CPSC 340: Machine Learning and Data Mining

More Deep Learning

Fall 2021

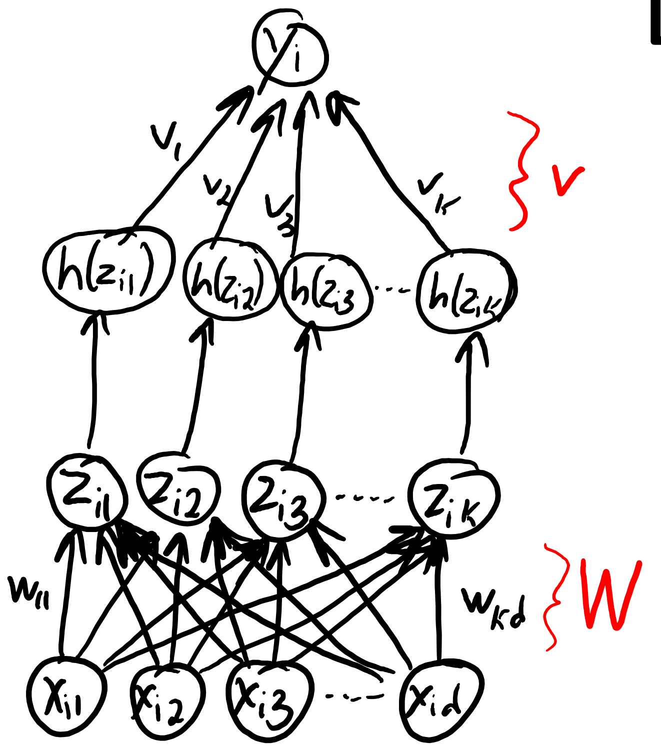
Admin

- Course surveys
  - Please fill them out
  - We care deeply about your education, so we take them very seriously
  - You will be able to evaluate the class overall, and then Mijung and I separately
  - Please use the text boxes to also let us know about the “lecture specialization experiment” [where we each specialized in half the lectures]
  - As always, please remember we’re real people, so both praise and critical feedback are great. Please avoid personal, hurtful, or unconstructive negative comments.

- A6 out: due April 8 (our last class)

Last Time: Deep Learning

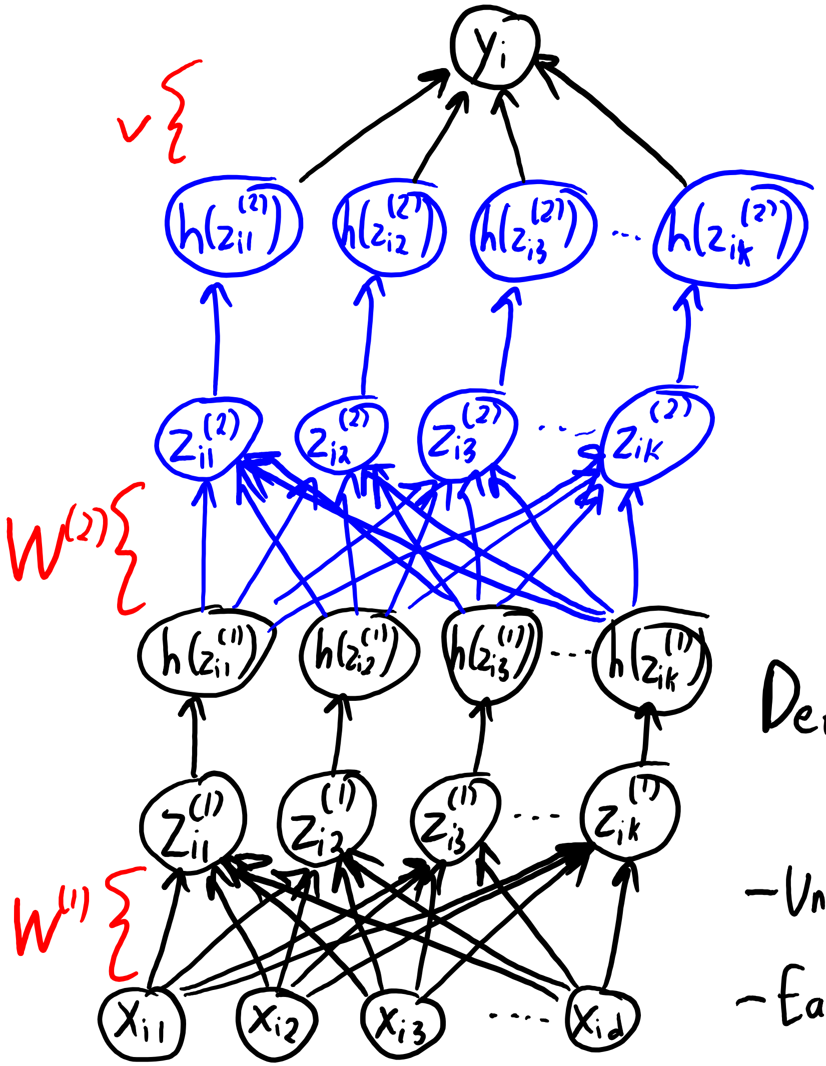
Neural network:

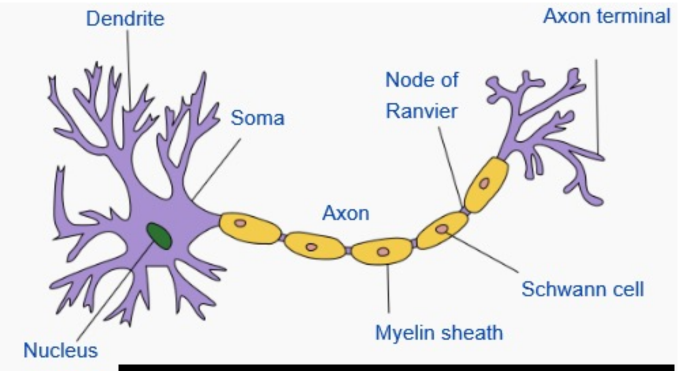


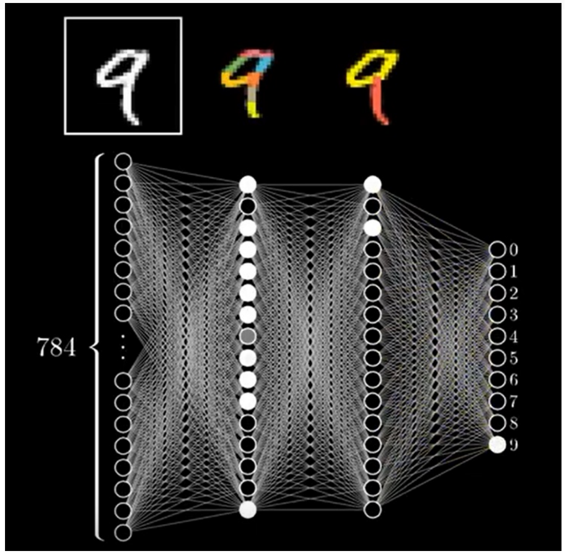
$$y_i = v^T h(Wx_i)$$

Learn 'W' and 'v' together.

- learn features for supervised learning.
- Non-linear 'h' makes it a universal approximator for large 'K'







Deep neural networks:

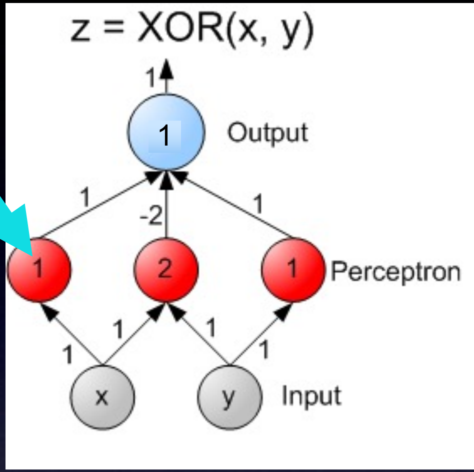
$$y_i = v^T h(W^{(2)} h(W^{(1)} x_i))$$

- Unprecedented performance on difficult problems.
- Each layer combines "parts" from previous layer.

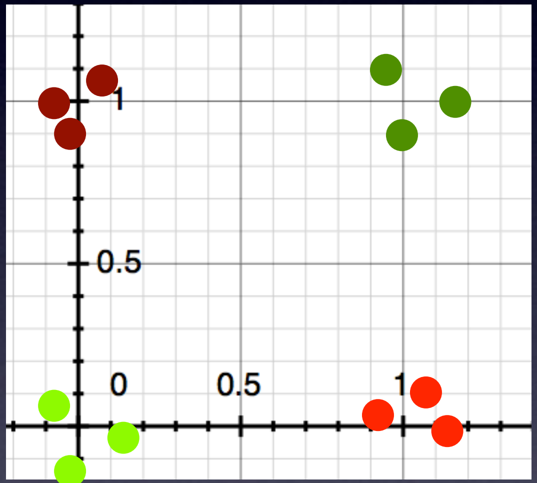
https://en.wikipedia.org/wiki/Neuron
https://www.youtube.com/watch?v=aircAruvnKk

Neural Networks

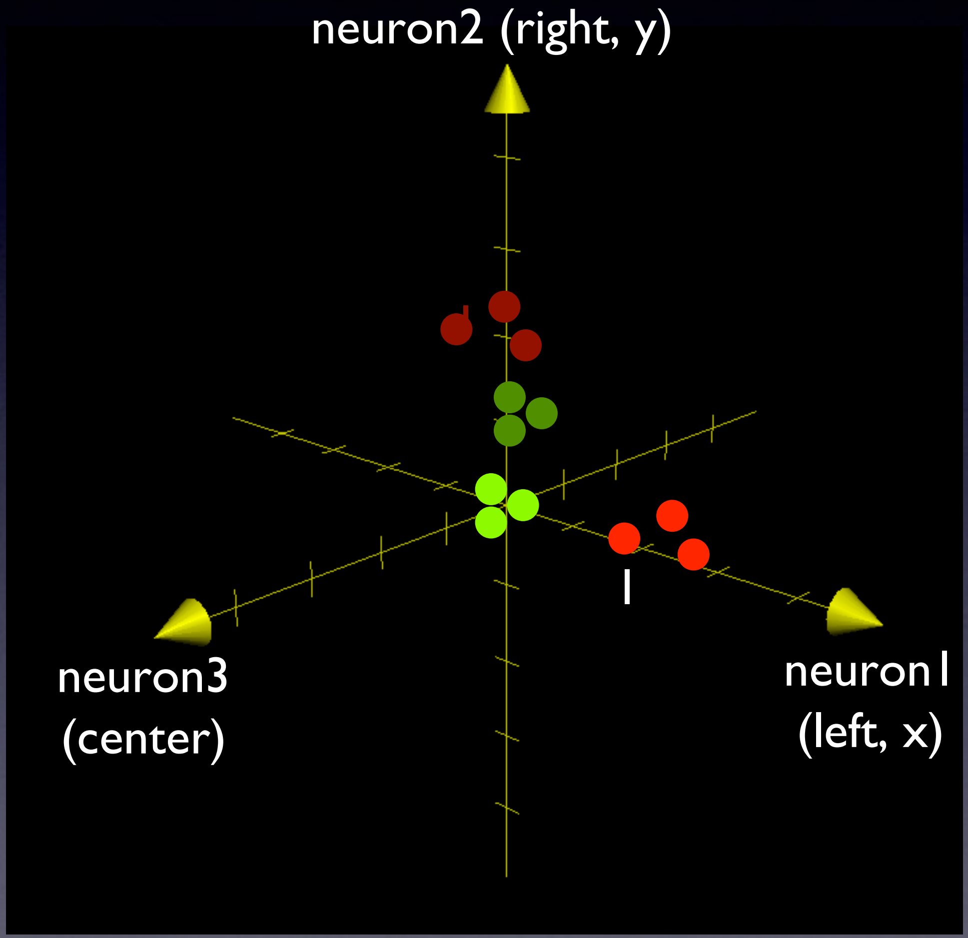
Outputs 1 if >= number in node



2D



Non-Linear Mapping



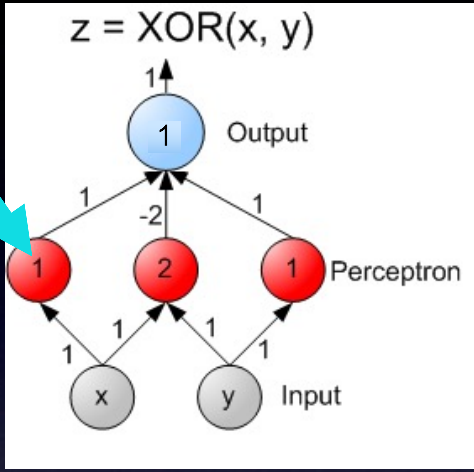
3D

x	y	Left	Center	Right	Output
1	1				
1	0				
0	1				
0	0				

Outputs of each node

Neural Networks

Outputs 1 if >= number in node



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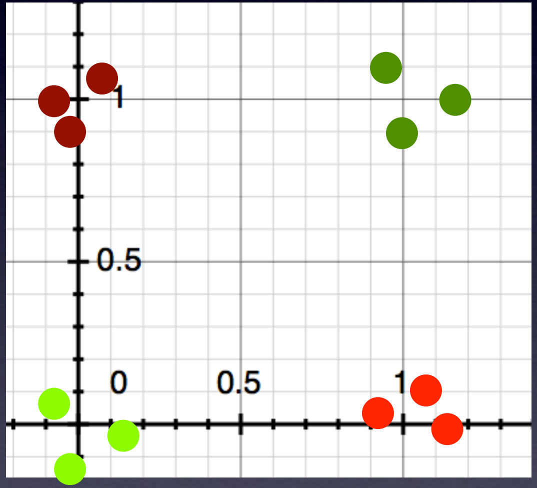

