CSE 5526: Introduction to Neural Networks

MLP Tips

MLP design parameters

- Several parameters to choose when designing an MLP (best to evaluate empirically)
- Number of hidden layers
- Number of units in each hidden layer
- Activation function
- Error function

Optimization tricks

- For a given network, local minima of the cost function are possible
- Many tricks exist to try to find better local minima
  - Momentum: mix in gradient from step
  - Weight initialization: small random values
  - Stopping criterion: early stopping
  - Learning rate annealing: start with large , slowly shrink
  - Second order methods: use a separate for each parameter or pair of parameters based on local curvature
  - Randomization of training example order
  - Regularization, i.e., terms in E(w) that only depend on w

Learning rate control: momentum

- To ease oscillating weights due to large η, some inertia (momentum) of weight update is added

$$\Delta w_{ji}(n) = \eta \delta_j y_i + \alpha \Delta w_{ji}(n-1), \qquad 0 < \alpha < 1$$

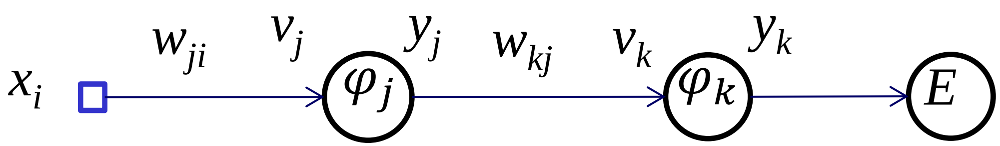
  - In the downhill situation, $\Delta w_{ji}(n) \approx \frac{\eta}{1-\alpha} \delta_j y_i$
    - thus accelerating learning by a factor of $1/(1 - \alpha)$
  - In the oscillating situation, it smooths weight change, thus stabilizing oscillations

Input pre-processing

- Remove mean
  - Avoids extra update steps to learn it
- Divide by standard deviation
  - Or whiten by multiplying by the square root of the covariance matrix
  - Make dimensions commensurate
  - Scales curvature of error surface to be less canyon-like

Weight initialization

- Consider a network with one hidden layer and a single output neuron
- What happens if we initialize all weights to 0?



$$y_k = \varphi\left(\sum_j w_{kj}\, \varphi\left(\sum_i w_{ji} x_i\right)_j\right)_k$$

