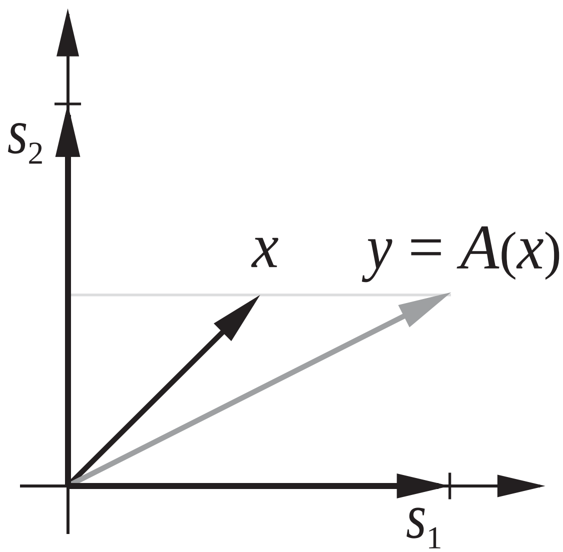
Part I
Eigen Transformation

Eigenvalues and Eigenvectors

Let $\mathcal{A}:X \rightarrow X$ be a linear transformation. Those vectors $z \in X$, which are not equal to zero, and those scalars λ which satisfy

$$\mathcal{A}(z) = \lambda\, z$$

are called eigenvectors and eigenvalues, respectively.



Can you find an eigenvector for this transformation?

Computing the Eigenvalues

$$\mathbf{A}\mathbf{z} = \lambda \mathbf{z}$$

$$[\mathbf{A} - \lambda \mathbf{I}]\mathbf{z} = \mathbf{0} \quad \Rightarrow \quad \left| [\mathbf{A} - \lambda \mathbf{I}] \right| = 0$$

Skewing example (45°):

$$\mathbf{A} = \begin{bmatrix} 1 & 1 \\ 0 & 1 \end{bmatrix} \qquad \left| \begin{bmatrix} 1-\lambda & 1 \\ 0 & 1-\lambda \end{bmatrix} \right| = 0 \qquad (1-\lambda)^2 = 0 \qquad \begin{matrix} \lambda_1 = 1 \\ \lambda_2 = 1 \end{matrix}$$

$$\begin{bmatrix} 1-\lambda & 1 \\ 0 & 1-\lambda \end{bmatrix} \mathbf{z} = \begin{bmatrix} 0 \\ 0 \end{bmatrix} \qquad \begin{bmatrix} 0 & 1 \\ 0 & 0 \end{bmatrix} \mathbf{z}_1 = \begin{bmatrix} 0 & 1 \\ 0 & 0 \end{bmatrix} \begin{bmatrix} z_{11} \\ z_{21} \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \end{bmatrix} \qquad z_{21} = 0 \qquad \mathbf{z}_1 = \begin{bmatrix} 1 \\ 0 \end{bmatrix}$$

For this transformation there is only one eigenvector.

Diagonalization

Perform a change of basis (similarity transformation) using the eigenvectors as the basis vectors. If the eigenvalues are distinct, the new matrix will be diagonal.

$$\mathbf{B} = \left[\mathbf{z}_1 \ \mathbf{z}_2 \ \dots \ \mathbf{z}_n\right]$$

$\{\mathbf{z}_1, \mathbf{z}_2, \dots, \mathbf{z}_n\}$ Eigenvectors

$\{\lambda_1, \lambda_2, \dots, \lambda_n\}$ Eigenvalues

$$[\mathbf{B}^{-1}\mathbf{A}\mathbf{B}] = \begin{bmatrix} \lambda_1 & 0 & \dots & 0 \\ 0 & \lambda_2 & \dots & 0 \\ \vdots & \vdots & & \vdots \\ 0 & 0 & \dots & \lambda_n \end{bmatrix}$$

Example

$$\mathbf{A} = \begin{bmatrix} 1 & 1 \\ 1 & 1 \end{bmatrix}$$

$$\left| \begin{bmatrix} 1-\lambda & 1 \\ 1 & 1-\lambda \end{bmatrix} \right| = 0 \qquad \lambda^2 - 2\lambda = (\lambda)(\lambda - 2) = 0 \qquad \begin{matrix} \lambda_1 = 0 \\ \lambda_2 = 2 \end{matrix} \qquad \begin{bmatrix} 1-\lambda & 1 \\ 1 & 1-\lambda \end{bmatrix} \mathbf{z} = \begin{bmatrix} 0 \\ 0 \end{bmatrix}$$

$$\lambda_1 = 0 \Longrightarrow \begin{bmatrix} 1 & 1 \\ 1 & 1 \end{bmatrix} \mathbf{z}_1 = \begin{bmatrix} 1 & 1 \\ 1 & 1 \end{bmatrix} \begin{bmatrix} z_{11} \\ z_{21} \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \end{bmatrix} \qquad z_{21} = -z_{11} \qquad \mathbf{z}_1 = \begin{bmatrix} 1 \\ -1 \end{bmatrix}$$

$$\lambda_2 = 2 \Longrightarrow \begin{bmatrix} -1 & 1 \\ 1 & -1 \end{bmatrix} \mathbf{z}_1 = \begin{bmatrix} -1 & 1 \\ 1 & -1 \end{bmatrix} \begin{bmatrix} z_{12} \\ z_{22} \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \end{bmatrix} \qquad z_{22} = z_{12} \qquad \mathbf{z}_2 = \begin{bmatrix} 1 \\ 1 \end{bmatrix}$$

Diagonal Form: $\mathbf{A}' = [\mathbf{B}^{-1}\mathbf{A}\mathbf{B}] = \begin{bmatrix} 1/2 & -1/2 \\ 1/2 & 1/2 \end{bmatrix} \begin{bmatrix} 1 & 1 \\ 1 & 1 \end{bmatrix} \begin{bmatrix} 1 & 1 \\ -1 & 1 \end{bmatrix} = \begin{bmatrix} 0 & 0 \\ 0 & 2 \end{bmatrix}$

Part II
Response Surfaces

Taylor Series Expansion

$$F(x) = F(x^*) + \frac{d}{dx}F(x)\Big|_{x = x^*}(x - x^*)$$

$$+ \frac{1}{2}\frac{d^2}{dx^2}F(x)\Bigg|_{x = x^*}(x - x^*)^2 + \cdots$$

$$+ \frac{1}{n!}\frac{d^n}{dx^n}F(x)\Bigg|_{x = x^*}(x - x^*)^n + \cdots$$

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Example

$$F(x) = e^{-x}$$

Taylor series of $F(x)$ about $x^* = 0$:

$$F(x) = e^{-x} = e^{-0} - e^{-0}(x-0) + \frac{1}{2}e^{-0}(x-0)^2 - \frac{1}{6}e^{-0}(x-0)^3 + \dots$$