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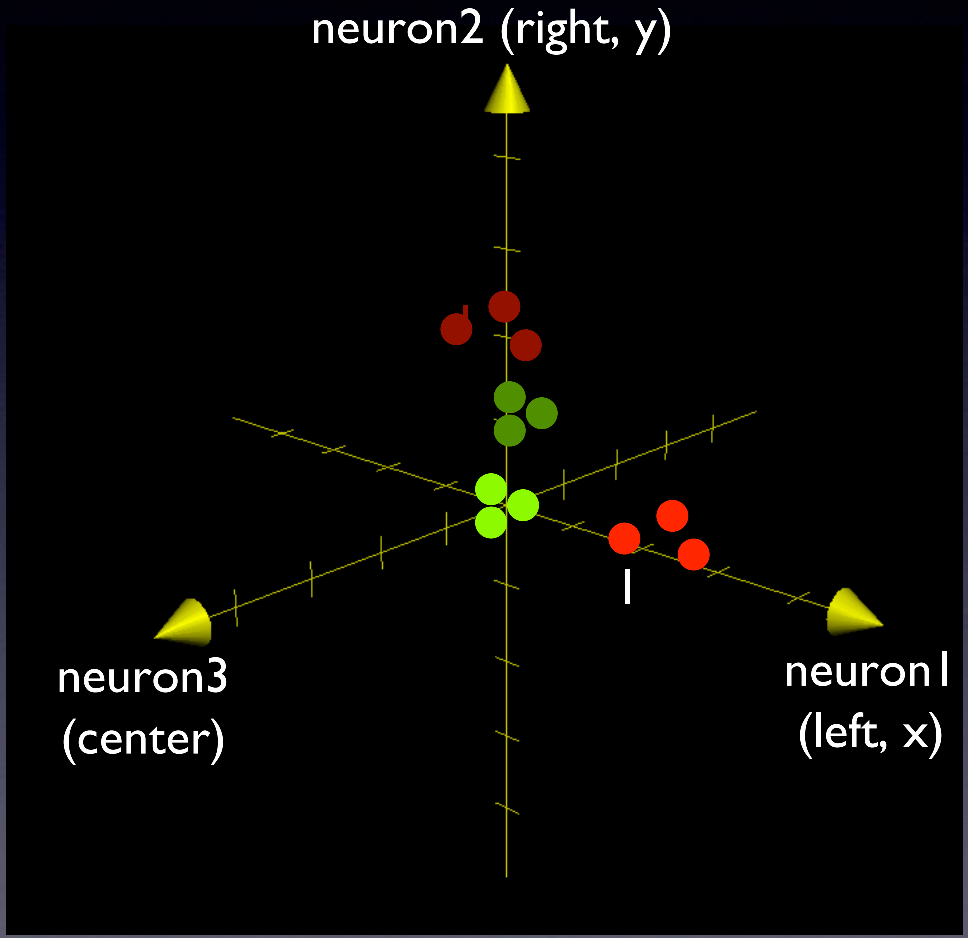
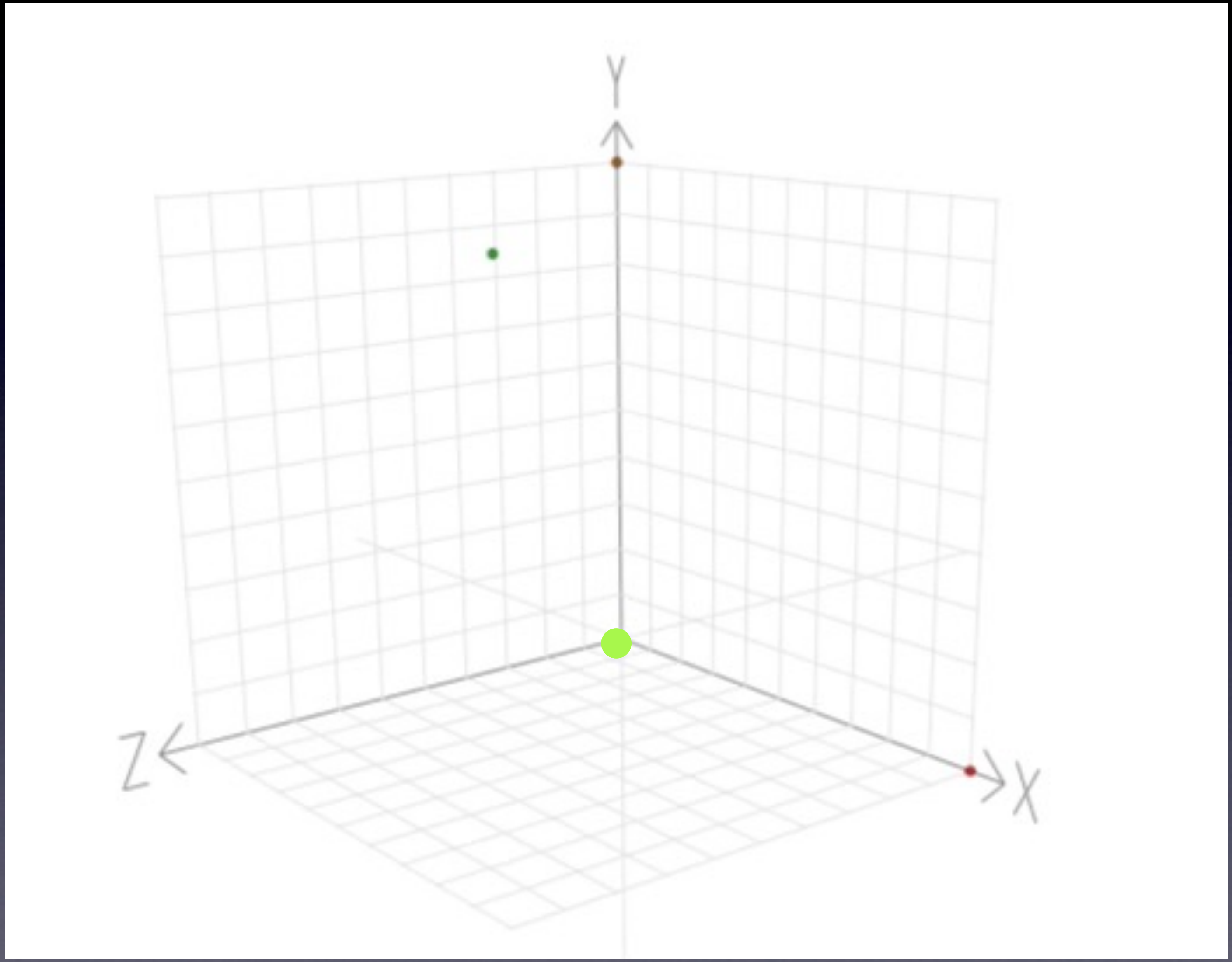


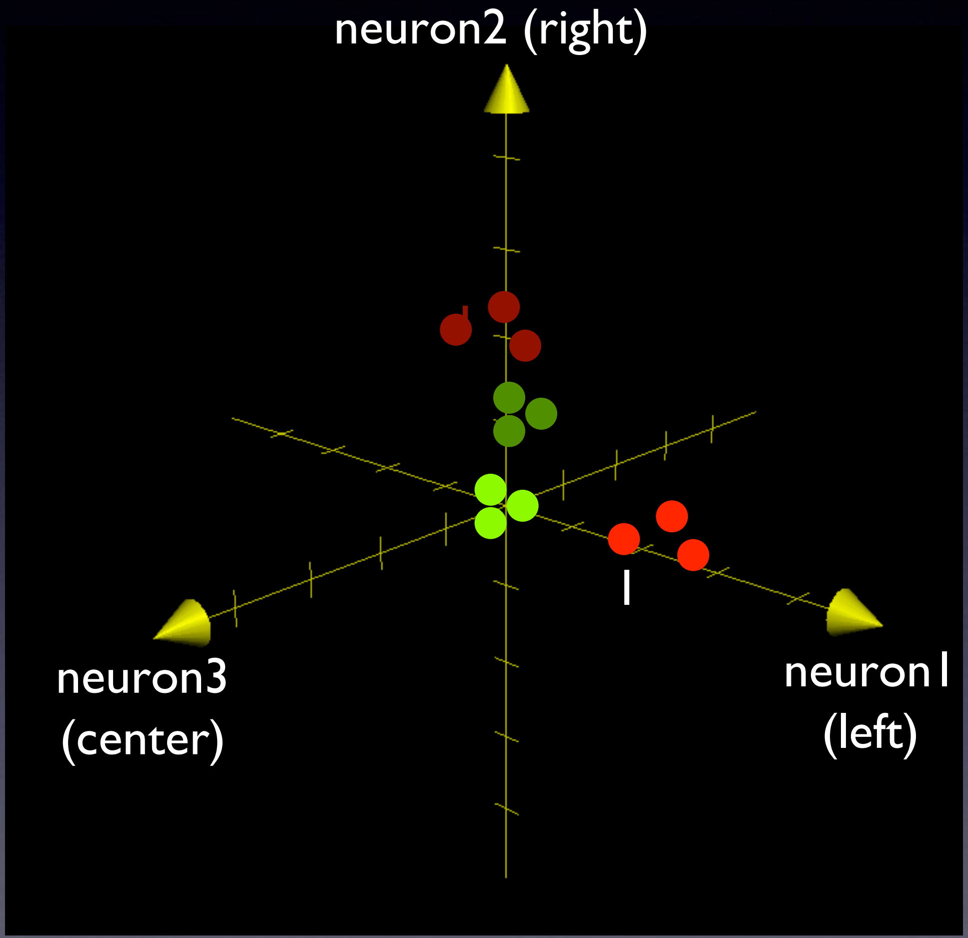
3D

Outputs of each node

x	y	Left	Center	Right	Output
1	1	1	1	1	0
1	0	1	0	0	1
0	1	0	0	1	1
0	0	0	0	0	0

Neural Networks





3D

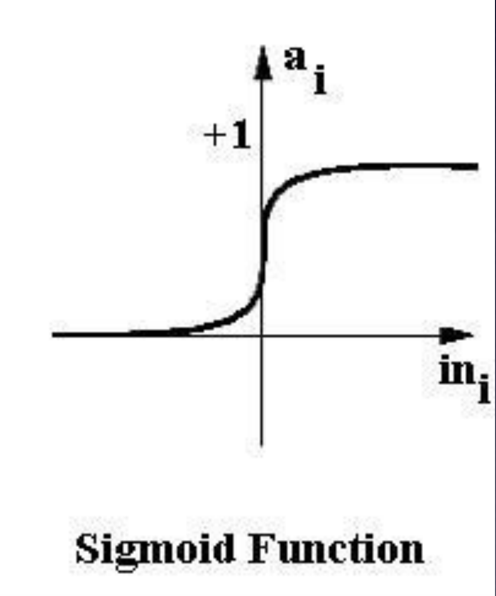
Neural Networks

- Cover's theorem: "The probability that classes are linearly separable increases when the features are nonlinearly mapped to a higher dimensional feature space." [Coover 1965]
- The output layer requires linear separability.
- The purpose of the hidden layers is to make the problem linearly separable!

From: http://130.236.96.13/edu/courses/TBMI26/pdfs/lectures/le5.pdf

Neural Networks

- Multi-layer networks thus allow “non-linear regression”



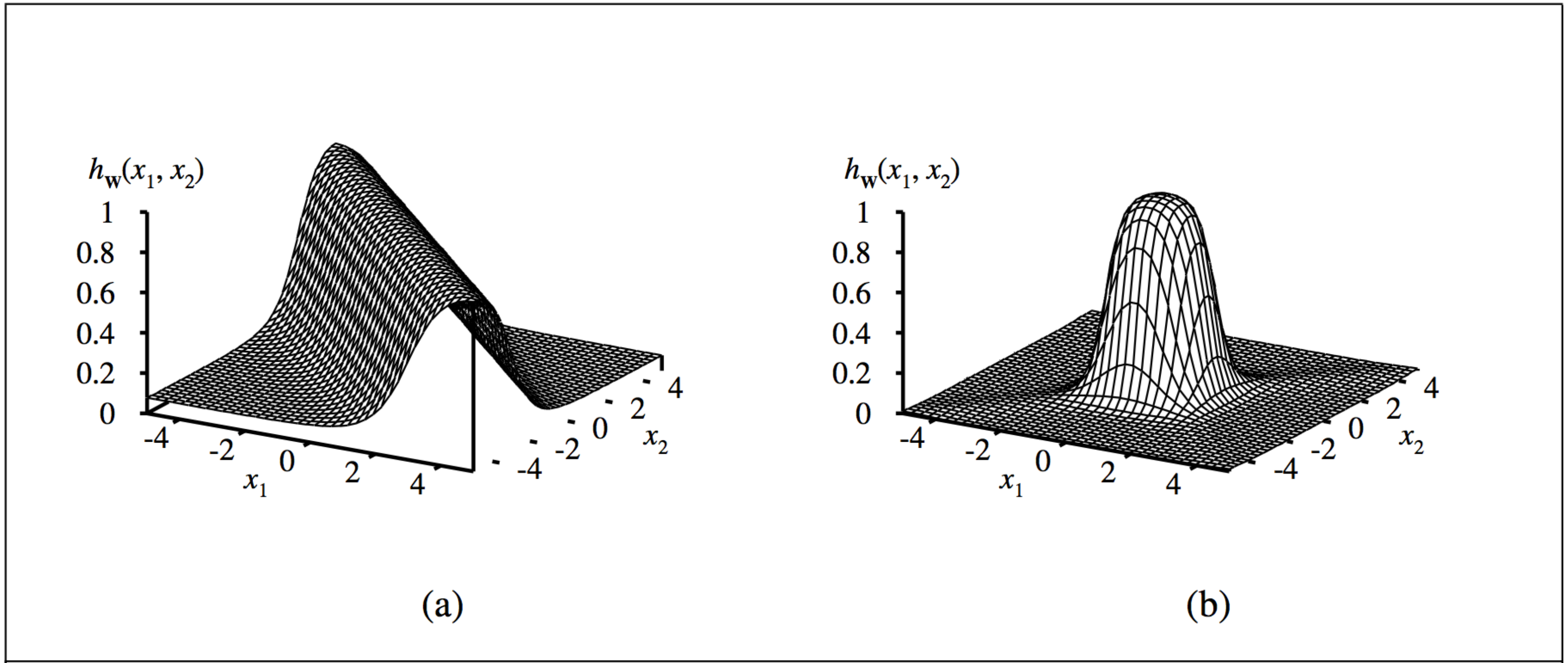


Figure 18.23 (a) The result of combining two opposite-facing soft threshold functions to produce a ridge. (b) The result of combining two ridges to produce a bump.

Neural Networks

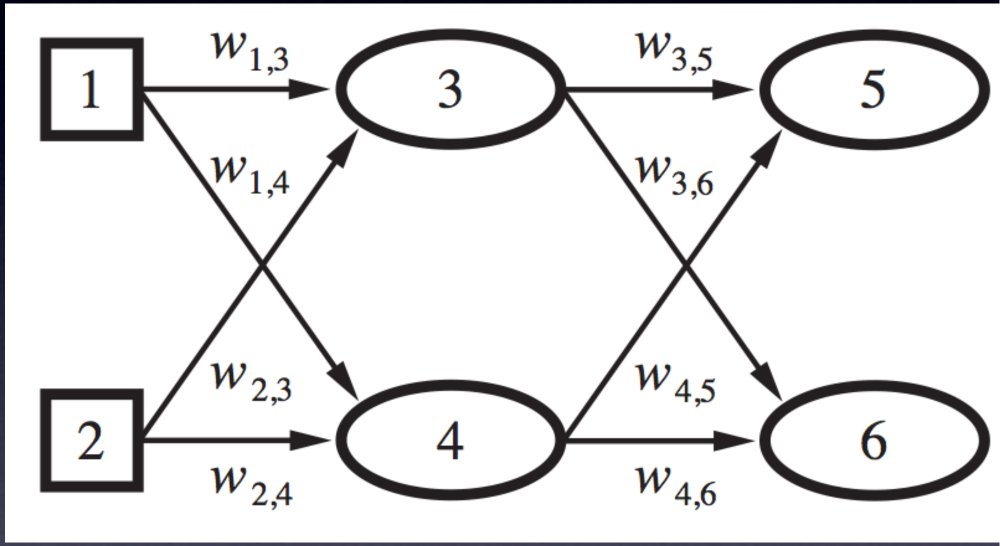
- Multi-layer networks thus allow “non-linear regression”
- Single hidden layer (often very large):
  - can represent any continuous function
- Two hidden layers:
  - can represent any discontinuous function

Neural Networks

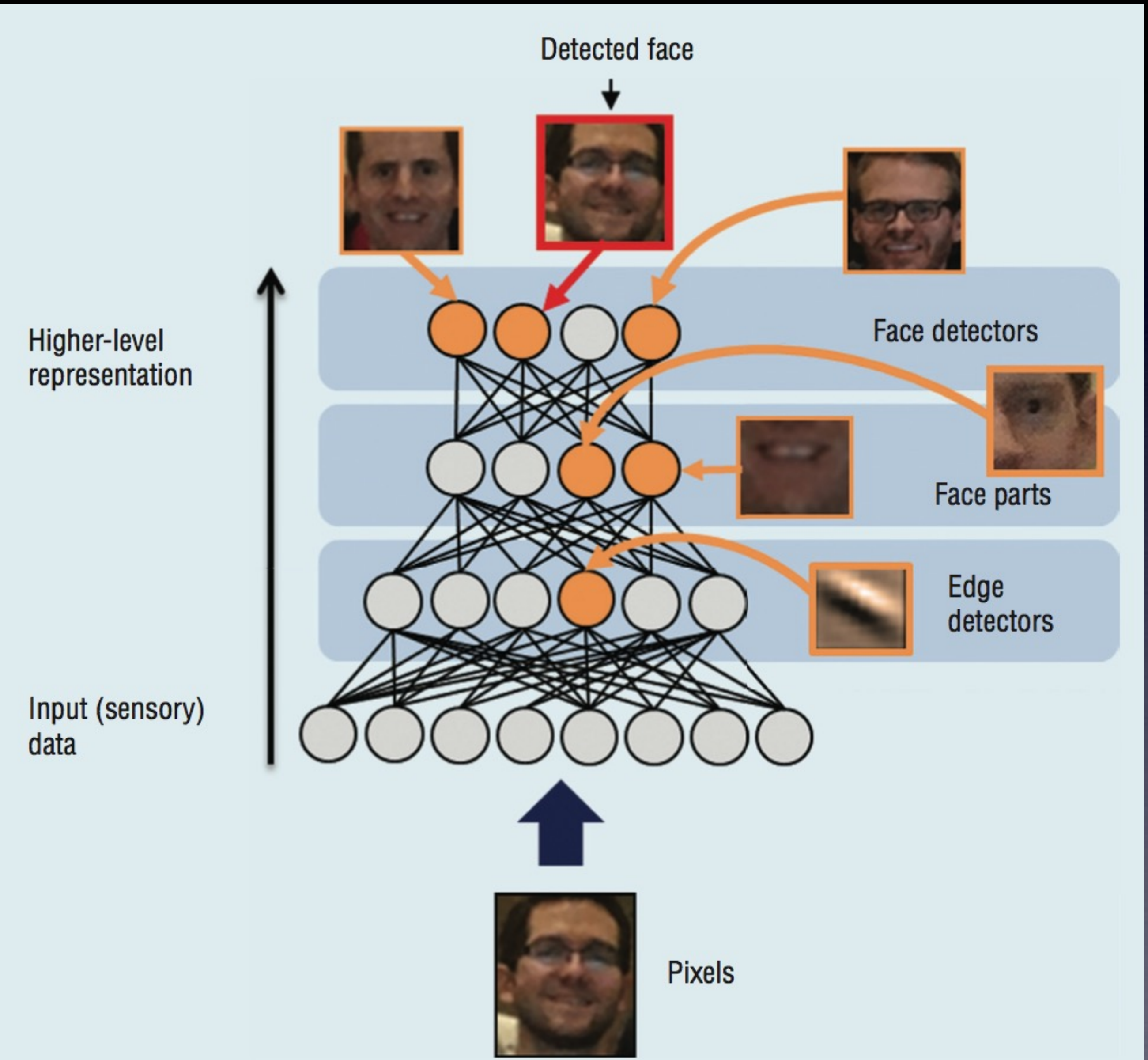
- Multi-layer networks thus allow “non-linear regression”
- Single hidden layer (often very large):
  - can represent any continuous function
- Two hidden layers:
  - can represent any discontinuous function
- But how do we train them?

