Regression prediction:



 $E(\mathbf{w}) = \frac{1}{2N} \sum_{n=1}^{\infty} \left(h^2(\mathbf{x}_n) - \mathbf{y}_n \right)^2$

Input Layer Hidden Layer Output Layer

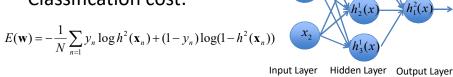
Cost Functions: Classification

- As with linear & logistic regression, to train a Neural Net we'll need a cost function.
 - And training data D={x,y} pairs....
- Classification prediction:

$$h^{2}(\mathbf{x}) = h(w_{10}^{2} + w_{11}^{2}h_{1}^{1} + w_{12}^{2}h_{2}^{1} + w_{13}^{2}h_{3}^{1})$$

= $\sigma(w_{10}^{2} + w_{11}^{2}h_{1}^{1} + w_{12}^{2}h_{2}^{1} + w_{13}^{2}h_{3}^{1})$

• Classification cost:



Computing the Cost

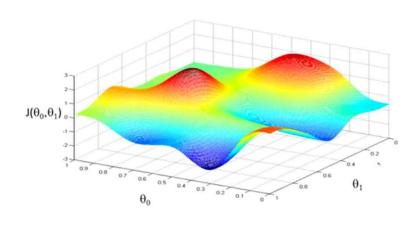
- To train NN, find weights to minimise the cost.
- We know how to write code to compute E(w)
 - 1. Do the "forward propagation" and make predictions.
 - 2. Use predictions to compute cost.
- But how to minimise it efficiently?

$$h^2(\mathbf{x}) = \mathbf{w}^2 h^1(\mathbf{W}^1 \mathbf{x})$$
 $h^2(\mathbf{x}) = \sigma(\mathbf{w}^2 h^1(\mathbf{W}^1 \mathbf{x}))$

$$E(\mathbf{w}) = \frac{1}{2N} \sum_{n=1}^{\infty} \left(h^2(\mathbf{x}_n) - \mathbf{y}_n \right)^2 \quad E(\mathbf{w}) = -\frac{1}{N} \sum_{n=1}^{\infty} y_n \log h^2(\mathbf{x}_n) + (1 - y_n) \log(1 - h^2(\mathbf{x}_n))$$

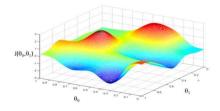
Minimising the Cost

Cost is Non-Convex



Neural Net Cost is Non Convex

- Cost is Non-Convex:
 - No global minima.
 - Require iterative gradient methods to train.
 - Gradient descent will only converge to local minima.



How to Optimise Cost?

- For Linear/Logistic regression, each weight had a straightforward derivative.
- For neural net, complicated by many layers of interdependent weights.

$$h^{2}(\mathbf{x}) = \mathbf{w}^{2}h^{1}(\mathbf{W}^{1}\mathbf{x}) \qquad \qquad h^{2}(\mathbf{x}) = \sigma(\mathbf{w}^{2} \ h^{1}(\mathbf{W}^{1}\mathbf{x}))$$

$$E(\mathbf{w}) = \frac{1}{2N} \sum_{n=1}^{\infty} \left(h^{2}(\mathbf{x}_{n}) - \mathbf{y}_{n}\right)^{2} \qquad E(\mathbf{w}) = -\frac{1}{N} \sum_{n=1}^{\infty} y_{n} \log h^{2}(\mathbf{x}_{n}) + (1 - y_{n}) \log(1 - h^{2}(\mathbf{x}_{n}))$$

Backpropagation Algorithm

- Derivative of cost wrt any weight w_{ii}:
 - Depends on activation: the linear combination of inputs before non-linearity.
 - Activation:
 - Every neuron does something like: $a_j = \sum_i w_{ji} z_j$ – (z may inputs or previous layer's outputs)
 - Before doing non-linearity: $h(a_i)$
 - Weight update via activations:

$$\frac{\partial E(\mathbf{w})}{\partial w_{ji}} = \frac{\partial E(\mathbf{w})}{\partial a_j} \frac{\partial a_j}{\partial w_{ji}} \implies \frac{\partial a_j}{\partial w_{ji}} = z_i \quad \frac{\partial E(\mathbf{w})}{\partial a_j} = \delta_j \implies \frac{\partial E(\mathbf{w})}{\partial w_{ji}} = \delta_j z_i$$

