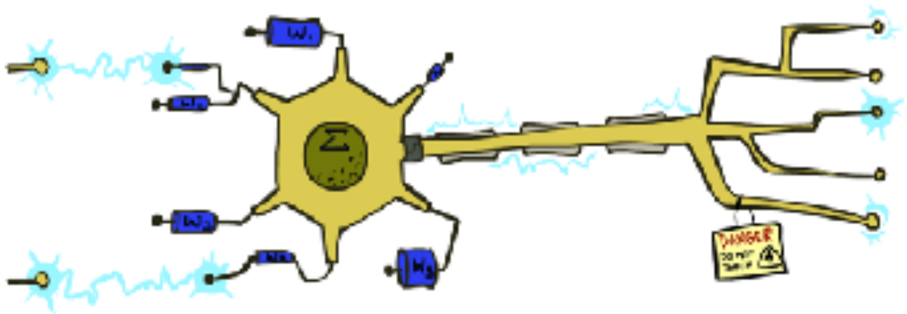
Machine Learning Systems

Lecture 8: Optimization and Neural Networks

Pooyan Jamshidi

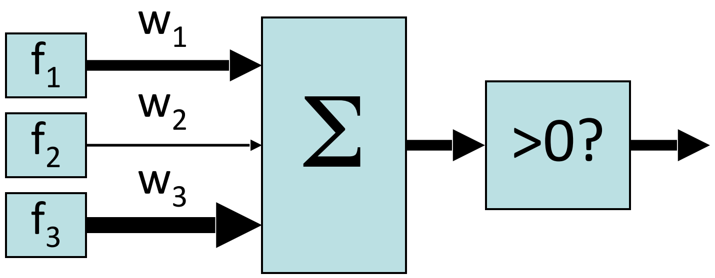
Reminder: Linear Classifiers

- 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



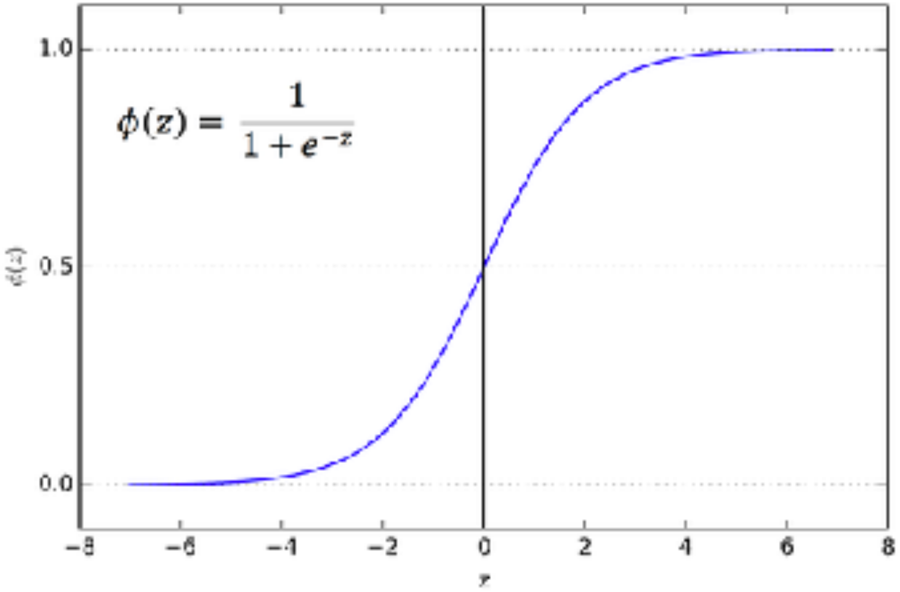
[These slides are mostly based on those of Dan Klein and Pieter Abbeel for CS188 Intro to AI at UC Berkeley, ai.berkeley.edu]

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:

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

with:

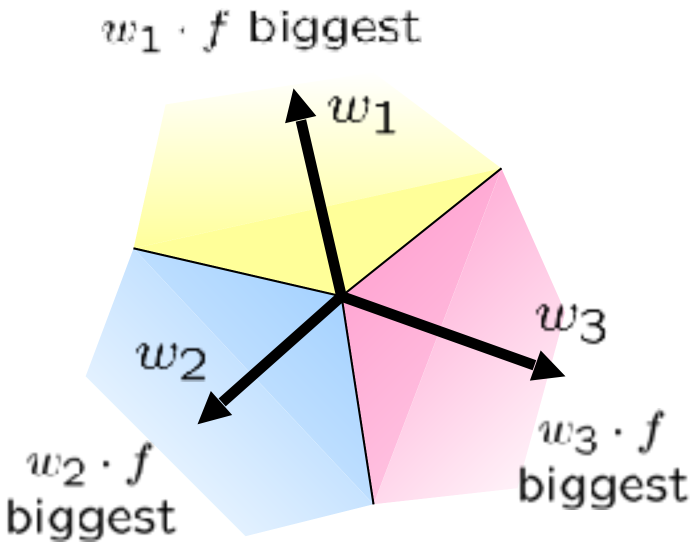
$$P(y^{(i)} = +1|x^{(i)}; w) = \frac{1}{1 + e^{-w \cdot f(x^{(i)})}}$$

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

= 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:

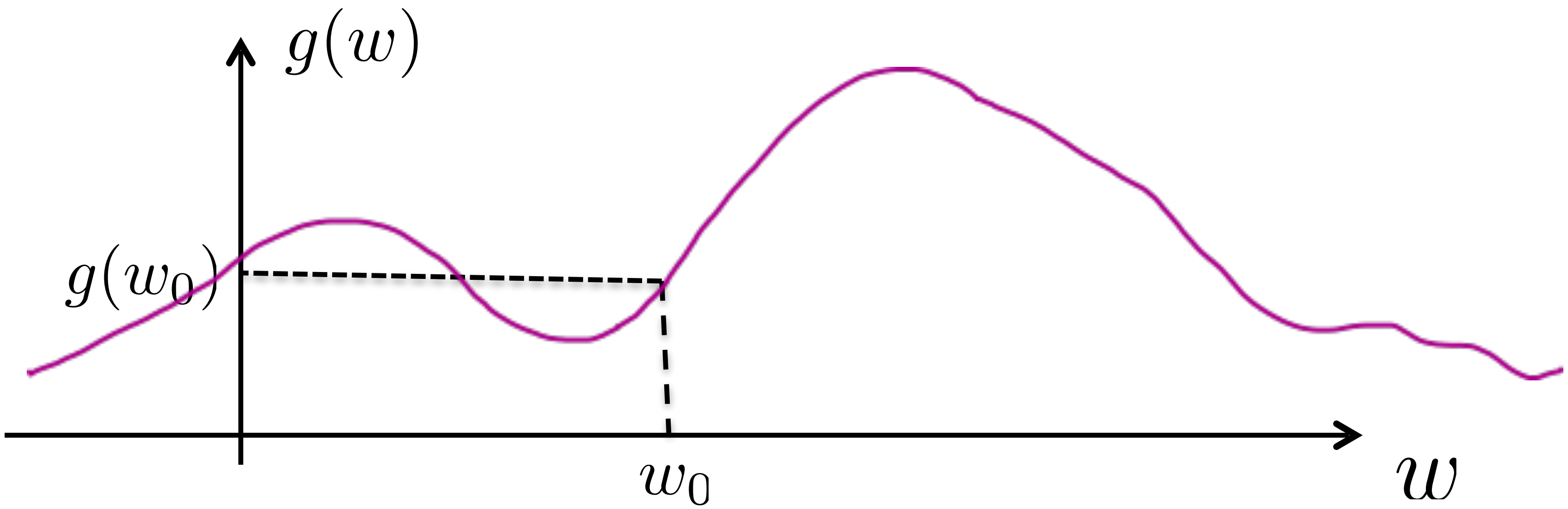
$$\max_w \quad ll(w) = \max_w \quad \sum_i \log P(y^{(i)}|x^{(i)}; w)$$

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

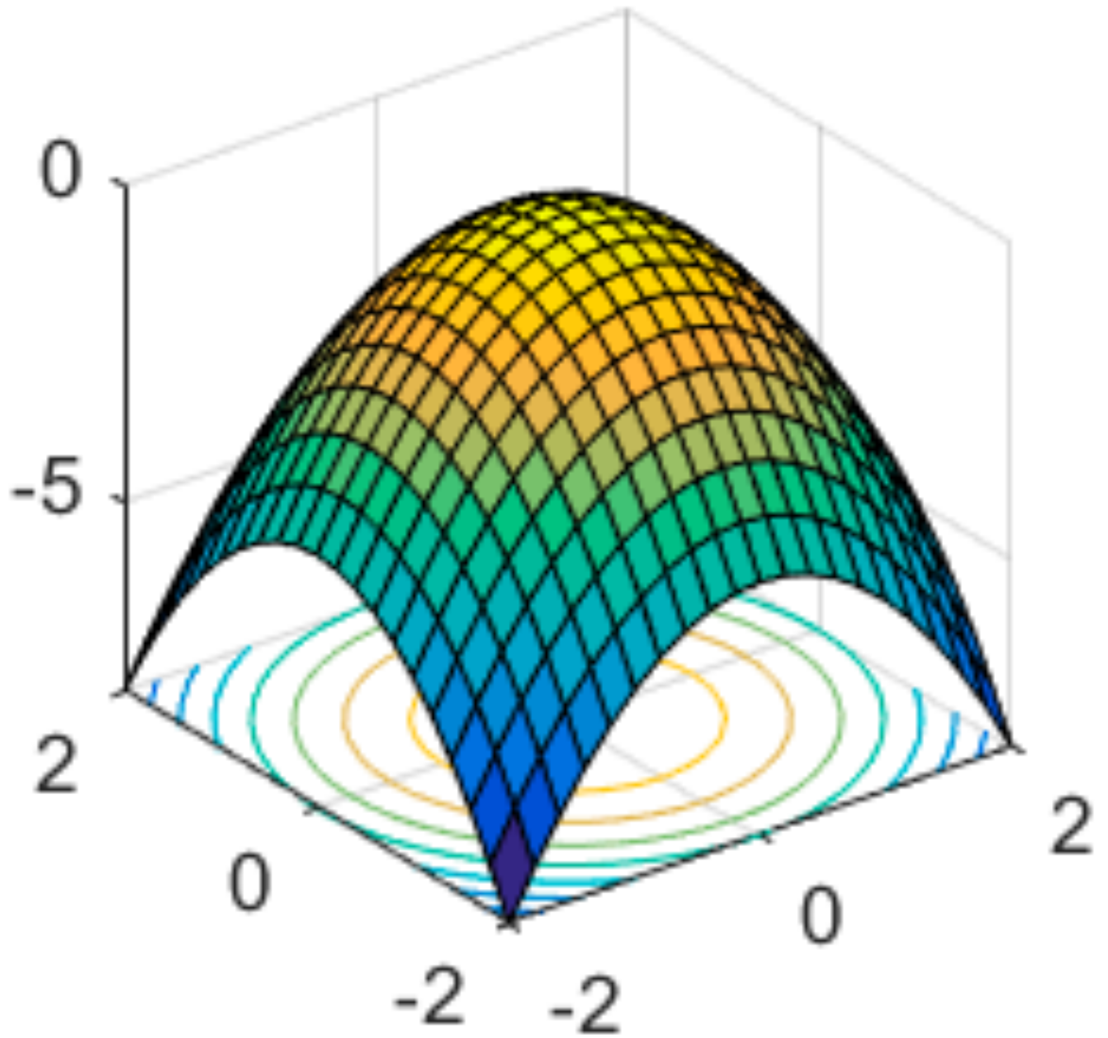
- What's particularly tricky when hill-climbing for multiclass logistic regression?
  - Optimization over a continuous space
    - Infinitely many neighbors!
    - How to do this efficiently?