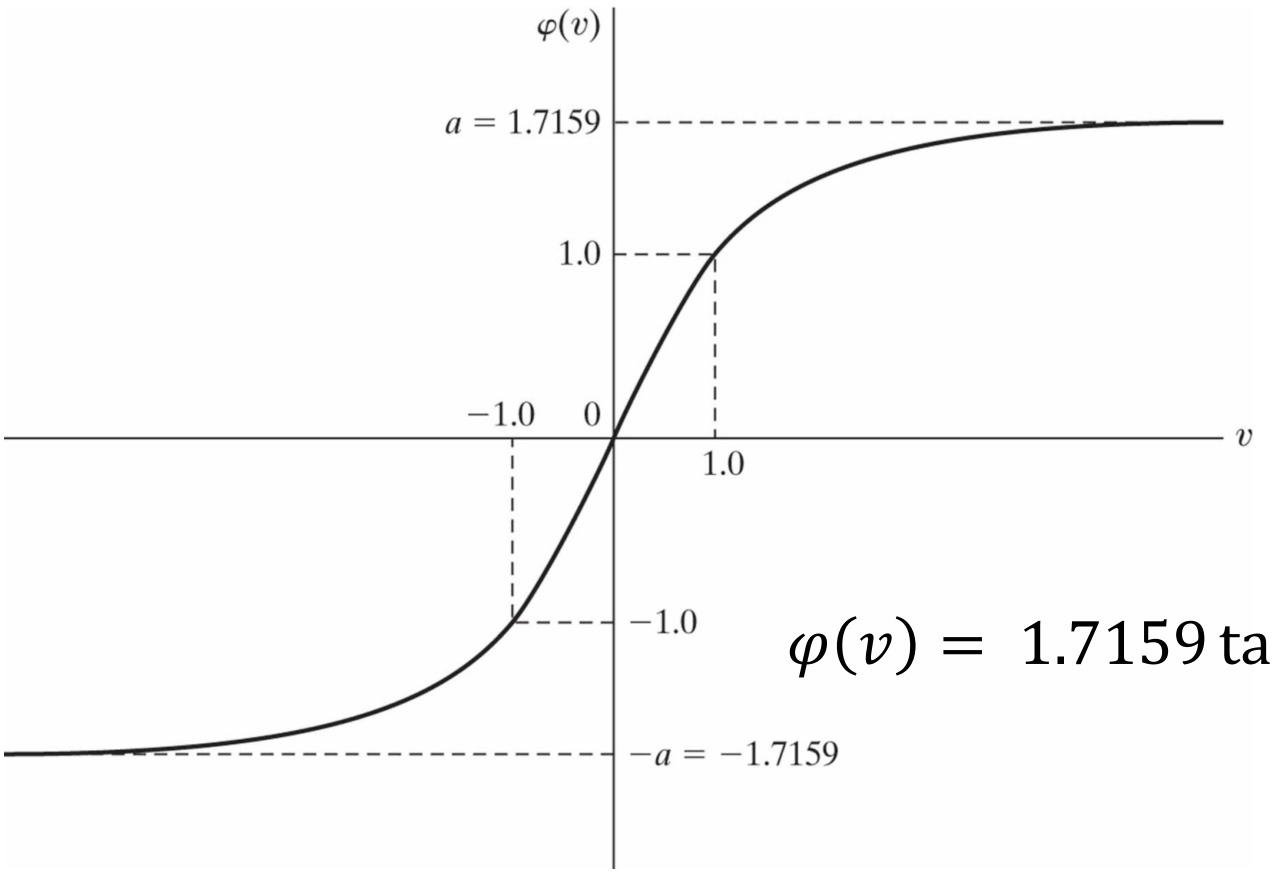
$$\frac{\partial}{\partial w_{kj}} E(\boldsymbol{w}) = -e_k \varphi'(v_k) y_j$$

$$\frac{\partial}{\partial w_{ji}} E(\boldsymbol{w}) = -e_j \varphi'(v_j) x_i$$

Weight initialization

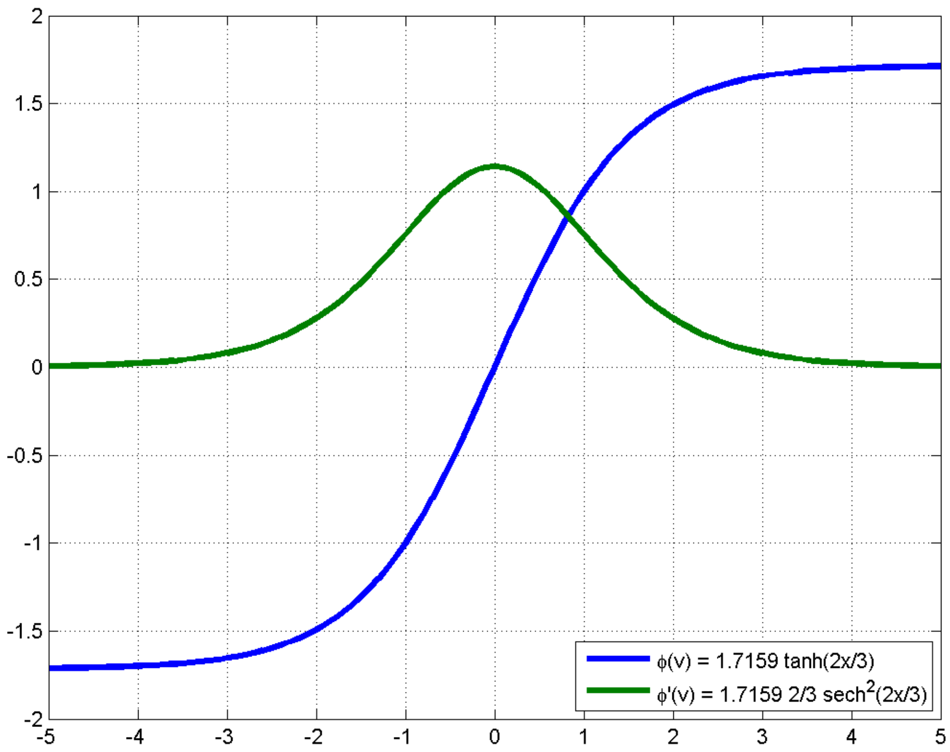
- Break symmetry by initializing with random values
- If inputs are normalized, they are uncorrelated, with zero-mean, and unit-variance
- Would like output to be approximately the same
- So inputs to sigmoid nonlinearity must be too

