Neural Networks

David Rosenberg

New York University

October 29, 2016

Objectives

- What are neural networks?
- How do they fit into our toolbox?
- When should we consider using them?

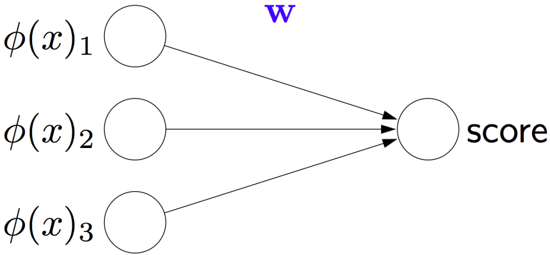
Linear Prediction Functions

- Linear prediction functions: SVM, ridge regression, Lasso
- Generate the feature vector $\phi(x)$ by hand.

From Percy Liang's "Lecture 3" slides from Stanford's CS221, Autumn 2014.

Linear Prediction Functions

- Linear prediction functions: SVM, ridge regression, Lasso
- Generate the feature vector $\phi(x)$ by hand.
- Learn weight vector w from data.



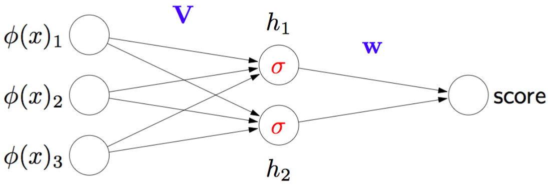
- So

$$\text{score} = w^T \phi(x)$$

From Percy Liang's "Lecture 3" slides from Stanford's CS221, Autumn 2014.

Neural Network

- Add an extra layer with a nonlinear transformation:



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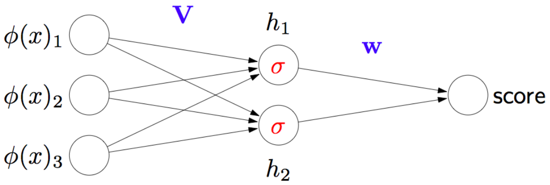

- We've introduced **hidden nodes** h_1 and h_2.

$$h_i = \sigma\left(v_i^T \phi(x)\right),$$

where σ is a nonlinear **activation function**. (We'll come back to this.)

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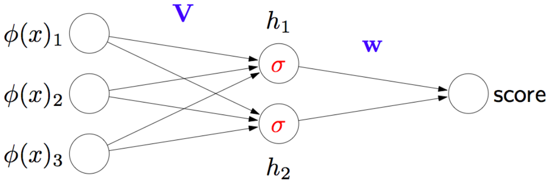
Neural Network



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$$\text{score} = w_1 h_1 + w_2 h_2$$

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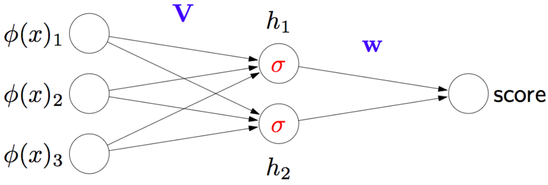

- Score is just

$$\begin{aligned} \text{score} &= w_1 h_1 + w_2 h_2 \\ &= w_1 \sigma(v_1^T \phi(x)) + w_2 \sigma\left(v_2^T \phi(x)\right) \end{aligned}$$

- This is the basic recipe.
  - We can add more hidden nodes.
  - We can add more hidden layers.

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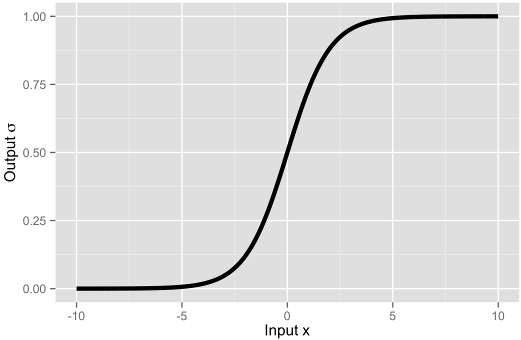
Activation Functions

- The **nonlinearity** of the activation function is a key ingredient.
- The **logistic sigmoid** function is one of the more commonly used:

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

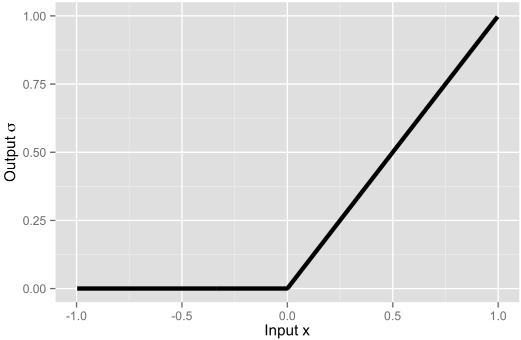


Activation Functions

- More recently, the **rectified linear** function has been very popular:

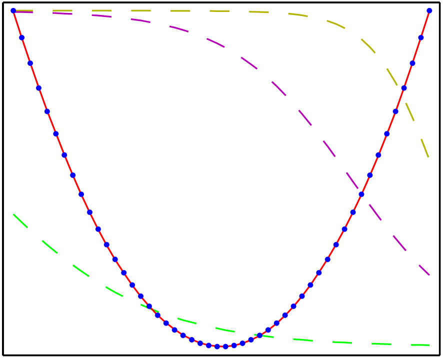
$$\sigma(x) = \max(0, x).$$

- "**RELU**" is much faster to calculate, and to calculate its derivatives.



Approximation Ability: $f(x) = x^2$

- 3 hidden units; logistic activation functions
- Blue dots are training points; Dashed lines are hidden unit outputs; Final output in Red.



From Bishop's *Pattern Recognition and Machine Learning*, Fig 5.3

Approximation Ability: $f(x) = \sin(x)$

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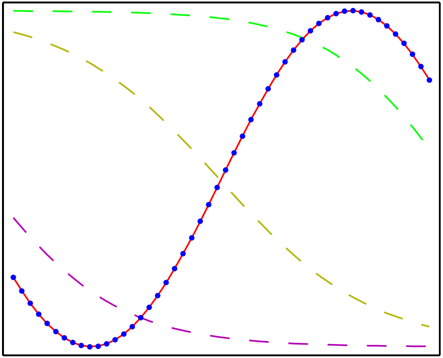

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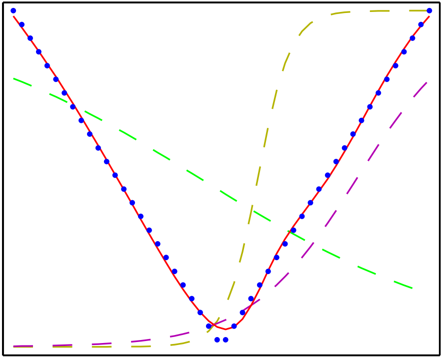

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Approximation Ability: $f(x) = 1(x > 0)$

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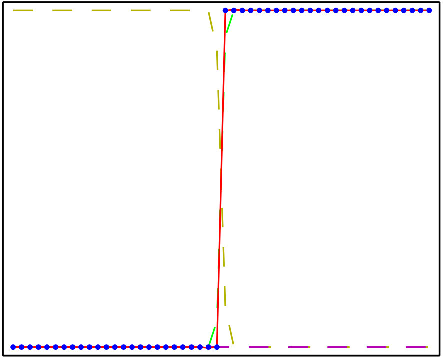

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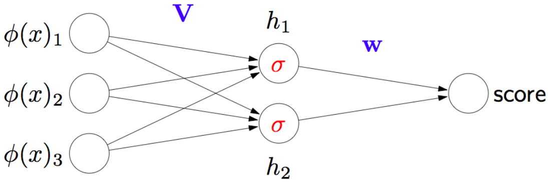
Neural Network: Hidden Nodes as Learned Features



- Can interpret h_1 and h_2 as nonlinear features learned from data.

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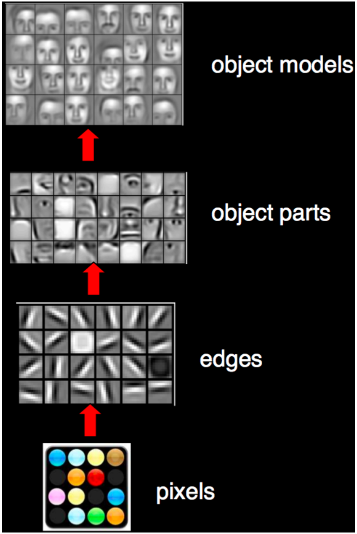
Facial Recognition: Learned Features



From Andrew Ng's CS229 Deep Learning slides

Neural Network: The Hypothesis Space

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- Functions in $\mathcal{F}$ **parameterized by the weights between nodes**.

