10707
Deep Learning

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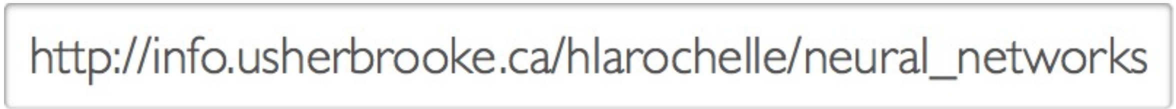
Neural Networks II

Neural Networks Online Course

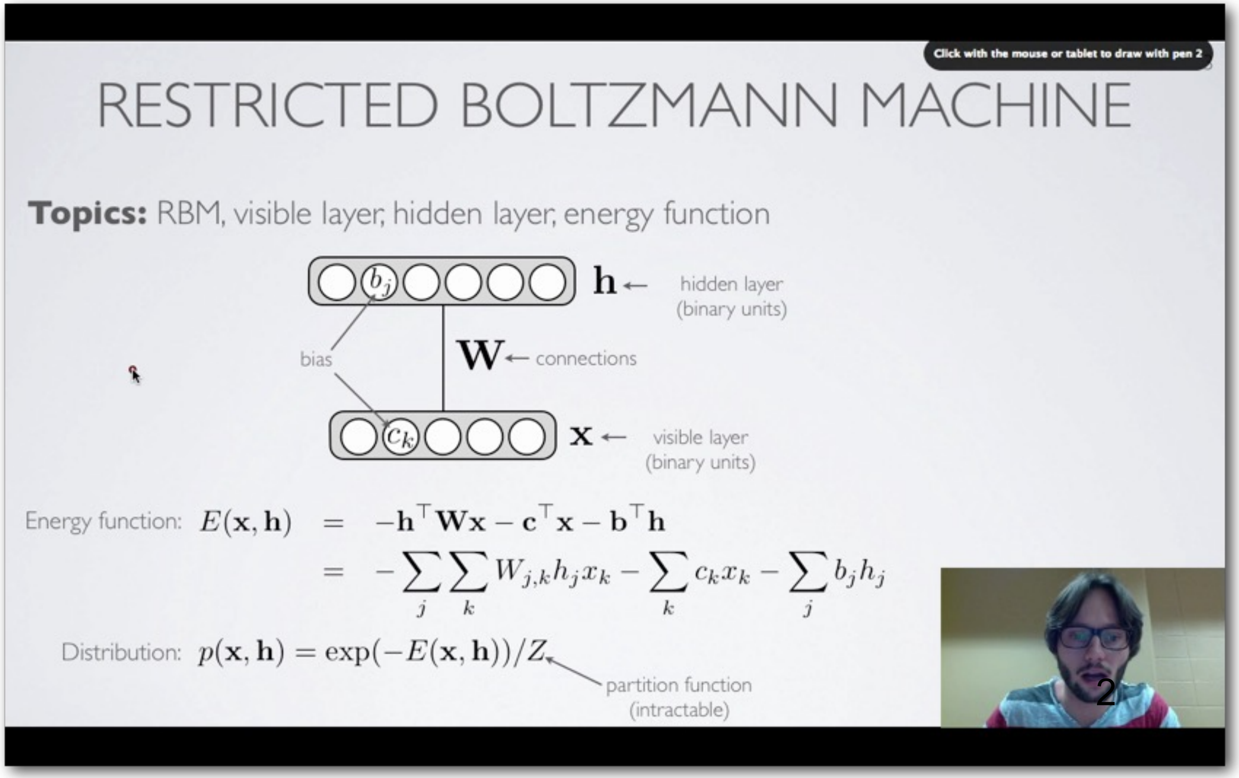
- **Disclaimer**: Much of the material and slides for this lecture were borrowed from Hugo Larochelle's class on Neural Networks: https://sites.google.com/site/deeplearningsummerschool2016/



http://info.usherbrooke.ca/hlarochelle/neural_networks

- Hugo's class covers many other topics: convolutional networks, neural language model, Boltzmann machines, autoencoders, sparse coding, etc.

- We will use his material for some of the other lectures.



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RESTRICTED BOLTZMANN MACHINE

Topics: RBM, visible layer, hidden layer, energy function

b_j
$\mathbf{h} \leftarrow$ hidden layer (binary units)
bias
$\mathbf{W} \leftarrow$ connections
c_k
$\mathbf{x} \leftarrow$ visible layer (binary units)

Energy function:
$$\begin{aligned} E(\mathbf{x},\mathbf{h}) &= -\mathbf{h}^\top \mathbf{W}\mathbf{x} - \mathbf{c}^\top \mathbf{x} - \mathbf{b}^\top \mathbf{h} \\ &= -\sum_j \sum_k W_{j,k} h_j x_k - \sum_k c_k x_k - \sum_j b_j h_j \end{aligned}$$

Distribution: $p(\mathbf{x},\mathbf{h}) = \exp(-E(\mathbf{x},\mathbf{h}))/Z$

partition function (intractable)

Initialization

- Initialize biases to 0
- For weights
  - Can not initialize weights to 0 with tanh activation
    - ➢ All gradients would be zero (saddle point)
  - Can not initialize all weights to the same value
    - ➢ All hidden units in a layer will always behave the same
    - ➢ Need to break symmetry
  - Sample $\mathbf{W}_{i,j}^{(k)}$ from $U\left[-b, b\right]$, where

$$b = \frac{\sqrt{6}}{\sqrt{H_k + H_{k-1}}}$$

Sample around 0 and break symmetry

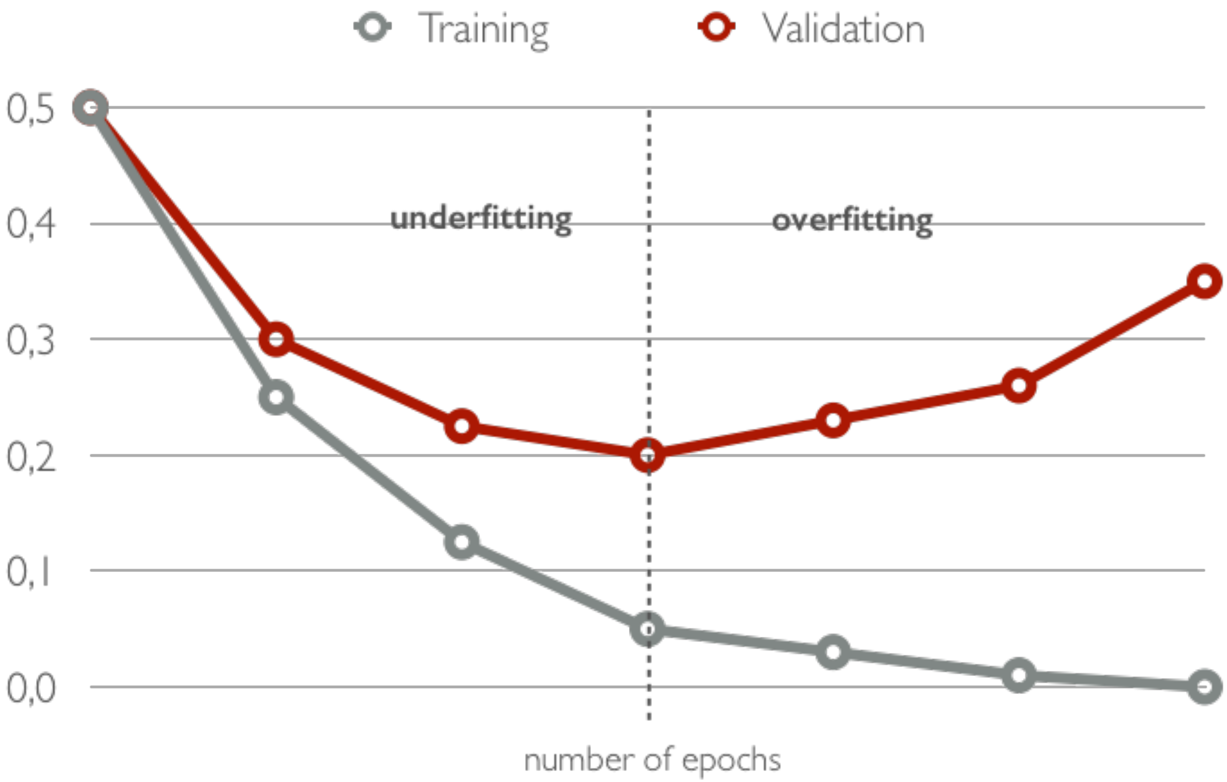
Size of $\mathbf{h}^{(k)}(\mathbf{x})$

Model Selection

- Training Protocol:
  - Train your model on the Training Set $\mathcal{D}^{\mathrm{train}}$
  - For model selection, use Validation Set $\mathcal{D}^{\mathrm{valid}}$
    - Hyper-parameter search: hidden layer size, learning rate, number of iterations/epochs, etc.
  - Estimate generalization performance using the Test Set $\mathcal{D}^{\mathrm{test}}$
- Remember: Generalization is the behavior of the model on **unseen examples**.

Early Stopping

- To select the number of epochs, stop training when validation set error increases (with some look ahead).