Hyperbolic tangent function



$$\varphi(v) = 1.7159 \tanh\left(\frac{2}{3}v\right)$$

Hyperbolic tangent function



Weight initialization

$$\sigma_{y_i}^2 = E_x\{y_i^2\} = E_x\left\{\varphi^2\left(\sum_j w_{ij}x_j\right)\right\}$$

$$\approx E_x\left\{\left(\sum_j w_{ij}x_j\right)^2\right\} \approx \sum_j w_{ij}^2 E_x\{x_j^2\}$$

$$= \sum_{j=1}^{m} w_{ij}^2$$

- So in order to make $\sigma_{y_i}^2 = 1$
  - Initialize w_{ij} randomly with $\sigma_w^2 = \frac{1}{m}$

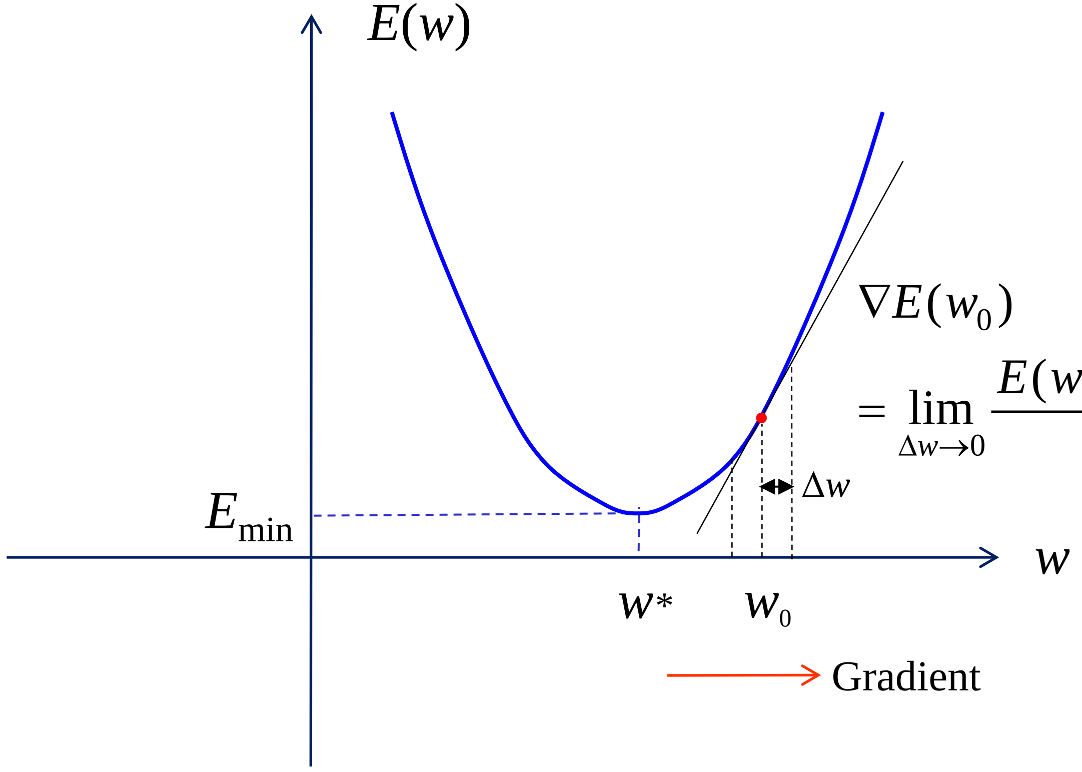
Debugging: Gradient checking

- Is your backpropagation code working properly?
  - I.e., is it computing the right gradient?
- Backpropagation computes

$$\nabla_{\mathbf{w}} E(\boldsymbol{x}_p; \boldsymbol{w}) = \left[\frac{\partial E}{\partial w_{111}}, \frac{\partial E}{\partial w_{121}}, \dots, \frac{\partial E}{\partial w_{NML}}\right]$$

