CS598PS – Machine Learning for Signal Processing

Deep Learning and Stochastic Neural Models

4 November 2020

Today's lecture

- Shallow vs. Deep learning
- Stochastic neural models
  - Deep learning structures
- Tricks that enable deep learning

“Shallow” models

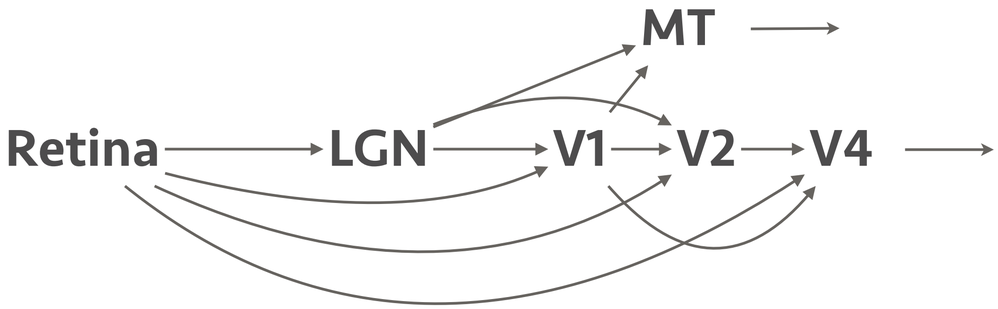
- Most models we used so far were “shallow”

$$\mathbf{y} = \mathbf{W} \cdot \mathbf{x}$$

- Single level of processing (PCA, linear classifier, …)
  - Allows us to use simple representations of the input
    - e.g. linear features, likelihoods, etc.

Looking for depth

- The way we think is inherently hierarchical (i.e. “deep”)
  - e.g. remember the perceptual pathways?
    - Features of features of features, …



  - We don’t really make algorithms like that
    - Maybe we should!

Trying to get some depth

- How about we try multilayer PCA?

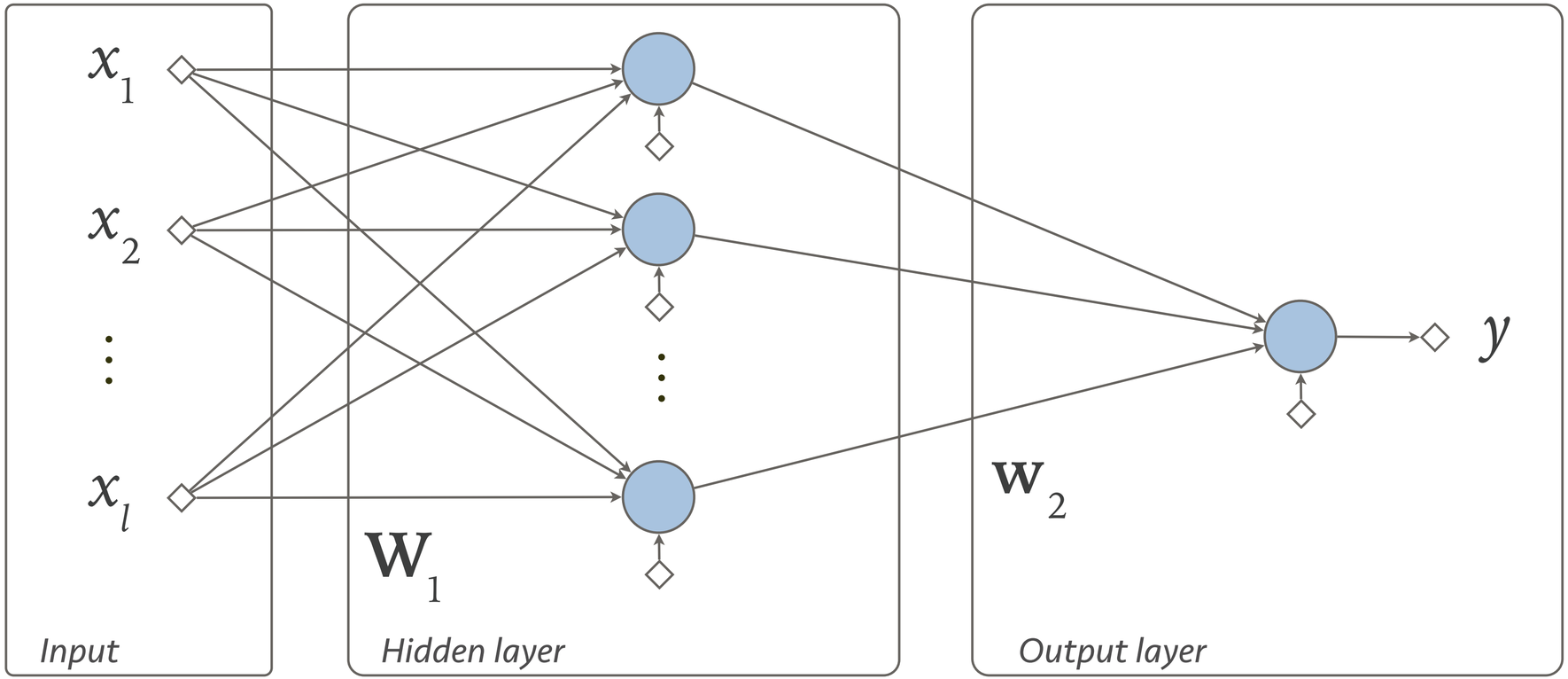
$$\mathbf{y} = \mathbf{W}_1 \cdot \mathbf{W}_2 \cdot \mathbf{x}$$

  - $\mathbf{W}_1$ can contain eigenvectors of eigenvectors!
    - Is that a good idea?

- Not really, $\mathbf{W}_1 = \mathbf{I}$ since $\mathbf{W}_2 \cdot \mathbf{x}$ is whitened already
  - Also with other linear approaches, extra layers make no sense
    - They all collapse to a single linear transform

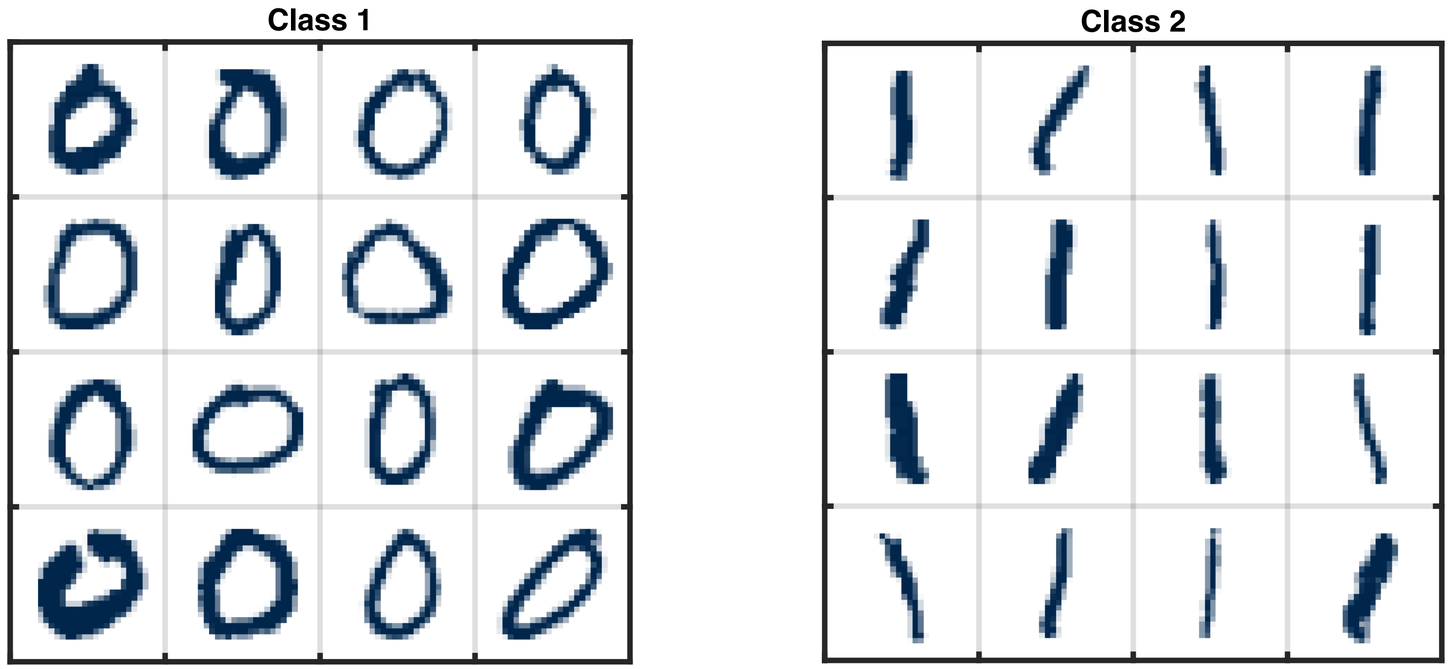
Revisiting the neural net

- An example of a "deep" architecture



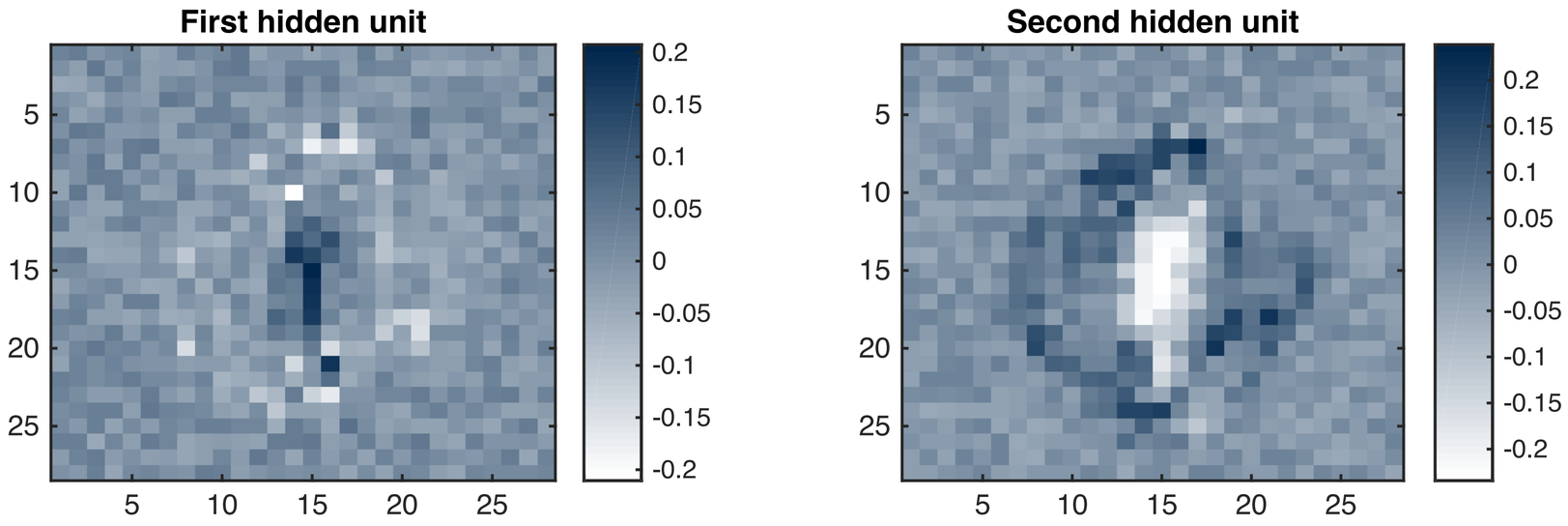
Example classifier

- A “0” vs. “1” digit classifier
  - 2-layer neural net with 2 hidden units and one output



Learned weights

- First layer is a “feature” transform
- Second layer is a simple classifier



The magic ingredient is the non-linearity

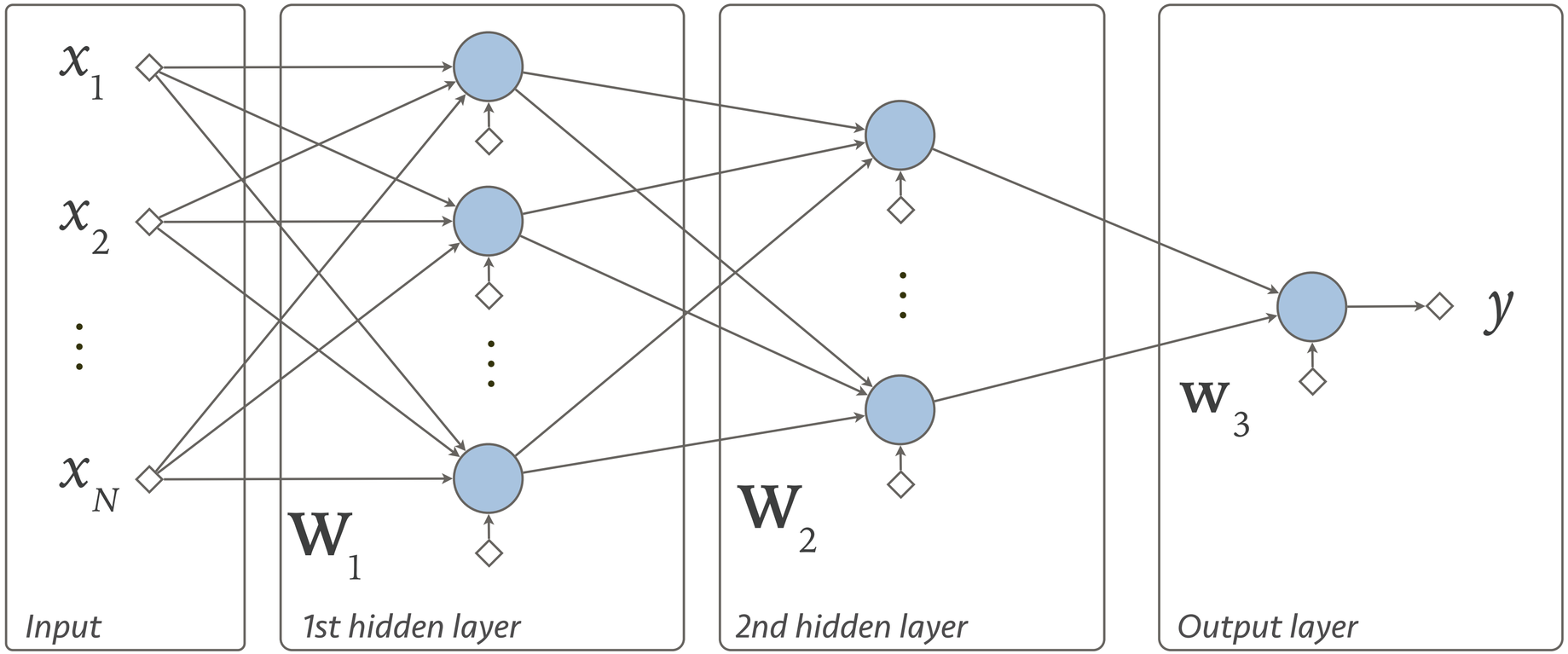
- At every layer we apply a sigmoid:

$$\mathbf{y} = \mathrm{g}\left(\mathbf{W}_1 \cdot \mathrm{g}\left(\mathbf{W}_2 \cdot \mathbf{x}\right)\right)$$

- This allows us to meaningfully *stack* transforms
  - And hence obtain a deep architecture

Multiple levels of features

- First layer contains low-level features, second layer contains mid-level features, …, final layer is a classifier



Arbitrarily deep architectures

- We can stack as many transforms as we like
  - The goal is to find rich representations
  - Thus we make a "deep" model

- The goal is to get features of features of features of ...
  - "Like the brain does"

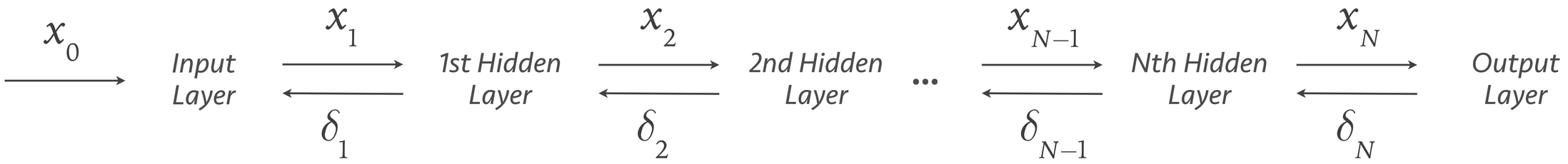
Whoa, wait a minute ...