Tricks of the Trade:

- Normalizing your (real-valued) data:
  - for each dimension x_i subtract its training set mean
  - divide each dimension x_i by its training set standard deviation
  - this can speed up training

- Decreasing the learning rate: As we get closer to the optimum, take smaller update steps:

  i. start with large learning rate (e.g. 0.1)
  ii. maintain until validation error stops improving
  iii. divide learning rate by 2 and go back to (ii)

Mini-batch, Momentum

- Make updates based on a mini-batch of examples (instead of a single example):
  - the gradient is the average regularized loss for that mini-batch
  - can give a more accurate estimate of the gradient
  - can leverage matrix/matrix operations, which are more efficient

- Momentum: Can use an exponential average of previous gradients:

$$\overline{\nabla}_{\boldsymbol{\theta}}^{(t)} = \nabla_{\boldsymbol{\theta}} l(\mathbf{f}(\mathbf{x}^{(t)}), y^{(t)}) + \beta \overline{\nabla}_{\boldsymbol{\theta}}^{(t-1)}$$

  - can get pass plateaus more quickly, by “gaining momentum”

Adapting Learning Rates

- Updates with adaptive learning rates ("one learning rate per parameter")

  - Adagrad: learning rates are scaled by the square root of the cumulative sum of squared gradients

$$\gamma^{(t)} = \gamma^{(t-1)} + \left(\nabla_\theta l(\mathbf{f}(\mathbf{x}^{(t)}), y^{(t)})\right)^2 \qquad \overline{\nabla}_\theta^{(t)} = \frac{\nabla_\theta l(\mathbf{f}(\mathbf{x}^{(t)}), y^{(t)})}{\sqrt{\gamma^{(t)} + \epsilon}}$$

  - RMSProp: instead of cumulative sum, use exponential moving average

$$\gamma^{(t)} = \beta\gamma^{(t-1)} + (1-\beta)\left(\nabla_\theta l(\mathbf{f}(\mathbf{x}^{(t)}), y^{(t)})\right)^2$$

$$\overline{\nabla}_\theta^{(t)} = \frac{\nabla_\theta l(\mathbf{f}(\mathbf{x}^{(t)}), y^{(t)})}{\sqrt{\gamma^{(t)} + \epsilon}}$$

  - Adam: essentially combines RMSProp with momentum

Gradient Checking

- To debug your implementation of fprop/bprop, you can compare with a finite-difference approximation of the gradient:

$$\frac{\partial f(x)}{\partial x} \approx \frac{f(x+\epsilon)-f(x-\epsilon)}{2\epsilon}$$

- ➢ $f(x)$ would be the loss
- ➢ x would be a parameter
- ➢ $f(x+\epsilon)$ would be the loss if you add ϵ to the parameter
- ➢ $f(x-\epsilon)$ would be the loss if you subtract ϵ to the parameter

Debugging on Small Dataset

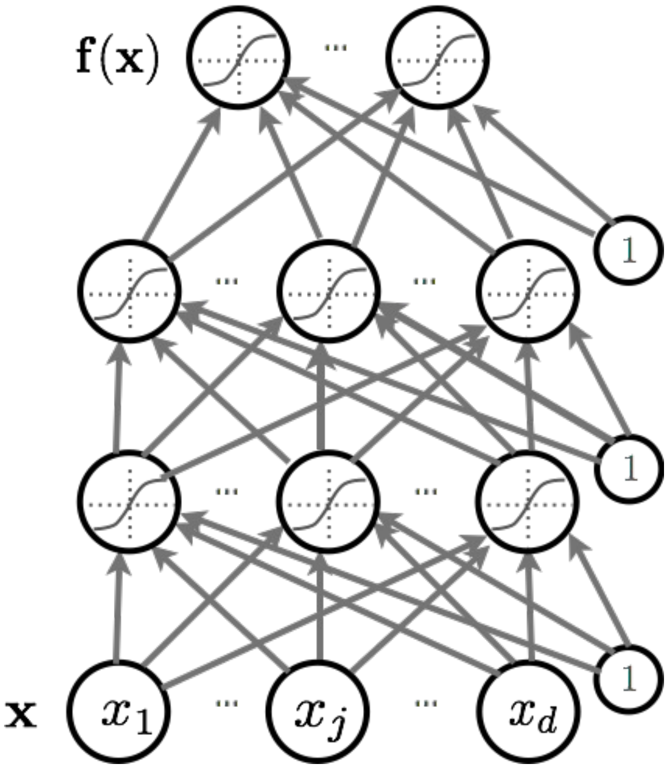
- If not, investigate the following situations:
  - ➢ Are some of the units saturated, even before the first update?
    - scale down the initialization of your parameters for these units
    - properly normalize the inputs
  - ➢ Is the training error bouncing up and down?
    - decrease the learning rate
- This does not mean that you have computed gradients correctly:
  - ➢ You could still overfit with some of the gradients being wrong

Feedforward Neural Networks

- How neural networks predict f(x) given an input x:
  - Forward propagation
  - Types of units
  - Capacity of neural networks

- How to train neural nets:
  - Loss function
  - Backpropagation with gradient descent

- More recent techniques:
  - Dropout
  - Batch normalization
  - Unsupervised Pre-training



Feedforward Neural Networks

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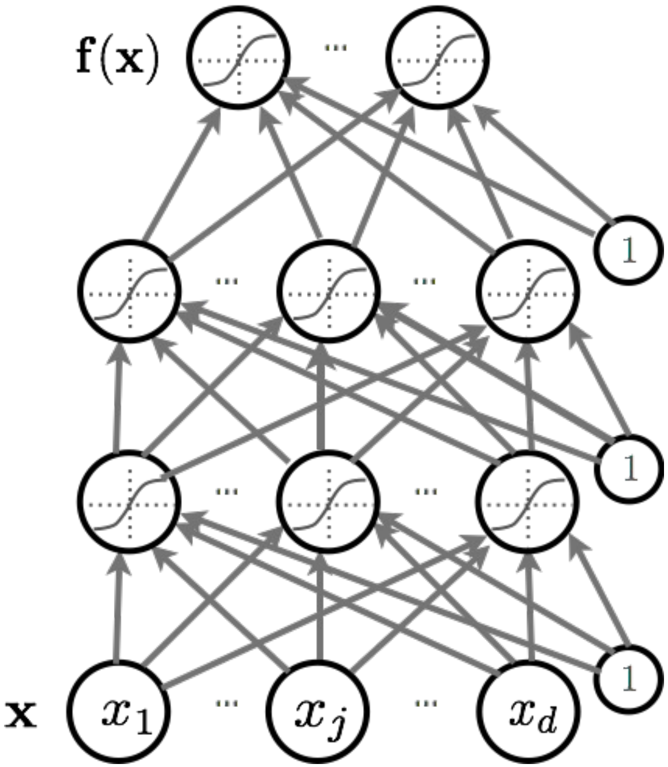


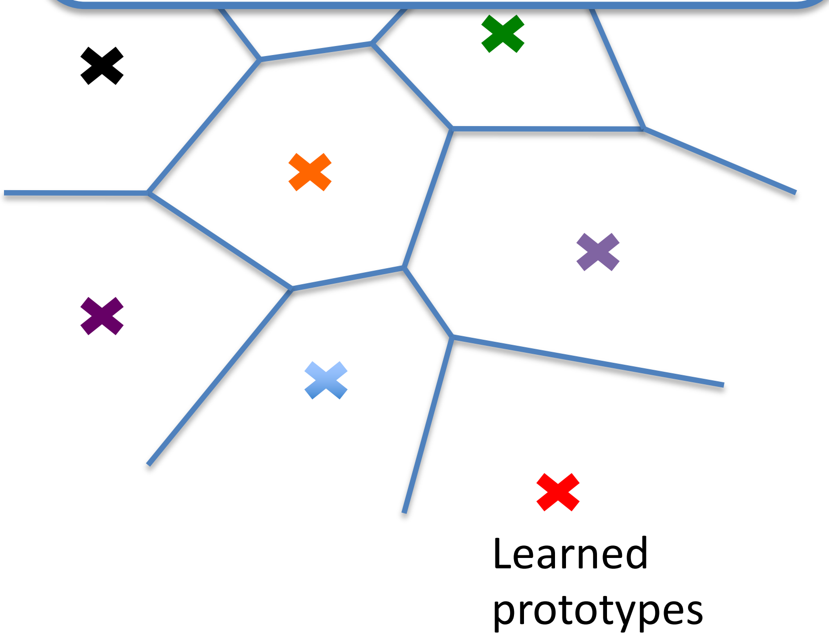
Learning Distributed Representations

- Deep learning is research on learning models with multilayer representations
  - ➢ multilayer (feed-forward) neural networks
  - ➢ multilayer graphical model (deep belief network, deep Boltzmann machine)
- Each layer learns "distributed representation"
  - ➢ Units in a layer are not mutually exclusive
    - each unit is a separate feature of the input
    - two units can be "active" at the same time
  - ➢ Units do not correspond to a partitioning (clustering) of the inputs
    - in clustering, an input can only belong to a single cluster

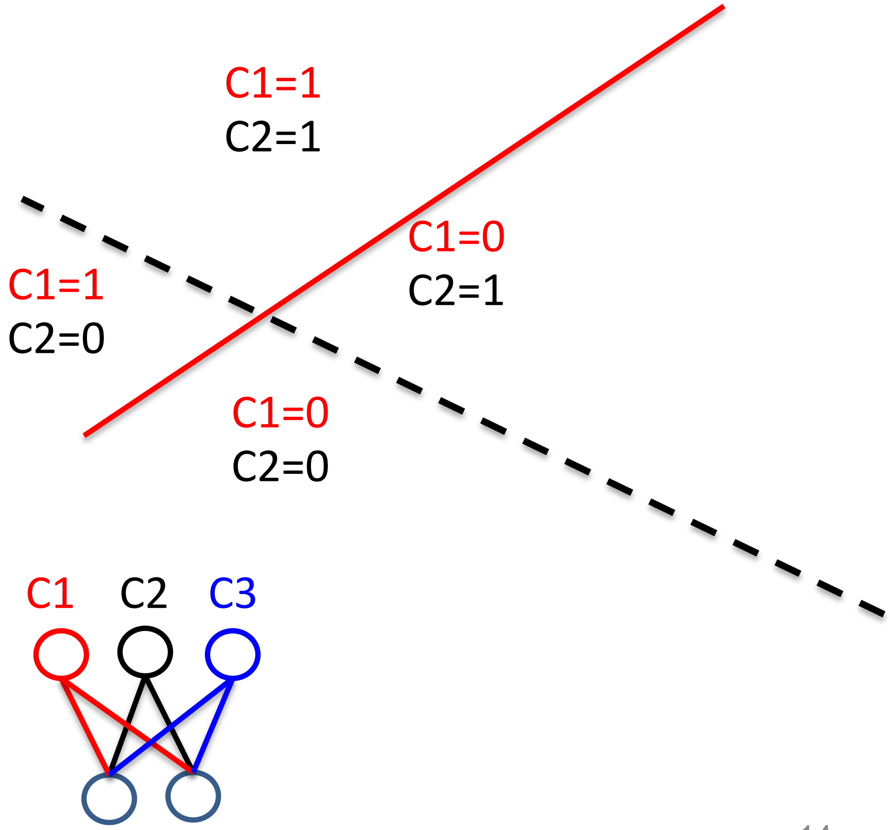
Local vs. Distributed Representations

- Clustering, Nearest Neighbors, RBF SVM, local density estimators

- Parameters for each region.
- # of regions is linear with # of parameters.



