Network-independent tricks

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Overview

- Activation Units
- Loss Functions
- Initialization
- Regularization
- Optimization
- Model selection
- Other Tricks:
  - Debugging
  - Batch Normalization

NEURAL NETWORK

Topics: multilayer neural network

- Could have L hidden layers:
  - layer pre-activation for $k>0$ $(\mathbf{h}^{(0)}(\mathbf{x}) = \mathbf{x})$

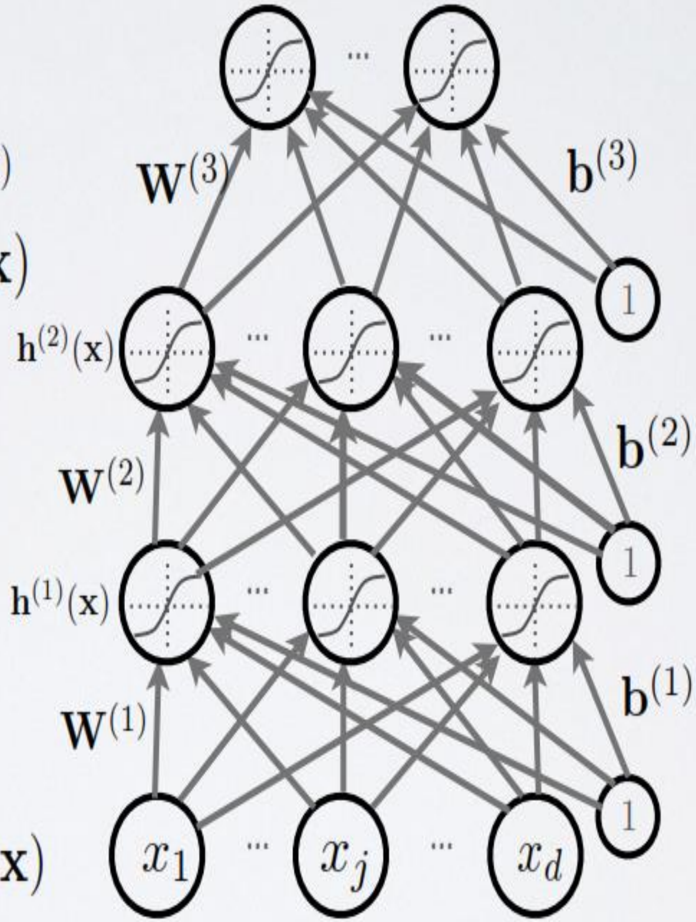
    $$\mathbf{a}^{(k)}(\mathbf{x}) = \mathbf{b}^{(k)} + \mathbf{W}^{(k)}\mathbf{h}^{(k-1)}(\mathbf{x})$$

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

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

  - output layer activation ($k=L+1$):

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



MACHINE LEARNING

Topics: empirical risk minimization, regularization

- Empirical risk minimization
  - framework to design learning algorithms

$$\arg\min_{\boldsymbol{\theta}} \frac{1}{T} \sum_t l(f(\mathbf{x}^{(t)}; \boldsymbol{\theta}), y^{(t)}) + \lambda \Omega(\boldsymbol{\theta})$$

  - $l(f(\mathbf{x}^{(t)}; \boldsymbol{\theta}), y^{(t)})$ is a loss function
  - $\Omega(\boldsymbol{\theta})$ is a regularizer (penalizes certain values of $\boldsymbol{\theta}$)
- Learning is cast as optimization
  - ideally, we'd optimize classification error, but it's not smooth
  - loss function is a surrogate for what we truly should optimize (e.g. upper bound)

MACHINE LEARNING

Topics: stochastic gradient descent (SGD)

