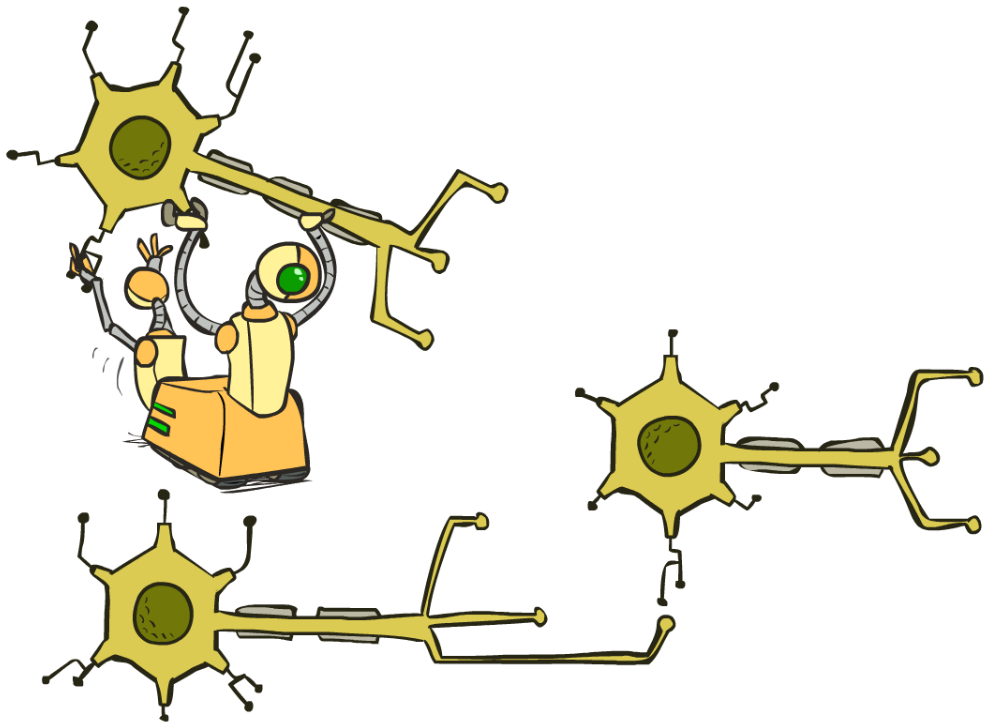
CS 188: Artificial Intelligence

Optimization and Neural Nets



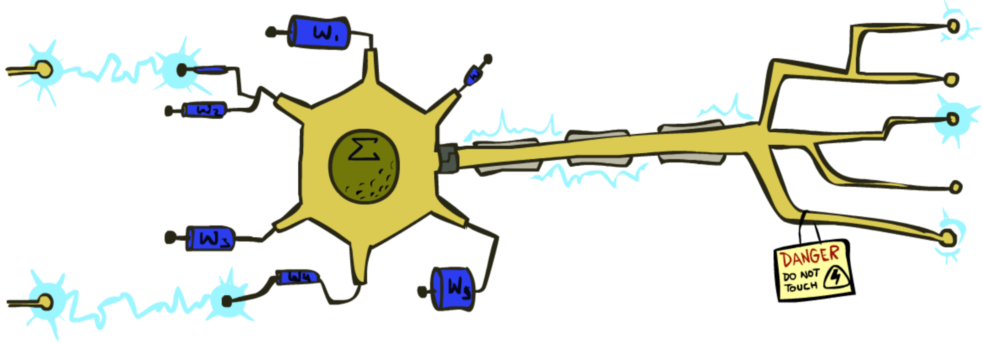
Instructors: John Canny and Oliver Grillmeyer --- University of California, Berkeley

Announcements

- Project 5 (last project)
  - Due Friday 4/25 at 11:59pm
- HW9
  - Due Wednesday 4/16 at 11:59pm
- HW10 (last homework)
  - Due Wednesday 4/23 at 11:59pm
- Final Exam
  - Thursday 5/15 at 3:00-6:00pm

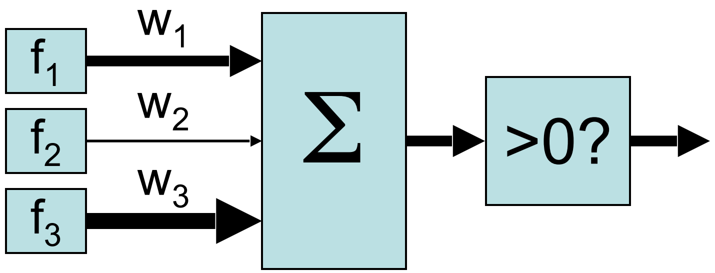
Refresher: Linear Classifiers

- 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

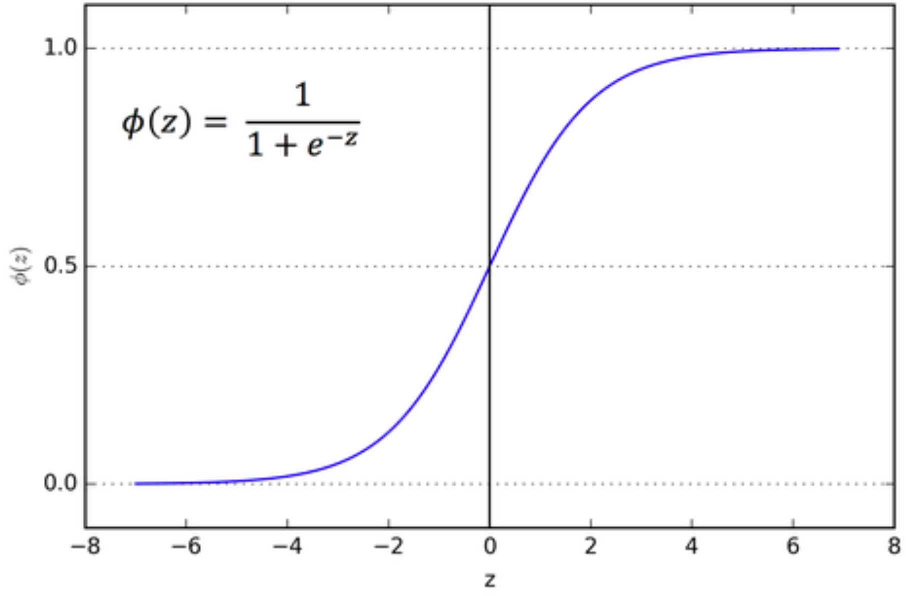


How to get probabilistic decisions?

- 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:

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

with:

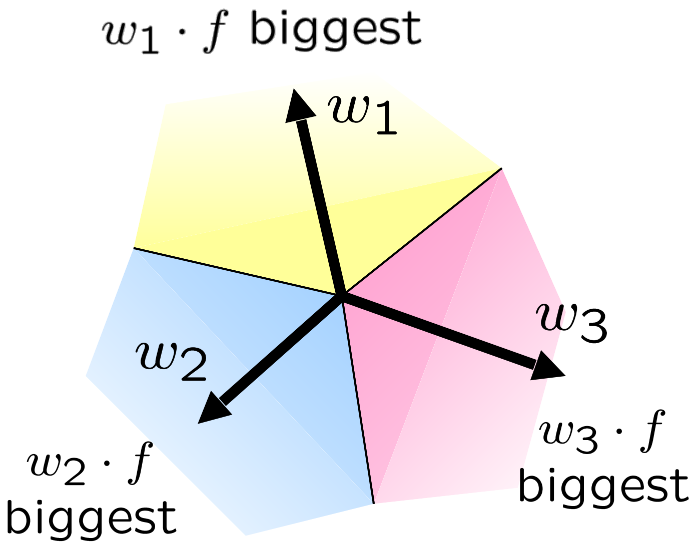
$$P(y^{(i)} = +1|x^{(i)};w) = \frac{1}{1+e^{-w\cdot f(x^{(i)})}}$$

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

= 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:

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

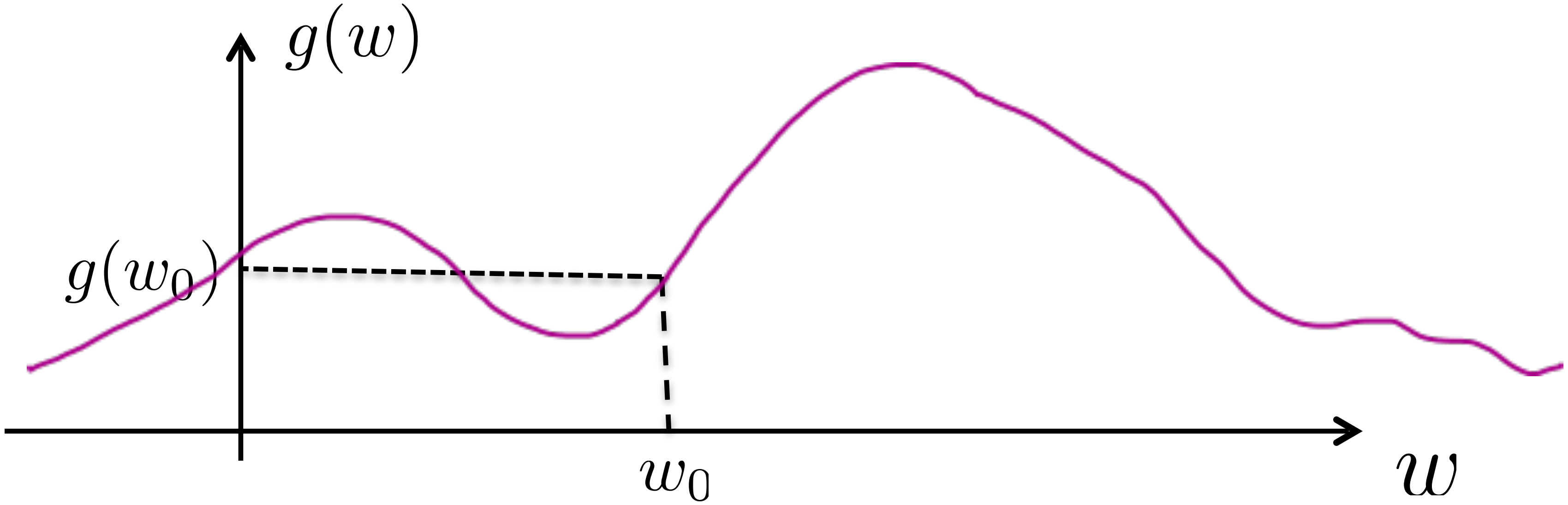
= Multi-Class Logistic Regression

Today's lecture: Choosing weights

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

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

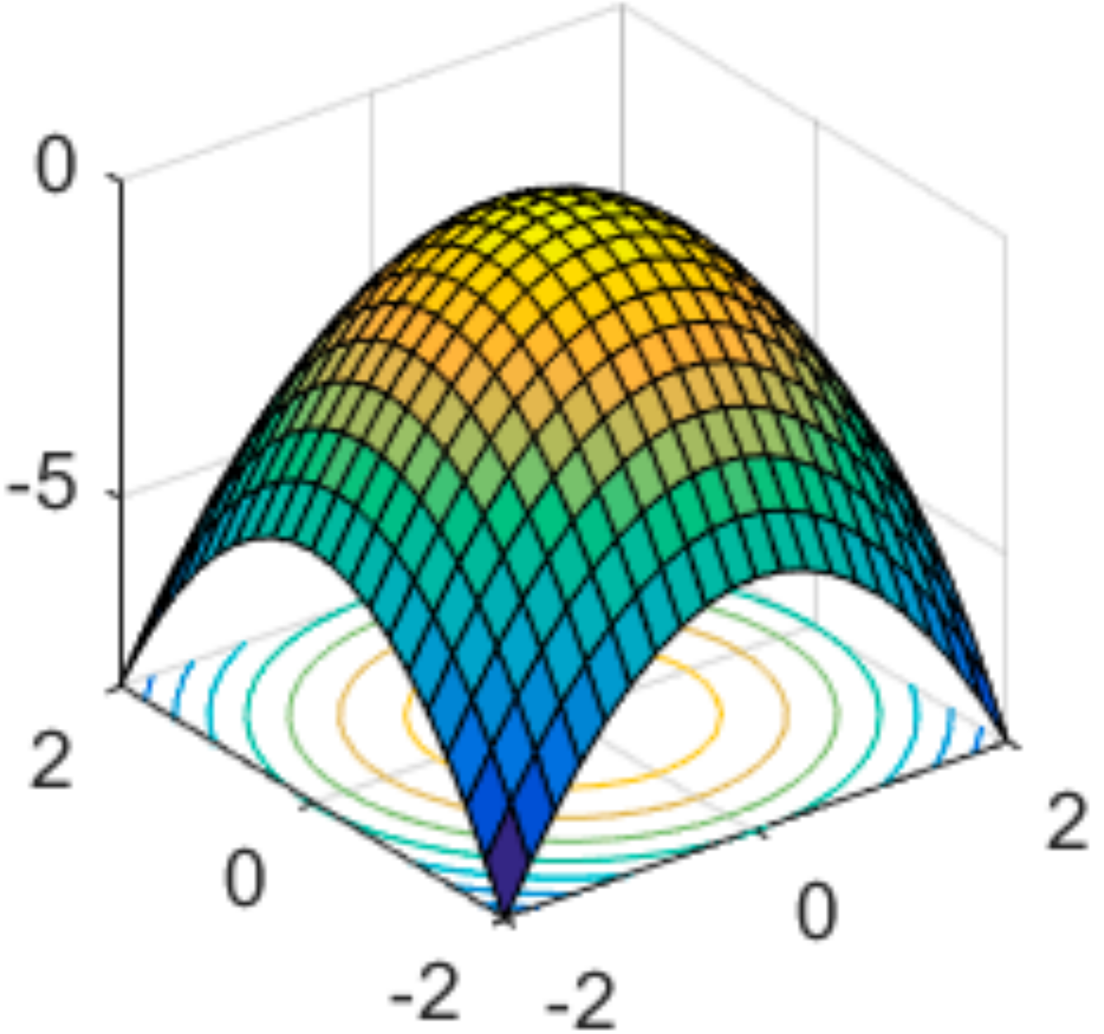
1-D Optimization



- 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

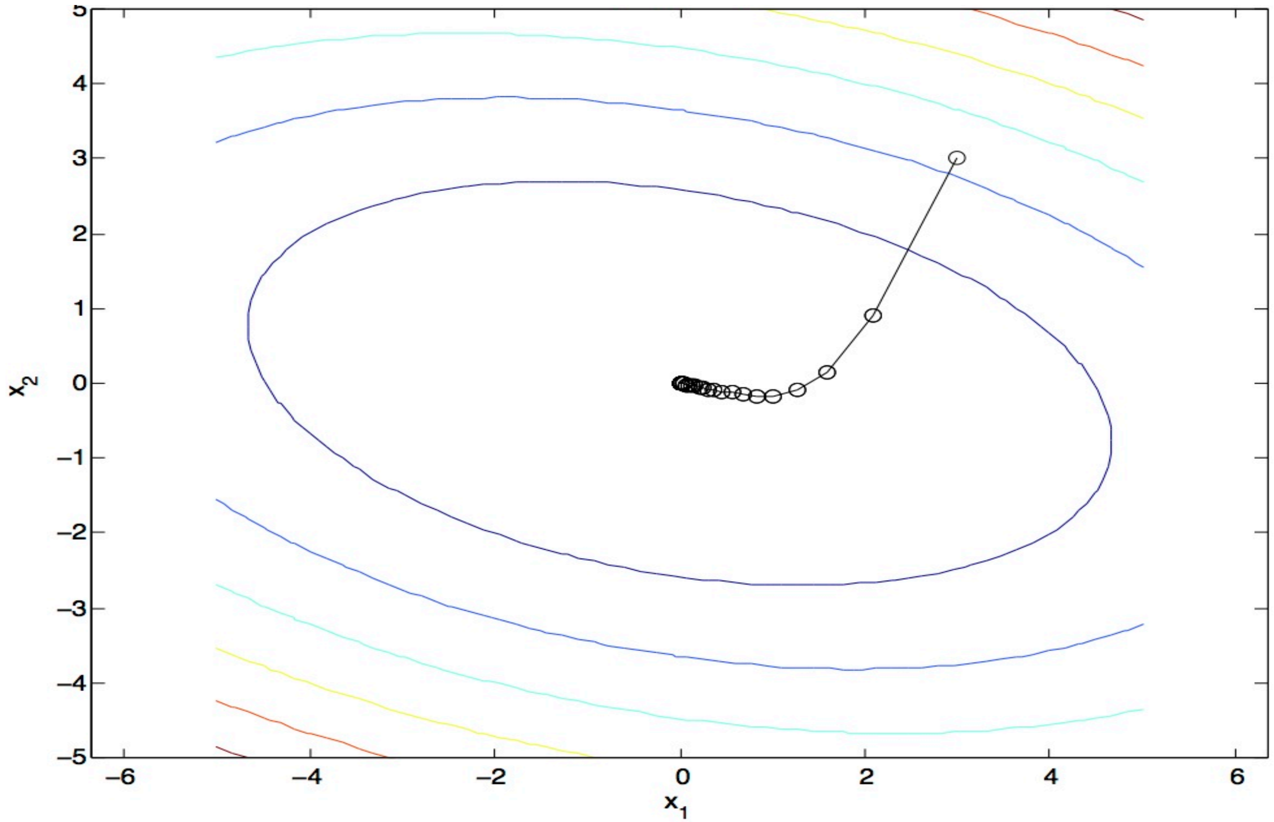
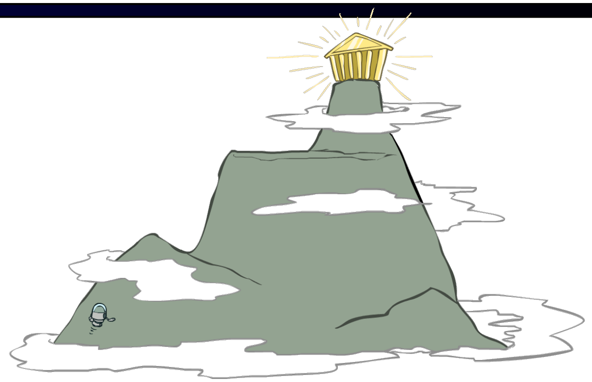


Figure source: Mathworks

What is the Steepest Direction?



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

- 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: $$\max_{\Delta:\Delta_1^2+\Delta_2^2\leq\varepsilon} \quad g(w) + \frac{\partial g}{\partial w_1}\Delta_1 + \frac{\partial g}{\partial w_2}\Delta_2$$
- Recall: $$\max_{\Delta:\|\Delta\|\leq\varepsilon} \Delta^\top a \quad \rightarrow \quad \Delta = \varepsilon\frac{a}{\|a\|}$$
- 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

