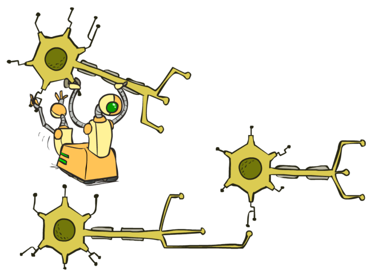
CS 188: Artificial Intelligence

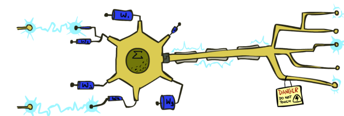
Optimization and Neural Nets



Instructors: Pieter Abbeel and Dan Klein --- University of California, Berkeley

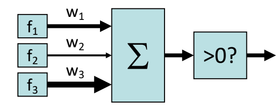
Reminder: Linear Classifiers

- Inputs are feature values
- Each feature has a weight
- Sum is the activation



$$\text{activation}_w(x) = \sum_i w_i \cdot f_i(x) = w \cdot f(x)$$

- If the activation is:
  - Positive, output +1
  - Negative, output -1

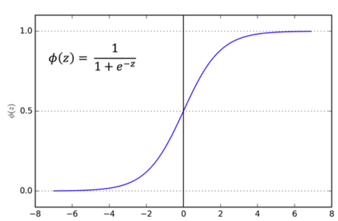


How to get probabilistic decisions?

- Activation: $z = w \cdot f(x)$
- If $z = w \cdot f(x)$ very positive → want probability going to 1
- If $z = w \cdot f(x)$ very negative → want probability going to 0

- Sigmoid function

$$\phi(z) = \frac{1}{1 + e^{-z}}$$



Best w?

- Maximum likelihood estimation:

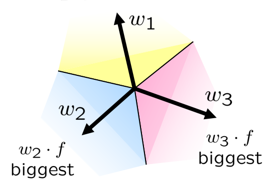
$$\max_w \; ll(w) = \max_w \; \sum_i \log P(y^{(i)}|x^{(i)}; w)$$

with:
$$P(y^{(i)} = +1|x^{(i)}; w) = \frac{1}{1 + e^{-w \cdot f(x^{(i)})}}$$
$$P(y^{(i)} = -1|x^{(i)}; w) = 1 - \frac{1}{1 + e^{-w \cdot f(x^{(i)})}}$$

= Logistic Regression

Multiclass Logistic Regression

- Multi-class linear classification
  - A weight vector for each class: w_y
  - Score (activation) of a class y: $w_y \cdot f(x)$
  - Prediction w/highest score wins: $y = \arg\max_y \; w_y \cdot f(x)$



- How to make the scores into probabilities?

$$\underbrace{z_1, z_2, z_3}_{\text{original activations}} \rightarrow \underbrace{\frac{e^{z_1}}{e^{z_1}+e^{z_2}+e^{z_3}}, \frac{e^{z_2}}{e^{z_1}+e^{z_2}+e^{z_3}}, \frac{e^{z_3}}{e^{z_1}+e^{z_2}+e^{z_3}}}_{\text{softmax activations}}$$

Best w?

- Maximum likelihood estimation:

$$\max_w \quad ll(w) = \max_w \quad \sum_i \log P(y^{(i)}|x^{(i)};w)$$

with: $$P(y^{(i)}|x^{(i)};w) = \frac{e^{w_{y^{(i)}} \cdot f(x^{(i)})}}{\sum_y e^{w_y \cdot f(x^{(i)})}}$$

= Multi-Class Logistic Regression

This Lecture

- Optimization
  - i.e., how do we solve:

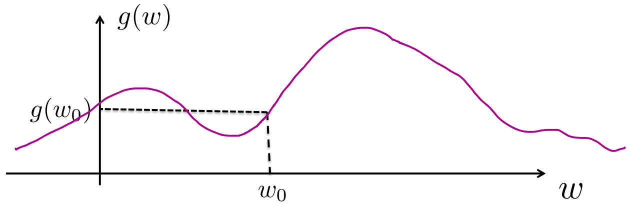
$$\max_w \quad ll(w) = \max_w \quad \sum_i \log P(y^{(i)}|x^{(i)};w)$$

Hill Climbing

- Recall from CSPs lecture: simple, general idea
  - Start wherever
  - Repeat: move to the best neighboring state
  - If no neighbors better than current, quit

