

Neural Networks

David Rosenberg

New York University

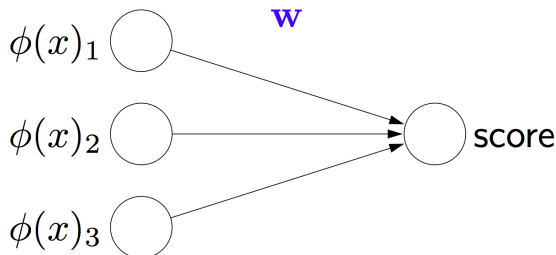
November 1, 2015

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. ()



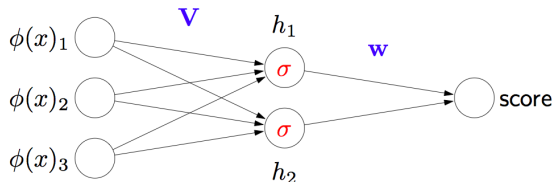
- So

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

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

Neural Network

- Add an extra layer with a nonlinear transformation:

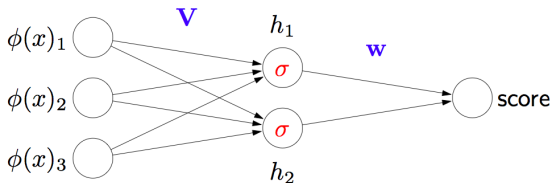


- We've introduced **hidden nodes** h_1 and h_2 .

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

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

Neural Network



- Score is just

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

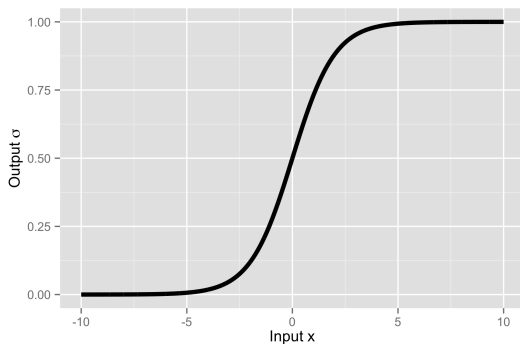
- This is the basic recipe.
 - We can add more hidden nodes.
 - We can add more hidden layers.

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:

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

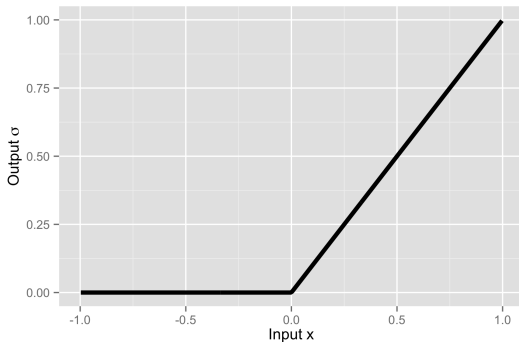


Activation Functions

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

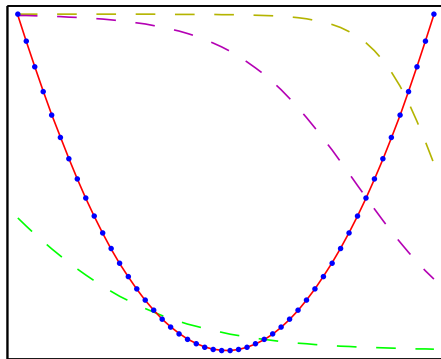
$$\sigma(x) = \max(0, x).$$

- Much faster to calculate, and to calculate its derivatives.



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

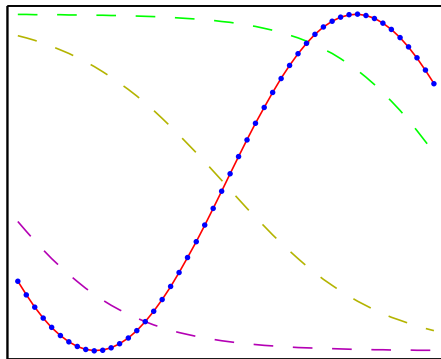
- 3 hidden units; logistic activation functions
- Blue dots are training points; Dashed lines are hidden unit outputs; Final output in Red.



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

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

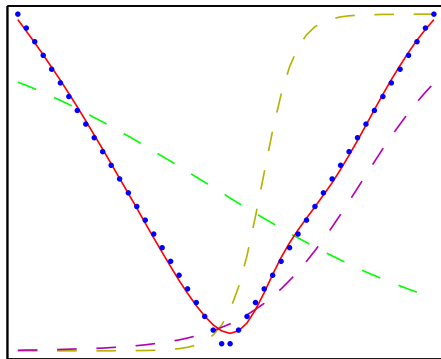
- 3 hidden units; logistic activation function
- Blue dots are training points; Dashed lines are hidden unit outputs; Final output in Red.



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

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

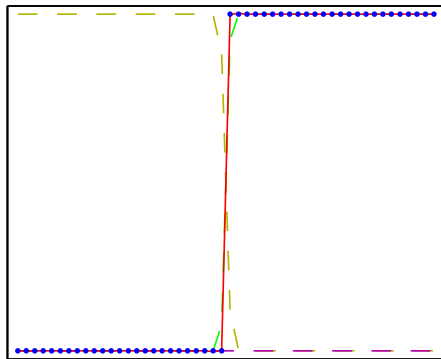
- 3 hidden units; logistic activation functions
- Blue dots are training points; Dashed lines are hidden unit outputs; Final output in Red.