- RBMs, Factor models, PCA, Sparse Coding, Deep models



Bengio, 2009, Foundations and Trends in Machine Learning

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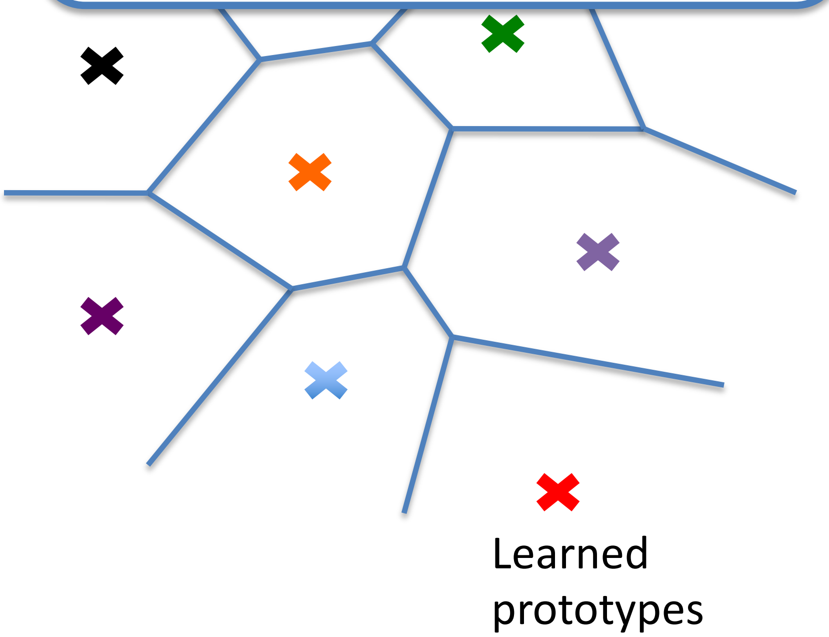

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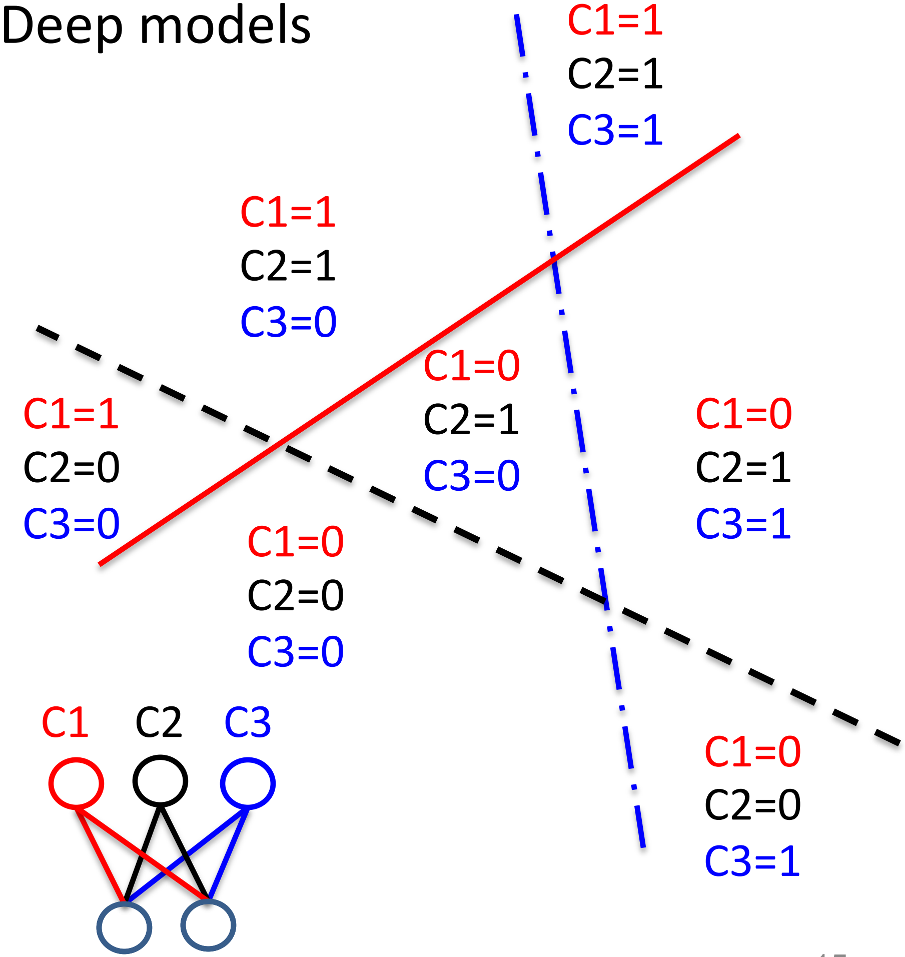

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Local vs. Distributed Representations

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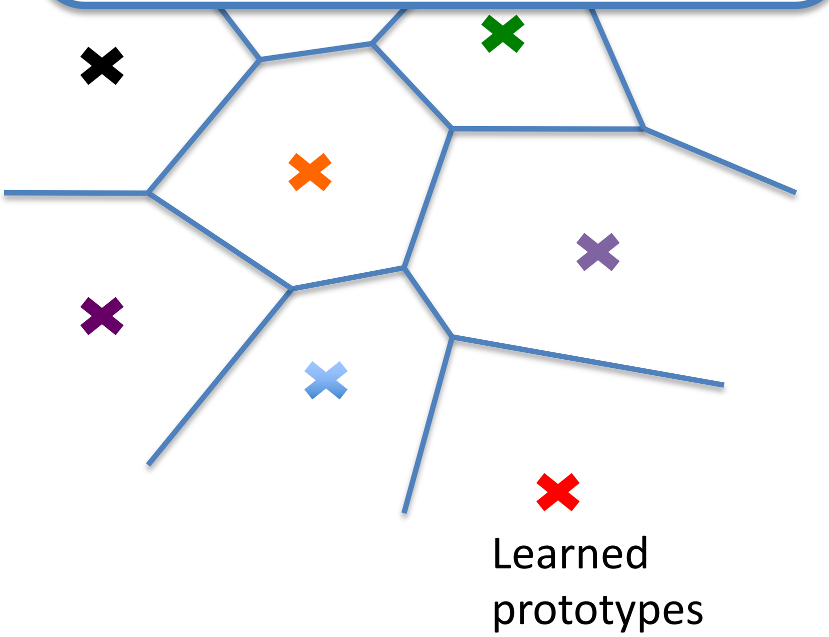
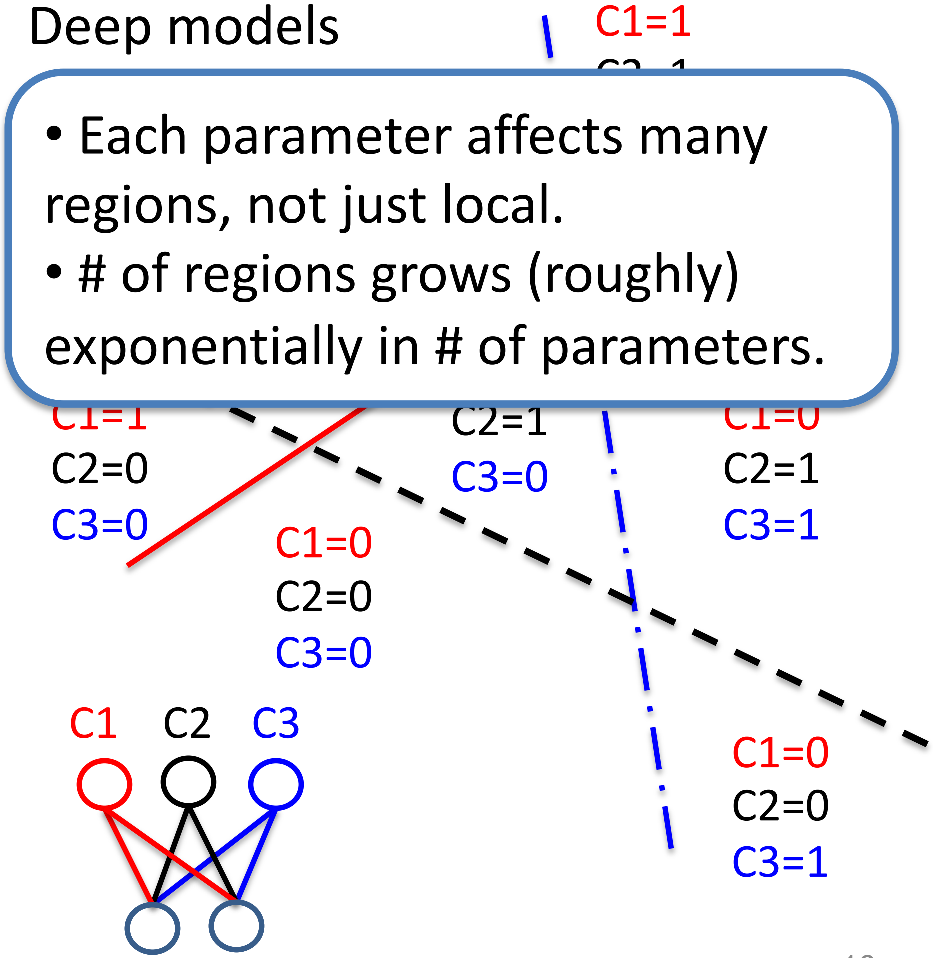


- RBMs, Factor models, PCA, Sparse Coding, Deep models

- Each parameter affects many regions, not just local.
- # of regions grows (roughly) exponentially in # of parameters.



