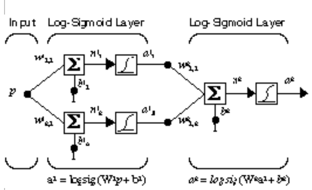
Variations on Backpropagation

Backprop Variations

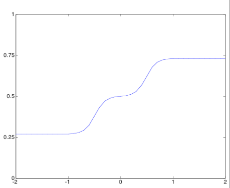
- Heuristic Modifications
  - Momentum
  - Variable Learning Rate
  - Quickprop
- Standard Numerical Optimization
  - Conjugate Gradient
  - Newton's Method (Levenberg-Marquardt)

Error Surface Example

Network Architecture



Nominal Function

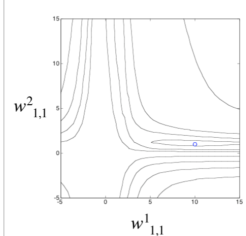


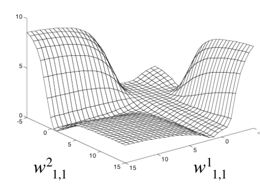
Parameter Values

$w^1_{1,1} = 10 \quad w^1_{2,1} = 10 \quad b^1_1 = -5 \quad b^1_2 = 5$

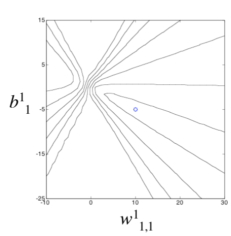
$w^2_{1,1} = 1 \quad w^2_{1,2} = 1 \quad b^2 = -1$

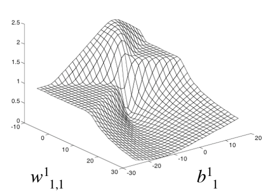
Squared Error vs. $w^1_{1,1}$ and $w^2_{1,1}$



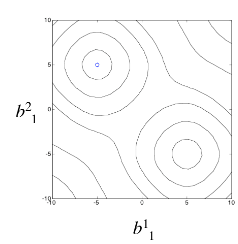


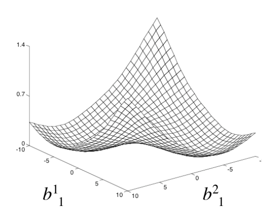
Squared Error vs. $w^1_{1,1}$ and b^1_1



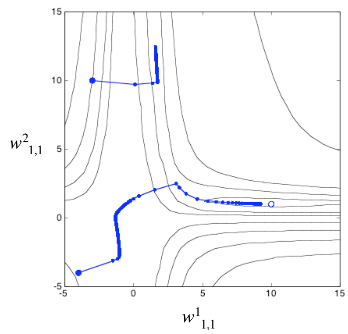


Squared Error vs. b^1_1 and b^1_2

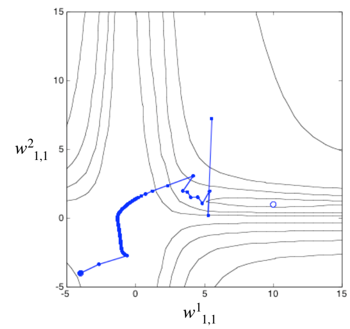




Convergence Example



Learning Rate Too Large



Momentum Backpropagation

Steepest Descent Backpropagation (SDBP)

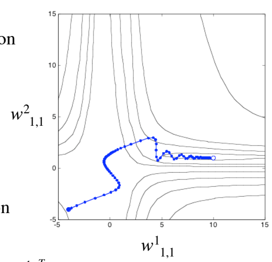
$$\square\mathbf{W}^m(k) = -\square\mathbf{s}^m(\mathbf{a}^{m-1})^T$$

$$\square\mathbf{b}^m(k) = -\square\mathbf{s}^m$$

Momentum Backpropagation (MOBP)

$$\square\mathbf{W}^m(k) = \square\square\mathbf{W}^m(k-1) - (1-\square)\square\mathbf{s}^m(\mathbf{a}^{m-1})^T$$

$$\square\mathbf{b}^m(k) = \square\square\mathbf{b}^m(k-1) - (1-\square)\square\mathbf{s}^m$$

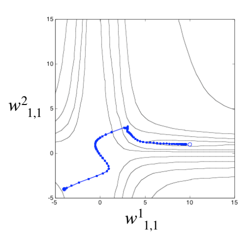


$\square = 0.8$

Variable Learning Rate (VLBP)

- If the squared error (over the entire training set) increases by more than some set percentage □ after a weight update, then the weight update is discarded, the learning rate is multiplied by some factor (1 > □ > 0), and the momentum coefficient □ is set to zero.
- If the squared error decreases after a weight update, then the weight update is accepted and the learning rate is multiplied by some factor □ > 1. If □ has been previously set to zero, it is reset to its original value.
- If the squared error increases by less than □, then the weight update is accepted, but the learning rate and the momentum coefficient are unchanged.