- Algorithm that performs updates after each example
  - initialize $\boldsymbol{\theta}$ $\left(\boldsymbol{\theta} \equiv \{\mathbf{W}^{(1)}, \mathbf{b}^{(1)}, \ldots, \mathbf{W}^{(L+1)}, \mathbf{b}^{(L+1)}\}\right)$
  - for N iterations
    - for each training example $(\mathbf{x}^{(t)}, y^{(t)})$
      - ✓ $\Delta = -\nabla_{\boldsymbol{\theta}} l(f(\mathbf{x}^{(t)}; \boldsymbol{\theta}), y^{(t)}) - \lambda \nabla_{\boldsymbol{\theta}} \Omega(\boldsymbol{\theta})$
      - ✓ $\boldsymbol{\theta} \leftarrow \boldsymbol{\theta} + \alpha\, \Delta$

  training epoch = iteration over **all** examples

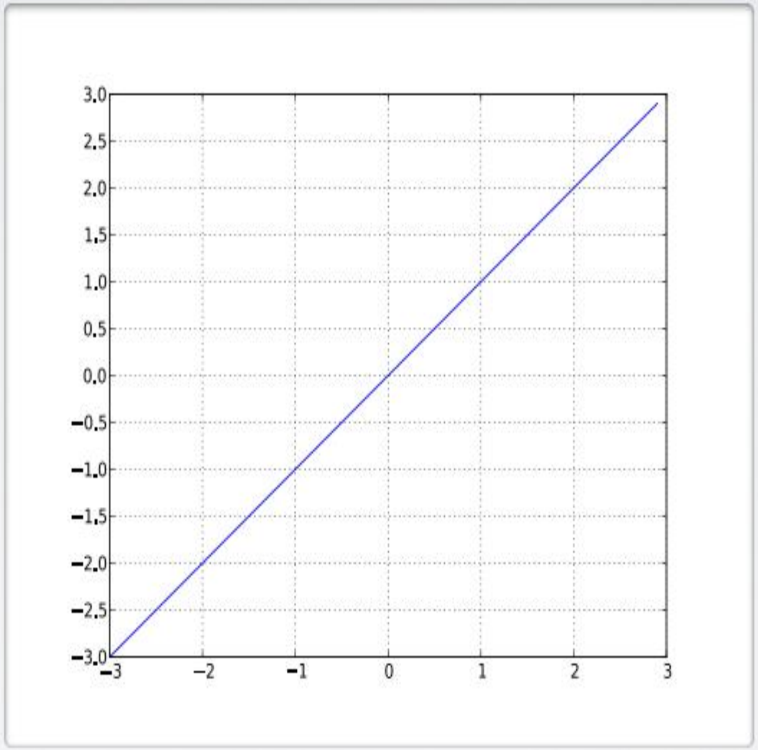
- To apply this algorithm to neural network training, we need
  - the loss function $l(\mathbf{f}(\mathbf{x}^{(t)}; \boldsymbol{\theta}), y^{(t)})$
  - a procedure to compute the parameter gradients $\nabla_{\boldsymbol{\theta}} l(\mathbf{f}(\mathbf{x}^{(t)}; \boldsymbol{\theta}), y^{(t)})$
  - the regularizer $\Omega(\boldsymbol{\theta})$ (and the gradient $\nabla_{\boldsymbol{\theta}} \Omega(\boldsymbol{\theta})$)

Activation Function

ACTIVATION FUNCTION

Topics: linear activation function

- Performs no input squashing
- Not very interesting...