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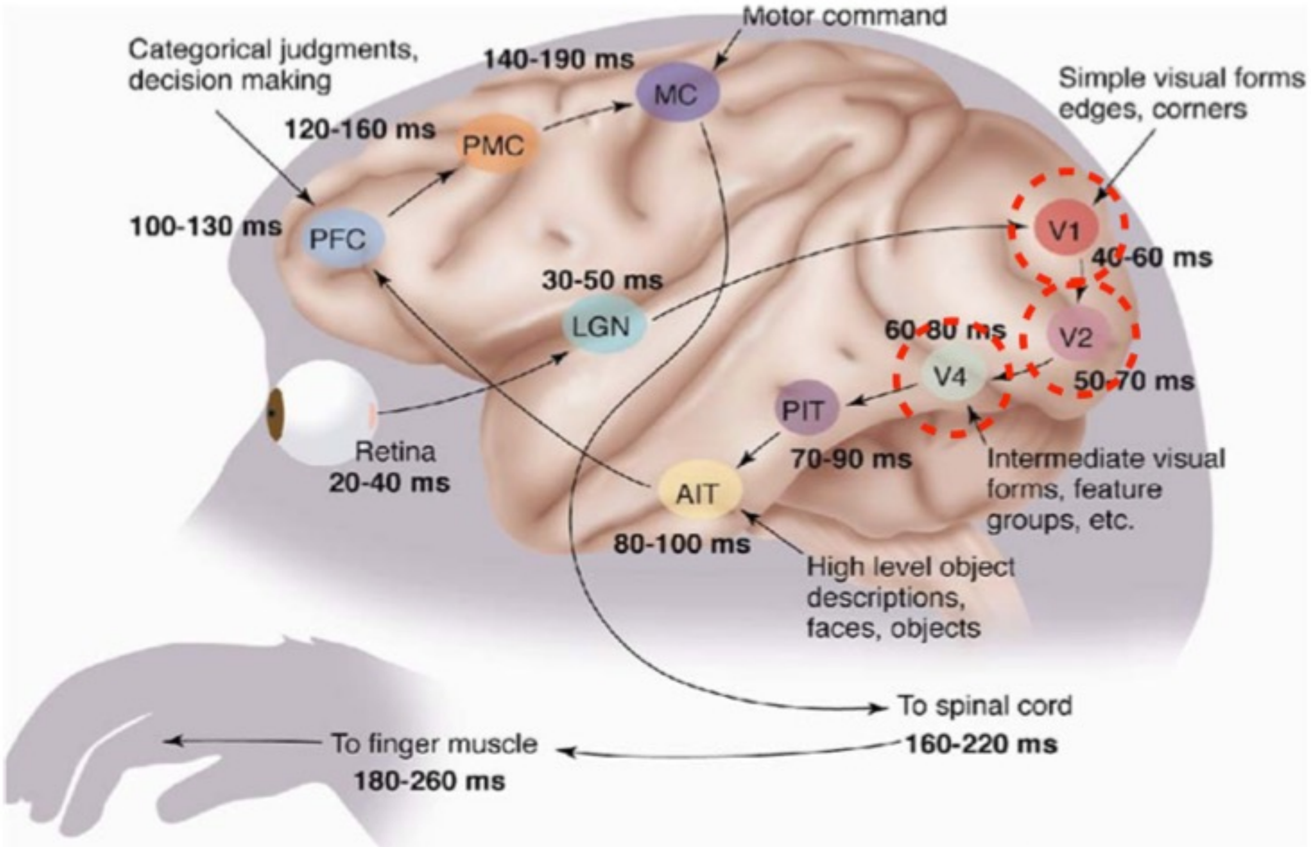
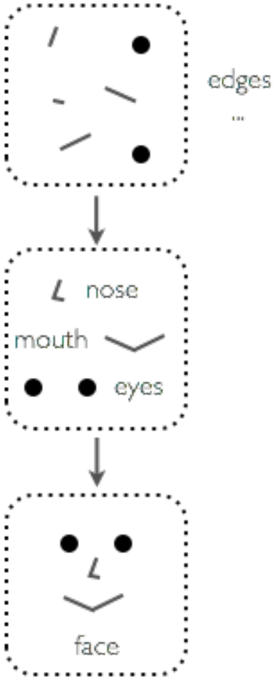
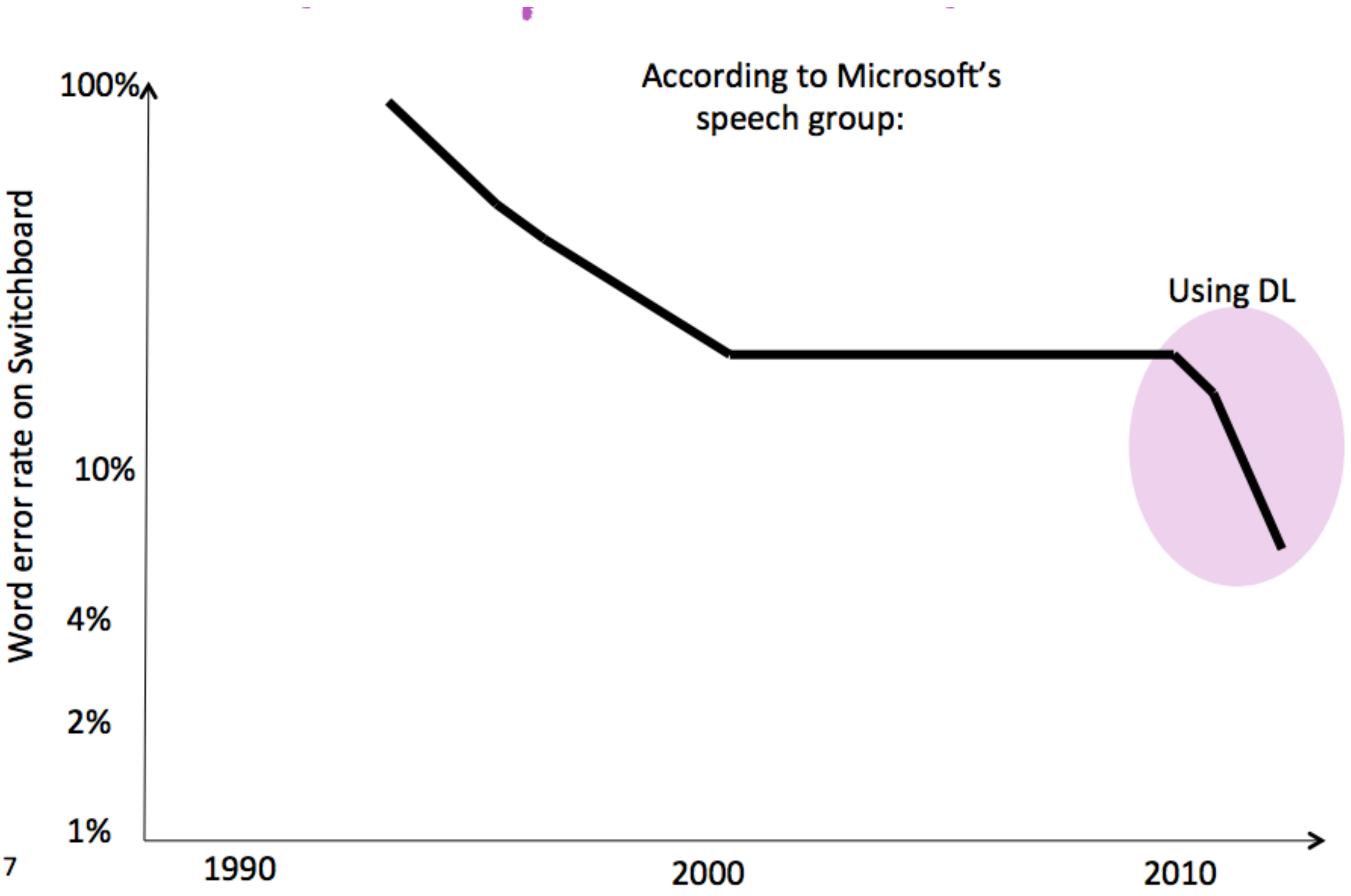
Inspiration from Visual Cortex



[picture from Simon Thorpe]

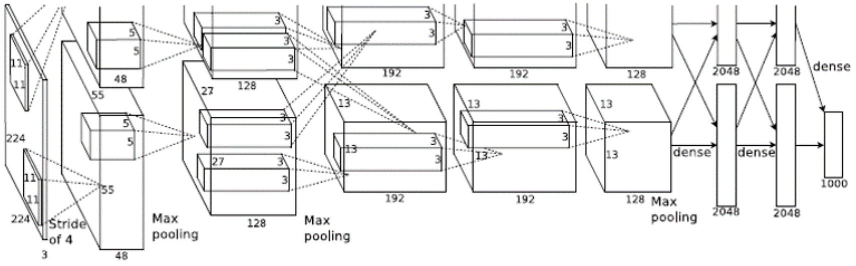


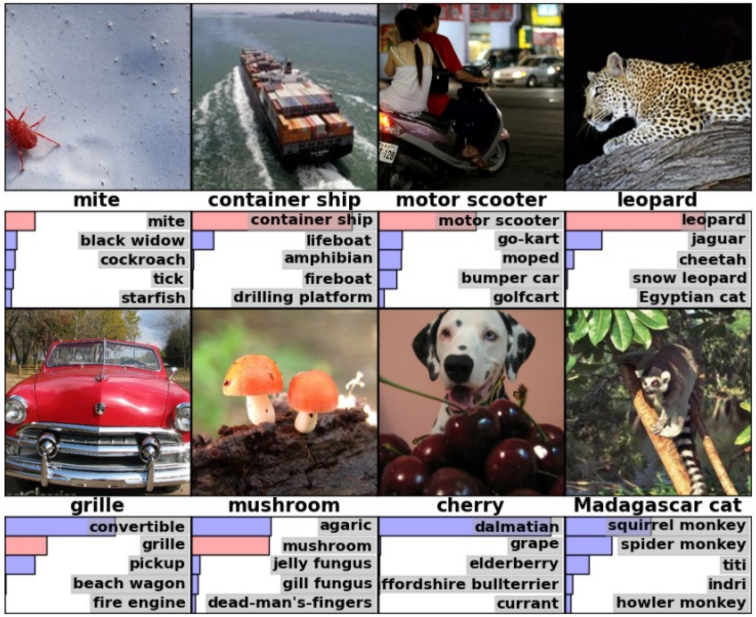
Success Story: Speech Recognition



Success Story: Image Recognition

- Deep Convolutional Nets for Vision (Supervised)