- You told us that three layers are enough for anything!
  - Why should we use more layers than that?
  - Aren't shallow models good enough?

- Yes, a shallow model is fine, but
  - There is no guarantee that you'll easily find the parameters!
  - Nor that you won't need a bazillion units

But there is a problem with depth

- Deep architectures have lots of parameters
  - In some cases in the billions!
- Typical neural net optimization becomes a problem



Vanishing gradient

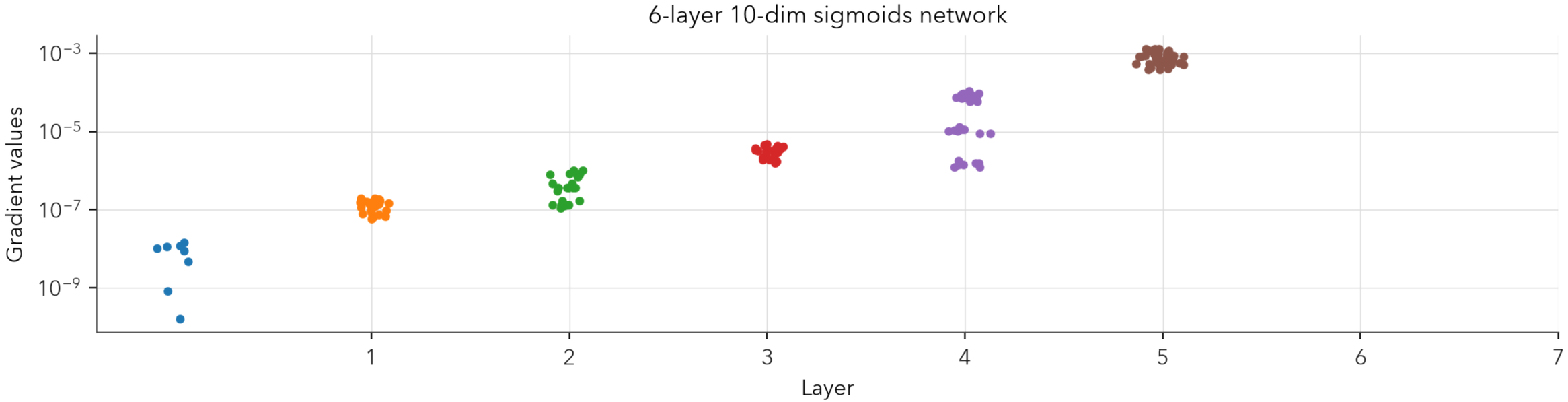
- As we calculate the gradient, we get smaller and smaller values propagating through each layer

Usually between {−1, 1}

$$\mathbf{x}_i = \mathrm{g}\left(\mathbf{W}_i \cdot \mathbf{x}_{i-1}\right)$$

Usually much smaller than 1

$$\delta_i = \left(\mathbf{W}_{i+1}^{\top} \cdot \delta_{i+1}\right) \cdot \mathrm{g}'\left(\mathbf{W}_i \cdot \mathbf{x}_{i-1}\right)$$



Problems with backpropagation

- Through many layers gradient becomes too small
  - We can't propagate errors through too many layers
- Potentially lots of local minima (due to lots of parameters)
  - Even with shallow networks this can be a problem
- Biologically it's a stretch
  - Does the visual cortex influence the retina?
  - Do we really have target values?

Desiderata

- We need a numerically stable learning procedure
- We like biological plausibility
  - Computations should be mostly local
  - We like distributed systems
- We thus need to move away from what we know

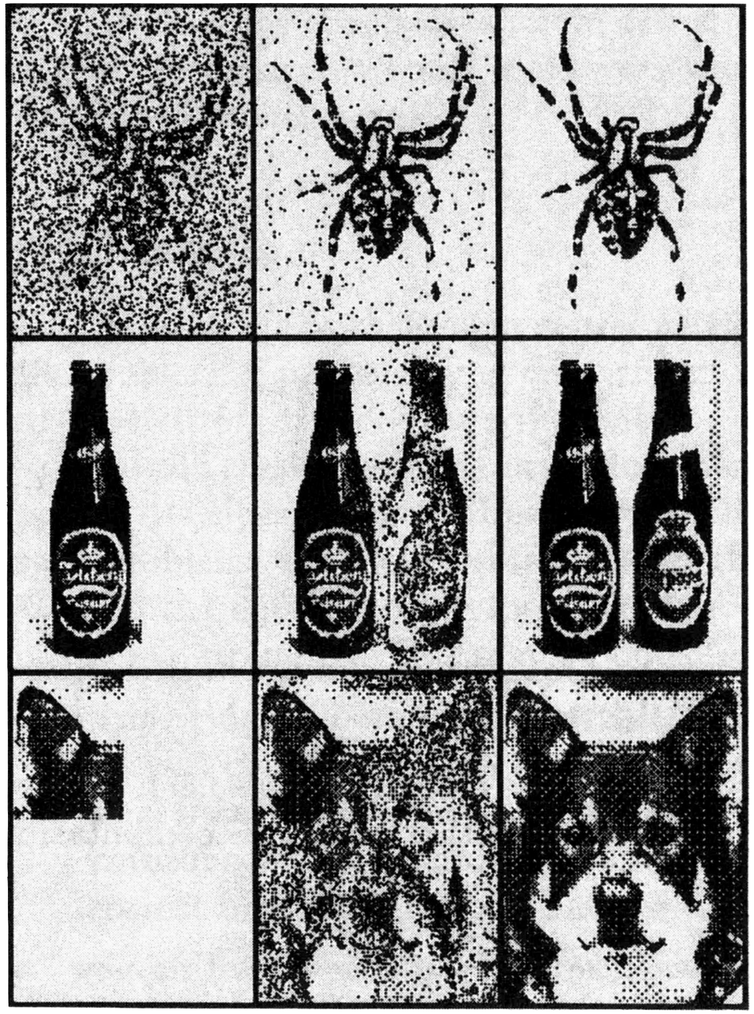
A digression

- A bit on stochastic neural networks
  - A different structure from what we've seen so far
  - Hopfield and Boltzmann models

- Strong influences from physics and neuroscience
  - One of the factors in the resurgence of neural nets

The Hopfield/Boltzmann networks

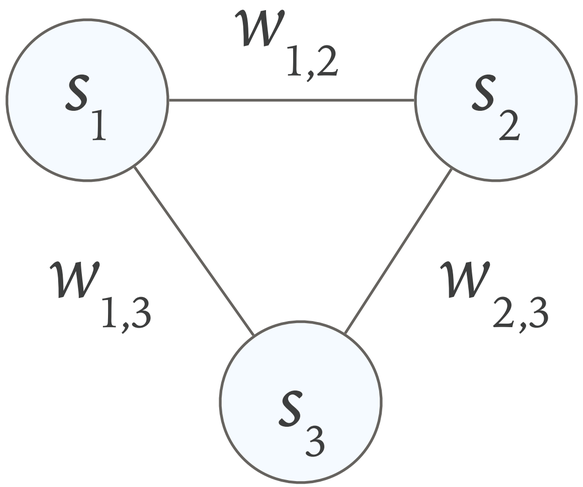
- Auto-associative memory
  - Learns patterns by finding stable equilibria
- Fully connected and recurrent
  - All nodes have binary states {0,1}
- Model can learn to recall patterns



Energy minimization

- Parameters: State $\mathbf{s}_i$, Weight $\mathbf{w}_{ij}$, Threshold θ_i
- After assigning patterns we minimize model "energy"

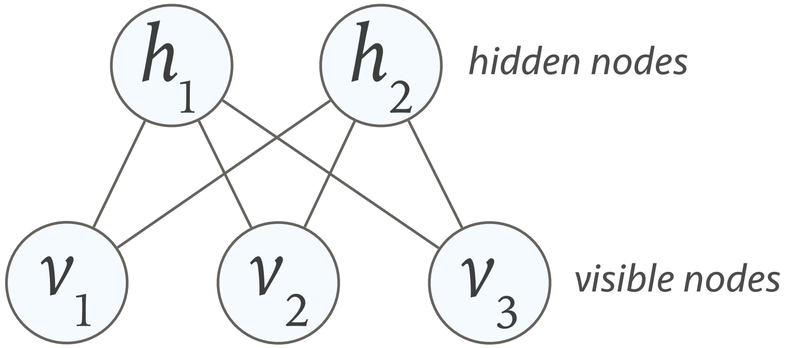
$$E = -\sum_{i<j} w_{i,j} s_i s_j + \sum_i \theta_i s_i$$



- Painful optimization problem!
  - Gradient solution for Hopfield
  - Stochastic solution for Boltzmann

The Restricted Boltzmann Machine (RBM)

- A more manageable form of Boltzmann machines
  - Two-layer, no intra-layer connections



- Visible and hidden nodes
  - Visible nodes represent known data
  - Hidden nodes are used for internal representation

- Easier to train and very useful for many tasks

Getting a handle on RBMs

- Define a *probability* of the network energy:

$$E(\mathbf{v},\mathbf{h}) = -\mathbf{a}^\top \cdot \mathbf{v} - \mathbf{b}^\top \cdot \mathbf{h} - \mathbf{h}^\top \cdot \mathbf{W} \cdot \mathbf{v}$$

$$P(v,h) = \frac{1}{Z} e^{-E(v,h)}$$

  - Z is a *partition function* and $\mathbf{a},\mathbf{b}$ are node biases

- We also define the node probabilities

$$P(h_i \mid v) = \mathrm{g}\left(b_i + \sum_j w_{i,j} v_j\right), \quad P(v_i \mid h) = \mathrm{g}\left(a_i + \sum_j w_{i,j} h_j\right)$$

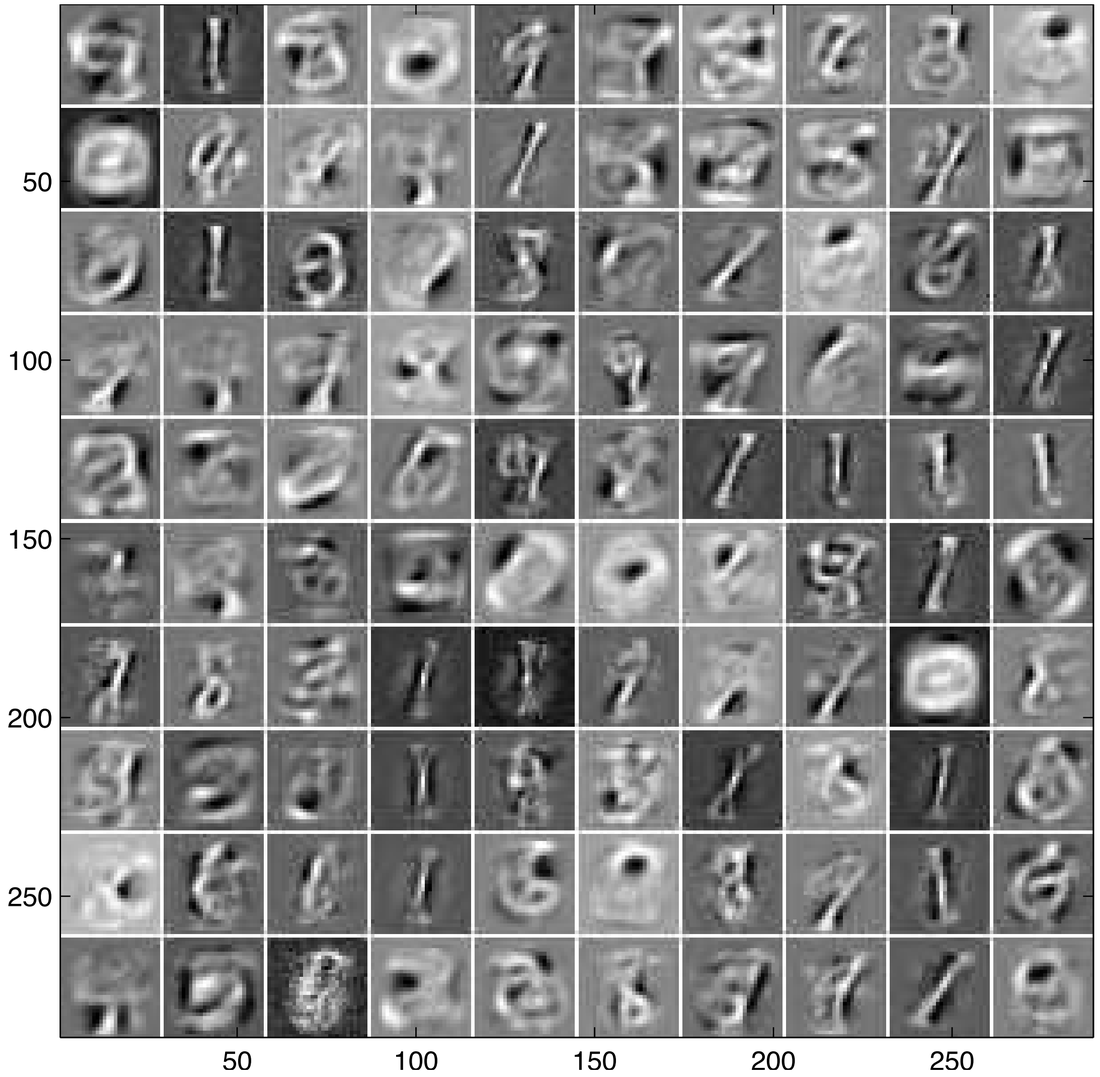
Contrastive Divergence learning

- Maximize product of all $P(\mathbf{v})$
  - 1) For a training sample v_1 compute hidden node probabilities
  - 2) Generate a hidden layer activation vector h_1 from above
  - 3) Go back and generate a new input vector v_2 based on h_1
  - 4) Go forth and generate a new activation vector h_2 from v_2
  - 5) Update corresponding $\mathbf{w}$ using: $\Delta \mathbf{w} \propto v_1 h_1 - v_2 h_2$

"Positive gradient" *"Negative gradient"*

So what does this do?