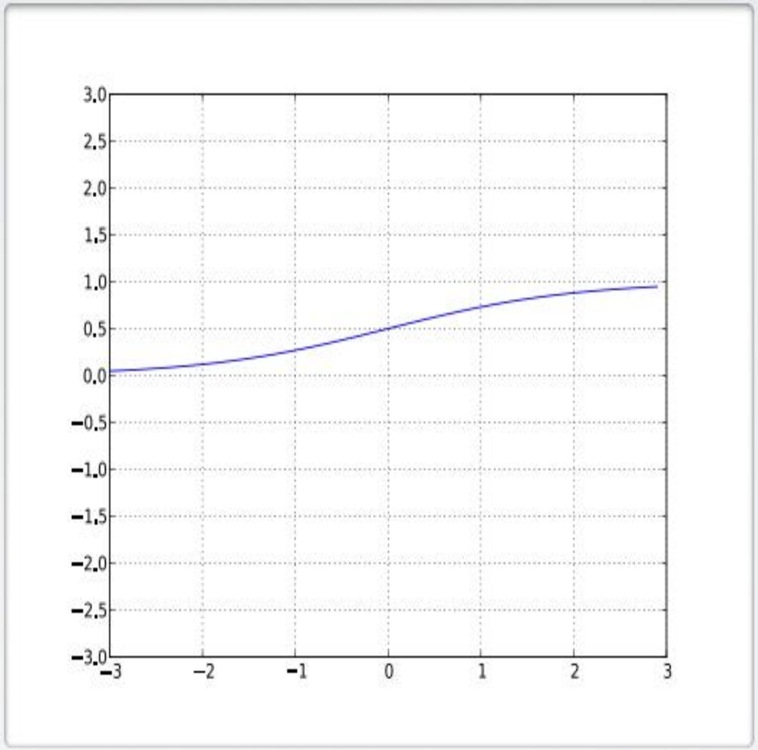


$$g(a) = a$$

ACTIVATION FUNCTION

Topics: sigmoid activation function

- Squashes the neuron's pre-activation between 0 and 1
- Always positive
- Bounded
- Strictly increasing

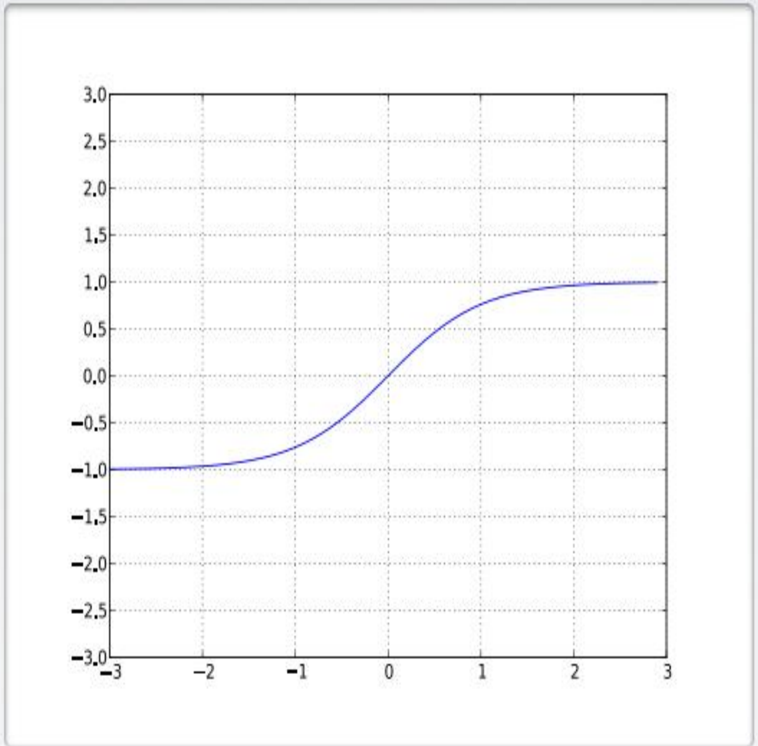


$$g(a) = \mathrm{sigm}(a) = \frac{1}{1+\exp(-a)}$$

ACTIVATION FUNCTION

Topics: hyperbolic tangent ("tanh") activation function

- Squashes the neuron's pre-activation between -1 and 1
- Can be positive or negative
- Bounded
- Strictly increasing

