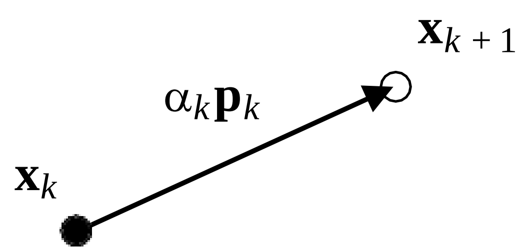
Performance Optimization (Performan Optimizasyonu Güncelleme Algoritmaları)

Basic Optimization Algorithm

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

or

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



$\mathbf{p}_k$ - Search Direction

α_k - Learning Rate

Steepest Descent

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 $F(\mathbf{x})$:

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

where

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

If we want the function to decrease:

$$\mathbf{g}_k^T \otimes\mathbf{x}_k = \alpha_k \mathbf{g}_k^T \mathbf{p}_k < 0$$

We can maximize the decrease by choosing:

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

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

Example

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

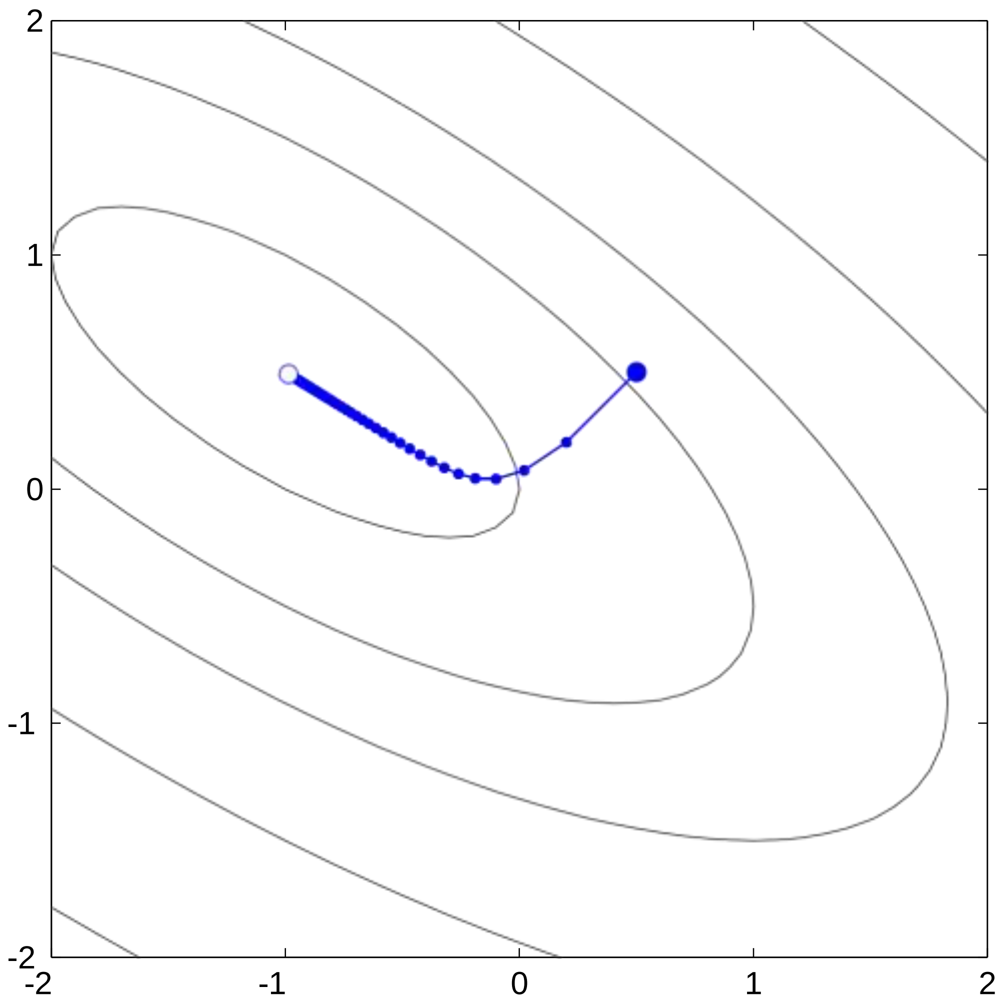
$$\mathbf{x}_0 = \begin{bmatrix} 0.5 \\ 0.5 \end{bmatrix} \qquad \alpha = 0.1$$