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

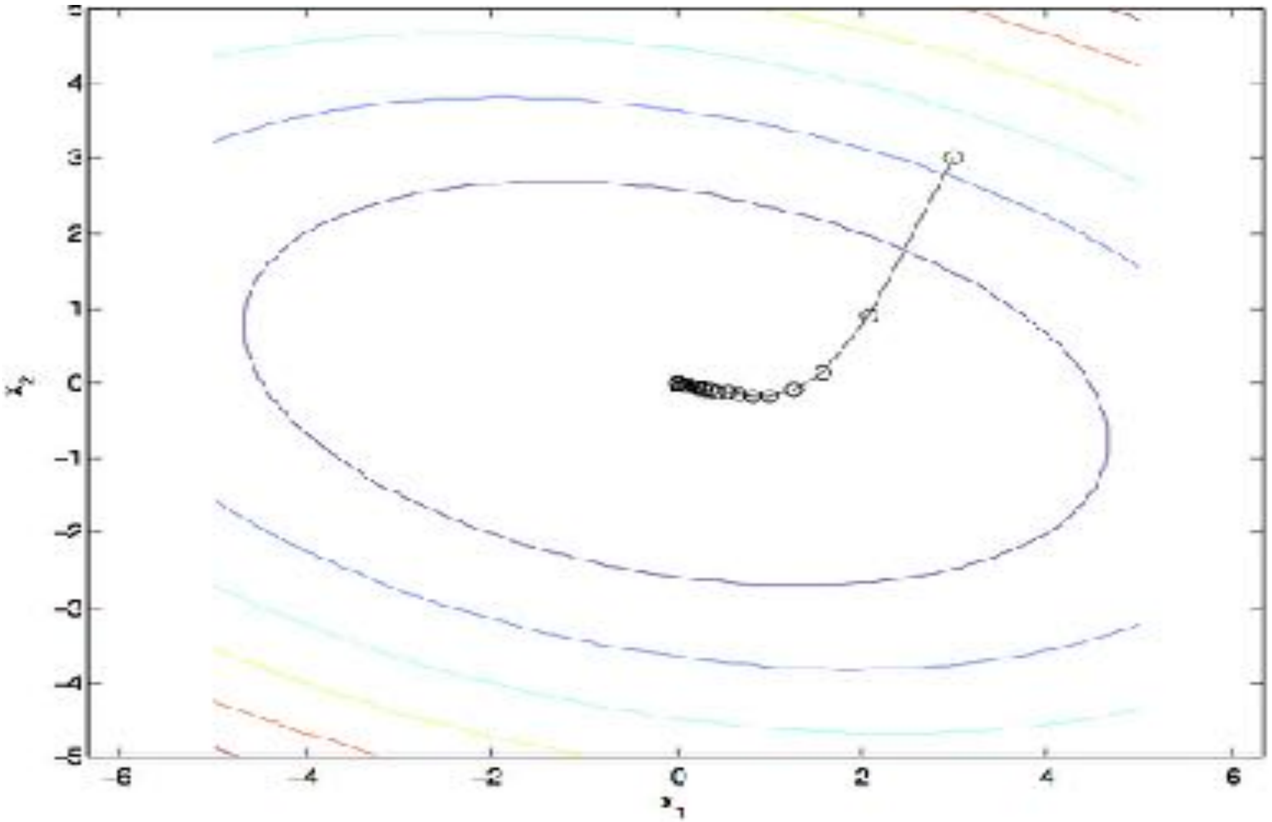
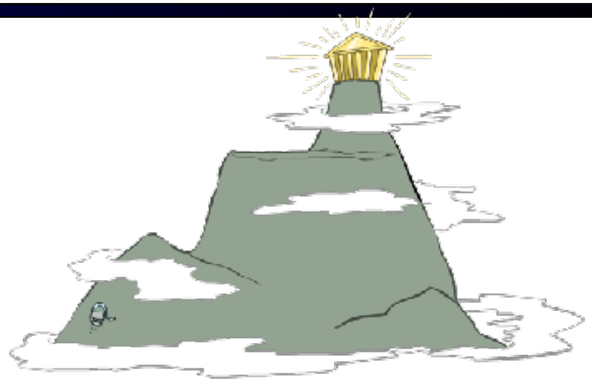


Figure source: Mathworks

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 Ascent 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: $$\max_{\Delta:\|\Delta\|\leq\varepsilon} \Delta^\top a \rightarrow \Delta = \varepsilon\frac{a}{\|a\|}$$
- 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

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

- 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

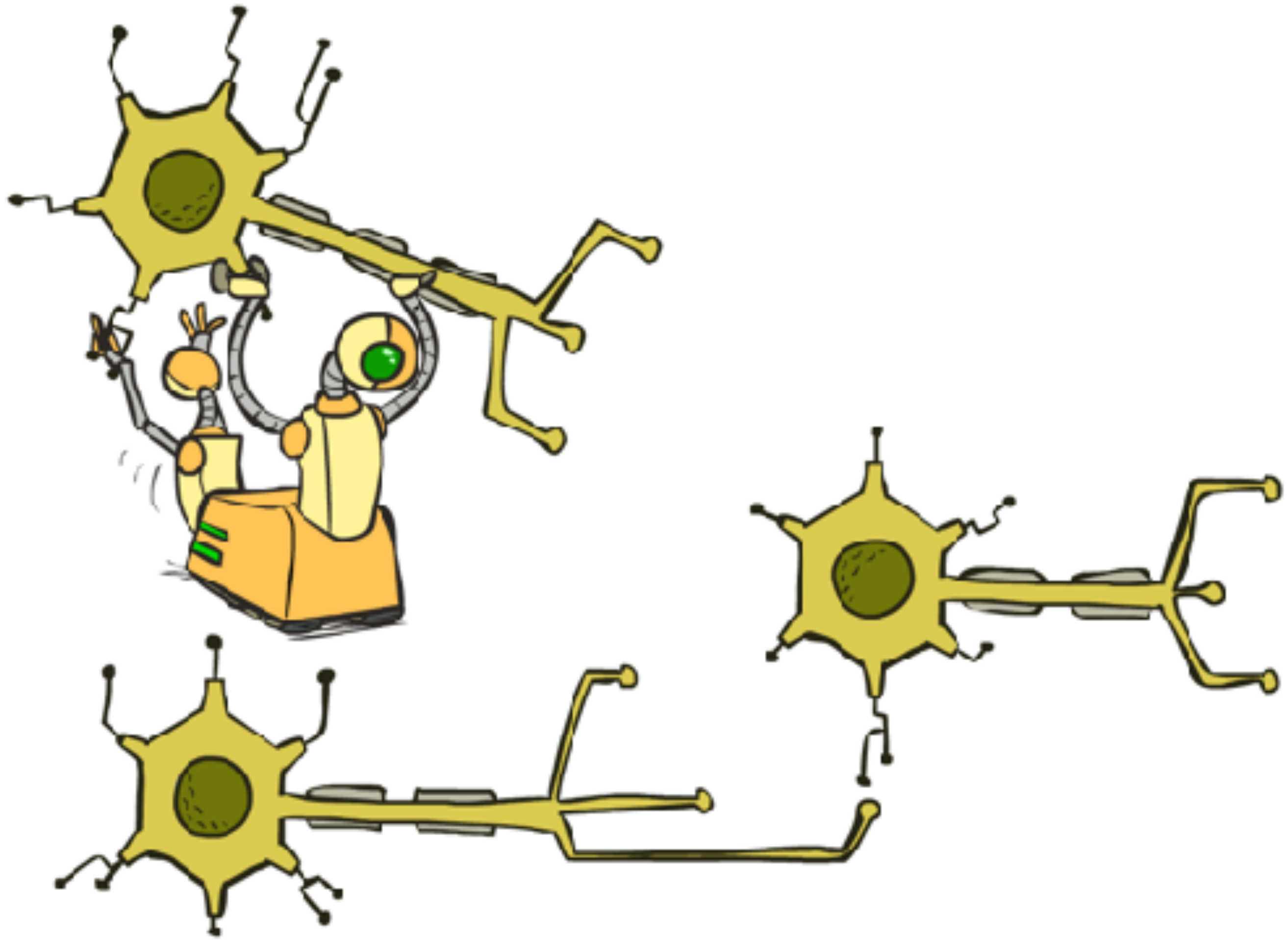
$$\max_w \quad ll(w) = \max_w \quad \sum_i \log P(y^{(i)}|x^{(i)}; w)$$

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`

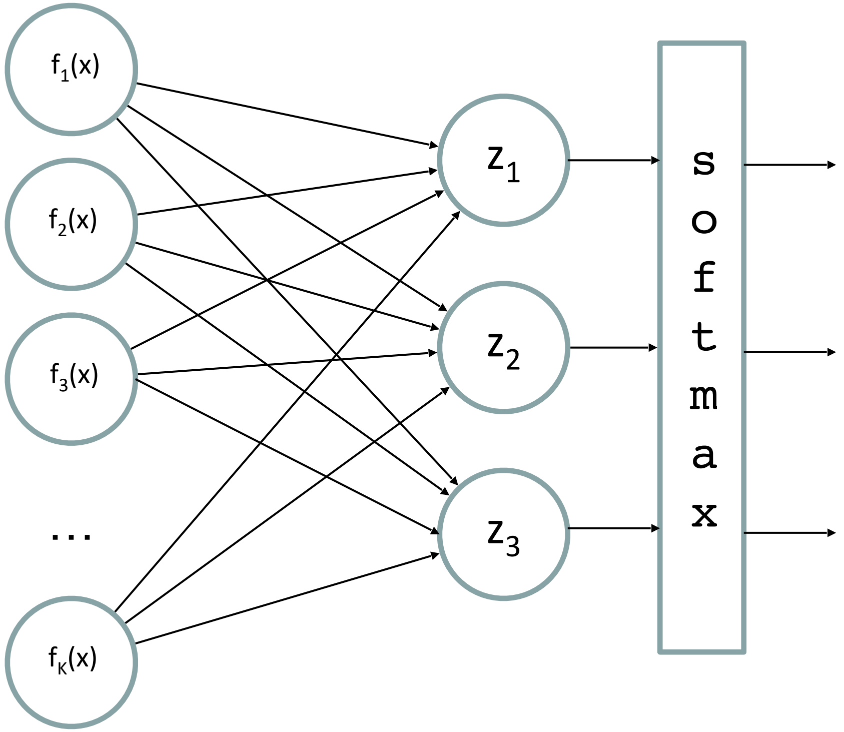
$$w \leftarrow w + \alpha * \sum_{j \in J} \nabla \log P(y^{(j)}|x^{(j)}; w)$$

