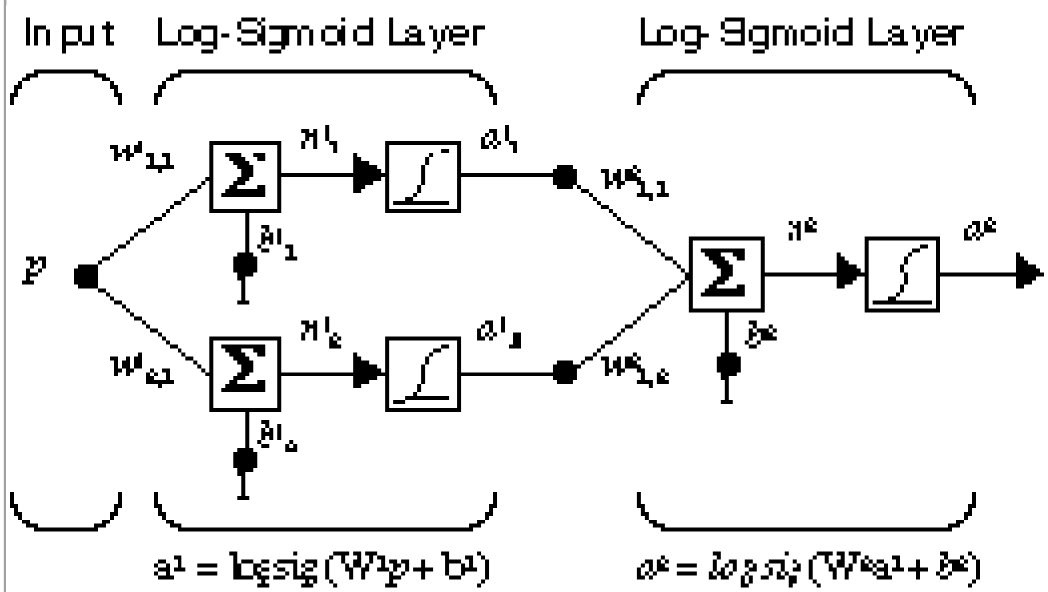
Variations on Backpropagation

Backprop Variations

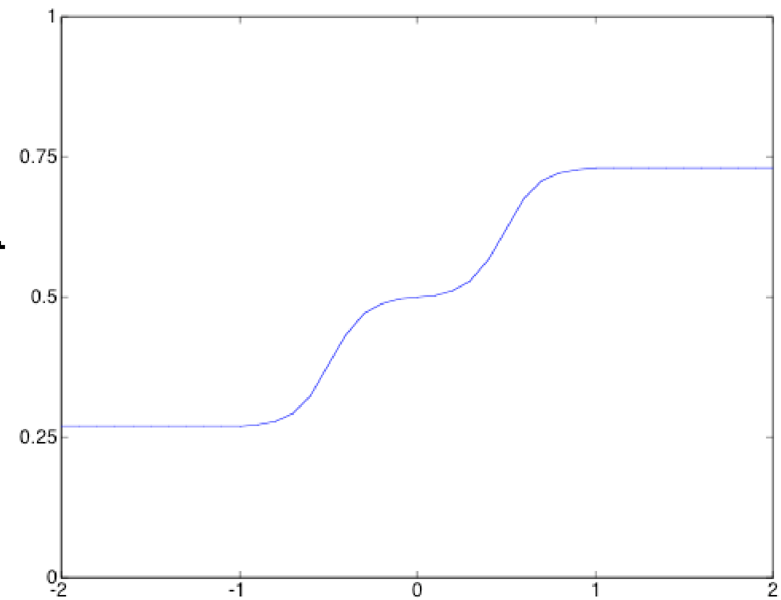
- Heuristic Modifications
  - Momentum
  - Variable Learning Rate
  - Quickprop
- Standard Numerical Optimization
  - Conjugate Gradient
  - Newton's Method (Levenberg-Marquardt)

Error Surface Example

Network Architecture



Nominal Function

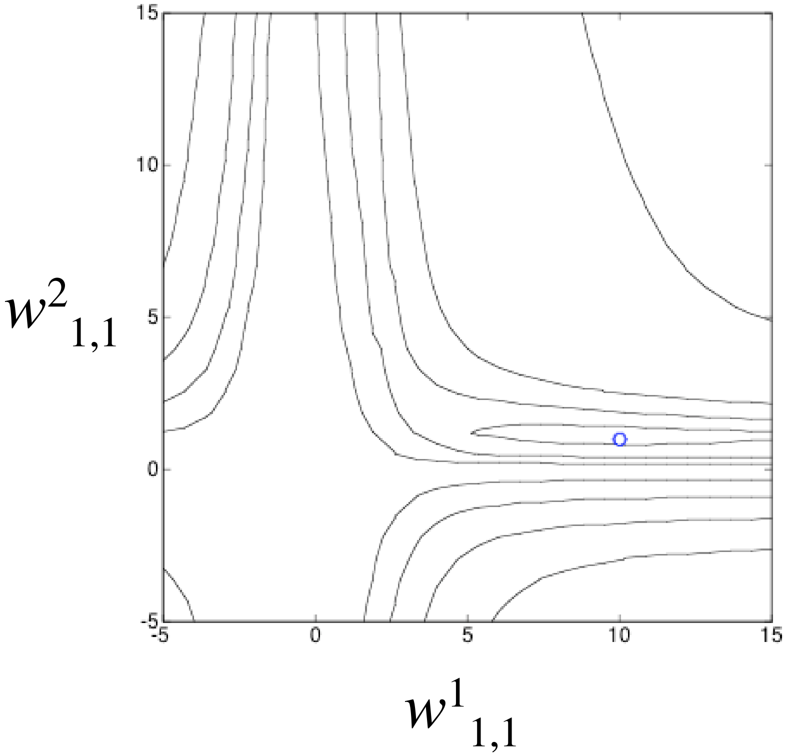


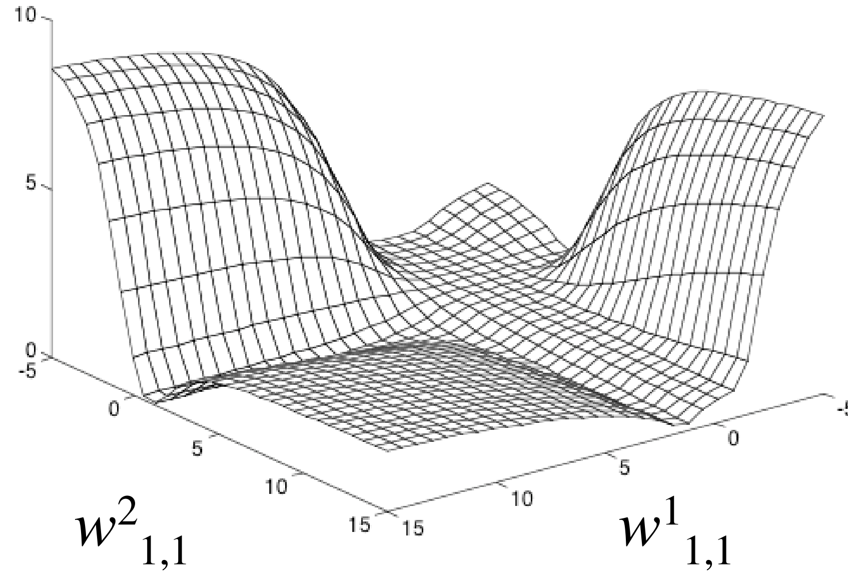
Parameter Values

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

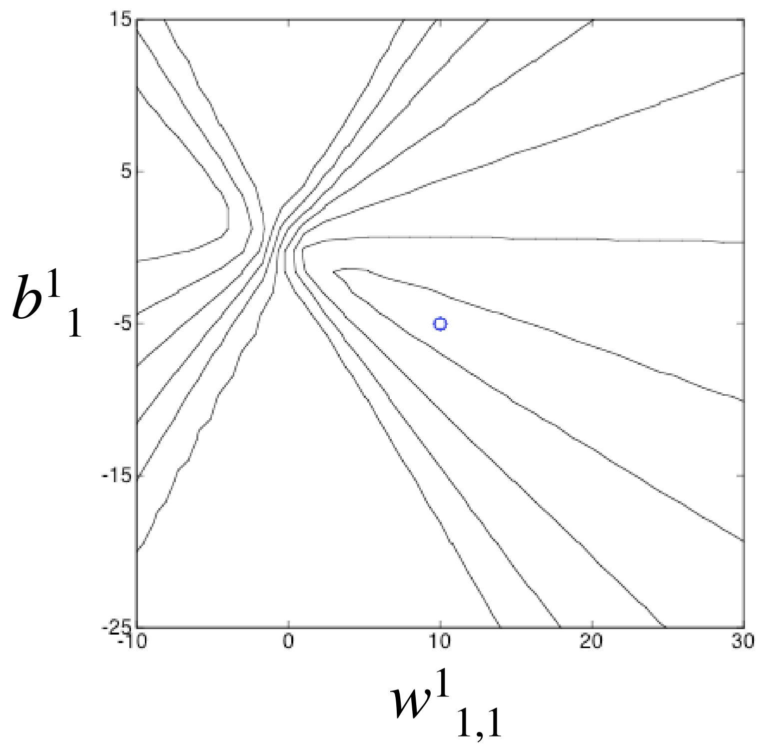
$$w^2_{1,1} = 1 \qquad w^2_{1,2} = 1 \qquad b^2 = -1$$