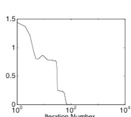
Example

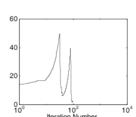


$\square = 1.05$

$\square = 0.7$

$\square = 4\%$





The remaining slides describe two method for accelerating backpropagation

- Conjugate Gradient method
- Levenberg-Marquardt method

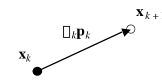
Steepest Descent (Gradient Descent) Review

Basic Optimization Algorithm

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

or

$$\Delta\mathbf{x}_k = (\mathbf{x}_{k+1} - \mathbf{x}_k) = \alpha_k \mathbf{p}_k$$



$\mathbf{p}_k$ - Search Direction

α_k - Learning Rate

Steepest Descent (Gradient Descent)

Choose the next step so that the function decreases:

$$F(\mathbf{x}_{k+1}) < F(\mathbf{x}_k)$$

For small changes in $\mathbf{x}$ we can approximate $F(\mathbf{x})$:

$$F(\mathbf{x}_{k+1}) = F(\mathbf{x}_k + \Delta\mathbf{x}_k) \approx F(\mathbf{x}_k) + \mathbf{g}_k^T \Delta\mathbf{x}_k$$

where

$$\mathbf{g}_k \equiv \nabla F(\mathbf{x})\big|_{\mathbf{x} = \mathbf{x}_k}$$

If we want the function to decrease:

$$\mathbf{g}_k^T \Delta\mathbf{x}_k = \alpha_k \mathbf{g}_k^T \mathbf{p}_k < 0 \quad \text{(learning rate*gradient*direction)}$$

We can maximize the decrease by choosing:

$$\mathbf{p}_k = -\mathbf{g}_k \quad \text{(direction = neg. gradient)}$$

$$\boxed{\mathbf{x}_{k+1} = \mathbf{x}_k - \alpha_k \mathbf{g}_k}$$

Example for an Analytic Function

$$F(\mathbf{x}) = x_1^2 + 2x_1x_2 + 2x_2^2 + x_1$$

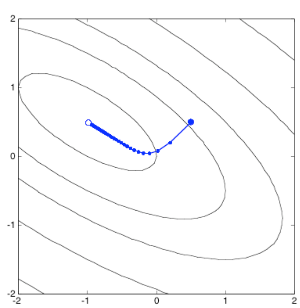
$$\mathbf{x}_0 = \begin{bmatrix} 0.5 \\ 0.5 \end{bmatrix} \qquad \alpha = 0.1$$

$$\nabla F(\mathbf{x}) = \begin{bmatrix} \frac{\partial}{\partial x_1} F(\mathbf{x}) \\ \frac{\partial}{\partial x_2} F(\mathbf{x}) \end{bmatrix} = \begin{bmatrix} 2x_1 + 2x_2 + 1 \\ 2x_1 + 4x_2 \end{bmatrix} \qquad \mathbf{g}_0 = \nabla F(\mathbf{x})\big|_{\mathbf{x} = \mathbf{x}_0} = \begin{bmatrix} 3 \\ 3 \end{bmatrix}$$

$$\mathbf{x}_1 = \mathbf{x}_0 - \alpha \mathbf{g}_0 = \begin{bmatrix} 0.5 \\ 0.5 \end{bmatrix} - 0.1 \begin{bmatrix} 3 \\ 3 \end{bmatrix} = \begin{bmatrix} 0.2 \\ 0.2 \end{bmatrix}$$

$$\mathbf{x}_2 = \mathbf{x}_1 - \alpha \mathbf{g}_1 = \begin{bmatrix} 0.2 \\ 0.2 \end{bmatrix} - 0.1 \begin{bmatrix} 1.8 \\ 1.2 \end{bmatrix} = \begin{bmatrix} 0.02 \\ 0.08 \end{bmatrix}$$

Plot



Note:
Lots of *small* steps

Conjugate Gradient Method

Minimizing Function *Along a Line*

Compute learning rate α_k to minimize $F(\mathbf{x}_k + \alpha_k \mathbf{p}_k)$

$\mathbf{p}_k$ is any chosen line direction, e.g. $-\mathbf{g}_k$ (negative gradient)

By Taylor expansion:

$$\frac{d}{d\alpha_k}(F(\mathbf{x}_k + \alpha_k \mathbf{p}_k)) = \nabla F(\mathbf{x})^T\Big|_{\mathbf{x}=\mathbf{x}_k} \mathbf{p}_k + \alpha_k \mathbf{p}_k^T \nabla^2 F(\mathbf{x})\Big|_{\mathbf{x}=\mathbf{x}_k} \mathbf{p}_k$$

Set derivative to 0 and solve for α_k:

$$\alpha_k = -\frac{\nabla F(\mathbf{x})^T\Big|_{\mathbf{x}=\mathbf{x}_k} \mathbf{p}_k}{\mathbf{p}_k^T \nabla^2 F(\mathbf{x})\Big|_{\mathbf{x}=\mathbf{x}_k} \mathbf{p}_k} = -\frac{\mathbf{g}_k^T \mathbf{p}_k}{\mathbf{p}_k^T \mathbf{A}_k \mathbf{p}_k}$$

is value where derivative is 0

where

$$\mathbf{A}_k \equiv \nabla^2 F(\mathbf{x})\Big|_{\mathbf{x}=\mathbf{x}_k} \qquad \text{(Hessian)}$$

This is the analytic version, which assumes we know the Hessian, which we often don't.

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Example

$$F(\mathbf{x}) = \frac{1}{2}\mathbf{x}^T \begin{bmatrix} 2 & 2 \\ 2 & 4 \end{bmatrix} \mathbf{x} + \begin{bmatrix} 1 & 0 \end{bmatrix} \mathbf{x} \qquad \mathbf{x}_0 = \begin{bmatrix} 0.5 \\ 0.5 \end{bmatrix}$$

$$\nabla F(\mathbf{x}) = \begin{bmatrix} \frac{\partial}{\partial x_1} F(\mathbf{x}) \\ \frac{\partial}{\partial x_2} F(\mathbf{x}) \end{bmatrix} = \begin{bmatrix} 2x_1 + 2x_2 + 1 \\ 2x_1 + 4x_2 \end{bmatrix} \qquad \mathbf{p}_0 = -\mathbf{g}_0 = -\nabla F(\mathbf{x})\Big|_{\mathbf{x}=\mathbf{x}_0} = \begin{bmatrix} -3 \\ -3 \end{bmatrix}$$

$$\alpha_0 = -\frac{\begin{bmatrix} 3 & 3 \end{bmatrix}\begin{bmatrix} -3 \\ -3 \end{bmatrix}}{\begin{bmatrix} -3 & -3 \end{bmatrix}\begin{bmatrix} 2 & 2 \\ 2 & 4 \end{bmatrix}\begin{bmatrix} -3 \\ -3 \end{bmatrix}} = 0.2 \qquad \mathbf{x}_1 = \mathbf{x}_0 - \alpha_0 \mathbf{g}_0 = \begin{bmatrix} 0.5 \\ 0.5 \end{bmatrix} - 0.2\begin{bmatrix} 3 \\ 3 \end{bmatrix} = \begin{bmatrix} -0.1 \\ -0.1 \end{bmatrix}$$