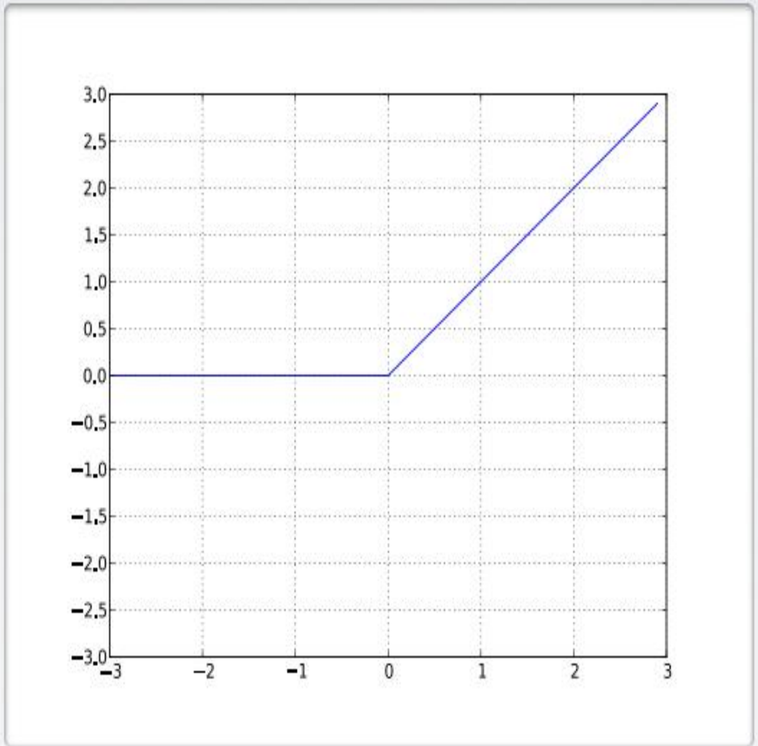


$$g(a) = \tanh(a) = \frac{\exp(a)-\exp(-a)}{\exp(a)+\exp(-a)} = \frac{\exp(2a)-1}{\exp(2a)+1}$$

ACTIVATION FUNCTION

Topics: rectified linear activation function

- Bounded below by 0 (always non-negative)
- Not upper bounded
- Strictly increasing
- Tends to give neurons with sparse activities



$$g(a) = \mathrm{reclin}(a) = \max(0, a)$$

LOSS FUNCTION

LOSS FUNCTION

Topics: loss function for classification

- Neural network estimates $f(\mathbf{x})_c = p(y = c|\mathbf{x})$
  - we could maximize the probabilities of $y^{(t)}$ given $\mathbf{x}^{(t)}$ in the training set

- To frame as minimization, we minimize the negative log-likelihood

natural log (ln)

$$l(\mathbf{f}(\mathbf{x}), y) = -\sum_c 1_{(y=c)} \log f(\mathbf{x})_c = -\log f(\mathbf{x})_y$$

  - we take the log to simplify for numerical stability and math simplicity
  - sometimes referred to as cross-entropy

INITIALIZATION

INITIALIZATION

Topics: initialization

- For biases
  - initialize all to 0
- For weights
  - Can't initialize weights to 0 with tanh activation
    - we can show that all gradients would then be 0 (saddle point)
  - Can't initialize all weights to the same value
    - we can show that all hidden units in a layer will always behave the same
    - need to break symmetry
  - Recipe: sample $\mathbf{W}_{i,j}^{(k)}$ from $U\left[-b, b\right]$ where $b = \frac{\sqrt{6}}{\sqrt{H_k + H_{k-1}}}$

    size of $\mathbf{h}^{(k)}(\mathbf{x})$
    - the idea is to sample around 0 but break symmetry
    - other values of b could work well (not an exact science) (see Glorot & Bengio, 2010)

MODEL SELECTION

MACHINE LEARNING

Topics: training, validation and test sets, generalization

- Training set $\mathcal{D}^{\text{train}}$ serves to train a model
- Validation set $\mathcal{D}^{\text{valid}}$ serves to select hyper-parameters
  - hidden layer size(s), learning rate, number of iterations/epochs, etc.
- Test set $\mathcal{D}^{\text{test}}$ serves to estimate the generalization performance (error)

- Generalization is the behavior of the model on **unseen examples**
  - this is what we care about in machine learning!

