# Training Multilayer Networks

Deep Learning

## Training Set

$$\{\mathbf{p}_1, \mathbf{t}_1\}, \{\mathbf{p}_2, \mathbf{t}_2\}, ..., \{\mathbf{p}_Q, \mathbf{t}_Q\}$$

## Network Response

$$\begin{aligned} \mathbf{a}_q^0 &= \mathbf{p}_q \\ \mathbf{a}_q^{m+1} &= \mathbf{f}^{m+1}\left(\mathbf{W}^{m+1}\mathbf{a}_q^m + \mathbf{b}^{m+1}\right) \text{ for } m = 0, 1, \ldots, M-1 \\ \mathbf{a}_q &= \mathbf{a}_q^M \end{aligned}$$

## Mean Square Error Performance Index

$$F(\mathbf{x}) = \frac{1}{QS^M} \sum_{q=1}^{Q} \sum_{i=1}^{S^M} \left(t_{i,q} - a_{i,q}^M\right)^2$$

## Cross Entropy Performance Index

$$a_{i,q} = P\{\mathbf{p}_q \text{ belongs to class } i\}$$

$$\mathbf{T} = \begin{bmatrix}\mathbf{t}_1 & \mathbf{t}_2 & \cdots & \mathbf{t}_Q\end{bmatrix}, \mathbf{P} = \begin{bmatrix}\mathbf{p}_1 & \mathbf{p}_2 & \cdots & \mathbf{p}_Q\end{bmatrix}$$

Likelihood Function

$$P\{\mathbf{T} \mid \mathbf{P}\} = \prod_{q=1}^{Q} \prod_{i=1}^{S^M} a_{i,q}^{t_{i,q}}$$

Negative Log Likelihood – Cross Entropy

$$F(\mathbf{x}) = -\sum_{q=1}^{Q} \sum_{i=1}^{S^M} t_{i,q} \ln a_{i,q}$$

## Approximate performance index

2nd order Taylor series expansion (quadratic)

$$F(\mathbf{x}) \cong F(\mathbf{x}^*) + \nabla F(\mathbf{x})^T|_{\mathbf{x}^*} (\mathbf{x} - \mathbf{x}^*) + \frac{1}{2} (\mathbf{x} - \mathbf{x}^*)^T \nabla^2 F(\mathbf{x})|_{\mathbf{x}^*} (\mathbf{x} - \mathbf{x}^*)$$

Gradient – Direction of increasing $F(\mathbf{x})$

$$\nabla F(\mathbf{x}) = \begin{bmatrix} \frac{\partial F(\mathbf{x})}{\partial x_1} & \frac{\partial F(\mathbf{x})}{\partial x_2} & \cdots & \frac{\partial F(\mathbf{x})}{\partial x_n} \end{bmatrix}^T$$

Hessian – Curvature of $F(\mathbf{x})$

$$\nabla^2 F(\mathbf{x}) = \begin{bmatrix} \frac{\partial^2 F(\mathbf{x})}{\partial x_1^2} & \frac{\partial^2 F(\mathbf{x})}{\partial x_1 \partial x_2} & \cdots & \frac{\partial^2 F(\mathbf{x})}{\partial x_1 \partial x_n} \\ \frac{\partial^2 F(\mathbf{x})}{\partial x_2 \partial x_1} & \frac{\partial^2 F(\mathbf{x})}{\partial x_2^2} & \cdots & \frac{\partial^2 F(\mathbf{x})}{\partial x_1 \partial x_n} \\ \vdots & \vdots & \ddots & \vdots \\ \frac{\partial^2 F(\mathbf{x})}{\partial x_n \partial x_1} & \frac{\partial^2 F(\mathbf{x})}{\partial x_n \partial x_2} & \cdots & \frac{\partial^2 F(\mathbf{x})}{\partial x_n^2} \end{bmatrix}$$

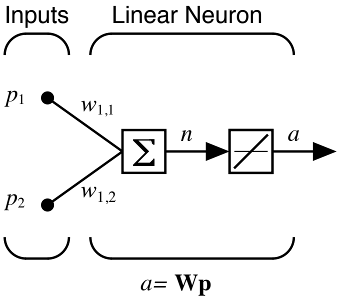
## General optimization algorithm

$$\mathbf{x}_{k+1} = \mathbf{x}_k + \alpha_k \mathbf{p}_k$$

- The search direction at iteration $k$ is $\mathbf{p}_k$.
- The learning rate is $\alpha_k$.
- For small learning rates, the largest reduction in $F(\mathbf{x})$ is obtained by setting $\mathbf{p}_k = -\nabla F(\mathbf{x}_k)$, the negative of the gradient direction. This is called the *steepest descent*, or gradient descent algorithm.