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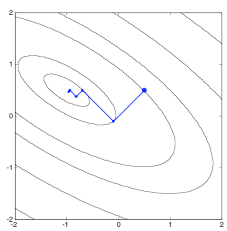
Successive Line Minimizations with different directions



$$\frac{d}{d\alpha_k}F(\mathbf{x}_k + \alpha_k \mathbf{p}_k) = \frac{d}{d\alpha_k}F(\mathbf{x}_{k+1}) = \nabla F(\mathbf{x})^T\Big|_{\mathbf{x}=\mathbf{x}_{k+1}} \frac{d}{d\alpha_k}[\mathbf{x}_k + \alpha_k \mathbf{p}_k]$$

$$= \nabla F(\mathbf{x})^T\Big|_{\mathbf{x}=\mathbf{x}_{k+1}} \mathbf{p}_k = \mathbf{g}_{k+1}^T \mathbf{p}_k$$

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Conjugate Vectors

$$F(\mathbf{x}) = \frac{1}{2}\mathbf{x}^T \mathbf{A}\mathbf{x} + \mathbf{d}^T\mathbf{x} + c$$

A set of vectors is mutually *conjugate* with respect to a positive definite Hessian matrix **A** if

$$\mathbf{p}_k^T \mathbf{A} \mathbf{p}_j = 0 \qquad k \neq j$$

One set of conjugate vectors consists of the eigenvectors of **A**.

$$\mathbf{z}_k^T \mathbf{A} \mathbf{z}_j = \lambda_j \mathbf{z}_k^T \mathbf{z}_j = 0 \qquad k \neq j$$

(The eigenvectors of symmetric matrices are orthogonal.)

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For *Quadratic* Functions

$$\nabla F(\mathbf{x}) = \mathbf{A}\mathbf{x} + \mathbf{d}$$

$$\nabla^2 F(\mathbf{x}) = \mathbf{A}$$

The change in the gradient at iteration k is

$$\Delta\mathbf{g}_k = \mathbf{g}_{k+1} - \mathbf{g}_k = (\mathbf{A}\mathbf{x}_{k+1} + \mathbf{d}) - (\mathbf{A}\mathbf{x}_k + \mathbf{d}) = \mathbf{A}\Delta\mathbf{x}_k$$

where

$$\Delta\mathbf{x}_k = (\mathbf{x}_{k+1} - \mathbf{x}_k) = \alpha_k \mathbf{p}_k$$

The conjugacy conditions can be rewritten

$$\alpha_k \mathbf{p}_k^T \mathbf{A} \mathbf{p}_j = \Delta\mathbf{x}_k^T \mathbf{A} \mathbf{p}_j = \Delta\mathbf{g}_k^T \mathbf{p}_j = 0 \qquad k \neq j$$

This does not require knowledge of the Hessian matrix.

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Forming *Conjugate* Directions

Choose the initial search direction as the negative of the gradient:

$$\mathbf{p}_0 = -\mathbf{g}_0$$

Choose subsequent search directions to be *conjugate*:

$$\mathbf{p}_k = -\mathbf{g}_k + \beta_k \mathbf{p}_{k-1}$$

where β_k is chosen by *one of these formulae*:

$$\beta_k = \frac{\Delta\mathbf{g}_{k-1}^T \mathbf{g}_k}{\Delta\mathbf{g}_{k-1}^T \mathbf{p}_{k-1}} \quad \textbf{or} \quad \beta_k = \frac{\mathbf{g}_k^T \mathbf{g}_k}{\mathbf{g}_{k-1}^T \mathbf{g}_{k-1}} \quad \textbf{or} \quad \beta_k = \frac{\Delta\mathbf{g}_{k-1}^T \mathbf{g}_k}{\mathbf{g}_{k-1}^T \mathbf{g}_{k-1}}$$

Hestnes & Steiffel — Fletcher-Reeves — Polak & Ribiere

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Conjugate Gradient algorithm

- The first search direction is the negative of the gradient.

$$\mathbf{p}_0 = -\mathbf{g}_0$$

- Select the learning rate to minimize along the line.

$$\alpha_k = -\frac{\nabla F(\mathbf{x})^T\big|_{\mathbf{x}=\mathbf{x}_k}\mathbf{p}_k}{\mathbf{p}_k^T\nabla^2 F(\mathbf{x})\big|_{\mathbf{x}=\mathbf{x}_k}\mathbf{p}_k} = -\frac{\mathbf{g}_k^T\mathbf{p}_k}{\mathbf{p}_k^T\mathbf{A}_k\mathbf{p}_k}$$

(For quadratic functions only.)

- Select the next search direction using

$$\mathbf{p}_k = -\mathbf{g}_k + \beta_k\mathbf{p}_{k-1}$$

- If the algorithm has not converged, return to second step.
- If the function were quadratic, it would be minimized in n steps.