MODEL SELECTION

Topics: grid search, random search

- To search for the best configuration of the hyper-parameters:
  - you can perform a grid search
    - specify a set of values you want to test for each hyper-parameter
    - try all possible configurations of these values
  - you can perform a random search (Bergstra and Bengio, 2012)
    - specify a distribution over the values of each hyper-parameters (e.g. uniform in some range)
    - sample independently each hyper-parameter to get configurations
  - bayesian optimization or sequential model-based optimization ...
- Use a validation set performance to select the best configuration
- You can go back and refine the grid/distributions if needed

FIGHTING OVERFITTING

REGULARIZATION

Topics: L2 regularization

$$\Omega(\boldsymbol{\theta}) = \sum_k \sum_i \sum_j \left(W_{i,j}^{(k)}\right)^2 = \sum_k ||\mathbf{W}^{(k)}||_F^2$$

- Gradient: $\nabla_{\mathbf{W}^{(k)}} \Omega(\boldsymbol{\theta}) = 2\mathbf{W}^{(k)}$

- Only applied on weights, not on biases (weight decay)
- Can be interpreted as having a Gaussian prior over the weights

REGULARIZATION

Topics: L1 regularization

$$\Omega(\boldsymbol{\theta}) = \sum_k \sum_i \sum_j |W_{i,j}^{(k)}|$$

- Gradient: $\nabla_{\mathbf{W}^{(k)}} \Omega(\boldsymbol{\theta}) = \text{sign}(\mathbf{W}^{(k)})$
  - where $\text{sign}(\mathbf{W}^{(k)})_{i,j} = 1_{\mathbf{W}_{i,j}^{(k)} > 0} - 1_{\mathbf{W}_{i,j}^{(k)} < 0}$
- Also only applied on weights
- Unlike L2, L1 will push certain weights to be exactly 0
- Can be interpreted as having a Laplacian prior over the weights

KNOWING WHEN TO STOP

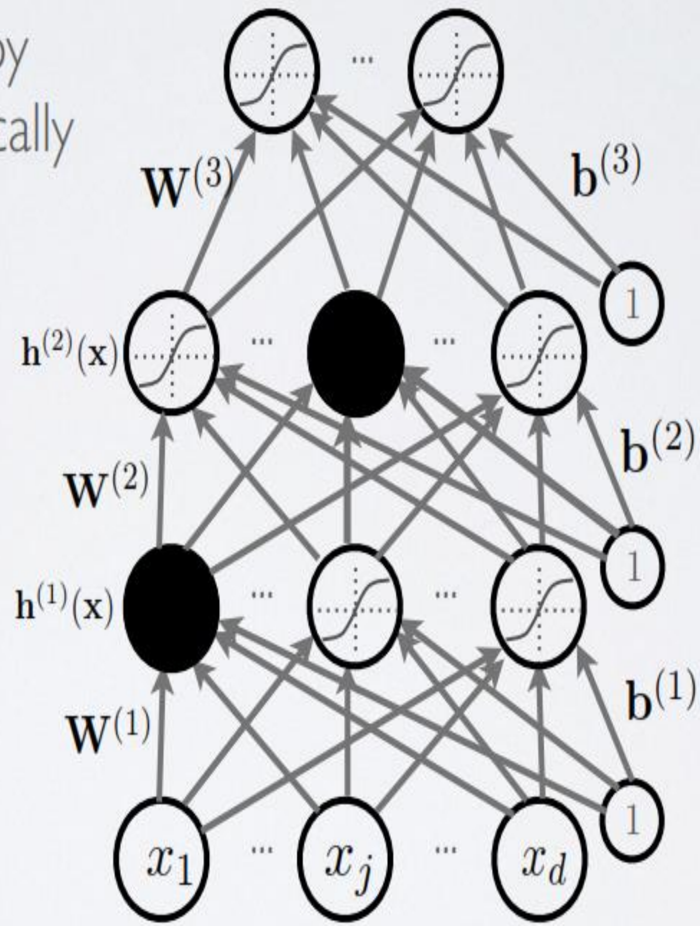
Topics: early stopping

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

DROPOUT

Topics: dropout

- 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

Topics: dropout

- Use random binary masks $\mathbf{m}^{(k)}$
  - layer pre-activation for $k>0$ $(\mathbf{h}^{(0)}(\mathbf{x}) = \mathbf{x})$