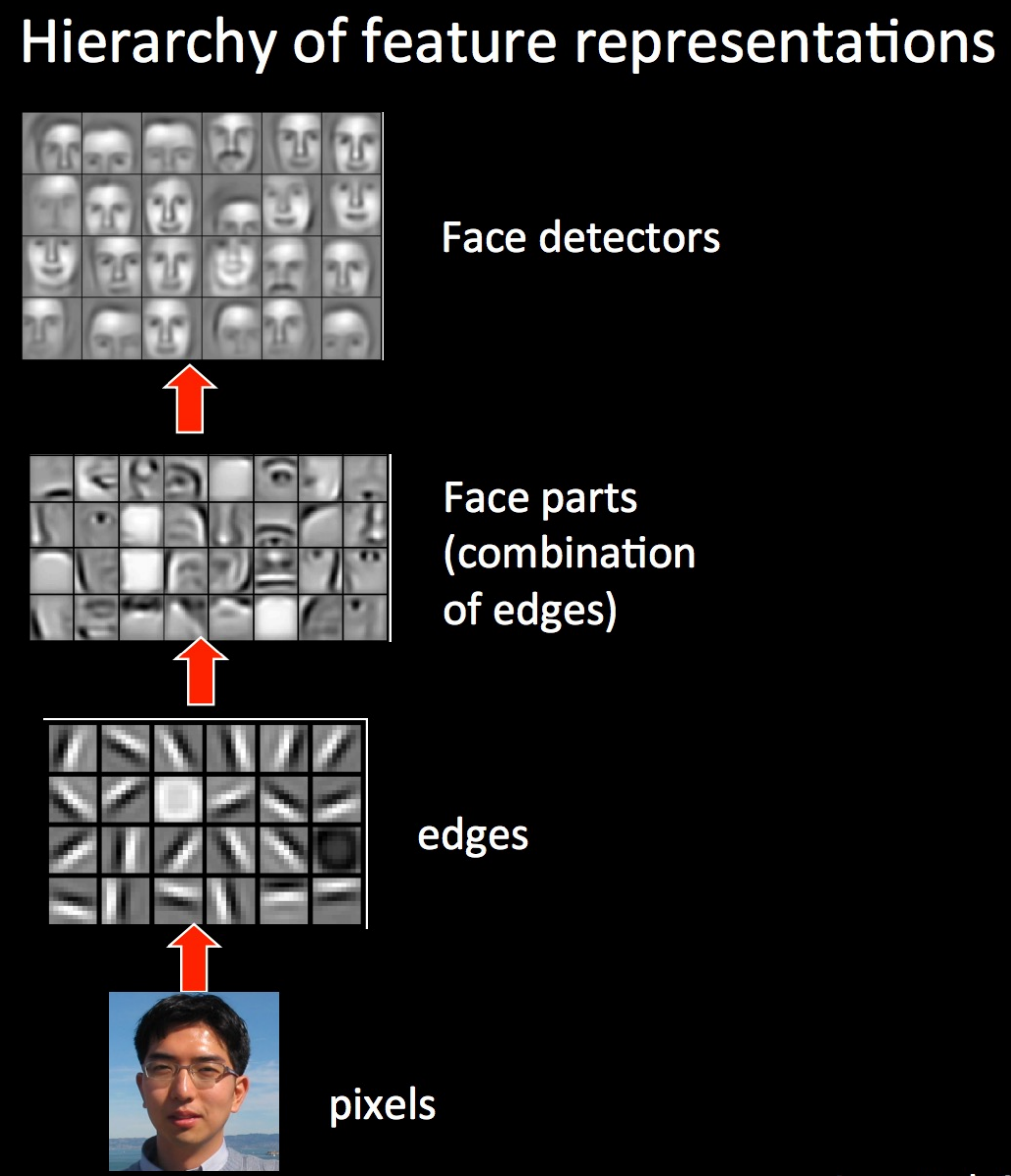
Training Multi-Layer Neural Networks

- General Idea: Propagate the error backwards
- Called Backpropagation



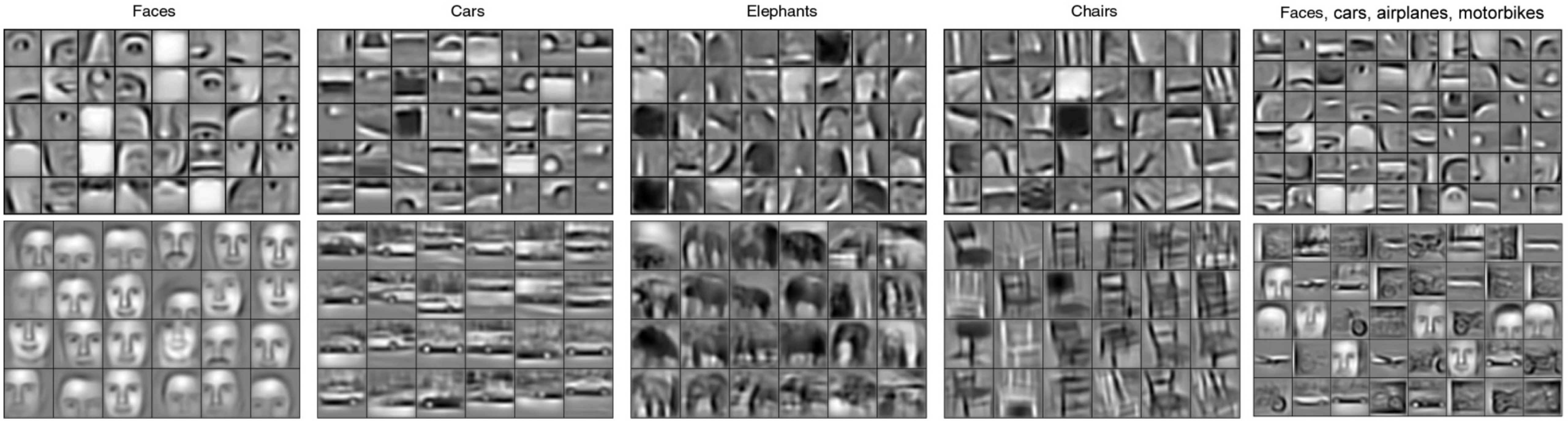
Hierarchically composed feature representations





Lee et al, 2009.

Learning features relevant to the data

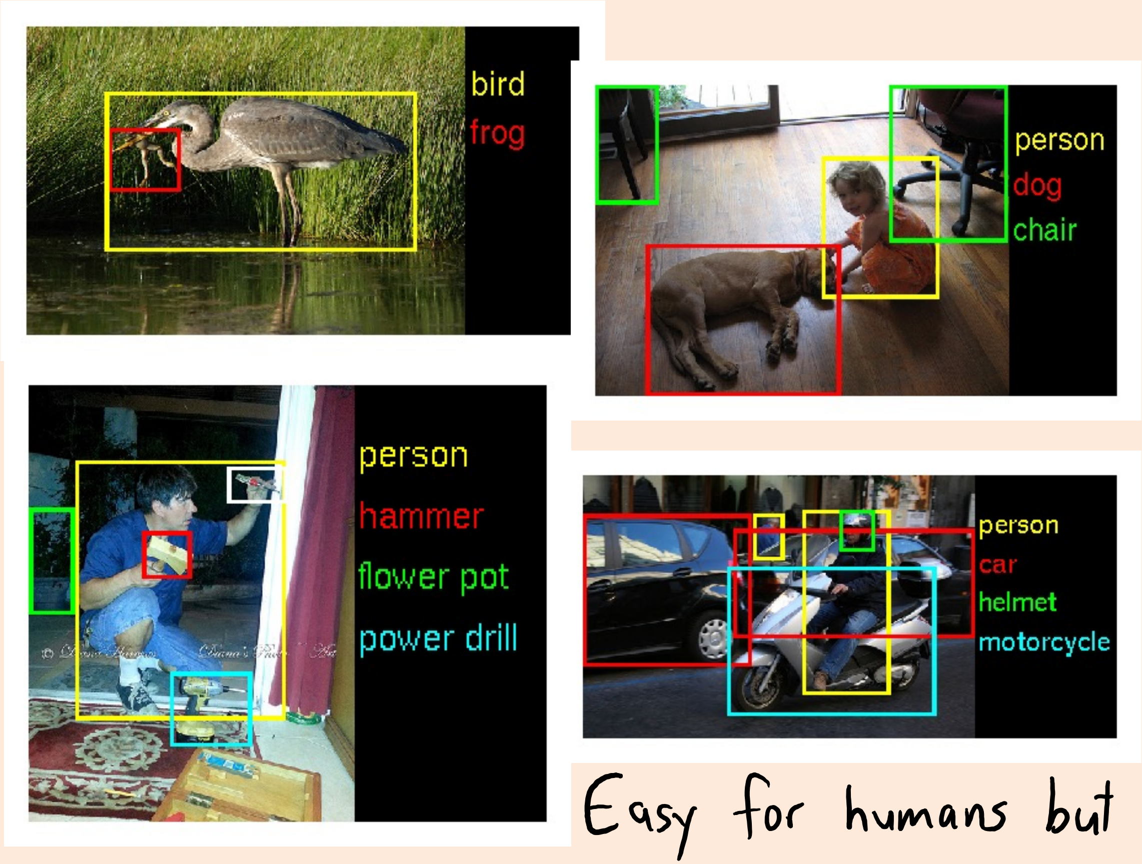


Lee et al. 2007

bonus!

ImageNet Challenge

- Millions of labeled images, 1000 object classes.



Easy for humans but hard for computers.

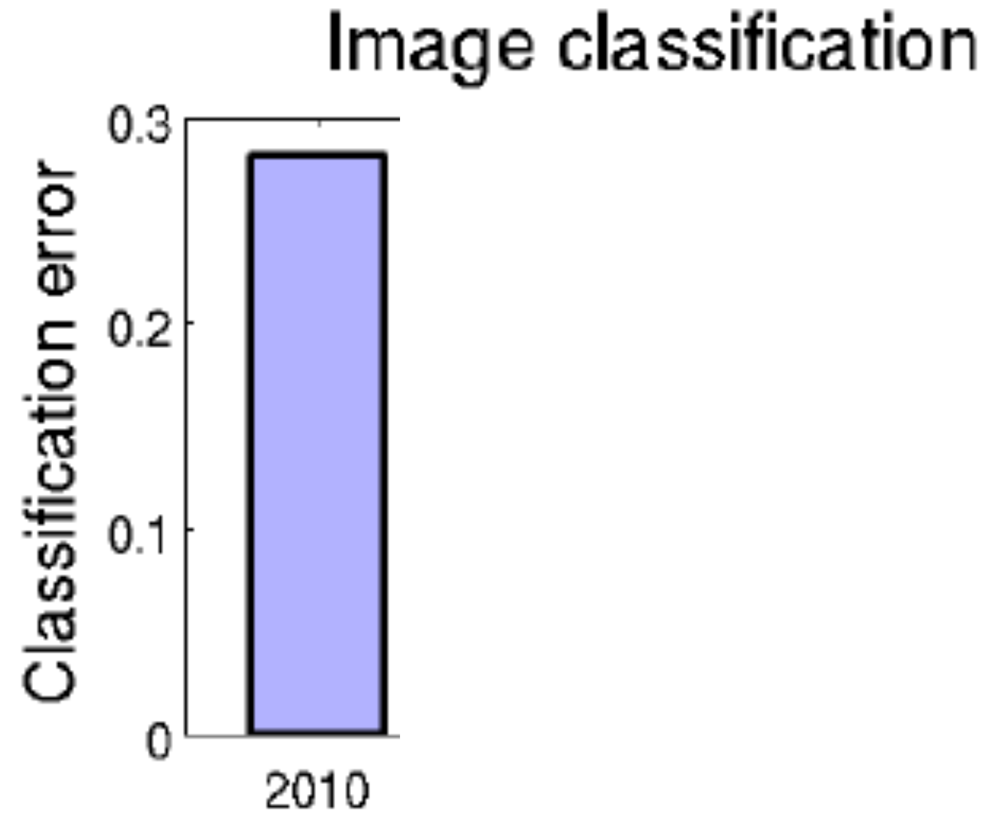
http://www.image-net.org/challenges/LSVRC/2014/

bonus!

ImageNet Challenge

- Object detection task:
  - Single label per image.
  - Humans: ~5% error.

Syberian Husky   Canadian Husky



https://ischlag.github.io/2016/04/05/important-ILSVRC-achievements/
http://arxiv.org/pdf/1409.0575v3.pdf
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bonus!

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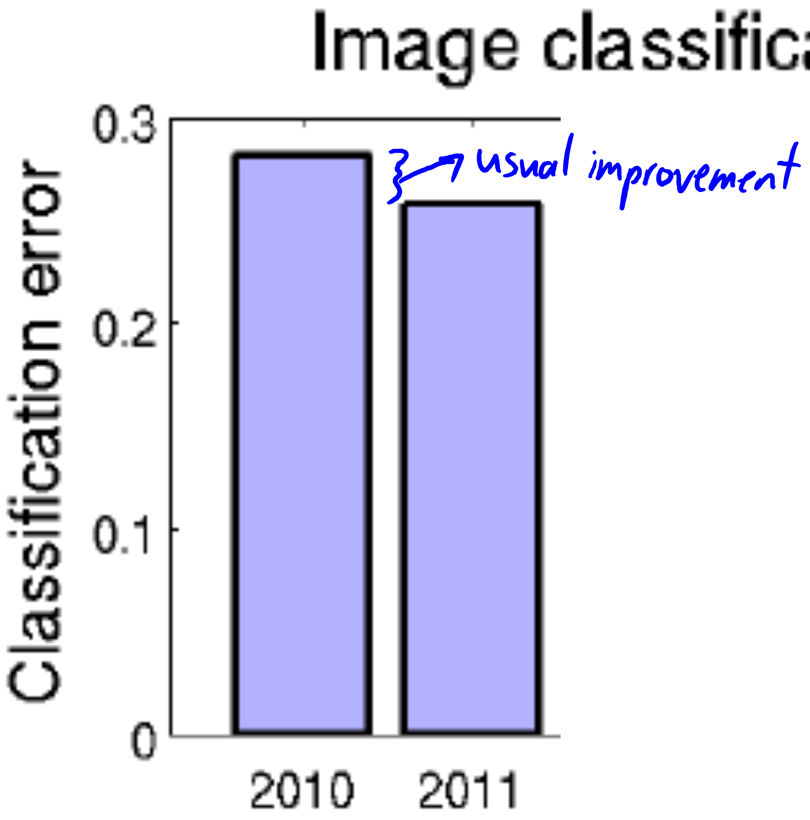