Neural Networks



Multi-class Logistic Regression

- = special case of neural network

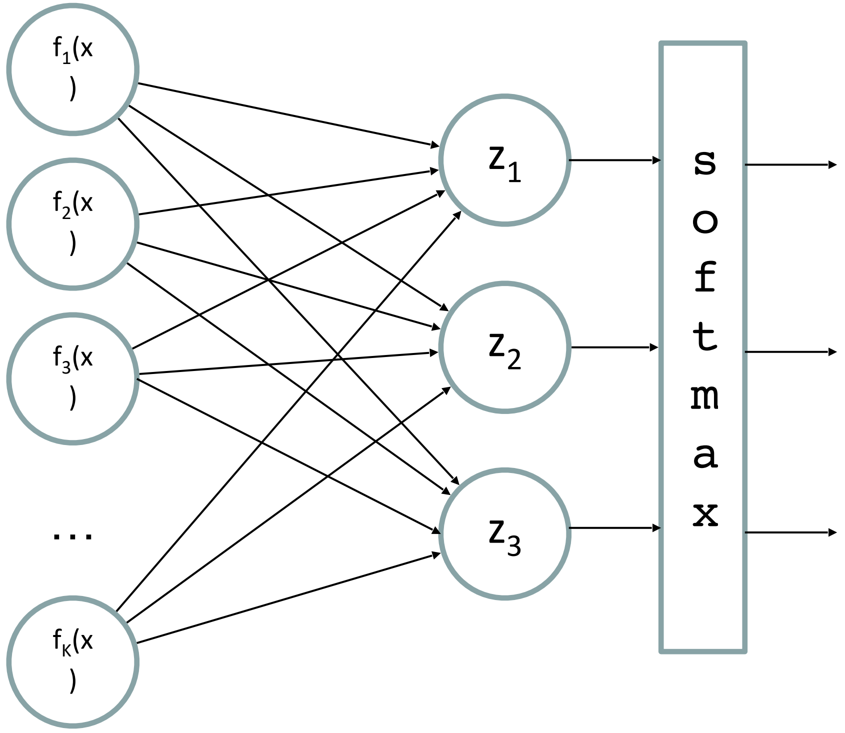


$$P(y_1|x;w) = \frac{e^{z_1}}{e^{z_1} + e^{z_2} + e^{z_3}}$$

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

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

Deep Neural Network = Also learn the features!



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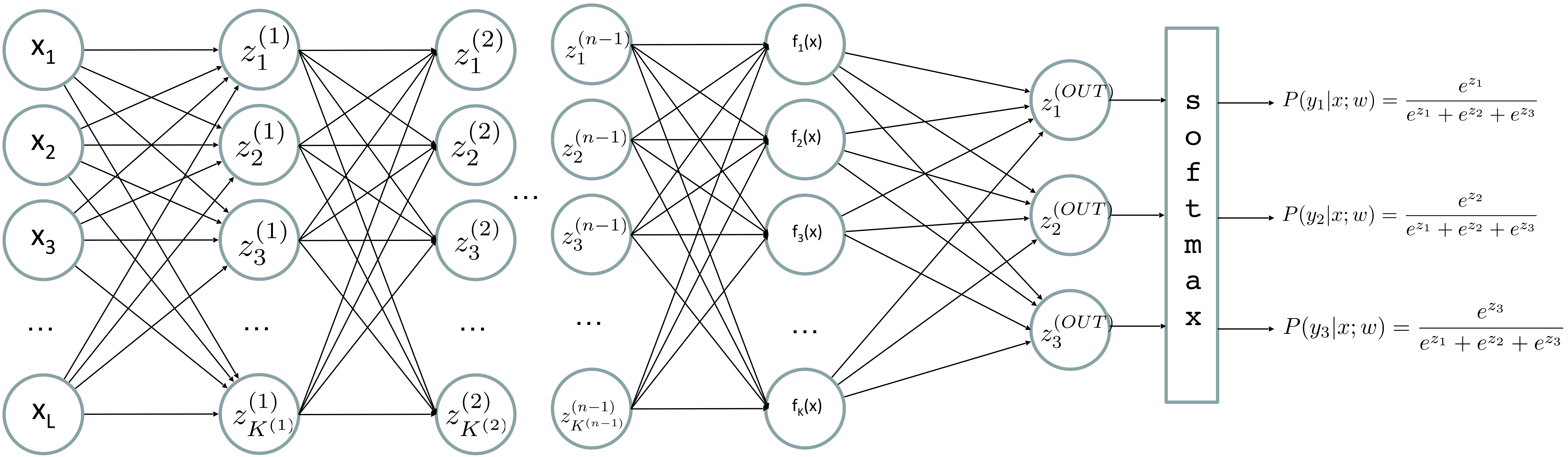
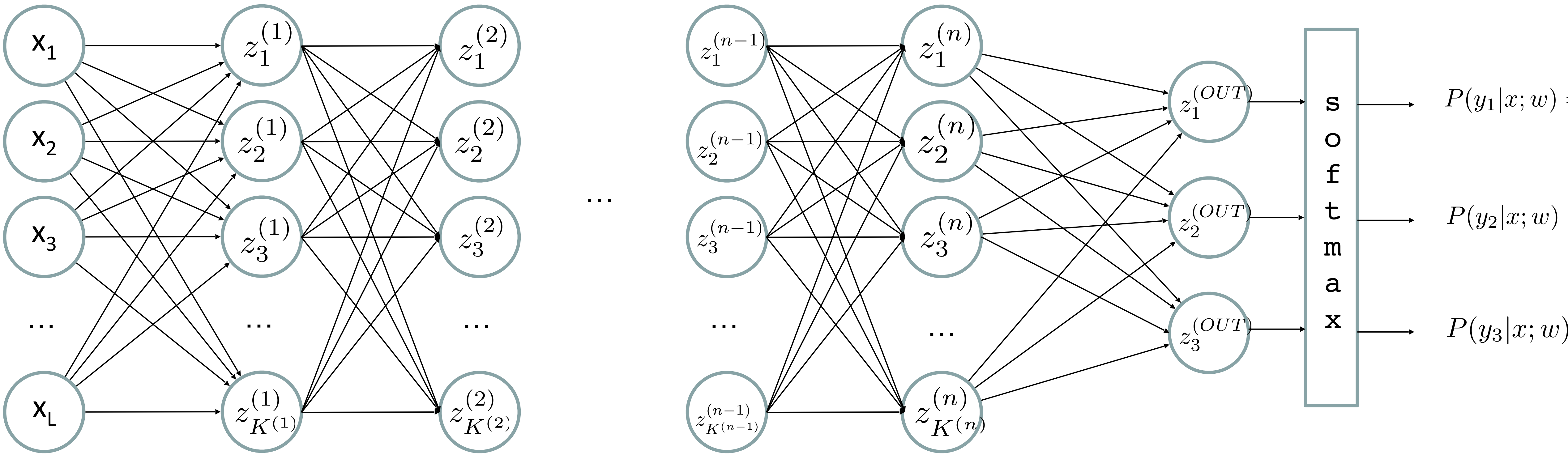
Deep Neural Network = Also learn the features!



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

g = nonlinear activation function

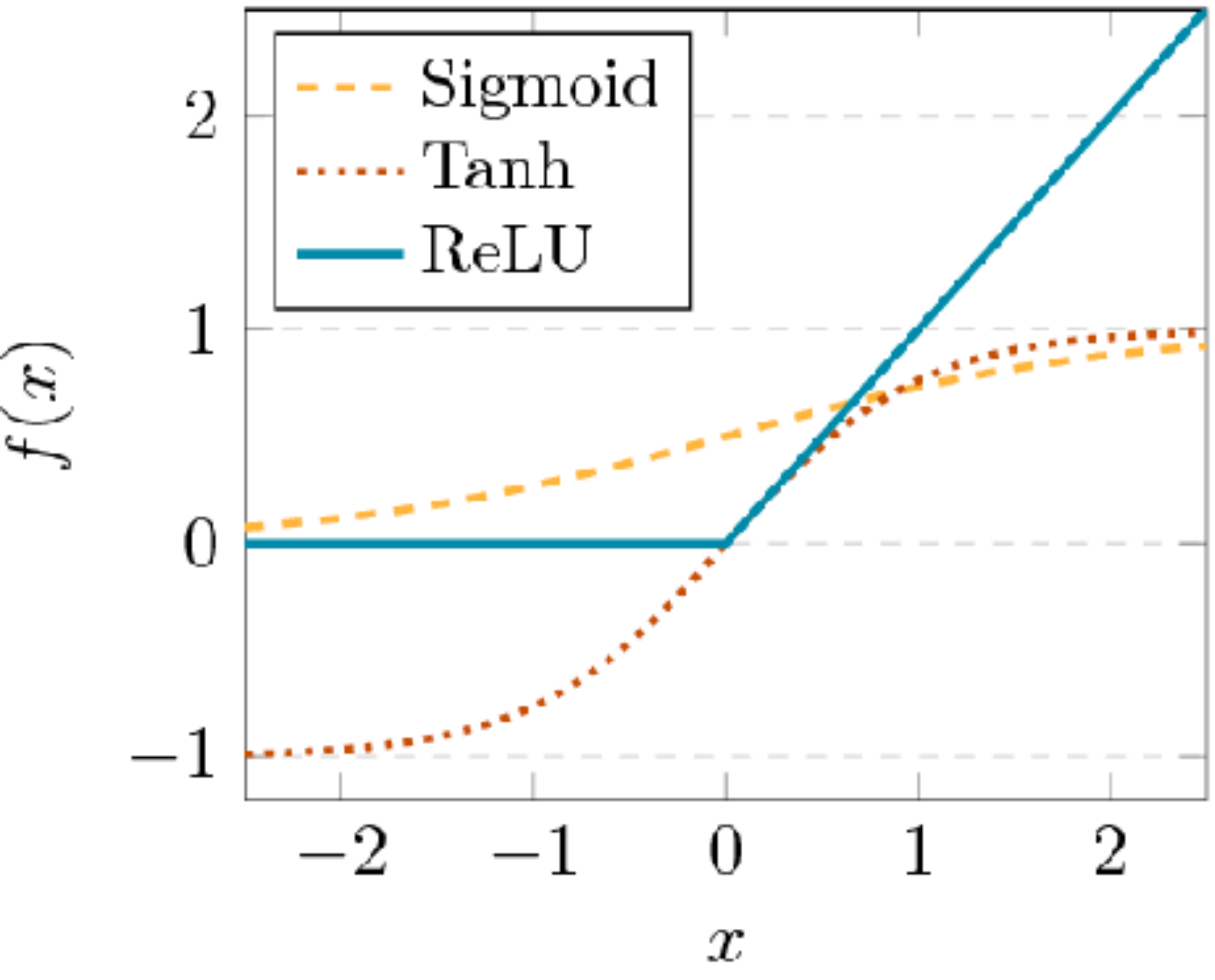
Deep Neural Network = Also learn the features!