Backpropagation Algorithm

- Iterate:
 - Propagate forward to find activations a and h(a) of all internal and output units. [Done]
 - Evaluate error term δ for output units [TBD].
 - Backpropagate output δs to obtain internal δs .

$$\delta_j = h'(a_j) \sum_k w_{kj} \delta_k$$
 Activ. Must be differentiable!

– Use δ s to get a gradient update for each weight:

$$\frac{\partial E(\mathbf{w})}{\partial w_{ji}} = \delta_j z_i \quad \frac{\partial E(\mathbf{w})}{\partial w_{ki}} = \delta_k z_j$$

Output Error Term: Regression

- $\frac{\partial E(\mathbf{w})}{\partial a_k} = \delta_k$ • Output error term:
- For linear regression:
 - Cost: Square Deviation
 - Activation: Identity.

$$E_n(\mathbf{w}) = 0.5 \left(h(a_j) - y \right)^2 \qquad \frac{\partial E_n(\mathbf{w})}{\partial a_k} = h'(a_k) \left(h(a_k) - y \right)$$

$$h(a_k) = a_k$$
 $h'(a_k) = 1$ $\frac{\partial E_n(\mathbf{w})}{\partial a_k} = \delta_k = (h(a_k) - y)$

Output Error Term: Binary Classifier

- Output error term: $\frac{\partial E(\mathbf{w})}{\partial a_k} = \delta_k$
- For binary classifier
 - Cost: Square Devation (or cross-entropy)
 - Activation: Sigmoid.

$$E_n(\mathbf{w}) = 0.5 (h(a_k) - y)^2$$

$$\frac{\partial E_n(\mathbf{w})}{\partial a_k} = h'(a_k) (h(a_k) - y)$$

$$E_{n}(\mathbf{w}) = 0.5 (h(a_{k}) - y)^{2} \qquad \frac{\partial E_{n}(\mathbf{w})}{\partial a_{k}} = h'(a_{k}) (h(a_{k}) - y)$$

$$h(a) = \sigma(a) = 1/(1 + e^{-a}) \qquad \frac{\partial E_{n}(\mathbf{w})}{\partial a_{k}} = \sigma'(a_{k}) (\sigma(a_{k}) - y)$$

$$h'(a) = \sigma'(a) = \sigma(a)(1 - \sigma(a))$$

Summary: Regression

• Iterate:

- Propagate forward to find activations a and h(a) of all internal and output units: $h^2(\mathbf{x}) = \mathbf{w}^2 h^1(\mathbf{W}^1 \mathbf{x})$
- Evaluate error term δ for output units: $\delta_k = \left(h(a_k) y\right)$
- Backpropagate output δs to obtain internal δs .

$$\delta_j = h'(a_j) \sum w_{kj} \delta_k$$

– Use δ s to get a gradient update for each weight:

$$\frac{\partial E(\mathbf{w})}{\partial w^{(1)}_{ii}} = \delta_j x_i \quad \frac{\partial E(\mathbf{w})}{\partial w^{(2)}_{ki}} = \delta_k h^{(1)}_{ji}$$

Summary: Binary Classification

• Iterate:

- Propagate forward to find activations a and h(a) of all internal and output units: $h^2(\mathbf{x}) = \sigma(\mathbf{w}^2 \ h^1(\mathbf{W}^1\mathbf{x}))$
- Evaluate error term δ for output units:

$$\delta_k = \sigma'(a_k) \big(\sigma(a_k) - y \big)$$

- Backpropagate output δs to obtain internal δs .

$$\delta_j = h'(a_j) \sum_k w_{kj} \delta_k$$

– Use δs to get a gradient update for each weight:

$$\frac{\partial E(\mathbf{w})}{\partial w^{(1)}_{ji}} = \delta_j x_i \quad \frac{\partial E(\mathbf{w})}{\partial w^{(2)}_{kj}} = \delta_k h^{(1)}_{ji}$$

Training Overview

- Implement forward propagation to get h(x) for any x.
- Implement cost function computation.
- Implement backpropagation to compute partial derivatives.
- Iterate forward & backward propagation.