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

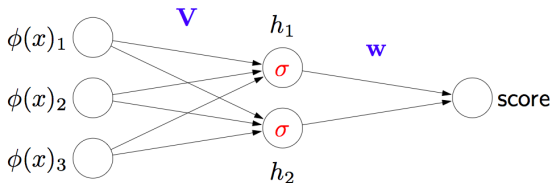
Approximation Ability: $f(x) = 1(x > 0)$

- 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

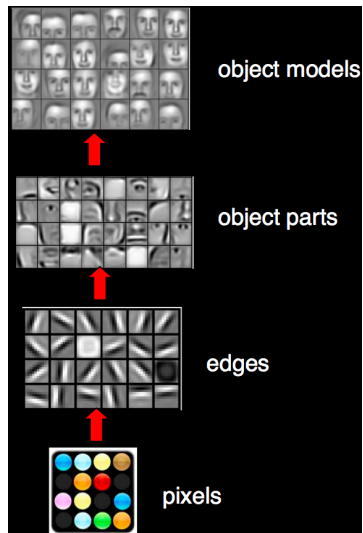
Neural Network: Hidden Nodes as Learned Features



- 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 (but so many to choose from)
- Example neural network hypothesis space:

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

- 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: **stochastic gradient descent**.

Neural Network: Objective Function

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

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

- Objective with square loss is then

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

- 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 SGD gradient
- Mathematically, it's not necessary.
- With lots of chain rule, you can 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, 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:

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

- 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 $\text{patience} = 10000$.
 - Whenever we find a minimum at iteration T ,
 - Set $\text{patience} \leftarrow \text{patience} + cT$, for some constant c .
 - Then run at least patience extra iterations 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:

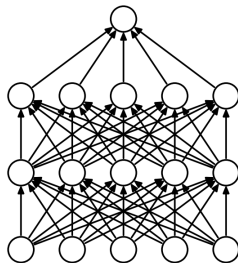
$$\|w\|_2 \leq c.$$

- 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.

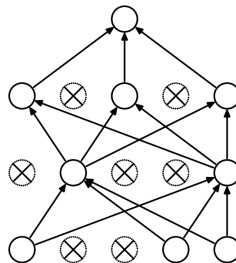
See <http://www.cs.toronto.edu/~rsalakhu/papers/srivastava14a.pdf> for details.

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

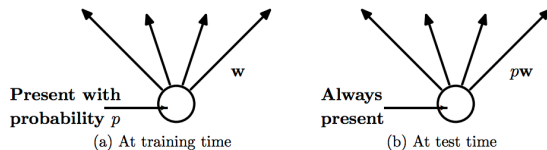


(b) After applying dropout.

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 .



- 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

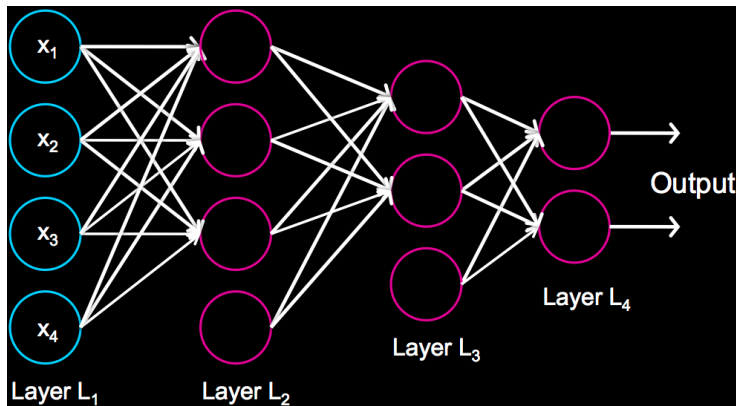
Figure from <http://www.cs.toronto.edu/~rsalakhu/papers/srivastava14a.pdf>.

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 $y_i \in \{1, \dots, K\}$:

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

- K output scores: $f_1(x), \dots, f_K(x)$. 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):

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

where $y_{ik} = 1(y_i = k)$.

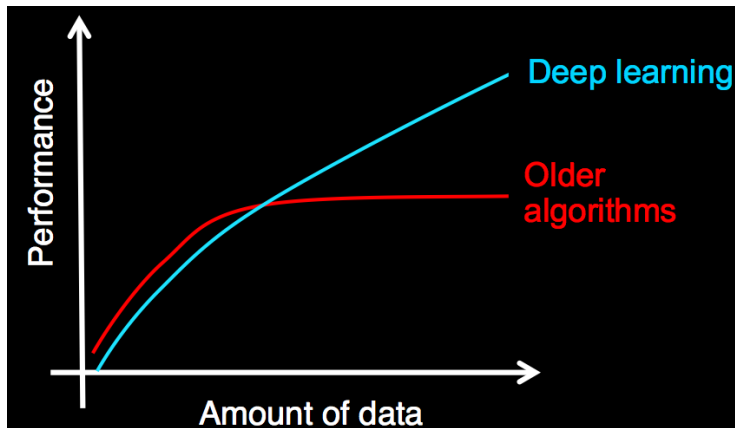
- We'll discuss this further when we talk about exponential families and generalized linear models.

OverFeat: Features

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

Google Brain



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

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. Check out “word2vec”
<https://code.google.com/p/word2vec/>.
 - Represents words and phrases using real-valued vectors.
 - Potentially much better than bag of words.