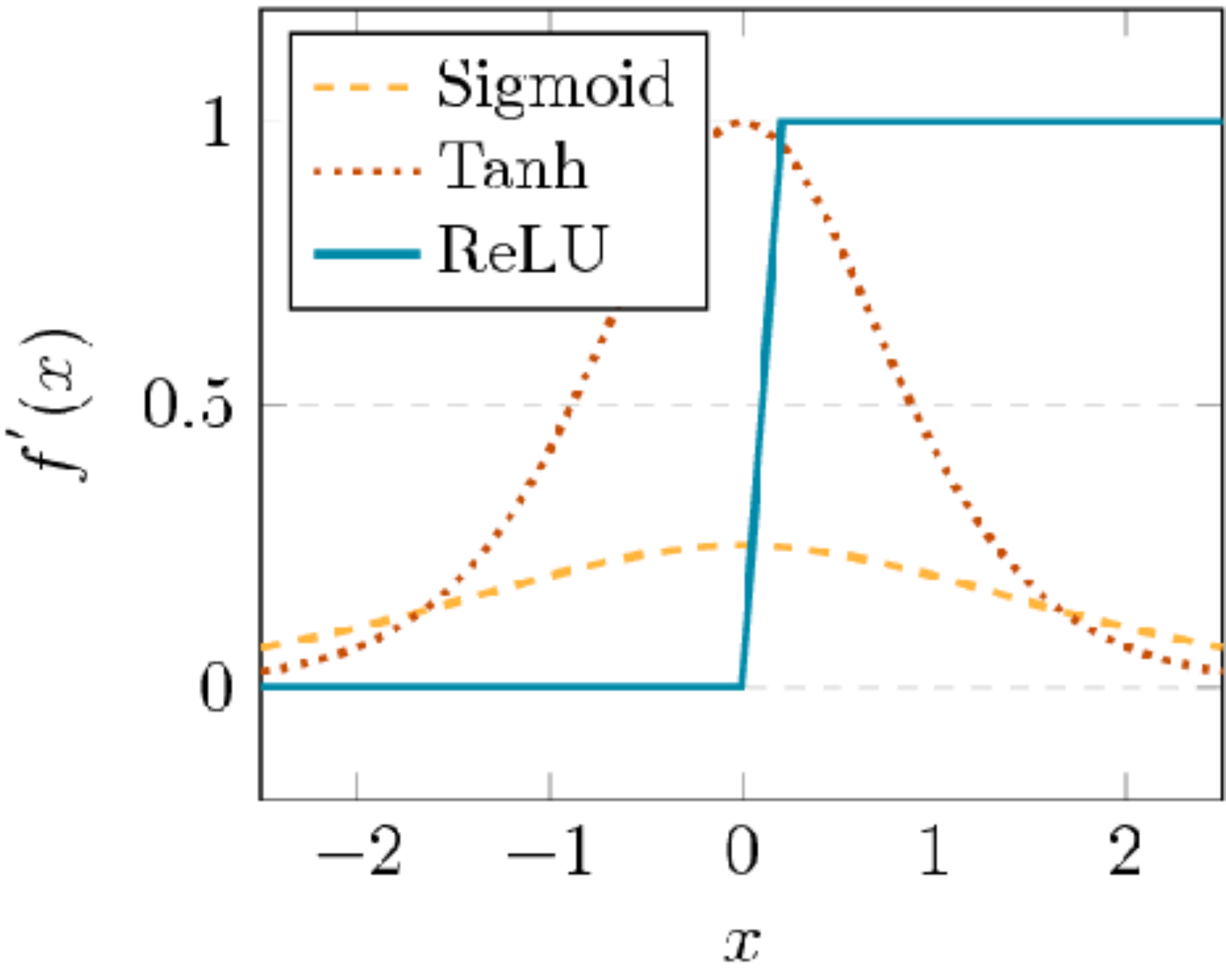
$$z_i^{(k)} = g\left(\sum_j W_{i,j}^{(k-1,k)} z_j^{(k-1)}\right)$$

g = nonlinear activation function

Common Activation Functions



(a) Activation functions



(b) Derivatives

Deep Neural Network: Also Learn the Features!

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

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

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*

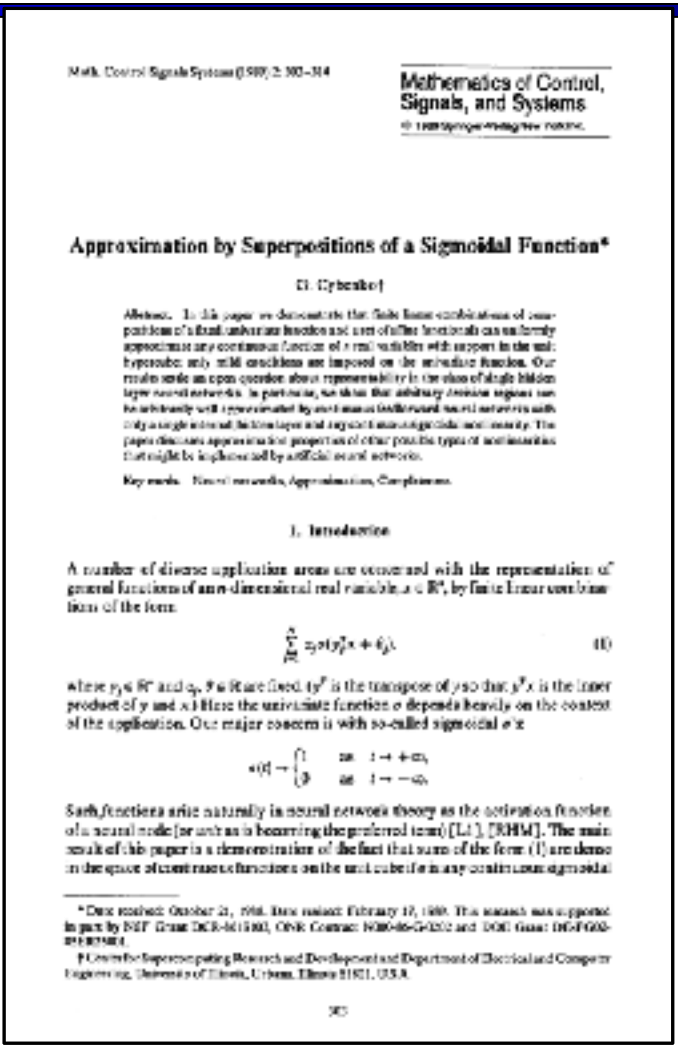
Hornik theorem 1: Whenever the activation function is *bounded and nonconstant*, then, for any finite measure μ, standard multilayer feedforward networks can approximate any function in $L^p(\mu)$ (the space of all functions on R^k such that $\int_{R^k} |f(x)|^p d\mu(x) < \infty$) arbitrarily well, provided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



Math. Control Signals Systems (1989) 2: 303–314

Mathematics of Control, Signals, and Systems

Approximation by Superpositions of a Sigmoidal Function*

G. Cybenko†

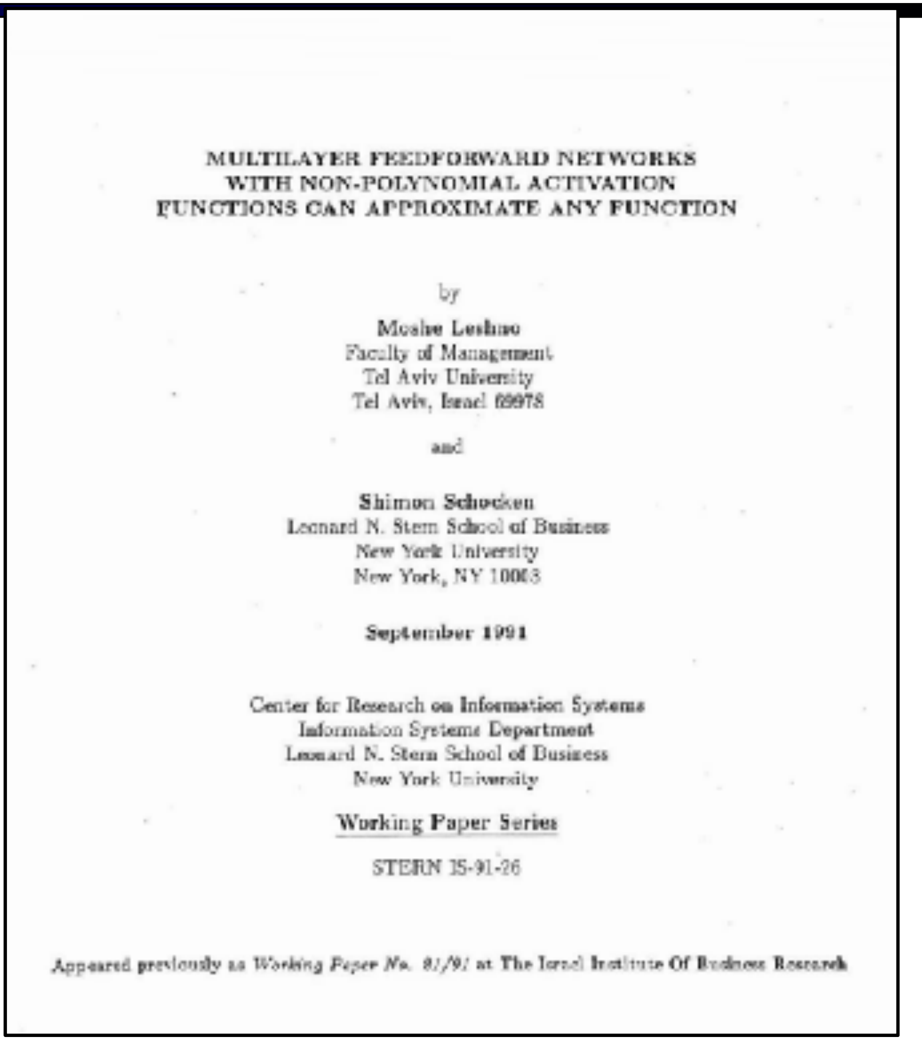
1. Introduction

ORIGINAL CONTRIBUTION

Approximation Capabilities of Multilayer Feedforward Networks

KURT HORNIK

1. INTRODUCTION



MULTILAYER FEEDFORWARD NETWORKS
WITH NON-POLYNOMIAL ACTIVATION
FUNCTIONS CAN APPROXIMATE ANY FUNCTION

by

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September 1991

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Functions Can Approximate Any Function”

Fun Neural Net Demo Site

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

How about computing all the derivatives?