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

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

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

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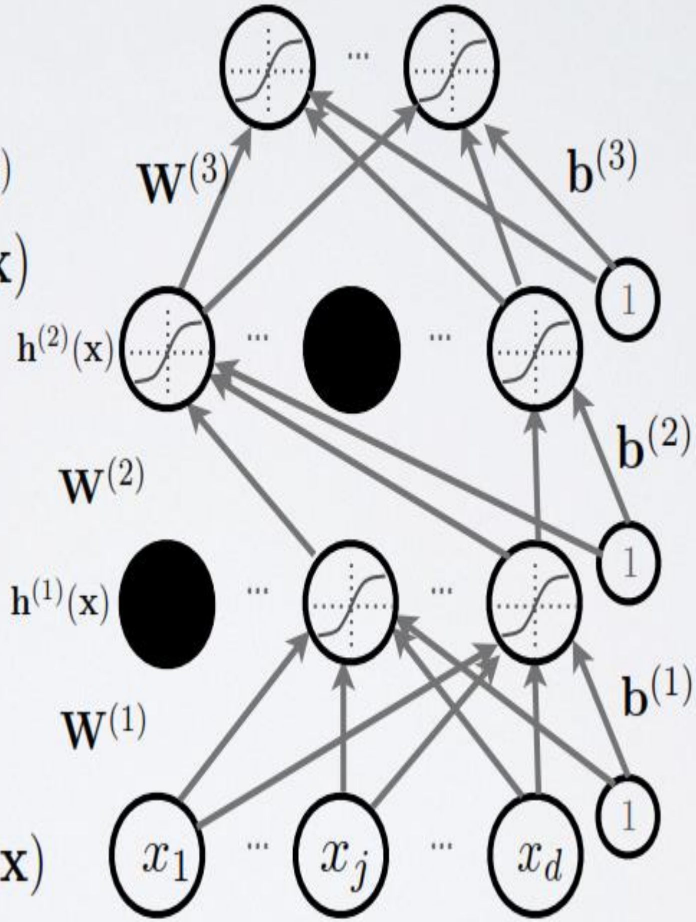


DROPOUT

Topics: test time classification

- 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, can show this is 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
  - Improving neural networks by preventing co-adaptation of feature detectors. Hinton, Srivastava, Krizhevsky, Sutskever and Salakhutdinov, 2012.

UNSUPERVISED PRE-TRAINING

Topics: unsupervised pre-training

- Solution: initialize hidden layers using unsupervised learning
  - force network to represent latent structure of input distribution