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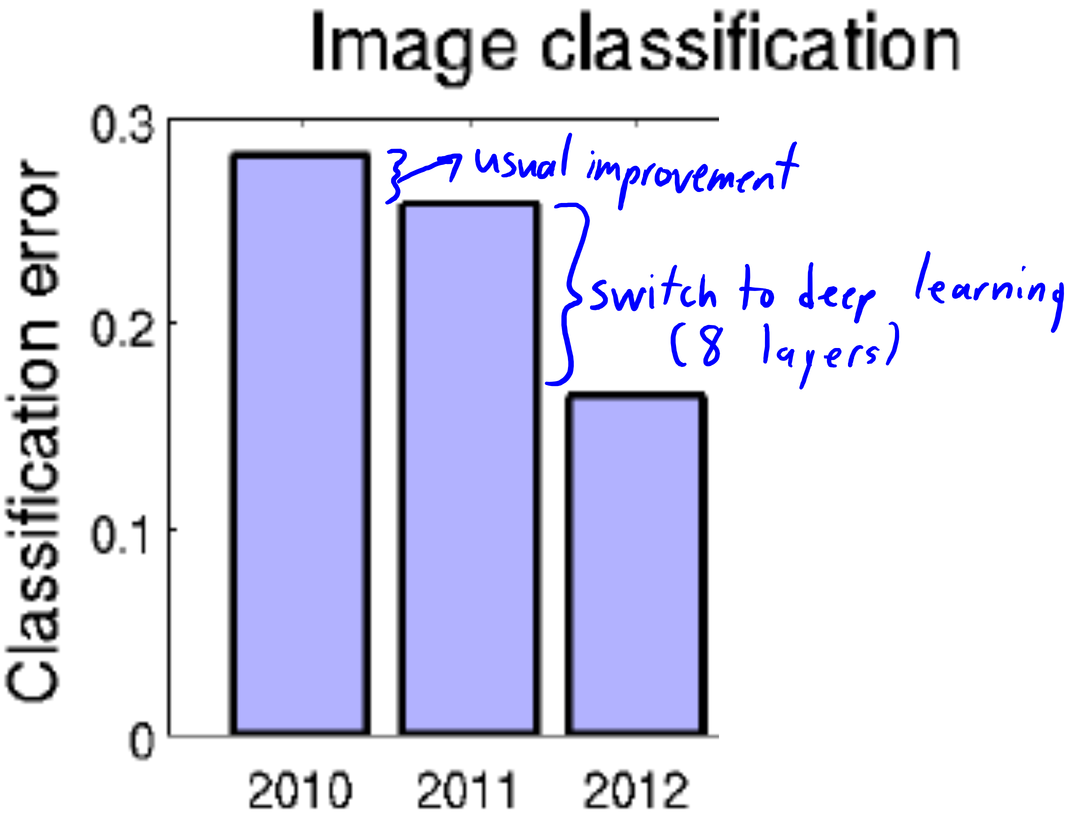

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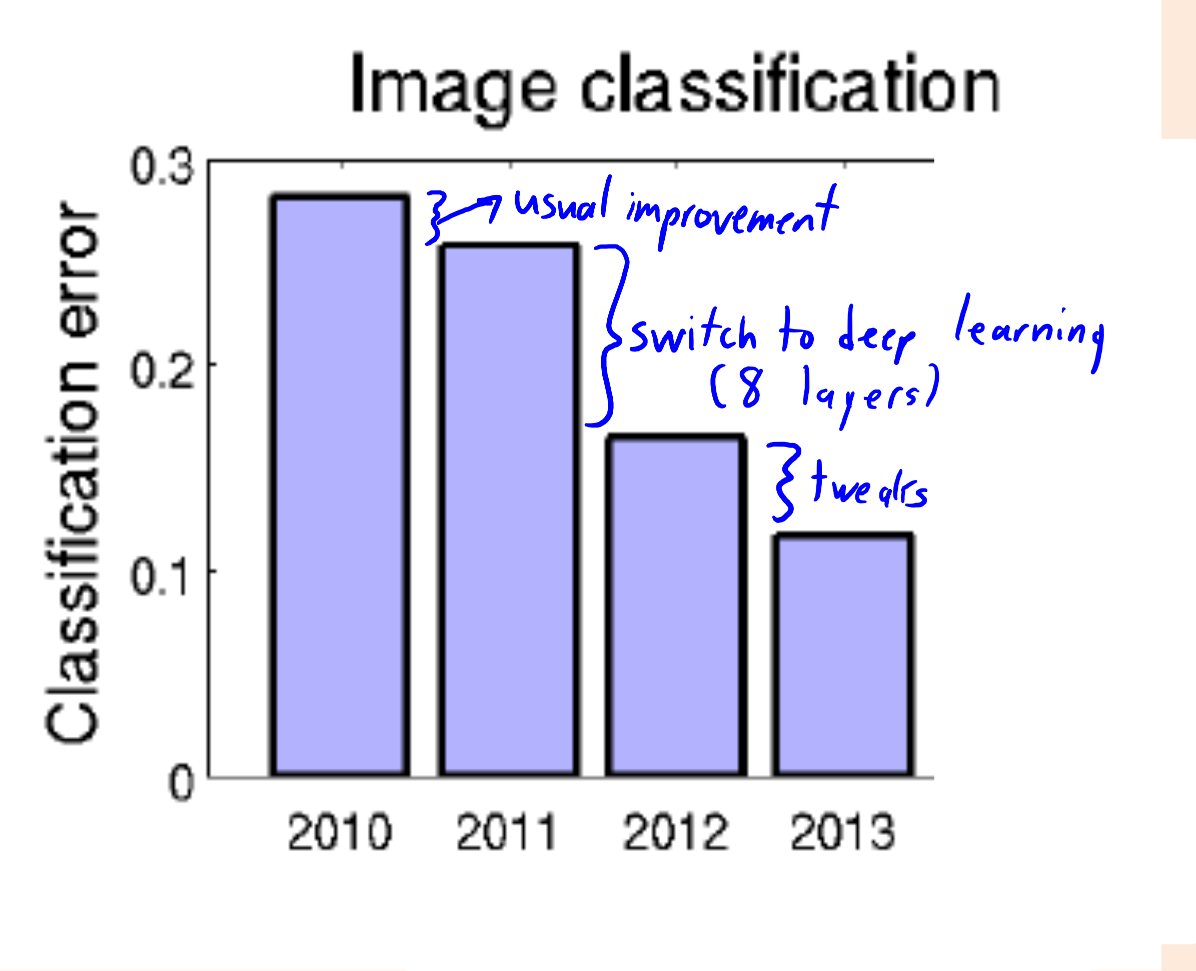

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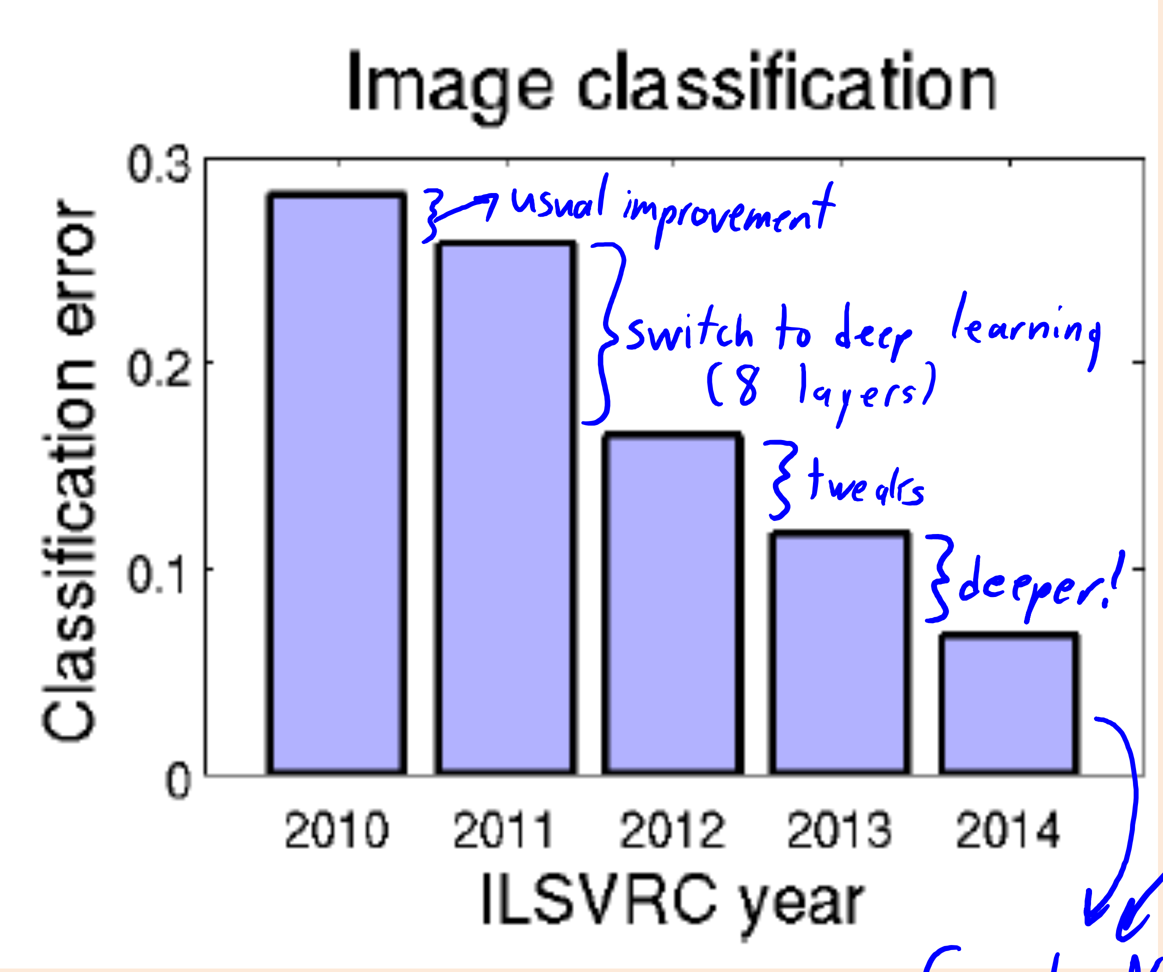
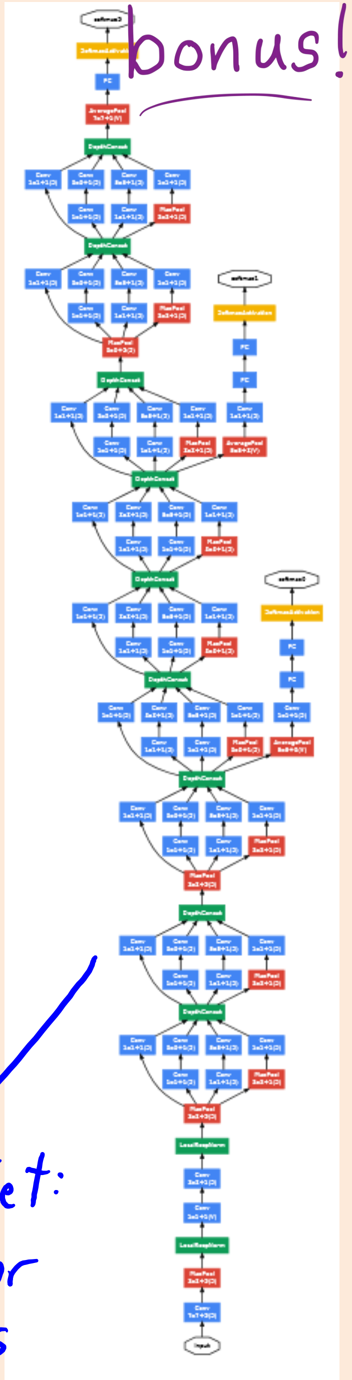




bonus!

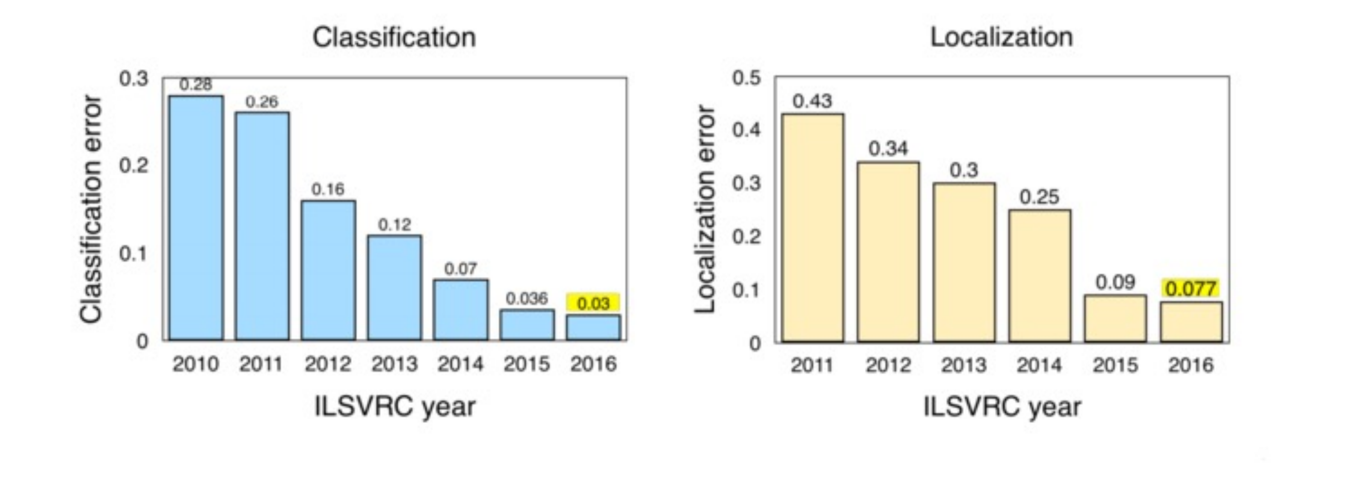
GoogLeNet:
6.7% error
22 layers

https://ischlag.github.io/2016/04/05/important-ILSVRC-achievements/
http://arxiv.org/pdf/1409.0575v3.pdf
http://arxiv.org/pdf/1409.4842v1.pdf

bonus!

ImageNet Challenge

- Object detection task:
  - Single label per image.
  - Humans: ~5% error.
- 2015: Won by Microsoft Asia
  - 3.6% error.
  - 152 layers, introduced “ResNets”.
  - Also won “localization” (finding location of objects in images).
- 2016: Chinese University of Hong Kong:
  - Ensembles of previous winners and other existing methods.
- 2017: fewer entries, organizers decided this would be last year.



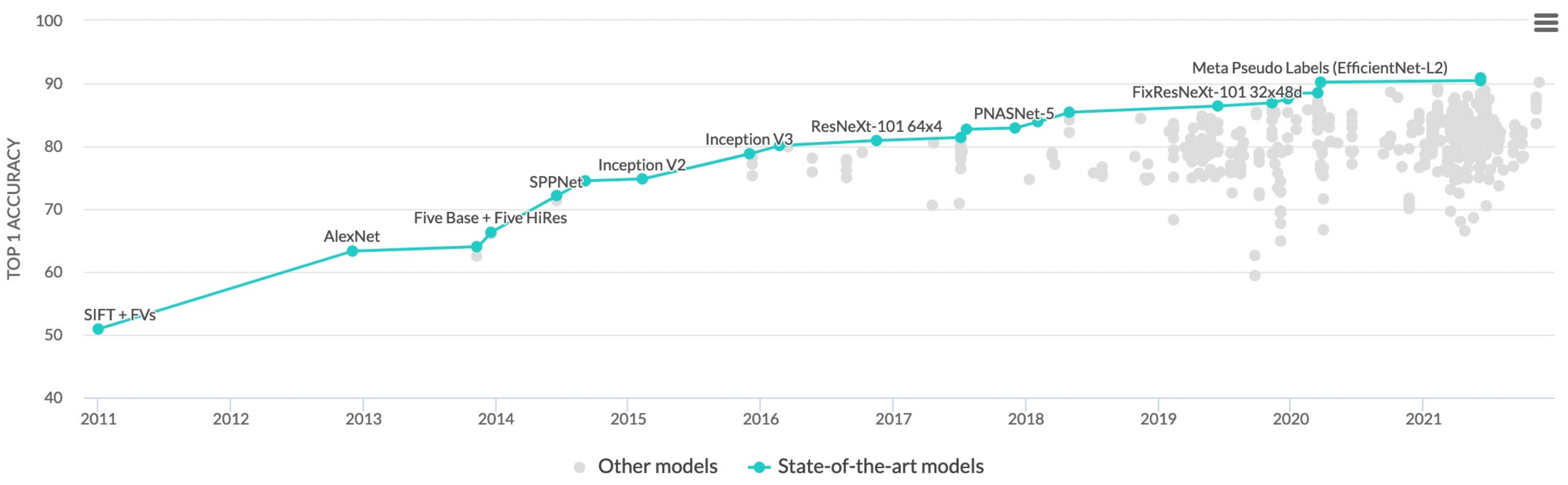
http://www.themtank.org/a-year-in-computer-vision

bonus!

Image Classification on ImageNet

Leaderboard Dataset

View Top 1 Accuracy by Date for All models



https://paperswithcode.com/sota/image-classification-on-imagenet

(pause)

Deep Learning Practicalities

- This lecture focus on deep learning practical issues:
  - Backpropagation to compute gradients.
  - Stochastic gradient training.
  - Regularization to avoid overfitting.

- Next couple lectures:
  - Special 'W' restrictions to further avoid overfitting (especially on images).

But first: Adding Bias Variables

- Recall fitting line regression with a bias:

$$\hat{y}_i = \sum_{j=1}^{d} w_j x_{ij} + \beta$$

  – We avoided this by adding a column of ones to X.