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- Optimization method of choice: **mini-batch gradient descent**.
  - In practice, lots of little tweaks; see e.g. AdaGrad and Adam

Neural Network: Objective Function

- In our simple network, the output score is given by

$$f(x) = w_1\sigma(v_1^T\phi(x)) + w_2\sigma\left(v_2^T\phi(x)\right)$$

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- Note: $J(w,v)$ is **not convex**.
    - makes optimization much more difficult
    - accounts for many of the "tricks of the trade"

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  - an efficient way to compute the gradient
- Nice introduction to this perspective:
  - Stanford CS221 Lecture 3, Slides 63-96
  - `http://web.stanford.edu/class/cs221/lectures/learning2.pdf`

Neural Network Regularization

- Neural networks are very expressive.
- Correspond to big hypothesis spaces.
- Many approaches are used for regularization.

Tikhonov Regularization? Sure.

- Can add an ℓ_2 and/or ℓ_1 regularization terms to our objective:

$$J(w,v) = \sum_{i=1}^{n} \left(y_i - f_{w,v}(x_i)\right)^2 + \lambda_1 \|w\|^2 + \lambda_2 \|v\|^2$$

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- In neural network literature, this is often called **weight decay**.

Regularization by Early Stopping

- As we train, check performance on validation set every once in a while.

See `http://arxiv.org/pdf/1206.5533v2.pdf` for details.

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- Don't stop immediately after validation error goes back up.
- The "**patience**" parameter: the number training rounds to continue after finding a minimum of validation error.
    - Start with patience $= 10000$.
    - Whenever we find a minimum at iteration T,
        - Set patience $\leftarrow$ patience $+ cT$, for some constant c.
        - Then run at least patience extra iterations before stopping.

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Max-Norm Regularization

- **Max-norm regularization**: Enforce max norm of incoming weight vector at every hidden node to be bounded:

$$\|w\|_2 \leqslant c.$$

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- Why?
  - There are heuristic justifications, but proof is in the performance.
  - We'll see below.

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Dropout for Regularization

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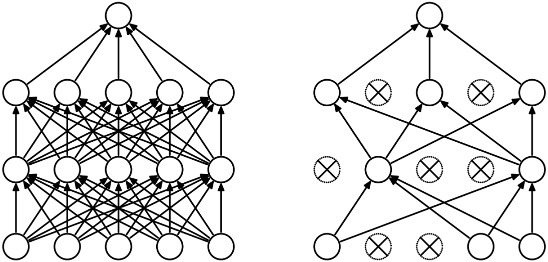

(a) Standard Neural Net (b) After applying dropout.

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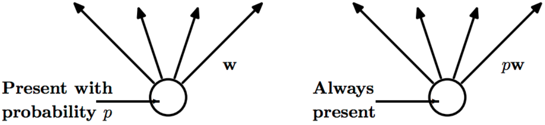
Dropout for Regularization

- At prediction time
  - all nodes are present
  - outgoing weights are multiplied by p.



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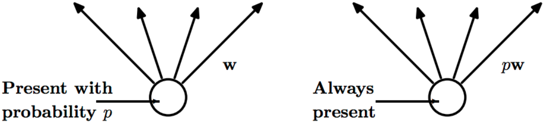

(a) At training time (b) At test time

- Dropout probability set using a validation set, or just set at 0.5.
  - Closer to 0.8 usually works better for input units.

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Dropout: Why might this help?

- Since any node may randomly disappear,
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  - forced to "spread the knowledge" across the nodes.
- Each hidden only gets a randomly chosen sample of its inputs,
  - so won't become too reliant on any single input.
  - More robust.

Dropout: Does it help?

Method	**Unit Type**	**Architecture**	**Error %**
Standard Neural Net (Simard et al., 2003)	Logistic	2 layers, 800 units	1.60
SVM Gaussian kernel	NA	NA	1.40
Dropout NN	Logistic	3 layers, 1024 units	1.35
Dropout NN	ReLU	3 layers, 1024 units	1.25
Dropout NN + max-norm constraint	ReLU	3 layers, 1024 units	1.06
Dropout NN + max-norm constraint	ReLU	3 layers, 2048 units	1.04
Dropout NN + max-norm constraint	ReLU	2 layers, 4096 units	1.01
Dropout NN + max-norm constraint	ReLU	2 layers, 8192 units	0.95
Dropout NN + max-norm constraint (Goodfellow et al., 2013)	Maxout	2 layers, (5×240) units	0.94