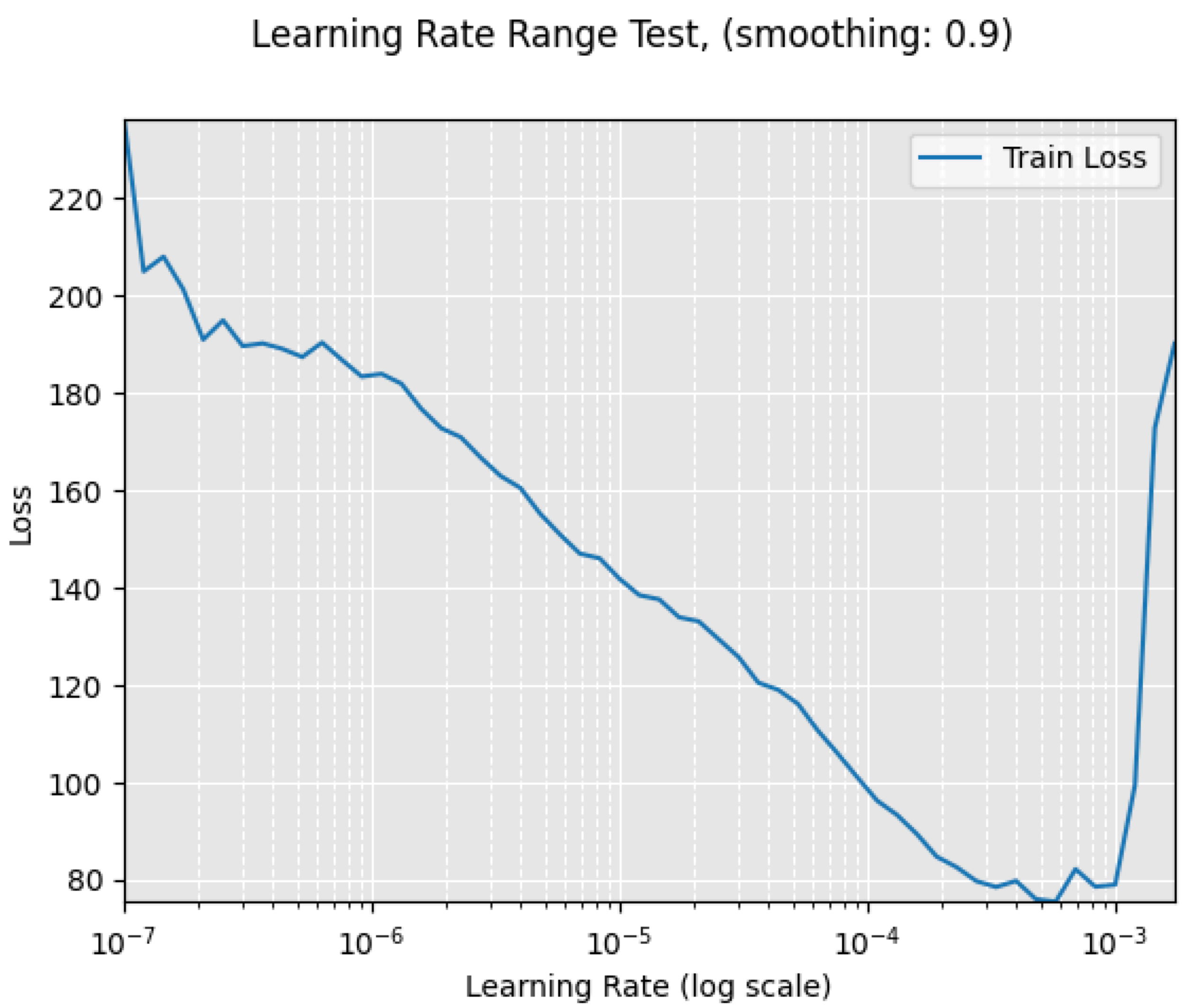
```
▪ init  w
▪ for iter = 1, 2, …
```

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

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

Learning Rate Finder

- Calculate a good learning rate by trying learning rates over a range of possible values
- Plot the training loss at each of these epochs
- Pick a learning rate where the loss is declining the most before it hits the minimum: 5x10^-5 - 3x10^-4



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

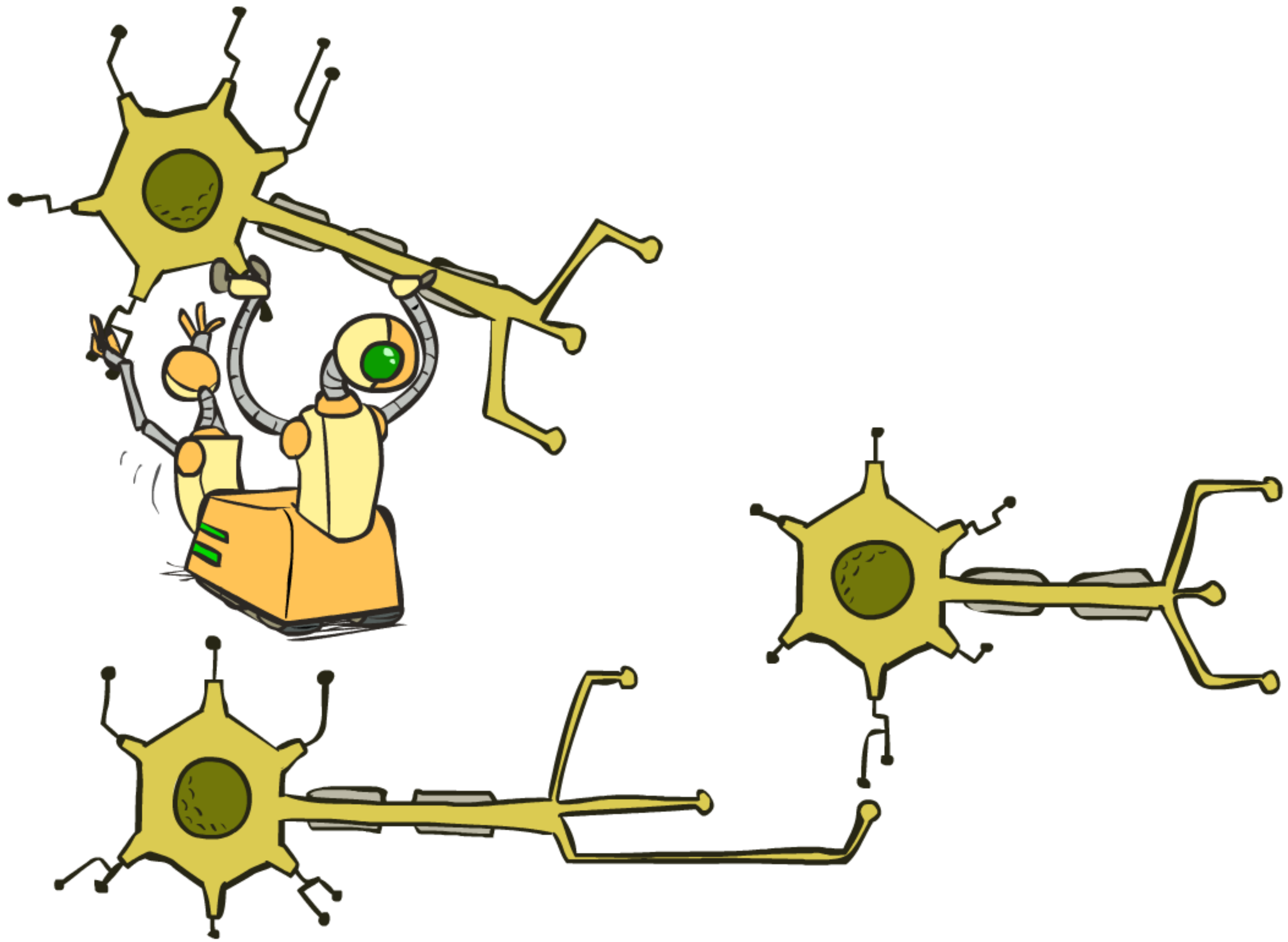
- init w
- for iter = 1, 2, …
  - pick random subset of training examples J

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

How about computing all the derivatives?

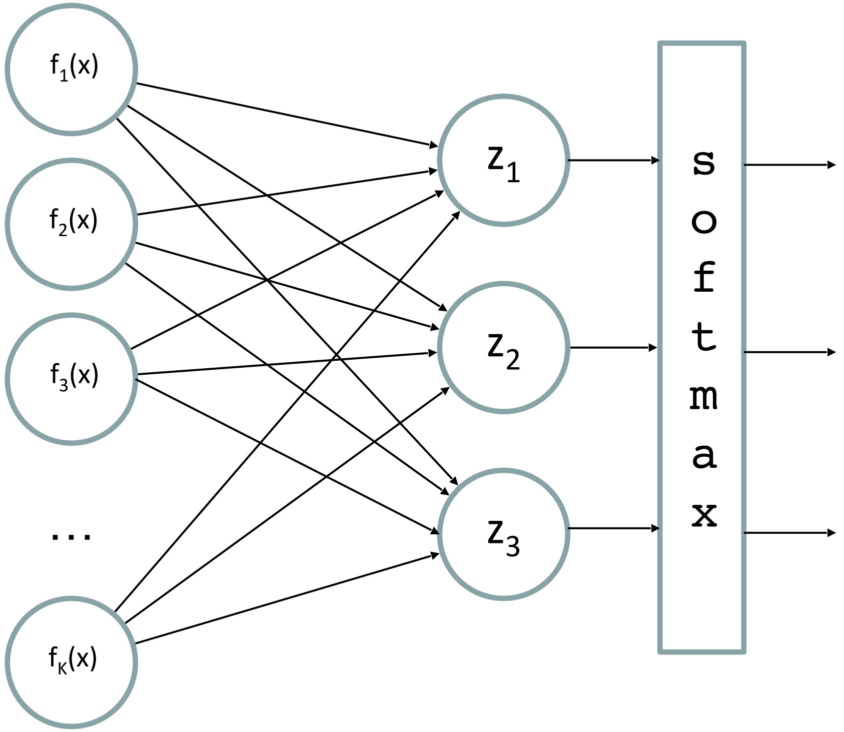
- We'll talk about that once we covered neural networks, which are a generalization of logistic regression

Neural Networks



Multi-class Logistic Regression

- = special case of neural network

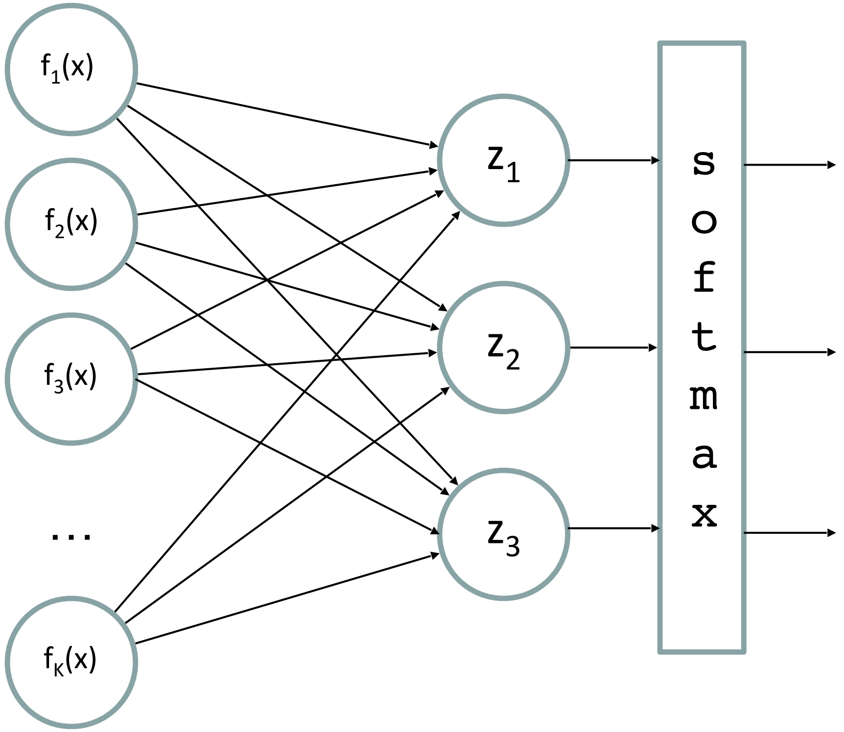


$$P(y_1|x;w) = \frac{e^{z_1}}{e^{z_1} + e^{z_2} + e^{z_3}}$$

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

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

Deep Neural Network = Also learn the features!