- In neural networks we often want a bias on the output:

$$\hat{y}_i = \sum_{c=1}^{k} v_c h(w_c^T x_i) + \beta$$

- But we also often also include biases on each z_{ic}:

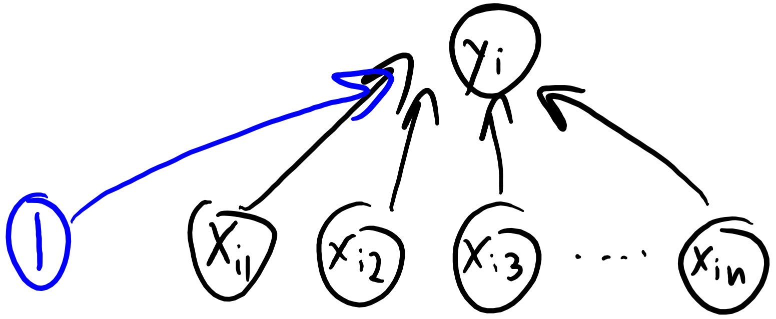
$$\hat{y}_i = \sum_{c=1}^{k} v_c h(w_c^T x_i + \beta_c) + \beta$$

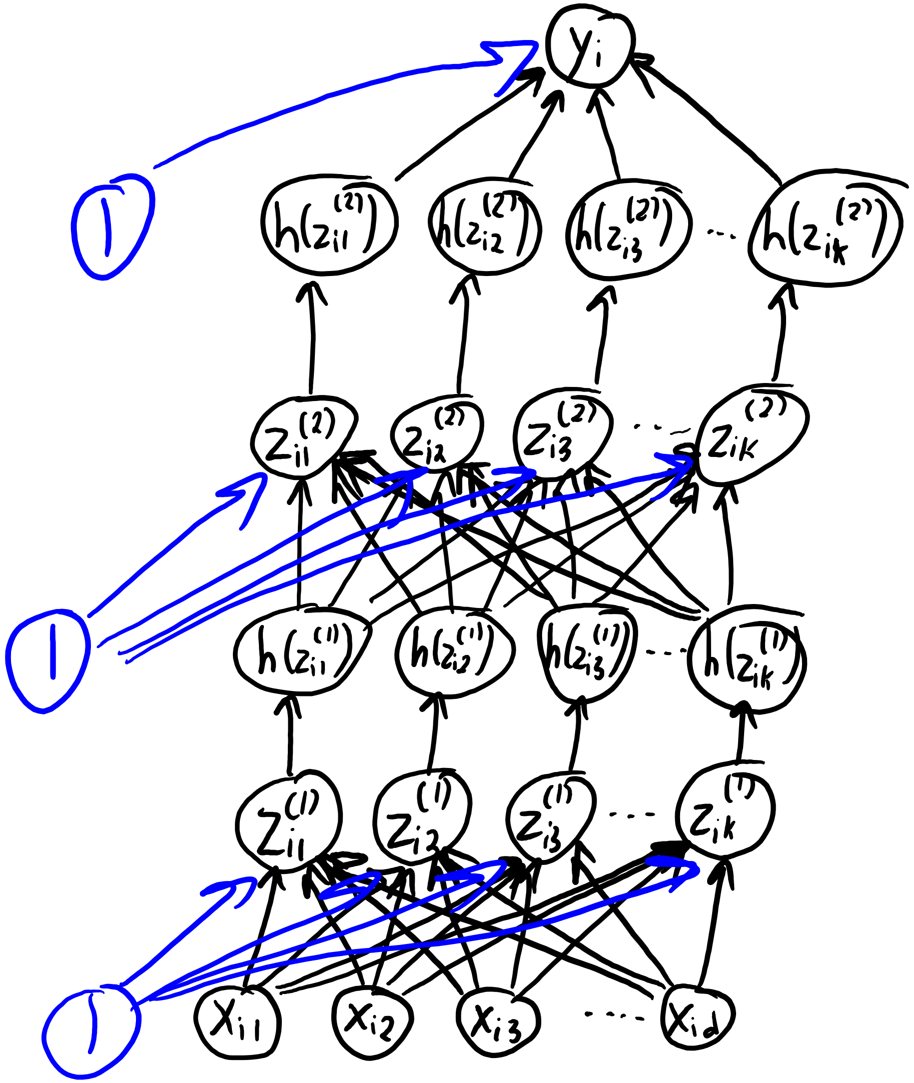
  – A bias towards this $h(z_{ic})$ being either 0 or 1.

- Equivalent to adding to vector $h(z_i)$ an extra value that is always 1.
  – For sigmoids, you could equivalently make one row of w_c be equal to 0.

But first: Adding Bias Variables

Linear model with bias:





Artificial Neural Networks

- With squared loss and 1 hidden layer, our objective function is:

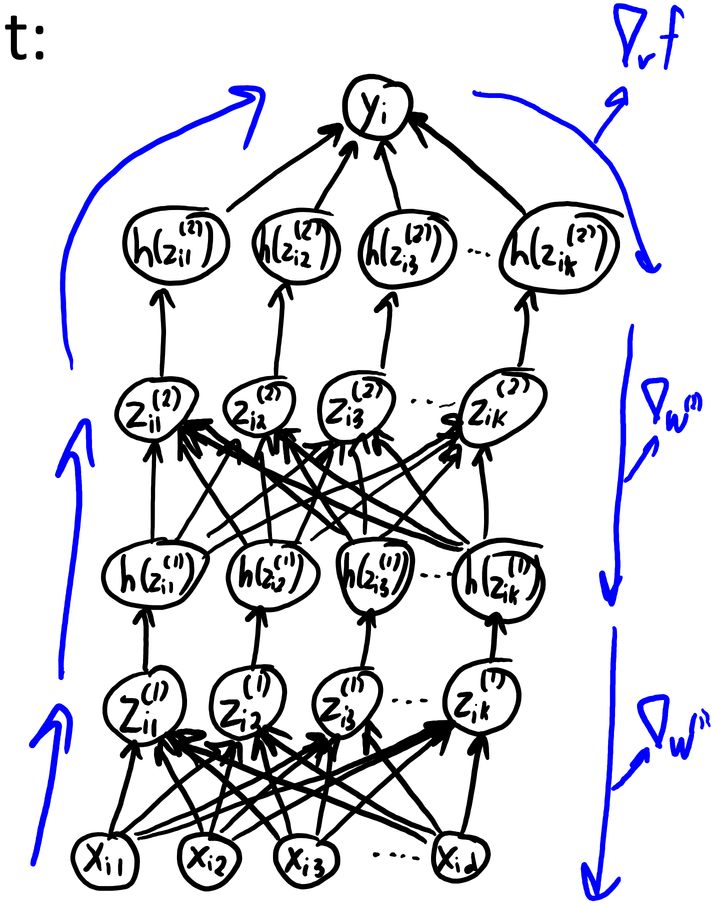
$$f(v, W) = \frac{1}{2}\sum_{i=1}^{n}\left(v^T h(Wx_i) - y_i\right)^2$$

- Usual training procedure: stochastic gradient.
  - Compute gradient of random example 'i', update both 'v' and 'W'.
  - Highly non-convex and can be difficult to tune.

- Computing the gradient is known as "backpropagation".
  - Video giving motivation here.

Backpropagation

- Overview of how we compute neural network gradient:
  - Forward propagation:
    - Compute $z_i^{(1)}$ from x_i.
    - Compute $z_i^{(2)}$ from $z_i^{(1)}$.
    - …
    - Compute $\hat{y}_i$ from $z_i^{(m)}$, and use this to compute error.
  - Backpropagation:
    - Compute gradient with respect to regression weights 'v'.
    - Compute gradient with respect to $z_i^{(m)}$ weights $W^{(m)}$.
    - Compute gradient with respect to $z_i^{(m-1)}$ weights $W^{(m-1)}$.
    - …
    - Compute gradient with respect to $z_i^{(1)}$ weights $W^{(1)}$.
- "Backpropagation" is the chain rule plus some bookkeeping for speed.



bonus!

Backpropagation

- Instead of the next few bonus slides, I HIGHLY recommend watching this video from former UBC master's student Andrej Karpathy (now director of AI and Autopilot Vision at Tesla)
  - https://www.youtube.com/watch?v=i94OvYb6noo

Backpropagation

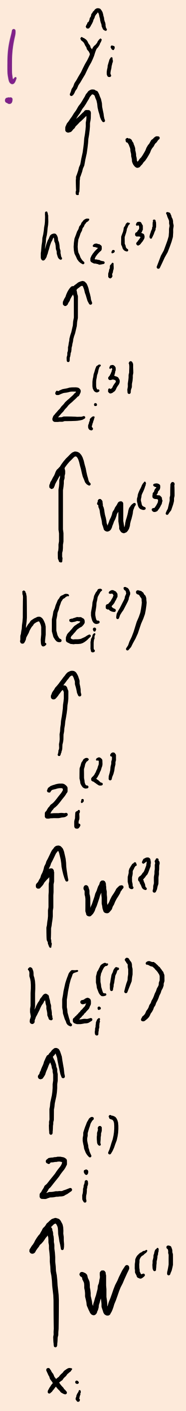
bonus!

- Let's illustrate backpropagation in a simple setting:
  - 1 training example, 3 hidden layers, 1 hidden "unit" in layer.

$$f(W^{(1)},W^{(2)},W^{(3)},v) = \frac{1}{2}(\underbrace{\hat{y}_i - y_i}_{r})^2 \quad \text{where} \quad \hat{y}_i = vh(W^{(3)}h(W^{(2)}h(W^{(1)}x_i)))$$

$$\frac{\partial f}{\partial v} = r\, h(W^{(3)}h(W^{(2)}h(W^{(1)}x_i))) = r\, h(z_i^{(3)})$$

$$\frac{\partial f}{\partial W^{(3)}} = r\, v h'(W^{(3)}h(W^{(2)}h(W^{(1)}x_i)))\, h(W^{(2)}h(W^{(1)}x_i)) = r\, v h'(z_i^{(3)})\, h(z_i^{(2)})$$



bonus!

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$$\frac{\partial f}{\partial W^{(2)}} = r\, v h'(W^{(3)} h(W^{(2)} h(W^{(1)} x_i)))\, W^{(3)} h'(W^{(2)} h(W^{(1)} x_i))\, h(W^{(1)} x_i) = \underbrace{r^{(3)} W^{(3)} h'(z_i^{(2)})}_{r^{(2)}}\, h(z_i^{(1)})$$

$$\frac{\partial f}{\partial W^{(1)}} = r\, v h'(W^{(3)} h(W^{(2)} h(W^{(1)} x_i)))\, W^{(3)} h'(W^{(2)}(W^{(1)} x_i))\, W^{(2)} h'(W^{(1)} x_i)\, x_i = r^{(2)} W^{(2)} h'(z_i^{(1)})\, x_i$$

bonus!

Backpropagation

- Let's illustrate backpropagation in a simple setting:
  - 1 training example, 3 hidden layers, 1 hidden "unit" in layer.

$$\frac{\partial f}{\partial v} = r\, h(z_i^{(3)})$$

$$\frac{\partial f}{\partial W^{(3)}} = r\; v\, h'(z_i^{(3)})\, h(z_i^{(2)})$$

$$\frac{\partial f}{\partial W^{(2)}} = r^{(3)}\, W^{(3)}\, h'(z_i^{(2)})\, h(z_i^{(1)})$$

$$\frac{\partial f}{\partial W^{(1)}} = r^{(2)}\, W^{(2)}\, h'(z_i^{(1)})\, x_i$$

$$\frac{\partial f}{\partial v_c} = r\, h(z_{ic}^{(3)})$$

$$\frac{\partial f}{\partial W^{(3)}_{c'c}} = r\, v_c\, h'(z_{ic'}^{(3)})\, h(z_{ic}^{(2)})$$

$$\frac{\partial f}{\partial W^{(2)}_{c'c}} = \left[\sum_{c''=1}^{k} r^{(3)}_{c''}\, W^{(3)}_{c''c'}\right] h'(z_{ic'}^{(2)})\, h(z_{ic}^{(1)})$$

$$\frac{\partial f}{\partial W^{(1)}_{cj}} = \left[\sum_{c''=1}^{k} r^{(2)}_{c''}\, W^{(2)}_{c''c}\right] h'(z_{ic}^{(1)})\, x_j$$

  - Only the first 'r' changes if you use a different loss.
  - With multiple hidden units, you get extra sums.
    - Efficient if you store the sums rather than computing from scratch.

Backpropagation

- I've marked those backprop math slides as bonus.
- Do you need to know how to do this?
  - Exact details are probably not vital (there are many implementations).
  - "Automatic differentiation" is now standard and has same cost.
  - But understanding basic idea helps you know what can go wrong.
    - Or give hints about what to do when you run out of memory.
  - See discussion here by a neural network expert (Andrej!)

- You should know cost of backpropagation:
  - Forward pass dominated by matrix multiplications by $W^{(1)}$, $W^{(2)}$, $W^{(3)}$, and 'v'.
    - If have 'm' layers and all z_i have 'k' elements, cost would be $O(dk + mk^2)$.
  - Backward pass has same cost as forward pass.

Multi-class / Multi-label networks

- For 'k' labels, replace 'v' by a matrix with 'k' columns
  - "Top" of a neural network is just a linear model (with learned 'z_i')…
  - …so we can do all the same tricks we already learned
  - Can still do backprop the same way
- Multi-class: we already learned the softmax loss!
  - Often called "cross entropy" by neural network people
  - Reason is, well, it's the cross-entropy: $\mathrm{H}(\mathrm{p}, \hat{p}) = \sum_i p_i \log \hat{p}_i$
- Multi-label: add up logistic loss (or whatever) on each output
  - In linear models, this was like running separate regressions
  - Here, we learn the 'z_i' for all labels at once, so it can help to do together

Deep Learning Vocabulary

- "Deep learning": Models with many hidden layers.
  - Usually neural networks.
- "Neuron": node in the neural network graph.
  - "Visible unit": feature.
  - "Hidden unit": latent factor z_{ic} or $h(z_{ic})$.
- "Activation function": non-linear transform.
- "Activation": $h(z_i)$.
- "Backpropagation": compute gradient of neural network.
  - Sometimes "backpropagation" means "training with SGD".
- "Weight decay": L2-regularization.
- "Cross entropy": softmax loss.
- "Learning rate": SGD step-size.
- "Learning rate decay": using decreasing step-sizes.
- "Vanishing/Exploding gradient": gradient becoming real small/big for deep net

(pause)

ImageNet Challenge and Optimization

- ImageNet challenge:
  – Use millions of images to recognize 1000 objects.
- ImageNet organizer visited UBC summer 2015.
- “Besides huge dataset/model/cluster, what is the most important?”
  1. Image transformations (translation, rotation, scaling, lighting, etc.).
  2. Optimization.
- Why would optimization be so important?
  – Neural network objectives are highly non-convex (and worse with depth).
  – Optimization has huge influence on quality of model.

Stochastic Gradient Training

- Standard training method is stochastic gradient (SG):
  - Choose a random example 'i'.
  - Use backpropagation to get gradient with respect to all parameters.
  - Take a small step in the negative gradient direction.
- Challenging to make SG work:
  - Often doesn't work as a "black box" learning algorithm.
  - But people have developed a lot of tricks/modifications to make it work.
- Highly non-convex, so are the problem local mimina?
  - Some empirical/theoretical evidence that local minima are not the problem.
  - If the network is "deep" and "wide" enough, we think all local minima are good.
  - But it can be hard to get SG to close to a local minimum in reasonable time.

Parameter Initialization

- Parameter initialization is crucial:
  - Can't initialize weights in same layer to same value, or units will stay the same.
    - Architecture is symmetric, so gradient would be the same for every hidden unit in the layer, so they'd all just always stay doing the exact same thing.
  - Can't initialize weights too large, it will take too long to learn.
- A traditional random initialization:
  - Initialize bias variables to 0.
  - Sample from standard normal, divided by 10^5 (0.00001*randn).
    - w = .00001*randn(k,1)
  - Performing multiple initializations does not seem to be important (except maybe with very small networks).