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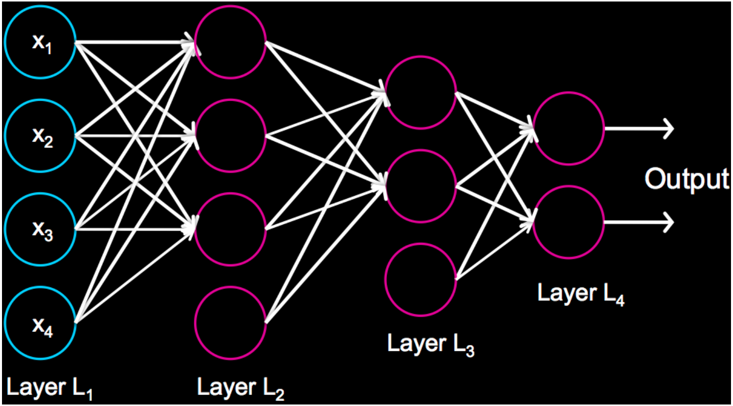
How big a network?

- How many hidden units?
- With proper regularization, too many doesn't hurt.
  - Except in computation time.

Multiple Output Neural Networks

- Very easy to add extra outputs to neural network structure.



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- We have two tasks:
    - Does the image have a cat?
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- Can have one output for each task.
- Seems plausible that basic pixel features would be shared by tasks.
- Learn them on the same neural network – benefit both tasks.

Single Task with "Extra Tasks"

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- No related tasks? Another trick:
  - Choose any input feature.
  - Change it's value to zero.
  - Make the prediction problem to predict the value of that feature.
  - Can help make model more robust (not depending too heavily on any single input).

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- Old days: train each output separately, e.g. with square loss.

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- Joint loss function (cross-entropy/deviance):

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  where $y_{ik} = 1(y_i = k)$.
- Same loss as for multinomial logistic regression.

OverFeat: Features

- OverFeat is a neural network for image classification
  - Trained on the huge ImageNet dataset
  - Lots of computing resources into training the network.

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- All those hidden layers of the network are very valuable **features**.
  - Paper: "*CNN Features off-the-shelf: an Astounding Baseline for Recognition*"
  - Showed that using features from OverFeat makes it easy to achieve state-of-the-art performance on new vision tasks.

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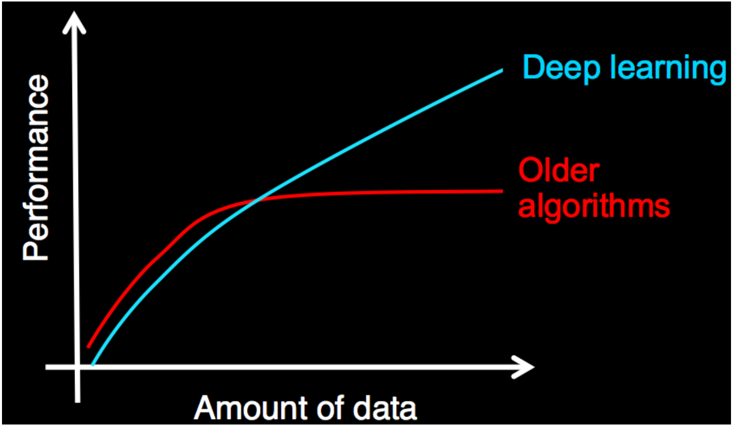
Neural Networks Benefit from Big Data



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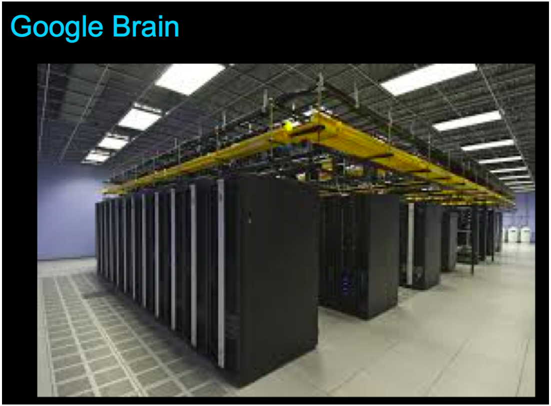
Big Data Requires Big Resources

- Best results always involve GPU processing.
- Typically on huge networks.



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  - All state of the art methods use neural networks
- Natural Language problems?
  - Maybe. Check out "word2vec" `https://code.google.com/p/word2vec/`.
  - Represents words using real-valued vectors.
    - Potentially much better than bag of words.