- Example on digit data
- 28×28 visible nodes
  - Set each pattern to a digit
- 100 hidden nodes
- $\mathbf{W}$ is 784×100
  - i.e. 100 “basis” functions

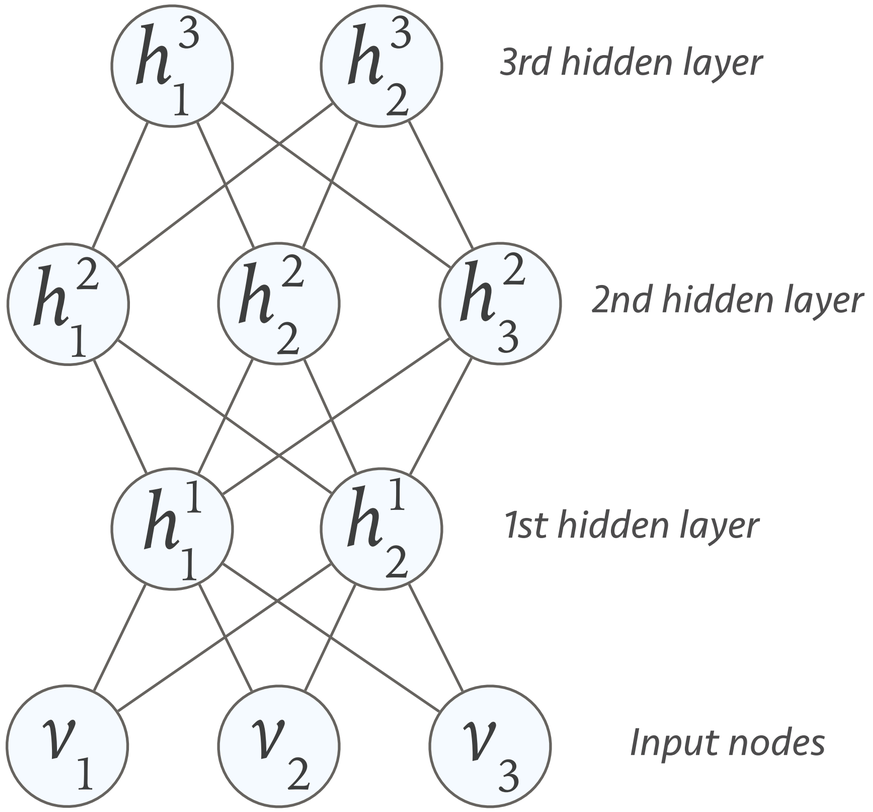


Back to deep learning

- The RBM is a shallow learner
- But we can use it to connect multiple layers
  - Treat each layer in a multi-layer input as an RBM
- The big idea: Train locally, group globally
  - This helps computational complexity and is biologically plausible

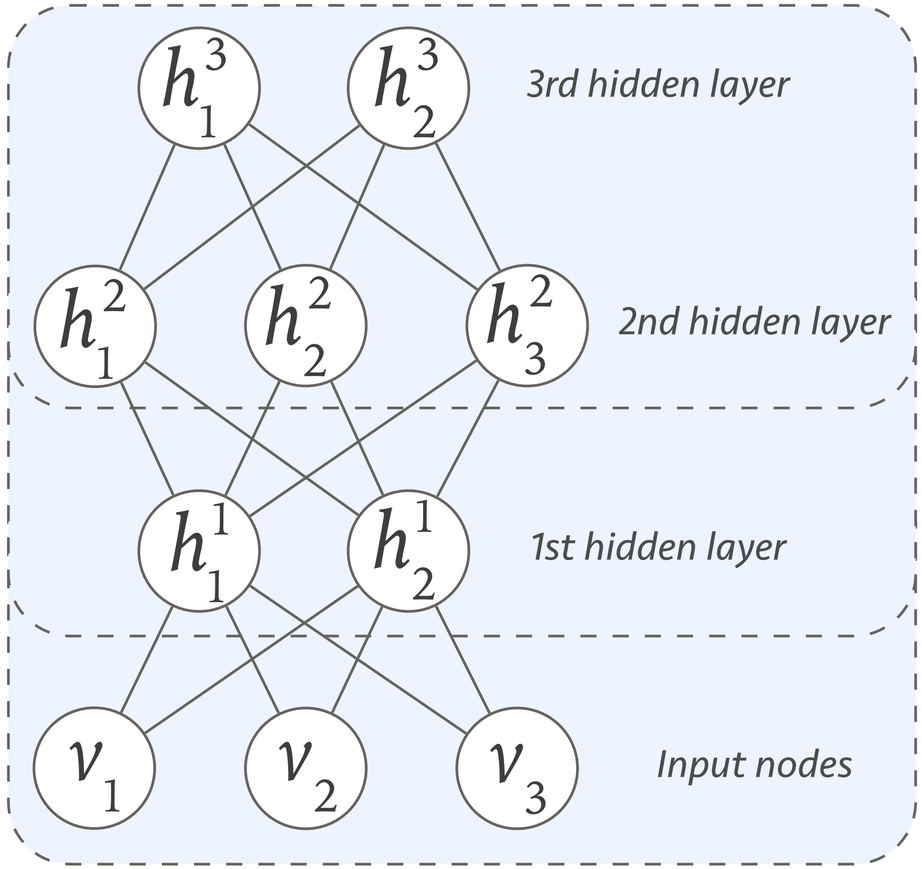
Deep Belief Networks (DBN)

- A stack of multiple RBMs
  - A deep generative model
- Initial weights are set using RBM training
- Further refinement using backpropagation



Greedy learning

- Step 1: Train an RBM for first layer
  - Visible nodes are the inputs
- Step 2: Fix hidden layer
  - Pretend it's visible and train next layer
- Step 3: Keep going



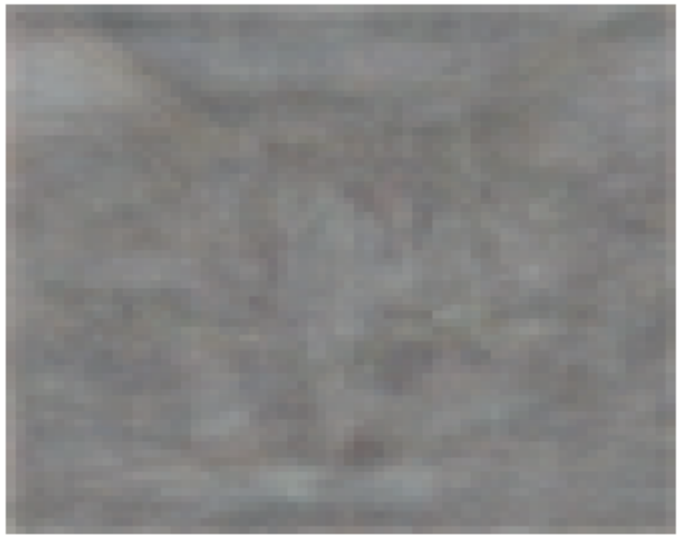
So what is it good for?

- We can learn complex representations of data
  - Learn a deep model with multiple feature levels
- We can learn to classify
  - Use visible nodes to represent classes
- Example simulations on digit data:
  - Hinton's Neural Network Simulation (Generative)
    - Demo: https://www.youtube.com/watch?v=KuPai0ogiHk#t=47s
  - 10 labels / 2000 l3 units / 500 l2 units / l1 500 units / 784 pixels

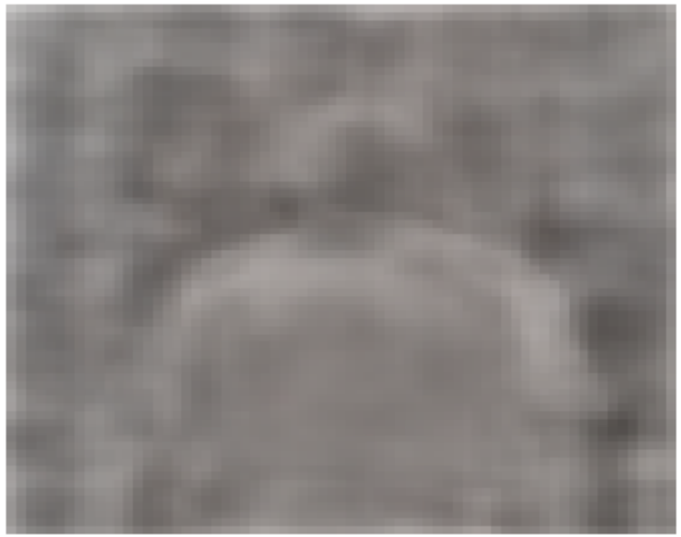
Some well-known press exposure

- A billion weights network trained on 10M YouTube frames
  - 1,000 machines for 3 days!
- Conclusion: YouTube has lots of cats! :)
  - and that we can get some great features that way

The cat neuron



The human body neuron

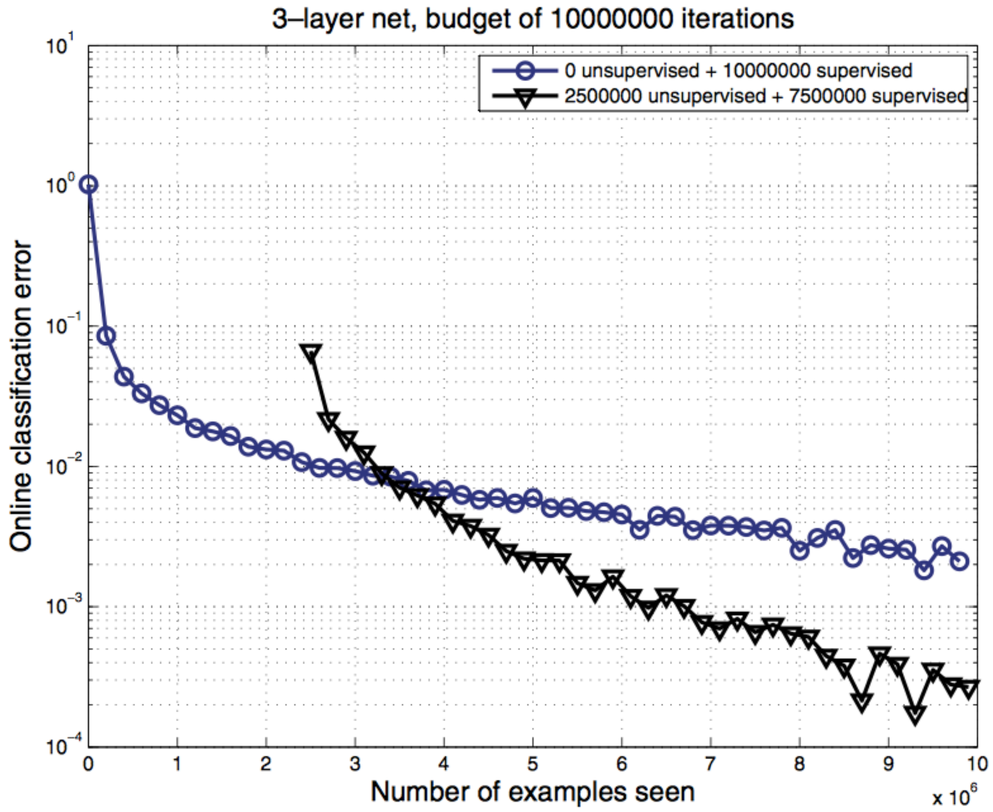


Helping out backpropagation

- We can also use this approach to learn large networks
  - e.g. a multiple layer classification network
- Use greedy learning to find initial values for weights
  - Treat each layer set as an RBM
- Once trained use as initial values for backprop

The importance of a good start

- Find “sensible” weight values
  - Don’t start from irrelevant points
- Starts from a space that is well-tuned to the data at hand
- Reduces the amount of required computations



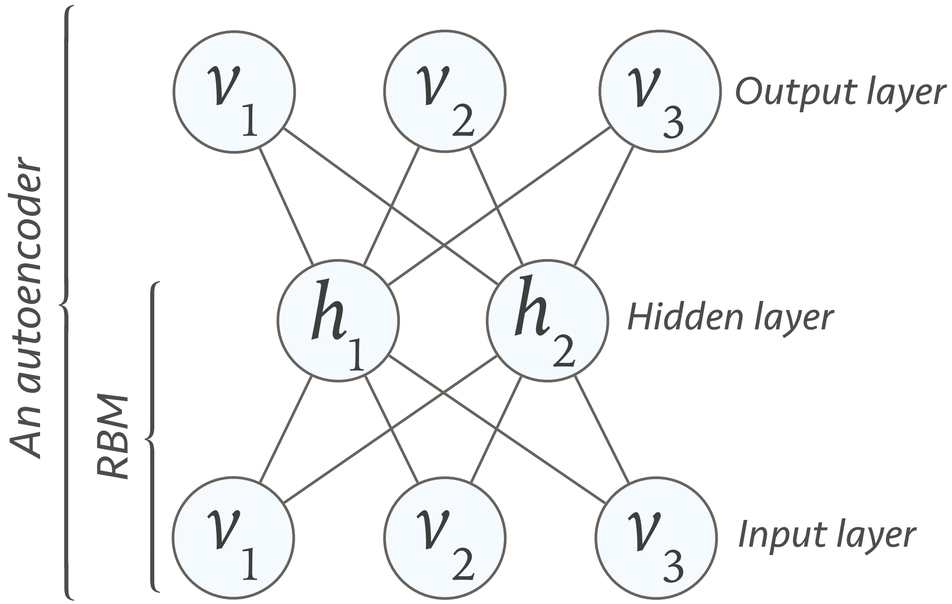
Ugh, that RBM business is difficult …

- There's no reason to stick to RBMs
  - The math is a little tricky and the optimization costly
- Instead we could use another type of "shallow" learner
  - But it has to have a structure conducive to what we want
    - E.g. overcomplete ICA so that we can have more output nodes
- Or we can use an *autoencoder*

Autoencoders

- A very simple approach to designing a shallow non-linear feature extractor

- Try to learn an identity mapping
  - but we won’t make it that easy!
  - We won't give it enough resources



More formally

- Neural net autoencoders
  - Series of layers that lead to a lower dimensional latent representation

$$\mathbf{h} = \mathrm{g}\left(\mathbf{W}_e \cdot \mathbf{x} + \mathbf{b}_e\right) \in \mathbb{R}^K$$

$$\hat{\mathbf{x}} = \mathrm{g}\left(\mathbf{W}_d \cdot \mathbf{h} + \mathbf{b}_d\right) \in \mathbb{R}^{M>K}$$

or

$$\mathbf{h} = \mathrm{g}\left(\mathbf{W}_{e_2} \cdot \mathrm{g}\left(\mathbf{W}_{e_1} \cdot \mathbf{x} + \mathbf{b}_{e_1}\right) + \mathbf{b}_{e_2}\right)$$

$$\hat{\mathbf{x}} = \mathrm{g}\left(\mathbf{W}_{d_2} \cdot \mathrm{g}\left(\mathbf{W}_{d_1} \cdot \mathbf{h} + \mathbf{b}_{d_1}\right) + \mathbf{b}_{d_2}\right)$$

  - And we can just learn this with plain backpropagation

Ways to constraint an autoencoder

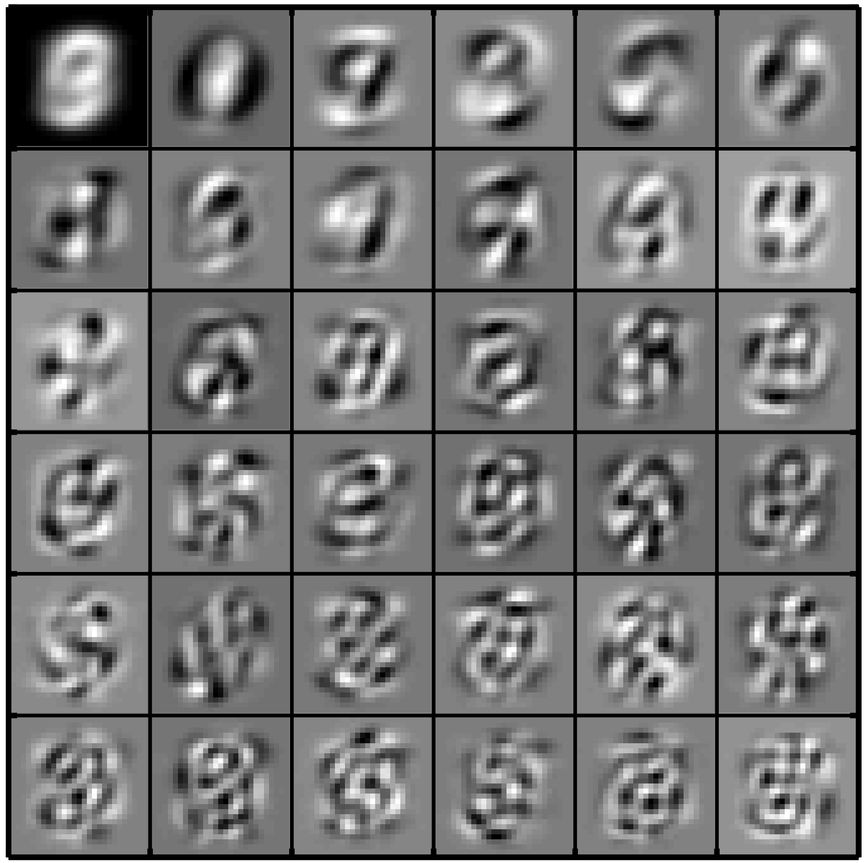
- Restrict the number of hidden nodes
  - Creates an information bottleneck
    - Resulting in an informative low-rank representation
- Go to higher dimensions but use sparsity
  - Creates informative “bases” and projects to high-D space
- Add some structure to the form of the layers
  - e.g. orthogonality, independence, non-negativity, etc.