Summary

- Training neural nets:
 - Use backpropagation to minimise their cost function.
 - Errors at later nodes are backpropagated to compute errors at earlier nodes.
 - Errors at each node give gradient update for that node.

Overview

- Neural Nets Intro
- From Neurons to Neural Nets
- Multi-Layer Neural Nets for Non-Linear Functions
- Neural Net Prediction Details
- Training Neural Nets
- More considerations

Batch vs Online

- Updates in past couple slides are gradients
 WRT one single input n.
 - Online Gradient Descent:
 - Iterate over data *n*, and weights *w*(*i*,*j*):

$$w_{ji} = w_{ji} - \alpha \frac{\partial E_n(\mathbf{w})}{\partial w_{ji}}$$

- Batch Gradient Descent:
 - Iterate over weights w(i,j):

$$w_{ji} = w_{ji} - \alpha \sum_{n} \frac{\partial E_{n}(\mathbf{w})}{\partial w_{ji}}$$

Gradient Checking

- When implementing gradient-descent algorithms like backprop....
- May be useful to check correctness of your derivatives numerically. $\frac{\partial E(\mathbf{w})}{\partial w_{ji}} = \delta_j h_i$ Should be equal
- Can implement finite difference numerical differentiation to check them

$$\frac{\partial E_n(\mathbf{w})}{\partial w_{ji}} = \frac{E_n(w_{ji} + \varepsilon) - E_n(w_{ji} - \varepsilon)}{2\varepsilon}$$

 I.e., perturb the current weight and re-compute the network's error. Get gradient from this change in error.

Gradient Checking

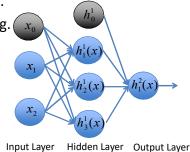
- Aside: You could also implement gradient descent by numerical differentiation, but slow!
 - Each forward propagation costs O(W).
 - Each weight must be perturbed individually at cost O(W).
- $=> Overall cost O(W^2)$

$$\frac{\partial E_n(\mathbf{w})}{\partial w_{ji}} = \frac{E_n(w_{ji} + \varepsilon) - E_n(w_{ji} - \varepsilon)}{2\varepsilon}$$

 I.e., perturb the current weight and re-compute the network's error. Get gradient from this change in error.

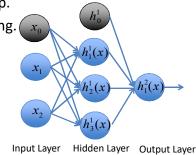
Initialization

- For gradient methods need to pick initial weight vectors **w**.
 - Zero initialization:
 - Every hidden unit gets the same input.
 - Nothing different to backprop.
 - Network never learns anything.



Initialization => Symmetry Breaking

- For gradient methods need to pick initial weight vectors **w**.
 - Zero initialization:
 - Every hidden unit gets the same input.
 - Nothing different to backprop.
 - Network never learns anything.
- Solution:
 - Init randomly in $[-\varepsilon, \varepsilon]$



Local Minima

- Neural Net costs are not Convex
- Solutions:
 - 1. Accept local minima.
 - 2. Online rather than batch gradient descent may help jitter out of minima.
 - Repeatedly restart from different random initial conditions, take the best performing network. (Expensive)
 - 4. ...momentum, etc.