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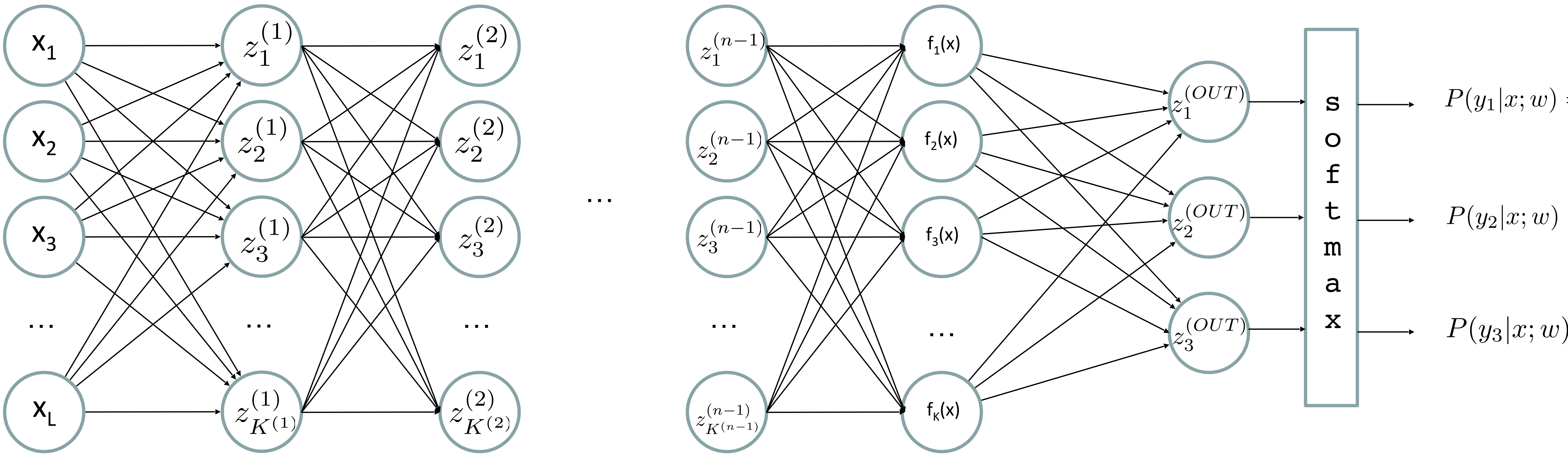
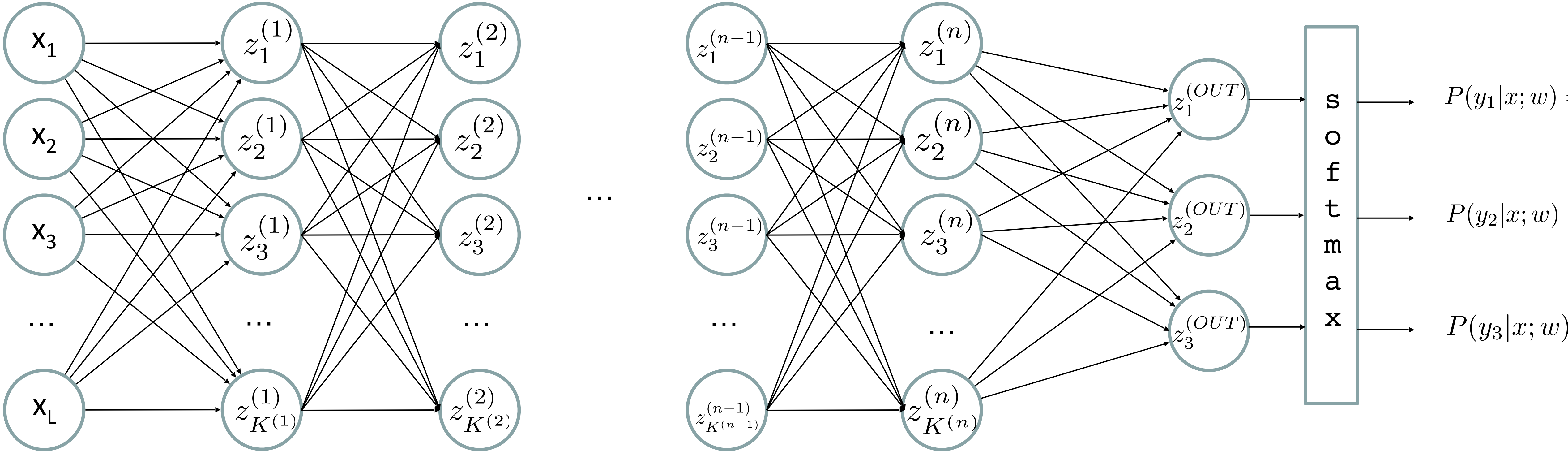
Deep Neural Network = Also learn the features!



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

g = nonlinear activation function

Deep Neural Network = Also learn the features!

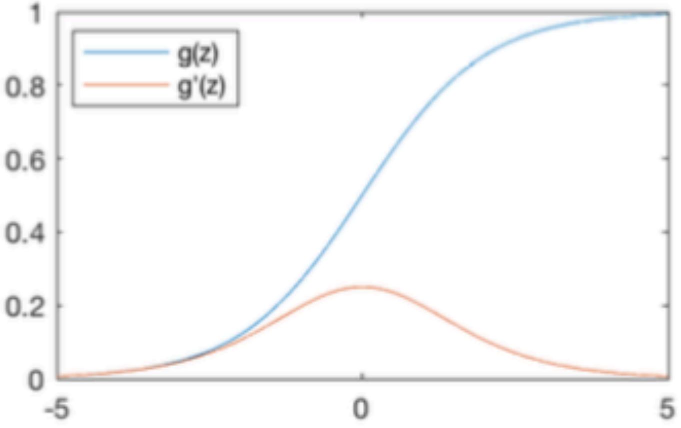


$$z_i^{(k)} = g\left(\sum_j W_{i,j}^{(k-1,k)} z_j^{(k-1)}\right)$$

g = nonlinear activation function

Common Activation Functions

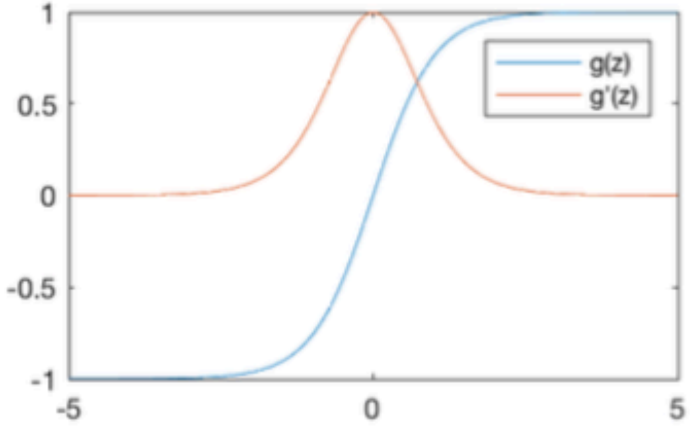
Sigmoid Function



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

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

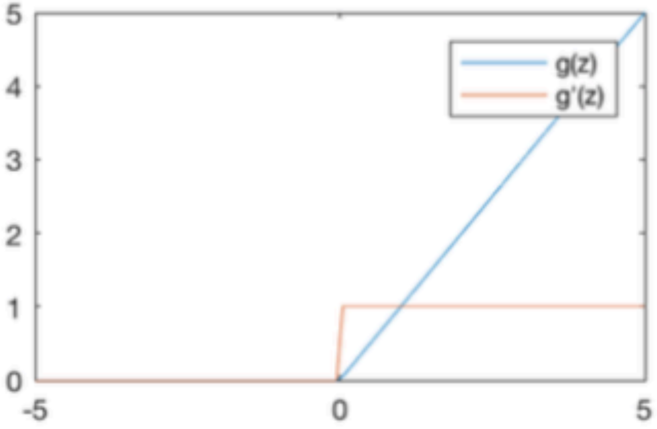
Hyperbolic Tangent



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

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

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:

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

- Much larger weight vector to learn
- Keep training (adjust weights with gradient ascent) until we meet our performance criteria or validation set performance starts decreasing

Neural Networks Properties

- Theorem (Universal Function Approximators). A two-layer neural network (input layer, hidden layer, and outputs) 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*

<u>**Hornik theorem 1:**</u> 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.

<u>**Hornik theorem 2:**</u> 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.

- <u>In words:</u> 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†

Abstract. In this paper we demonstrate that finite linear combinations of compositions of a fixed, univariate function and a set of affine functionals can uniformly approximate any continuous function of n real variables with support in the unit hypercube; only mild conditions are imposed on the univariate function. Our results settle an open question about representability in the class of single hidden layer neural networks. In particular, we show that arbitrary decision regions can be arbitrarily well approximated by continuous feedforward neural networks with only a single internal, hidden layer and any continuous sigmoidal nonlinearity. The paper discusses approximation properties of other possible types of nonlinearities that might be implemented by artificial neural networks.