$$F(x) = 1 - x + \frac{1}{2}x^2 - \frac{1}{6}x^3 + \dots$$

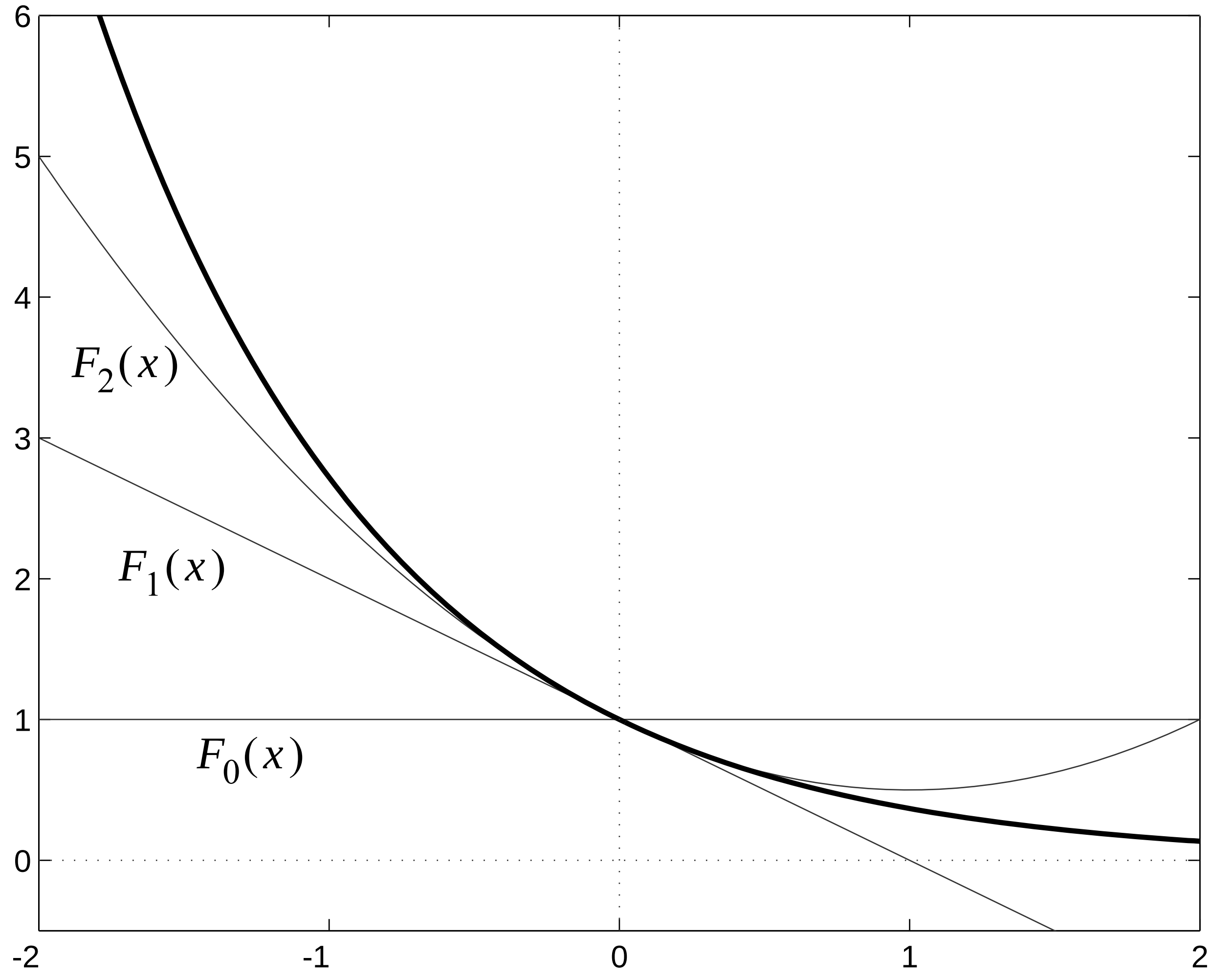
Taylor series approximations:

$$F(x) \approx F_0(x) = 1$$

$$F(x) \approx F_1(x) = 1 - x$$

$$F(x) \approx F_2(x) = 1 - x + \frac{1}{2}x^2$$

Plot of Approximations



Vector Case

$$F(\mathbf{x}) = F(x_1, x_2, \dots, x_n)$$

$$F(\mathbf{x}) = F(\mathbf{x}^*) + \frac{\partial}{\partial x_1} F(\mathbf{x})\Big|_{\mathbf{x} = \mathbf{x}^*} (x_1 - x_1^*) + \frac{\partial}{\partial x_2} F(\mathbf{x})\Big|_{\mathbf{x} = \mathbf{x}^*} (x_2 - x_2^*)$$

$$+ \dots + \frac{\partial}{\partial x_n} F(\mathbf{x})\Big|_{\mathbf{x} = \mathbf{x}^*} (x_n - x_n^*) + \frac{1}{2} \frac{\partial^2}{\partial x_1^2} F(\mathbf{x})\Big|_{\mathbf{x} = \mathbf{x}^*} (x_1 - x_1^*)^2$$

$$+ \frac{1}{2} \frac{\partial^2}{\partial x_1 \partial x_2} F(\mathbf{x})\Big|_{\mathbf{x} = \mathbf{x}^*} (x_1 - x_1^*)(x_2 - x_2^*) + \dots$$

Matrix Form

$$F(\mathbf{x}) = F(\mathbf{x}^*) + \nabla F(\mathbf{x})^T\Big|_{\mathbf{x}=\mathbf{x}^*}(\mathbf{x}-\mathbf{x}^*)$$

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

Gradient

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

Hessian

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

Directional Derivatives

First derivative (slope) of $F(\mathbf{x})$ along x_i axis: $\partial F(\mathbf{x}) / \partial x_i$

(ith element of gradient)

Second derivative (curvature) of $F(\mathbf{x})$ along x_i axis: $\partial^2 F(\mathbf{x}) / \partial x_i^2$

(i,i element of Hessian)

First derivative (slope) of $F(\mathbf{x})$ along vector $\mathbf{p}$: $$\frac{\mathbf{p}^T \nabla F(\mathbf{x})}{\|\mathbf{p}\|}$$

Second derivative (curvature) of $F(\mathbf{x})$ along vector $\mathbf{p}$: $$\frac{\mathbf{p}^T \nabla^2 F(\mathbf{x}) \mathbf{p}}{\|\mathbf{p}\|^2}$$

Example

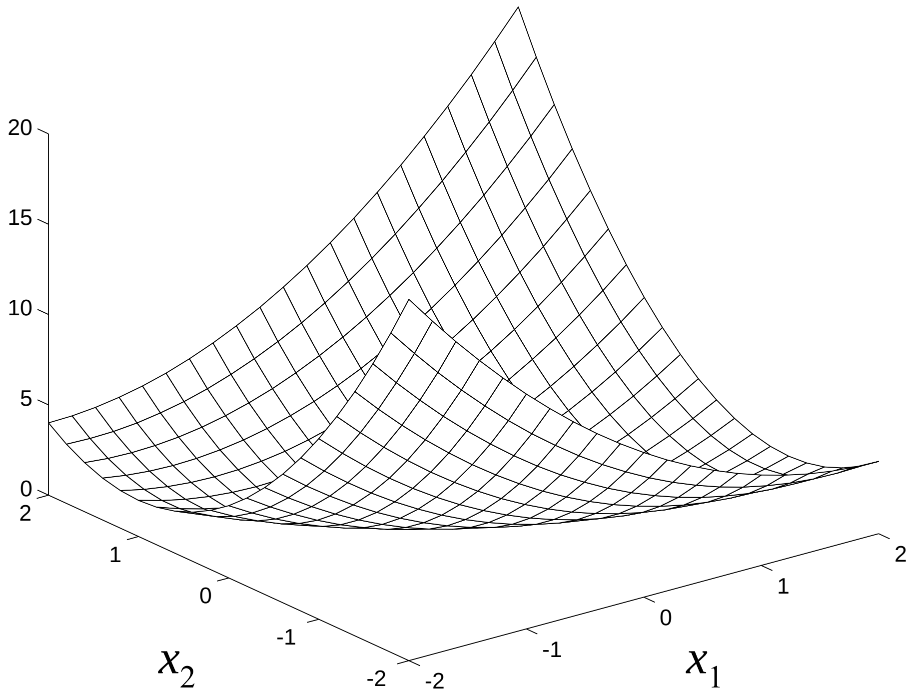
$$F(\mathbf{x}) = x_1^2 + 2x_1x_2 + 2x_2^2$$

$$\mathbf{x}^* = \begin{bmatrix} 0.5 \\ 0 \end{bmatrix} \qquad \mathbf{p} = \begin{bmatrix} 1 \\ -1 \end{bmatrix}$$