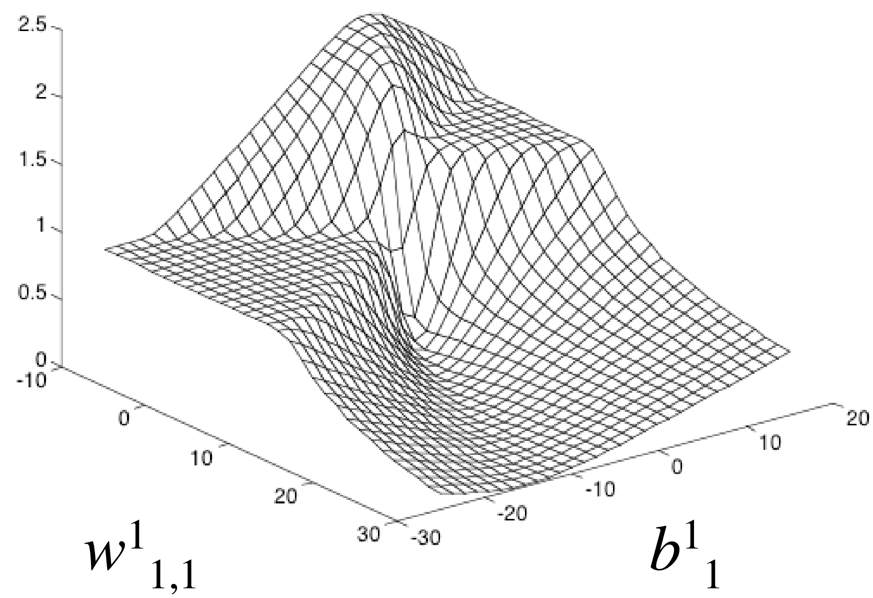
Squared Error vs. $w^1_{1,1}$ and $w^2_{1,1}$