Key words. Neural networks, Approximation, Completeness.

1. Introduction

A number of diverse application areas are concerned with the representation of general functions of an n-dimensional real variable, $x \in \mathbb{R}^n$, by finite linear combinations of the form

$$\sum_{j=1}^{N} \alpha_j \sigma(y_j^{\mathrm{T}} x + \theta_j), \tag{1}$$

where $y_j \in \mathbb{R}^n$ and $\alpha_j, \theta \in \mathbb{R}$ are fixed. (y^{T} is the transpose of y so that $y^{\mathrm{T}}x$ is the inner product of y and x.) Here the univariate function σ depends heavily on the context of the application. Our major concern is with so-called sigmoidal σ's:

$$\sigma(t) \to \begin{cases} 1 & \text{as} \quad t \to +\infty, \\ 0 & \text{as} \quad t \to -\infty. \end{cases}$$

Such functions arise naturally in neural network theory as the activation function of a neural node (or *unit* as is becoming the preferred term) [L1], [RHM]. The main result of this paper is a demonstration of the fact that sums of the form (1) are dense in the space of continuous functions on the unit cube if σ is any continuous sigmoidal

* Date received: October 21, 1988. Date revised: February 17, 1989. This research was supported in part by NSF Grant DCR-8619103, ONR Contract N000-86-G-0202 and DOE Grant DE-FG02-85ER25001.

† Center for Supercomputing Research and Development and Department of Electrical and Computer Engineering, University of Illinois, Urbana, Illinois 61801, U.S.A.

Neural Networks, Vol. 4, pp. 251–257, 1991

0893-6080/91 $3.00 + .00

ORIGINAL CONTRIBUTION

Approximation Capabilities of Multilayer Feedforward Networks

KURT HORNIK

Technische Universität Wien, Vienna, Austria

(*Received 30 January* 1990; *revised and accepted 25 October* 1990)

Abstract—*We show that standard multilayer feedforward networks with as few as a single hidden layer and arbitrary bounded and nonconstant activation function are universal approximators with respect to $L^p(\mu)$ performance criteria, for arbitrary finite input environment measures μ, provided only that sufficiently many hidden units are available. If the activation function is continuous, bounded and nonconstant, then continuous mappings can be learned uniformly over compact input sets. We also give very general conditions ensuring that networks with sufficiently smooth activation functions are capable of arbitrarily accurate approximation to a function and its derivatives.*

Keywords—Multilayer feedforward networks, Activation function, Universal approximation capabilities, Input environment measure, $L^p(\mu)$ approximation, Uniform approximation, Sobolev spaces, Smooth approximation.

1. INTRODUCTION

The approximation capabilities of neural network architectures have recently been investigated by many authors, including Carroll and Dickinson (1989), Cybenko (1989), Funahashi (1989), Gallant and White (1988), Hecht-Nielsen (1989), Hornik, Stinchcombe, and White (1989, 1990), Irie and Miyake (1988), Lapedes and Farber (1988), Stinchcombe and White (1989, 1990). (This list is by no means complete.)

If we think of the network architecture as a rule for computing values at l output units given values at k input units, hence implementing a class of mappings from R^k to R^l, we can ask how well arbitrary mappings from R^k to R^l can be approximated by the network, in particular, if as many hidden units as required for internal representation and computation may be employed.

How to measure the accuracy of approximation depends on how we measure closeness between functions, which in turn varies significantly with the specific problem to be dealt with. In many applications, it is necessary to have the network perform *simultaneously* well on all input samples taken from some compact input set X in R^k. In this case, closeness is measured by the uniform distance between functions on X, that is,

$$\rho_{\mu,X}(f, g) = \sup_{x \in X} |f(x) - g(x)|.$$

In other applications, we think of the inputs as random variables and are interested in the *average performance* where the average is taken with respect to the input environment measure μ, where $\mu(R^k) < \infty$. In this case, closeness is measured by the $L^p(\mu)$ distances

$$\rho_{p,\mu}(f, g) = \left[\int_{R^k} |f(x) - g(x)|^p \, d\mu(x) \right]^{1/p},$$

$1 \le p < \infty$, the most popular choice being $p = 2$, corresponding to mean square error.

Of course, there are many more ways of measuring closeness of functions. In particular, in many applications, it is also necessary that the *derivatives* of the approximating function implemented by the network closely resemble those of the function to be approximated, up to some order. This issue was first taken up in Hornik et al. (1990), who discuss the sources of need of smooth functional approximation in more detail. Typical examples arise in robotics (learning of smooth movements) and signal processing (analysis of chaotic time series); for a recent application to problems of nonparametric inference in statistics and econometrics, see Gallant and White (1989).

All papers establishing certain approximation ca-

Requests for reprints should be sent to Kurt Hornik, Institut für Statistik und Wahrscheinlichkeitstheorie, Technische Universität Wien, Wiedner Hauptstraße 8-10/107, A-1040 Wien, Austria.

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

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Fun Neural Net Demo Site

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

How about computing all the derivatives?

- Derivatives tables:

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

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

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

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

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

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

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

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

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

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

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

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

$$\frac{d}{dx}\left[\log_a u\right]=\log_a e\frac{1}{u}\frac{du}{dx}$$

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

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

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

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

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

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

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

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

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

[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

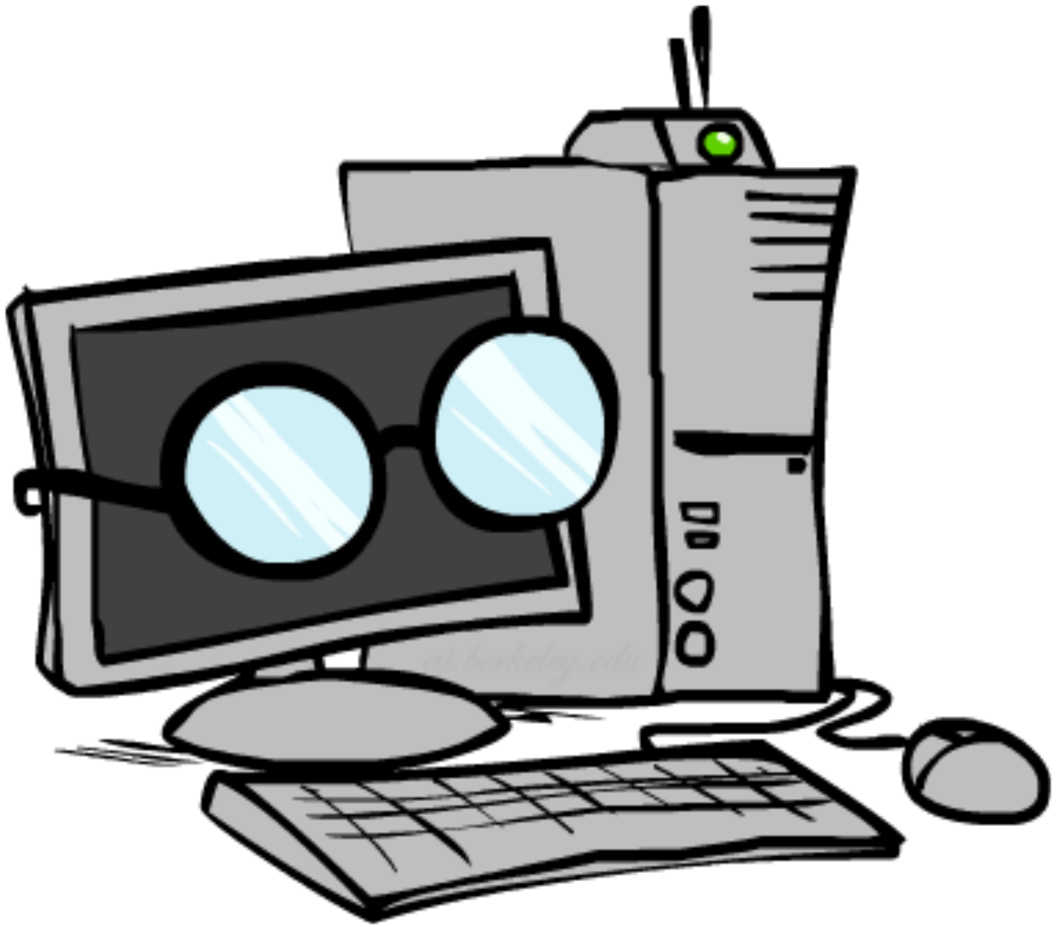
- Optimize probability of label given input $\max_w \; ll(w) = \max_w \; \sum_i \log P(y^{(i)}|x^{(i)};w)$

- 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")