Neural net PCA *Neural net ICA* *Neural net NMF*

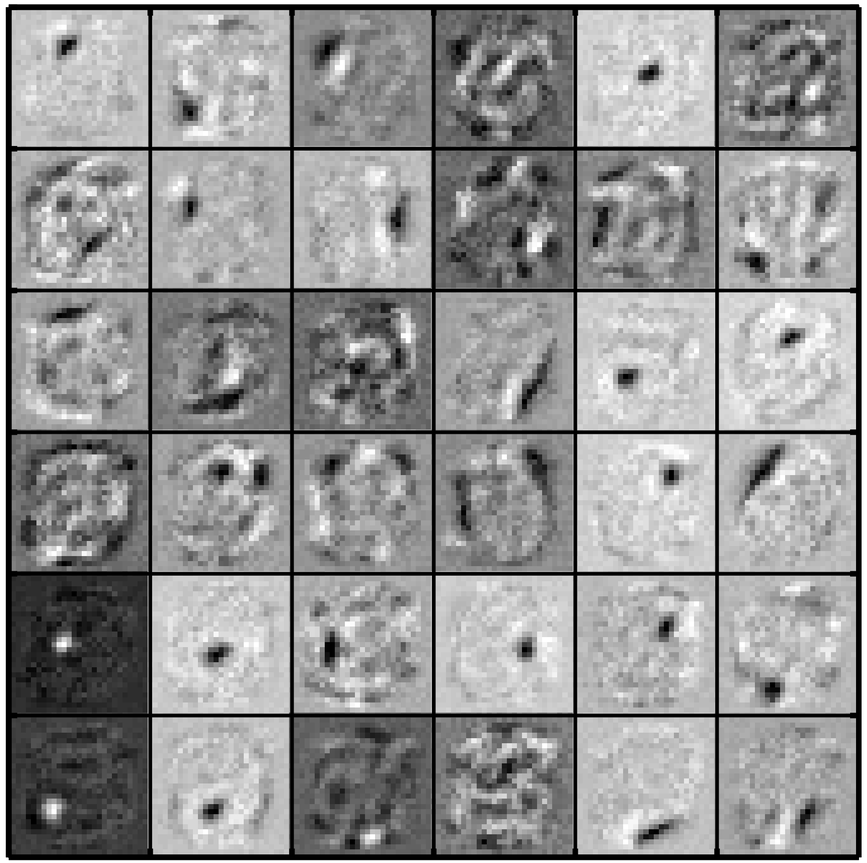
Example case

- Unconstrained AE on digit data

PCA

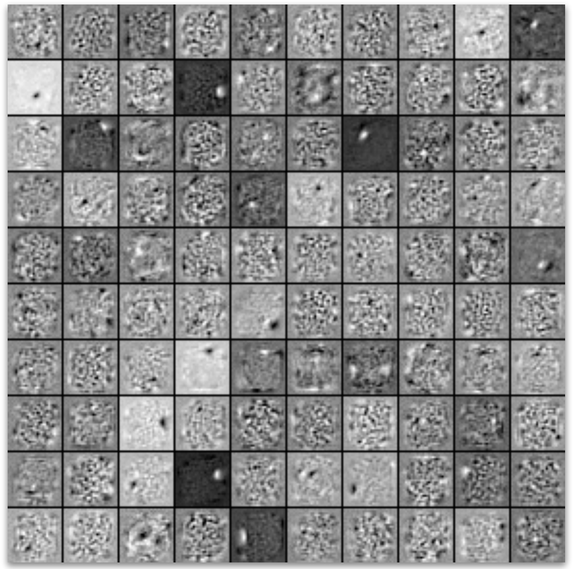


Autoencoder

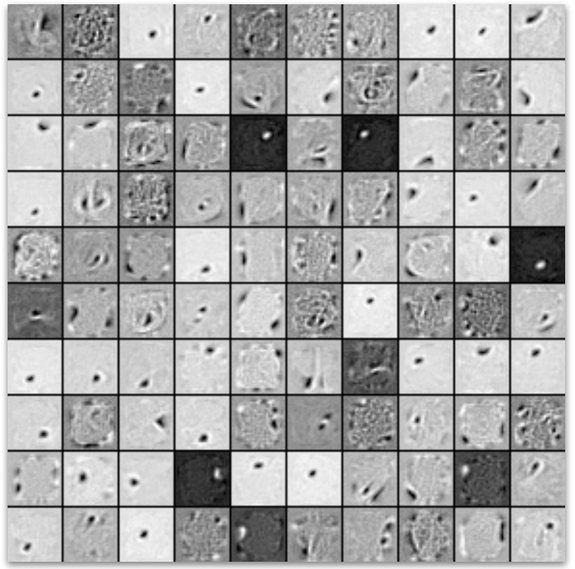


Noisy autoencoders

- Find a “robust” representation
  - But stochastically corrupt the input
  - e.g. adding noise, removing random bits, transform it in non-linear ways, etc.



- Now the input is not always the same as the output
  - We need robust features that map all the noisy inputs to the proper output

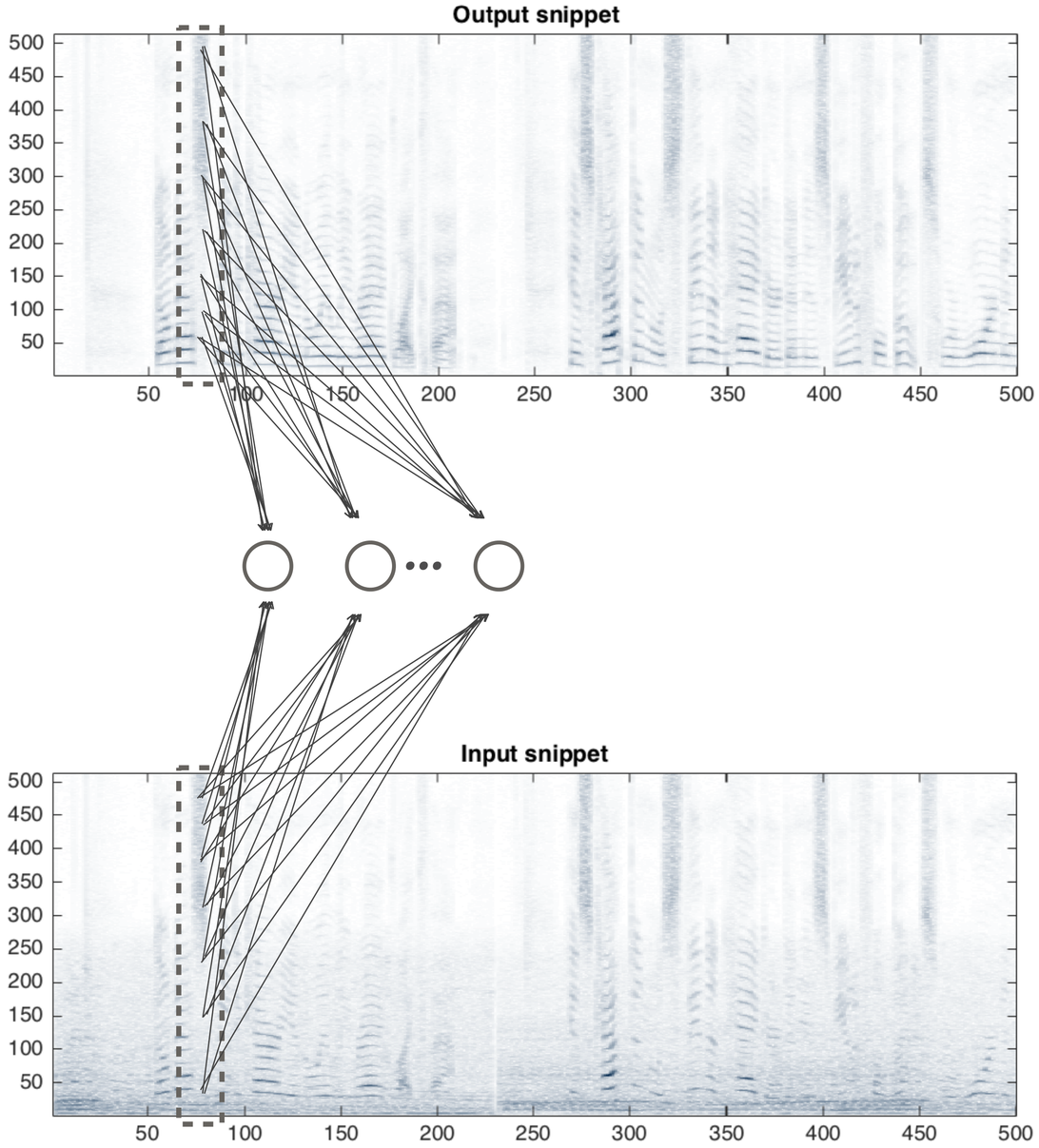


Noisy autoencoders for enhancement

- We can also use noisy autoencoders to clean signals
  - Learn to predict a desirable output for a noisy input
- Can be used for multiple enhancement tasks
  - Removing noise, recovering higher resolution, …
- Generate noisy/clean training data and learn a network

Toy example: Speech denoising

- Trained on 30sec inputs
  - Speech + street noise
  - Known speaker
  - Takes 30sec to train
    - on a laptop (2-3sec with GPU)
- Parameters
  - 1024pt spectra
  - 1 hidden layer, 100 nodes
  - Leaky ReLU activations

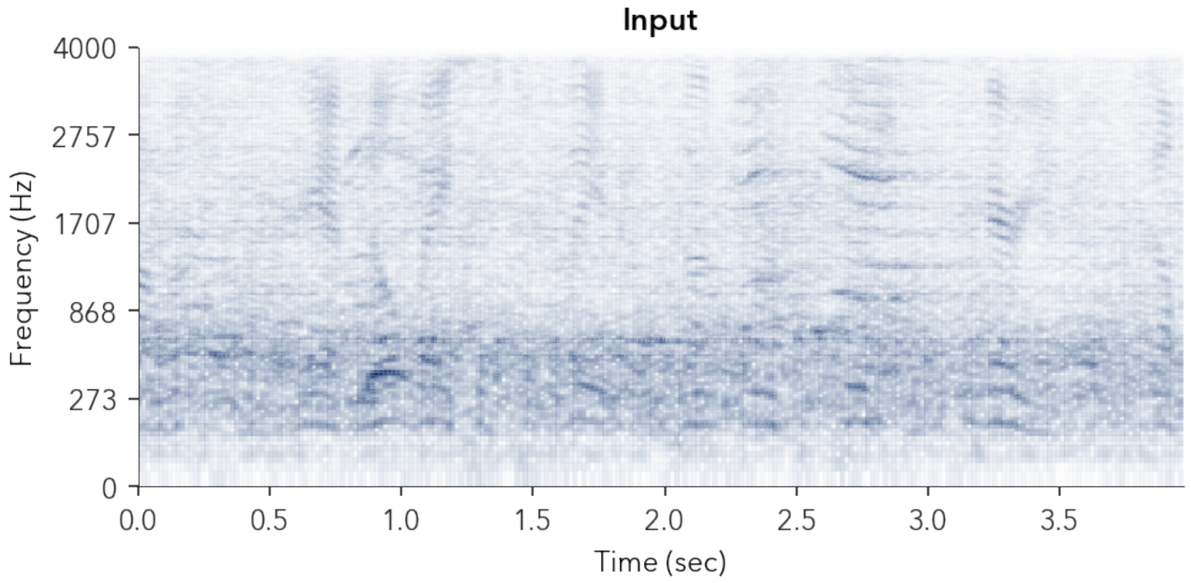


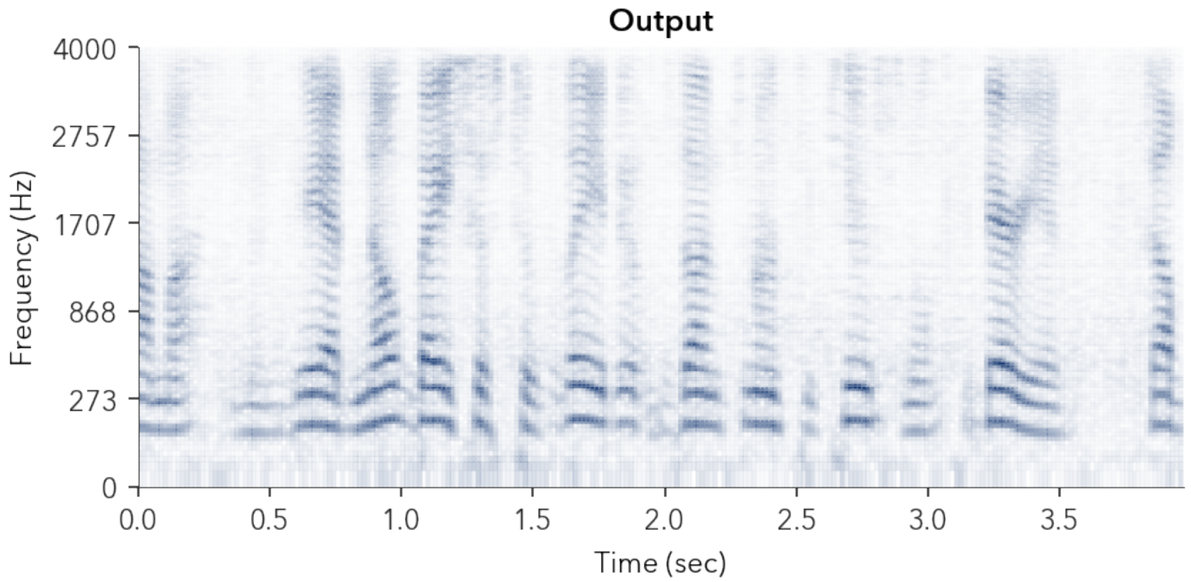
Runtime denoising

- Very lightweight process
  - ~300x real-time
    - 0.01sec in this case
- Works better than NMF
  - But cannot generalize to new noise types!