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Example

$$F(\mathbf{x}) = \frac{1}{2}\mathbf{x}^T\begin{bmatrix}2 & 2\\ 2 & 4\end{bmatrix}\mathbf{x} + \begin{bmatrix}1 & 0\end{bmatrix}\mathbf{x} \qquad \mathbf{x}_0 = \begin{bmatrix}0.5\\ 0.5\end{bmatrix}$$

$$\nabla F(\mathbf{x}) = \begin{bmatrix}\frac{\partial}{\partial x_1}F(\mathbf{x})\\ \frac{\partial}{\partial x_2}F(\mathbf{x})\end{bmatrix} = \begin{bmatrix}2x_1 + 2x_2 + 1\\ 2x_1 + 4x_2\end{bmatrix} \qquad \mathbf{p}_0 = -\mathbf{g}_0 = -\nabla F(\mathbf{x})\big|_{\mathbf{x}=\mathbf{x}_0} = \begin{bmatrix}-3\\ -3\end{bmatrix}$$

$$\alpha_0 = -\frac{\begin{bmatrix}3 & 3\end{bmatrix}\begin{bmatrix}-3\\ -3\end{bmatrix}}{\begin{bmatrix}-3 & -3\end{bmatrix}\begin{bmatrix}2 & 2\\ 2 & 4\end{bmatrix}\begin{bmatrix}-3\\ -3\end{bmatrix}} = 0.2 \qquad \mathbf{x}_1 = \mathbf{x}_0 - \alpha_0\mathbf{g}_0 = \begin{bmatrix}0.5\\ 0.5\end{bmatrix} - 0.2\begin{bmatrix}3\\ 3\end{bmatrix} = \begin{bmatrix}-0.1\\ -0.1\end{bmatrix}$$

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Example

$$\mathbf{g}_1 = \nabla F(\mathbf{x})\big|_{\mathbf{x}=\mathbf{x}_1} = \begin{bmatrix}2 & 2\\ 2 & 4\end{bmatrix}\begin{bmatrix}-0.1\\ -0.1\end{bmatrix} + \begin{bmatrix}1\\ 0\end{bmatrix} = \begin{bmatrix}0.6\\ -0.6\end{bmatrix}$$

$$\beta_1 = \frac{\mathbf{g}_1^T\mathbf{g}_1}{\mathbf{g}_0^T\mathbf{g}_0} = \frac{\begin{bmatrix}0.6 & -0.6\end{bmatrix}\begin{bmatrix}0.6\\ -0.6\end{bmatrix}}{\begin{bmatrix}3 & 3\end{bmatrix}\begin{bmatrix}3\\ 3\end{bmatrix}} = \frac{0.72}{18} = 0.04$$

$$\mathbf{p}_1 = -\mathbf{g}_1 + \beta_1\mathbf{p}_0 = \begin{bmatrix}-0.6\\ 0.6\end{bmatrix} + 0.04\begin{bmatrix}-3\\ -3\end{bmatrix} = \begin{bmatrix}-0.72\\ 0.48\end{bmatrix}$$

$$\alpha_1 = -\frac{\begin{bmatrix}0.6 & -0.6\end{bmatrix}\begin{bmatrix}-0.72\\ 0.48\end{bmatrix}}{\begin{bmatrix}-0.72 & 0.48\end{bmatrix}\begin{bmatrix}2 & 2\\ 2 & 4\end{bmatrix}\begin{bmatrix}-0.72\\ 0.48\end{bmatrix}} = -\frac{-0.72}{0.576} = 1.25$$

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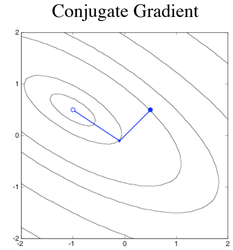
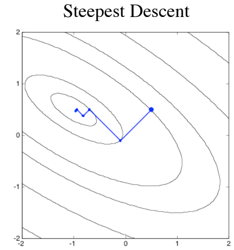
Plots

$$\mathbf{x}_2 = \mathbf{x}_1 + \alpha_1\mathbf{p}_1 = \begin{bmatrix}-0.1\\ -0.1\end{bmatrix} + 1.25\begin{bmatrix}-0.72\\ 0.48\end{bmatrix} = \begin{bmatrix}-1\\ 0.5\end{bmatrix}$$

Conjugate Gradient



Steepest Descent



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Line Minimization for General Functions (not necessarily quadratic)

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Numerical Line Minimization

- First locate an **interval** containing the minimum.
- Then reduce the interval's width successively, until the interval is sufficiently small that we are close enough to the minimum.

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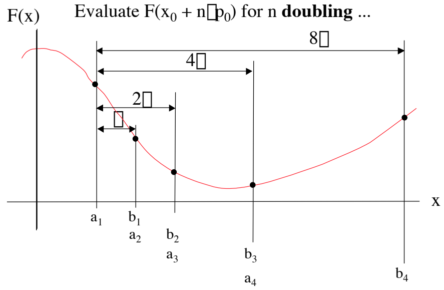
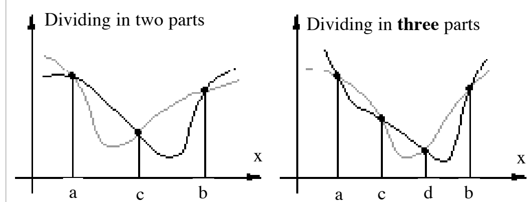
Interval Location to Bracket Minimum

Evaluate $F(x_0 + n\varepsilon p_0)$ for n **doubling** ...



Stop when two successive increases occur.

Interval Reduction



Interval **not reduced**.

Minimum is not between a and c

⇒ **eliminate** a-c.