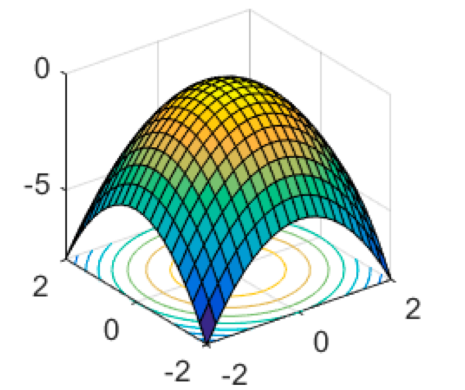
- What's particularly tricky when hill-climbing for multiclass logistic regression?
  - Optimization over a continuous space
    - Infinitely many neighbors!
    - How to do this efficiently?

1-D Optimization



- Could evaluate $g(w_0 + h)$ and $g(w_0 - h)$
  - Then step in best direction
- Or, evaluate derivative: $\frac{\partial g(w_0)}{\partial w} = \lim_{h \to 0} \frac{g(w_0 + h) - g(w_0 - h)}{2h}$
  - Tells which direction to step into

2-D Optimization



Source: offconvex.org

Gradient Ascent

- Perform update in uphill direction for each coordinate
- The steeper the slope (i.e. the higher the derivative) the bigger the step for that coordinate
- E.g., consider: $g(w_1, w_2)$
  - Updates:

$$w_1 \leftarrow w_1 + \alpha * \frac{\partial g}{\partial w_1}(w_1, w_2)$$

$$w_2 \leftarrow w_2 + \alpha * \frac{\partial g}{\partial w_2}(w_1, w_2)$$

  - Updates in vector notation:

$$w \leftarrow w + \alpha * \nabla_w g(w)$$

with: $\nabla_w g(w) = \begin{bmatrix} \frac{\partial g}{\partial w_1}(w) \\ \frac{\partial g}{\partial w_2}(w) \end{bmatrix}$ **= gradient**

Gradient Ascent

- Idea:
  - Start somewhere
  - Repeat: Take a step in the gradient direction

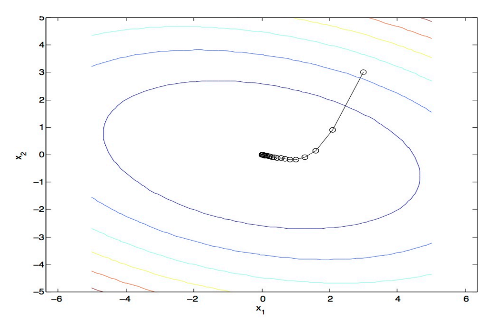


Figure source: Mathworks

What is the Steepest Direction?

$$\max_{\Delta:\Delta_1^2+\Delta_2^2\leq\varepsilon} g(w+\Delta)$$

- First-Order Taylor Expansion: $g(w+\Delta) \approx g(w) + \frac{\partial g}{\partial w_1}\Delta_1 + \frac{\partial g}{\partial w_2}\Delta_2$
- Steepest Descent Direction: $\max_{\Delta:\Delta_1^2+\Delta_2^2\leq\varepsilon} g(w) + \frac{\partial g}{\partial w_1}\Delta_1 + \frac{\partial g}{\partial w_2}\Delta_2$
- Recall: $\max_{\Delta:\|\Delta\|\leq\varepsilon} \Delta^\top a$ → $\Delta = \varepsilon \frac{a}{\|a\|}$
- Hence, solution: $\Delta = \varepsilon \frac{\nabla g}{\|\nabla g\|}$ **Gradient direction = steepest direction!** $\nabla g = \begin{bmatrix} \frac{\partial g}{\partial w_1} \\ \frac{\partial g}{\partial w_2} \end{bmatrix}$

Gradient in n dimensions

$$\nabla g = \begin{bmatrix} \frac{\partial g}{\partial w_1} \\ \frac{\partial g}{\partial w_2} \\ \cdots \\ \frac{\partial g}{\partial w_n} \end{bmatrix}$$

Optimization Procedure: Gradient Ascent

- `init` w
- `for iter = 1, 2, …`

$$w \leftarrow w + \alpha * \nabla g(w)$$

- α: learning rate --- tweaking parameter that needs to be chosen carefully
- How? Try multiple choices
  - Crude rule of thumb: update changes w about 0.1 – 1 %