Input mixture

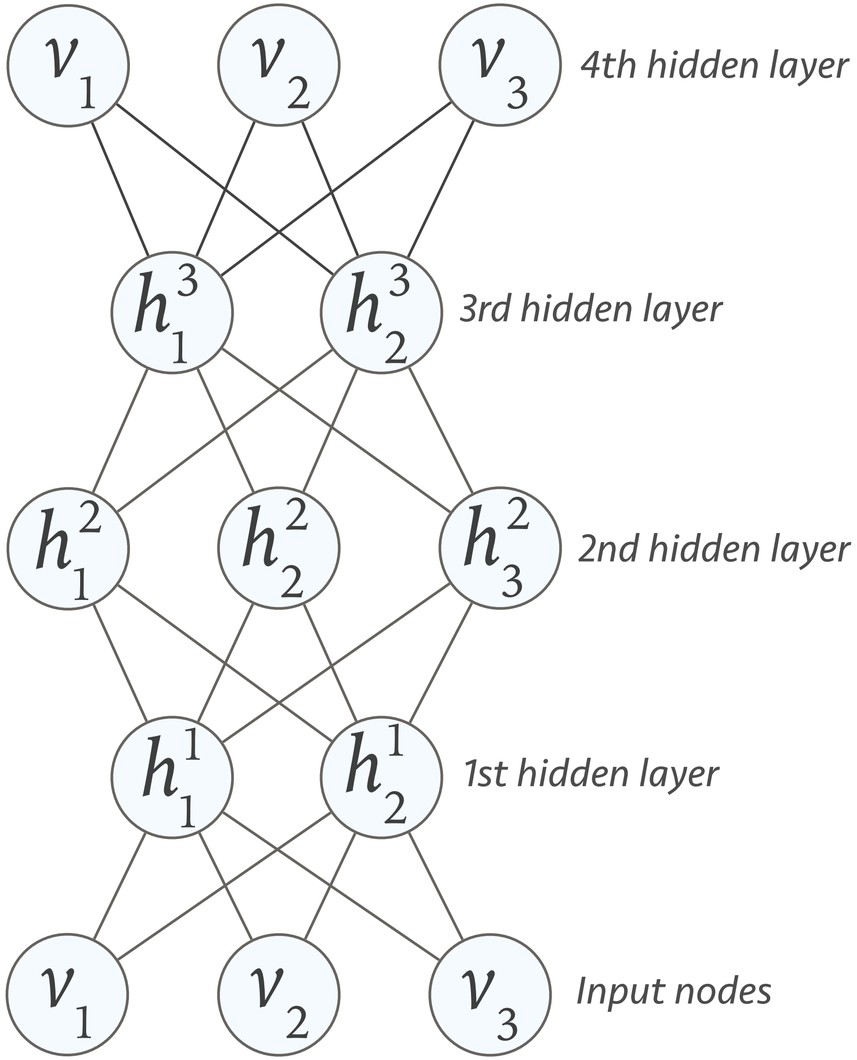
Predicted output





Stacked autoencoders

- Similar to DBNs
  - Multiple-layer architecture
  - Train each layer separately
    - Stack them all in the end
- Can also be used to classify
  - Once trained, add a classification layer and refine with backprop



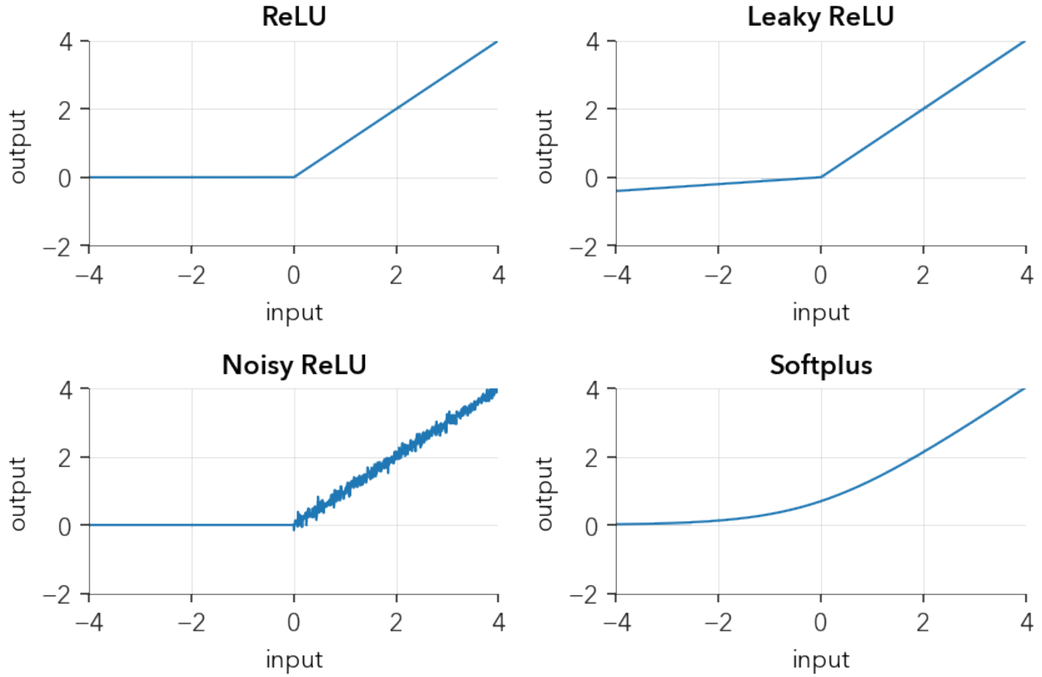
So what's new from the 90's?

- The cynical view: Not much
  - We have more data and faster processors
    - So we can train deeper models with more data

- But, we now have many more tricks of the trade
  - Better activations, smarter training strategies, many little tricks to assist better convergence, more elaborate models than before
  - Many techniques to avoid vanishing gradients

Modern activation functions

- Rectified Linear Units (ReLU's)
  - Instead of a sigmoid use: $y_i = \max(0, x_i)$
  - Much faster since there is minimal computation
    - Leaky versions: $y_i = x_i \text{ if } x_i > 0 \text{ else } a\, x_i$
    - Noisy versions: $y_i = \max(0, x_i + n_i), \ldots$
  - Doesn't saturate as much
- Softplus: $y_i = \log(1 + e^{x_i})$
  - "Softer" version of ReLU



Dropout for better training

- Drop-out training
  - Randomly “turn off” units at every training iteration
    - Usually 50%
  - Puts pressure on units to be useful

- Results in a more robust networks
  - Equivalent to training multiple nets with shared weights, but slightly different connectivity patterns

Updating the weights

- Gradient descent

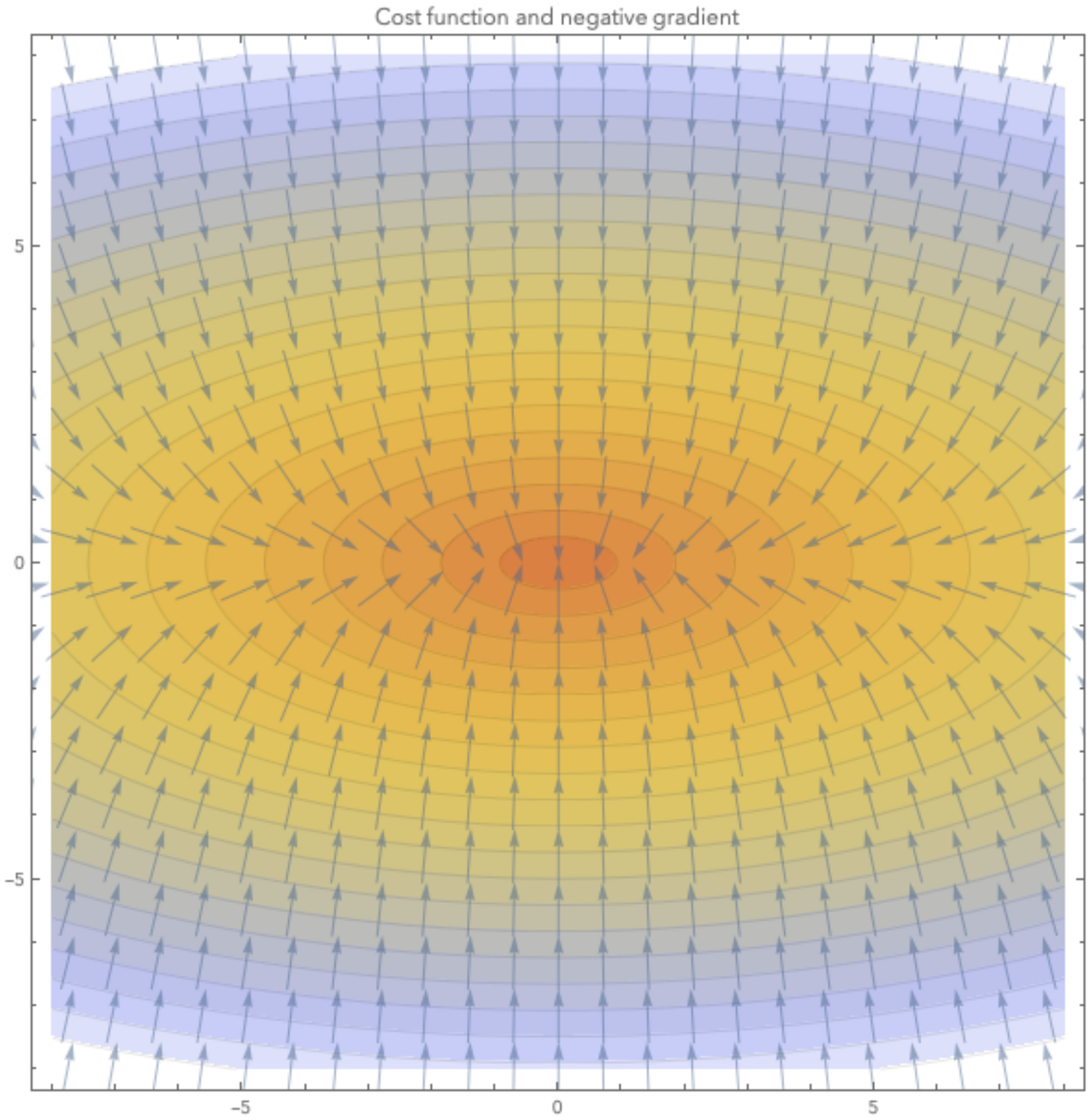
$$\mathbf{w}_{t+1} = \mathbf{w}_t - \eta \nabla f(\mathbf{w}_t)$$

Learning rate → η

$\mathbf{w}_t$ ← *Parameters*

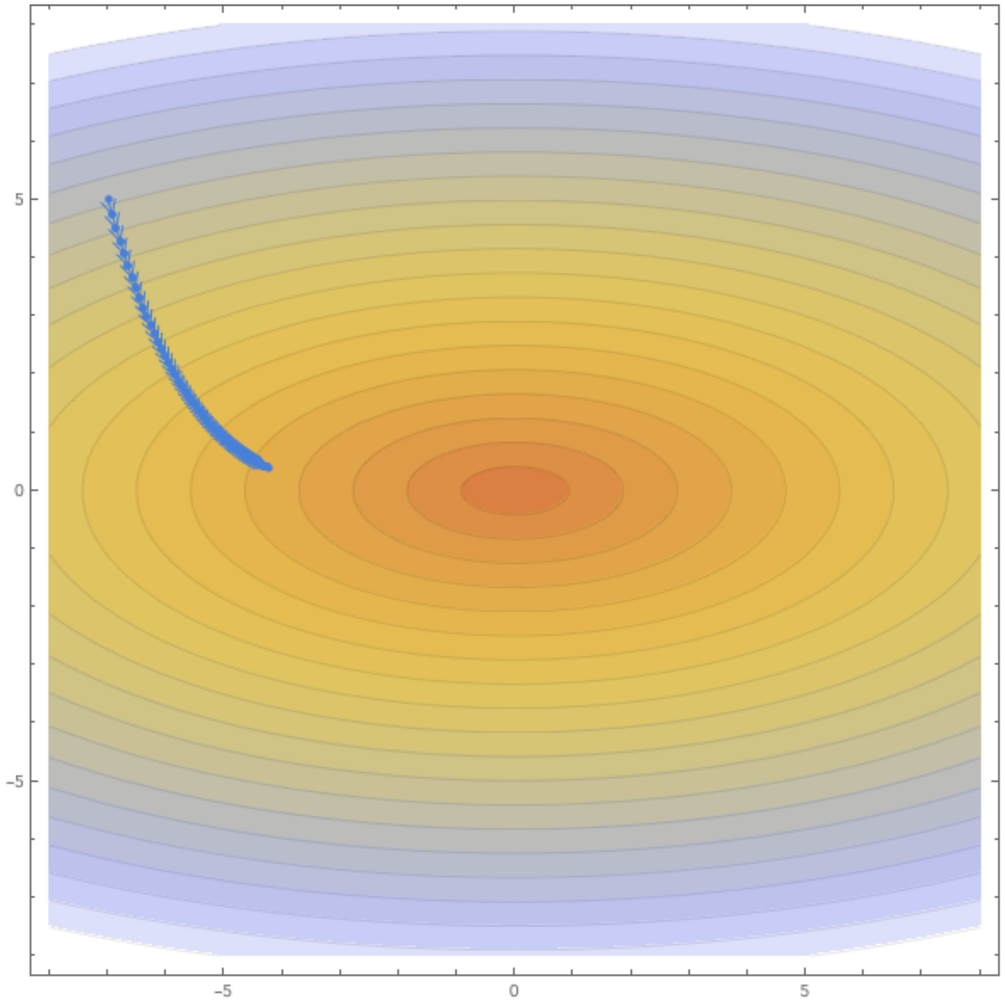
$\nabla f(\mathbf{w}_t)$ ← *Neural network*

- η is learning rate
  - How much to move along
  - Usually $\eta = 0.01$-ish
- We can also average over multiple passes (batch)