Golden Section (Fibonacci) Search

$\tau = 0.618$

Set $c_1 = a_1 + (1-\tau)(b_1 - a_1)$, $F_c = F(c_1)$

$d_1 = b_1 - (1-\tau)(b_1 - a_1)$, $F_d = F(d_1)$

For k=1,2, ... repeat

If $F_c < F_d$ then

Set $a_{k+1} = a_k$; $b_{k+1} = d_k$; $d_{k+1} = c_k$

$c_{k+1} = a_{k+1} + (1-\tau)(b_{k+1} - a_{k+1})$

$F_d = F_c$; $F_c = F(c_{k+1})$

else

Set $a_{k+1} = c_k$; $b_{k+1} = b_k$; $c_{k+1} = d_k$

$d_{k+1} = b_{k+1} - (1-\tau)(b_{k+1} - a_{k+1})$

$F_c = F_d$; $F_d = F(d_{k+1})$

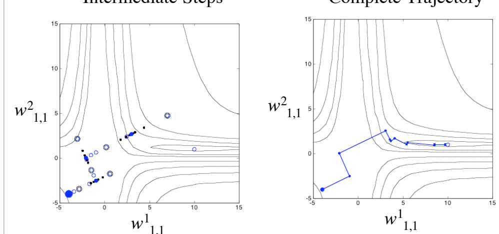
end

end until $b_{k+1} - a_{k+1} < tol$

Conjugate Gradient BP (CGBP)

Intermediate Steps

Complete Trajectory



Levenberg-Marquardt Method (blends Newton's method with steepest descent)

Probably the fastest known method for training (but storage intensive)

Newton's Method

$$\mathbf{x}_{k+1} = \mathbf{x}_k - \mathbf{A}_k^{-1}\mathbf{g}_k$$

$$\mathbf{A}_k \equiv \nabla^2 F(\mathbf{x})\big|_{\mathbf{x}=\mathbf{x}_k} \qquad \mathbf{g}_k \equiv \nabla F(\mathbf{x})\big|_{\mathbf{x}=\mathbf{x}_k}$$

If the performance index is a sum of squares function:

$$F(\mathbf{x}) = \sum_{i=1}^{N} v_i^2(\mathbf{x}) = \mathbf{v}^T(\mathbf{x})\mathbf{v}(\mathbf{x})$$

then the jth element of the gradient is

$$[\nabla F(\mathbf{x})]_j = \frac{\partial F(\mathbf{x})}{\partial x_j} = 2\sum_{i=1}^{N} v_i(\mathbf{x})\frac{\partial v_i(\mathbf{x})}{\partial x_j}$$

Newton's Method

$$F(\mathbf{x}_{k+1}) = F(\mathbf{x}_k + \Delta\mathbf{x}_k) \approx F(\mathbf{x}_k) + \mathbf{g}_k^T \Delta\mathbf{x}_k + \frac{1}{2}\Delta\mathbf{x}_k^T \mathbf{A}_k \Delta\mathbf{x}_k$$

Take the gradient of this second-order approximation and set it equal to zero to find the stationary point:

$$\mathbf{g}_k + \mathbf{A}_k \Delta\mathbf{x}_k = \mathbf{0}$$

$$\Delta\mathbf{x}_k = -\mathbf{A}_k^{-1}\mathbf{g}_k$$

$$\boxed{\mathbf{x}_{k+1} = \mathbf{x}_k - \mathbf{A}_k^{-1}\mathbf{g}_k}$$

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Example

$$F(\mathbf{x}) = x_1^2 + 2x_1x_2 + 2x_2^2 + x_1$$

$$\mathbf{x}_0 = \begin{bmatrix} 0.5 \\ 0.5 \end{bmatrix}$$

$$\nabla F(\mathbf{x}) = \begin{bmatrix} \frac{\partial}{\partial x_1}F(\mathbf{x}) \\ \frac{\partial}{\partial x_2}F(\mathbf{x}) \end{bmatrix} = \begin{bmatrix} 2x_1 + 2x_2 + 1 \\ 2x_1 + 4x_2 \end{bmatrix}$$

$$\mathbf{g}_0 = \nabla F(\mathbf{x})\Big|_{\mathbf{x}=\mathbf{x}_0} = \begin{bmatrix} 3 \\ 3 \end{bmatrix}$$

$$\mathbf{A} = \begin{bmatrix} 2 & 2 \\ 2 & 4 \end{bmatrix}$$

$$\mathbf{x}_1 = \begin{bmatrix} 0.5 \\ 0.5 \end{bmatrix} - \begin{bmatrix} 2 & 2 \\ 2 & 4 \end{bmatrix}^{-1} \begin{bmatrix} 3 \\ 3 \end{bmatrix} = \begin{bmatrix} 0.5 \\ 0.5 \end{bmatrix} - \begin{bmatrix} 1 & -0.5 \\ -0.5 & 0.5 \end{bmatrix} \begin{bmatrix} 3 \\ 3 \end{bmatrix} = \begin{bmatrix} 0.5 \\ 0.5 \end{bmatrix} - \begin{bmatrix} 1.5 \\ 0 \end{bmatrix} = \begin{bmatrix} -1 \\ 0.5 \end{bmatrix}$$

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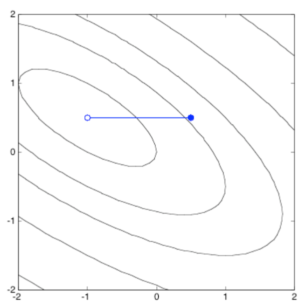
Plot



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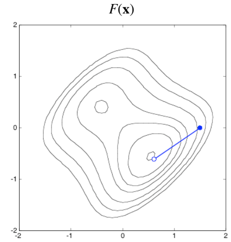
Non-Quadratic Example