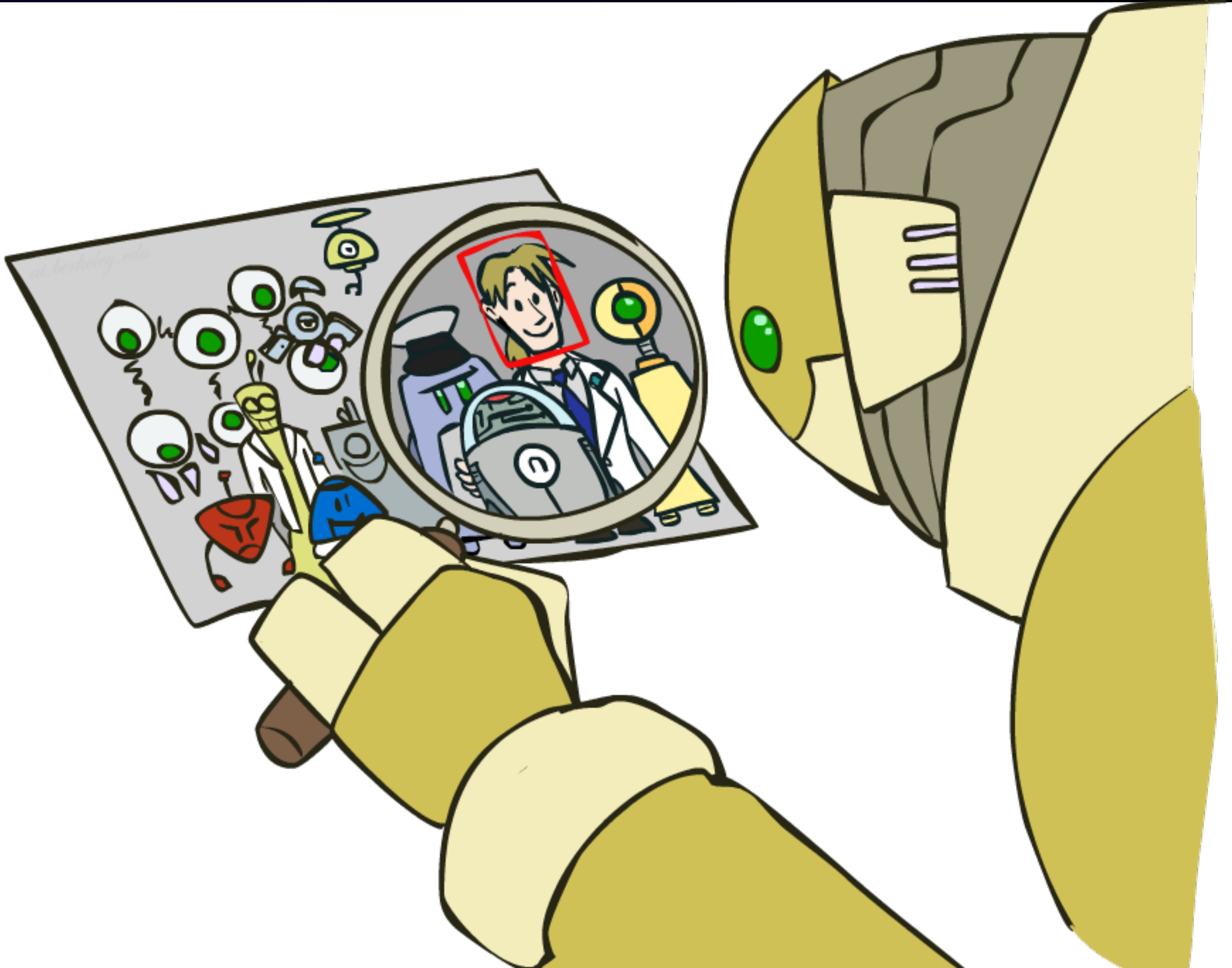
- Deep neural nets
  - Last layer = still logistic regression
  - Now also many more layers before this last layer
    - = computing the features
    - → the features are learned rather than hand-designed
  - Universal function approximation theorem
    - `If` neural net is large enough
    - `Then`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

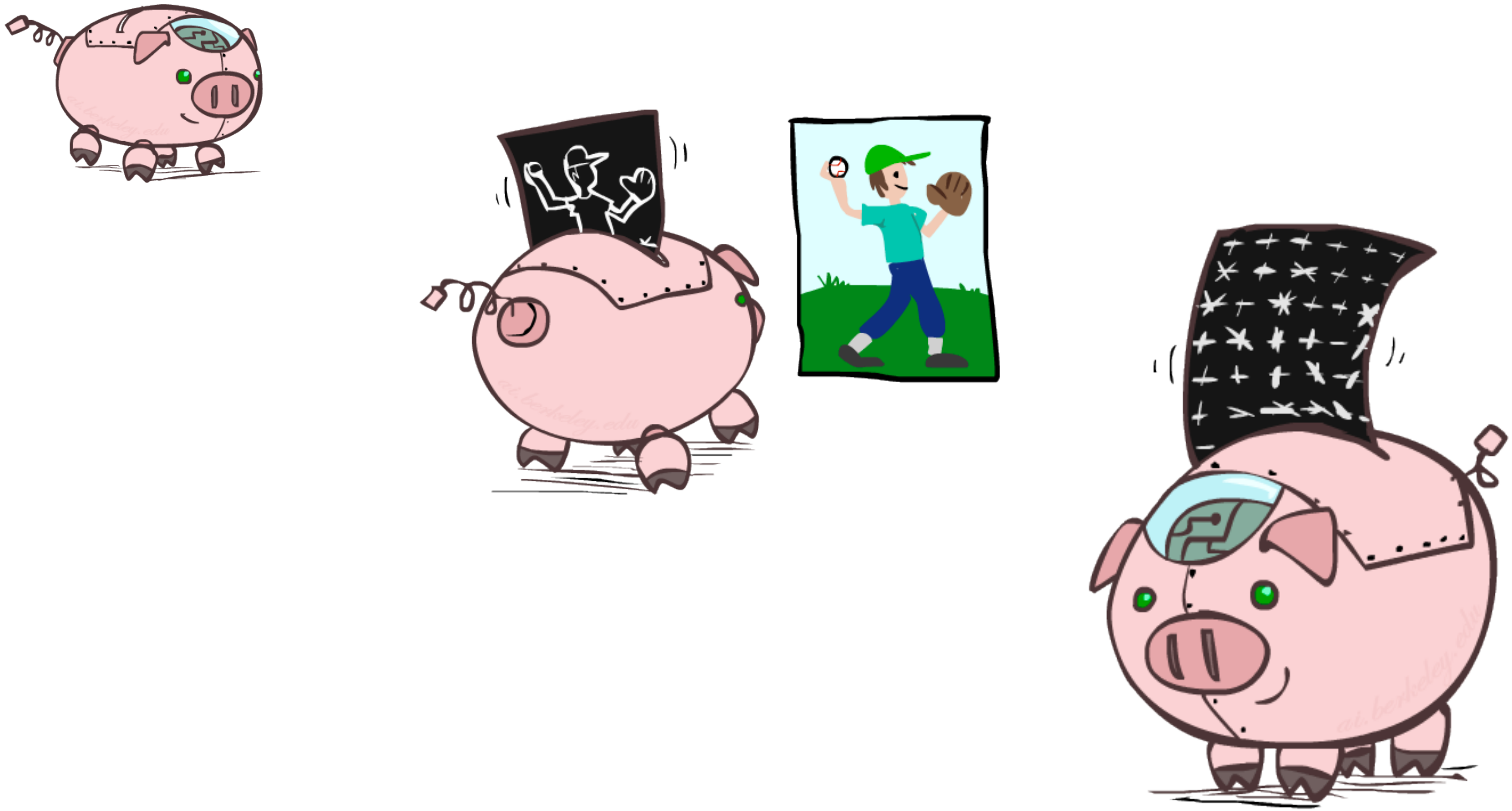
Computer Vision



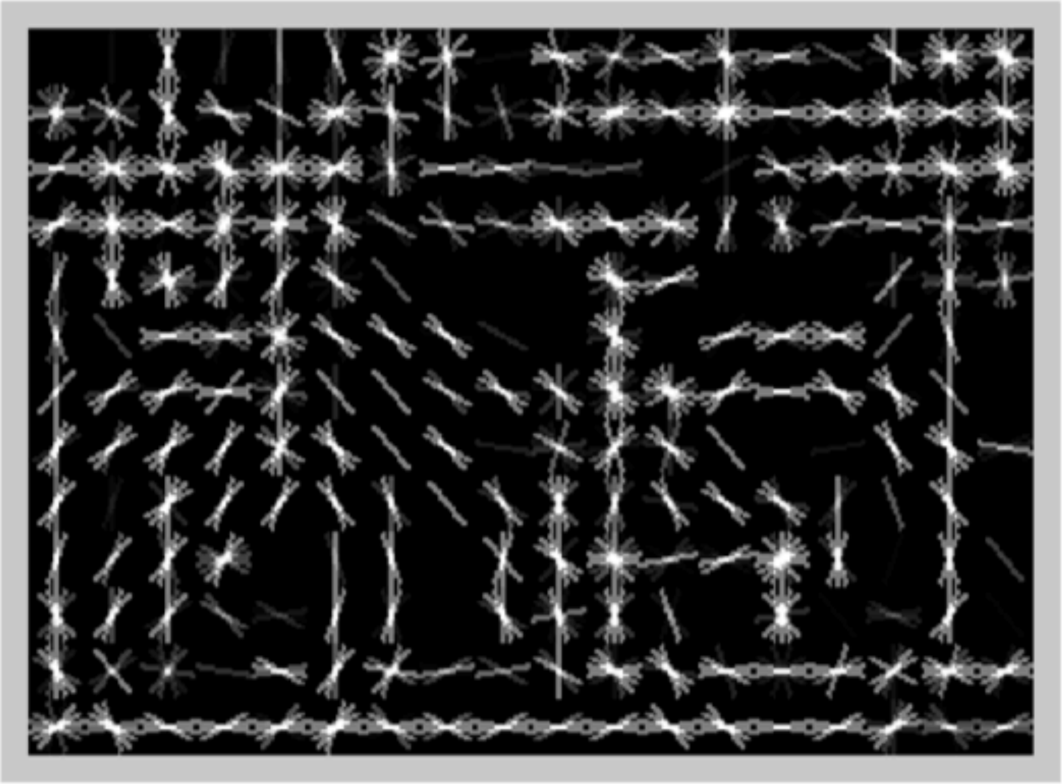
Object Detection



Manual Feature Design



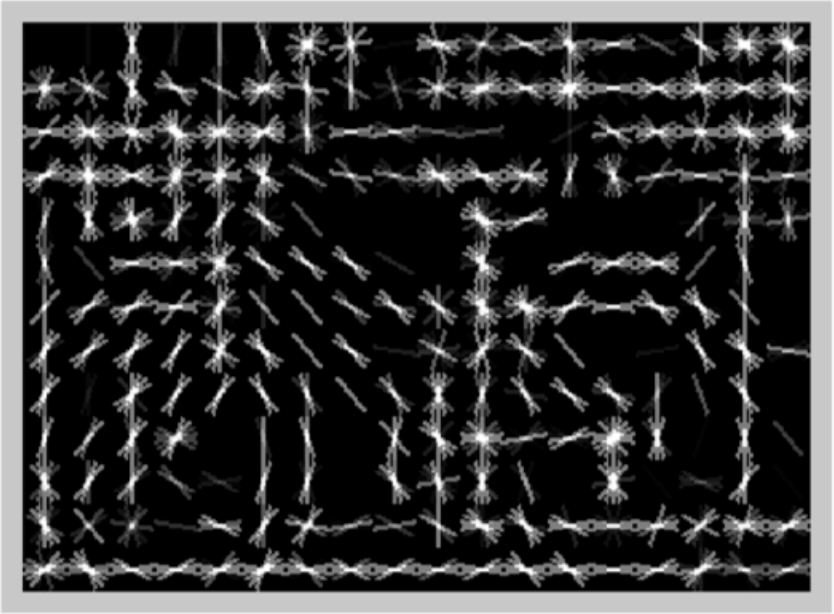
Features and Generalization



[HoG: Dalal and Triggs, 2005]