Batch Gradient Ascent on the Log Likelihood Objective

$$\max_w \; ll(w) = \max_w \; \underbrace{\sum_i \log P(y^{(i)}|x^{(i)};w)}_{g(w)}$$

- `init` w
- `for iter = 1, 2, …`

$$w \leftarrow w + \alpha * \sum_i \nabla \log P(y^{(i)}|x^{(i)};w)$$

Stochastic Gradient Ascent on the Log Likelihood Objective

$$\max_w \quad ll(w) = \max_w \quad \sum_i \log P(y^{(i)}|x^{(i)};w)$$

Observation: once gradient on one training example has been computed, might as well incorporate before computing next one

- init w
- for iter = 1, 2, …
  - pick random j

$$w \leftarrow w + \alpha * \nabla \log P(y^{(j)}|x^{(j)};w)$$

Mini-Batch Gradient Ascent on the Log Likelihood Objective

$$\max_w \quad ll(w) = \max_w \quad \sum_i \log P(y^{(i)}|x^{(i)};w)$$

Observation: gradient over small set of training examples (=mini-batch) can be computed in parallel, might as well do that instead of a single one

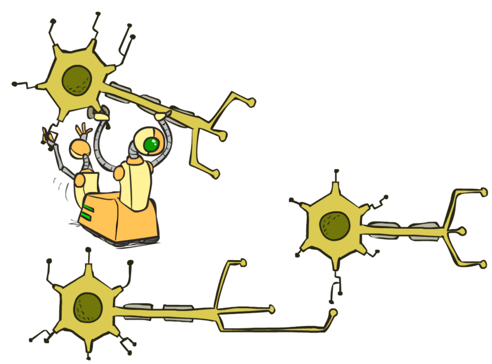
- init w
- for iter = 1, 2, …
  - pick random subset of training examples J

$$w \leftarrow w + \alpha * \sum_{j \in J} \nabla \log P(y^{(j)}|x^{(j)};w)$$

How about computing all the derivatives?

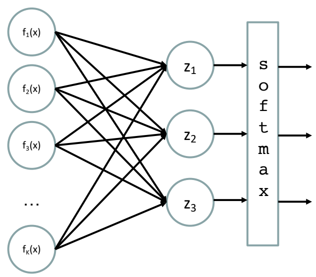
- We'll talk about that once we covered neural networks, which are a generalization of logistic regression

Neural Networks



Multi-class Logistic Regression

- = special case of neural network

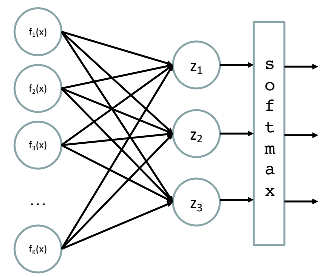


$$P(y_1|x;w) = \frac{e^{z_1}}{e^{z_1}+e^{z_2}+e^{z_3}}$$

$$P(y_2|x;w) = \frac{e^{z_2}}{e^{z_1}+e^{z_2}+e^{z_3}}$$

$$P(y_3|x;w) = \frac{e^{z_3}}{e^{z_1}+e^{z_2}+e^{z_3}}$$

Deep Neural Network = Also learn the features!



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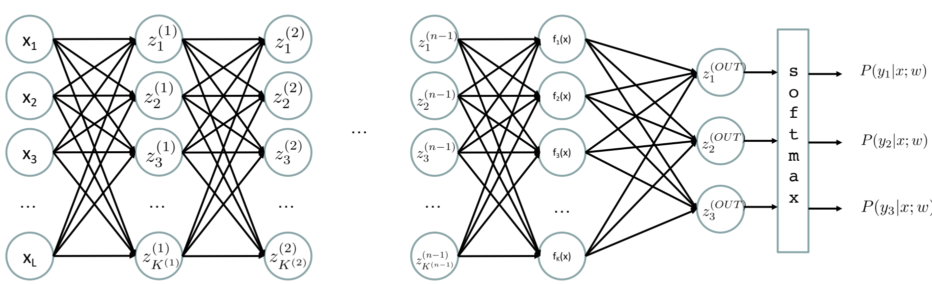
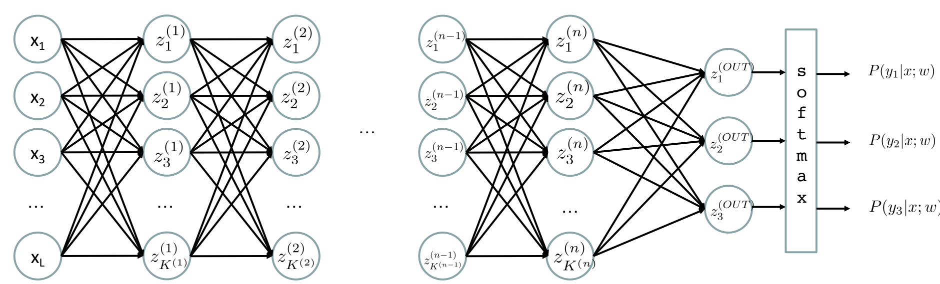
Deep Neural Network = Also learn the features!