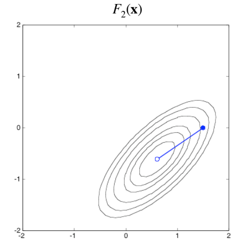
$$F(\mathbf{x}) = (x_2 - x_1)^4 + 8x_1x_2 - x_1 + x_2 + 3$$

Stationary Points: $\mathbf{x}^1 = \begin{bmatrix} -0.42 \\ 0.42 \end{bmatrix}$ $\mathbf{x}^2 = \begin{bmatrix} -0.13 \\ 0.13 \end{bmatrix}$ $\mathbf{x}^3 = \begin{bmatrix} 0.55 \\ -0.55 \end{bmatrix}$

$F(\mathbf{x})$



$F_2(\mathbf{x})$



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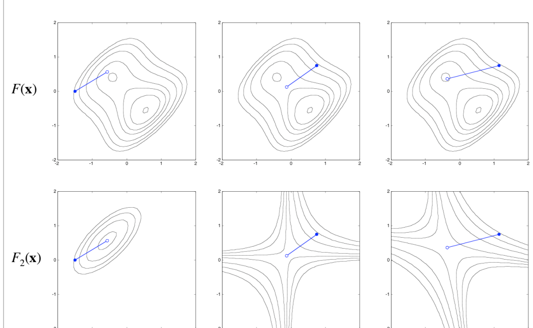
Different Initial Conditions



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Matrix Form

The gradient can be written in matrix form as a matrix-vector product:

$$\nabla F(\mathbf{x}) = 2\mathbf{J}^T(\mathbf{x})\mathbf{v}(\mathbf{x})$$

where $\mathbf{J}$ is the Jacobian matrix:

$$\mathbf{J}(\mathbf{x}) = \begin{bmatrix} \frac{\partial v_1(\mathbf{x})}{\partial x_1} & \frac{\partial v_1(\mathbf{x})}{\partial x_2} & \dots & \frac{\partial v_1(\mathbf{x})}{\partial x_n} \\ \frac{\partial v_2(\mathbf{x})}{\partial x_1} & \frac{\partial v_2(\mathbf{x})}{\partial x_2} & \dots & \frac{\partial v_2(\mathbf{x})}{\partial x_n} \\ \vdots & \vdots & & \vdots \\ \frac{\partial v_N(\mathbf{x})}{\partial x_1} & \frac{\partial v_N(\mathbf{x})}{\partial x_2} & \dots & \frac{\partial v_N(\mathbf{x})}{\partial x_n} \end{bmatrix}$$

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Hessian represents Curvature Express in terms of Jacobian:

$$[\nabla^2 F(\mathbf{x})]_{k,j} = \frac{\partial^2 F(\mathbf{x})}{\partial x_k \partial x_j} = 2\sum_{i=1}^{N}\left\{\frac{\partial v_i(\mathbf{x})}{\partial x_k}\frac{\partial v_i(\mathbf{x})}{\partial x_j} + v_i(\mathbf{x})\frac{\partial^2 v_i(\mathbf{x})}{\partial x_k \partial x_j}\right\}$$

$$\nabla^2 F(\mathbf{x}) = 2\mathbf{J}^T(\mathbf{x})\mathbf{J}(\mathbf{x}) + 2\mathbf{S}(\mathbf{x})$$

$$\mathbf{S}(\mathbf{x}) = \sum_{i=1}^{N} v_i(\mathbf{x})\nabla^2 v_i(\mathbf{x})$$

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Gauss-Newton Method

Approximate the Hessian matrix as:

$$\nabla^2 F(\mathbf{x}) \cong 2\mathbf{J}^T(\mathbf{x})\mathbf{J}(\mathbf{x})$$

Newton's method becomes:

$$\mathbf{x}_{k+1} = \mathbf{x}_k - [2\mathbf{J}^T(\mathbf{x}_k)\mathbf{J}(\mathbf{x}_k)]^{-1} 2\mathbf{J}^T(\mathbf{x}_k)\mathbf{v}(\mathbf{x}_k)$$

$$= \mathbf{x}_k - [\mathbf{J}^T(\mathbf{x}_k)\mathbf{J}(\mathbf{x}_k)]^{-1}\mathbf{J}^T(\mathbf{x}_k)\mathbf{v}(\mathbf{x}_k)$$

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Levenberg-Marquardt

Gauss-Newton approximates the Hessian by:

$$\mathbf{H} = \mathbf{J}^T\mathbf{J}$$

This matrix may be singular, but can be made invertible as follows:

$$\mathbf{G} = \mathbf{H} + \mu\mathbf{I}$$

If the eigenvalues and eigenvectors of **H** are:

$$\{\lambda_1, \lambda_2, \ldots, \lambda_n\} \qquad \{\mathbf{z}_1, \mathbf{z}_2, \ldots, \mathbf{z}_n\}$$

then

$$\mathbf{G}\mathbf{z}_i = [\mathbf{H} + \mu\mathbf{I}]\mathbf{z}_i = \mathbf{H}\mathbf{z}_i + \mu\mathbf{z}_i = \lambda_i\mathbf{z}_i + \mu\mathbf{z}_i = \overbrace{(\lambda_i + \mu)}^{\text{Eigenvalues of } \mathbf{G}}\mathbf{z}_i$$

$$\boxed{\mathbf{x}_{k+1} = \mathbf{x}_k - [\mathbf{J}^T(\mathbf{x}_k)\mathbf{J}(\mathbf{x}_k) + \mu_k\mathbf{I}]^{-1}\mathbf{J}^T(\mathbf{x}_k)\mathbf{v}(\mathbf{x}_k)}$$