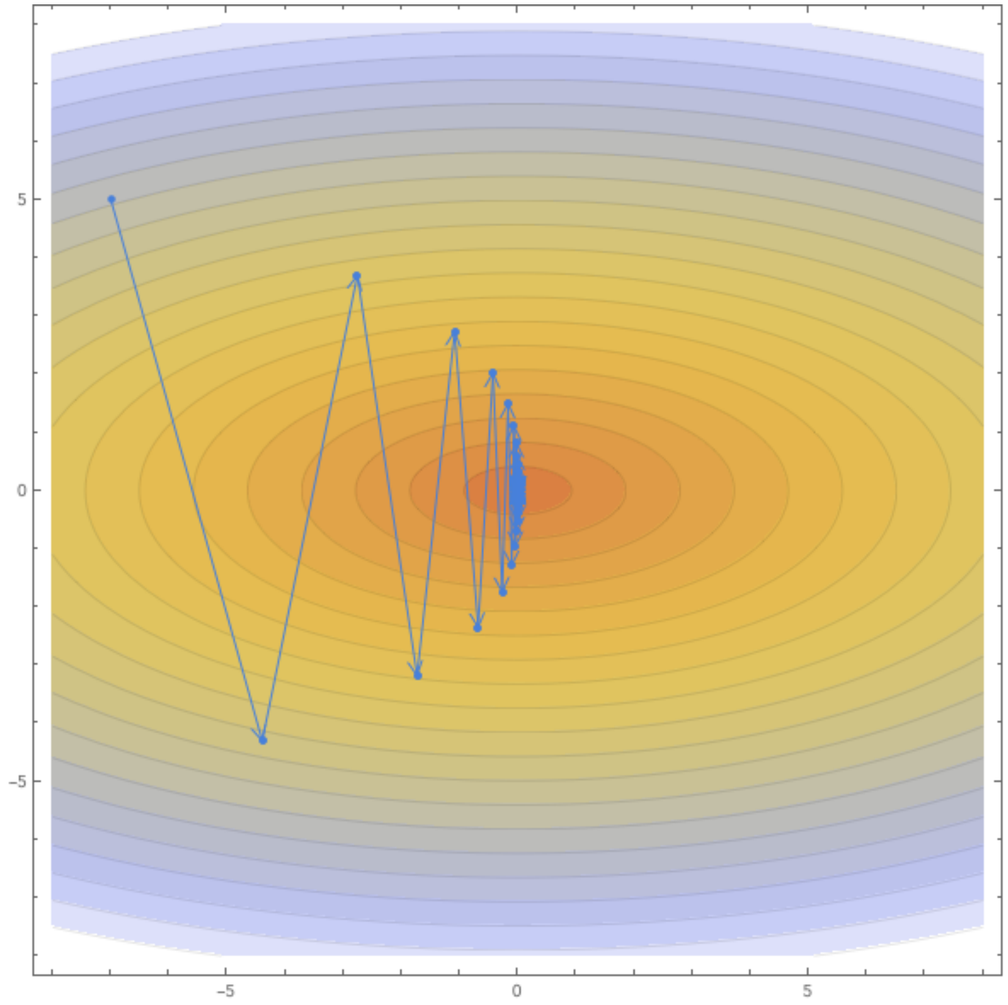


Some problems

Small learning rate ⟶ slow convergence



Large learning rate ⟶ erratic movements



Momentum

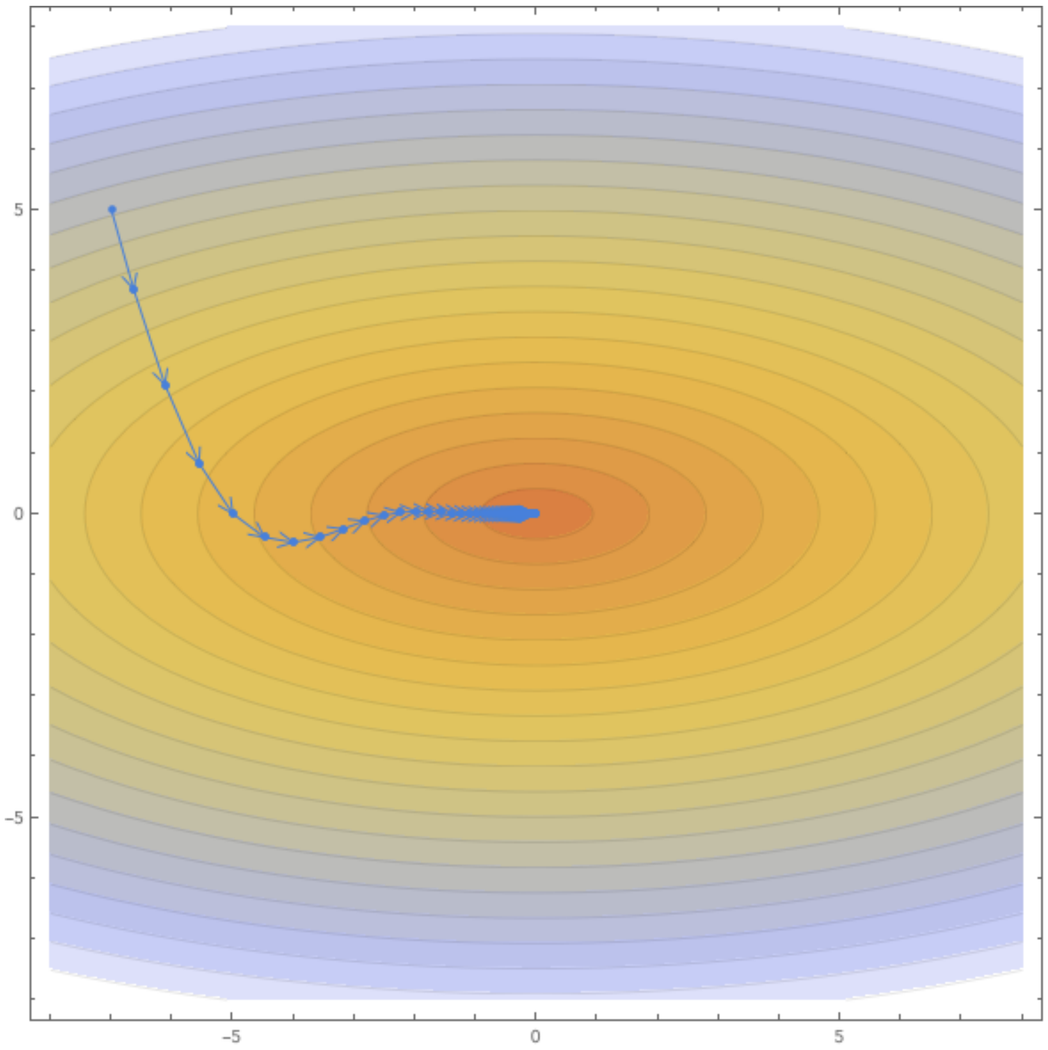
- Lowpass filter the gradient
  - Removes jerkiness
  - Reinforces consistent movements

$$\mathbf{u}_t = \eta \nabla f(\mathbf{w}_t) + \mu \mathbf{u}_{t-1}$$

$$\mathbf{w}_{t+1} = \mathbf{w}_t - \mathbf{u}_t$$

  - Usually $\mu = 0.9$-ish

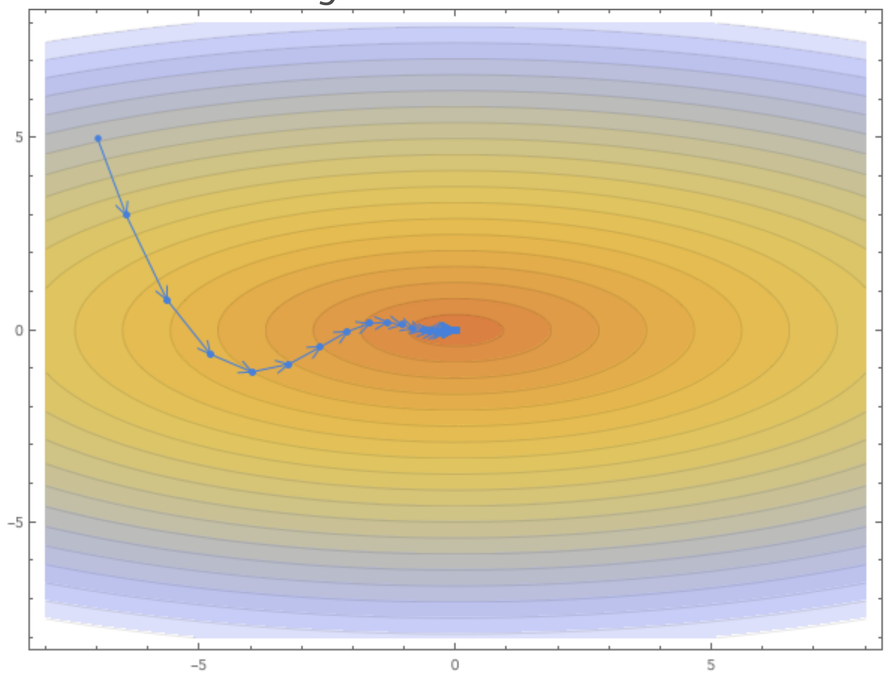
Momentum smooths update track



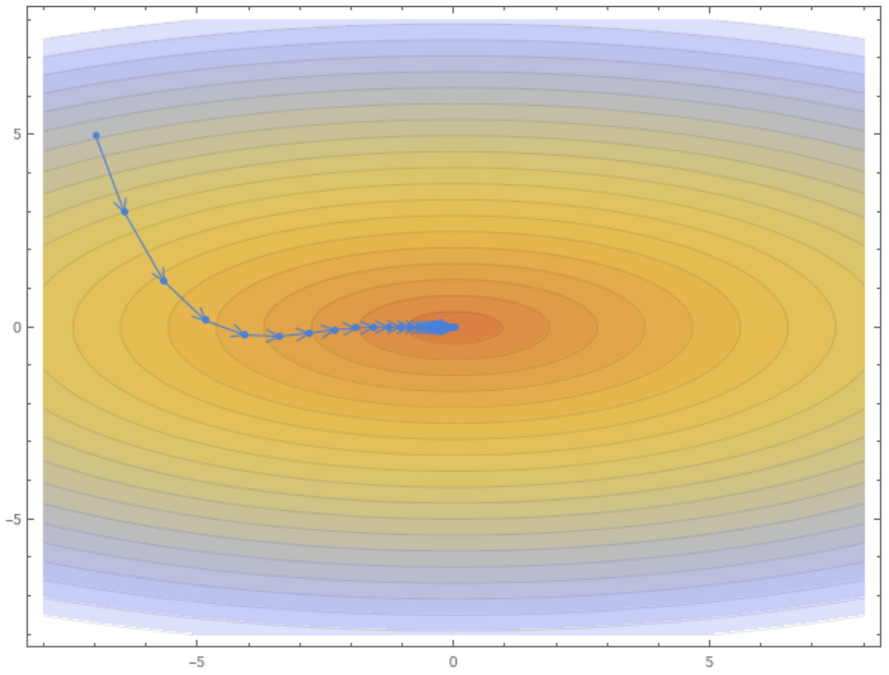
Nesterov accelerated gradient

- Momentum is not quite right
  - We use the gradient without accounting for momentum offset
  - Instead do: $\mathbf{u}_t = \eta \nabla f(\mathbf{w}_t - \mu \mathbf{u}_{t-1}) + \mu \mathbf{u}_{t-1}$

Regular momentum



Nesterov



Per-parameter learning rate

- Use a different rate for each parameter's update
  - *Adagrad*: penalize consistently large updates
    - Move faster on flatter dimensions, cautiously on bumpy ones

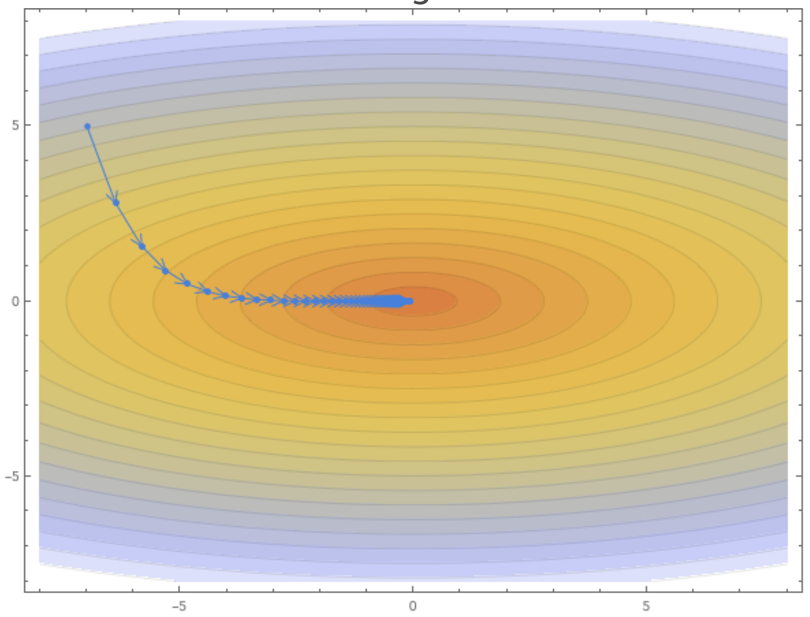
Adagrad

$$\mathbf{g}_{t+1} = \mathbf{g}_t + \nabla f(\mathbf{w}_t)^2$$

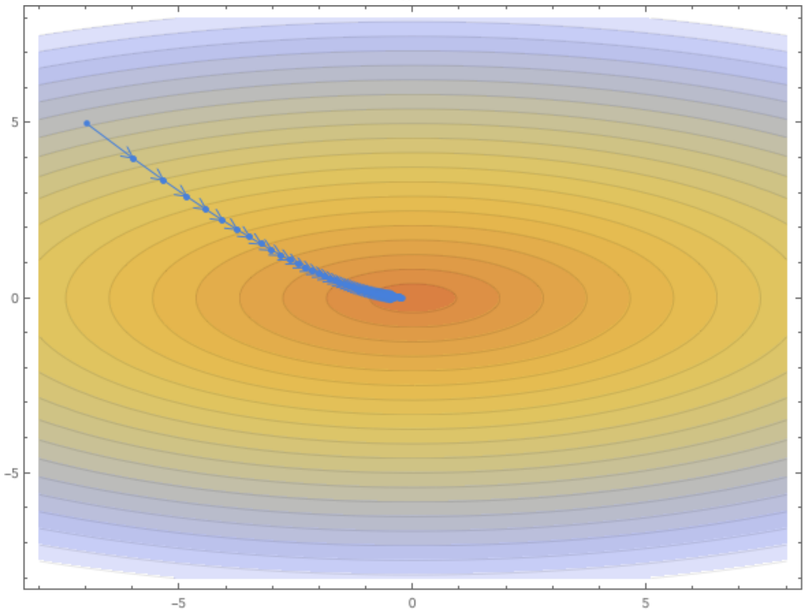
$$\mathbf{w}_{t+1} = \mathbf{w}_t - \eta \frac{\nabla f(\mathbf{w}_t)}{\sqrt{\sum_{k=0}^{t+1} \mathbf{g}_k^2}}$$

Divide each parameter's update by accumulated amount of past updates

Unscaled gradient



Adagrad



Embellishments

- Adagrad slows down to a halt after a while
  - Scaling becomes increasingly larger, updates tend to zero
  - *RMSprop* resolves that with an online estimate
  - *Adam* additionally smooths gradient (with a momentum)

RMSprop

$$\mathbf{g}_{t+1} = \gamma \mathbf{g}_t + (1-\gamma) \nabla f(\mathbf{w}_t)^2$$

$$\mathbf{w}_{t+1} = \mathbf{w}_t - \eta \frac{\nabla f(\mathbf{w}_t)}{\sqrt{\mathbf{g}_{t+1}}}$$

Same as Adagrad, but get online estimate of $\mathbf{g}$

Adam

$$\mathbf{m}_{t+1} = \beta_1 \mathbf{m}_t + (1-\beta_1) \nabla f(\mathbf{w}_t)$$

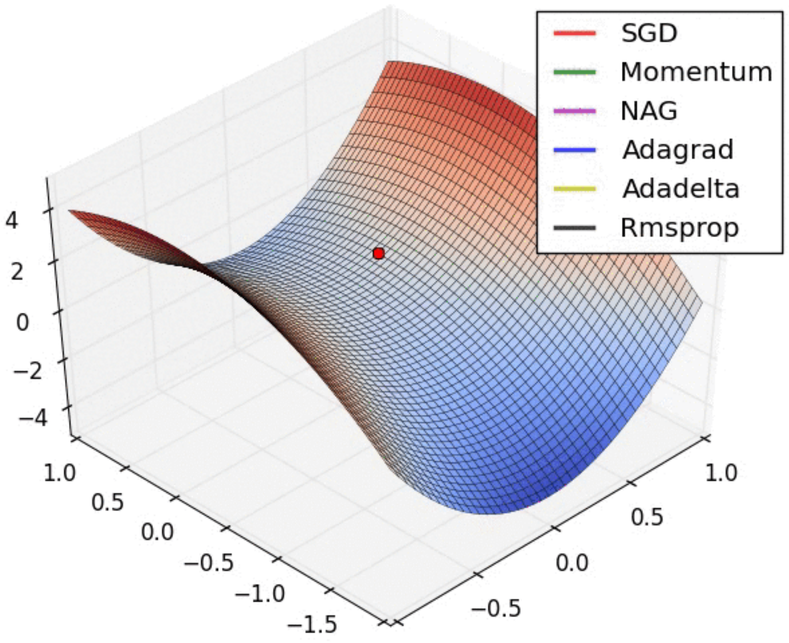
$$\mathbf{g}_{t+1} = \beta_2 \mathbf{g}_t + (1-\beta_2) \nabla f(\mathbf{w}_t)^2$$