$$z_i^{(k)} = g(\sum_j W_{i,j}^{(k-1,k)} z_j^{(k-1)})$$

g = nonlinear activation function

Deep Neural Network = Also learn the features!



$$z_i^{(k)} = g(\sum_j W_{i,j}^{(k-1,k)} z_j^{(k-1)})$$

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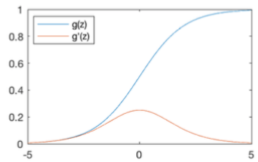
Common Activation Functions

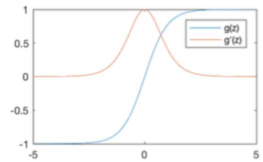
Sigmoid Function



$$g(z) = \frac{1}{1+e^{-z}}$$

$$g'(z) = g(z)(1-g(z))$$

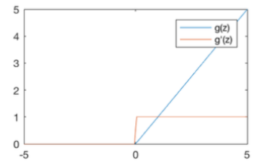
Hyperbolic Tangent



$$g(z) = \frac{e^{z}-e^{-z}}{e^{z}+e^{-z}}$$

$$g'(z) = 1 - g(z)^2$$

Rectified Linear Unit (ReLU)



$$g(z) = \max(0, z)$$

$$g'(z) = \begin{cases} 1, & z > 0 \\ 0, & \text{otherwise} \end{cases}$$

[source: MIT 6.S191 introtodeeplearning.com]

Deep Neural Network: Also Learn the Features!

- Training the deep neural network is just like logistic regression:

$$\max_w \quad ll(w) = \max_w \quad \sum_i \log P(y^{(i)} | x^{(i)}; w)$$

just w tends to be a much, much larger vector ☺

→just run gradient ascent
+ stop when log likelihood of hold-out data starts to decrease

Neural Networks Properties

- Theorem (Universal Function Approximators). A two-layer neural network with a sufficient number of neurons can approximate any continuous function to any desired accuracy.
- Practical considerations
  - Can be seen as learning the features
  - Large number of neurons
    - Danger for overfitting
    - (hence early stopping!)

Universal Function Approximation Theorem*

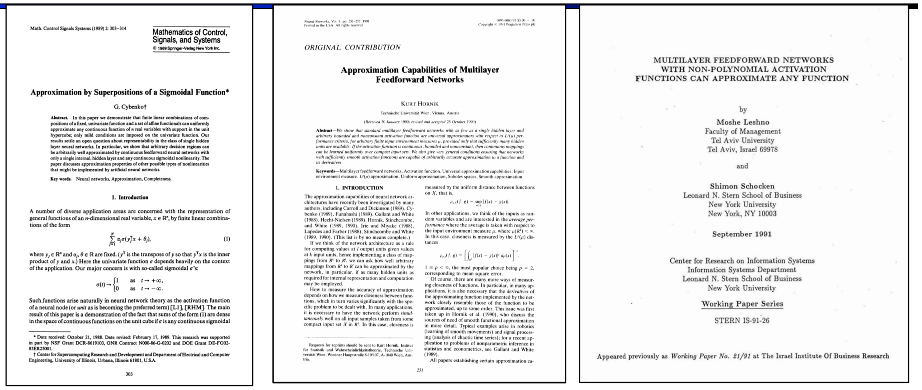
Hornik theorem 1: Whenever the activation function is *bounded and nonconstant*, then, for any finite measure μ, standard multilayer feedforward networks can approximate any function in $L^p(\mu)$ (the space of all functions on R^k such that $\int_{R^k} |f(x)|^p d\mu(x) < \infty$) arbitrarily well, provided that sufficiently many hidden units are available.