- Derivatives tables:

$$\frac{d}{dx}(a)=0$$

$$\frac{d}{dx}(x)=1$$

$$\frac{d}{dx}(au)=a\frac{du}{dx}$$

$$\frac{d}{dx}(u+v-w)=\frac{du}{dx}+\frac{dv}{dx}-\frac{dw}{dx}$$

$$\frac{d}{dx}(uv)=u\frac{dv}{dx}+v\frac{du}{dx}$$

$$\frac{d}{dx}\left(\frac{u}{v}\right)=\frac{1}{v}\frac{du}{dx}\quad\frac{u}{v^2}\frac{dv}{dx}$$

$$\frac{d}{dx}(u^n)=nu^{n-1}\frac{du}{dx}$$

$$\frac{d}{dx}(\sqrt{u})-\frac{1}{2\sqrt{u}}\frac{du}{dx}$$

$$\frac{d}{dx}\left(\frac{1}{u}\right)=\quad\frac{1}{u^2}\frac{du}{dx}$$

$$\frac{d}{dx}\left(\frac{1}{u^n}\right)=-\frac{n}{u^{n+1}}\frac{du}{dx}$$

$$\frac{d}{dx}\left[f(u)\right]=\frac{d}{du}\left[f(u)\right]\frac{du}{dx}$$

$$\frac{d}{dx}[\ln u]=\frac{d}{dx}[\log_e u]=\frac{1}{u}\frac{du}{dx}$$

$$\frac{d}{dx}[\log_a u]-\log_a e\frac{1}{u}\frac{du}{dx}$$

$$\frac{d}{dx}e^u=e^u\frac{du}{dx}$$

$$\frac{d}{dx}a^u=a^u\ln a\frac{du}{dx}$$

$$\frac{d}{dx}(u^v)-vu^{v-1}\frac{du}{dx}+\ln u\quad u^v\frac{dv}{dx}$$

$$\frac{d}{dx}\sin u=\cos u\frac{du}{dx}$$

$$\frac{d}{dx}\cos u=-\sin u\frac{du}{dx}$$

$$\frac{d}{dx}\tan u=\sec^2 u\frac{du}{dx}$$

$$\frac{d}{dx}\cot u=-\csc^2 u\frac{du}{dx}$$

$$\frac{d}{dx}\sec u=\sec u\tan u\frac{du}{dx}$$

$$\frac{d}{dx}\csc u=-\csc u\cot u\frac{du}{dx}$$

[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

Summary of Key Ideas

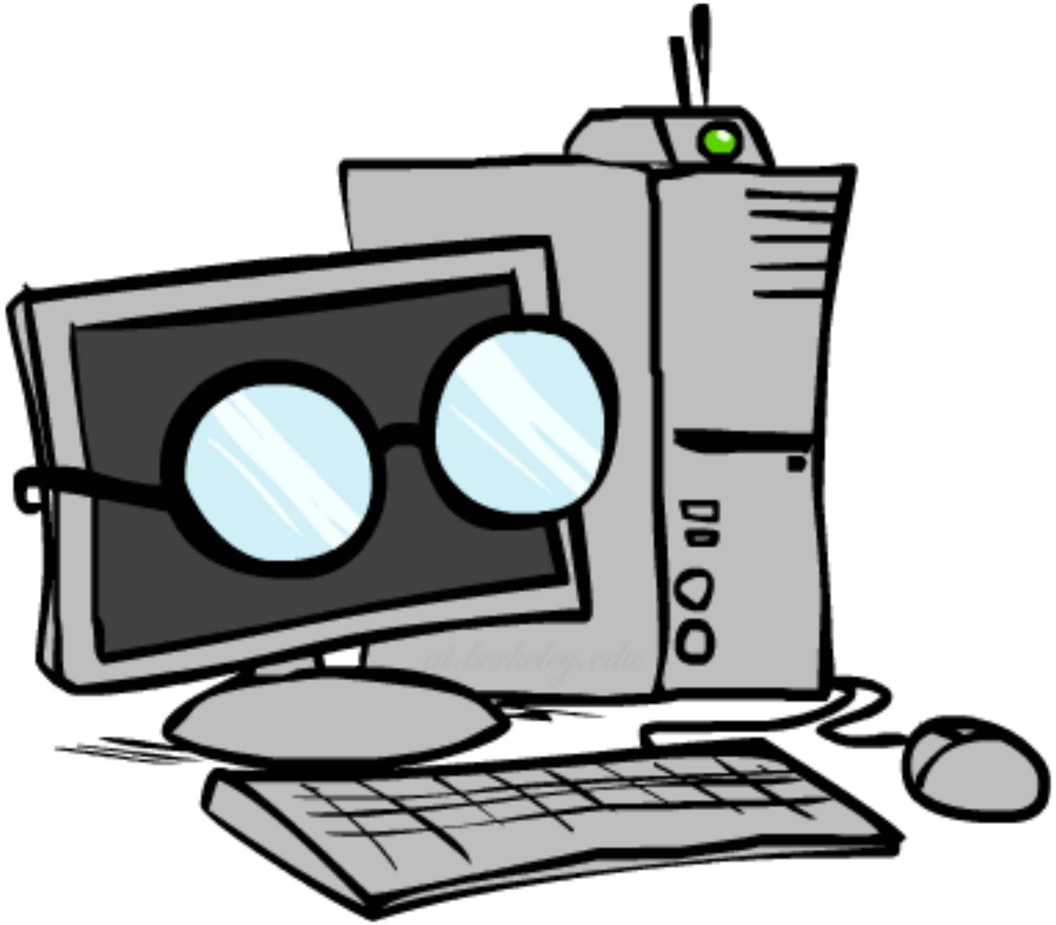
- Optimize probability of label given input $\max_w \quad ll(w) = \max_w \quad \sum_i \log P(y^{(i)}|x^{(i)};w)$

- 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")

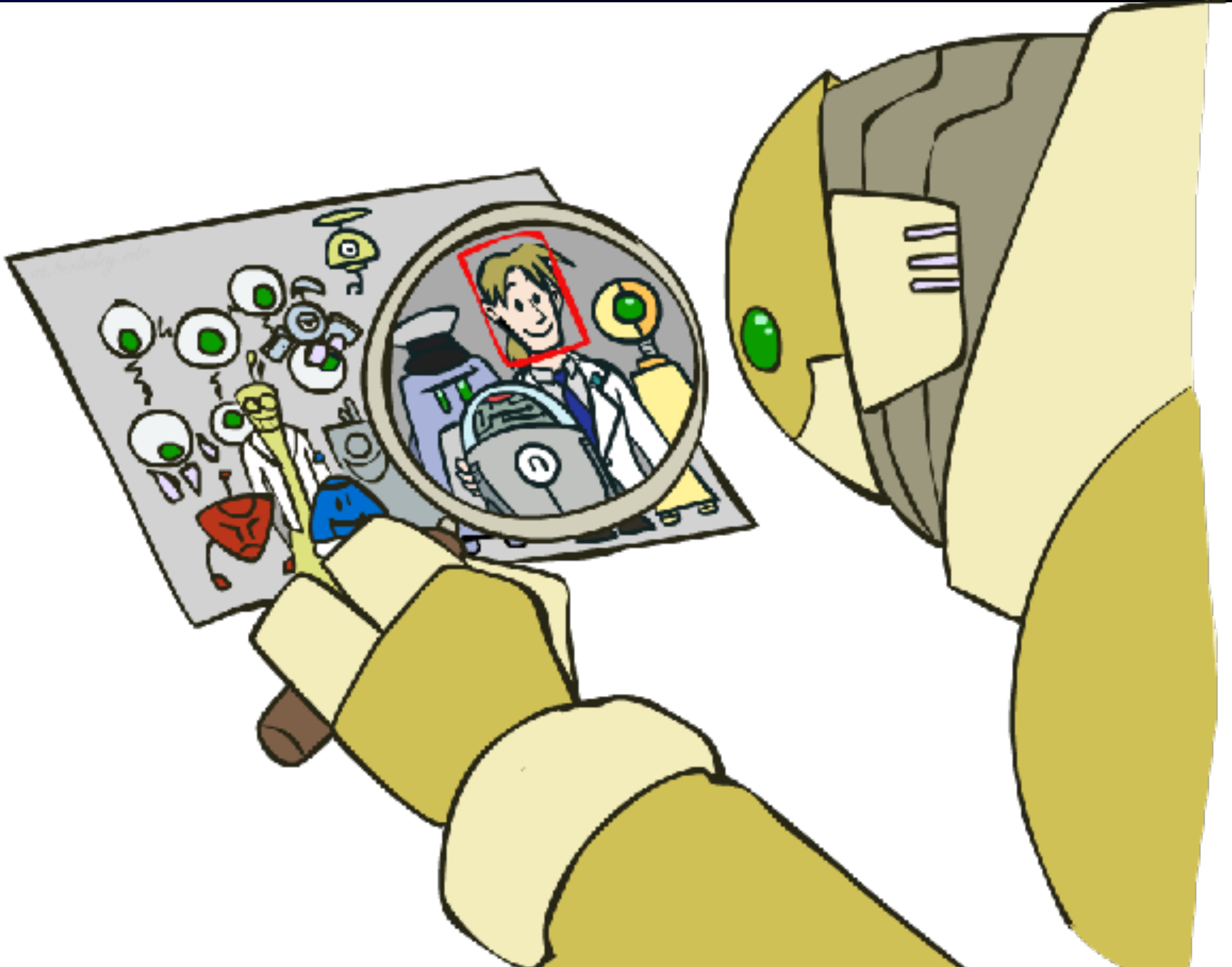
- Deep neural nets
  - Last layer = still logistic regression
  - Now also many more layers before this last layer
    - = computing the features
    - → the features are learned rather than hand-designed
  - Universal function approximation theorem
    - `If` neural net is large enough
    - `Then` 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 well does it work?