$$\mathbf{x}_{k+1} = \mathbf{x}_k - \alpha \nabla F(\mathbf{x}_k)$$

## Example



$$\left\{\mathbf{p}_1 = \begin{bmatrix}-1\\2\end{bmatrix}, \mathbf{t}_1 = [-1]\right\}, \left\{\mathbf{p}_2 = \begin{bmatrix}2\\-1\end{bmatrix}, \mathbf{t}_2 = [-1]\right\}$$

$$\left\{\mathbf{p}_3 = \begin{bmatrix}0\\-1\end{bmatrix}, \mathbf{t}_3 = [1]\right\}, \left\{\mathbf{p}_4 = \begin{bmatrix}-1\\0\end{bmatrix}, \mathbf{t}_4 = [1]\right\}$$

## Example performance index

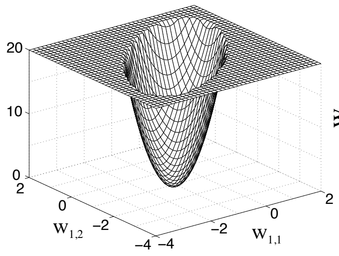
$$\mathbf{U} = \begin{bmatrix} \mathbf{p}_1^T \\ \mathbf{p}_2^T \\ \mathbf{p}_3^T \\ \mathbf{p}_4^T \end{bmatrix}, \mathbf{t} = \begin{bmatrix} t_1 \\ t_2 \\ t_3 \\ t_4 \end{bmatrix}, \mathbf{x} = \begin{bmatrix} w_{1,1} \\ w_{1,2} \end{bmatrix}$$

$$\begin{aligned} F(\mathbf{x}) &= \sum_{q=1}^{4} (t_q - a_q)^2 = (\mathbf{t} - \mathbf{U}\mathbf{x})^T (\mathbf{t} - \mathbf{U}\mathbf{x}) \\ &= \left(\mathbf{t}^T\mathbf{t} - 2\mathbf{t}^T\mathbf{U}\mathbf{x} + \mathbf{x}^T\mathbf{U}^T\mathbf{U}\mathbf{x}\right) \\ &= c + \mathbf{d}^T\mathbf{x} + \frac{1}{2}\mathbf{x}^T\mathbf{A}\mathbf{x} \\ \nabla F(\mathbf{x}) &= \mathbf{A}\mathbf{x} + \mathbf{d}, \nabla^2 F(\mathbf{x}) = \mathbf{A} \end{aligned}$$

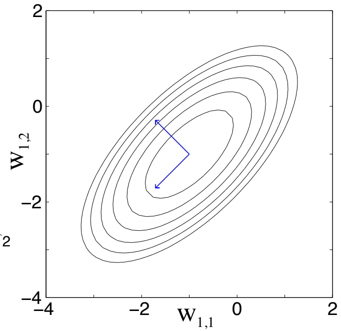
$$c = \mathbf{t}^T\mathbf{t}, \mathbf{d} = -2\mathbf{U}^T\mathbf{t}, \mathbf{A} = 2\mathbf{U}^T\mathbf{U}$$

# Example performance surface

$$\mathbf{U} = \begin{bmatrix} -1 & 2 \\ 2 & -1 \\ 0 & -1 \\ -1 & 0 \end{bmatrix}, \mathbf{t} = \begin{bmatrix} -1 \\ -1 \\ 1 \\ 1 \end{bmatrix}, \mathbf{A} = \begin{bmatrix} 12 & -8 \\ -8 & 12 \end{bmatrix}, \mathbf{d} = \begin{bmatrix} 4 \\ 4 \end{bmatrix}, c = 4$$