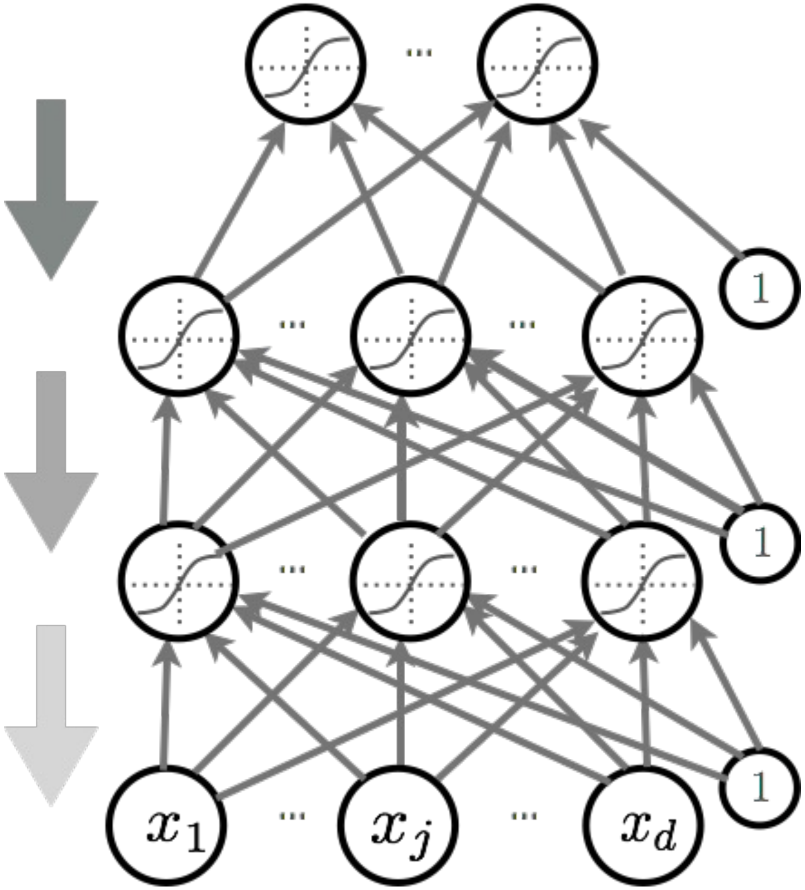


1.2 million training images
1000 classes

Why Training is Hard

- First hypothesis: Hard optimization problem (underfitting)
  - vanishing gradient problem
  - saturated units block gradient propagation

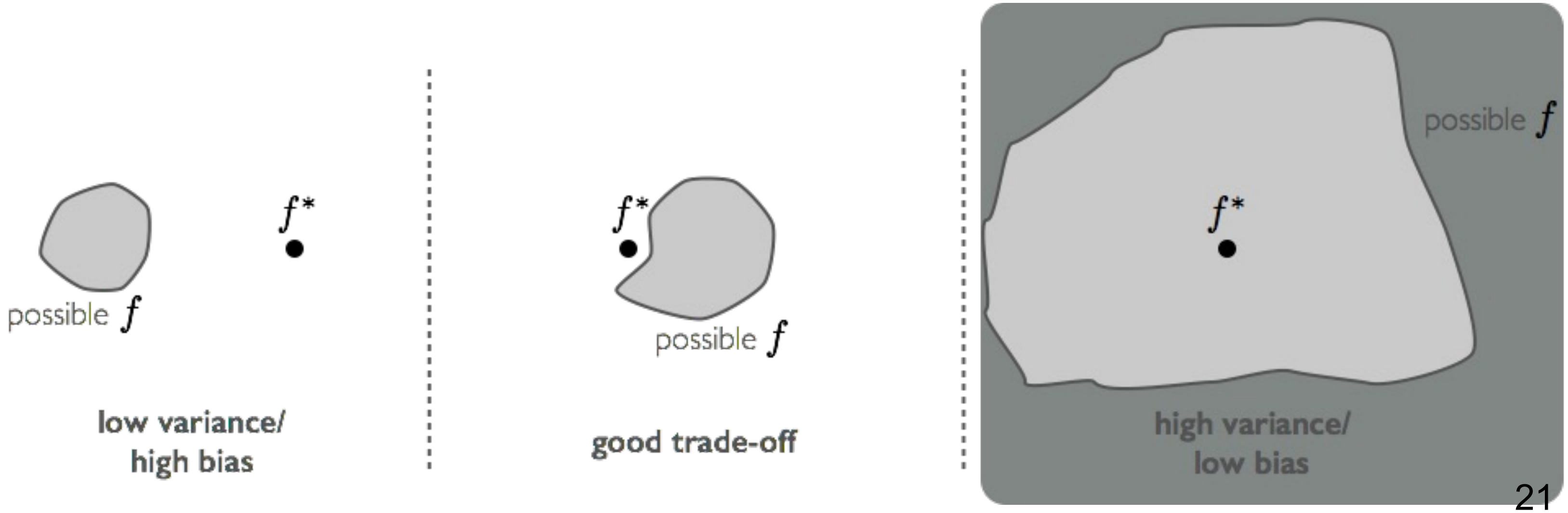
- This is a well known problem in recurrent neural networks



Why Training is Hard

- Second hypothesis: Overfitting
  - ➢ we are exploring a space of complex functions
  - ➢ deep nets usually have lots of parameters

- Might be in a high variance / low bias situation



Why Training is Hard

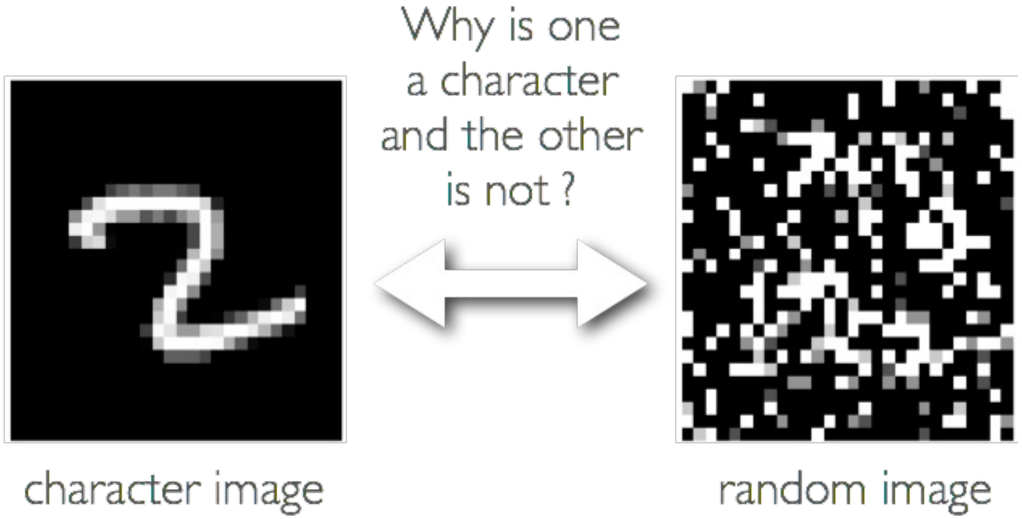
- First hypothesis (underfitting): better optimize
  - ➢ Use better optimization tools (e.g. batch-normalization, second order methods, such as KFAC)
  - ➢ Use GPUs, distributed computing.

- Second hypothesis (overfitting): use better regularization
  - ➢ Unsupervised pre-training
  - ➢ Stochastic drop-out training

- For many large-scale practical problems, you will need to use both: better optimization and better regularization!

Unsupervised Pre-training

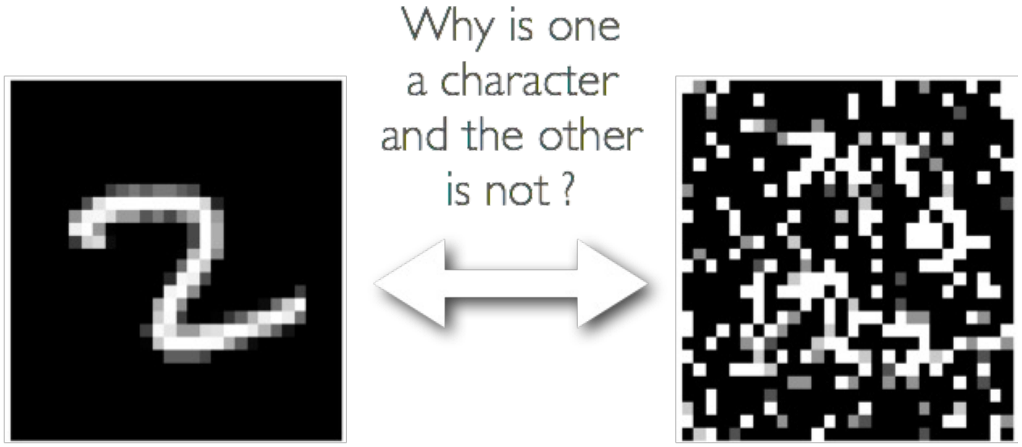
- Initialize hidden layers using unsupervised learning
  - ➢ Force network to represent latent structure of input distribution



  - ➢ Encourage hidden layers to encode that structure

Unsupervised Pre-training

- Initialize hidden layers using unsupervised learning
  - ➢ This is a harder task than supervised learning (classification)



Why is one a character and the other is not ?