character image

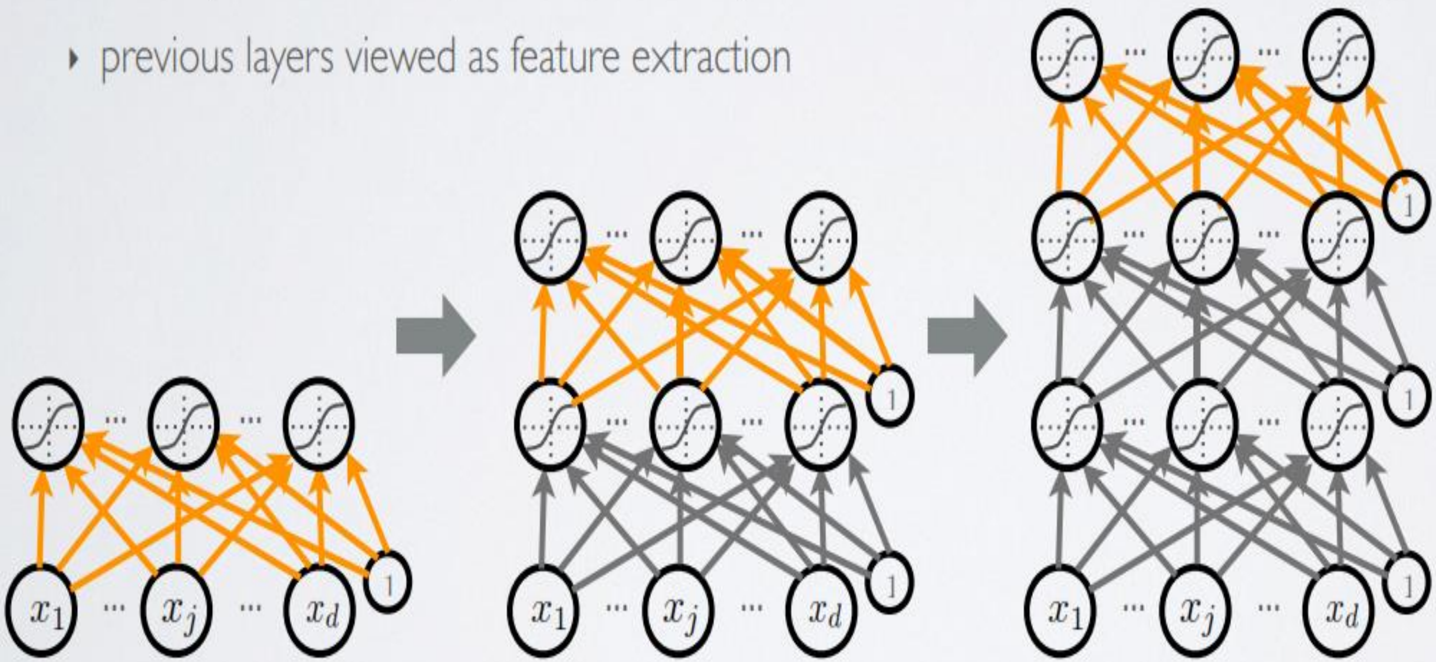
random image

  - encourage hidden layers to encode that structure

UNSUPERVISED PRE-TRAINING

Topics: unsupervised pre-training

- We will use a greedy, layer-wise procedure
  - train one layer at a time, from first to last, with unsupervised criterion
  - fix the parameters of previous hidden layers
  - previous layers viewed as feature extraction



UNSUPERVISED PRE-TRAINING

Topics: unsupervised pre-training

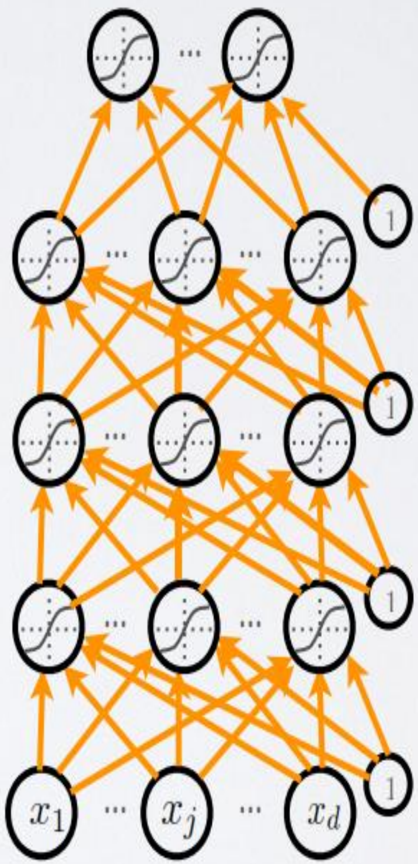
- We call this procedure unsupervised pre-training
  - **first layer:** find hidden unit features that are more common in training inputs than in random inputs
  - **second layer:** find *combinations* of hidden unit features that are more common than random hidden unit features
  - **third layer:** find *combinations of combinations* of ...
  - etc.

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

FINE-TUNING

Topics: 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 feed-forward 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



OPTIMIZATION

OTHER TRICKS OF THE TRADE

Topics: mini-batch, momentum

- Can update based on a mini-batch of example (instead of 1 example):
  - the gradient is the average regularized loss for that mini-batch
  - can give a more accurate estimate of the risk gradient
  - can leverage matrix/matrix operations, which are more efficient

- 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 through plateaus more quickly, by "gaining momentum"

OTHER TRICKS OF THE TRADE

Topics: Adagrad, RMSProp, Adam

- 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

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

  - **Adam**: essentially combines RMSProp with momentum

DEBUGGING

GRADIENT CHECKING

Topics: finite difference approximation

- 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

Topics: debugging on small dataset

- Next, make sure your model is able to (over)fit on a very small dataset (~50 examples)

- 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

- Note that this isn't a replacement for gradient checking
  - could still overfit with some of the gradients being wrong

BATCH NORMALIZATION

BATCH NORMALIZATION

Topics: batch normalization

- Normalizing the inputs will speed up training (Lecun et al. 1998)
  - could normalization also 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**