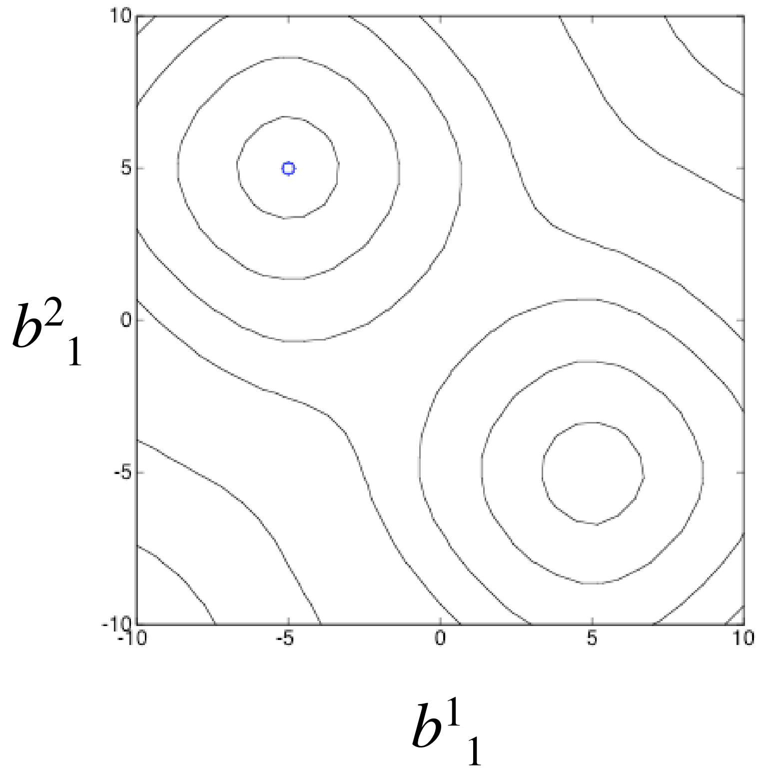


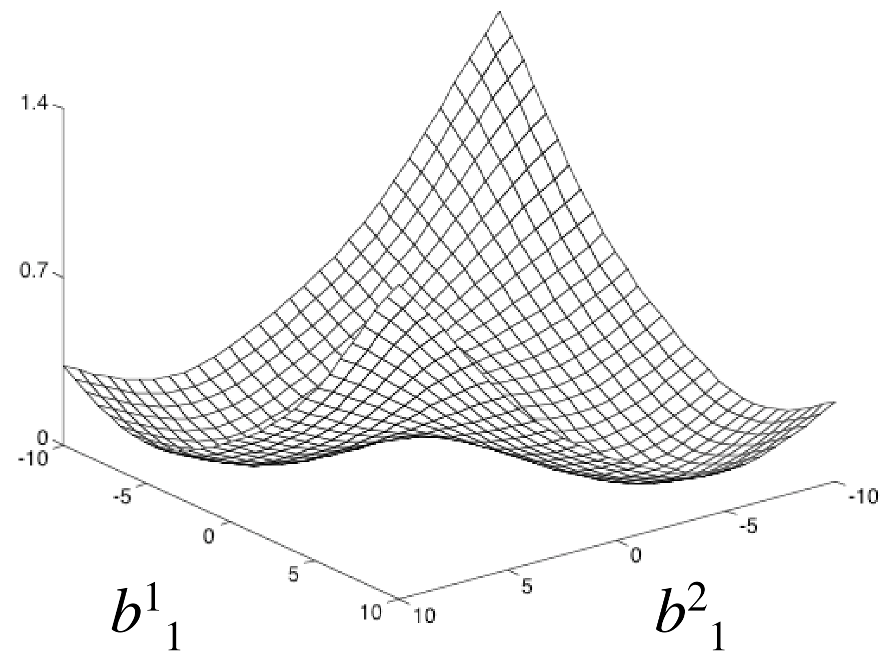
Squared Error vs. $w^1_{1,1}$ and b^1_1



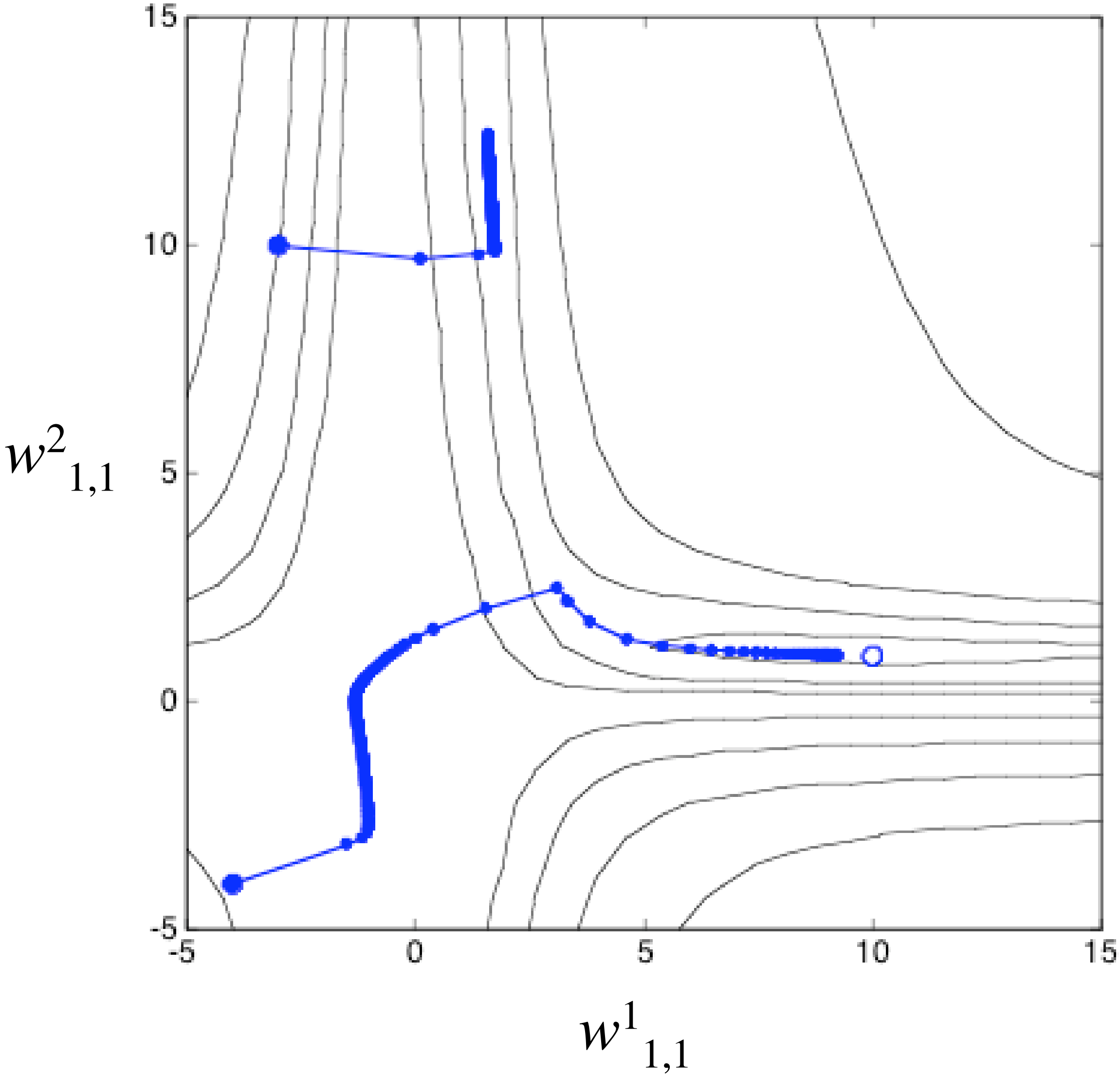


Squared Error vs. b^1_1 and b^1_2

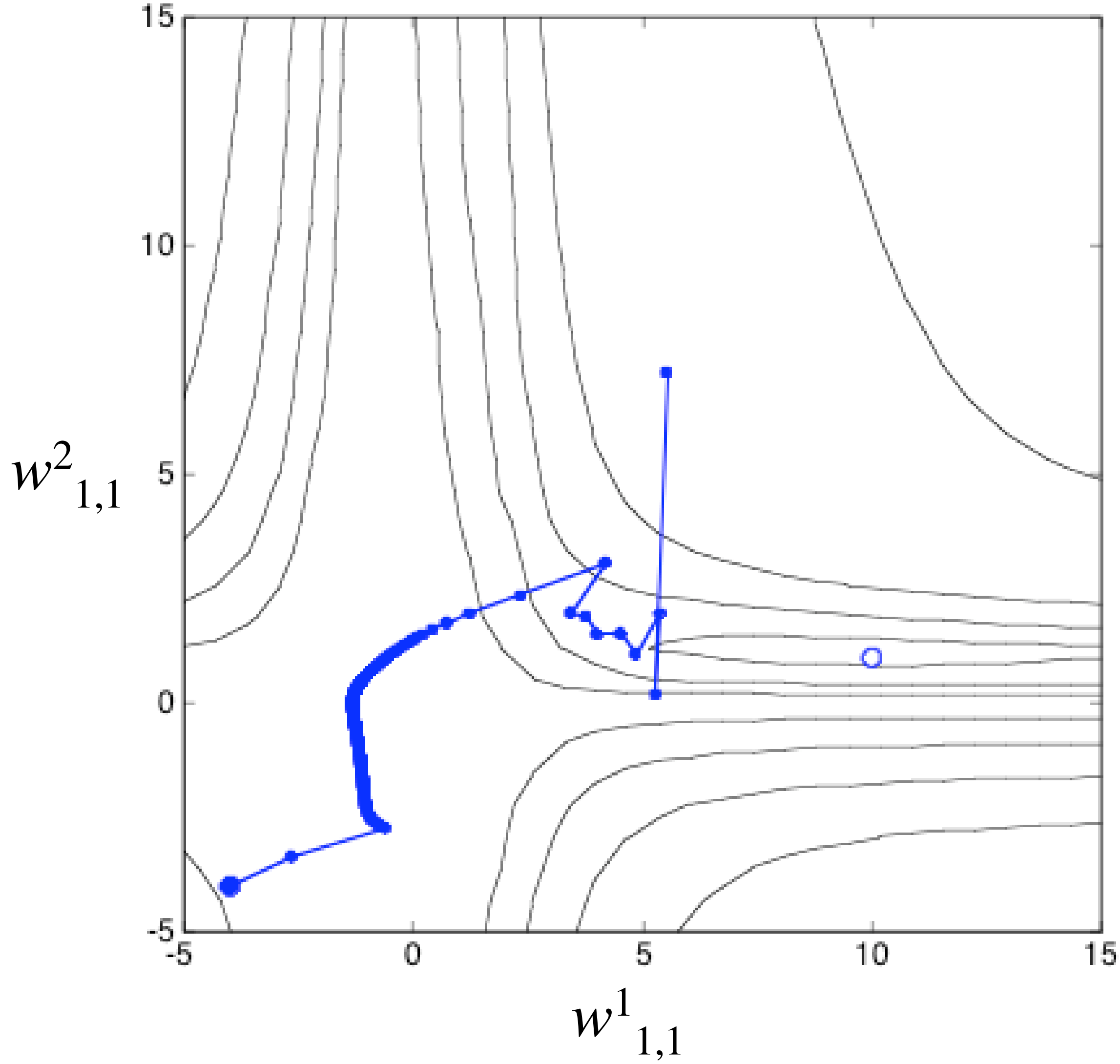




Convergence Example



Learning Rate Too Large



Momentum Backpropagation

Steepest Descent Backpropagation (SDBP)

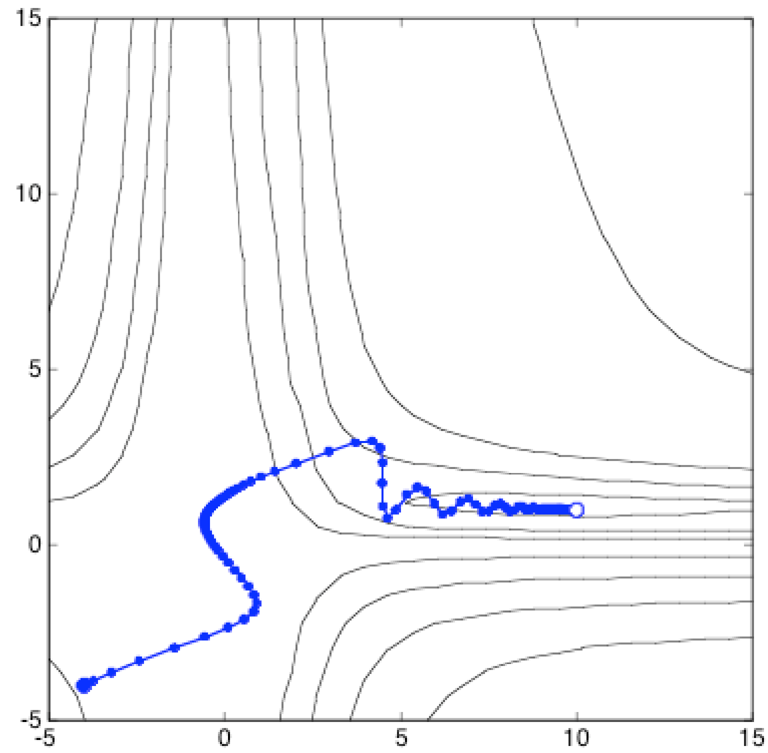
$$\Delta \mathbf{W}^m(k) = -\alpha \mathbf{s}^m (\mathbf{a}^{m-1})^T$$

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

Momentum Backpropagation (MOBP)

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

$$\Delta \mathbf{b}^m(k) = \gamma \Delta \mathbf{b}^m(k-1) - (1-\gamma)\alpha \mathbf{s}^m$$



$w^2_{1,1}$ vs. $w^1_{1,1}$

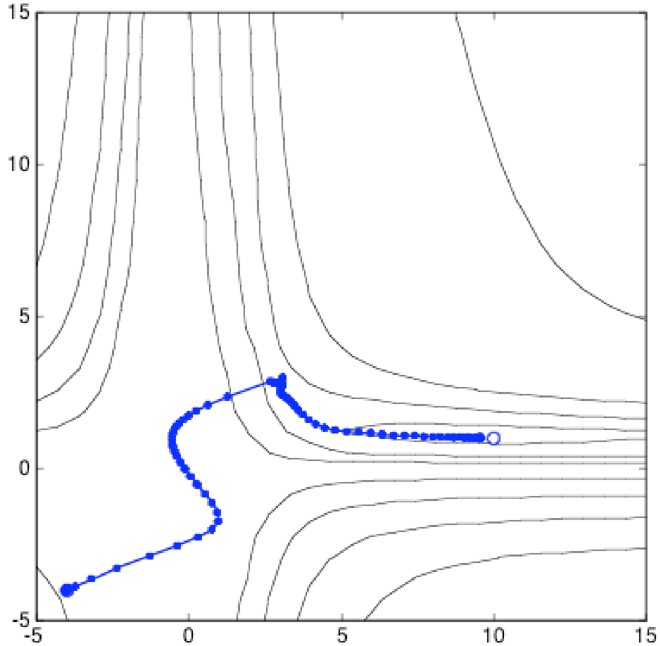
$$\gamma = 0.8$$

Variable Learning Rate (VLBP)

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

Example

$w^2_{1,1}$



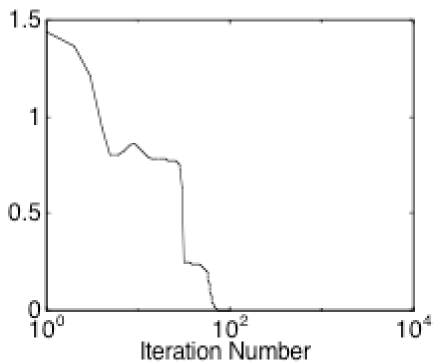
$w^1_{1,1}$

$\eta = 1.05$

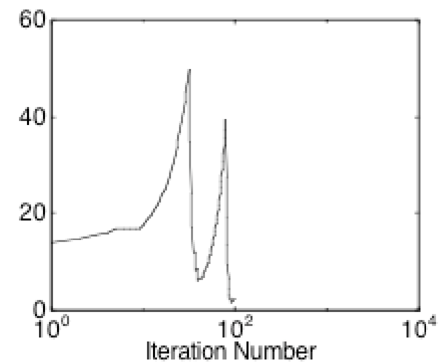
$\rho = 0.7$

$\zeta = 4\%$

MSE



Learning Rate



Two methods for accelerating backpropagation

- Conjugate Gradient method
- Levenberg-Marquardt method

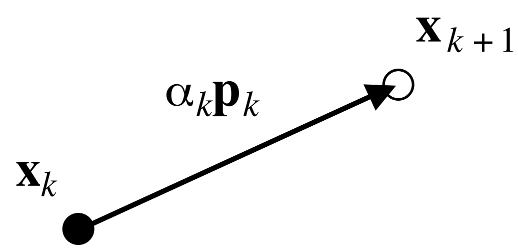
Gradient Descent Review

Basic Optimization Algorithm

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

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:

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

We can maximize the decrease by choosing:

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

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

Example for an Analytic Function

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

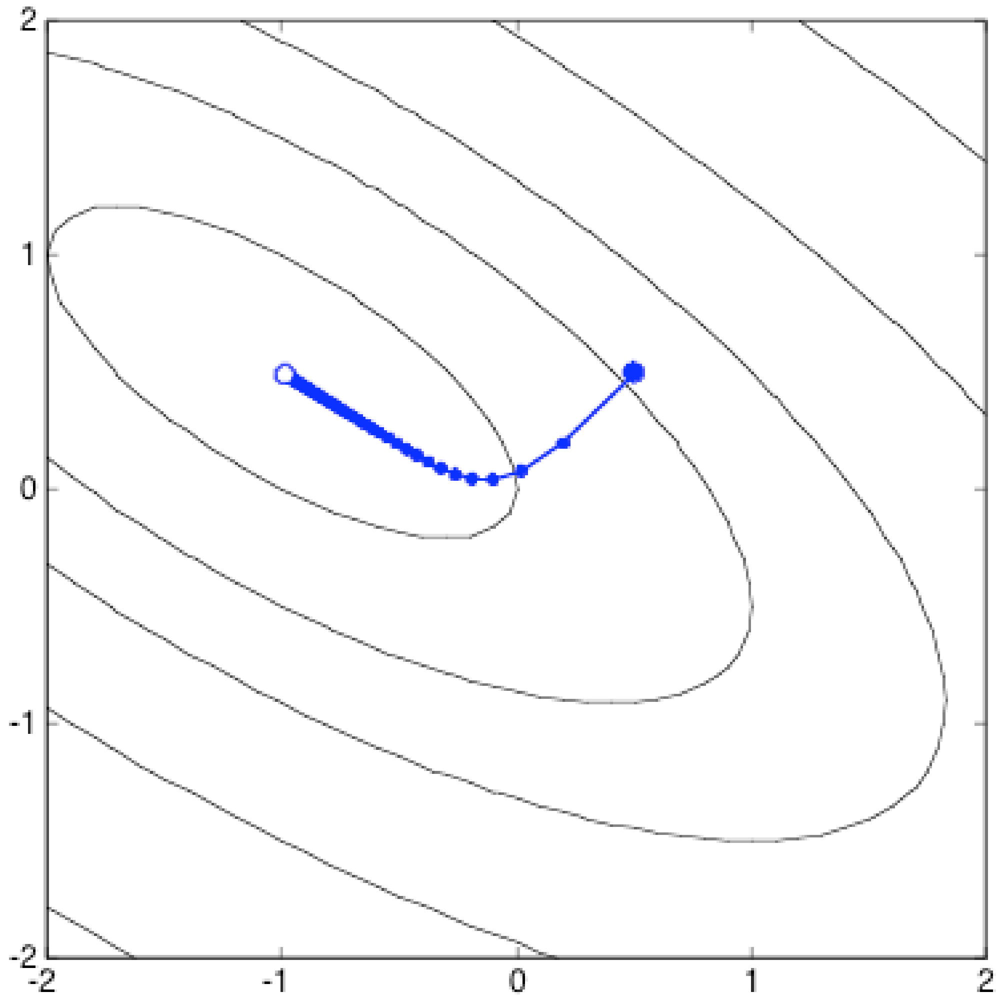
$$\mathbf{x}_0 = \begin{bmatrix} 0.5 \\ 0.5 \end{bmatrix} \qquad \alpha = 0.1$$

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

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

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

Steepest Descent Plot



Note:
Lots of *small* steps

Conjugate Gradient Method

Acceleration by Minimizing MSE Function *Along a Line*

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

$\boldsymbol{p}_k$ is **any chosen line direction**, e.g. -$\boldsymbol{g}_k$ (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, but we often don't. Later, we show how to minimize by search.

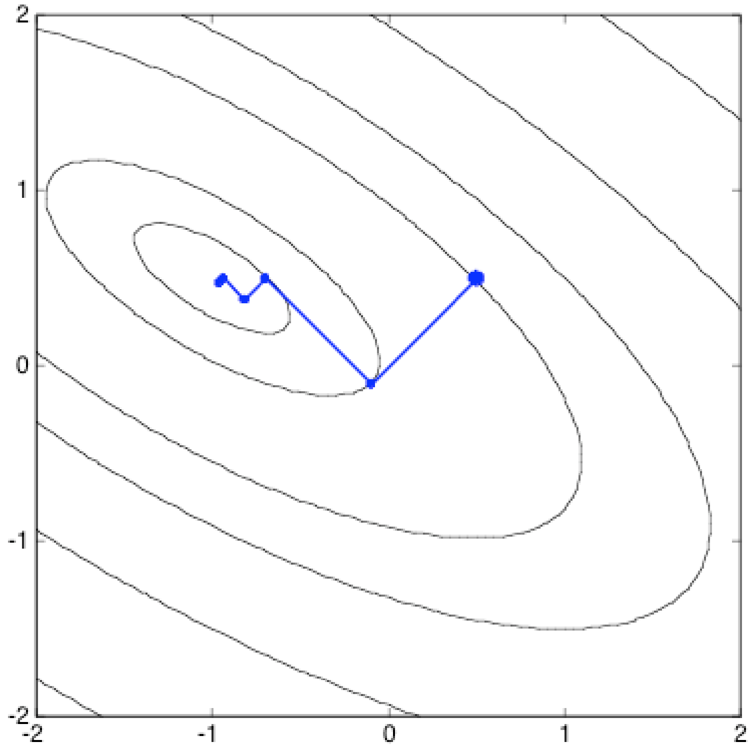
Example

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

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

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

Successive Line Minimizations with different directions



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

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

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 $\mathbf{p}_i$ is mutually *conjugate* with respect to a positive definite Hessian matrix **A** provided

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

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.)

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

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

the last term not requiring knowledge of the Hessian matrix A.

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 according to *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

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.

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

(e.g. 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, where n is the number of dimensions.

Example Analytic Solution, Quadratic

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

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

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

Example

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

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

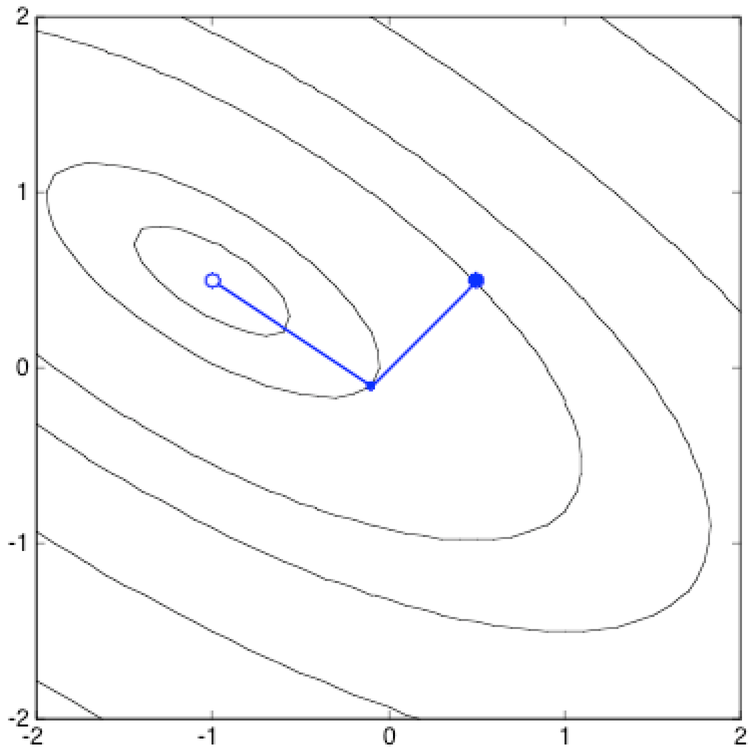
$$\mathbf{p}_1 = -\mathbf{g}_1 + \beta_1 \mathbf{p}_0 = \begin{bmatrix} -0.6 \\ 0.6 \end{bmatrix} + 0.04\begin{bmatrix} -3 \\ -3 \end{bmatrix} = \begin{bmatrix} -0.72 \\ 0.48 \end{bmatrix}$$

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

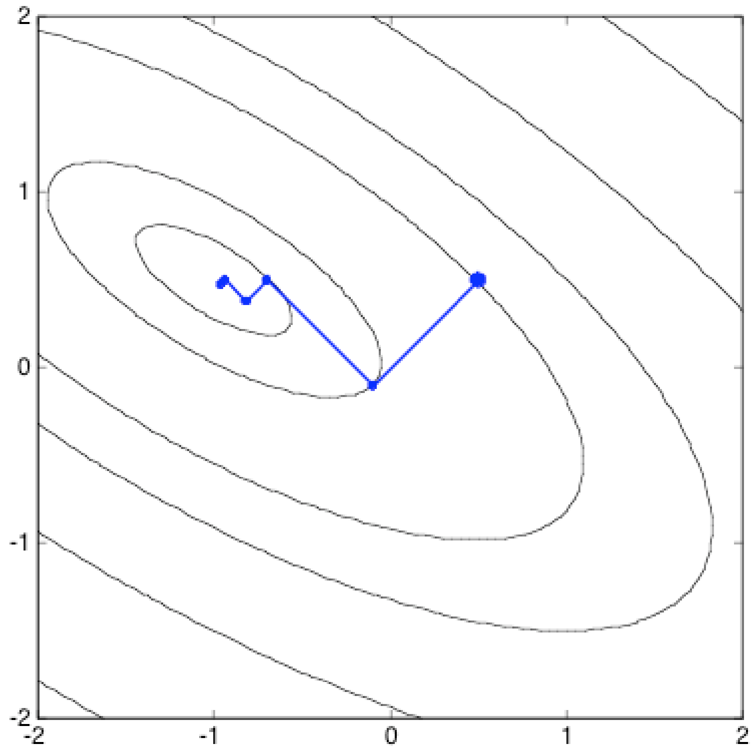
Conjugate Gradient vs. Steepest Descent Plots