Hornik theorem 2: Whenever the activation function is *continuous, bounded and nonconstant*, then, for arbitrary compact subsets $X \subseteq R^k$, standard multilayer feedforward networks can approximate any continuous function on X arbitrarily well with respect to uniform distance, provided that sufficiently many hidden units are available.

- In words: Given any continuous function f(x), if a 2-layer neural network has enough hidden units, then there is a choice of weights that allow it to closely approximate f(x).

Cybenko (1989) "Approximations by superpositions of sigmoidal functions"
Hornik (1991) "Approximation Capabilities of Multilayer Feedforward Networks"
Leshno and Schocken (1991) "Multilayer Feedforward Networks with Non-Polynomial Activation Functions Can Approximate Any Function"

Universal Function Approximation Theorem*



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Fun Neural Net Demo Site

- Demo-site:
  - http://playground.tensorflow.org/

How about computing all the derivatives?

- Derivatives tables:

$$\frac{d}{dx}(a)=0$$
$$\frac{d}{dx}(x)=1$$
$$\frac{d}{dx}(au)=a\frac{du}{dx}$$
$$\frac{d}{dx}(u+v-w)=\frac{du}{dx}+\frac{dv}{dx}-\frac{dw}{dx}$$
$$\frac{d}{dx}(uv)=u\frac{dv}{dx}+v\frac{du}{dx}$$
$$\frac{d}{dx}\left(\frac{u}{v}\right)=\frac{1}{v}\frac{du}{dx}-\frac{u}{v^2}\frac{dv}{dx}$$
$$\frac{d}{dx}(u^n)=nu^{n-1}\frac{du}{dx}$$
$$\frac{d}{dx}(\sqrt{u})=\frac{1}{2\sqrt{u}}\frac{du}{dx}$$
$$\frac{d}{dx}\left(\frac{1}{u}\right)=-\frac{1}{u^2}\frac{du}{dx}$$
$$\frac{d}{dx}\left(\frac{1}{u^n}\right)=-\frac{n}{u^{n+1}}\frac{du}{dx}$$
$$\frac{d}{dx}[f(u)]=\frac{d}{du}[f(u)]\frac{du}{dx}$$
$$\frac{d}{dx}[\ln u]=\frac{d}{dx}[\log_e u]=\frac{1}{u}\frac{du}{dx}$$
$$\frac{d}{dx}[\log_a u]=\log_a e\frac{1}{u}\frac{du}{dx}$$
$$\frac{d}{dx}e^u=e^u\frac{du}{dx}$$
$$\frac{d}{dx}a^u=a^u\ln a\frac{du}{dx}$$
$$\frac{d}{dx}(u^v)=vu^{v-1}\frac{du}{dx}+\ln u\; u^v\frac{dv}{dx}$$
$$\frac{d}{dx}\sin u=\cos u\frac{du}{dx}$$
$$\frac{d}{dx}\cos u=-\sin u\frac{du}{dx}$$
$$\frac{d}{dx}\tan u=\sec^2 u\frac{du}{dx}$$
$$\frac{d}{dx}\cot u=-\csc^2 u\frac{du}{dx}$$
$$\frac{d}{dx}\sec u=\sec u\tan u\frac{du}{dx}$$
$$\frac{d}{dx}\csc u=-\csc u\cot u\frac{du}{dx}$$

[source: http://hyperphysics.phy-astr.gsu.edu/hbase/Math/derfunc.html

How about computing all the derivatives?

- But neural net f is never one of those?
  - No problem: CHAIN RULE:

If $$f(x)=g(h(x))$$

Then $$f'(x)=g'(h(x))h'(x)$$

→ **Derivatives can be computed by following well-defined procedures**

Automatic Differentiation

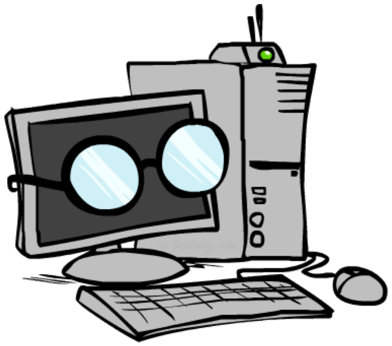
- Automatic differentiation software
  - e.g. Theano, TensorFlow, PyTorch, Chainer
  - Only need to program the function g(x,y,w)
  - Can automatically compute all derivatives w.r.t. all entries in w
  - This is typically done by caching info during forward computation pass of f, and then doing a backward pass = “backpropagation”
  - Autodiff / Backpropagation can often be done at computational cost comparable to the forward pass
- Need to know this exists
- How this is done? -- outside of scope of CS188