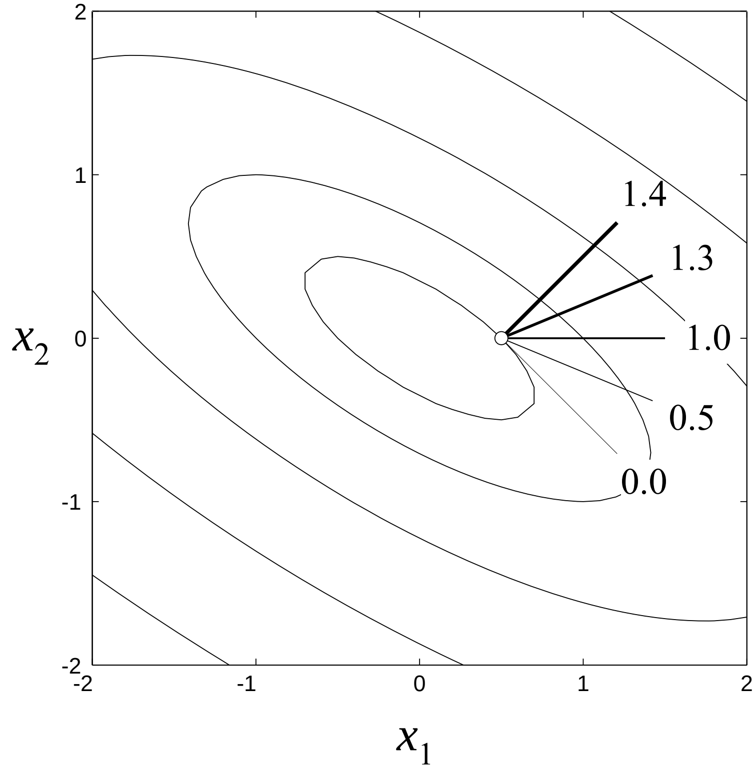
$$\nabla F(\mathbf{x})\Big|_{\mathbf{x}=\mathbf{x}^*} = \left.\begin{bmatrix} \frac{\partial}{\partial x_1}F(\mathbf{x}) \\ \frac{\partial}{\partial x_2}F(\mathbf{x}) \end{bmatrix}\right|_{\mathbf{x}=\mathbf{x}^*} = \left.\begin{bmatrix} 2x_1 + 2x_2 \\ 2x_1 + 4x_2 \end{bmatrix}\right|_{\mathbf{x}=\mathbf{x}^*} = \begin{bmatrix} 1 \\ 1 \end{bmatrix}$$

$$\frac{\mathbf{p}^T \nabla F(\mathbf{x})}{\|\mathbf{p}\|} = \frac{\begin{bmatrix} 1 & -1 \end{bmatrix}\begin{bmatrix} 1 \\ 1 \end{bmatrix}}{\left\|\begin{bmatrix} 1 \\ -1 \end{bmatrix}\right\|} = \frac{\begin{bmatrix} 0 \end{bmatrix}}{\sqrt{2}} = 0$$

Plots



Directional Derivatives



Minima

Strong Minimum

The point $\mathbf{x}^*$ is a strong minimum of $F(\mathbf{x})$ if a scalar $\delta > 0$ exists, such that $F(\mathbf{x}^*) < F(\mathbf{x}^* + \Delta\mathbf{x})$ for all $\Delta\mathbf{x}$ such that $\delta > \|\Delta\mathbf{x}\| > 0$.

Global Minimum

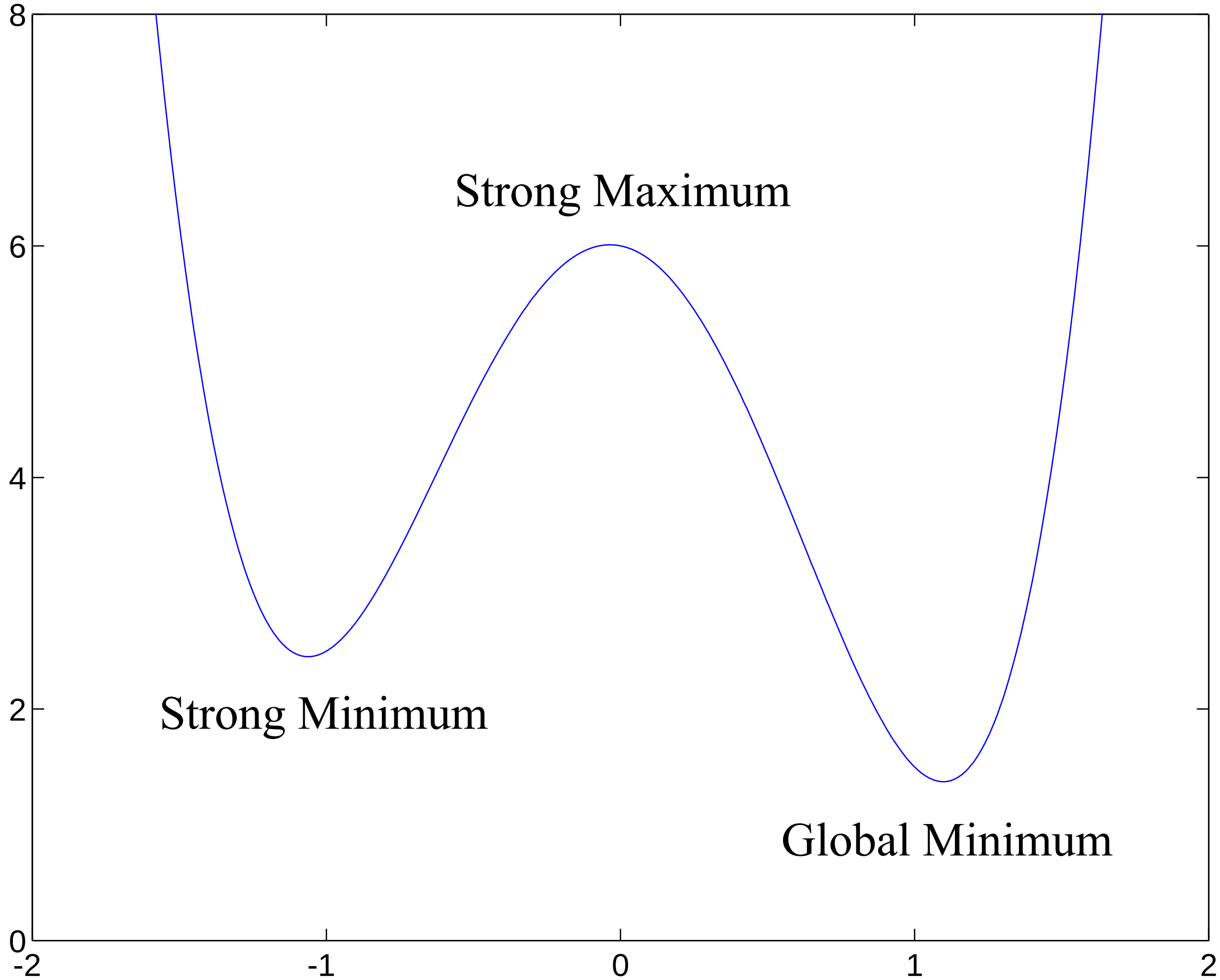
The point $\mathbf{x}^*$ is a unique global minimum of $F(\mathbf{x})$ if $F(\mathbf{x}^*) < F(\mathbf{x}^* + \Delta\mathbf{x})$ for all $\Delta\mathbf{x} \neq 0$.