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

Conjugate Gradient



Steepest Descent



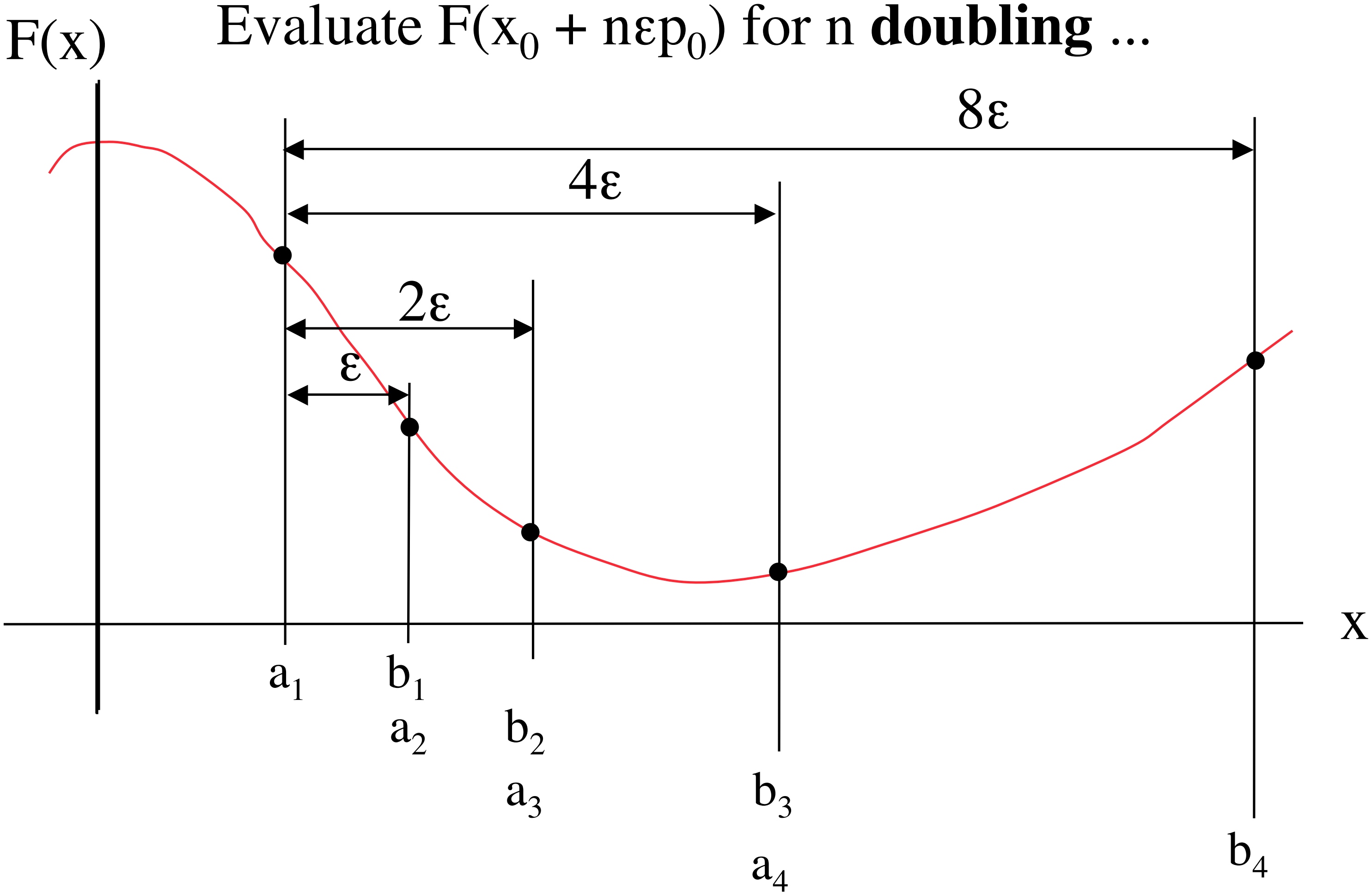
Heuristic for Line Minimization for General Functions (not necessarily quadratic)

Numerical Line Minimization

- Part 1: **Locate** an **interval** containing the minimum.
- Part 2: **Reduce** the interval's width successively, until the interval is sufficiently small that we are close enough to the minimum.

Part 1: Interval Location to Bracket Minimum

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

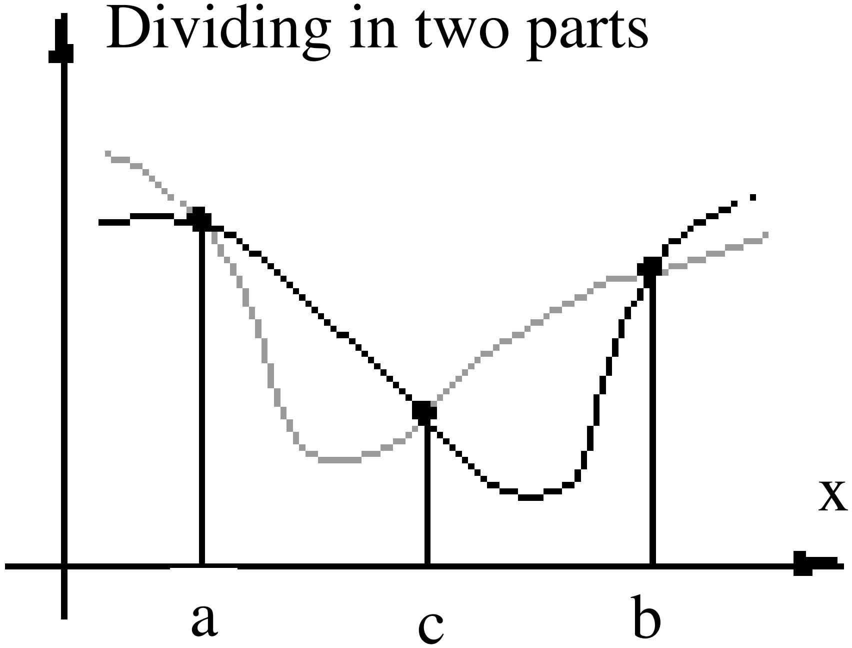


Stop when two successive increases occur.

Part 2: Interval Reduction

What doesn't help:

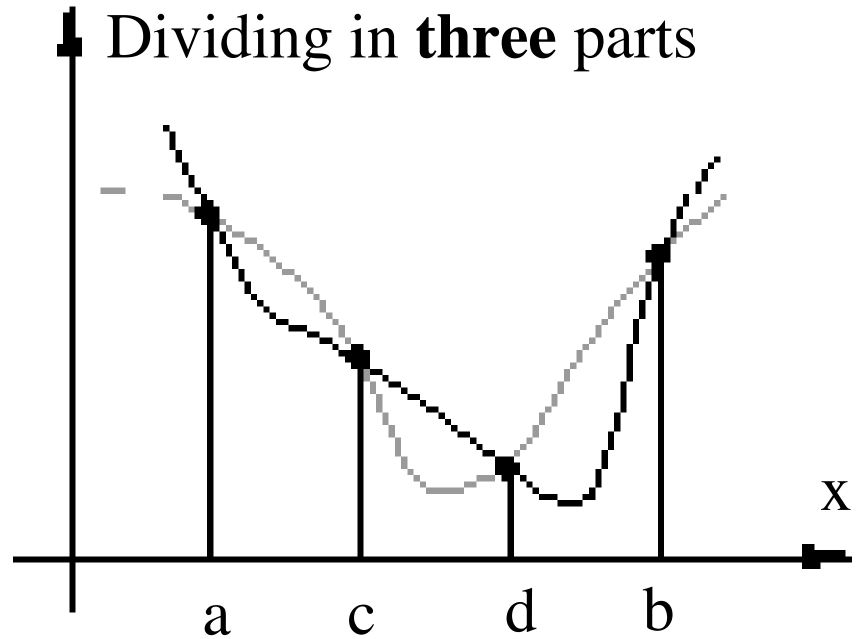
Dividing in two parts



Interval **not reduced**.

What does:

Dividing in **three** parts



Minimum is not between a and c
$\Rightarrow$ **eliminate** a-c.