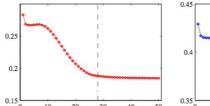
Overfitting in Neural Nets

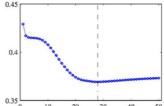
- Neural Nets can have lots of parameters (weights)
 - 10s of millions in practice!
 - Overfitting is a risk, especially if limited data.
- Solutions: Regularization:
 - Use L2 regularizer/weight decay as we did with linear/logistic regression (needs update to gradients)

Overfitting in Neural Nets

- Neural Nets can have lots of parameters (weights)
 - 10s of millions in practice!
 - Overfitting is a risk, especially if limited data.
- Solutions: Early Stopping:
 - At each iteration of gradient descent, check the network cost on validation set.
 - Stop once validation error starts to increase (although train error will still be decreasing)

Overfitting in Neural Nets



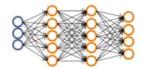


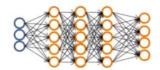
- Solutions: Early Stopping:
 - At each iteration of gradient descent, check the network cost on validation set.
 - Stop once validation error starts to increase (although train error will still be decreasing)

NN: Design Decisions

- Network Architecture
 - # of Hidden Layers.
 - # of Hidden Nodes.
- (# of input & output relatively easy)







- Cost function choice
- Activation function choice
- Learning rate

Training Overview (2)

- Choose architecture
- Initialize weights to small random numbers
- Implement forward propagation to get h(x) for any x.
- Implement cost function computation.
- Implement backpropagation to compute partial derivatives.
- Iterate forward & backward propagation.
- Use gradient checking to debug.
- Disable gradient checking once debugged.
- Early Stop training once validation error increasing.
- (Repeatedly retrain to try and find different local minima)

Overview

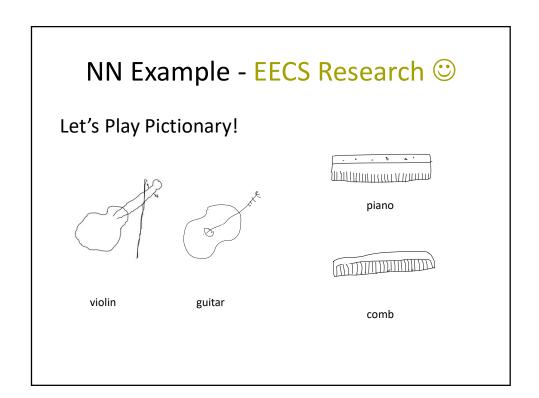
- Neural Nets Intro
- From Neurons to Neural Nets
- Multi-Layer Neural Nets for Non-Linear Functions
- Neural Net Prediction Details
- Training Neural Nets
- More considerations
- Resurgence and Deep Neural Nets

Why were NNs out of favor?

- Slow to train:
 - Vanilla gradient descent inefficient compared to convex optimisers (e.g., Kernel-SVM).
- Local minima & no better than alternatives:
 - Kernel-SVMs can do "equally good" non-linear classification and get global optimum quickly.
- Over-fitting:
 - Neural nets have lots of parameters.
 - They seemed easy to overfit, and tricky to regularize them.

Why are NNs back?

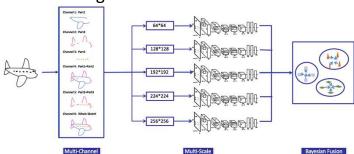
- Slow to train: Solved?
 - In ~2012, GPU computation used to speed up operations required for backprop x10-20 times (per GPU!) over CPU.
- Over-fitting: Solved?
 - "Big Data" in 2017 vast available databases can constrain vast number of parameters.
 - New regularization techniques: Dropout.
- Local minima: Doesn't matter?
 - With other stuff taken care of, local minima are usually pretty good.
- Technical advances:
 - RELU activation.
 - Deep neural nets can be better than shallow. (wide as well)
- Feature learning
 - Can input "raw data" an learn the features.



NN Example - EECS Research ©

Best Paper Prize: BMVC 2015!

- Our AI system plays superhuman level of pictionary!
 - Key components: Neural Net => Metric Learning => Nearest Neighbor.



NN Example - EECS Research ©

Best Paper Prize: BMVC 2015!

- Specs:
 - Eight layers (five convolutional).
 - "Only" 8.5 million parameters. (CF 144 mil).
 - Trained on 300M images with 32C Xenon CPU: 80 hours, or K40 GPU: 10 hours.