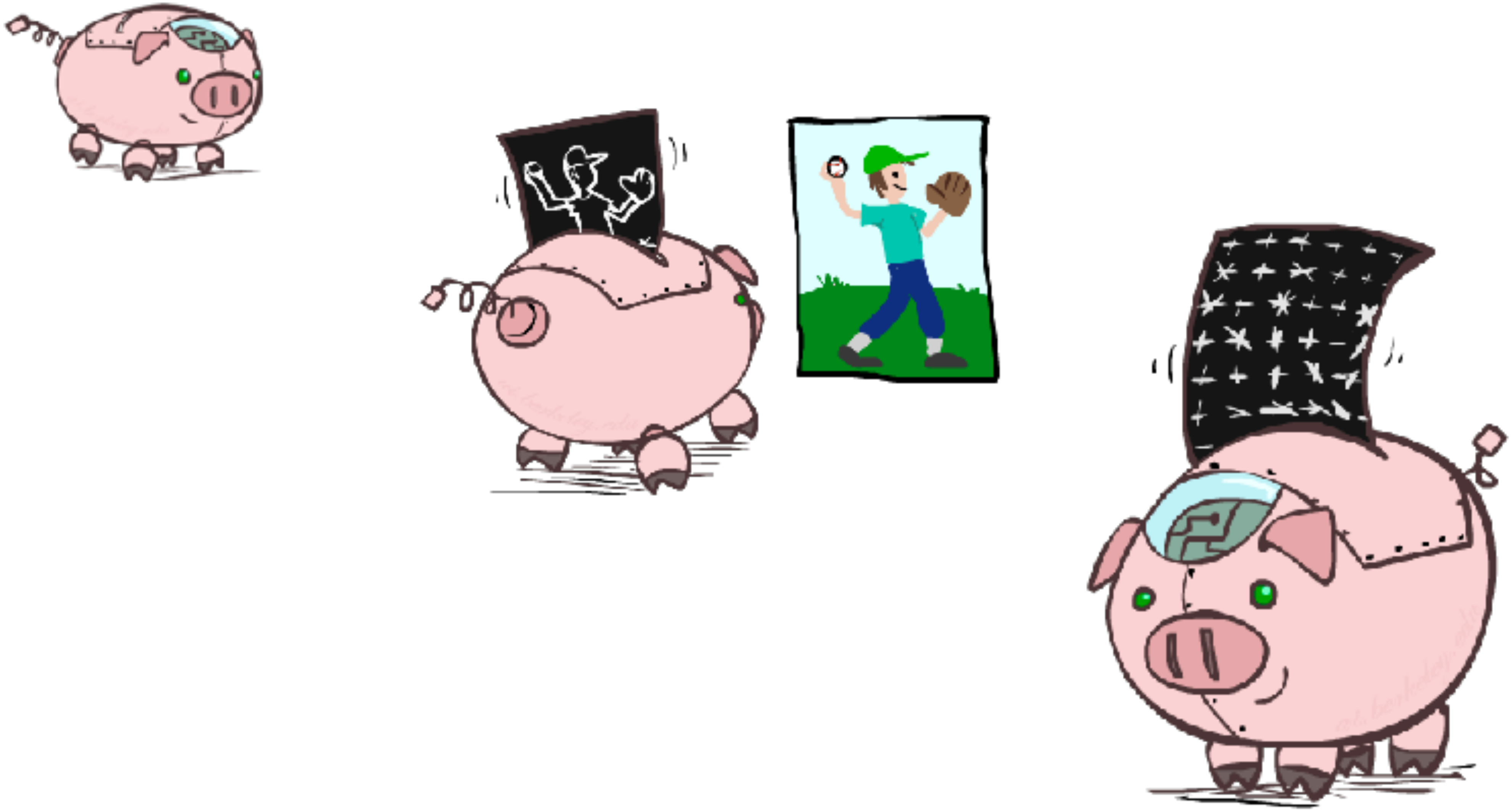
Computer Vision



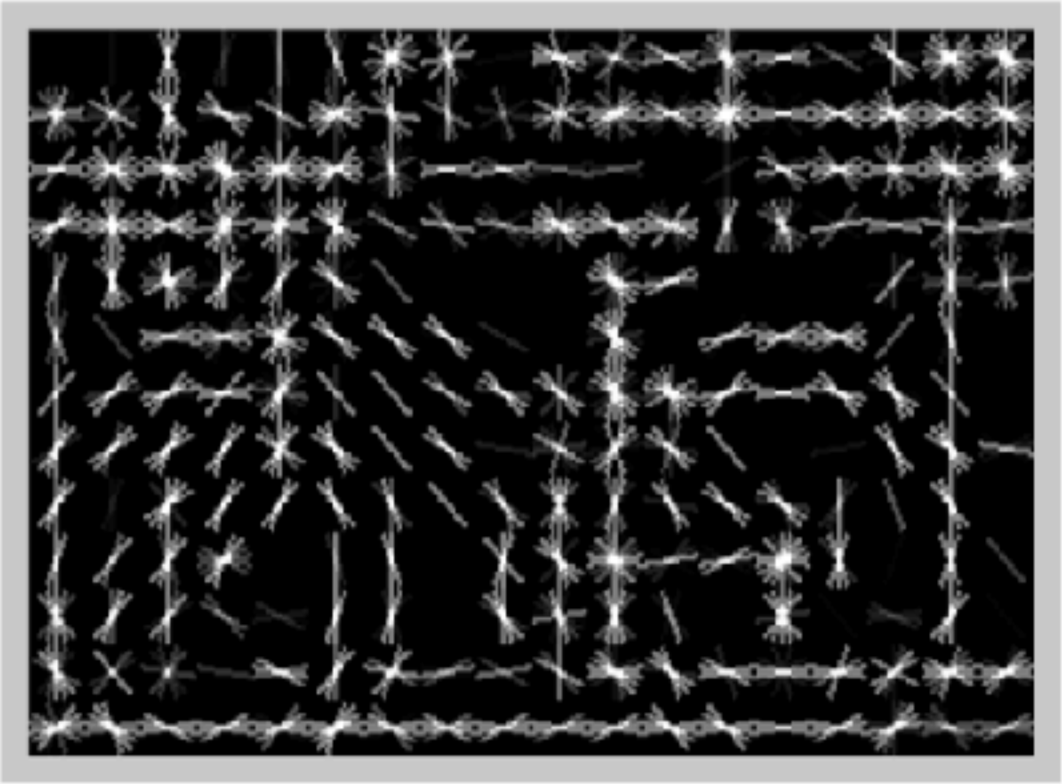
Object Detection



Manual Feature Design



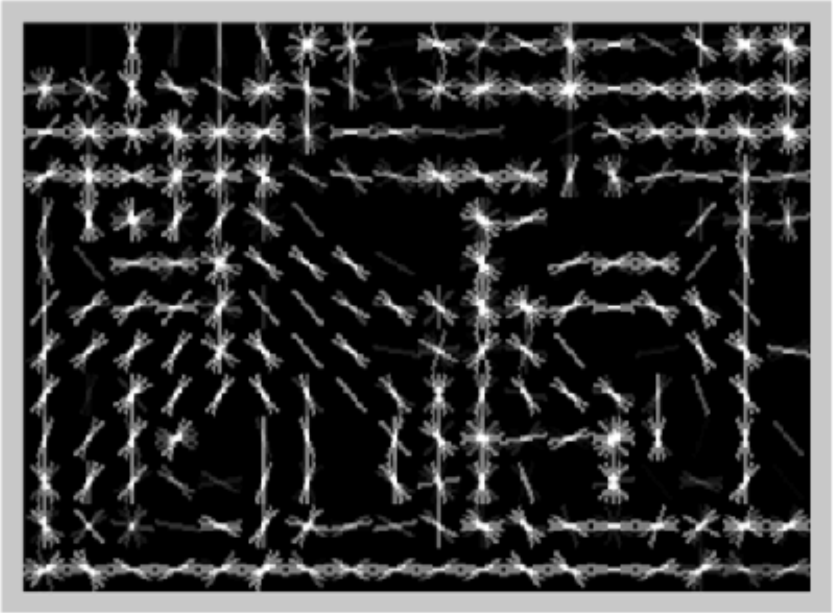
Features and Generalization



[HoG: Dalal and Triggs, 2005]

