Neural Networks

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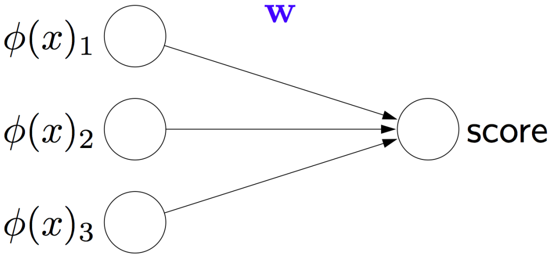
Objectives

- 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.
- Learn weight vector w from data.



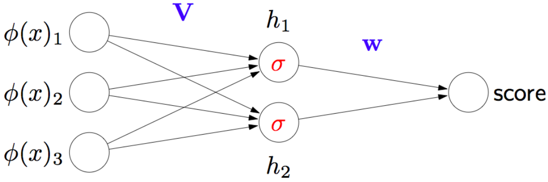
- So

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

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

Basic Neural Network (Multilayer Perceptron)

- Add an extra layer with a nonlinear transformation:



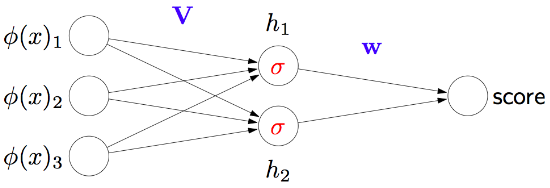
- We've introduced **hidden nodes** h_1 and h_2.

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

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

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

Basic Neural Network



- Score is just

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

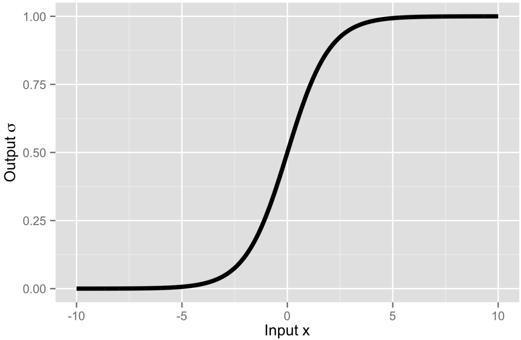
- This is the basic recipe.
  - We can add more hidden nodes.
  - We can add more hidden layers.

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

Activation Functions

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

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

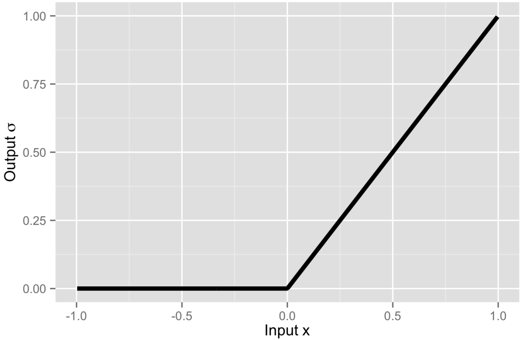


Activation Functions

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

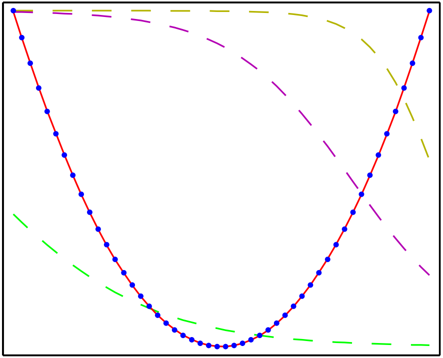
$$\sigma(x) = \max(0, x).$$

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



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

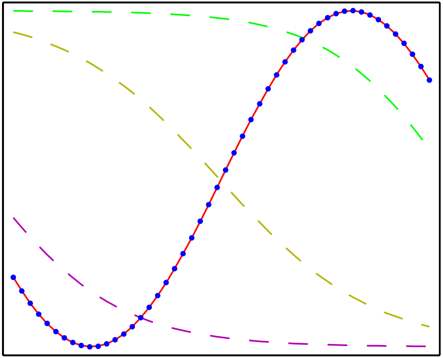
- 3 hidden units; logistic activation functions
- Blue dots are training points; Dashed lines are hidden unit outputs; Final output in Red.



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

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

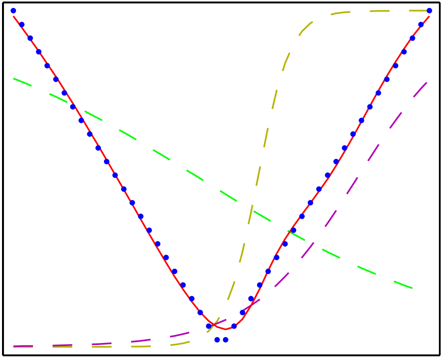
- 3 hidden units; logistic activation function
- Blue dots are training points; Dashed lines are hidden unit outputs; Final output in Red.