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Adjustment of μ_k

As $\mu_k \to 0$, LM becomes Gauss-Newton.

$$\mathbf{x}_{k+1} = \mathbf{x}_k - [\mathbf{J}^T(\mathbf{x}_k)\mathbf{J}(\mathbf{x}_k)]^{-1}\mathbf{J}^T(\mathbf{x}_k)\mathbf{v}(\mathbf{x}_k)$$

As $\mu_k \to \infty$, LM becomes Steepest Descent with small learning rate.

$$\mathbf{x}_{k+1} \cong \mathbf{x}_k - \frac{1}{\mu_k}\mathbf{J}^T(\mathbf{x}_k)\mathbf{v}(\mathbf{x}_k) = \mathbf{x}_k - \frac{1}{2\mu_k}\nabla F(\mathbf{x})$$

Steepest Descent is a default position: Begin with a small μ_k to use Gauss-Newton. If a step does not yield a smaller $F(\mathbf{x})$, then repeat the step with an **increased** μ_k until $F(\mathbf{x})$ is decreased. $F(\mathbf{x})$ must decrease eventually, since we will eventually be taking a very **small** step in the steepest descent direction.

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Application to Multilayer Network

The performance index for the multilayer network is:

$$F(\mathbf{x}) = \sum_{q=1}^{Q}(\mathbf{t}_q - \mathbf{a}_q)^T(\mathbf{t}_q - \mathbf{a}_q) = \sum_{q=1}^{Q}\mathbf{e}_q^T\mathbf{e}_q = \sum_{q=1}^{Q}\sum_{j=1}^{S^M}(e_{j,q})^2 = \sum_{i=1}^{N}(v_i)^2$$

Q = number of samples

The error vector is:

$$\mathbf{v}^T = \begin{bmatrix} v_1 & v_2 & \ldots & v_N \end{bmatrix} = \begin{bmatrix} e_{1,1} & e_{2,1} & \ldots & e_{S^M,1} & e_{1,2} & \ldots & e_{S^M,Q} \end{bmatrix}$$

S^M = number of outputs

The parameter vector is:

$$\mathbf{x}^T = \begin{bmatrix} x_1 & x_2 & \ldots & x_n \end{bmatrix} = \begin{bmatrix} w^1_{1,1} & w^1_{1,2} & \ldots & w^1_{S^1,R} & b^1_1 & \ldots & b^1_{S^1} & w^2_{1,1} & \ldots & b^M_{S^M} \end{bmatrix}$$

The dimensions of the two vectors are:

$$N = Q \times S^M \qquad n = S^1(R+1) + S^2(S^1+1) + \ldots + S^M(S^{M-1}+1)$$

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Jacobian Matrix for Levenberg-Marquardt

$$\mathbf{J}(\mathbf{x}) = \begin{bmatrix}
\frac{\partial e_{1,1}}{\partial w^1_{1,1}} & \frac{\partial e_{1,1}}{\partial w^1_{1,2}} & \ldots & \frac{\partial e_{1,1}}{\partial w^1_{S^1,R}} & \frac{\partial e_{1,1}}{\partial b^1_1} & \ldots \\
\frac{\partial e_{2,1}}{\partial w^1_{1,1}} & \frac{\partial e_{2,1}}{\partial w^1_{1,2}} & \ldots & \frac{\partial e_{2,1}}{\partial w^1_{S^1,R}} & \frac{\partial e_{2,1}}{\partial b^1_1} & \ldots \\
\vdots & \vdots & & \vdots & \vdots & \\
\frac{\partial e_{S^M,1}}{\partial w^1_{1,1}} & \frac{\partial e_{S^M,1}}{\partial w^1_{1,2}} & \ldots & \frac{\partial e_{e_{S^M,1}}}{\partial w^1_{S^1,R}} & \frac{\partial e_{e_{S^M,1}}}{\partial b^1_1} & \ldots \\
\frac{\partial e_{1,2}}{\partial w^1_{1,1}} & \frac{\partial e_{1,2}}{\partial w^1_{1,2}} & \ldots & \frac{\partial e_{1,2}}{\partial w^1_{S^1,R}} & \frac{\partial e_{1,2}}{\partial b^1_1} & \ldots \\
\vdots & \vdots & & \vdots & \vdots &
\end{bmatrix}$$

M rows for every input sample

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Computing the Jacobian

Steepest descent computes terms of the form:

$$\frac{\partial \hat{F}(\mathbf{x})}{\partial x_l} = \frac{\partial \mathbf{e}_q^T \mathbf{e}_q}{\partial x_l}$$

using the chain rule:

$$\frac{\partial \hat{F}}{\partial w_{i,j}^m} = \frac{\partial \hat{F}}{\partial n_i^m} \times \frac{\partial n_i^m}{\partial w_{i,j}^m}$$

where the sensitivity

$$s_i^m \equiv \frac{\partial \hat{F}}{\partial n_i^m}$$

is computed using backpropagation.