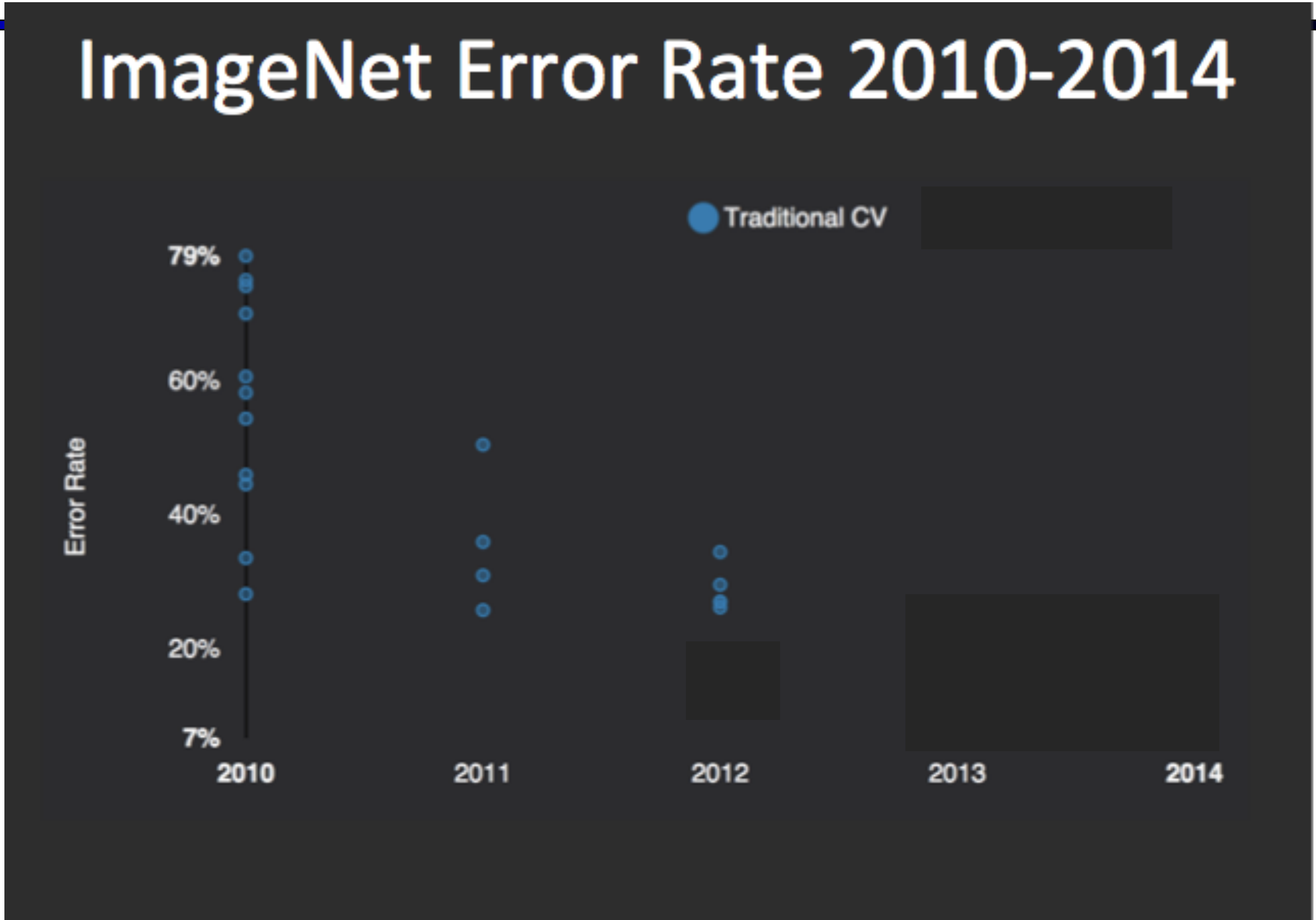
Features and Generalization

Image



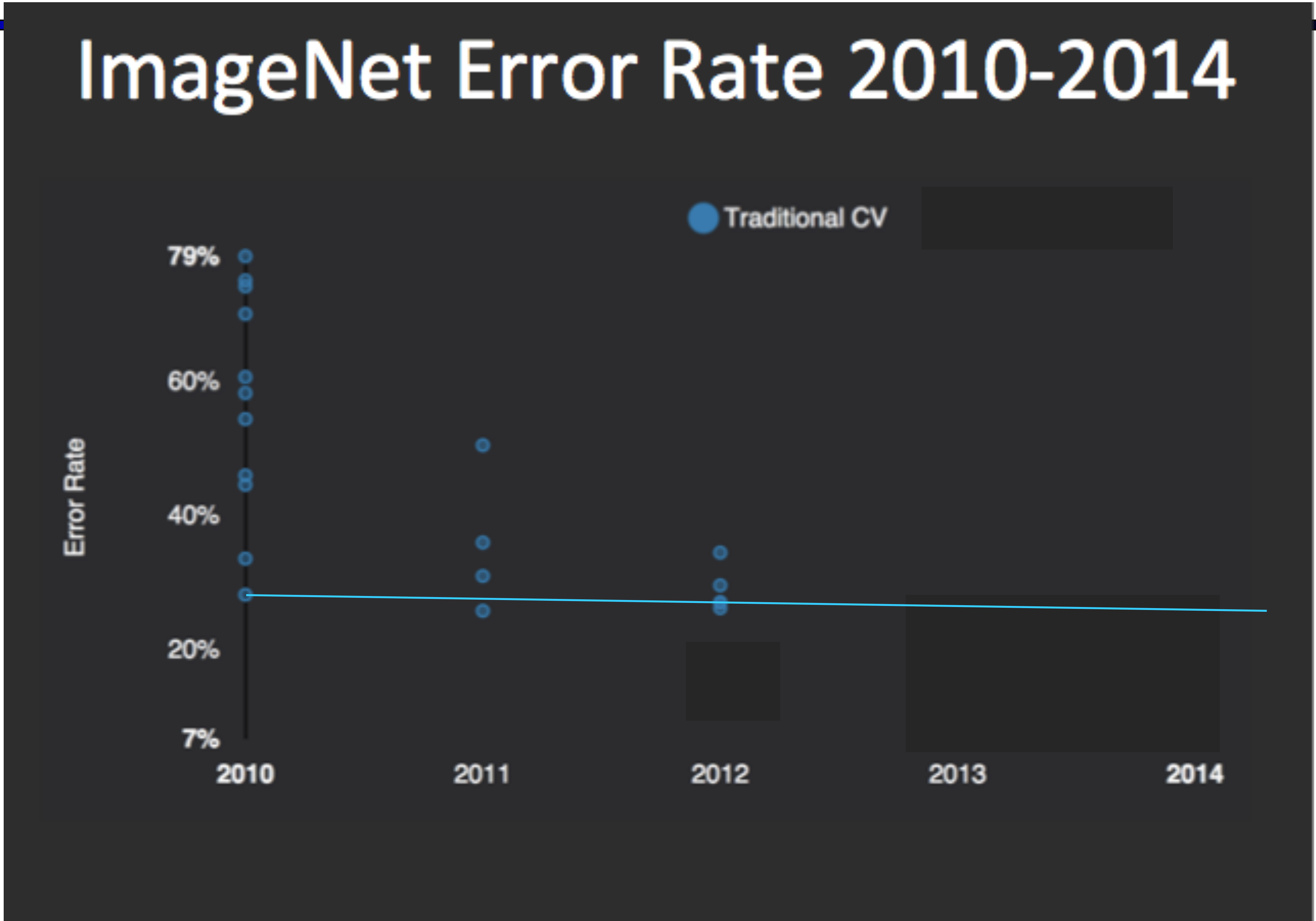
HoG

Performance



graph credit Matt Zeiler, Clarifai

Performance



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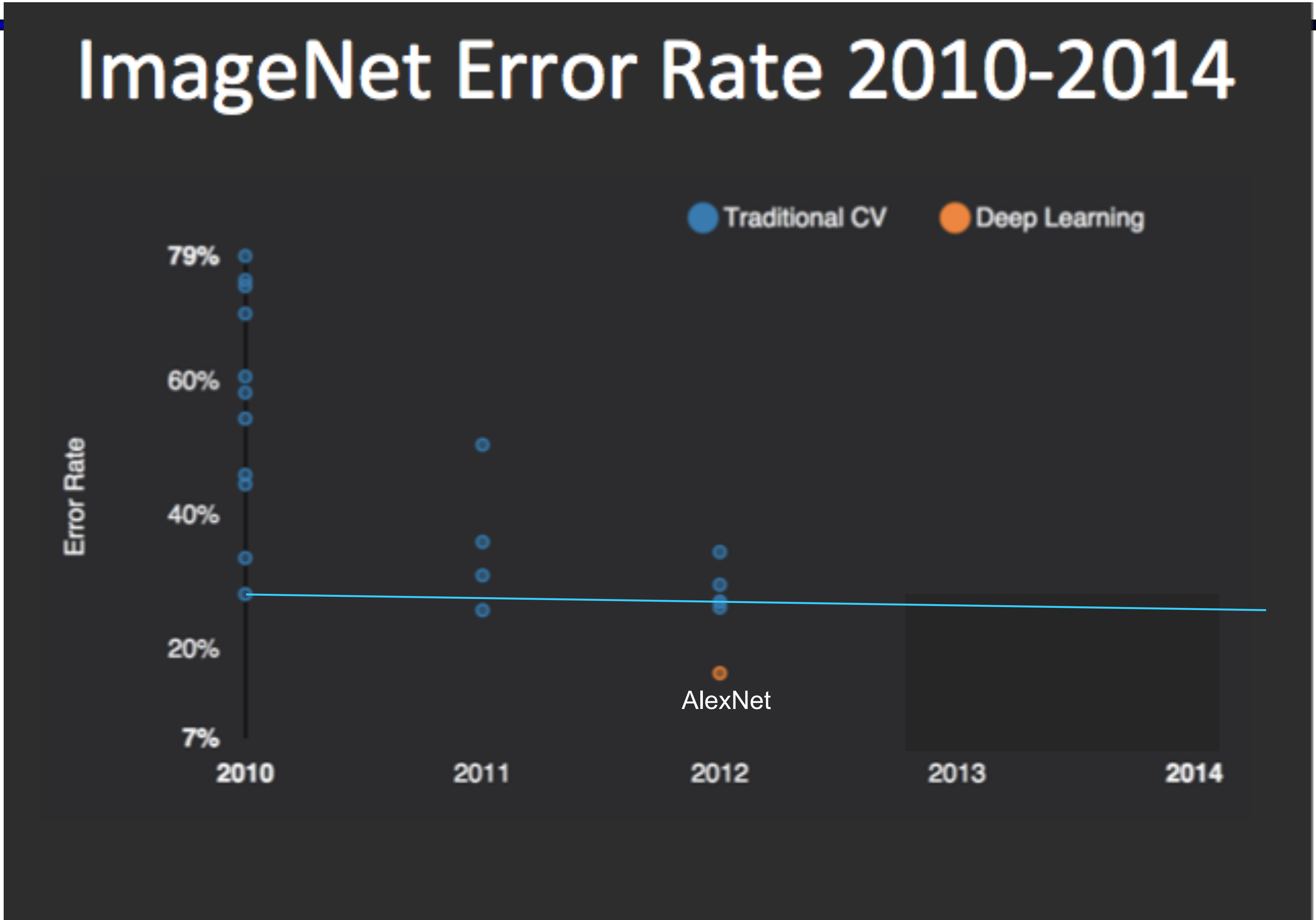
Performance



graph credit Matt Zeiler, Clarifai

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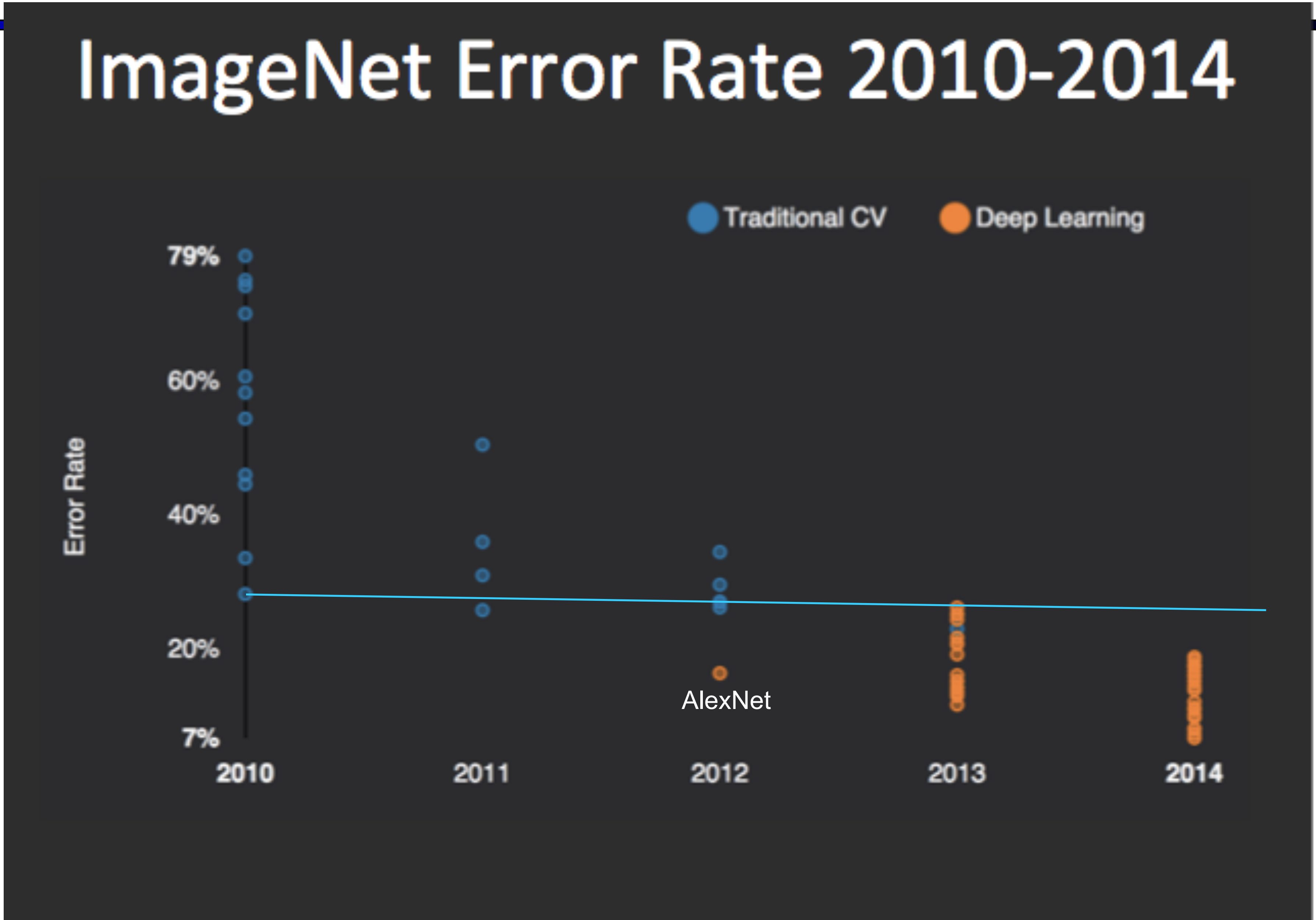