Summary of Key Ideas

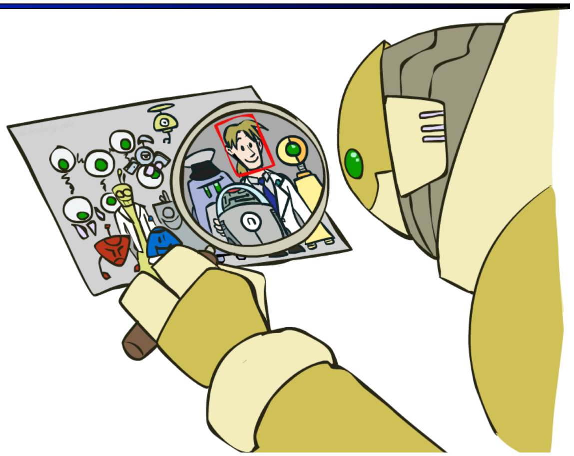
- Optimize probability of label given input $\max_w \; ll(w) = \max_w \; \sum_i \log P(y^{(i)}|x^{(i)}; w)$
- Continuous optimization
  - Gradient ascent:
    - Compute steepest uphill direction = gradient (= just vector of partial derivatives)
    - Take step in the gradient direction
    - Repeat (until held-out data accuracy starts to drop = “early stopping”)
- Deep neural nets
  - Last layer = still logistic regression
  - Now also many more layers before this last layer
    - = computing the features
    - → the features are learned rather than hand-designed
  - Universal function approximation theorem
    - `If` neural net is large enough
    - `Then` neural net can represent any continuous mapping from input to output with arbitrary accuracy
    - But remember: need to avoid overfitting / memorizing the training data → early stopping!
  - Automatic differentiation gives the derivatives efficiently (how? = outside of scope of 188)

How well does it work?

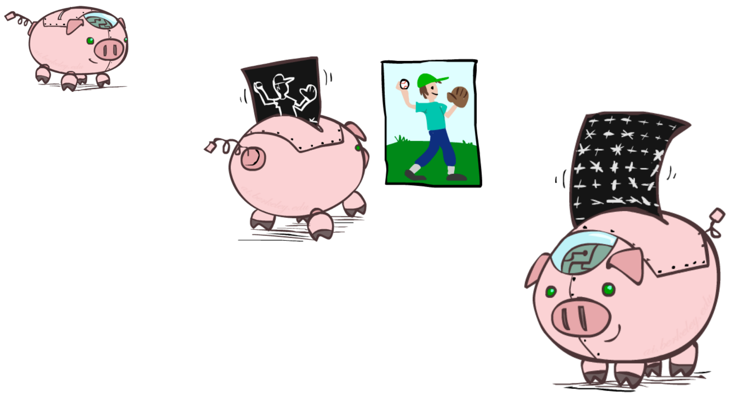
Computer Vision



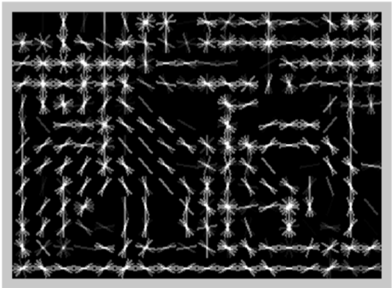
Object Detection



Manual Feature Design



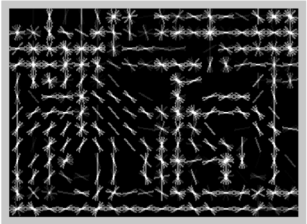
Features and Generalization



[HoG: Dalal and Triggs, 2005]