Weak Minimum

The point $\mathbf{x}^*$ is a weak minimum of $F(\mathbf{x})$ if it is not a strong minimum, and a scalar $\delta > 0$ exists, such that $F(\mathbf{x}^*) \le F(\mathbf{x}^* + \Delta\mathbf{x})$ for all $\Delta\mathbf{x}$ such that $\delta > \|\Delta\mathbf{x}\| > 0$.

Scalar Example

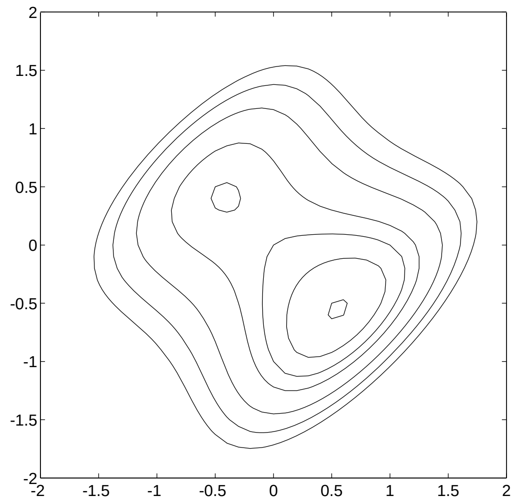
$$F(x) = 3x^4 - 7x^2 - \frac{1}{2}x + 6$$

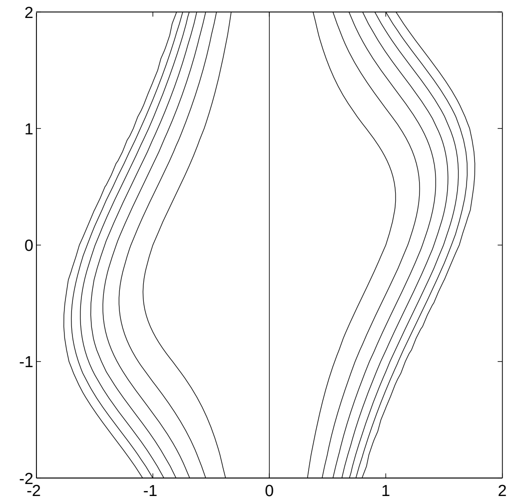


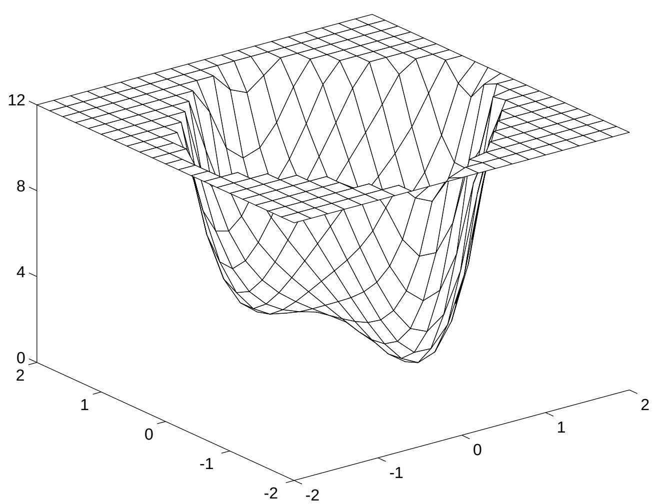
Vector Example

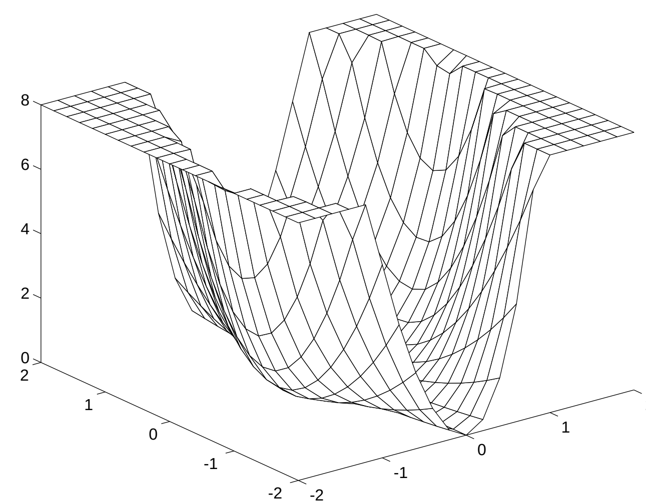
$$F(\mathbf{x}) = (x_2 - x_1)^4 + 8x_1x_2 - x_1 + x_2 + 3$$

$$F(\mathbf{x}) = (x_1^2 - 1.5x_1x_2 + 2x_2^2)x_1^2$$









First-Order Optimality Condition

$$F(\mathbf{x}) = F(\mathbf{x}^* + \Delta\mathbf{x}) = F(\mathbf{x}^*) + \nabla F(\mathbf{x})^T\Big|_{\mathbf{x}=\mathbf{x}^*}\Delta\mathbf{x} + \frac{1}{2}\Delta\mathbf{x}^T\nabla^2 F(\mathbf{x})\Big|_{\mathbf{x}=\mathbf{x}^*}\Delta\mathbf{x} + \cdots$$

$$\Delta\mathbf{x} = \mathbf{x} - \mathbf{x}^*$$

For small $\Delta\mathbf{x}$:

$$F(\mathbf{x}^* + \Delta\mathbf{x}) \cong F(\mathbf{x}^*) + \nabla F(\mathbf{x})^T\Big|_{\mathbf{x}=\mathbf{x}^*}\Delta\mathbf{x}$$

If $\mathbf{x}^*$ is a minimum, this implies:

$$\nabla F(\mathbf{x})^T\Big|_{\mathbf{x}=\mathbf{x}^*}\Delta\mathbf{x} \geq 0$$

If $\nabla F(\mathbf{x})^T\Big|_{\mathbf{x}=\mathbf{x}^*}\Delta\mathbf{x} > 0$ then $F(\mathbf{x}^* - \Delta\mathbf{x}) \cong F(\mathbf{x}^*) - \nabla F(\mathbf{x})^T\Big|_{\mathbf{x}=\mathbf{x}^*}\Delta\mathbf{x} < F(\mathbf{x}^*)$