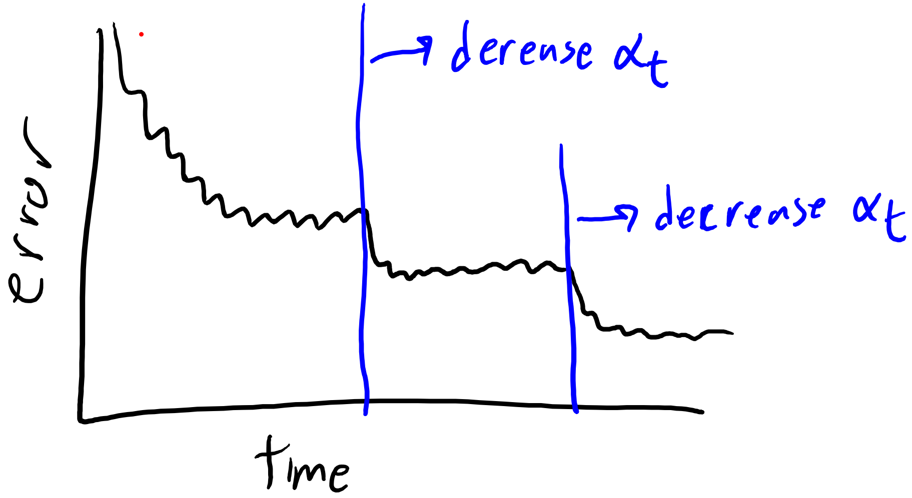
bonus!

Parameter Initialization

- Parameter initialization is crucial:
  - Can't initialize weights in same layer to same value, or they will stay same.
  - Can't initialize weights too large, it will take too long to learn.
- Also common to transform data in various ways:
  - Subtract mean, divide by standard deviation, "whiten", standardize y_i.
- More recent initializations try to standardize initial z_i:
  - Use different initialization in each layer.
  - Try to make variance of z_i the same across layers.
    - Popular approach is to sample from standard normal, divide by sqrt(2*nInputs).
  - Use samples from uniform distribution on [-b,b], where $b = \frac{\sqrt{6}}{\sqrt{k^{(m)} + k^{(m-1)}}}$

Setting the Step-Size

- Stochastic gradient is very sensitive to the step size in deep models.
- Common approach: manual "babysitting" of the step-size.
  - Run SG for a while with a fixed step-size.
  - Occasionally measure error and plot progress:



  - If error is not decreasing, decrease step-size.

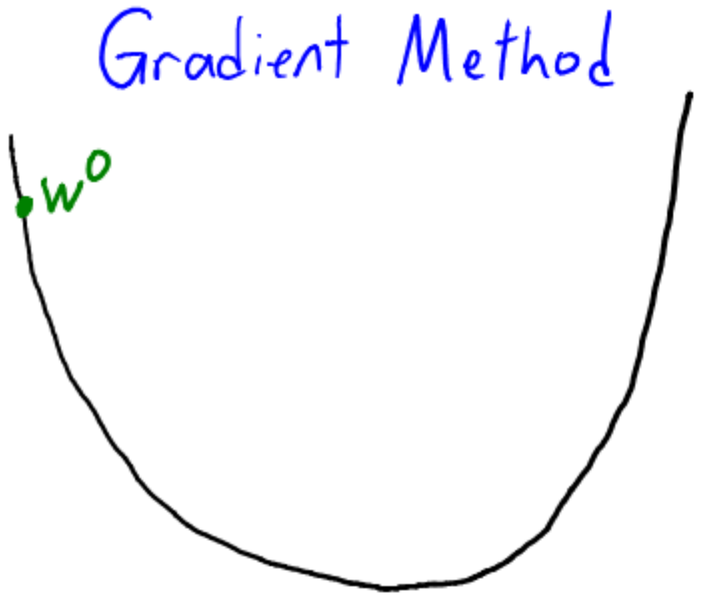
Setting the Step-Size

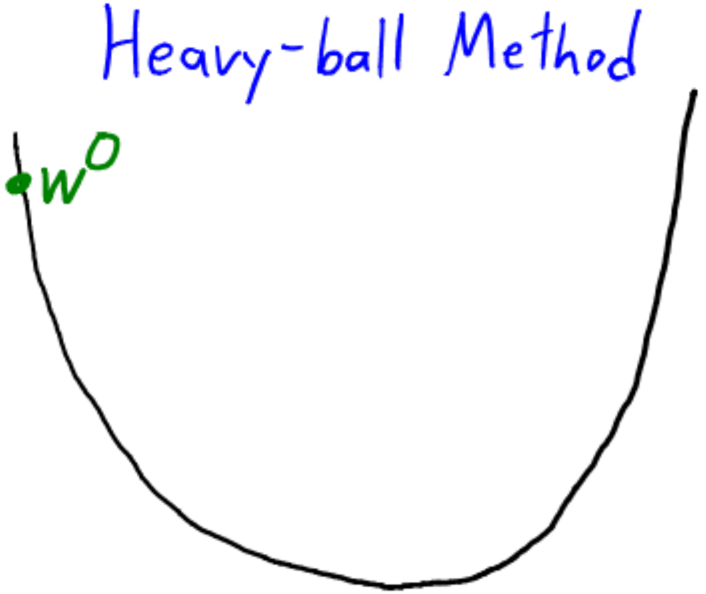
- Stochastic gradient is very sensitive to the step size in deep models.
- Bias step-size multiplier: use bigger step-size for the bias variables.
- Momentum (stochastic version of "heavy-ball" algorithm):
  - Add term that moves in previous direction:

$$w^{t+1} = w^t - \alpha^t \nabla f_i(w^t) + \underbrace{\beta^t (w^t - w^{t-1})}_{\text{keep going in the old direction}}$$

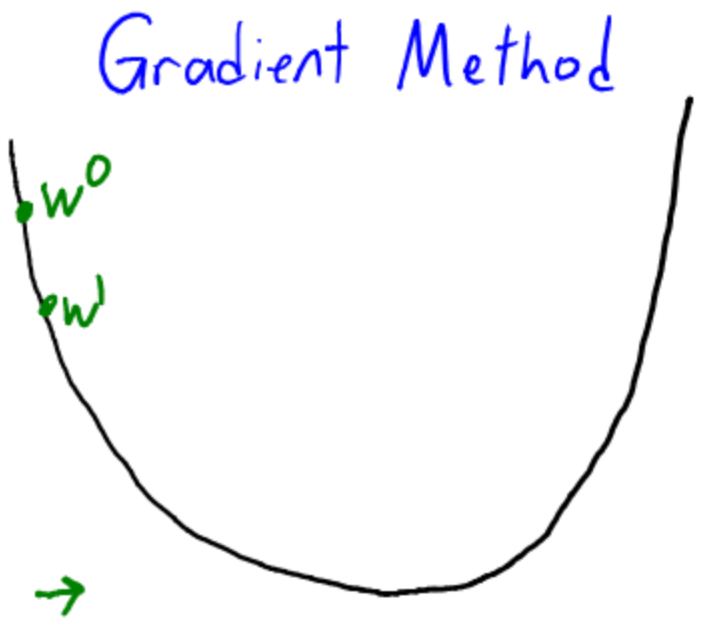
  - Usually $\beta^t = 0.9$.