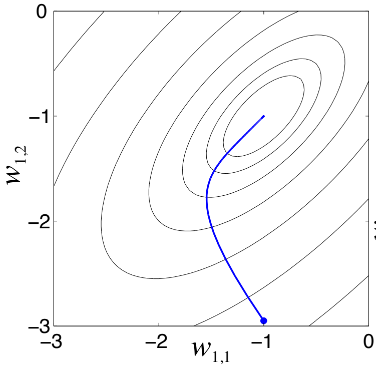
Performance surface



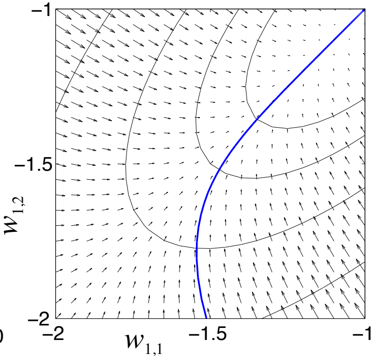
Contour plot

## Example steepest descent path

$$\mathbf{x}_{k+1} = \mathbf{x}_k - \alpha \nabla F(\mathbf{x}_k) = \mathbf{x}_k - 0.01\left(\mathbf{A}\mathbf{x}_k + \mathbf{d}\right) = \begin{bmatrix} 0.88 & 0.08 \\ 0.08 & 0.88 \end{bmatrix} \mathbf{x}_k + \begin{bmatrix} 0.04 \\ 0.04 \end{bmatrix}$$



Steepest descent path



Zoomed path with gradients

## Stochastic gradient

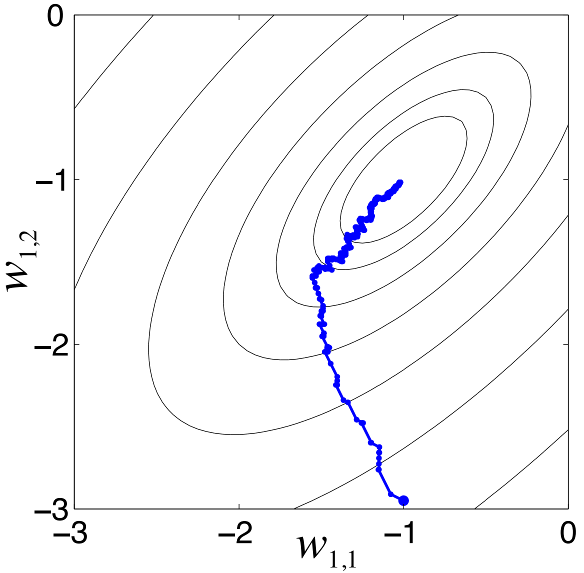
- Standard steepest descent is a batch algorithm, because the entire batch of data is used to compute the gradient.
- If we compute the gradient for one data point, it is an incremental, or stochastic algorithm.
- Mini-batches can also be used, where the algorithm operates on a subset of data – especially useful for large data sets.

$$\hat{F}(\mathbf{x}) = (t_k - a_k)^2$$
$$\nabla \hat{F}(\mathbf{x}) = -2\,(t_k - a_k)\,\nabla a_k = -2 e_k \mathbf{p}_k$$

### Stochastic gradient algorithm

$$\mathbf{x}_{k+1} = \mathbf{x}_k + 2\alpha e_k \mathbf{p}_k$$

## Stochastic gradient trajectory



## Adam algorithm (using curvature)

Smoothed gradient and smoothed squared gradient where $\mathbf{g}_k = \nabla F(\mathbf{x}_k)$

$$\begin{aligned}\mathbf{m}_{k+1} &= \beta_1 \mathbf{m}_k + (1-\beta_1)\mathbf{g}_k \\ \mathbf{v}_{k+1} &= \beta_2 \mathbf{v}_k + (1-\beta_2)\mathbf{g}_k \circ \mathbf{g}_k \\ \mathbf{m}_0 &= \mathbf{v}_0 = \mathbf{0}\end{aligned}$$

Correct for bias toward 0 $(0 < \beta_1, \beta_2 < 1)$

$$\begin{aligned}\hat{\mathbf{m}}_{k+1} &= \mathbf{m}_{k+1}/(1-\beta_1^{k+1}) \\ \hat{\mathbf{v}}_{k+1} &= \mathbf{v}_{k+1}/(1-\beta_2^{k+1})\end{aligned}$$

Final algorithm

$$\mathbf{x}_{k+1} = \mathbf{x}_k - \alpha \hat{\mathbf{m}}_{k+1} \oslash \left(\sqrt{\hat{\mathbf{v}}_{i+1}} + \epsilon\right)$$

## Gradient calculation in multilayer networks

- For multilayer networks, the error is not a direct function of weights in the hidden layers.
- To compute the necessary gradients we need to use the chain rule.
- The chain rule is implemented one component at a time (e.g., performance function, transfer function, weight function).