But this would imply that $\mathbf{x}^*$ is not a minimum. Therefore $\nabla F(\mathbf{x})^T\Big|_{\mathbf{x}=\mathbf{x}^*}\Delta\mathbf{x} = 0$

Since this must be true for every $\Delta\mathbf{x}$, $\boxed{\nabla F(\mathbf{x})\Big|_{\mathbf{x}=\mathbf{x}^*} = \mathbf{0}}$

Second-Order Condition

If the first-order condition is satisfied (zero gradient), then

$$F(\mathbf{x}^* + \Delta\mathbf{x}) = F(\mathbf{x}^*) + \frac{1}{2}\Delta\mathbf{x}^T \nabla^2 F(\mathbf{x})\Big|_{\mathbf{x} = \mathbf{x}^*} \Delta\mathbf{x} + \cdots$$

A strong minimum will exist at $\mathbf{x}^*$ if $\Delta\mathbf{x}^T \nabla^2 F(\mathbf{x})\Big|_{\mathbf{x} = \mathbf{x}^*} \Delta\mathbf{x} > 0$ for any $\Delta\mathbf{x} \neq \mathbf{0}$.

Therefore the Hessian matrix must be positive definite. A matrix **A** is positive definite if:

$$\boxed{\mathbf{z}^T \mathbf{A}\mathbf{z} > 0} \qquad \text{for any } \mathbf{z} \neq 0.$$

This is a **sufficient** condition for optimality.

A **necessary** condition is that the Hessian matrix be positive semidefinite. A matrix A is positive semidefinite if:

$$\boxed{\mathbf{z}^T \mathbf{A}\mathbf{z} \geq 0} \qquad \text{for any } \mathbf{z}.$$

Example

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

$$\nabla F(\mathbf{x}) = \begin{bmatrix} 2x_1 + 2x_2 + 1 \\ 2x_1 + 4x_2 \end{bmatrix} = \mathbf{0} \quad \Rightarrow \quad \mathbf{x}^* = \begin{bmatrix} -1 \\ 0.5 \end{bmatrix}$$

$$\nabla^2 F(\mathbf{x}) = \begin{bmatrix} 2 & 2 \\ 2 & 4 \end{bmatrix}$$

(Not a function of $\mathbf{x}$ in this case.)

To test the definiteness, check the eigenvalues of the Hessian. If the eigenvalues are all greater than zero, the Hessian is positive definite.

$$\left|\nabla^2 F(\mathbf{x}) - \lambda \mathbf{I}\right| = \left|\begin{bmatrix} 2-\lambda & 2 \\ 2 & 4-\lambda \end{bmatrix}\right| = \lambda^2 - 6\lambda + 4 = (\lambda - 0.76)(\lambda - 5.24)$$

$\lambda = 0.76, 5.24$ Both eigenvalues are positive, therefore <u>strong minimum</u>.

Quadratic Functions

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

Gradient and Hessian:

Useful properties of gradients:

$$\nabla(\mathbf{h}^T\mathbf{x}) = \nabla(\mathbf{x}^T\mathbf{h}) = \mathbf{h}$$

$$\nabla\mathbf{x}^T\mathbf{Q}\mathbf{x} = \mathbf{Q}\mathbf{x} + \mathbf{Q}^T\mathbf{x} = 2\mathbf{Q}\mathbf{x} \quad \text{(for symmetric } \mathbf{Q}\text{)}$$

Gradient of Quadratic Function:

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

Hessian of Quadratic Function:

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

Eigensystem of the Hessian

Consider a quadratic function which has a stationary point at the origin, and whose value there is zero.

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

Perform a similarity transform on the Hessian matrix, using the eigenvalues as the new basis vectors.

$$\mathbf{B} = \begin{bmatrix} \mathbf{z}_1 & \mathbf{z}_2 & \dots & \mathbf{z}_n \end{bmatrix}$$

Since the Hessian matrix is symmetric, its eigenvectors are orthogonal.

$$\mathbf{B}^{-1} = \mathbf{B}^T$$

$$\mathbf{A}' = [\mathbf{B}^T\mathbf{A}\mathbf{B}] = \begin{bmatrix} \lambda_1 & 0 & \dots & 0 \\ 0 & \lambda_2 & \dots & 0 \\ \vdots & \vdots & & \vdots \\ 0 & 0 & \dots & \lambda_n \end{bmatrix} = \Lambda$$

$$\mathbf{A} = \mathbf{B}\Lambda\mathbf{B}^T$$

Second Directional Derivative

$$\frac{\mathbf{p}^T \nabla^2 F(\mathbf{x})\mathbf{p}}{\|\mathbf{p}\|^2} = \frac{\mathbf{p}^T \mathbf{A}\mathbf{p}}{\|\mathbf{p}\|^2}$$

Represent **p** with respect to the eigenvectors (new basis):

$$\mathbf{p} = \mathbf{B}\mathbf{c}$$

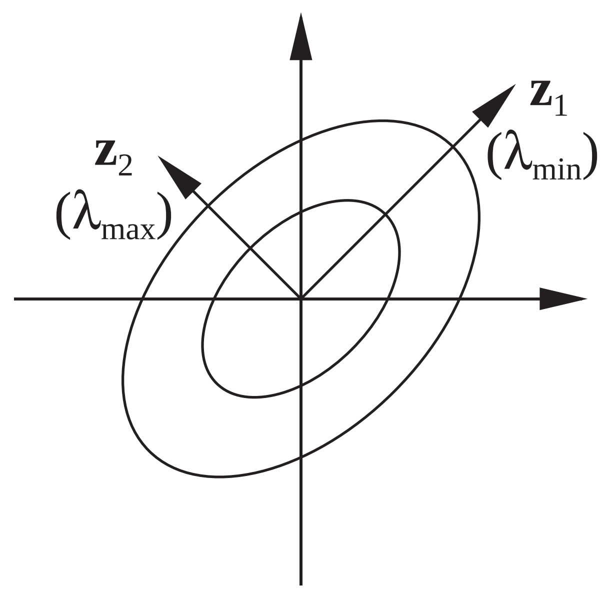
$$\frac{\mathbf{p}^T \mathbf{A}\mathbf{p}}{\|\mathbf{p}\|^2} = \frac{\mathbf{c}^T \mathbf{B}^T (\mathbf{B}\Lambda\mathbf{B}^T)\mathbf{B}\mathbf{c}}{\mathbf{c}^T \mathbf{B}^T \mathbf{B}\mathbf{c}} = \frac{\mathbf{c}^T \Lambda \mathbf{c}}{\mathbf{c}^T \mathbf{c}} = \frac{\sum_{i=1}^{n} \lambda_i c_i^2}{\sum_{i=1}^{n} c_i^2}$$

$$\lambda_{min} \le \frac{\mathbf{p}^T \mathbf{A}\mathbf{p}}{\|\mathbf{p}\|^2} \le \lambda_{max}$$

Eigenvector (Largest Eigenvalue)

$$\mathbf{p} = \mathbf{z}_{max} \qquad \mathbf{c} = \mathbf{B}^T\mathbf{p} = \mathbf{B}^T\mathbf{z}_{max} = \begin{bmatrix} 0 \\ 0 \\ \vdots \\ 0 \\ 1 \\ 0 \\ \vdots \\ 0 \end{bmatrix}$$

$$\frac{\mathbf{z}_{max}^T \mathbf{A} \mathbf{z}_{max}}{\|\mathbf{z}_{max}\|^2} = \frac{\sum_{i=1}^{n} \lambda_i c_i^2}{\sum_{i=1}^{n} c_i^2} = \lambda_{max}$$