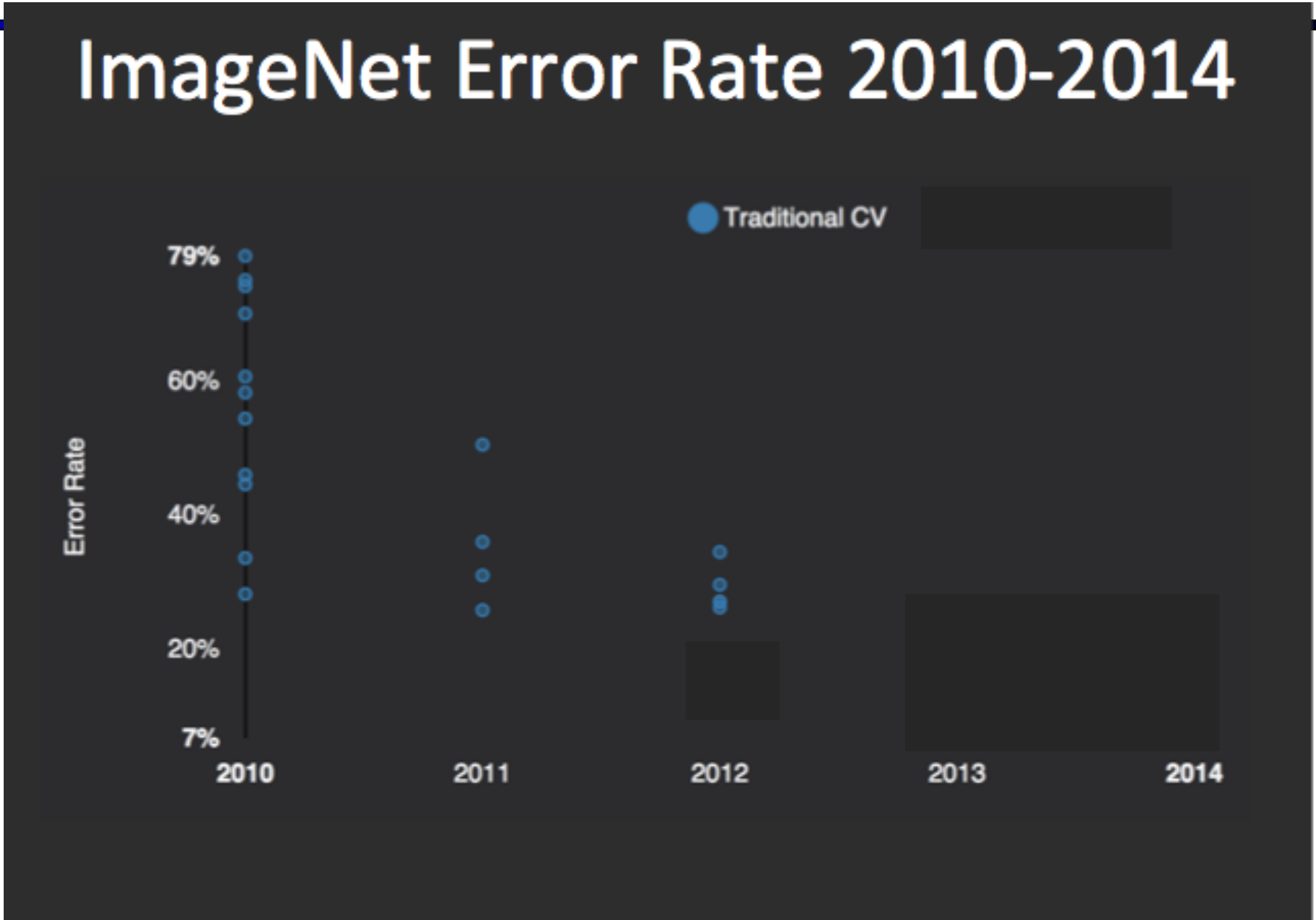
Features and Generalization

Image



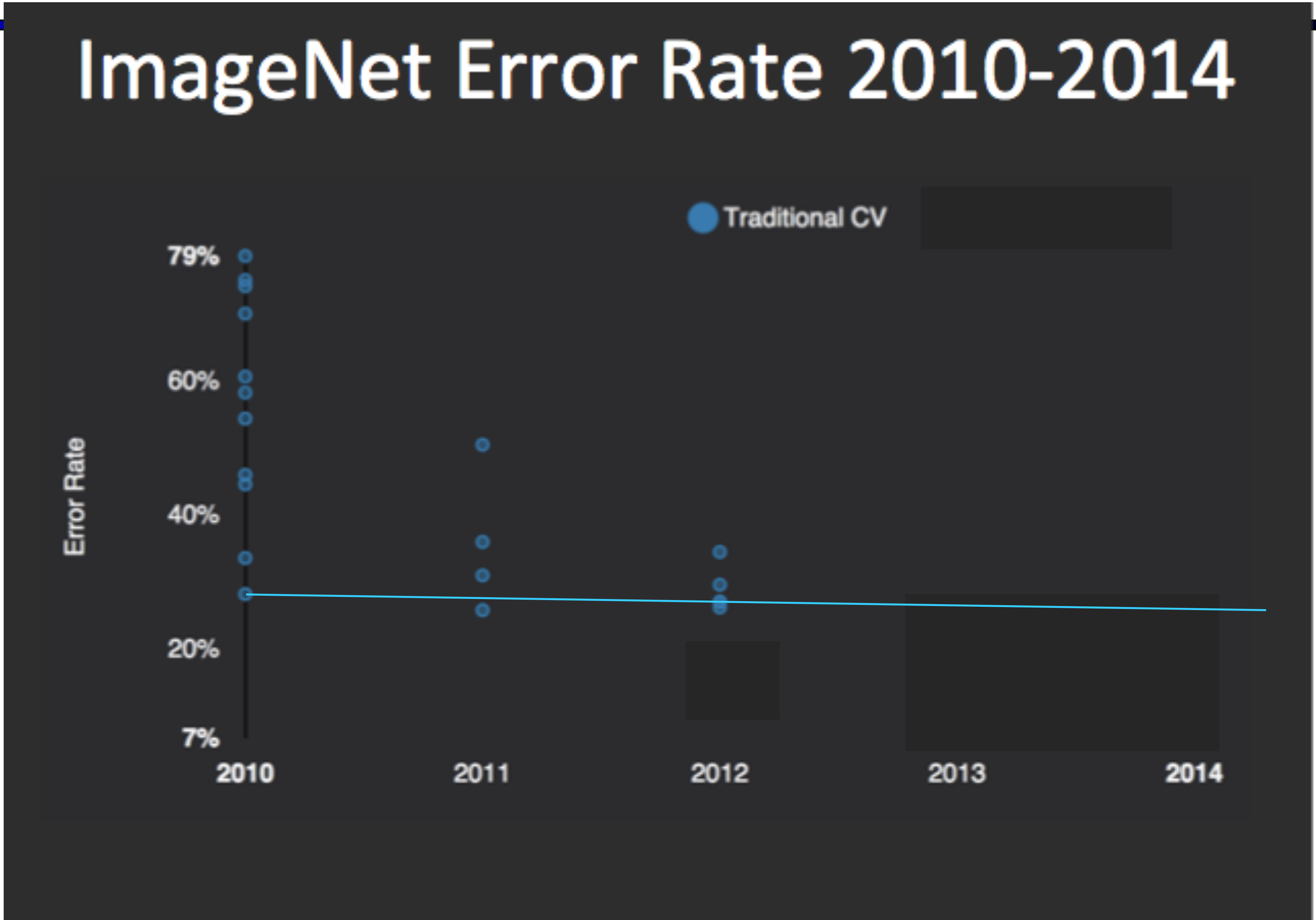
HoG

Performance



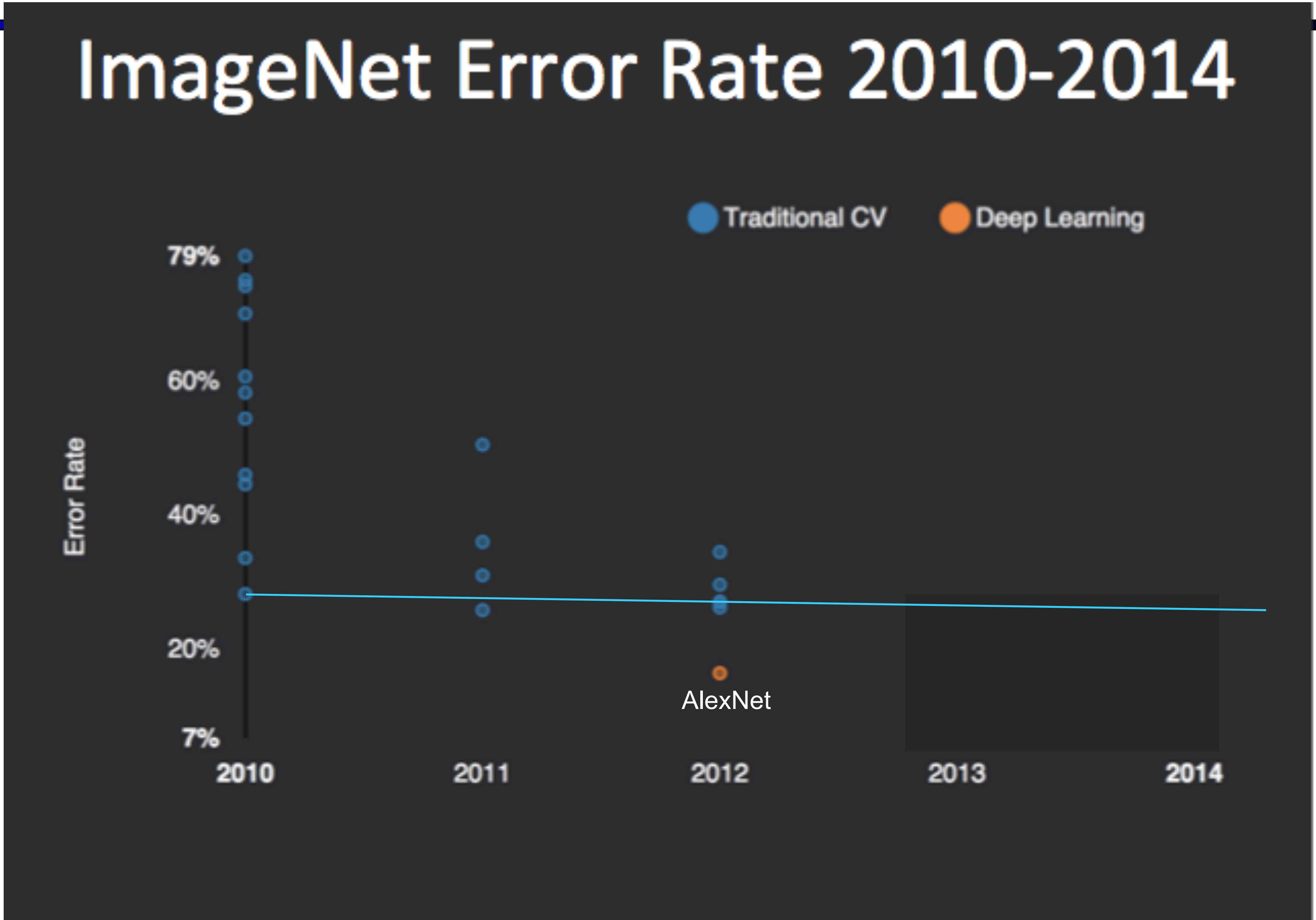
graph credit Matt Zeiler, Clarifai

Performance



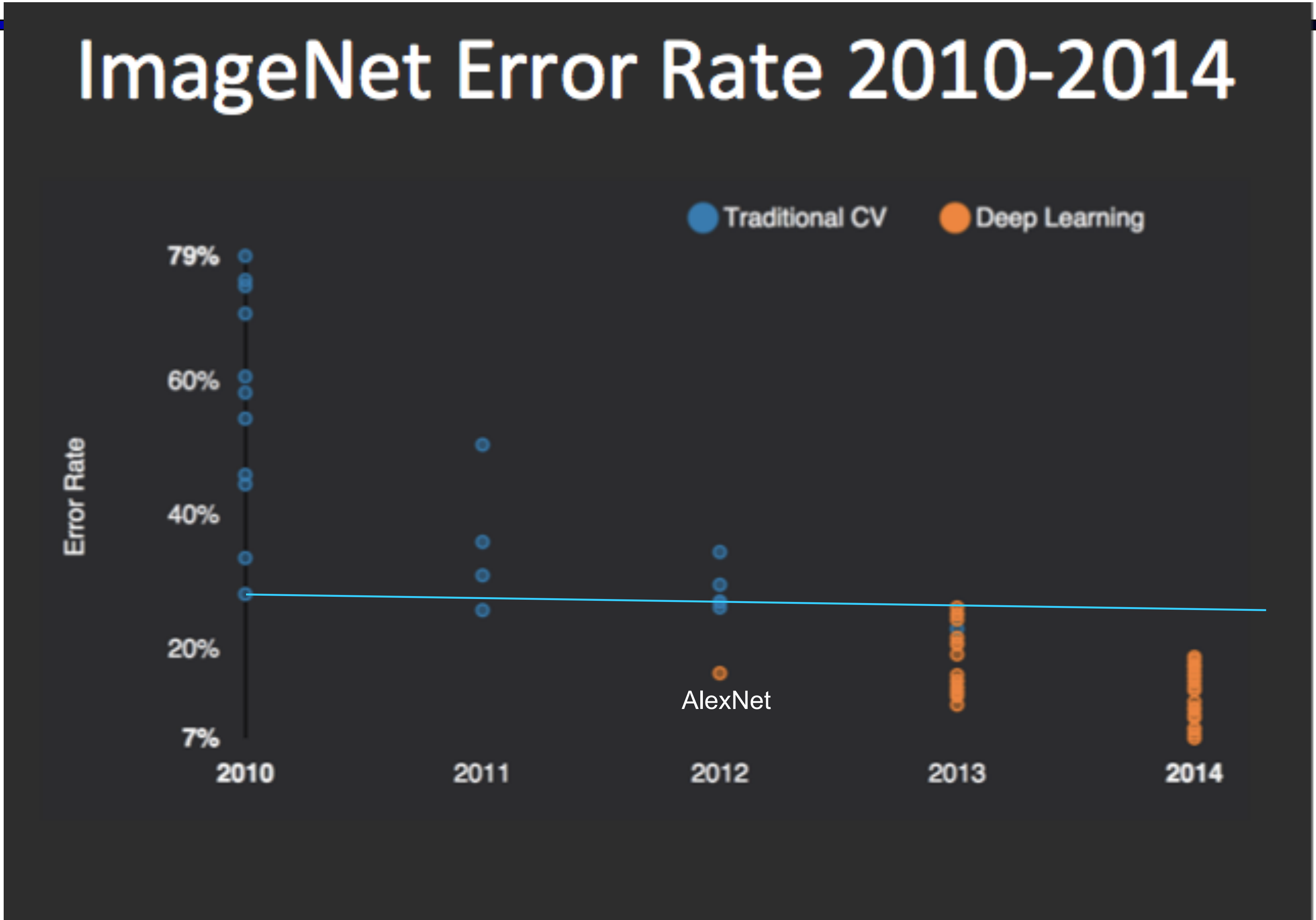
graph credit Matt Zeiler, Clarifai