  - where $w_{i_1 i_2 \ell}$ is the weight in layer ℓ connecting neurons i_1 and i_2
- Compute the gradient **numerically** and compare

Recall: Gradient illustration



$$\nabla E(w_0) = \lim_{\Delta w \to 0} \frac{E(w_0 + \Delta w) - E(w_0 - \Delta w)}{2\Delta w}$$

Debugging: Gradient checking

- One-sided numerical gradient:

$$\frac{\partial E}{\partial w_{i_1 i_2 \ell}} \approx \frac{1}{\delta}\left(E\left(\boldsymbol{x}_p; \boldsymbol{w} + \delta \mathbf{1}_{i_1 i_2 \ell}\right) - E\left(\boldsymbol{x}_p; \boldsymbol{w}\right)\right)$$

  - where $\mathbf{1}_{i_1 i_2 \ell}$ is a vector that is 1 at entry $i_1 i_2 \ell$ and 0 everywhere else and δ is a “small” constant
- Two-sided numerical gradient:

$$\frac{1}{2\delta}\left(E\left(\boldsymbol{x}_p; \boldsymbol{w} + \delta \mathbf{1}_{i_1 i_2 \ell}\right) - E\left(\boldsymbol{x}_p; \boldsymbol{w} - \delta \mathbf{1}_{i_1 i_2 \ell}\right)\right)$$

  - More accurate approximation
  - But requires twice as many evaluations of $E\left(\boldsymbol{x}_p; \boldsymbol{w}\right)$

Debugging: Gradient checking

- Complexity of backpropagation
  - 1 forward pass (O(1) multiply and add per weight)
  - 1 backward pass (O(1) multiply and add per weight)
- Complexity of numerical gradient
  - One-sided: 1 forward pass *per network weight*
    - So W+1 forward passes total
  - Two-sided: 2 forward passes *per network weight*
- So numerical gradient is good for checking correctness of backpropagation
  - But very slow to use in training, especially for large W