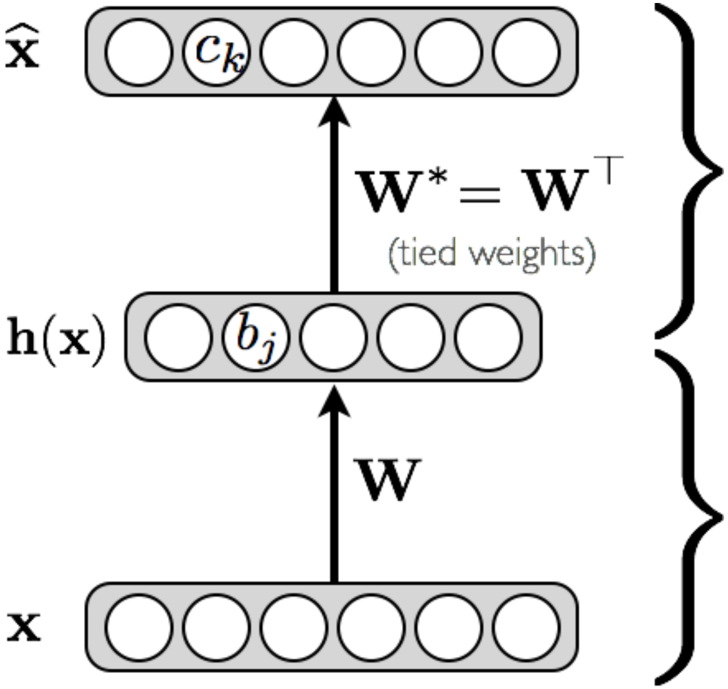
character image

random image

  - ➢ Hence we expect less overfitting

Autoencoders: Preview

- Feed-forward neural network trained to reproduce its input at the output layer



Decoder

$$\begin{aligned}\widehat{\mathbf{x}} &= o(\widehat{\mathbf{a}}(\mathbf{x}))\\ &= \underbrace{\mathrm{sigm}}_{\text{For binary units}}(\mathbf{c} + \mathbf{W}^*\mathbf{h}(\mathbf{x}))\end{aligned}$$

Encoder

$$\begin{aligned}\mathbf{h}(\mathbf{x}) &= g(\mathbf{a}(\mathbf{x}))\\ &= \mathrm{sigm}(\mathbf{b} + \mathbf{W}\mathbf{x})\end{aligned}$$

Autoencoders: Preview

- Loss function for binary inputs

$$l(f(\mathbf{x})) = -\sum_k \left(x_k \log(\widehat{x}_k) + (1 - x_k)\log(1 - \widehat{x}_k)\right)$$

➢ Cross-entropy error function $f(\mathbf{x}) \equiv \widehat{\mathbf{x}}$

- Loss function for real-valued inputs

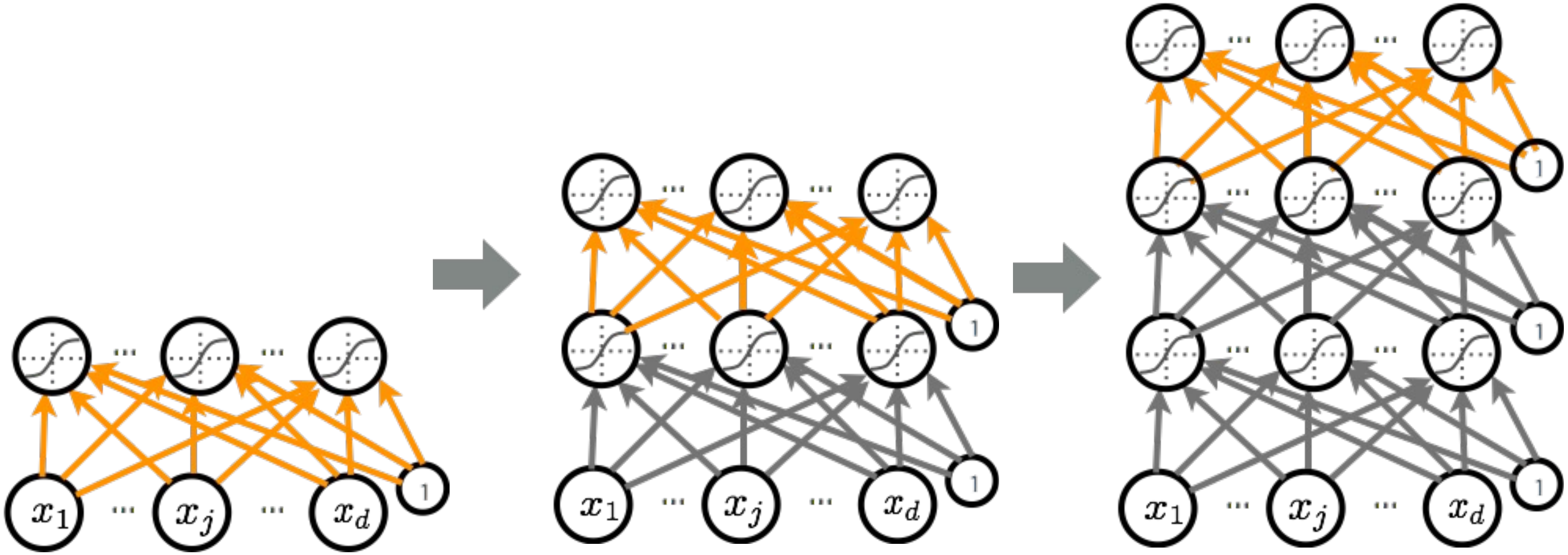
$$l(f(\mathbf{x})) = \frac{1}{2}\sum_k (\widehat{x}_k - x_k)^2$$

➢ sum of squared differences

➢ we use a linear activation function at the output

Pre-training

- We will use a greedy, layer-wise procedure
  - Train one layer at a time with unsupervised criterion
  - Fix the parameters of previous hidden layers
  - Previous layers can be viewed as feature extraction



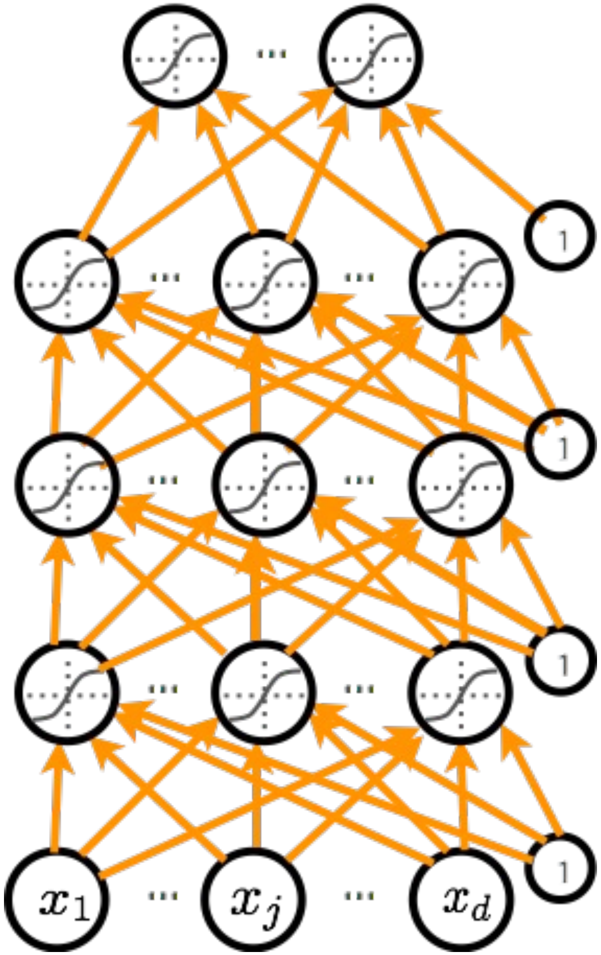
Pre-training

- Unsupervsed Pre-training
  - first layer: find hidden unit features that are more common in training inputs than in random inputs
  - second layer: find combinations of hidden unit features that are more common than random hidden unit features
  - third layer: find combinations of combinations of ...

- Pre-training initializes the parameters in a region such that the near local optima overfit less the data

Fine-tuning

- Once all layers are pre-trained
  - ➢ add output layer
  - ➢ train the whole network using supervised learning
- Supervised learning is performed as in a regular network
  - ➢ forward propagation, backpropagation and update
- We call this last phase fine-tuning
  - ➢ all parameters are “tuned” for the supervised task at hand
  - ➢ representation is adjusted to be more discriminative



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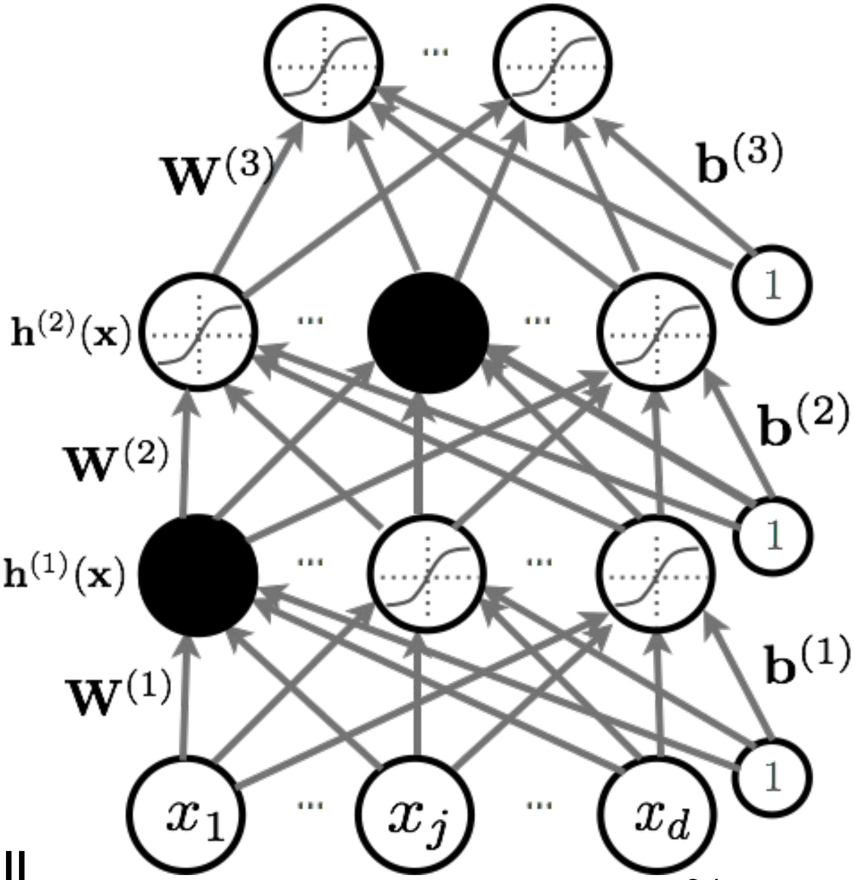
- For many large-scale practical problems, you will need to use both: better optimization and better regularization!