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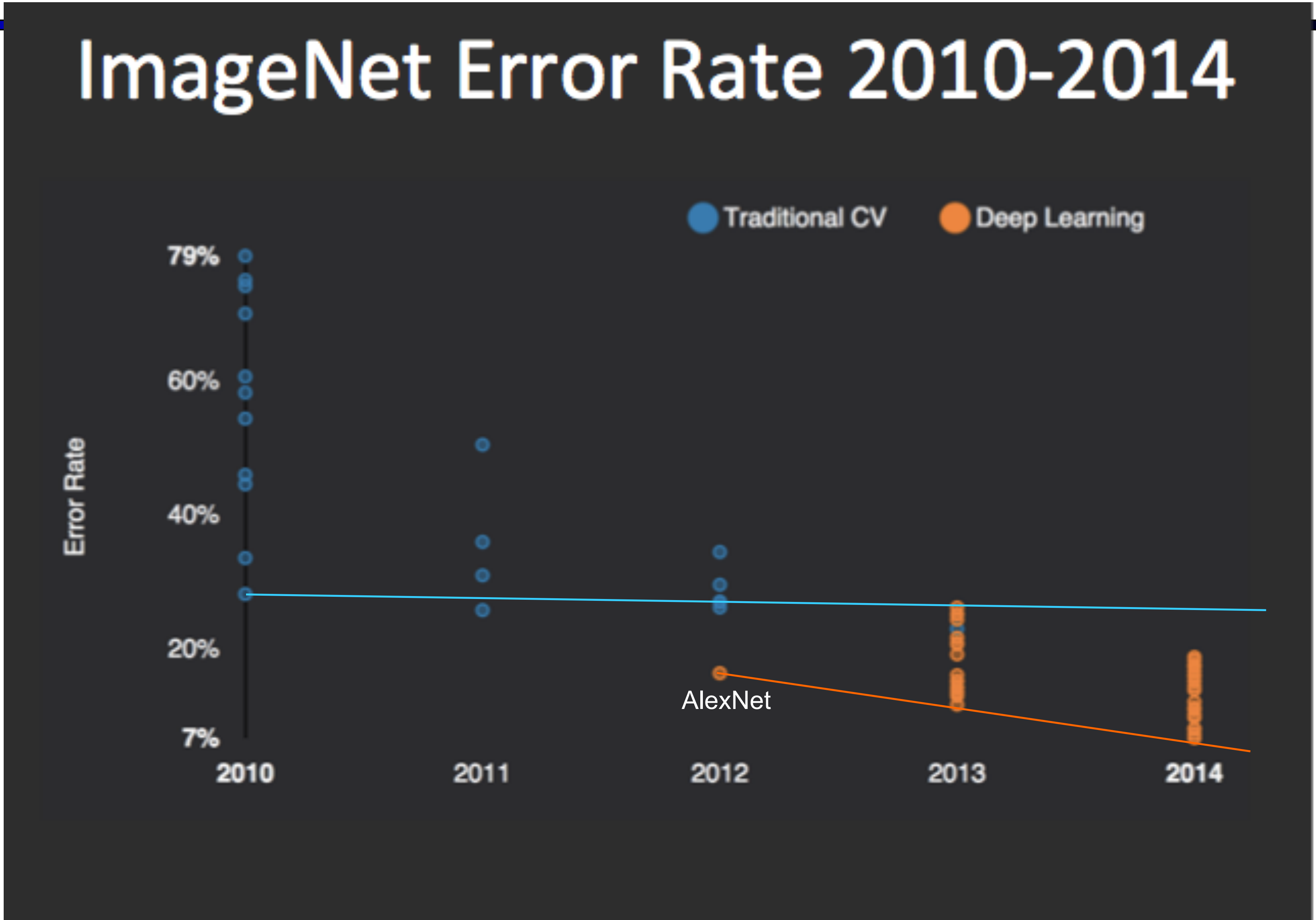


graph credit Matt Zeiler, Clarifai

MS COCO Image Captioning Challenge

"man in black shirt is playing guitar."

"construction worker in orange safety vest is working on road."

"two young girls are playing with lego toy."

"boy is doing backflip on wakeboard."

"girl in pink dress is jumping in air."

"black and white dog jumps over bar."

"young girl in pink shirt is swinging on swing."

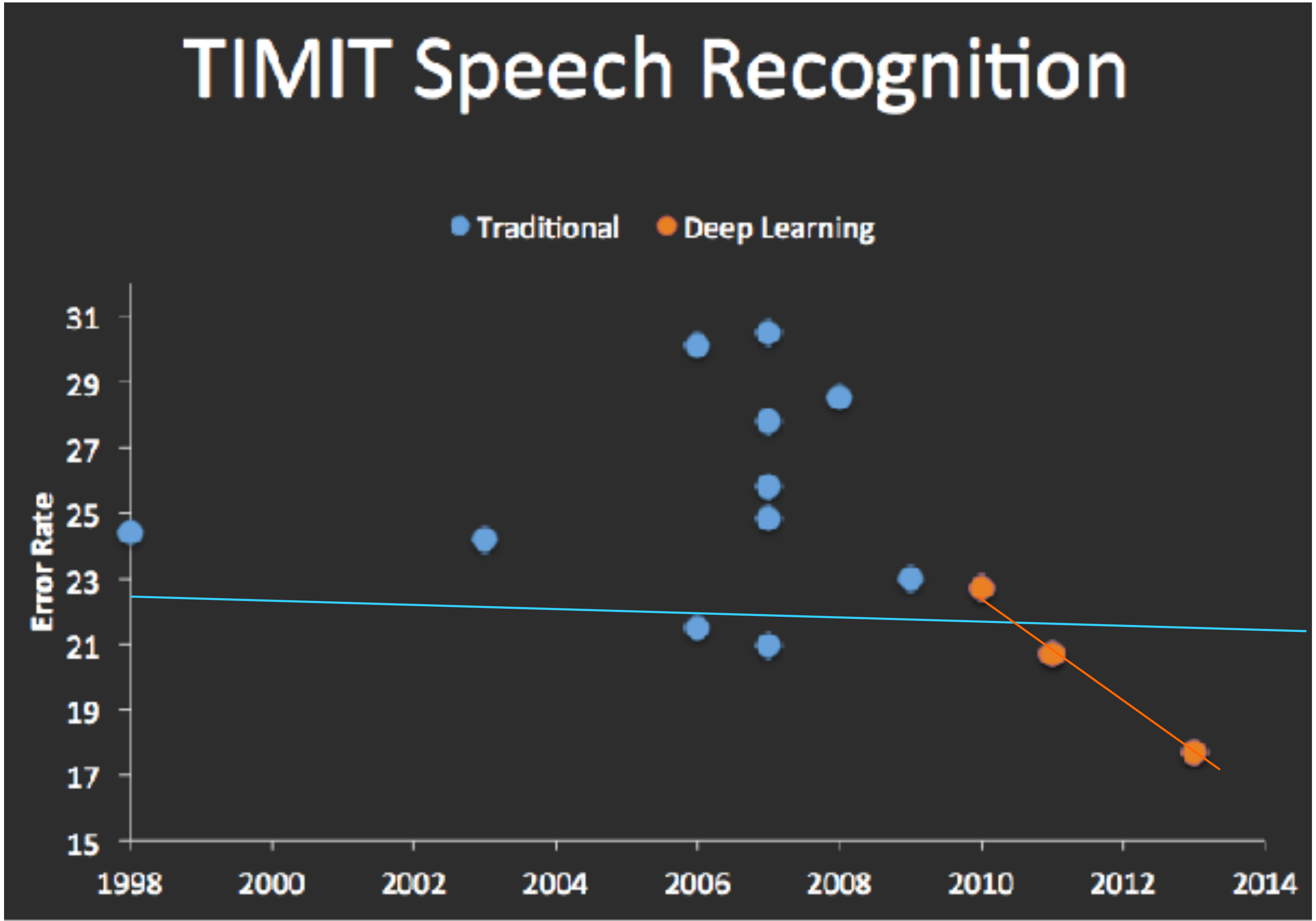
"man in blue wetsuit is surfing on wave."

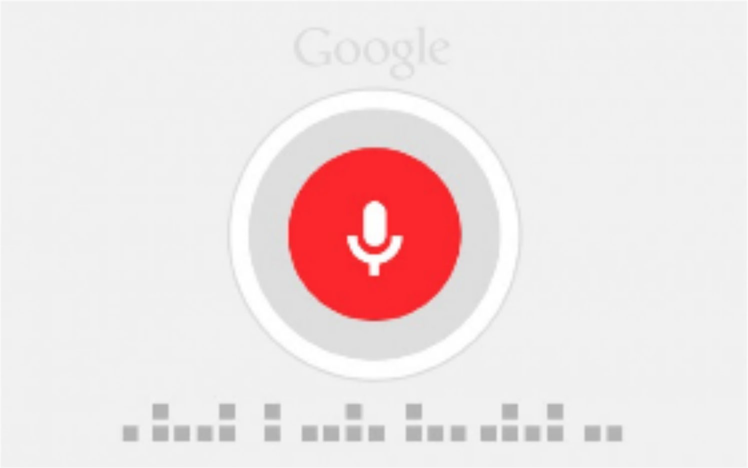
Karpathy & Fei-Fei, 2015; Donahue et al., 2015; Xu et al, 2015; many more

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)