Optimization of Function Evaluations: Fibonacci Search

$\tau = 0.618$

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

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

For k=1,2, ... repeat

If $F_c < F_d$ then

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

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

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

else

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

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

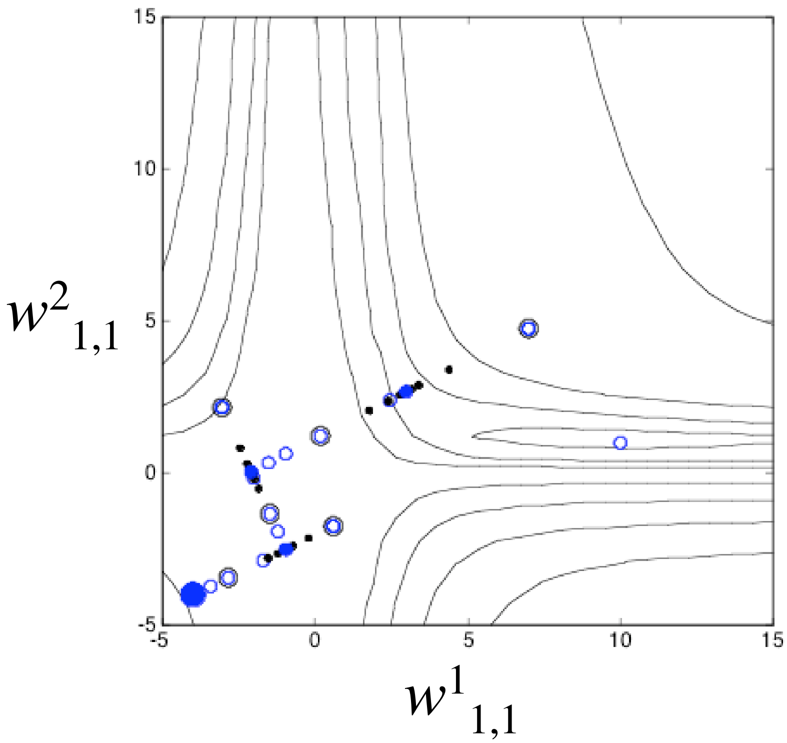
$F_c = F_d$; $F_d\text{=}F(d_{k+1})$

end

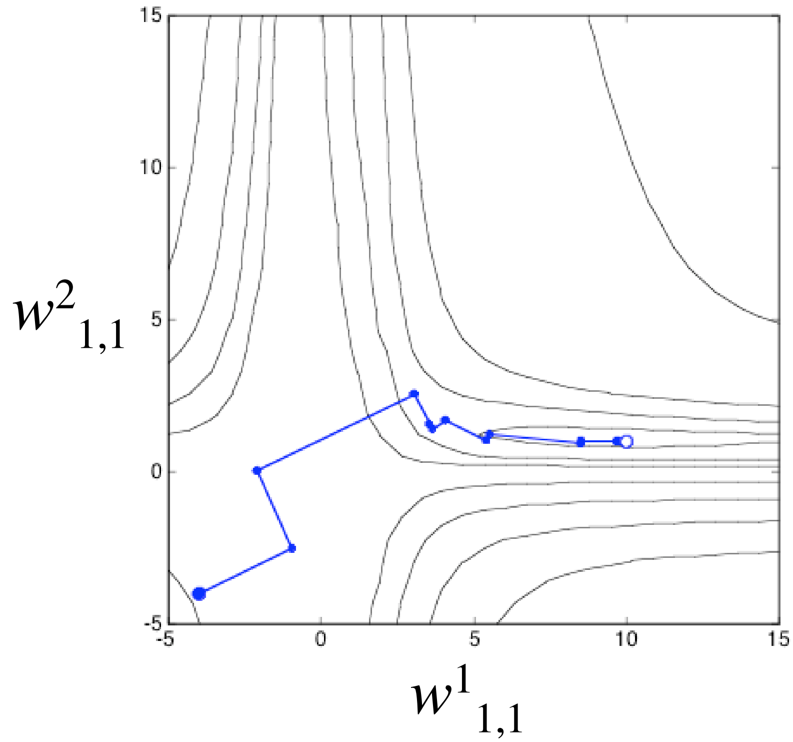
end until $b_{k+1} - a_{k+1} < tol$

Conjugate Gradient BP (CGBP)

Intermediate Steps



Complete Trajectory



Note on Conjugate Gradient

- CG is a **batch-mode** algorithm:
  - Average the gradient over all samples.

Newton's Method for Locating a Minimum

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

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

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 *j*th 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:

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

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

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

Example

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

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

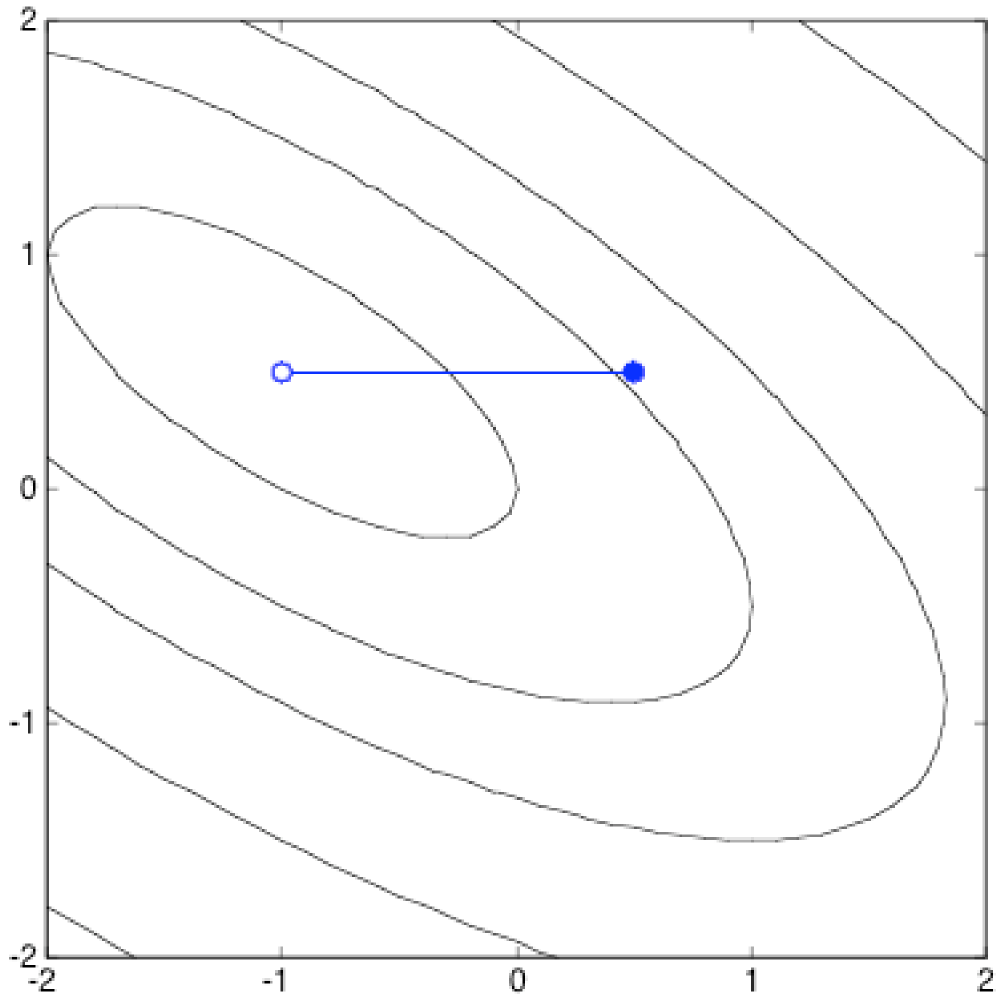
$$\nabla F(\mathbf{x}) = \begin{bmatrix} \frac{\partial}{\partial x_1} F(\mathbf{x}) \\ \frac{\partial}{\partial x_2} F(\mathbf{x}) \end{bmatrix} = \begin{bmatrix} 2x_1 + 2x_2 + 1 \\ 2x_1 + 4x_2 \end{bmatrix}$$