Dropout

- Key idea: Cripple neural network by removing hidden units stochastically

  - each hidden unit is set to 0 with probability 0.5
  - hidden units cannot co-adapt to other units
  - hidden units must be more generally useful

- Could use a different dropout probability, but 0.5 usually works well



Dropout

- Use random binary masks $m^{(k)}$
  - layer pre-activation for k>0

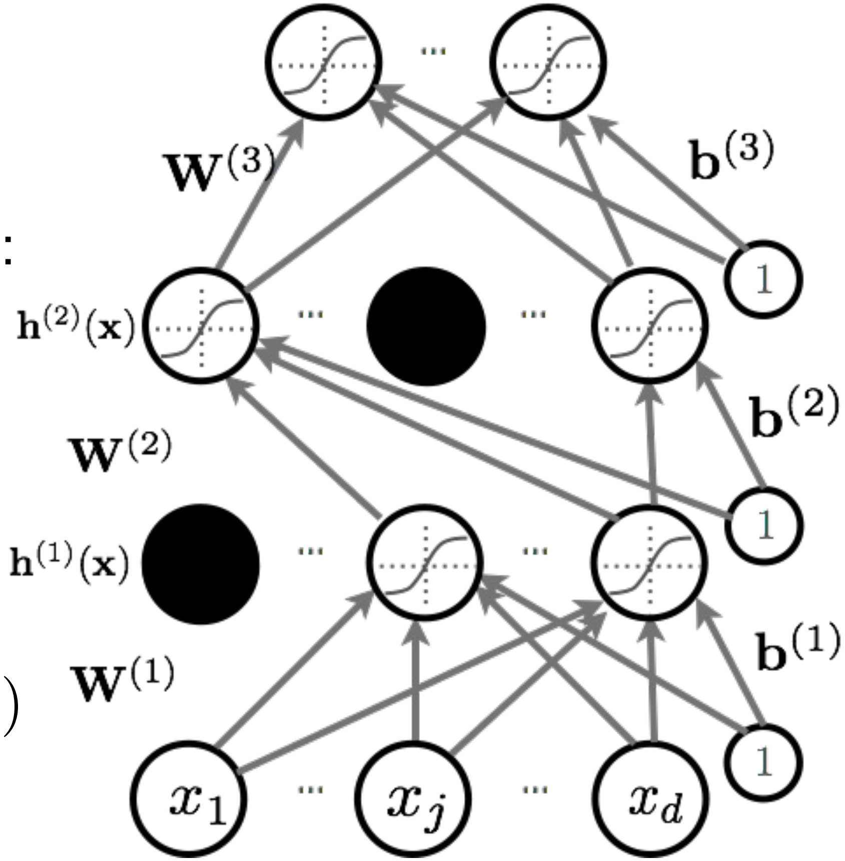
$$\mathbf{a}^{(k)}(\mathbf{x}) = \mathbf{b}^{(k)} + \mathbf{W}^{(k)}\mathbf{h}^{(k-1)}(\mathbf{x})$$

  - hidden layer activation (k=1 to L):

$$\mathbf{h}^{(k)}(\mathbf{x}) = \mathbf{g}(\mathbf{a}^{(k)}(\mathbf{x})) \odot \mathrm{m}^{(k)}$$

  - Output activation (k=L+1)

$$\mathbf{h}^{(L+1)}(\mathbf{x}) = \mathbf{o}(\mathbf{a}^{(L+1)}(\mathbf{x})) = \mathbf{f}(\mathbf{x})$$



Backpropagation Algorithm

- Perform forward propagation
- Compute output gradient (before activation):

$$\nabla_{\mathbf{a}^{(L+1)}(\mathbf{x})} -\log f(\mathbf{x})_y \quad \Longleftarrow \quad -\left(\mathbf{e}(y) - \mathbf{f}(\mathbf{x})\right)$$

Includes the mask m$^{(k-1)}$

- For k=L+1 to 1
  - Compute gradients w.r.t. the hidden layer parameters:

$$\nabla_{\mathbf{W}^{(k)}} -\log f(\mathbf{x})_y \quad \Longleftarrow \quad \left(\nabla_{\mathbf{a}^{(k)}(\mathbf{x})} -\log f(\mathbf{x})_y\right) \boxed{\mathbf{h}^{(k-1)}(\mathbf{x})^\top}$$

$$\nabla_{\mathbf{b}^{(k)}} -\log f(\mathbf{x})_y \quad \Longleftarrow \quad \nabla_{\mathbf{a}^{(k)}(\mathbf{x})} -\log f(\mathbf{x})_y$$

  - Compute gradients w.r.t. the hidden layer below:

$$\nabla_{\mathbf{h}^{(k-1)}(\mathbf{x})} -\log f(\mathbf{x})_y \quad \Longleftarrow \quad \mathbf{W}^{(k)^\top} \left(\nabla_{\mathbf{a}^{(k)}(\mathbf{x})} -\log f(\mathbf{x})_y\right)$$

  - Compute gradients w.r.t. the hidden layer below (before activation):

$$\nabla_{\mathbf{a}^{(k-1)}(\mathbf{x})} -\log f(\mathbf{x})_y \quad \Longleftarrow \quad \left(\nabla_{\mathbf{h}^{(k-1)}(\mathbf{x})} -\log f(\mathbf{x})_y\right) \odot \left[\ldots, g'(a^{(k-1)}(\mathbf{x})_j), \ldots\right]$$

Dropout at Test Time

- At test time, we replace the masks by their expectation
  - ➢ This is simply the constant vector 0.5 if dropout probability is 0.5
  - ➢ For single hidden layer: equivalent to taking the geometric average of all neural networks, with all possible binary masks

- Can be combined with unsupervised pre-training

- Beats regular backpropagation on many datasets

- Ensemble: Can be viewed as a geometric average of exponential number of networks.

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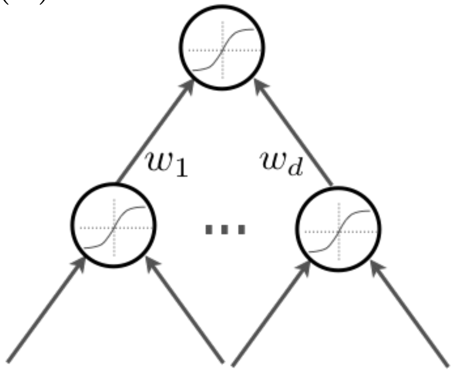
Batch Normalization

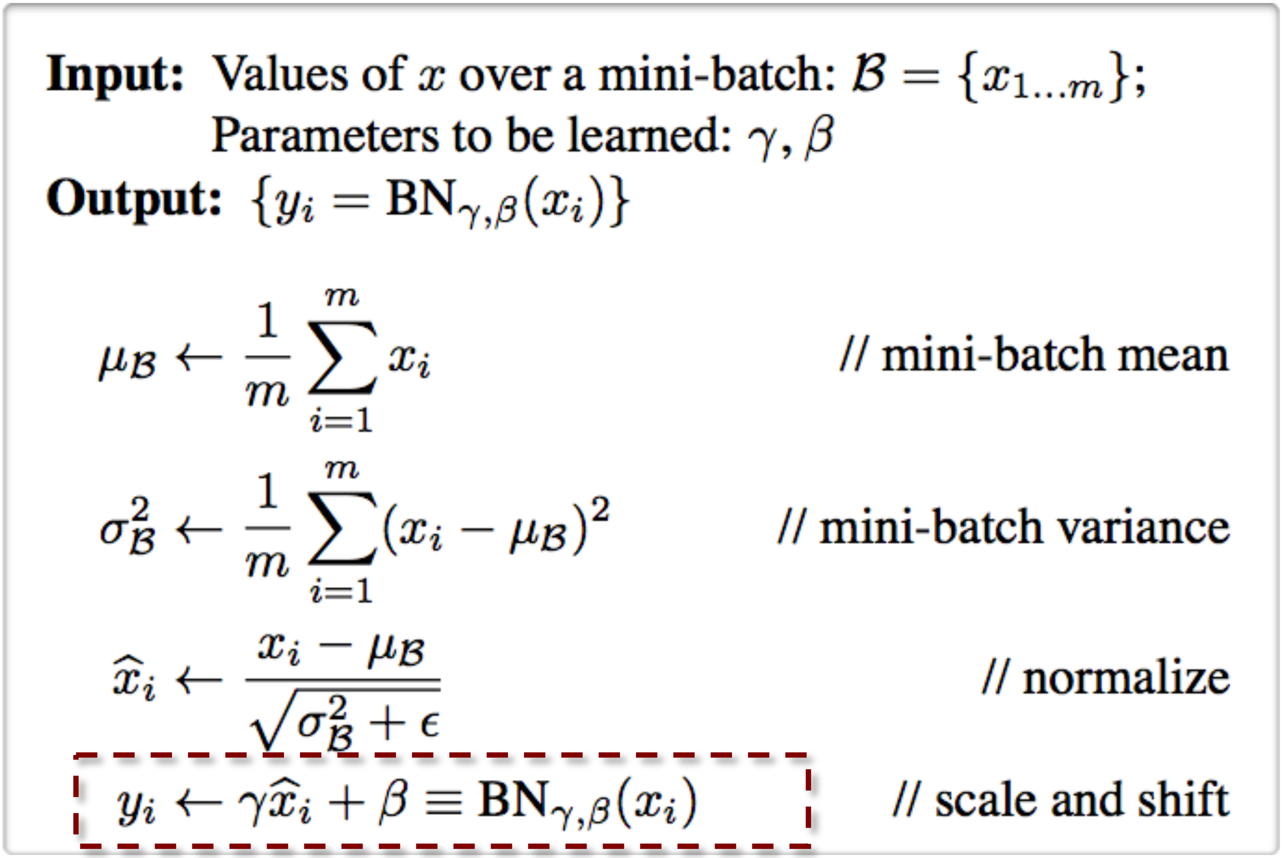
- Normalizing the inputs will speed up training (Lecun et al. 1998)
  - ➢ could normalization be useful at the level of the hidden layers?