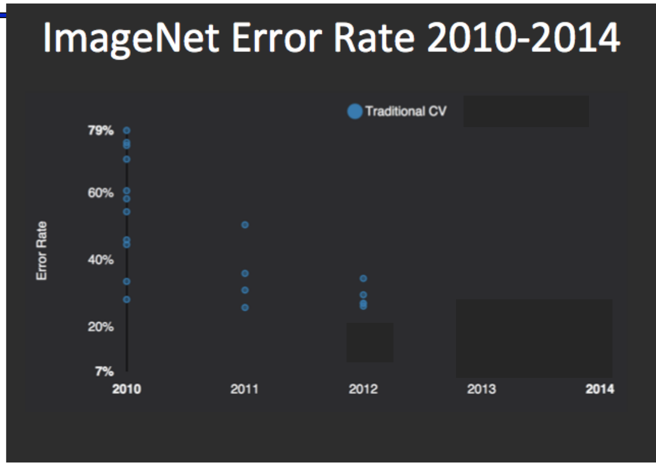
Features and Generalization

Image



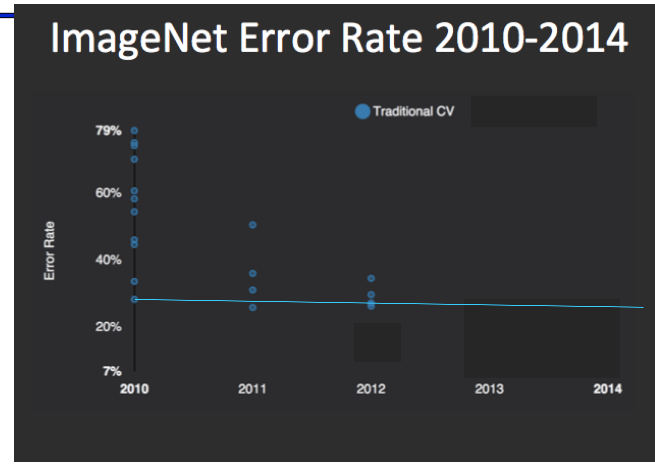
HoG

Performance



graph credit Matt Zeiler, Clarifai

Performance



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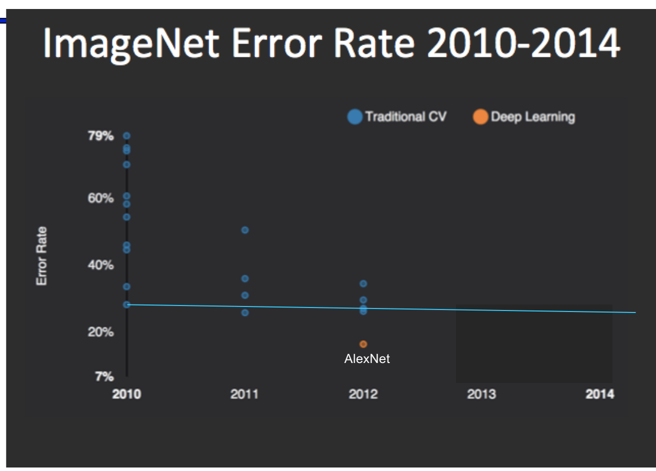

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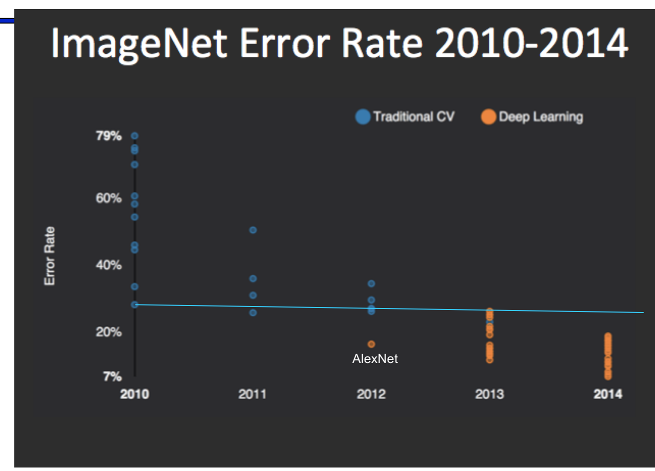