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

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

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

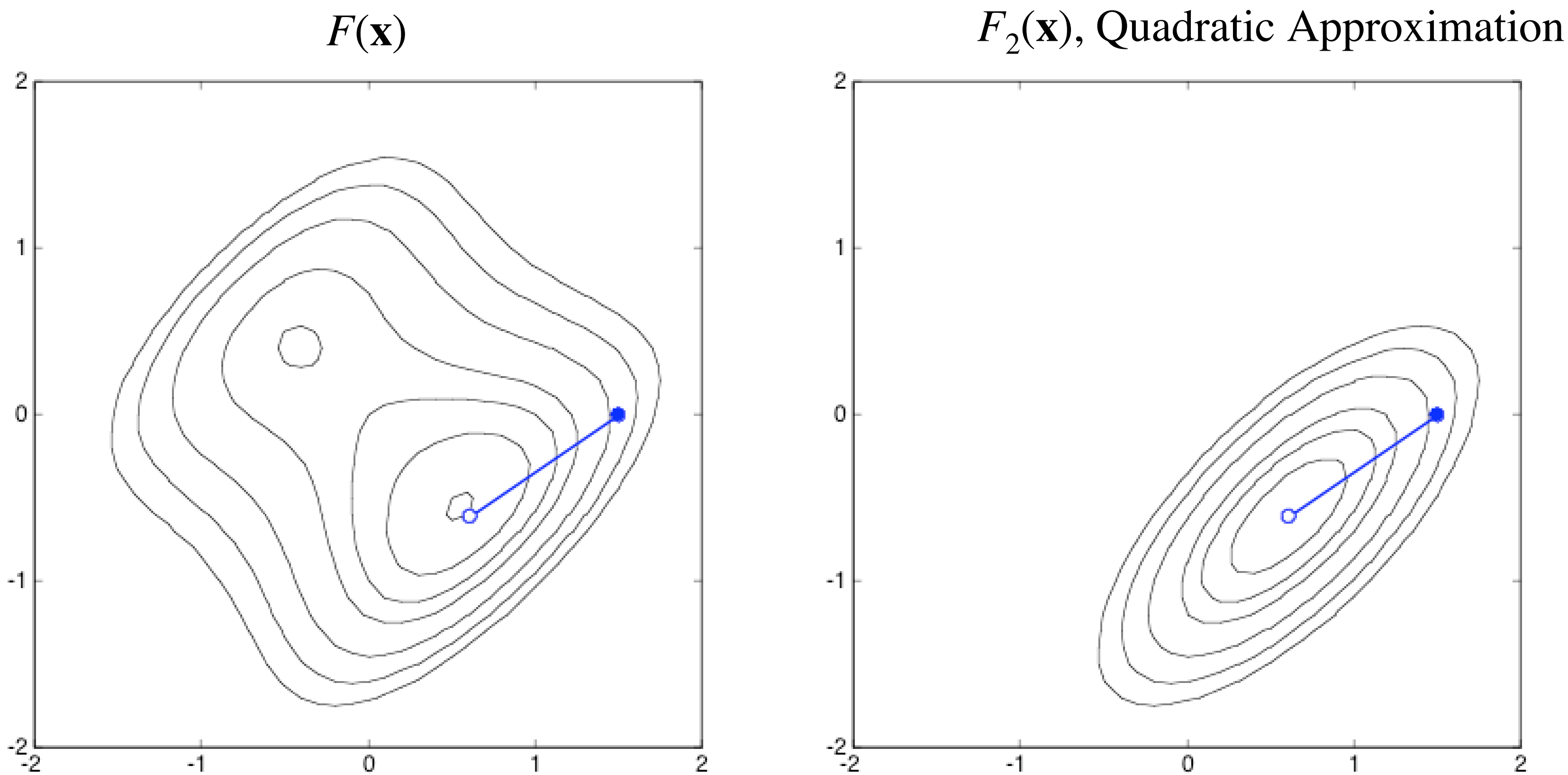
Plot of Newton's Method for a Quadratic



Non-Quadratic Example

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

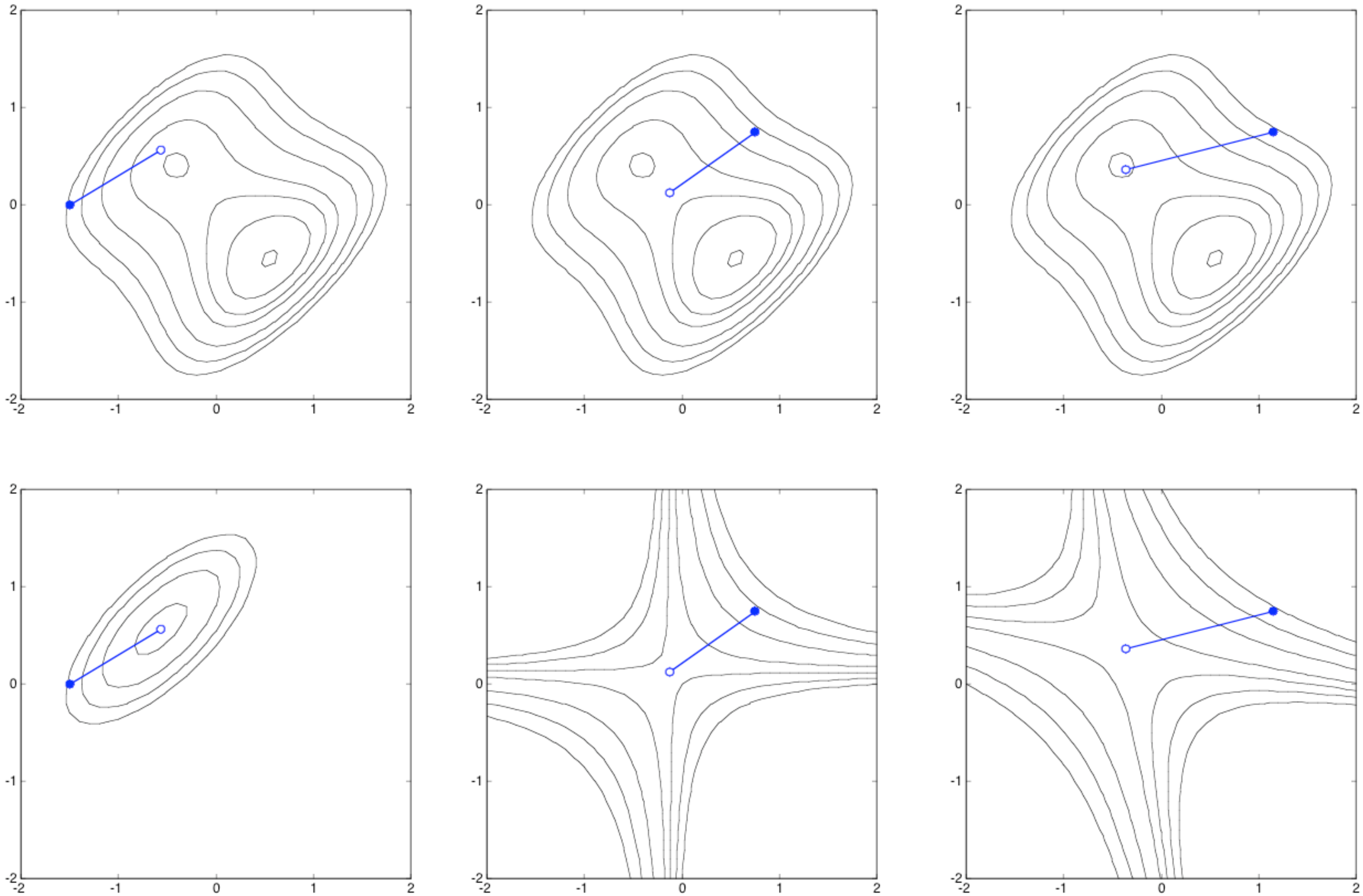
Stationary Points: $\mathbf{x}^1 = \begin{bmatrix} -0.42 \\ 0.42 \end{bmatrix}$ $\mathbf{x}^2 = \begin{bmatrix} -0.13 \\ 0.13 \end{bmatrix}$ $\mathbf{x}^3 = \begin{bmatrix} 0.55 \\ -0.55 \end{bmatrix}$



Different Initial Conditions and Quadratic Approximations to Each

$F(\mathbf{x})$

$F_2(\mathbf{x})$



Levenberg-Marquardt Method

(blends Newton's method with steepest descent)

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

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 **J** is the Jacobian matrix:

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

v are the error values for each component of each sample

Express Hessian, which represents Curvature, in terms of Jacobian:

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

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

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

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:

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

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

This method does not require calculating second derivatives.

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

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

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

Adjustment of μ_k

As $\mu_k \rightarrow 0$, 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 $\mu_k \rightarrow \infty$, LM becomes Steepest Descent with small learning rate.

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

Adjustment of μ_k

• **Steepest Descent is the 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.

Application to Multilayer Network

The performance index for the multilayer network is:

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

S^M = number of outputs,

Q = number of samples

The error vector is:

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

The parameter vector is:

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

The dimensions of the two vectors are:

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

Jacobian Matrix for Levenberg-Marquardt

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

M rows for every input sample

Repeated Q times

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):

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

we can compute the Jacobian as follows:

weight

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

bias

$$[\mathbf{J}]_{h,l} = \frac{\partial v_h}{\partial x_l} = \frac{\partial e_{k,q}}{\partial b^m_i} = \frac{\partial e_{k,q}}{\partial n^m_{i,q}} \times \frac{\partial n^m_{i,q}}{\partial b^m_i} = \tilde{s}^m_{i,h} \times \frac{\partial n^m_{i,q}}{\partial b^m_i} = \tilde{s}^m_{i,h}$$

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

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

$$\tilde{\mathbf{S}}^{m} = \left[\tilde{\mathbf{S}}_{1}^{m} \middle| \tilde{\mathbf{S}}_{2}^{m} \middle| \ldots \middle| \tilde{\mathbf{S}}_{Q}^{m} \right]$$

Q = number of samples

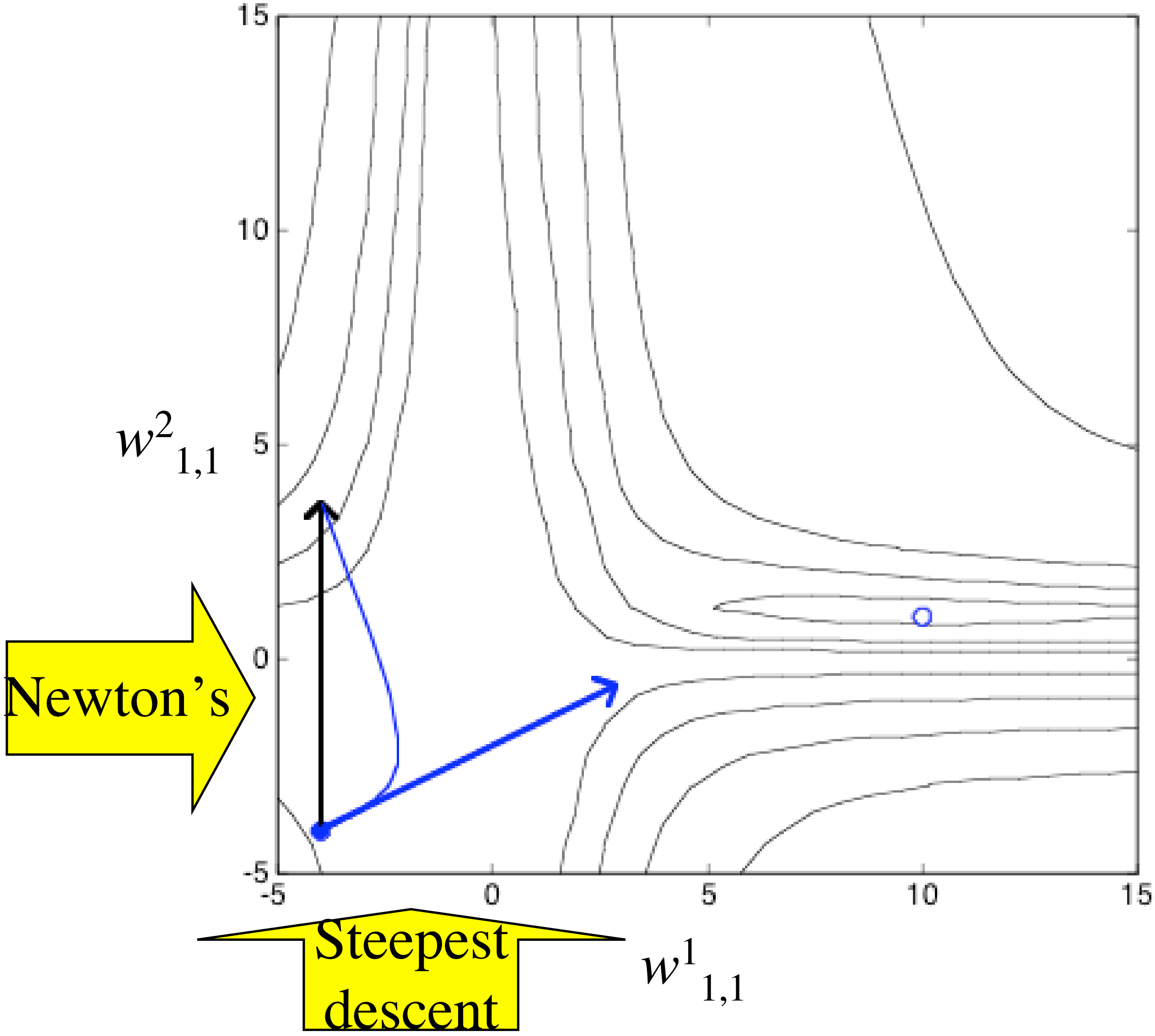
Levenberg-Marquardt Backpropagation

1. Present *all inputs* to the network and compute the corresponding network outputs and the errors. Compute the sum of squared errors over all inputs.
2. 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 using previous equations.
3. Invert the matrix in the following equation