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

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

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

Plot



Stable Learning Rates (Quadratic)

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

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

$$\mathbf{x}_{k+1} = \mathbf{x}_k - \alpha\mathbf{g}_k = \mathbf{x}_k - \alpha(\mathbf{A}\mathbf{x}_k + \mathbf{d}) \quad \Rightarrow \quad \mathbf{x}_{k+1} = \underbrace{[\mathbf{I} - \alpha\mathbf{A}]}_{\text{Stability is determined by the eigenvalues of this matrix.}}\mathbf{x}_k - \alpha\mathbf{d}$$

$$[\mathbf{I} - \alpha\mathbf{A}]\mathbf{z}_i = \mathbf{z}_i - \alpha\mathbf{A}\mathbf{z}_i = \mathbf{z}_i - \alpha\lambda_i\mathbf{z}_i = \underbrace{(1 - \alpha\lambda_i)}_{\text{Eigenvalues of } [\mathbf{I} - \alpha\mathbf{A}].}\mathbf{z}_i$$

(λ_i - eigenvalue of $\mathbf{A}$)

Stability Requirement:

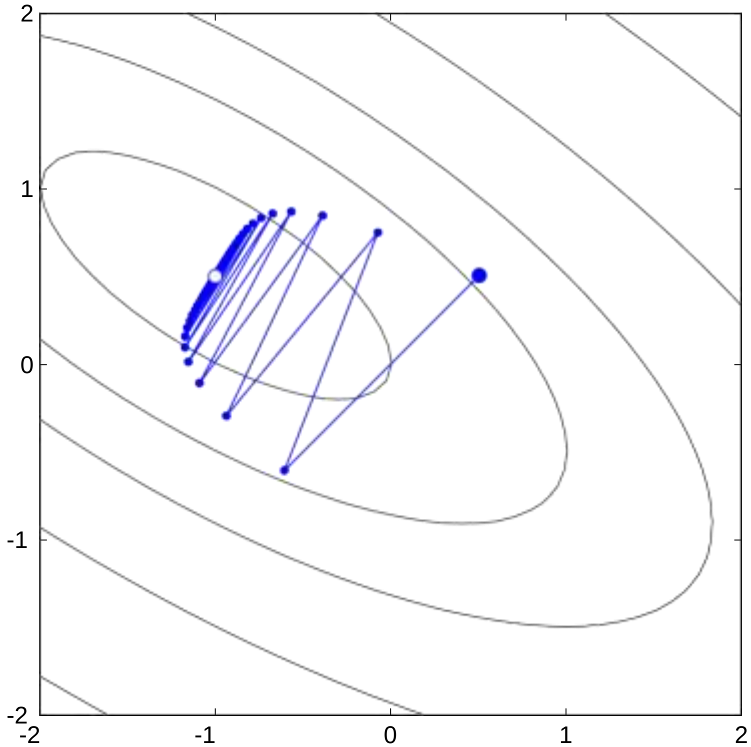
$$\left|(1 - \alpha\lambda_i)\right| < 1 \qquad \alpha < \frac{2}{\lambda_i} \qquad \boxed{\alpha < \frac{2}{\lambda_{max}}}$$