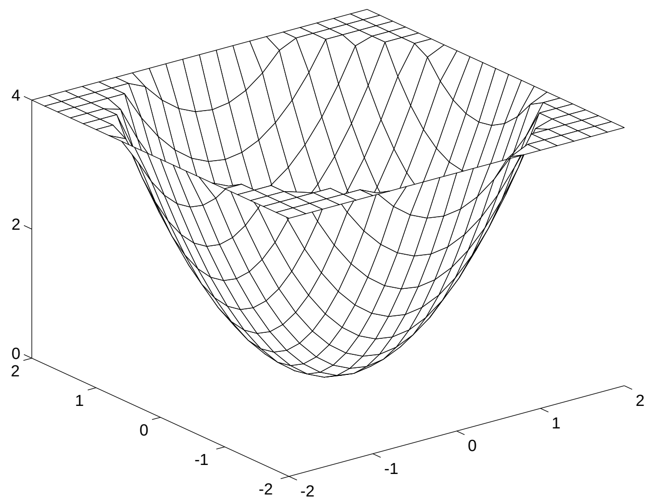
The eigenvalues represent curvature (second derivatives) along the eigenvectors (the principal axes).

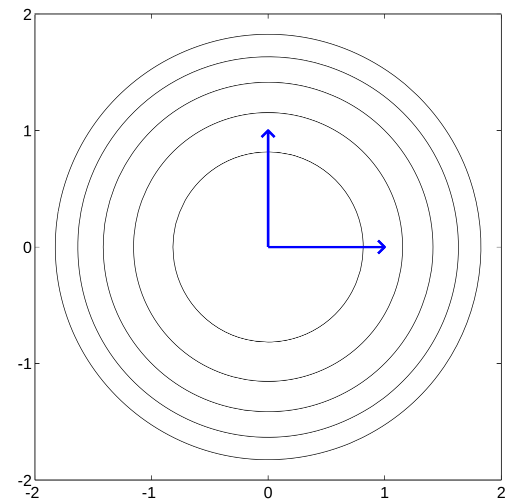
Circular Hollow

$$F(\mathbf{x}) = x_1^2 + x_2^2 = \frac{1}{2}\mathbf{x}^T \begin{bmatrix} 2 & 0 \\ 0 & 2 \end{bmatrix} \mathbf{x}$$

$$\nabla^2 F(\mathbf{x}) = \begin{bmatrix} 2 & 0 \\ 0 & 2 \end{bmatrix} \qquad \lambda_1 = 2 \qquad \mathbf{z}_1 = \begin{bmatrix} 1 \\ 0 \end{bmatrix} \qquad \lambda_2 = 2 \qquad \mathbf{z}_2 = \begin{bmatrix} 0 \\ 1 \end{bmatrix}$$

(Any two independent vectors in the plane would work.)

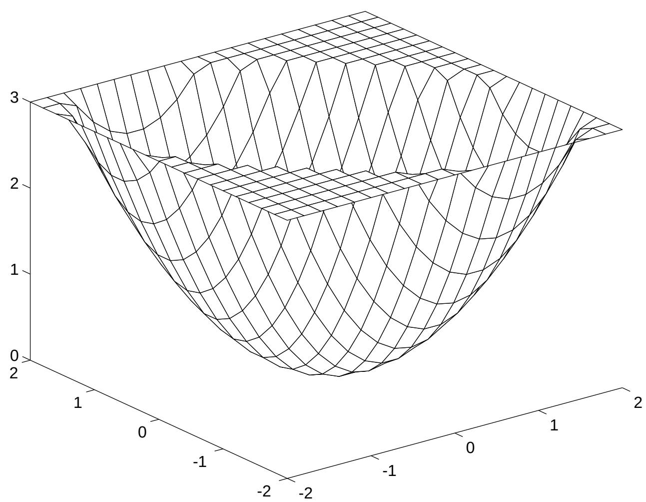


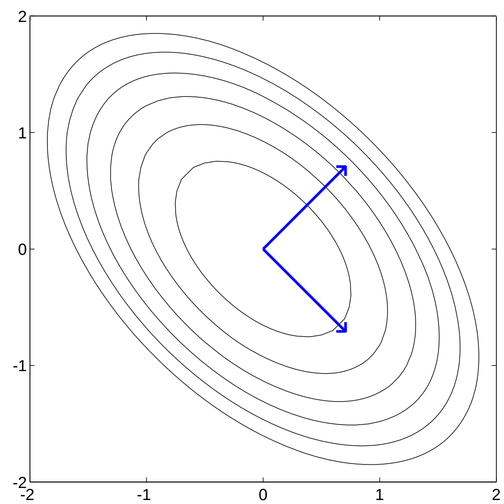


Elliptical Hollow

$$F(\mathbf{x}) = x_1^2 + x_1 x_2 + x_2^2 = \frac{1}{2}\mathbf{x}^T \begin{bmatrix} 2 & 1 \\ 1 & 2 \end{bmatrix} \mathbf{x}$$

$$\nabla^2 F(\mathbf{x}) = \begin{bmatrix} 2 & 1 \\ 1 & 2 \end{bmatrix} \qquad \lambda_1 = 1 \qquad \mathbf{z}_1 = \begin{bmatrix} 1 \\ -1 \end{bmatrix} \qquad \lambda_2 = 3 \qquad \mathbf{z}_2 = \begin{bmatrix} 1 \\ 1 \end{bmatrix}$$

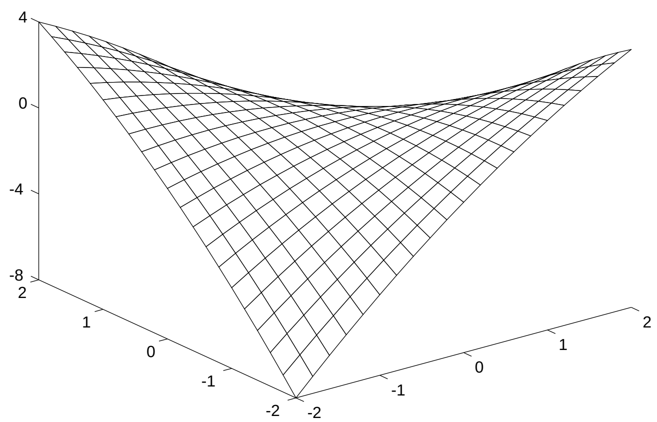


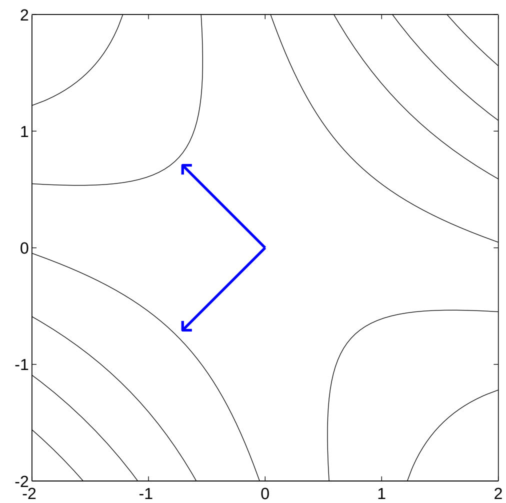


Elongated Saddle

$$F(\mathbf{x}) = -\frac{1}{4}x_1^2 - \frac{3}{2}x_1x_2 - \frac{1}{4}x_2^2 = \frac{1}{2}\mathbf{x}^T\begin{bmatrix}-0.5 & -1.5\\ -1.5 & -0.5\end{bmatrix}\mathbf{x}$$

$$\nabla^2 F(\mathbf{x}) = \begin{bmatrix}-0.5 & -1.5\\ -1.5 & -0.5\end{bmatrix} \qquad \lambda_1 = 1 \qquad \mathbf{z}_1 = \begin{bmatrix}-1\\ 1\end{bmatrix} \qquad \lambda_2 = -2 \qquad \mathbf{z}_2 = \begin{bmatrix}-1\\ -1\end{bmatrix}$$