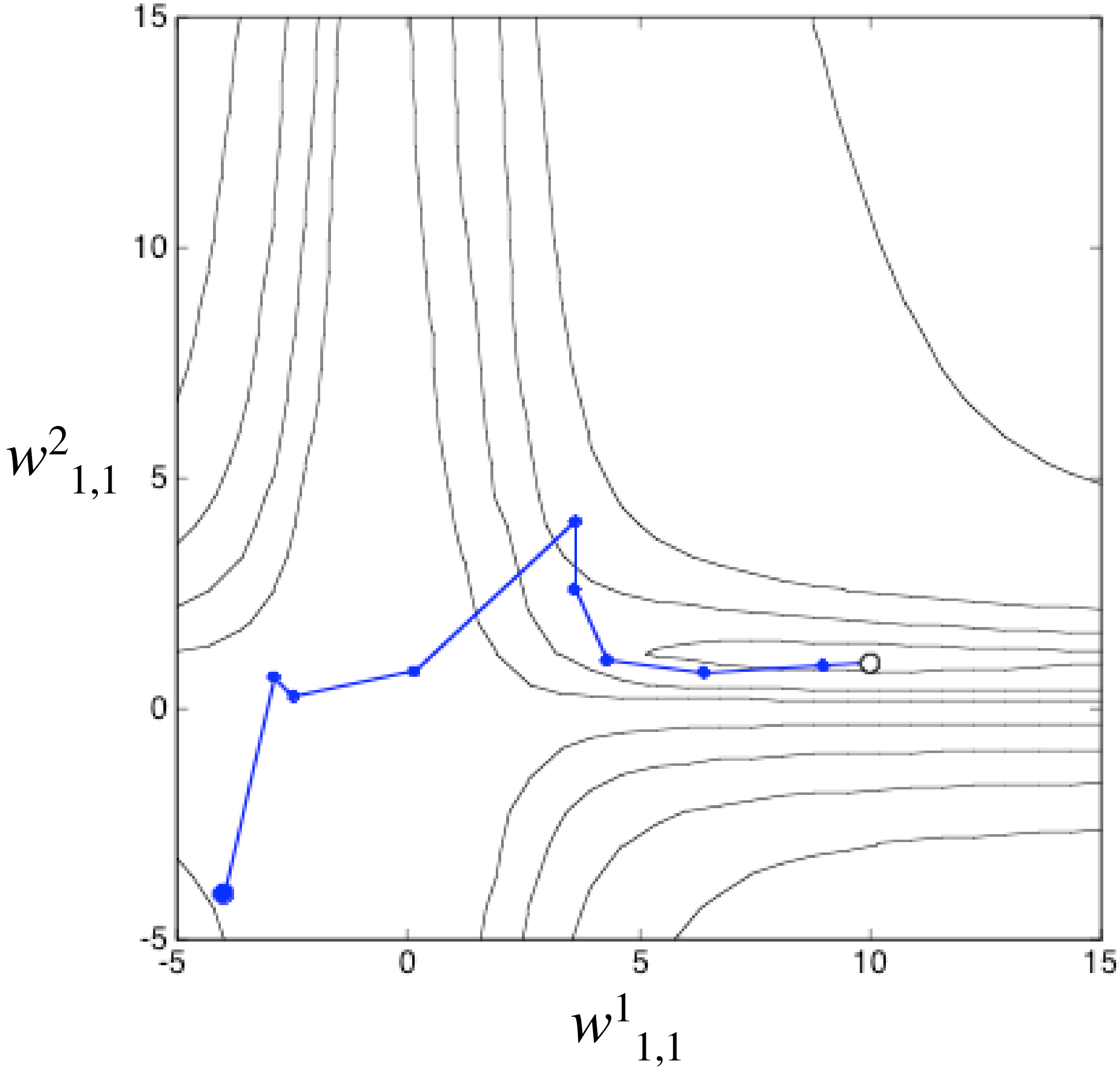
$$\mathbf{x}_{k+1} = \mathbf{x}_k - [\mathbf{J}^T(\mathbf{x}_k)\mathbf{J}(\mathbf{x}_k) + \mu_k \mathbf{I}]^{-1}\mathbf{J}^T(\mathbf{x}_k)\mathbf{v}(\mathbf{x}_k)$$

   to obtain the weight updates.
4. 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 υ, update the weights and go back to step 1. If the sum of squares is not reduced, then multiply μ_k by υ and go back to step 3.

Example LMBP Step



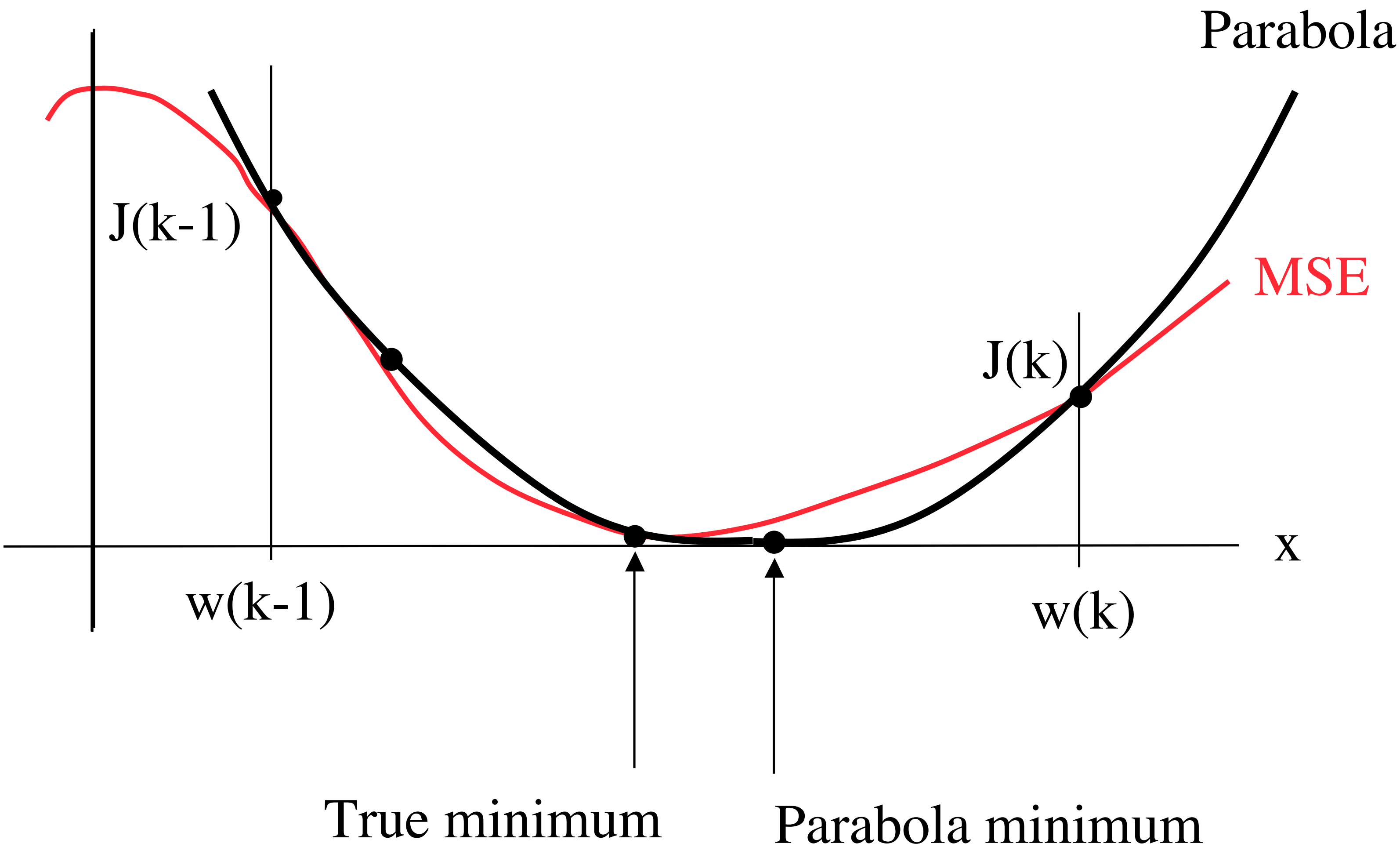
LMBP Trajectory



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 $\Delta w(k-1) = w(k) - w(k-1)$
- (continued next page)

Quickprop

- Set $J'(w(k+1)) = 0$, since we are looking for the parabolic **minimum** at the next step.
- Then $2a\, w(k+1) + b = 0$, 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 $w(k+1)$.