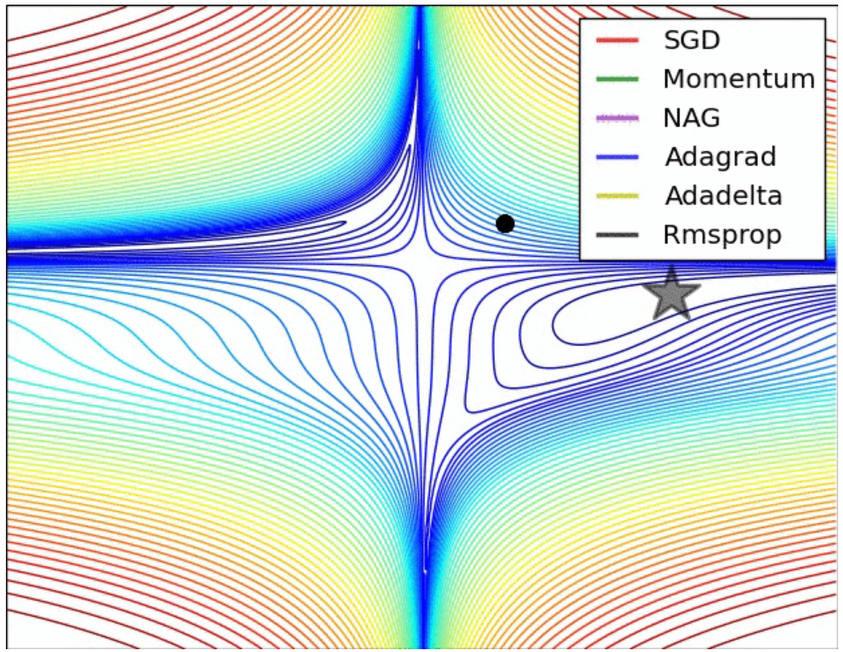
$$\mathbf{w}_{t+1} = \mathbf{w}_t - \eta \frac{\mathbf{m}_{t+1}}{\sqrt{\mathbf{g}_{t+1}}}$$

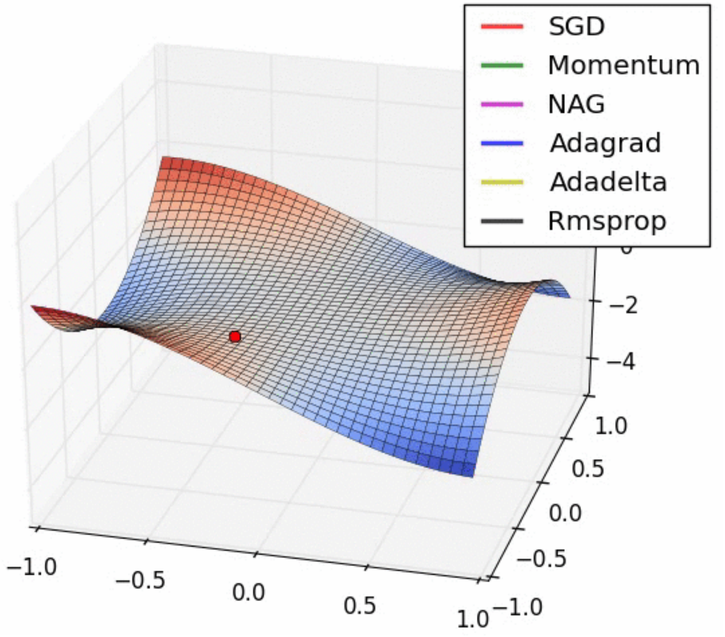
Same as RMSprop, get smooth estimate of gradient as well

What difference does it make?

- Alec Radford's excellent optimization animations:







http://imgur.com/a/Hqolp

Second-order updates

- We can also update using 2nd order methods:

$$\mathbf{w}_{t+1} = \mathbf{w}_t - \eta Hf(\mathbf{w}_t)^{-1} \nabla f(\mathbf{w}_t)$$

Hessian matrix *Gradient vector*

- Problems
  - Hessian is # parameters squared (i.e. a large matrix)
  - Computing its inverse is flaky and slow
- Alternatives (e.g. L-BFGS) exist, but can be inefficient
  - In practice, gradient methods are a better choice

Batch normalization

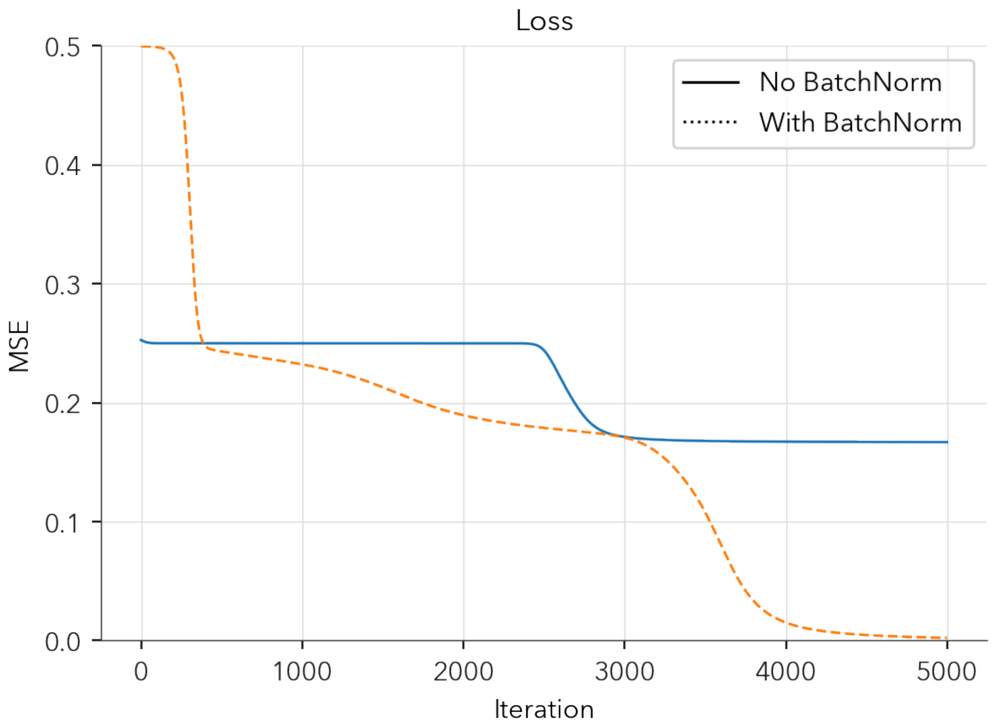
- We can also help the network by normalizing outputs
  - Scale and translate each batch:

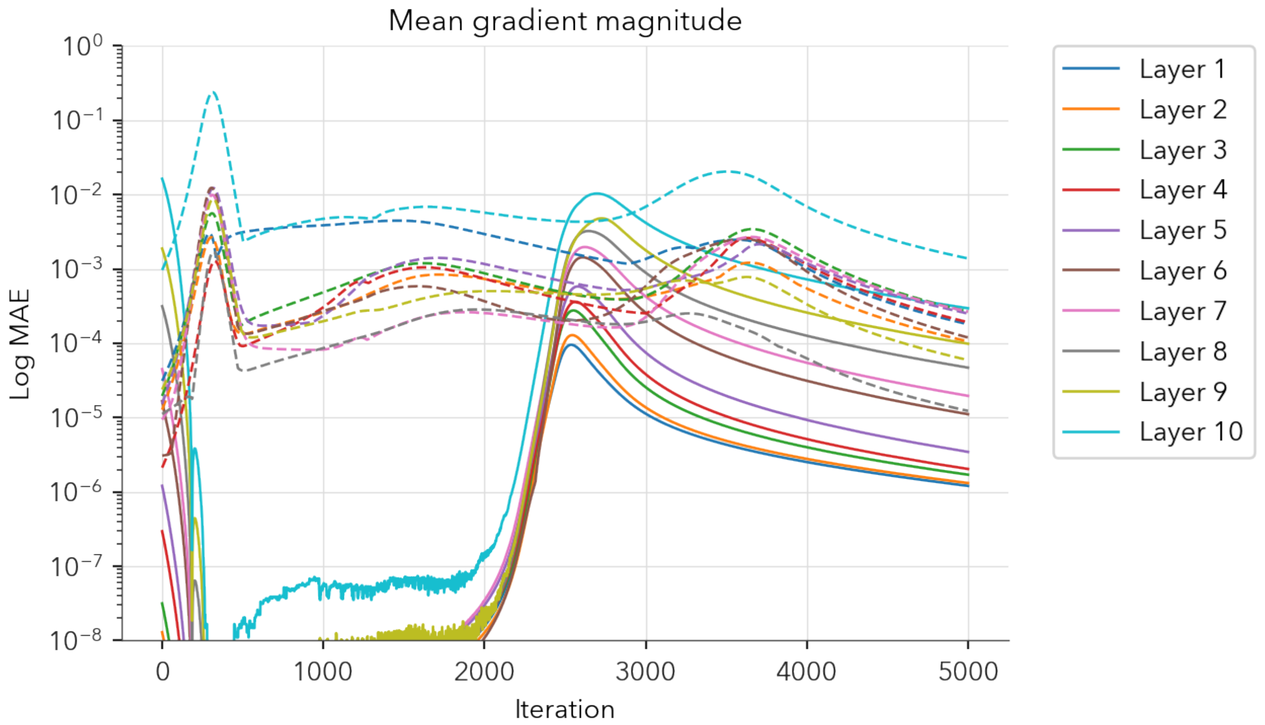
$$\mathbf{x}_i = \mathrm{g}\left(\mathbf{W}_i \cdot \mathbf{x}_{i-1}\right) \qquad \hat{\mathbf{x}}_i = \gamma \frac{\mathbf{x}_i - \mu_{\mathbf{x}_i}}{\sigma_{\mathbf{x}_i}} + \beta$$

    - Learn optimal parameters γ and β
    - Estimate μ and σ online from training data
- Ensures that layer's inputs do not saturate the layer
  - Saturating a layer results in small gradients

Effect of BatchNorm in training

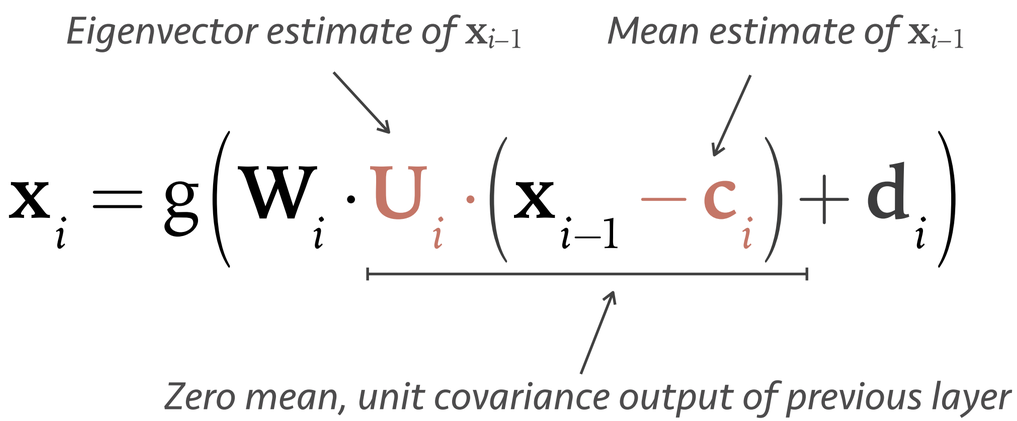
- Same network trained without and with BatchNorm
  - Using BatchNorm helps speed up convergence
  - Gradient magnitudes are more reasonable (in IEEE float format)





PRONG

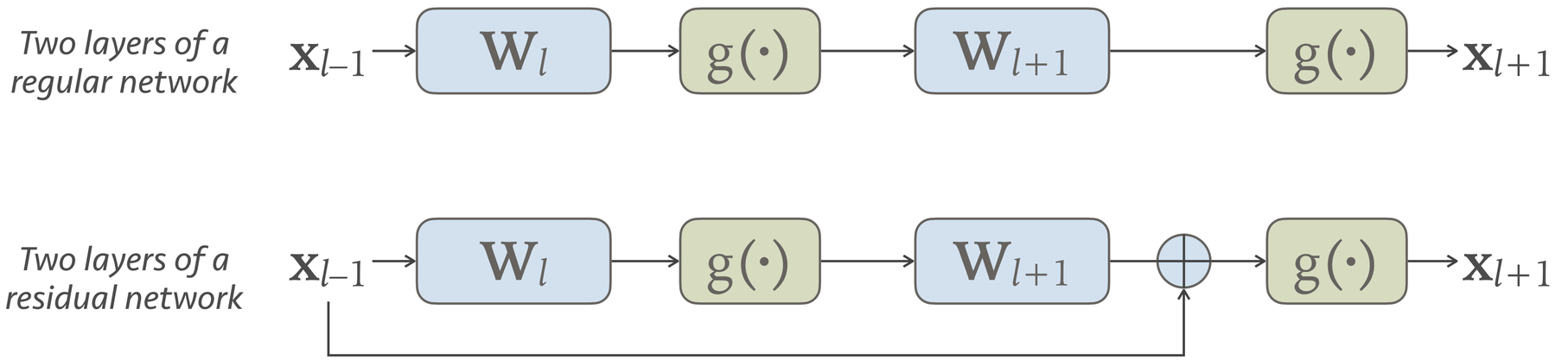
- Instead of BatchNorm, we can *whiten* the outputs!
  - Don't scale the variance, scale the covariance (like PCA)



- Simplifies optimization significantly (at a cost of course!)