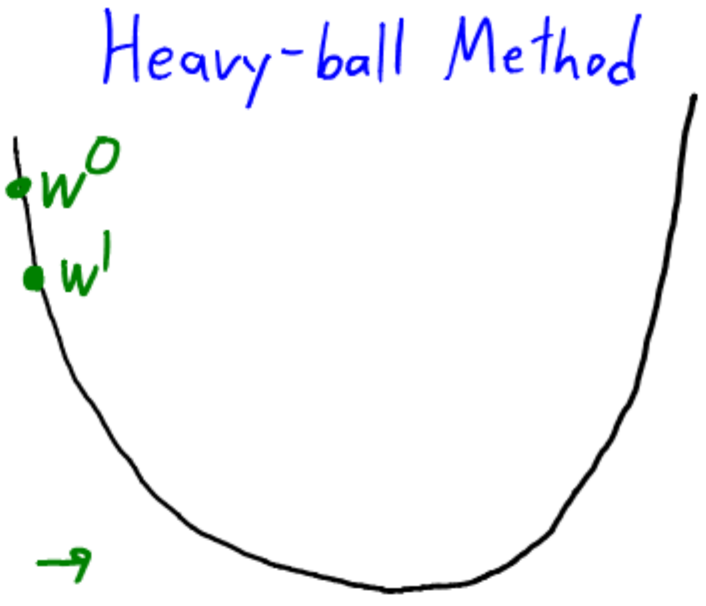
Gradient Descent vs. Heavy-Ball Method



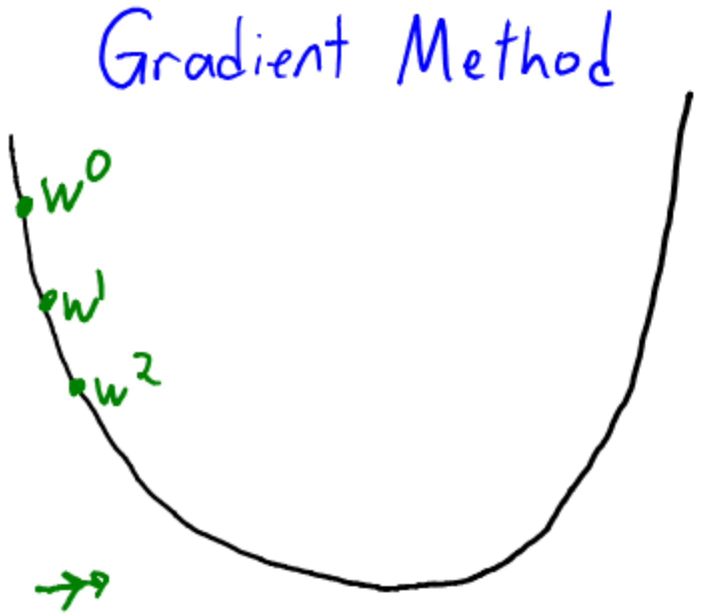


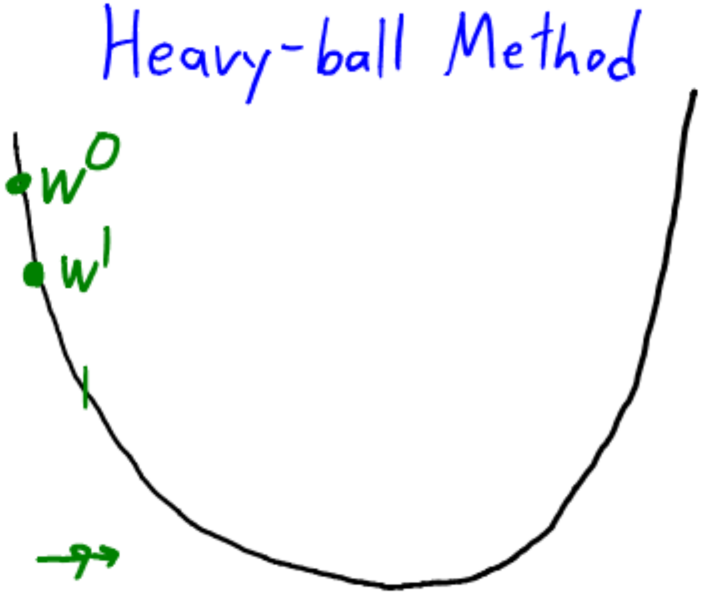
Gradient Descent vs. Heavy-Ball Method



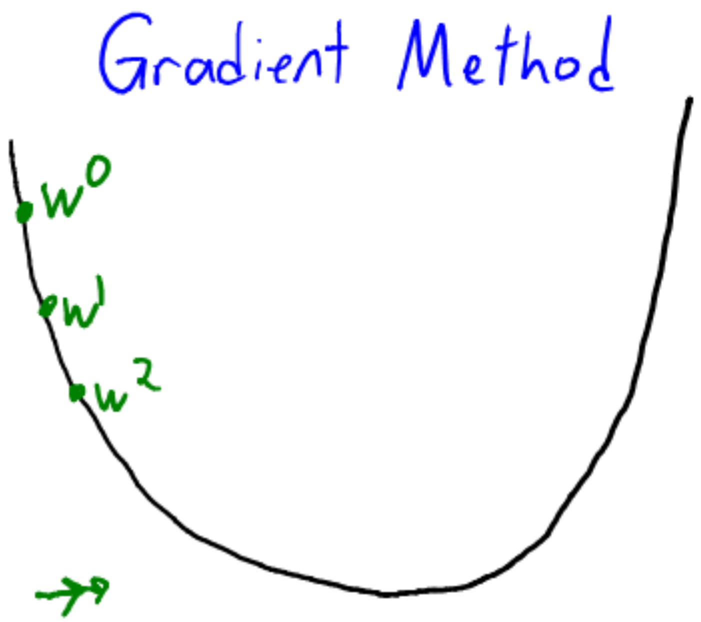


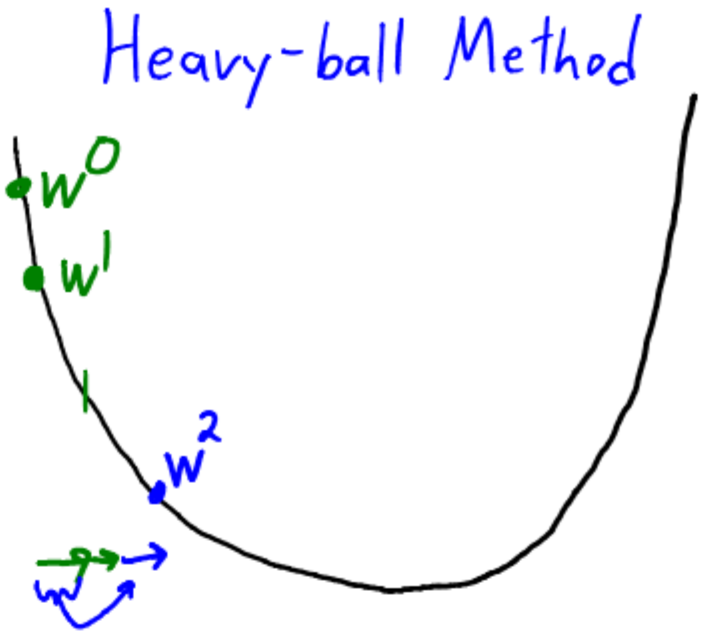
Gradient Descent vs. Heavy-Ball Method



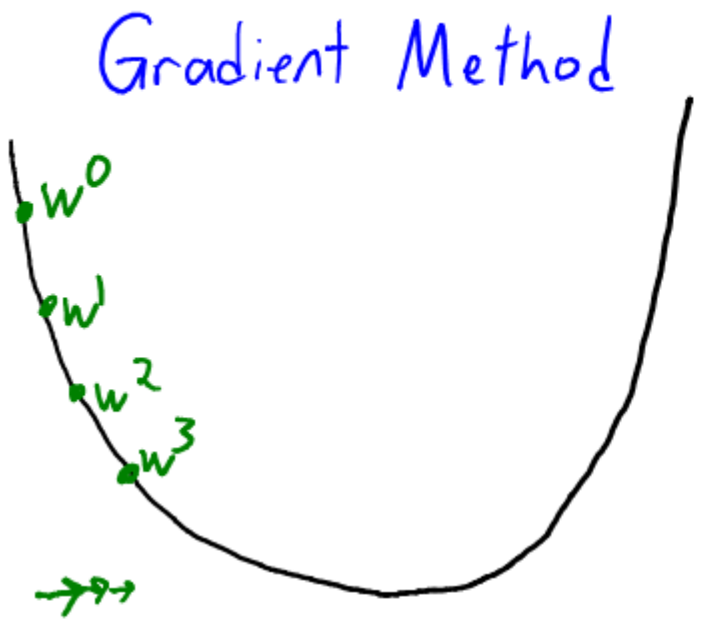


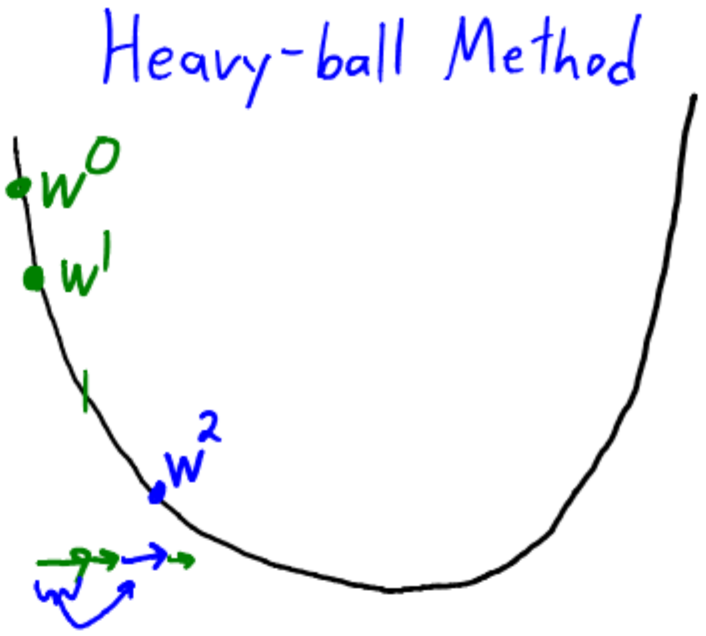
Gradient Descent vs. Heavy-Ball Method



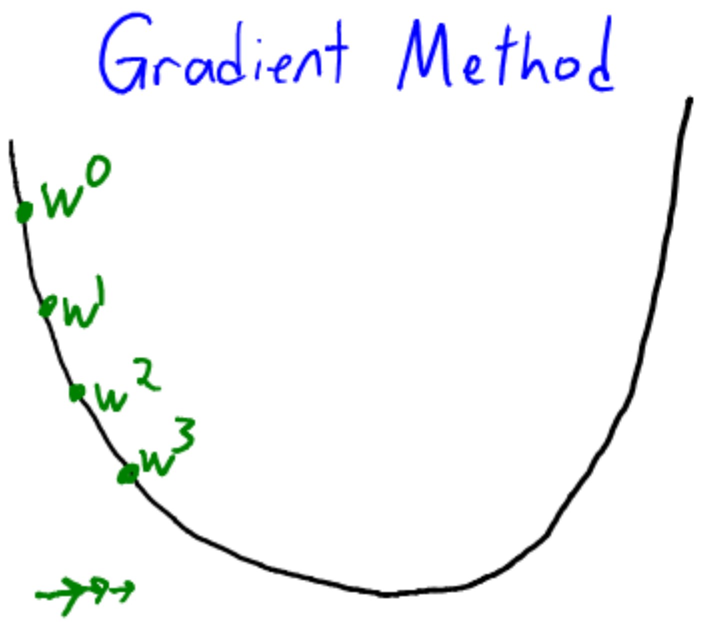


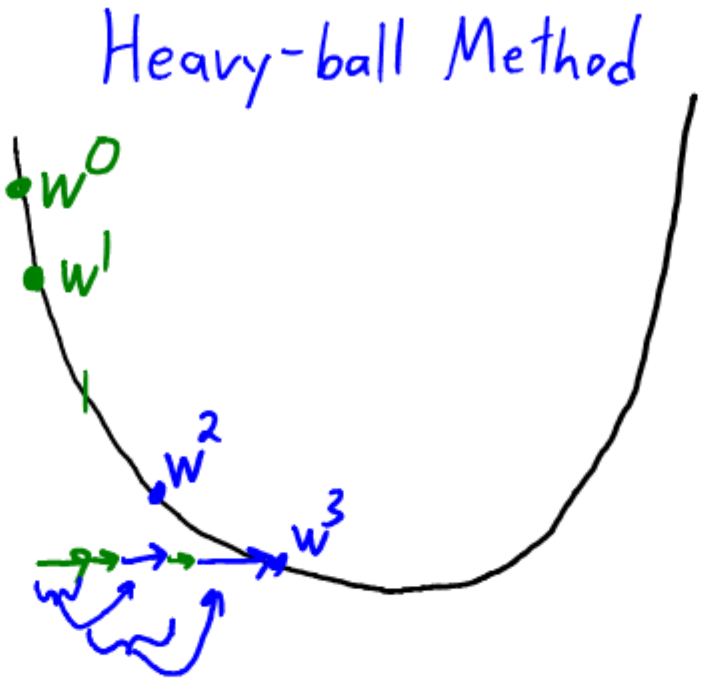
Gradient Descent vs. Heavy-Ball Method



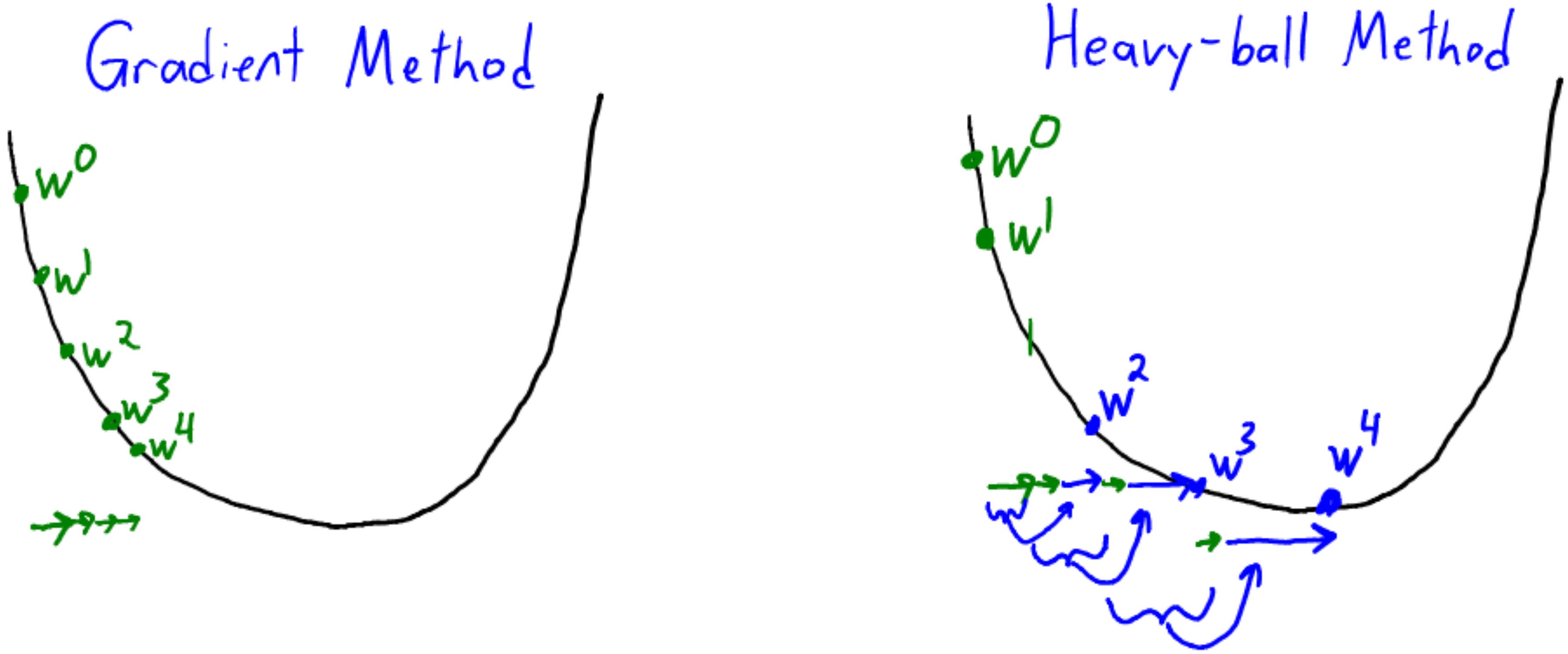


Gradient Descent vs. Heavy-Ball Method

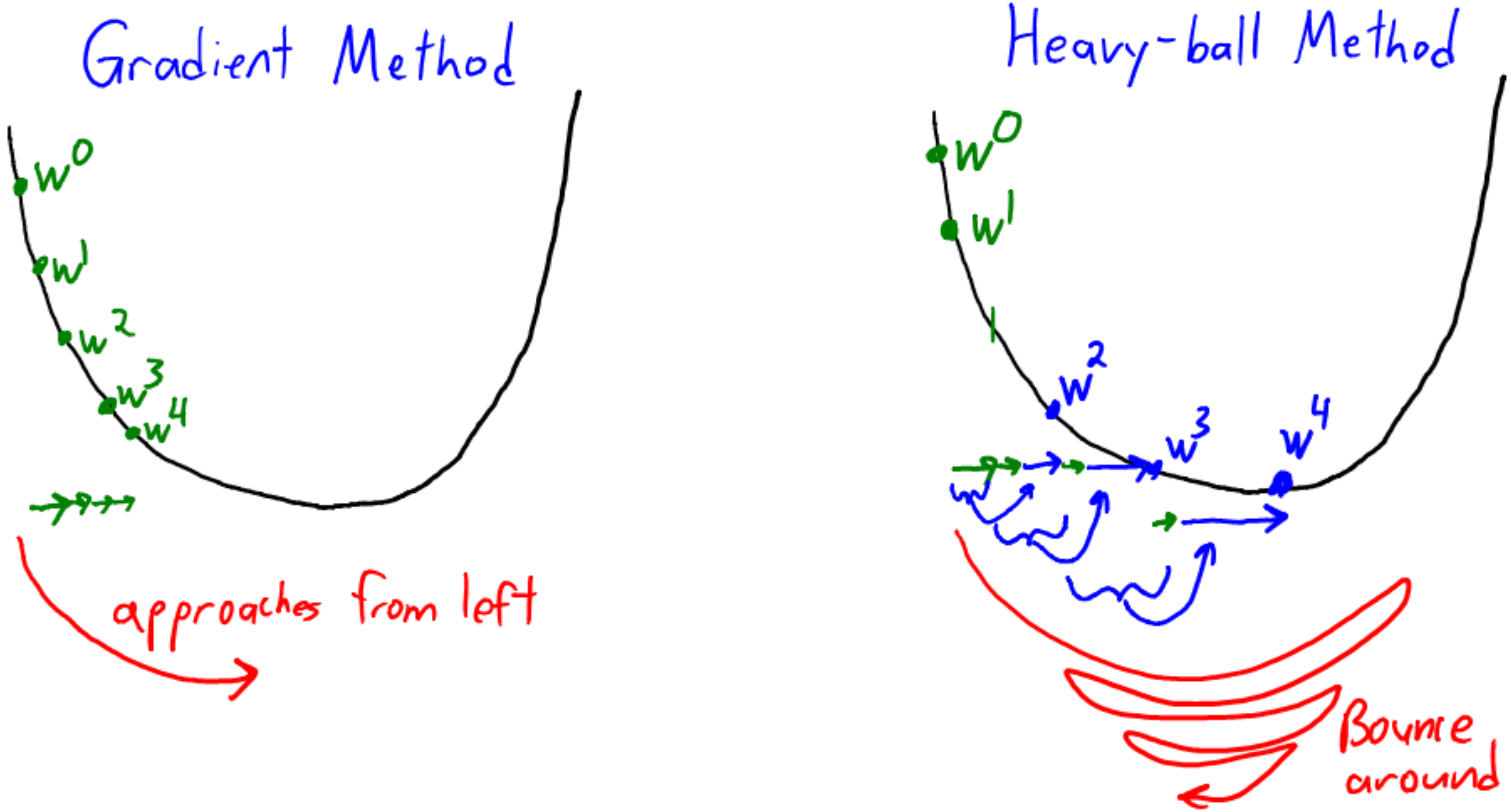




Gradient Descent vs. Heavy-Ball Method



Gradient Descent vs. Heavy-Ball Method



Good demo to check out: https://distill.pub/2017/momentum/

bonus!

Setting the Step-Size

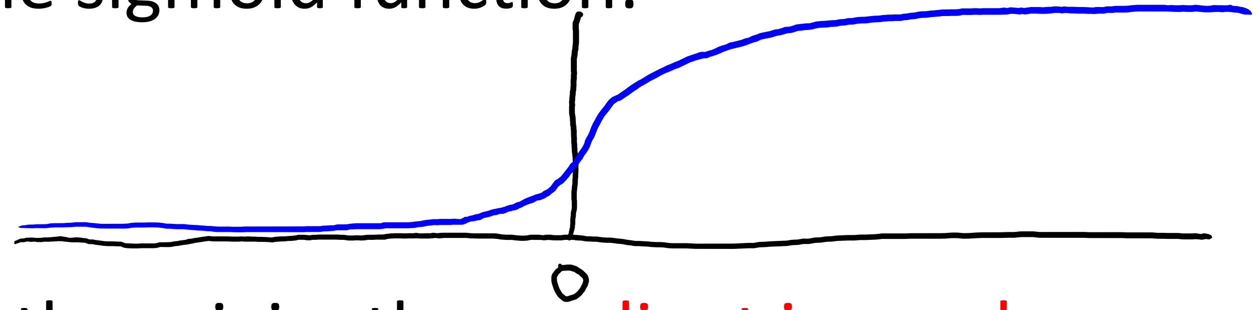
- Automatic method to set step size is Bottou trick:
  1. Grab a small set of training examples (maybe 5% of total).
  2. Do a binary search for a step size that works well on them.
  3. Use this step size for a long time (or slowly decrease it from there).

- Several recent methods using a step size for each variable:
  - AdaGrad, RMSprop, Adam (often work better "out of the box").
  - Some controversy versus plain stochastic gradient (often with momentum).
    - SGD can often get lower test error, even though it takes longer and requires more tuning of step-size.
- Batch size (number of random examples) also influences results.
  - Bigger batch sizes often give faster convergence but maybe to worse solutions?

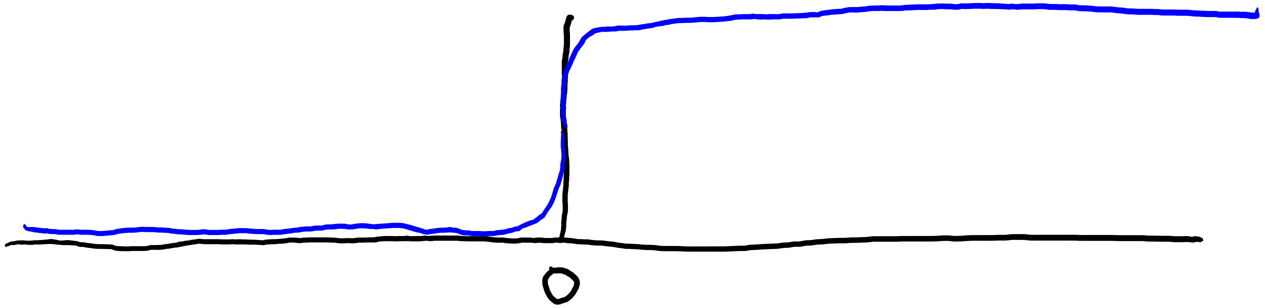
- Another recent trick is batch normalization:
  - Try to "standardize" the hidden units within the random samples as we go.
  - Held as example of deep learning "alchemy" (blog post here about deep learning claims).
    - Sounds science-ey and often works, but little theoretical understanding.

Vanishing Gradient Problem

- Consider the sigmoid function:



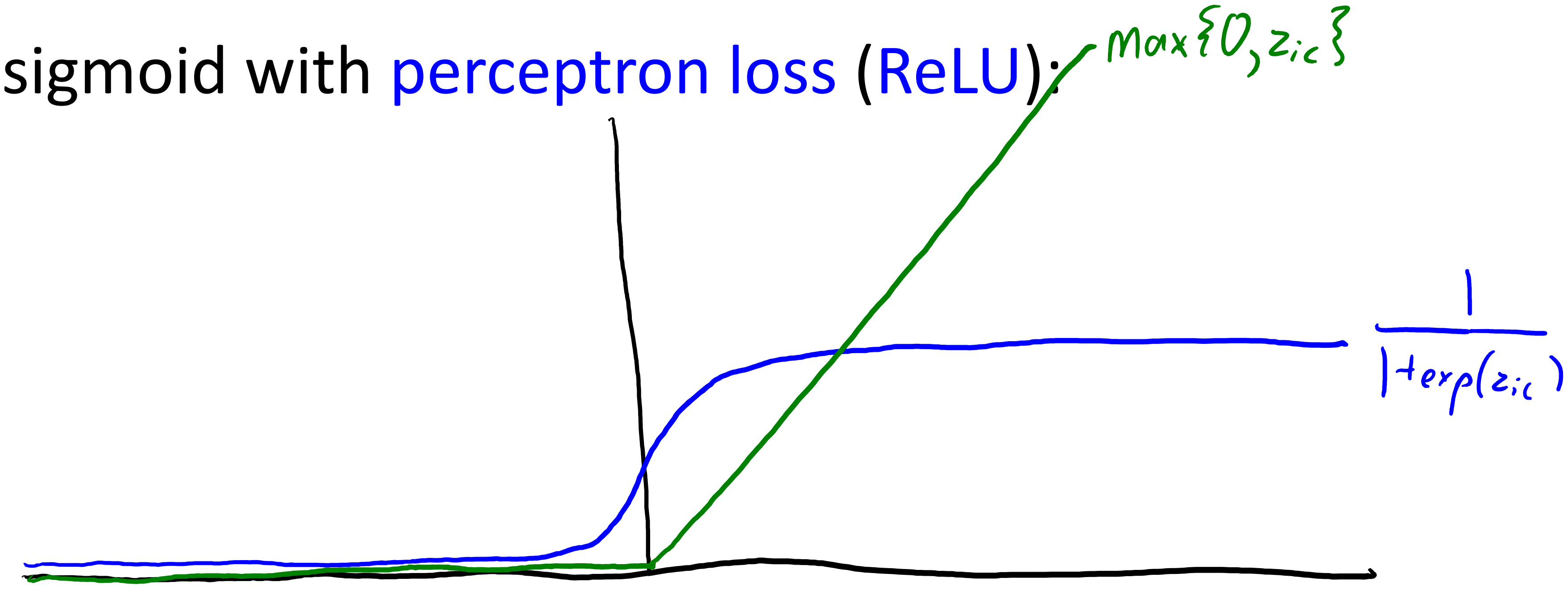
- Away from the origin, the gradient is nearly zero.
- The problem gets worse when you take the sigmoid of a sigmoid:



- In deep networks, many gradients can be nearly zero everywhere.