- Batch normalization is an attempt to do that (Ioffe and Szegedy, 2014)
  - ➢ each unit's pre-activation is normalized (mean subtraction, stddev division)
  - ➢ during training, mean and stddev is computed for each minibatch
  - ➢ backpropagation takes into account the normalization
  - ➢ at test time, the global mean / stddev is used

$$\mathbf{a}^{(k)}(\mathbf{x}) = \mathbf{b}^{(k)} + \mathbf{W}^{(k)}\mathbf{h}^{(k-1)}(\mathbf{x})$$



Batch Normalization



```
Input: Values of $x$ over a mini-batch: $\mathcal{B} = \{x_{1\ldots m}\}$;
       Parameters to be learned: $\gamma$, $\beta$
Output: $\{y_i = \mathrm{BN}_{\gamma,\beta}(x_i)\}$

    $\mu_\mathcal{B} \leftarrow \frac{1}{m}\sum_{i=1}^{m} x_i$                              // mini-batch mean
    $\sigma_\mathcal{B}^2 \leftarrow \frac{1}{m}\sum_{i=1}^{m}(x_i - \mu_\mathcal{B})^2$          // mini-batch variance
    $\widehat{x}_i \leftarrow \frac{x_i - \mu_\mathcal{B}}{\sqrt{\sigma_\mathcal{B}^2 + \epsilon}}$                       // normalize
    $\boxed{y_i \leftarrow \gamma\widehat{x}_i + \beta \equiv \mathrm{BN}_{\gamma,\beta}(x_i)}$            // scale and shift
```

Learned linear transformation to adapt to non-linear activation function (γ and β are trained)

Batch Normalization

- Why normalize the pre-activation?
  - ➢ can help keep the pre-activation in a non-saturating regime (though the linear transform $y_i \leftarrow \gamma \widehat{x}_i + \beta$ could cancel this effect)
- Why use minibatches?
  - ➢ since hidden units depend on parameters, can't compute mean/stddev once and for all
  - ➢ adds stochasticity to training, which might regularize

Batch Normalization

- How to take into account the normalization in backdrop?
  - ➢ derivative w.r.t. x_i depends on the partial derivative of both: the mean and stddev
  - ➢ must also update γ and β

- Why use the global mean and stddev at test time?
  - ➢ removes the stochasticity of the mean and stddev
  - ➢ requires a final phase where, from the first to the last hidden layer
    - propagate all training data to that layer
    - compute and store the global mean and stddev of each unit
  - ➢ for early stopping, could use a running average

Optimization Tricks

- SGD with momentum, batch-normalization, and dropout usually works very well

- Pick learning rate by running on a subset of the data
  - ➢ Start with large learning rate & divide by 2 until loss does not diverge
  - ➢ Decay learning rate by a factor of ~100 or more by the end of training

- Use ReLU nonlinearity

- Initialize parameters so that each feature across layers has similar variance. Avoid units in saturation.

[From Marc'Aurelio Ranzato, CVPR tutorial]

Improving Generalization

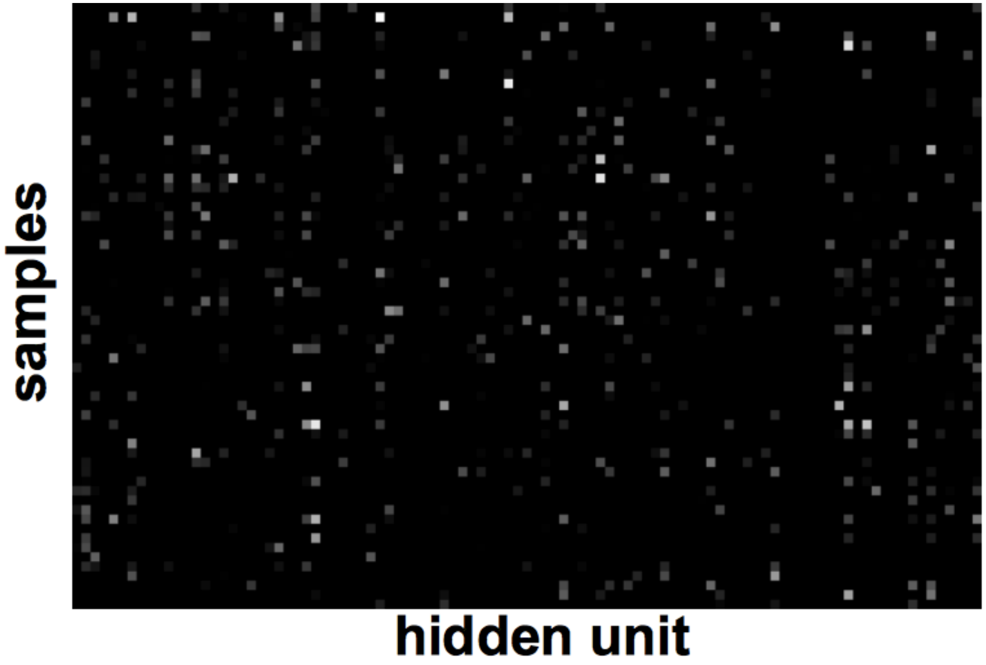
- Weight sharing (greatly reduce the number of parameters)
- Dropout
- Weight decay (L2, L1)
- Sparsity in the hidden units

[From Marc'Aurelio Ranzato, CVPR tutorial]

Visualization

- Check gradients numerically by finite differences

- Visualize features (features need to be uncorrelated) and have high variance



- Good training: hidden units are sparse across samples

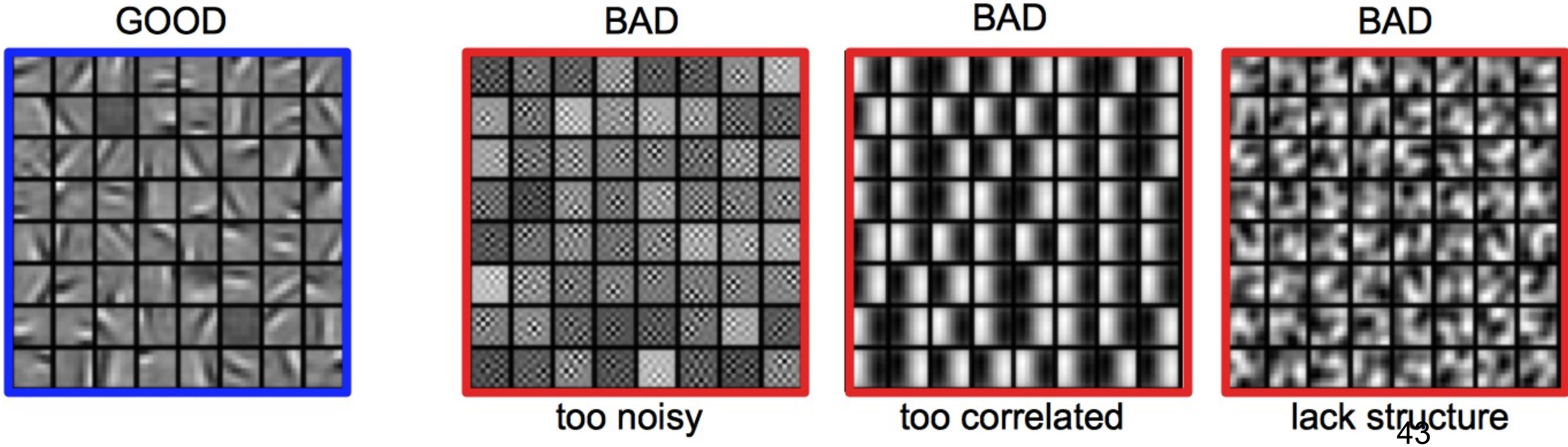
[From Marc'Aurelio Ranzato, CVPR tutorial]

Visualization

- Check gradients numerically by finite differences

- Visualize features (features need to be uncorrelated) and have high variance

- Visualize parameters: learned features should exhibit structure and should be uncorrelated and are uncorrelated

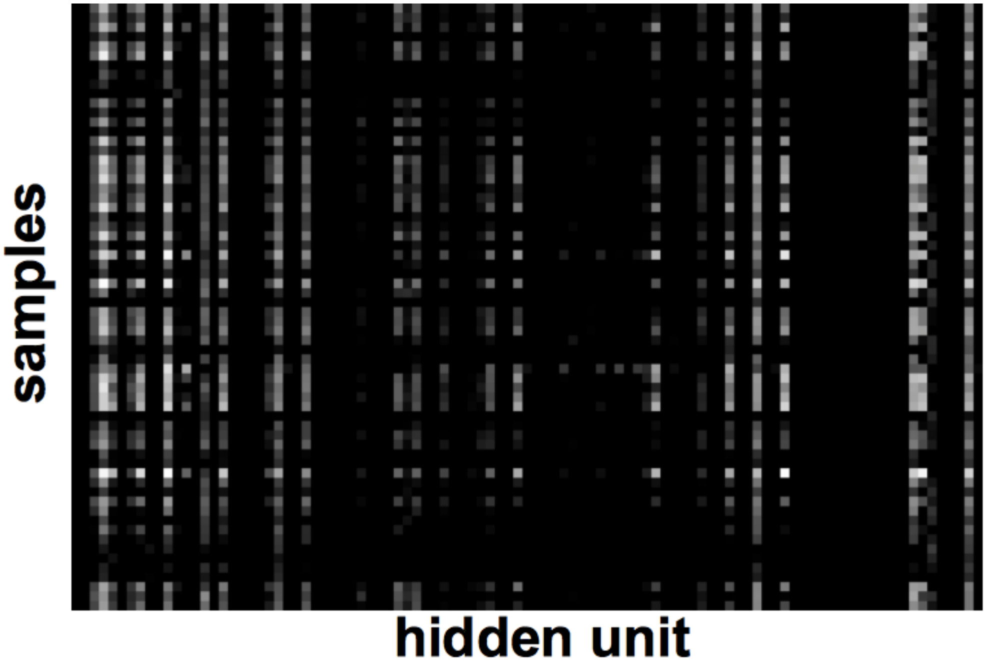


[From Marc'Aurelio Ranzato, CVPR tutorial]

Visualization

- Check gradients numerically by finite differences

- Visualize features (features need to be uncorrelated) and have high variance



- Bad training: many hidden units ignore the input and/or exhibit strong correlations

[From Marc'Aurelio Ranzato, CVPR tutorial]

Visualization

- Check gradients numerically by finite differences

- Visualize features (features need to be uncorrelated) and have high variance

- Visualize parameters: learned features should exhibit structure and should be uncorrelated and are uncorrelated

- Measure error on both training and validation set

- Test on a small subset of the data and check the error → 0.

[From Marc'Aurelio Ranzato, CVPR tutorial]

When it does not work

- Training diverges:
  - Learning rate may be too large → decrease learning rate
  - BPROP is buggy → numerical gradient checking
- Parameters collapse / loss is minimized but accuracy is low
  - Check loss function: Is it appropriate for the task you want to solve?
  - Does it have degenerate solutions?
- Network is underperforming
  - Compute flops and nr. params. → if too small, make net larger
  - Visualize hidden units/params → fix optimization
- Network is too slow
  - GPU,distrib. framework, make net smaller

[From Marc'Aurelio Ranzato, CVPR tutorial]