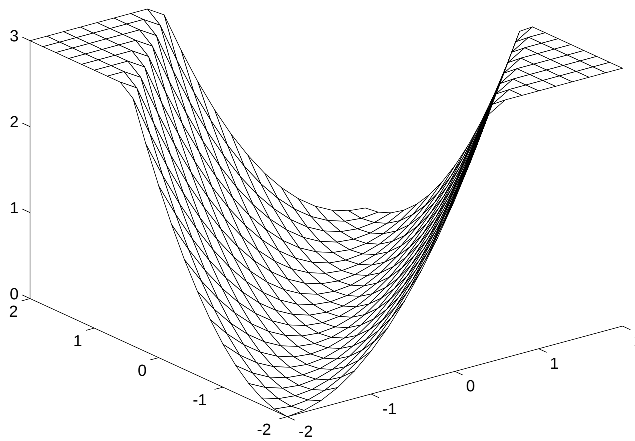


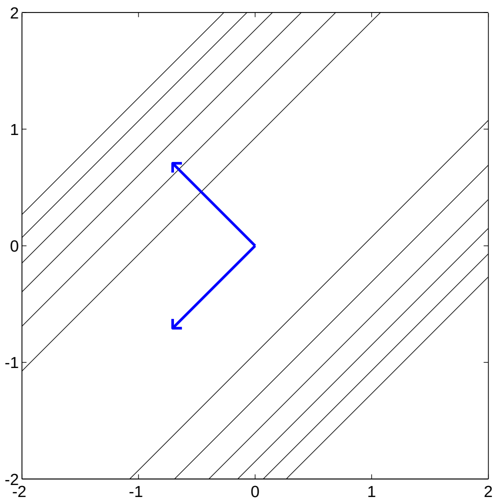


Stationary Valley

$$F(\mathbf{x}) = \frac{1}{2}x_1^2 - x_1x_2 + \frac{1}{2}x_2^2 = \frac{1}{2}\mathbf{x}^T\begin{bmatrix}1 & -1\\ -1 & 1\end{bmatrix}\mathbf{x}$$

$$\nabla^2 F(\mathbf{x}) = \begin{bmatrix}1 & -1\\ -1 & 1\end{bmatrix} \qquad \lambda_1 = 1 \qquad \mathbf{z}_1 = \begin{bmatrix}-1\\ 1\end{bmatrix} \qquad \lambda_2 = 0 \qquad \mathbf{z}_2 = \begin{bmatrix}-1\\ -1\end{bmatrix}$$





Quadratic Function Summary

- If the eigenvalues of the Hessian matrix are all positive, the function will have a single strong minimum.
- If the eigenvalues are all negative, the function will have a single strong maximum.
- If some eigenvalues are positive and other eigenvalues are negative, the function will have a single saddle point.
- If the eigenvalues are all nonnegative, but some eigenvalues are zero, then the function will either have a weak minimum or will have no stationary point.
- If the eigenvalues are all nonpositive, but some eigenvalues are zero, then the function will either have a weak maximum or will have no stationary point.

Stationary Point: $\mathbf{x}^* = -\mathbf{A}^{-1}\mathbf{d}$

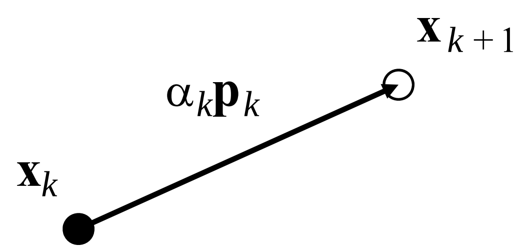
Part III
Performance Optimization

Basic Optimization Algorithm

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

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

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:

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

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

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

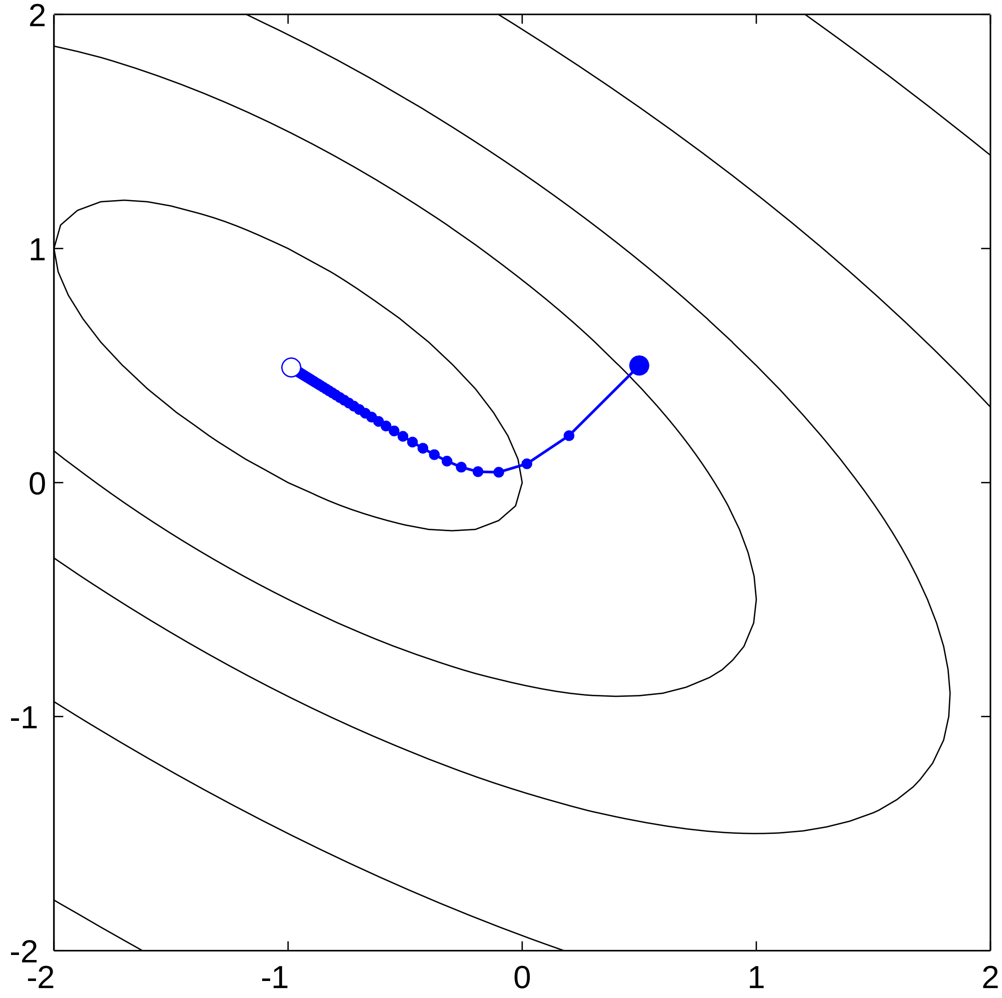
$$\mathbf{x}_0 = \begin{bmatrix} 0.5 \\ 0.5 \end{bmatrix} \qquad \alpha = 0.1$$