Example

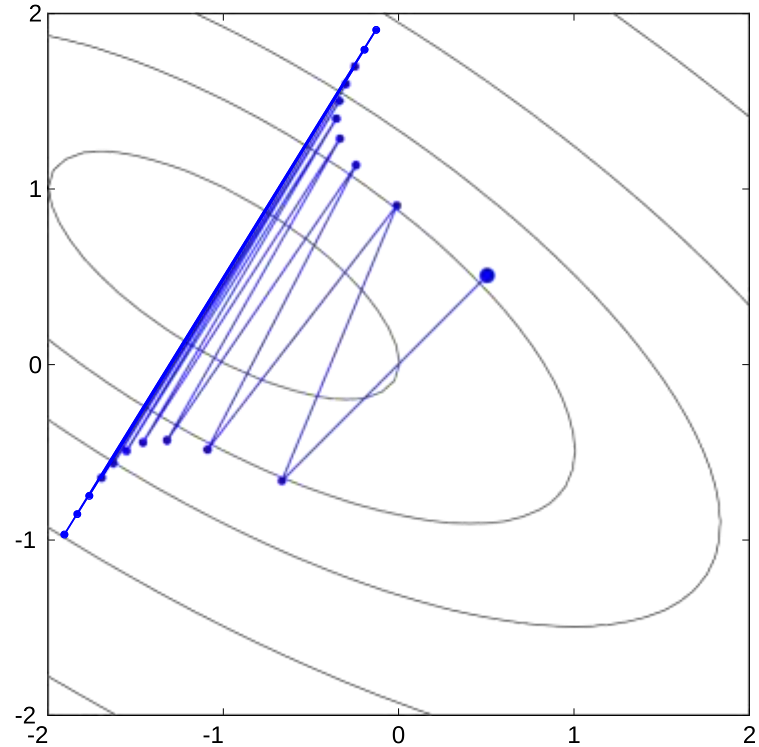
$$\mathbf{A} = \begin{bmatrix} 2 & 2 \\ 2 & 4 \end{bmatrix} \qquad \left\{ (\lambda_1 = 0.764),\ \mathbf{z}_1 = \begin{bmatrix} 0.851 \\ -0.526 \end{bmatrix} \right\}, \left\{ \lambda_2 = 5.24,\ \mathbf{z}_2 = \begin{bmatrix} 0.526 \\ 0.851 \end{bmatrix} \right\}$$

$$\alpha < \frac{2}{\lambda_{max}} = \frac{2}{5.24} = 0.38$$

$\alpha = 0.37$



$\alpha = 0.39$



Minimizing Along a Line

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

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

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

where

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

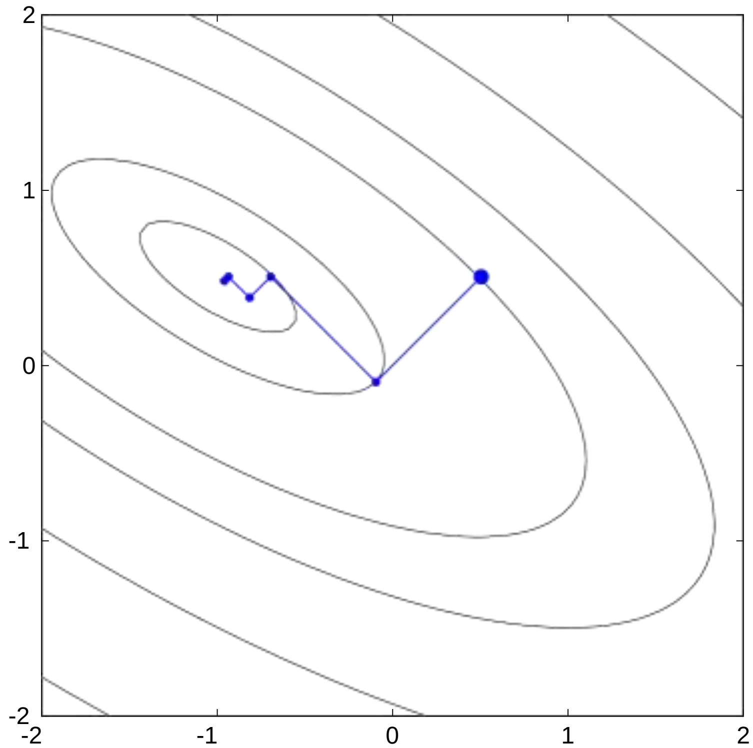
Example

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

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

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

Plot



Successive steps are orthogonal.