BATCH NORMALIZATION

Topics: batch normalization

- **Batch normalization**

Input: Values of x over a mini-batch: $\mathcal{B} = \{x_{1\ldots m}\}$;
Parameters to be learned: γ, β

Output: $\{y_i = \mathrm{BN}_{\gamma,\beta}(x_i)\}$

$$\mu_\mathcal{B} \leftarrow \frac{1}{m}\sum_{i=1}^{m} x_i \qquad \text{// mini-batch mean}$$

$$\sigma_\mathcal{B}^2 \leftarrow \frac{1}{m}\sum_{i=1}^{m} (x_i - \mu_\mathcal{B})^2 \qquad \text{// mini-batch variance}$$

$$\widehat{x}_i \leftarrow \frac{x_i - \mu_\mathcal{B}}{\sqrt{\sigma_\mathcal{B}^2 + \epsilon}} \qquad \text{// normalize}$$

$$\boxed{y_i \leftarrow \gamma \widehat{x}_i + \beta \equiv \mathrm{BN}_{\gamma,\beta}(x_i)} \qquad \text{// scale and shift}$$

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

BATCH NORMALIZATION

Topics: 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 (dropout not as useful)

BATCH NORMALIZATION

Topics: batch normalization

- How to take into account the normalization in backdrop?
  - derivative wrt x_i depends on the partial derivative of the mean and stddev
  - must also update γ and β
- Why use the global mean 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
    1. propagate all training data to that layer
    2. compute and store the global mean and stddev of each unit
  - for early stopping, could use a running average

Discussion

- Sigmoid Units are coming back thanks to BN.
- Initialization: Pre-training can help.
- Regularization: BN, Dropout, early stopping.
- Optimization: Adam, RMSPROP.
- Model selection: Random search or grid search.

THANK YOU!

DROPOUT

Topics: dropout backpropagation

- This assumes a forward propagation has been made before
  - compute output gradient (before activation)

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

  - for k from $L+1$ to 1

includes the mask $\mathrm{m}^{(k-1)}$

    - compute gradients of hidden layer parameter

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

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

    - compute gradient of hidden layer below

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

    - compute gradient of hidden layer below (before activation)

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

$$\frac{\partial \ell}{\partial \widehat{x}_i} = \frac{\partial \ell}{\partial y_i} \cdot \gamma$$

$$\frac{\partial \ell}{\partial \sigma_{\mathcal{B}}^2} = \sum_{i=1}^{m} \frac{\partial \ell}{\partial \widehat{x}_i} \cdot (x_i - \mu_{\mathcal{B}}) \cdot \frac{-1}{2}\left(\sigma_{\mathcal{B}}^2 + \epsilon\right)^{-3/2}$$

$$\frac{\partial \ell}{\partial \mu_{\mathcal{B}}} = \left(\sum_{i=1}^{m} \frac{\partial \ell}{\partial \widehat{x}_i} \cdot \frac{-1}{\sqrt{\sigma_{\mathcal{B}}^2+\epsilon}}\right) + \frac{\partial \ell}{\partial \sigma_{\mathcal{B}}^2} \cdot \frac{\sum_{i=1}^{m} -2(x_i - \mu_{\mathcal{B}})}{m}$$

$$\frac{\partial \ell}{\partial x_i} = \frac{\partial \ell}{\partial \widehat{x}_i} \cdot \frac{1}{\sqrt{\sigma_{\mathcal{B}}^2+\epsilon}} + \frac{\partial \ell}{\partial \sigma_{\mathcal{B}}^2} \cdot \frac{2(x_i - \mu_{\mathcal{B}})}{m} + \frac{\partial \ell}{\partial \mu_{\mathcal{B}}} \cdot \frac{1}{m}$$

$$\frac{\partial \ell}{\partial \gamma} = \sum_{i=1}^{m} \frac{\partial \ell}{\partial y_i} \cdot \widehat{x}_i$$

$$\frac{\partial \ell}{\partial \beta} = \sum_{i=1}^{m} \frac{\partial \ell}{\partial y_i}$$