$$\frac{\partial \hat{F}(\mathbf{x})}{\partial w_{i,j}^{m}} = \frac{\partial \hat{F}(\mathbf{x})}{\partial n_i^m}\frac{\partial n_i^m}{\partial w_{i,j}^{m}} = \frac{\partial \hat{F}(\mathbf{x})}{\partial n_i^m}\frac{\partial(\sum_{l=1}^{\mathrm{S}^{m-1}} w_{i,l}^m a_l^{m-1} + b_i^m)}{\partial w_{i,j}^{m}}$$

$$= \frac{\partial \hat{F}(\mathbf{x})}{\partial n_i^m} a_j^{m-1}$$

## Module derivatives

Derivative across transfer function

$$\frac{\partial \mathbf{a}^m}{\partial (\mathbf{n}^m)^T} = \dot{\mathbf{F}}^{\mathbf{m}}\left(\mathbf{n}^m\right) = \begin{bmatrix} \frac{\partial f_1^m(\mathbf{n}^m)}{\partial n_1^m} & \frac{\partial f_1^m(\mathbf{n}^m)}{\partial n_2^m} & \cdots & \frac{\partial f_1^m(\mathbf{n}^m)}{\partial n_{S^m}^m} \\ \frac{\partial f_2^m(\mathbf{n}^m)}{\partial n_1^m} & \frac{\partial f_2^m(\mathbf{n}^m)}{\partial n_2^m} & \cdots & \frac{\partial f_2^m(\mathbf{n}^m)}{\partial n_{S^m}^m} \\ \vdots & \vdots & \ddots & \vdots \\ \frac{\partial f_{S^m}^m(\mathbf{n}^m)}{\partial n_1^m} & \frac{\partial f_{S^m}^m(\mathbf{n}^m)}{\partial n_2^m} & \cdots & \frac{\partial f_{S^m}^m(\mathbf{n}^m)}{\partial n_{S^m}^m} \end{bmatrix}$$

Derivative across weight function

$$\frac{\partial \mathbf{n}^{m+1}}{\partial (\mathbf{a}^m)^T} = \frac{\partial [\mathbf{W}^{m+1}\mathbf{a}^m + \mathbf{b}^{m+1}]}{\partial (\mathbf{a}^m)^T} = \mathbf{W}^{m+1}$$

## Example transfer function derivatives

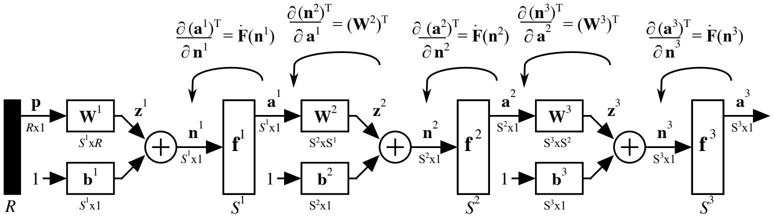
### Poslin

$$\dot{\mathbf{F}}^{\mathbf{m}}(\mathbf{n}^m) = \begin{bmatrix} \text{hardlim}(n_1^m) & 0 & \cdots & 0 \\ 0 & \text{hardlim}(n_2^m) & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & \text{hardlim}(n_{S^m}^m) \end{bmatrix}$$

### Softmax

$$\dot{\mathbf{F}}^{\mathbf{m}}(\mathbf{n}^m) = \begin{bmatrix} a_1^m \left(\sum_{i=1}^{S^m} a_i^m - a_1^m\right) & -a_1^m a_2^m & \cdots & -a_1^m a_{S^m}^m \\ -a_2^m a_1^m & a_2^m \left(\sum_{i=1}^{S^m} a_i^m - a_2^m\right) & \cdots & -a_2^m a_{S^m}^m \\ \vdots & \vdots & \ddots & \vdots \\ -a_{S^m}^m a_1^m & -a_{S^m}^m a_2^m & \cdots & a_{S^m}^m \left(\sum_{i=1}^{S^m} a_i^m - a_{S^m}^m\right) \end{bmatrix}$$