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

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

Newton's Method

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

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

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

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

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

Example

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

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

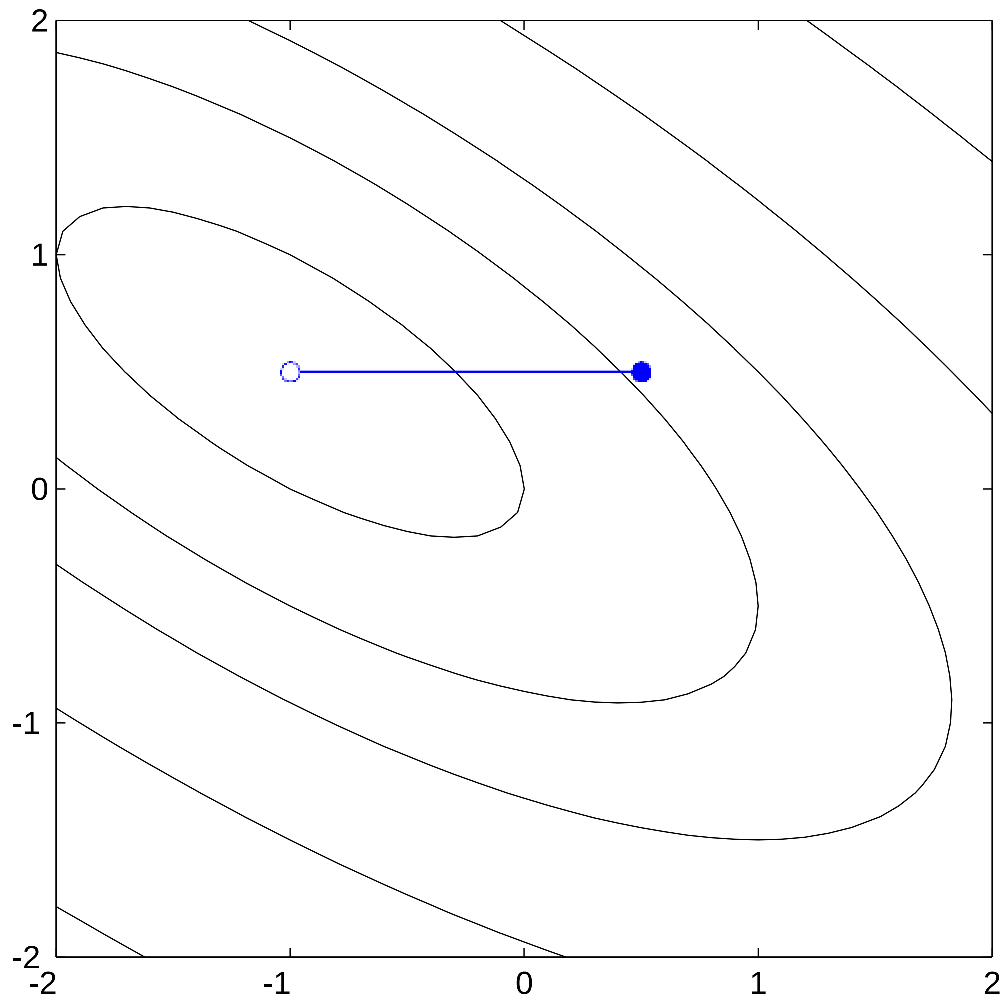
$$\nabla F(\mathbf{x}) = \begin{bmatrix} \frac{\partial}{\partial x_1} F(\mathbf{x}) \\ \frac{\partial}{\partial x_2} F(\mathbf{x}) \end{bmatrix} = \begin{bmatrix} 2x_1 + 2x_2 + 1 \\ 2x_1 + 4x_2 \end{bmatrix}$$