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

Approximation Ability: $f(x) = |x|$

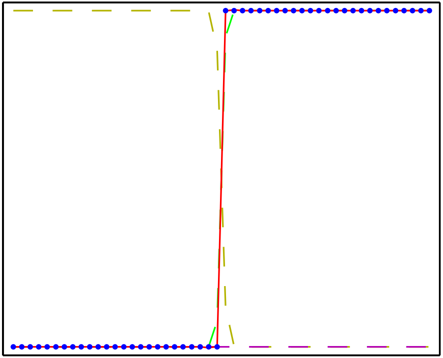
- 3 hidden units; logistic activation functions
- Blue dots are training points; Dashed lines are hidden unit outputs; Final output in Red.



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

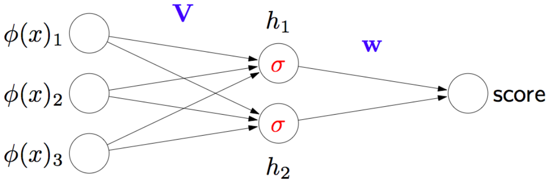
Approximation Ability: $f(x) = 1(x > 0)$

- 3 hidden units; logistic activation function
- 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

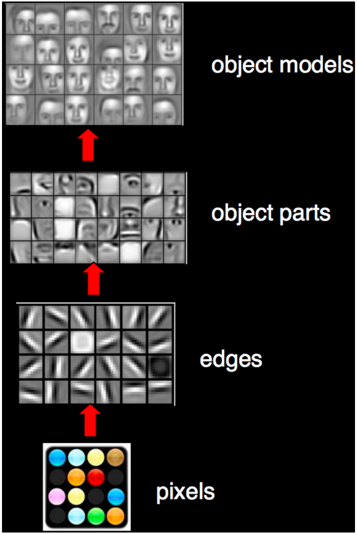
Neural Network: Hidden Nodes as Learned Features



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

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

Facial Recognition: Learned Features



From Andrew Ng's CS229 Deep Learning slides

Neural Network: The Hypothesis Space

- What hyperparameters describe a neural network?
  - Number of layers
  - Number of nodes in each hidden layer
  - Activation function (many to choose from)
- Example neural network hypothesis space:

$$\mathcal{F} = \left\{ f : \mathbf{R}^d \to \mathbf{R} \mid f \text{ is a NN with 2 hidden layers, 500 nodes in each} \right\}$$

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

Neural Network: Loss Functions and Learning

- Neural networks give a **new hypothesis space**.
- But we can use all the **same loss functions** we've used before.
- Optimization method of choice: **mini-batch SGD**.
  - 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

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

- Objective with square loss is then

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

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

Learning with Back-Propagation

- Back-propagation is an **algorithm** for computing the gradient
- With lots of chain rule, you could also work out the gradient by hand.
- Back-propagation is
  - a clean way to organize the computation of the gradient
  - an efficient way to compute the gradient
- Nice introduction to this perspective:
  - Stanford CS221 Lecture 3 (2016), Slides 75-94

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:

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

- 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.
- 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 step T,
    - Set patience $\leftarrow$ patience $+ cT$, for some constant c.
    - Then run at least patience extra steps before stopping.

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

Max-Norm Regularization

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

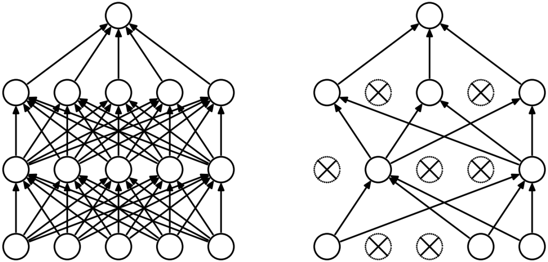
$$\|w\|_2 \leqslant c.$$

- Project any w that's too large onto ball of radius c.
- It's like ℓ_2-complexity control, but locally at each node.
- Why?
  - There are heuristic justifications, but proof is in the performance.
  - We'll see below.

See http://www.cs.toronto.edu/~rsalakhu/papers/srivastava14a.pdf for details.

Dropout for Regularization

- A recent trick for improving generalization performance is **dropout**.
- A fixed probability p is chosen.
- Before every stochastic gradient step,
  - each node is selected for "dropout" with probability p
  - a dropout node is removed, along with its links
  - after the stochastic gradient step, all nodes are restored.

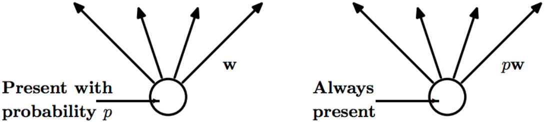


(a) Standard Neural Net (b) After applying dropout.

Figure from http://www.cs.toronto.edu/~rsalakhu/papers/srivastava14a.pdf.

Dropout for Regularization

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



(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.

Figure from http://www.cs.toronto.edu/~rsalakhu/papers/srivastava14a.pdf.

Dropout: Why might this help?