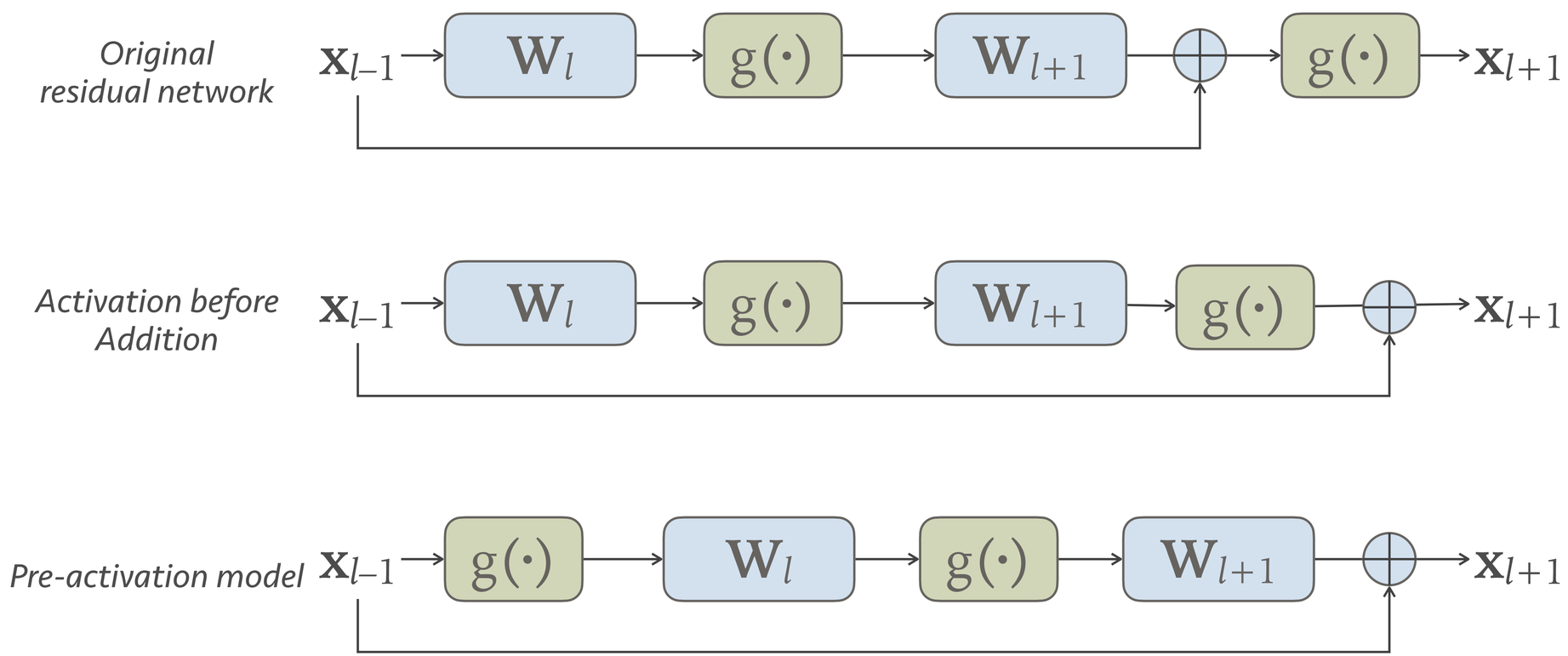
Residual nets

- Really deep networks do not train as well
  - Gradients vanish after backpropagating too many layers
- R*esidual* nets bypass this problem
  - Add preceding layer's inputs to future layer's outputs
  - Effectively "shallows" network and facilitates convergence



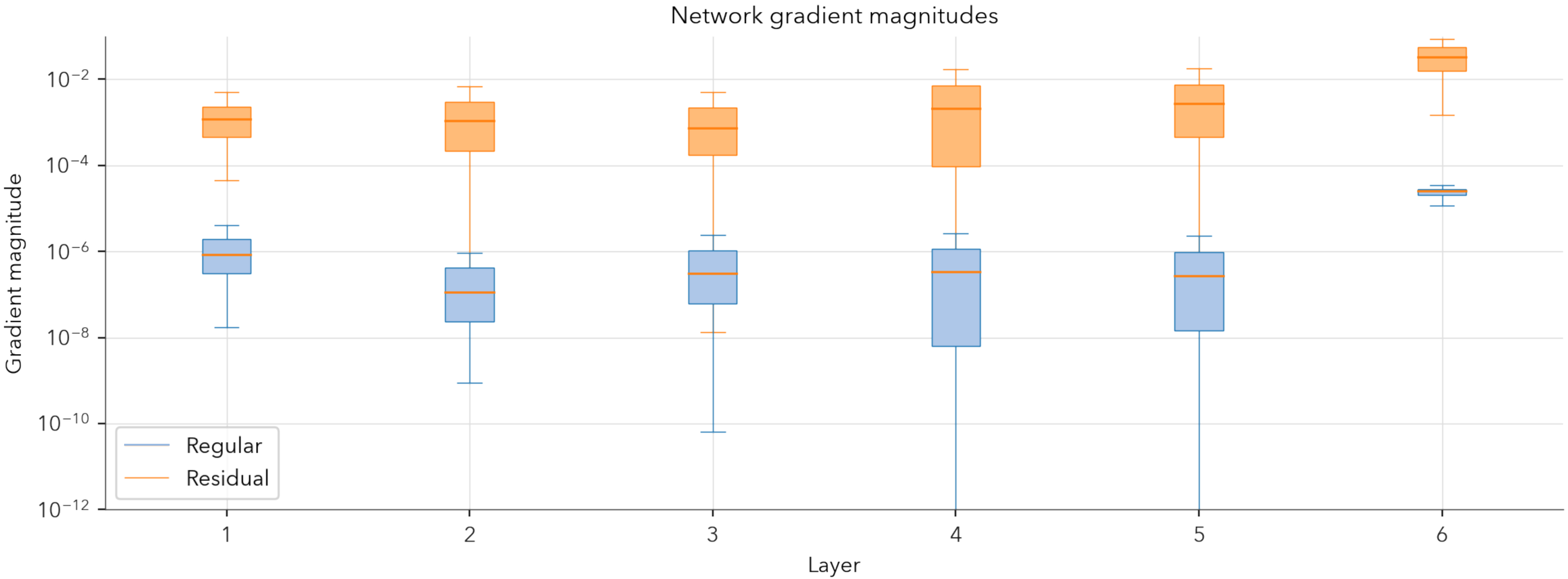
Residual net variations

- Subsequent tweaking of the original idea
  - Can also use various BatchNorms in between



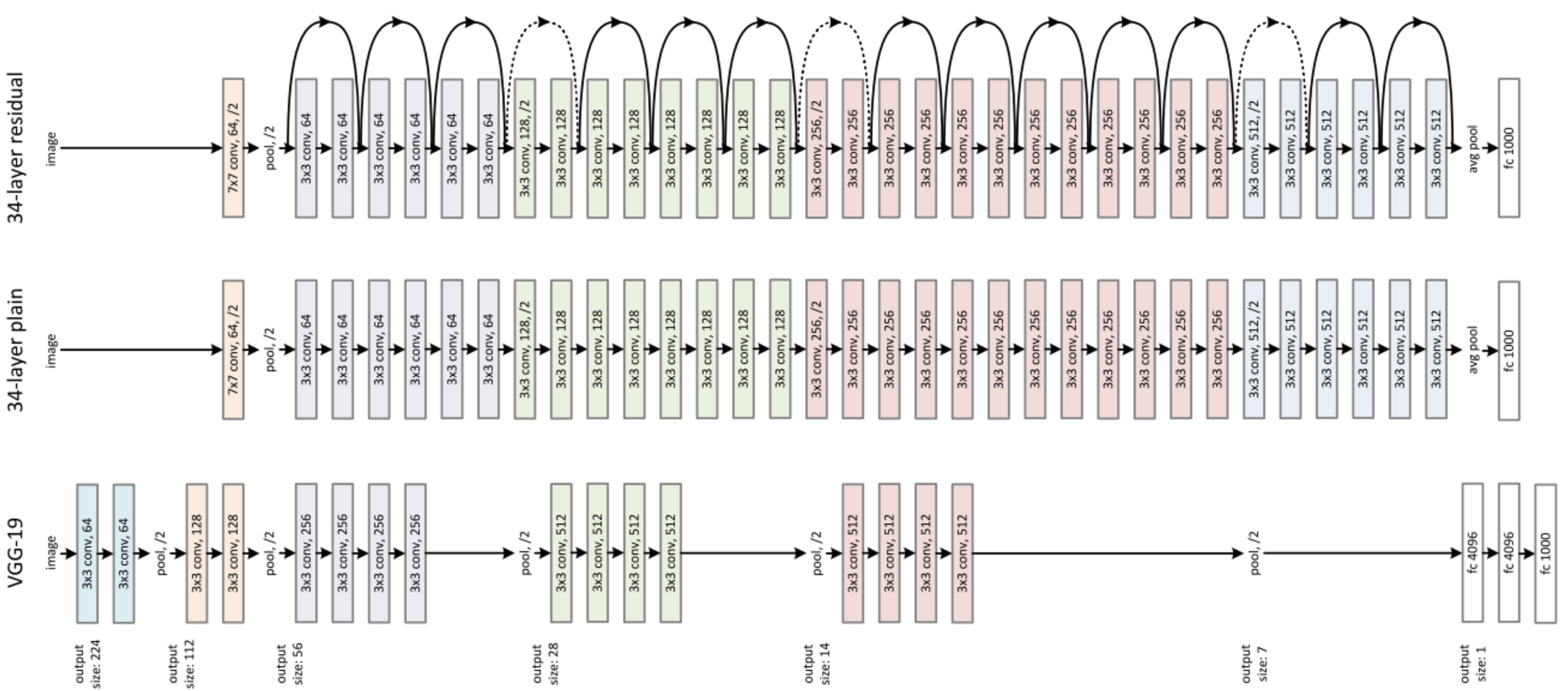
Effect of residual nets

- Results in more usable gradient values
  - Allows for the design of networks with hundreds of layers



ResNets in practice

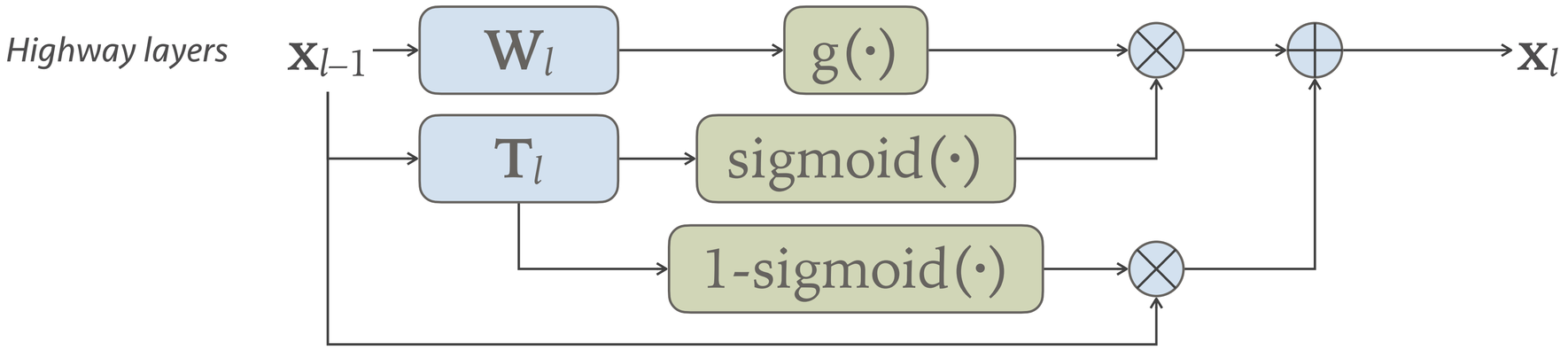
- This is the small one!



Highway networks

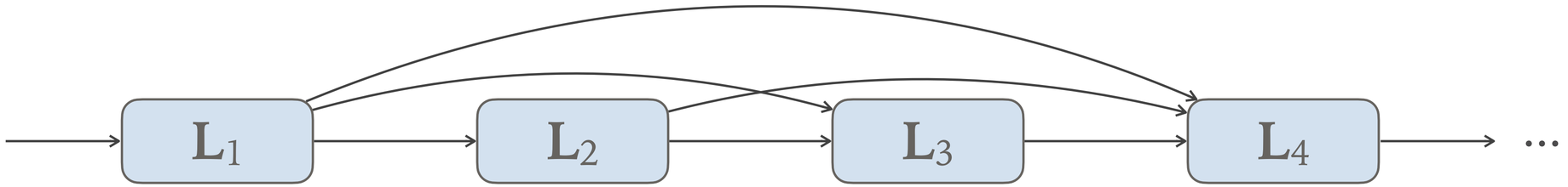
- Generalizing the residual network idea
  - Add a data-driven gate to the skip connection

$$\mathbf{x}_l = g\left(\mathbf{W}_l \cdot \mathbf{x}_{l-1}\right)\text{sigmoid}\left(\mathbf{T}_l \cdot \mathbf{x}_{l-1}\right) + \mathbf{x}_{l-1}\left(1 - \text{sigmoid}\left(\mathbf{T}_l \cdot \mathbf{x}_{l-1}\right)\right)$$



DenseNets

- And why not go all out and connect all layers?
  - Unlike previous approaches, we use past outputs as extra input dimensions to the subsequent layers
  - A drawback: we need a lot more memory!



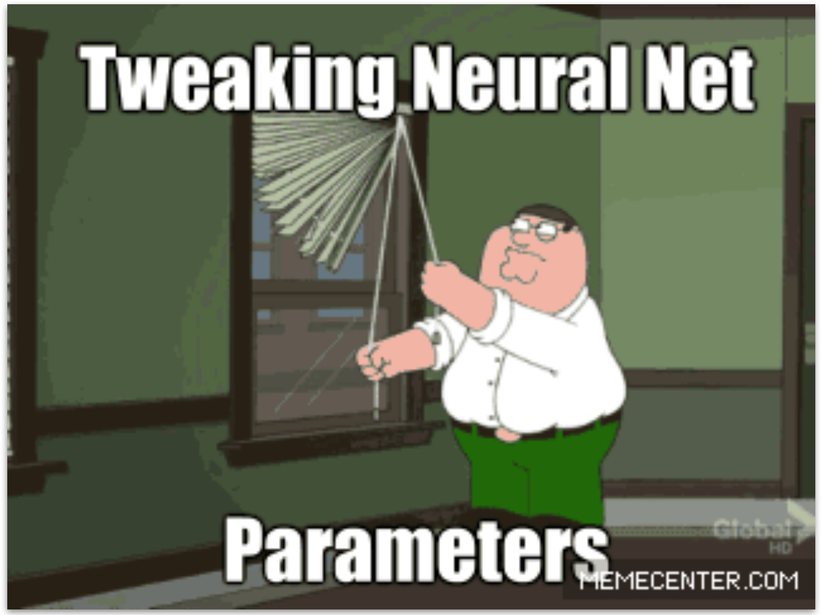
  - Advantage: Gradients propagate nicely through network

Model Compression

- Is being shallow necessary?
  - Remember that three layers should be all we need
- Using a deep structure tends to facilitate training
  - Despite the introduction of many more parameters
- Train shallow networks to mimic trained deep networks
  - Train a deep network, generate a lot of outputs for random inputs and use them as training data for a shallow network

So what's the verdict?

- Good news:
  - Very powerful and flexible approaches
  - Potential biological(ish) plausibility
    - And computability implications



- Bad news:
  - Too flexible, picking right structure is very much an art
  - Cumbersome and potentially finicky training procedures

Progression to remember

- Try a linear model: $\mathbf{x}_1 = \mathbf{W} \cdot \mathbf{x}_0 + \mathbf{b}$
  - PCA, linear classifiers, etc
- Try a non-linear model: $\mathbf{x}_1 = \mathrm{g}\left(\mathbf{W} \cdot \mathbf{x}_0 + \mathbf{b}\right)$
  - Quadratic classifiers, logistic regression, non-linear models
- Try an (increasingly) deeper model: $\mathbf{x}_i = \mathrm{g}\left(\mathbf{W}_i \cdot \mathbf{x}_{i-1} + \mathbf{b}_i\right)$
  - Try this lecture's material to get convergence
- Then try next lecture's models …

Recap

- Stochastic shallow networks
  - Boltzmann machine
- Deep learning concepts
- Common deep architectures and tricks
  - Optimization schemes, residuals, highways,

More material

- “Deep Learning”, the book:
  - http://www.deeplearningbook.org
  - (no PDF but you can read online)

- A Fast Learning Algorithm for Deep Belief Nets
  - http://www.cs.toronto.edu/~hinton/absps/fastnc.pdf

Next lecture

- Deep Learning on Time Series
  - Convolutional and Recurrent architectures
  - Sequence learning

- Neural Generative models
  - VAEs & GANs