Performance



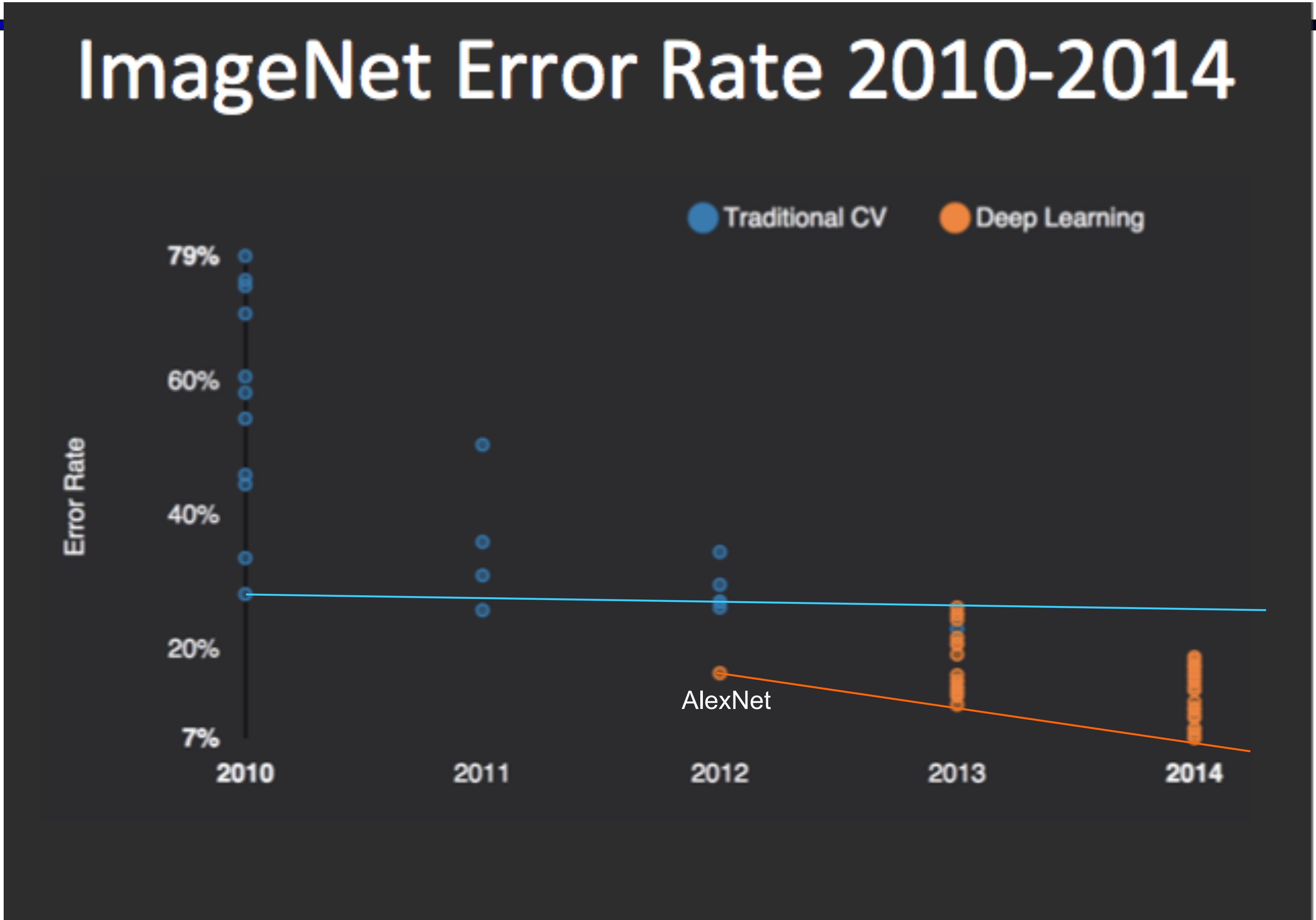
graph credit Matt Zeiler, Clarifai

Performance



graph credit Matt Zeiler, Clarifai

Performance



graph credit Matt Zeiler, Clarifai

Next Lectures

- Neural Net Applications wrap-up
- Formalizing Learning
- Decision Trees
- Thursday: Transformers