## Multilayer chain rule (backpropagation)


$\frac{\partial (\mathbf{a}^1)^T}{\partial \mathbf{n}^1} = \dot{\mathbf{F}}(\mathbf{n}^1)$
$\frac{\partial (\mathbf{n}^2)^T}{\partial \mathbf{a}^1} = (\mathbf{W}^2)^T$
$\frac{\partial (\mathbf{a}^2)^T}{\partial \mathbf{n}^2} = \dot{\mathbf{F}}(\mathbf{n}^2)$
$\frac{\partial (\mathbf{n}^3)^T}{\partial \mathbf{a}^2} = (\mathbf{W}^3)^T$
$\frac{\partial (\mathbf{a}^3)^T}{\partial \mathbf{n}^3} = \dot{\mathbf{F}}(\mathbf{n}^3)$
p
Rx1
R
1
W1
S1xR
b1
S1x1
z1
n1
S1x1
f1
S1
a1
S1x1
1
W2
S2xS1
b2
S2x1
z2
n2
S2x1
f2
S2
a2
S2x1
1
W3
S3xS2
b3
S3x1
z3
n3
S3x1
f3
S3
a3
S3x1

$$\frac{\partial \hat{F}(\mathbf{x})}{\partial \mathbf{n}^1} = \frac{\partial \mathbf{a}^1}{\partial \mathbf{n}^1} \times \frac{\partial \mathbf{n}^2}{\partial \mathbf{a}^1} \times \frac{\partial \mathbf{a}^2}{\partial \mathbf{n}^2} \times \frac{\partial \mathbf{n}^3}{\partial \mathbf{a}^2} \times \frac{\partial \mathbf{a}^3}{\partial \mathbf{n}^3} \times \frac{\partial \hat{F}(\mathbf{x})}{\partial \mathbf{a}^3}$$

$$\frac{\partial \hat{F}(\mathbf{x})}{\partial \mathbf{n}^m} = \frac{\partial \mathbf{a}^m}{\partial \mathbf{n}^m} \times \frac{\partial \mathbf{n}^{m+1}}{\partial \mathbf{a}^m} \times \frac{\partial \hat{F}(\mathbf{x})}{\partial \mathbf{n}^{m+1}} = \dot{\mathbf{F}}(\mathbf{n}^m)(\mathbf{W}^{m+1})^T \frac{\partial \hat{F}(\mathbf{x})}{\partial \mathbf{n}^{m+1}}$$

## Initializing backpropagation

### For Mean Square Error

$$\frac{\partial \hat{F}(\mathbf{x})}{\partial n_i^M} = \sum_{j=1}^{S^M} \frac{\partial \hat{F}(\mathbf{x})}{\partial a_j^M} \frac{\partial a_j^M}{\partial n_i^M} = \frac{1}{S^M} \sum_{j=1}^{S^M} \frac{\partial \left(t_j - a_j^M\right)^2}{\partial a_j^M} \frac{\partial a_j^M}{\partial n_i^M}$$

$$\frac{\partial \hat{F}(\mathbf{x})}{\partial n_i^M} = \frac{-2}{S^M} \sum_{j=1}^{S^M} \left(t_j - a_j^M\right) \frac{\partial a_j^M}{\partial n_i^M}$$

$$= \frac{-2}{S^M} \sum_{j=1}^{S^M} e_j \frac{\partial a_j^M}{\partial n_i^M}$$

$$\frac{\partial \hat{F}(\mathbf{x})}{\partial \mathbf{n}^M} = \frac{\partial (\mathbf{a}^M)^T}{\partial \mathbf{n}^M} \frac{\partial \hat{F}(\mathbf{x})}{\partial \mathbf{a}^M} = \frac{-2}{S^M} \dot{\mathbf{F}}^{\mathbf{M}} \left(\mathbf{n}^m\right) \mathbf{e}$$

## Summary of multilayer stochastic gradient

If we define the sensitivity to be

$$\mathbf{s}^m \triangleq \frac{\partial \hat{F}(\mathbf{x})}{\partial \mathbf{n}^m}$$

Then the stochastic gradient for mean square error can be computed as

$$\begin{aligned}
\mathbf{s}^M &= \frac{-2}{S^M}\dot{\mathbf{F}}^{\mathbf{M}}\left(\mathbf{n}^m\right)\mathbf{e} \\
\mathbf{s}^m &= \dot{\mathbf{F}}(\mathbf{n}^m)(\mathbf{W}^{m+1})^T\mathbf{s}^{m+1} \\
\frac{\partial \hat{F}(\mathbf{x})}{\partial w_{i,j}^m} &= s_i^m a_j^{m-1} \\
\frac{\partial \hat{F}(\mathbf{x})}{\partial b_i^m} &= s_i^m
\end{aligned}$$