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

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

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

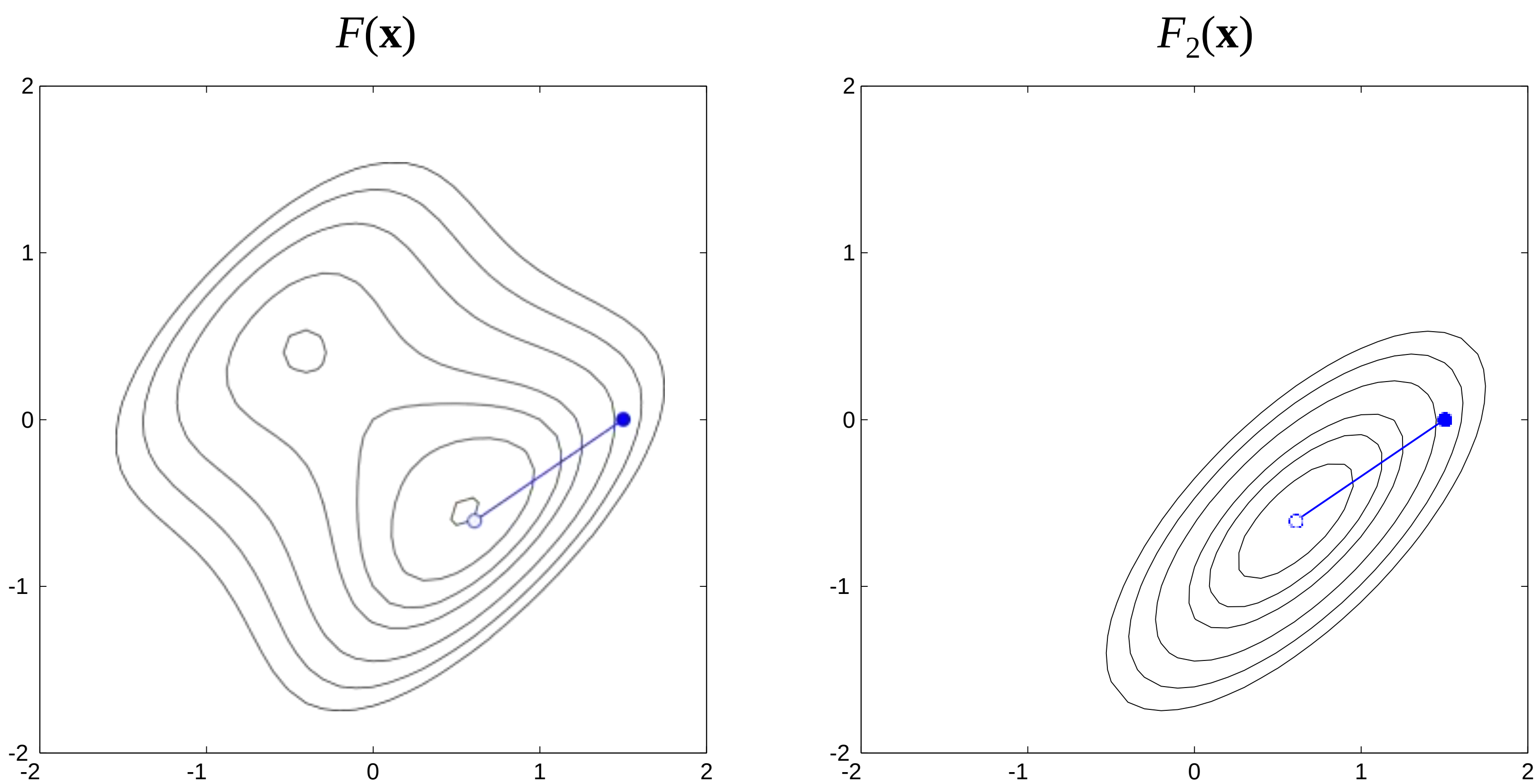
Plot



Non-Quadratic Example

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

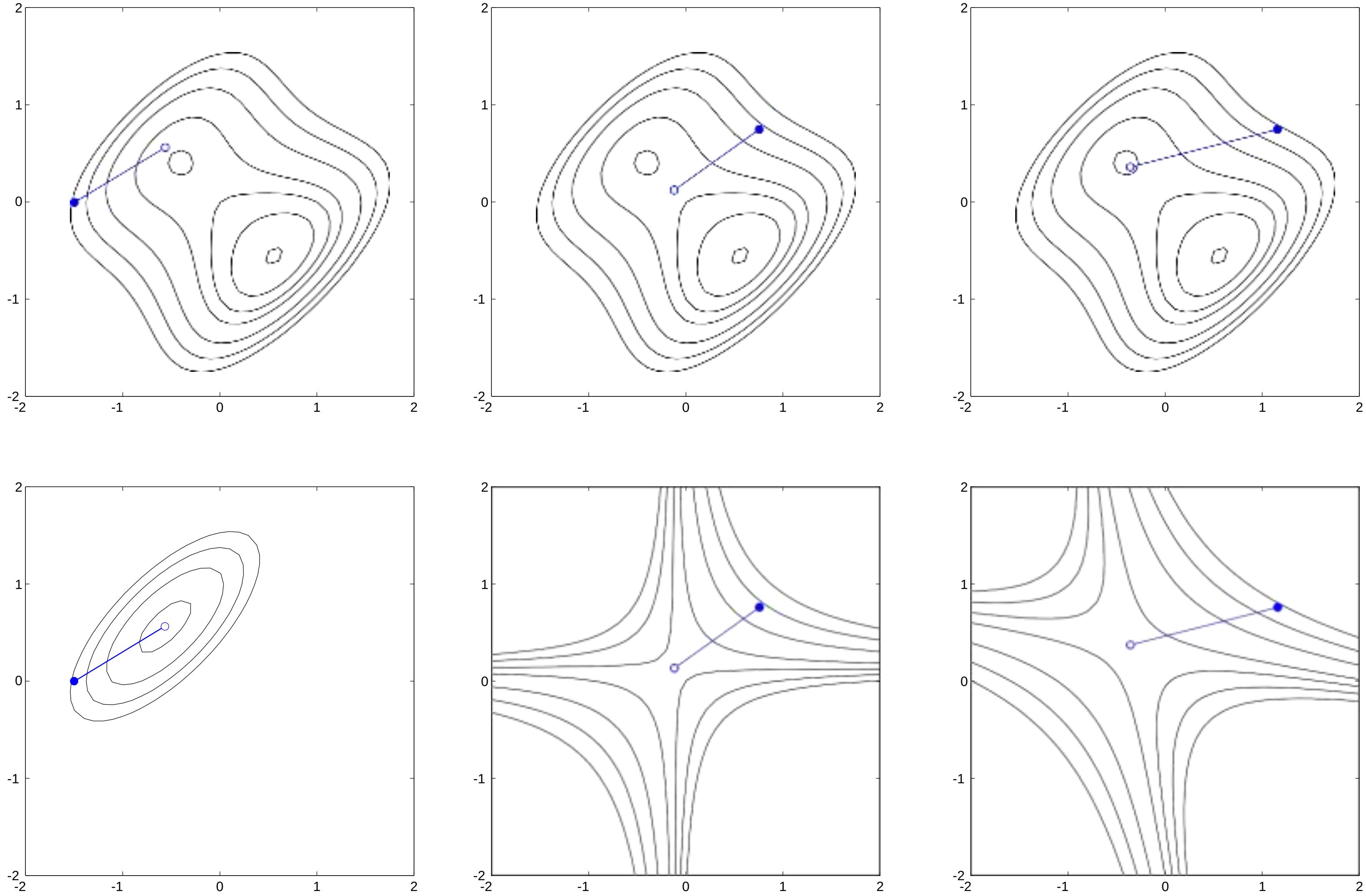
Stationary Points: $\mathbf{x}^1 = \begin{bmatrix} -0.42 \\ 0.42 \end{bmatrix}$ $\mathbf{x}^2 = \begin{bmatrix} -0.13 \\ 0.13 \end{bmatrix}$ $\mathbf{x}^3 = \begin{bmatrix} 0.55 \\ -0.55 \end{bmatrix}$



Different Initial Conditions

$F(\mathbf{x})$

$F_2(\mathbf{x})$



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 <u>conjugate</u> 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.)

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

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

where

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

The conjugacy conditions can be rewritten

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

This does not require knowledge of the Hessian matrix.

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

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

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.)

- 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.
- A quadratic function will be minimized in n steps.

Example

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

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

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

Example

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

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

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

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

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