- Since any node may randomly disappear,
  - 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

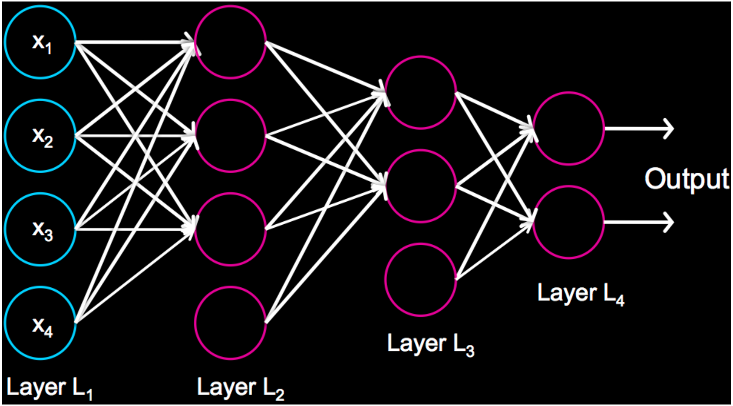
Figure from http://www.cs.toronto.edu/~rsalakhu/papers/srivastava14a.pdf.

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.



From Andrew Ng's CS229 Deep Learning slides (http://cs229.stanford.edu/materials/CS229-DeepLearning.pdf)

Multitask Learning

- Suppose $\mathcal{X} = \{\text{Natural Images}\}$.
- We have two tasks:
    - Does the image have a cat?
    - Does the image have a dog?
- 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"

- Only one task we're interested in.
- Gather data from related tasks.
- Train them along with the task you're interested in.
- 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).

Multiclass Classification

- Could make each class a separate task / output.
- Suppose we have K classes.
- Use a one-hot encoding of each $y_i \in \{1, \ldots, K\}$:

$$y_i = (y_{i1}, \ldots, y_{ik}) \text{ with } y_{ik} = 1(y_i = k).$$

- K output scores: $f_1(x), \ldots, f_K(x)$. Each f_k is trained to predict 1 if class is k, 0 otherwise.
- Predict with $f^*(x) = \arg\max_k [f_k(x)]$.
- Old days: train each output separately, e.g. with square loss.

Multiclass Classification: Cross-Entropy Loss

- Network can do better if it "knows" that classes are mutually exclusive.
- Need to introduce a joint loss across the outputs.
- Joint loss function (cross-entropy/deviance):

$$\ell(w,v) = -\sum_{i=1}^{n}\sum_{i=1}^{K} y_{ik}\log f_k(x_i),$$

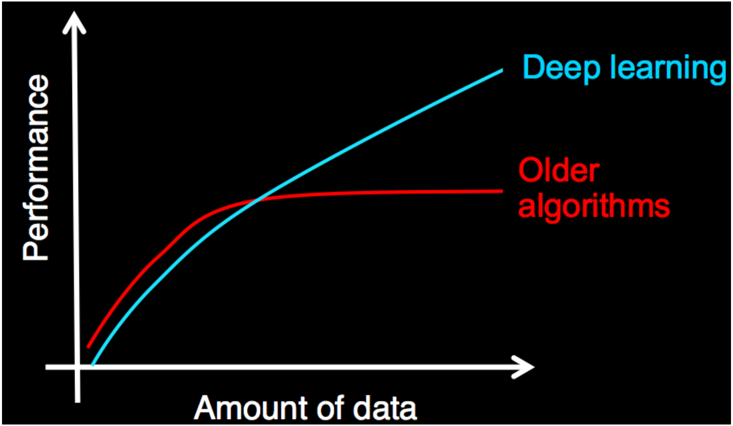
  where $y_{ik} = 1(y_i = k)$.
- This is the negative log-likelihood we get for softmax predictions in multinomial logistic regression.

OverFeat: Features

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

OverFeat code is at https://github.com/sermanet/OverFeat

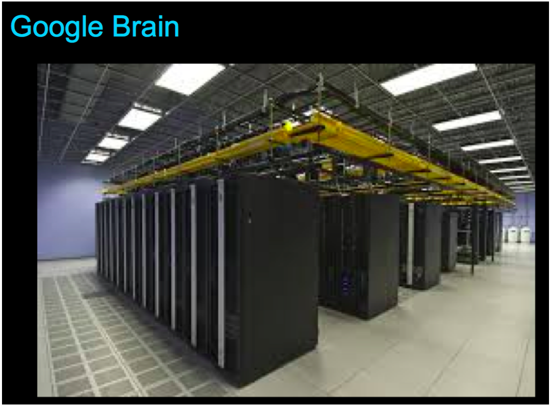
Neural Networks Benefit from Big Data



From Andrew Ng's CS229 Deep Learning slides (http://cs229.stanford.edu/materials/CS229-DeepLearning.pdf)

Big Data Requires Big Resources

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



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Neural Networks: When to Use?

- Computer vision problems
  - All state of the art methods use neural networks
- Speech recognition
  - All state of the art methods use neural networks
- Natural Language problems
  - Maybe. State-of-the-art, but not as large a margin.
  - Check out "word2vec" https://code.google.com/p/word2vec/.
  - Represents words using real-valued vectors.
    - Potentially much better than bag of words.