For the Jacobian we need to compute terms of the form:

$$[\mathbf{J}]_{h,l} = \frac{\partial v_h}{\partial x_l} = \frac{\partial e_{k,q}}{\partial x_l}$$

Marquardt Sensitivity

If we define a Marquardt sensitivity (q is the sample's index):

$$\tilde{s}_{i,h}^m \equiv \frac{\partial v_h}{\partial n_{i,q}^m} = \frac{\partial e_{k,q}}{\partial n_{i,q}^m} \qquad h = (q-1)S^M + k$$

we can compute the Jacobian as follows:

weight

$$[\mathbf{J}]_{h,l} = \frac{\partial v_h}{\partial x_l} = \frac{\partial e_{k,q}}{\partial w_{i,j}^m} = \frac{\partial e_{k,q}}{\partial n_{i,q}^m} \times \frac{\partial n_{i,q}^m}{\partial w_{i,j}^m} = \tilde{s}_{i,h}^m \times \frac{\partial n_{i,q}^m}{\partial w_{i,j}^m} = \tilde{s}_{i,h}^m \times a_{j,q}^{m-1}$$

bias

$$[\mathbf{J}]_{h,l} = \frac{\partial v_h}{\partial x_l} = \frac{\partial e_{k,q}}{\partial b_i^m} = \frac{\partial e_{k,q}}{\partial n_{i,q}^m} \times \frac{\partial n_{i,q}^m}{\partial b_i^m} = \tilde{s}_{i,h}^m \times \frac{\partial n_{i,q}^m}{\partial b_i^m} = \tilde{s}_{i,h}^m$$

Computing the Sensitivities

Initialization

$$\tilde{s}_{i,h}^M = \frac{\partial v_h}{\partial n_{i,q}^M} = \frac{\partial e_{k,q}}{\partial n_{i,q}^M} = \frac{\partial (t_{k,q} - a_{k,q}^M)}{\partial n_{i,q}^M} = -\frac{\partial a_{k,q}^M}{\partial n_{i,q}^M}$$

$$\tilde{s}_{i,h}^M = \begin{cases} -\dot{f}^M(n_{i,q}^M) & \text{for } i = k \\ 0 & \text{for } i \neq k \end{cases}$$

$$\tilde{\mathbf{S}}_q^M = -\dot{\mathbf{F}}^M(\mathbf{n}_q^M)$$

Backpropagation

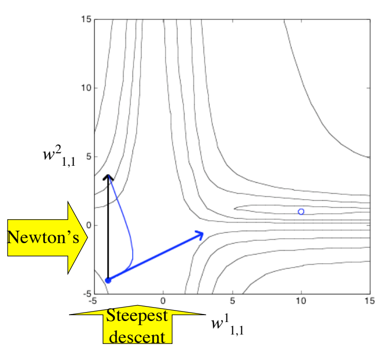
$$\tilde{\mathbf{S}}_q^m = \dot{\mathbf{F}}^m(\mathbf{n}_q^m)(\mathbf{W}^{m+1})^T \tilde{\mathbf{S}}_q^{m+1}$$

$$\tilde{\mathbf{S}}^m = \left[\tilde{\mathbf{S}}_1^m \middle| \tilde{\mathbf{S}}_2^m \middle| \ldots \middle| \tilde{\mathbf{S}}_Q^m \right] \qquad \text{Q = number of samples}$$

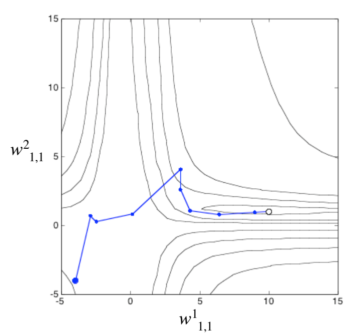
Levenberg-Marquardt Backpropagation

- Present *all inputs* to the network and compute the corresponding network outputs and the errors. Compute the sum of squared errors over all inputs.
- Compute the Jacobian matrix. Calculate the sensitivities with the backpropagation algorithm, after initializing. Augment the individual matrices into the Marquardt sensitivities. Compute the elements of the Jacobian matrix.
- Solve to obtain the change in the weights.
- Recompute the sum of squared errors with the new weights. If this new sum of squares is smaller than that computed in step 1, then divide μ_k by ϑ, update the weights and go back to step 1. If the sum of squares is not reduced, then multiply μ_k by ϑ and go back to step 3.

Example LMBP Step



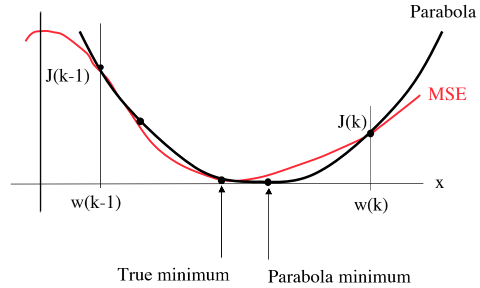
LMBP Trajectory



Quickprop
Scott Fahlman, CMU

- This is an optimization of backpropagation based on Newton's method.
- It is applicable when, between two steps, the **gradient** has decreased in magnitude and has **changed sign**.
- Then a **parabolic estimate** of the MSE is used to determine the weights for the next step.

Quickprop, step k, in 1 dimension



Quickprop

- Assume a parabola:
  $J(w) = aw^2 + bw + c$
- First derivative is a line:
  $\partial J / \partial w = 2aw + b$
  abbreviate $\partial J / \partial w$ as $J'(w)$.
- To find: value of $w(k+1)$ such that $J'(w(k+1)) = 0$.
- We have
  $J'(w(k)) = 2aw(k) + b$
  $J'(w(k-1)) = 2aw(k-1) + b$
- Solving for a and b in terms of the other quantities:
  $2a = [J'(w(k))-J'(w(k-1))]/ \Delta w(k-1)$
  $b = J'(w(k)) - [(J'(w(k))-J'(w(k-1)))w(k) / \Delta w(k-1)]$
  where $\Delta w(k-1) = w(k) - w(k-1)$

Quickprop

- Set $J'(w(k+1)) = 0$, since we are looking for the parabolic **minimum** at the next step.
- Then $2aw(k+1) + b = 0$, i.e. $w(k+1) = -b/2a$.
- Substituting in previous equations, we get

$w(k+1) =$

$$w(k) + [J'(w(k)) \Delta w(k-1)] /[J'(w(k-1)) - J'(w(k))]$$

as the choice for $w(k+1)$.