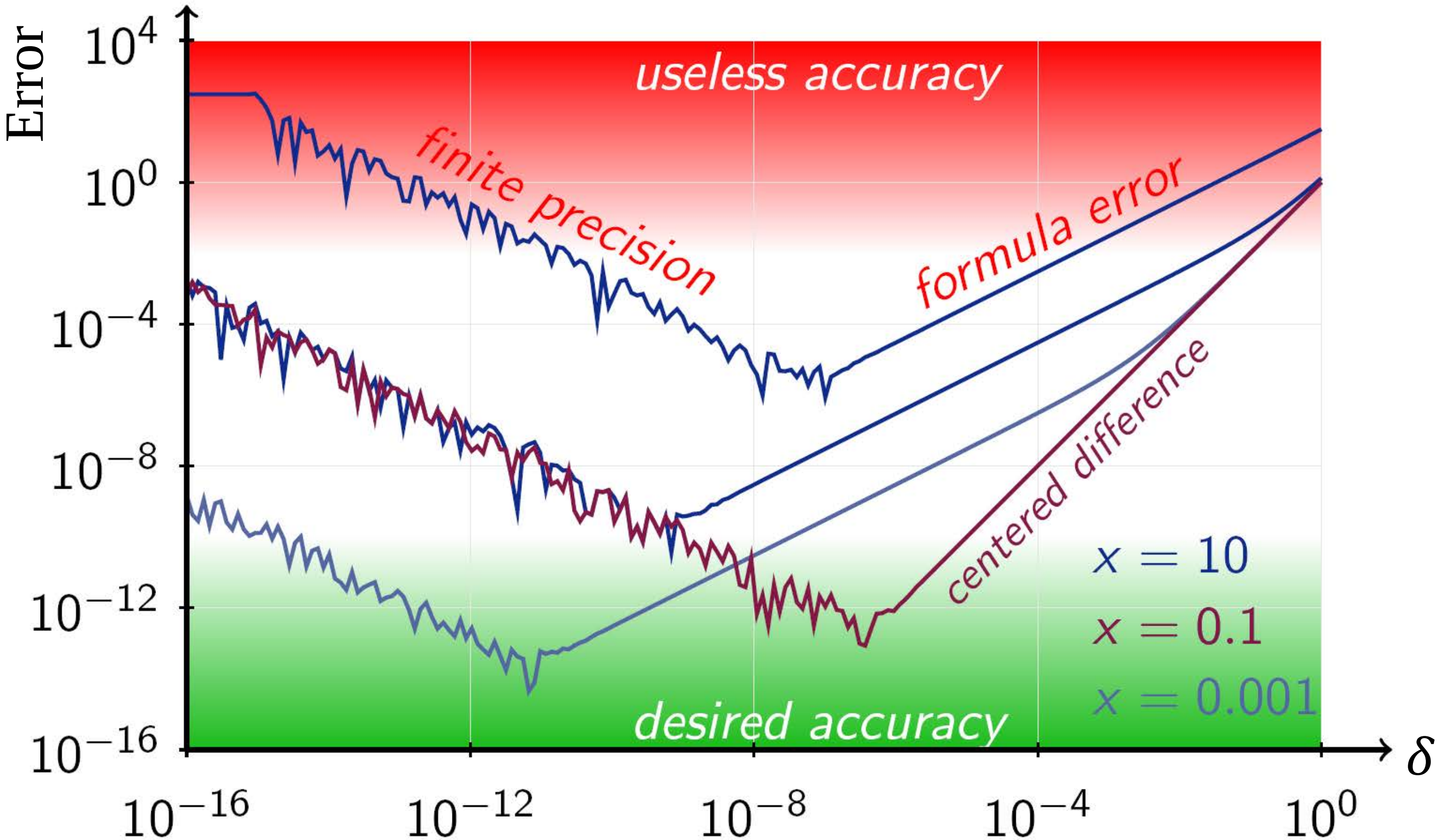
Gradient checking procedure

- Select an example data point, $\boldsymbol{x}_p$, initialize $\boldsymbol{w}$
- Compute the gradient of $E(\boldsymbol{x}_p; \boldsymbol{w})$ using backprop
  - Gives a vector of derivatives, one for each weight in the network
- Compute the gradient numerically
  - Evaluate $E(\boldsymbol{x}_p; \boldsymbol{w})$
  - Loop over each weight in the network
    - Evaluate $E(\boldsymbol{x}_p; \boldsymbol{w} + \delta \mathbf{1}_{i_1 i_2 \ell})$, compute partial derivative
- If they are not the same, look for patterns as a function of i_1, i_2, ℓ, etc

How to select δ?

- δ too big means derivative might be different at $E\left(\boldsymbol{x}_p; \boldsymbol{w} + \delta \mathbf{1}_{i_1 i_2 \ell}\right)$ and $E\left(\boldsymbol{x}_p; \boldsymbol{w}\right)$
  - Leading to a bad estimate using the above formulas
- δ too small runs into numerical issues
  - Need to be aware of limitations of floating point math
  - For δ too small, $1 + \delta = 1$
  - This might be around 1e-16, depending on the data type (e.g., float, double)
  - So $\delta =$ 1e-8 might be reasonable

How to select δ?



"AbsoluteErrorNumericalDifferentiationExample" by Berland - Self-made using TikZ, Beamer and LaTeX. Licensed under Public domain via Wikimedia Commons - http://commons.wikimedia.org/wiki/File:AbsoluteErrorNumericalDifferentiationExample.png #mediaviewer/File:AbsoluteErrorNumericalDifferentiationExample.png