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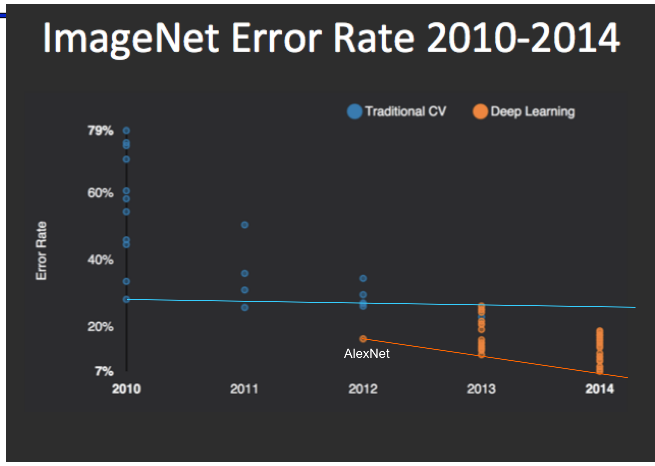
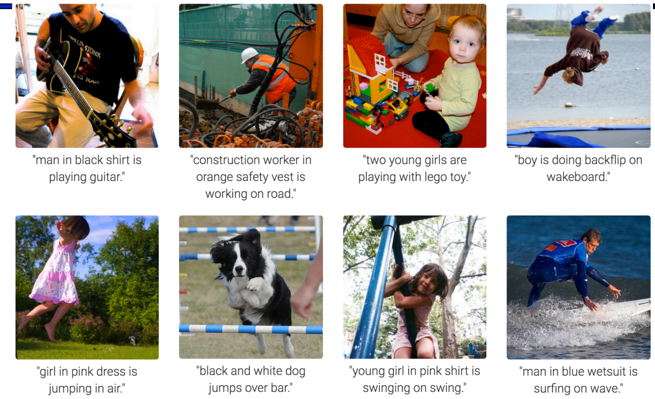


graph credit Matt Zeiler, Clarifai

MS COCO Image Captioning Challenge

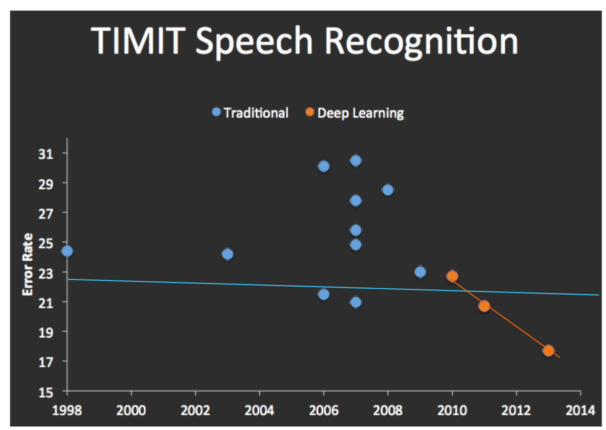


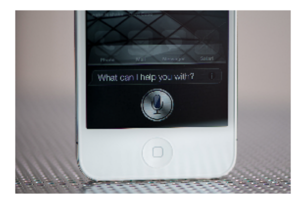
Karpathy & Fei-Fei, 2015; Donahue et al., 2015; Xu et al, 2015; many more

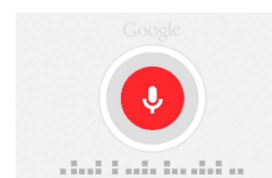
Visual QA Challenge

Stanislaw Antol, Aishwarya Agrawal, Jiasen Lu, Margaret Mitchell, Dhruv Batra, C. Lawrence Zitnick, Devi Parikh

Speech Recognition



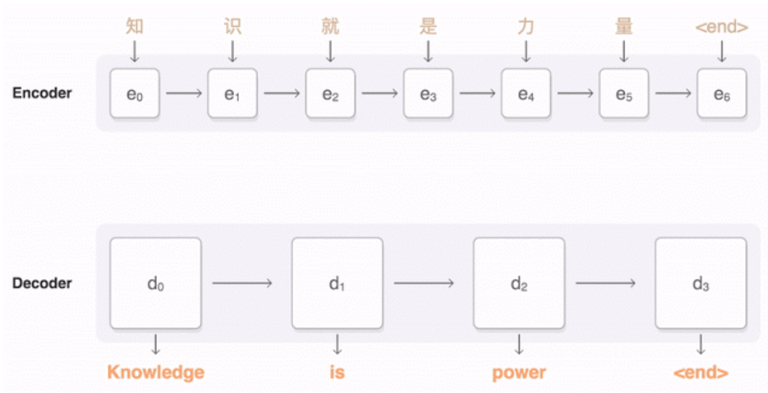




graph credit Matt Zeiler, Clarifai

Machine Translation

Google Neural Machine Translation (in production)



Next: More Neural Net Applications!