Rectified Linear Units (ReLU)

- Replace sigmoid with perceptron loss (ReLU):

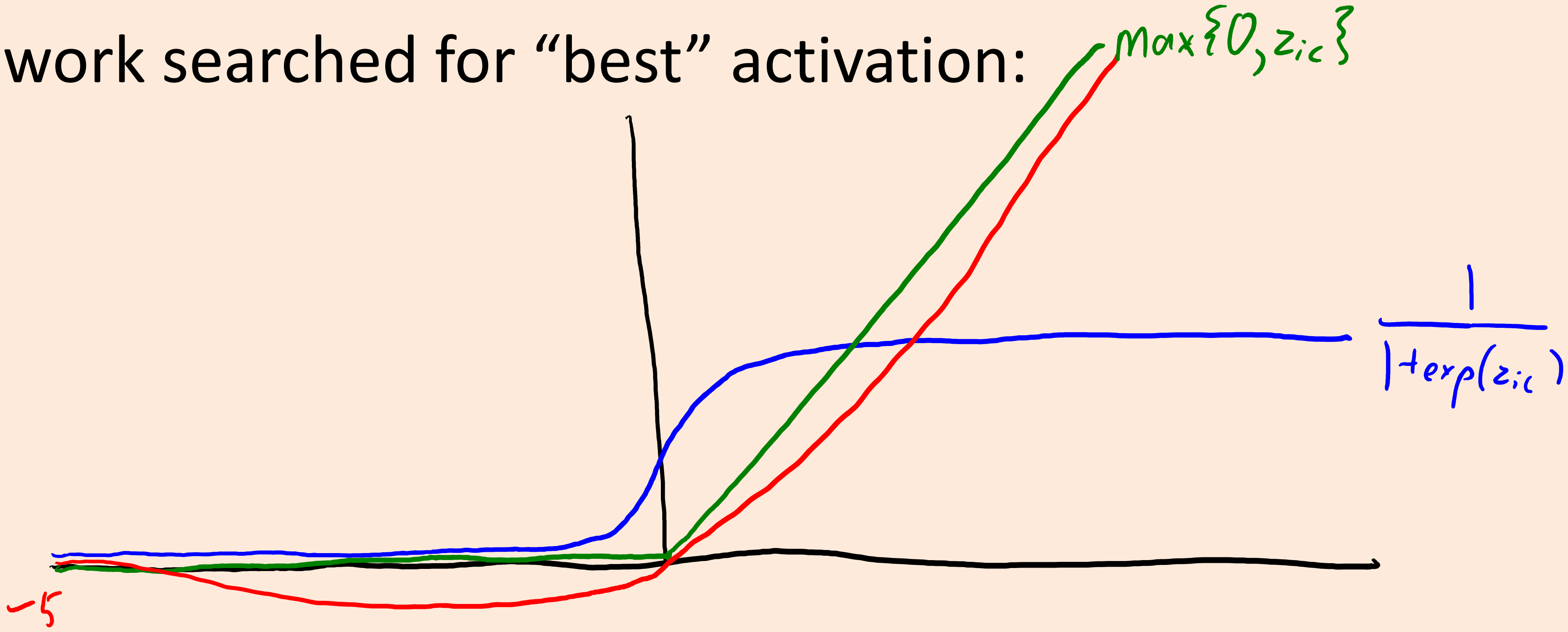


- Just sets negative values z_{ic} to zero.
  - Fixes vanishing gradient problem.
  - Gives sparser activations.
  - Not really simulating binary signal, but could be simulating "rate coding".

bonus!

"Swish" Activation

- Recent work searched for "best" activation:



- Found that $z_{ic}/(1+\exp(-z_{ic}))$ worked best ("swish" function).
  - A bit weird because it allows negative values and is non-monotonic.
  - But basically the same as ReLU when not close to 0.

Summary

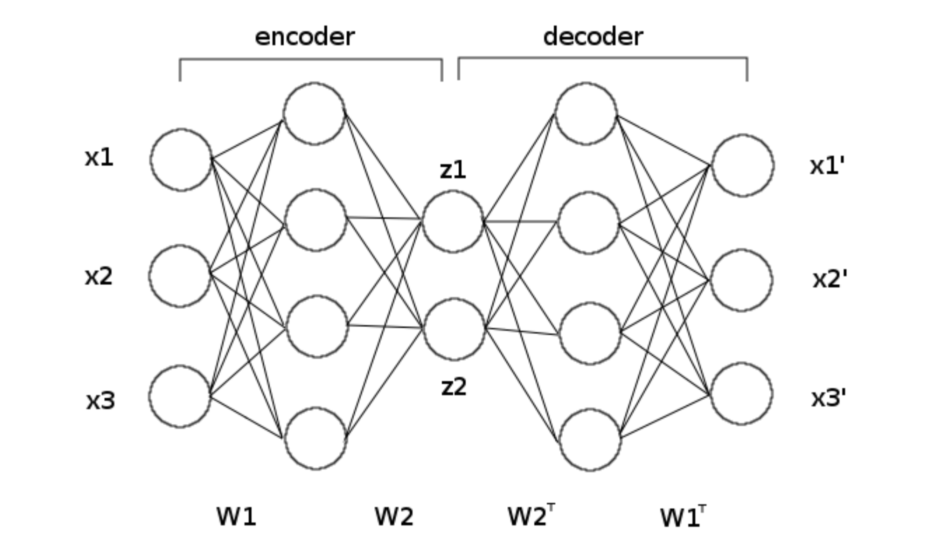
- Unprecedented performance on difficult pattern recognition tasks.
- Backpropagation computes neural network gradient via chain rule.
- Parameter initialization is crucial to neural net performance.
- Optimization and step size are crucial to neural net performance.
  - “Babysitting”, momentum.
- ReLU avoid “vanishing gradients”.

- Next lectures: The most important idea in computer vision?

bonus!

Autoencoders

- Autoencoders are an unsupervised deep learning model:
  - Use the inputs as the output of the neural network.



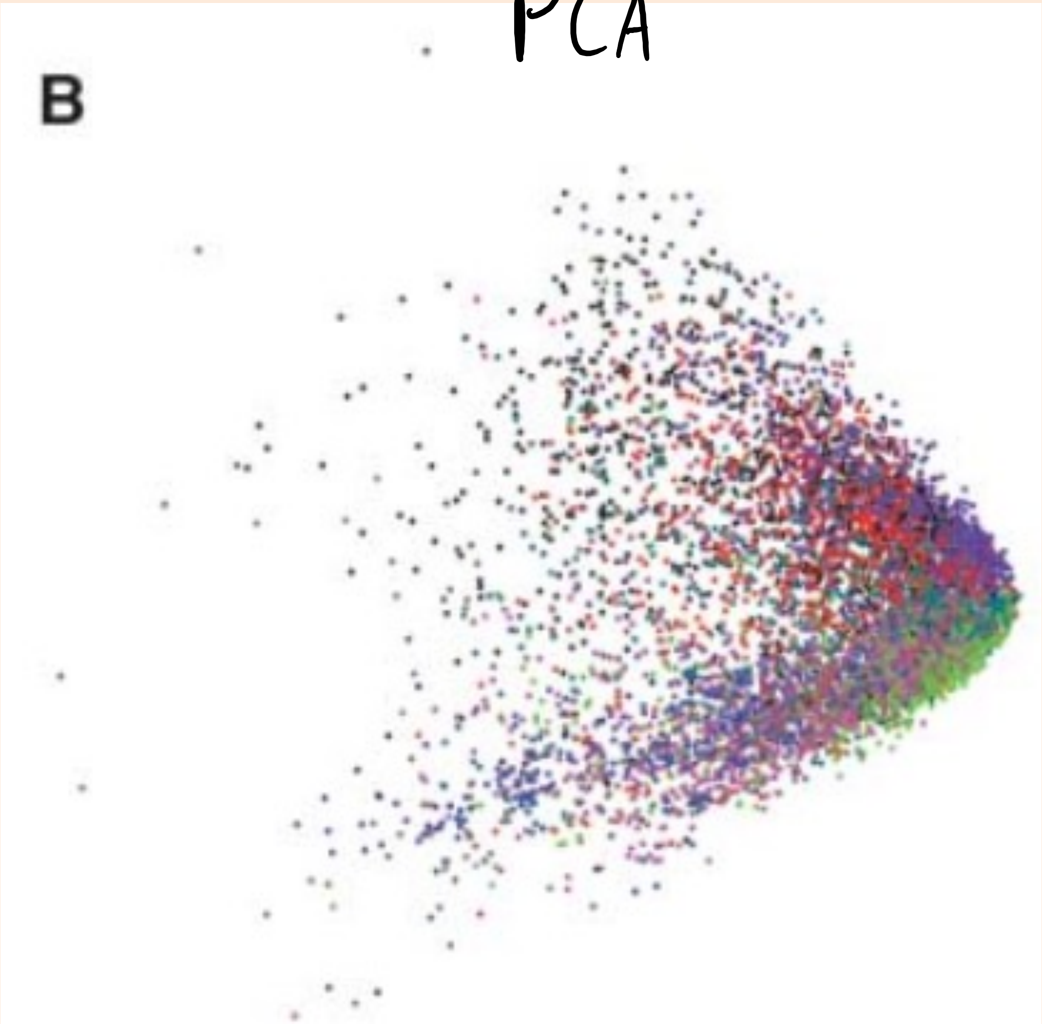
  - Middle layer could be latent features in non-linear latent-factor model.
    - Can do outlier detection, data compression, visualization, etc.
  - A non-linear generalization of PCA.
    - Equivalent to PCA if you don't have non-linearities.

http://inspirehep.net/record/1252540/plots

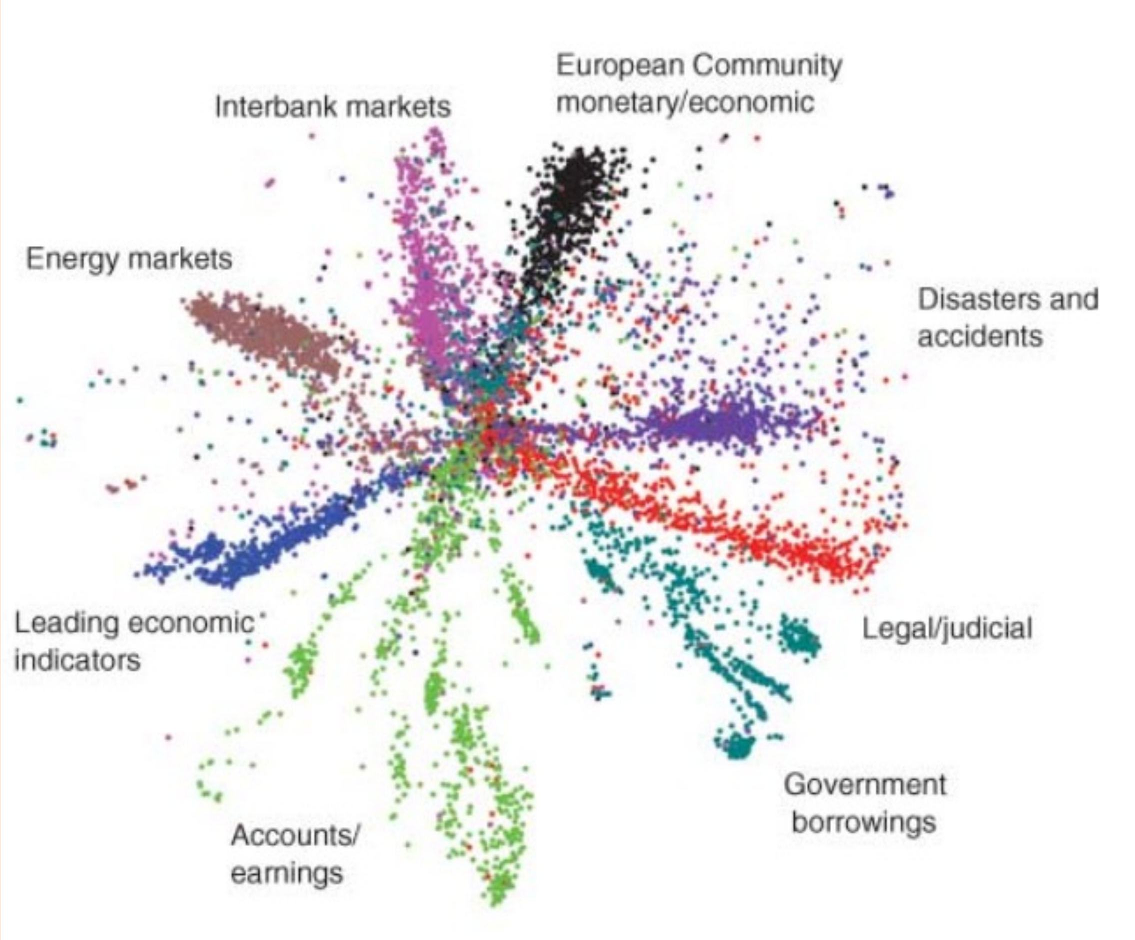
bonus!

Autoencoders

PCA



Autoencoder

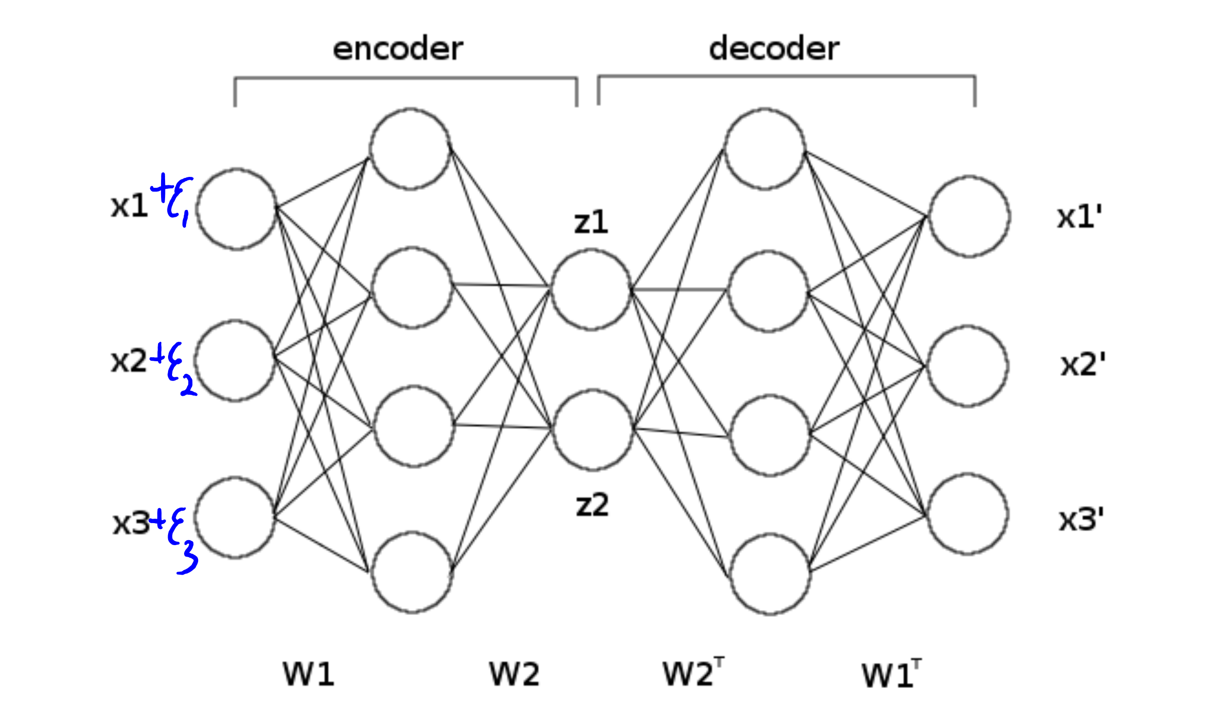


https://www.cs.toronto.edu/~hinton/science.pdf

bonus!

Denoising Autoencoder

- Denoising autoencoders add noise to the input:



  - Learns a model that can remove the noise.

http://inspirehep.net/record/1252540/plots