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

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

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

Plot



Stable Learning Rates (Quadratic)

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

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

$$\mathbf{x}_{k+1} = \mathbf{x}_k - \alpha\mathbf{g}_k = \mathbf{x}_k - \alpha(\mathbf{A}\mathbf{x}_k + \mathbf{d}) \Rightarrow \mathbf{x}_{k+1} = [\mathbf{I} - \alpha\mathbf{A}]\mathbf{x}_k - \alpha\mathbf{d}$$

Stability is determined by the eigenvalues of this matrix.

$$[\mathbf{I} - \alpha\mathbf{A}]\mathbf{z}_i = \mathbf{z}_i - \alpha\mathbf{A}\mathbf{z}_i = \mathbf{z}_i - \alpha\lambda_i\mathbf{z}_i = (1 - \alpha\lambda_i)\mathbf{z}_i$$

(λ_i - eigenvalue of **A**)

Eigenvalues of [**I** - α**A**].

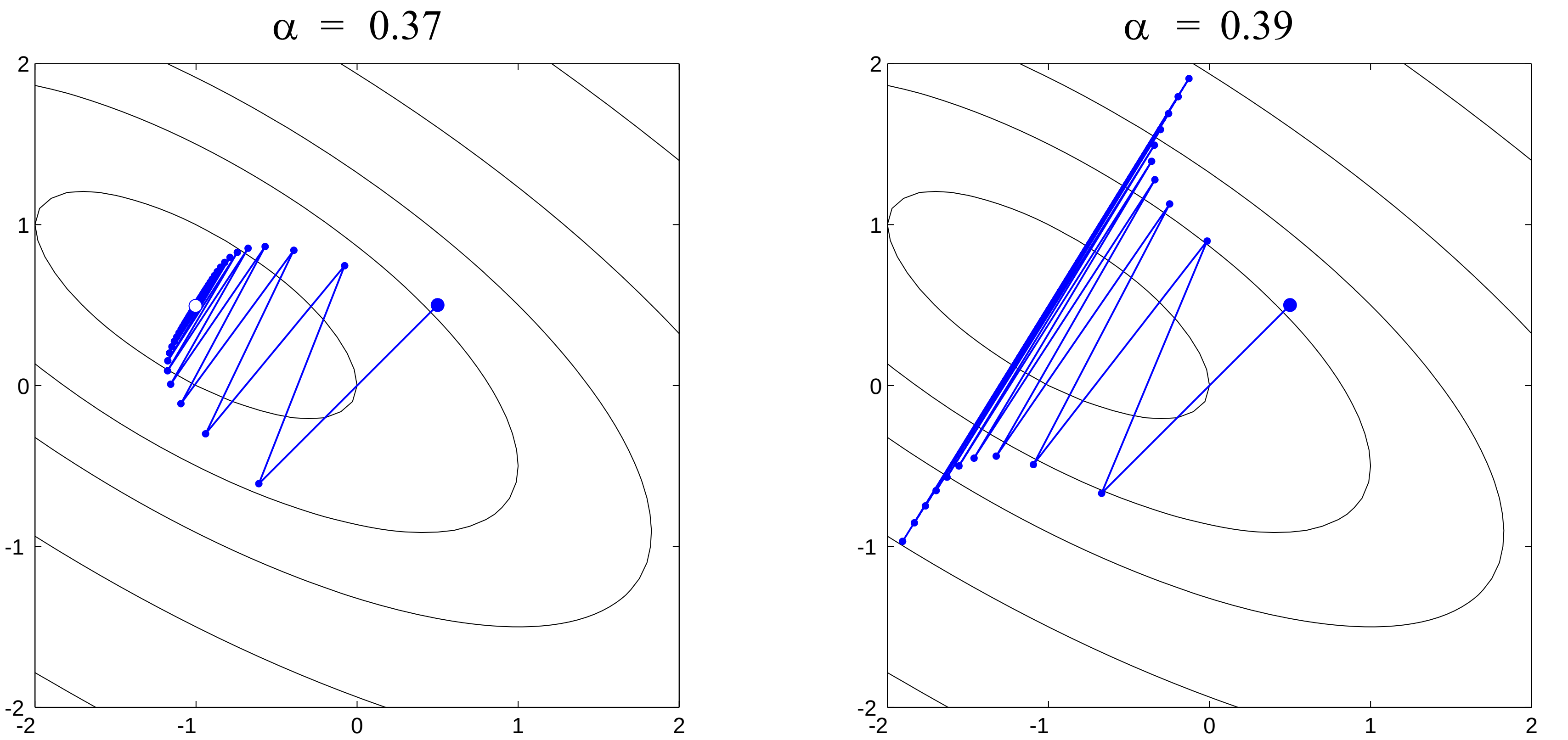
Stability Requirement:

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

Example

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

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



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

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

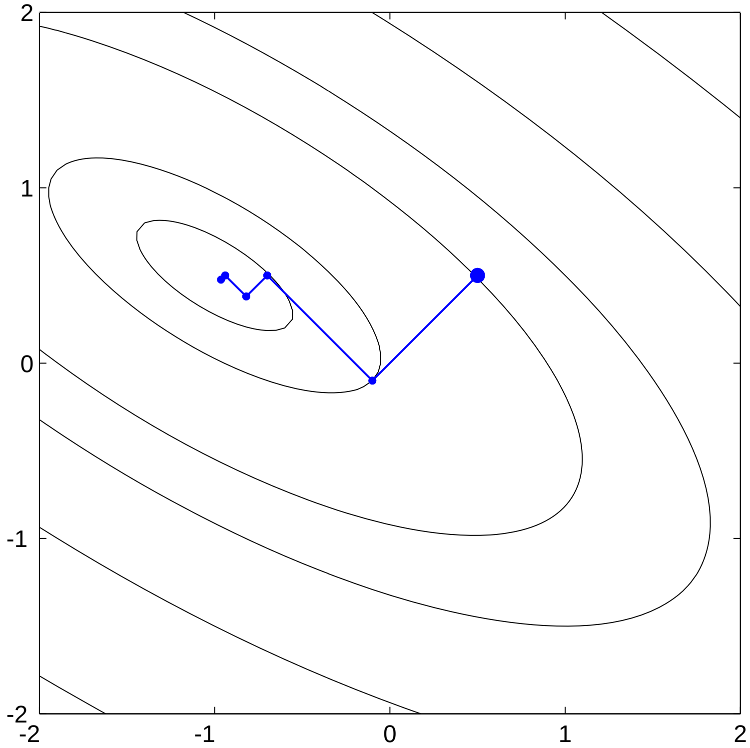
Example

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

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

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

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

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

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

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

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

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

Example

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

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

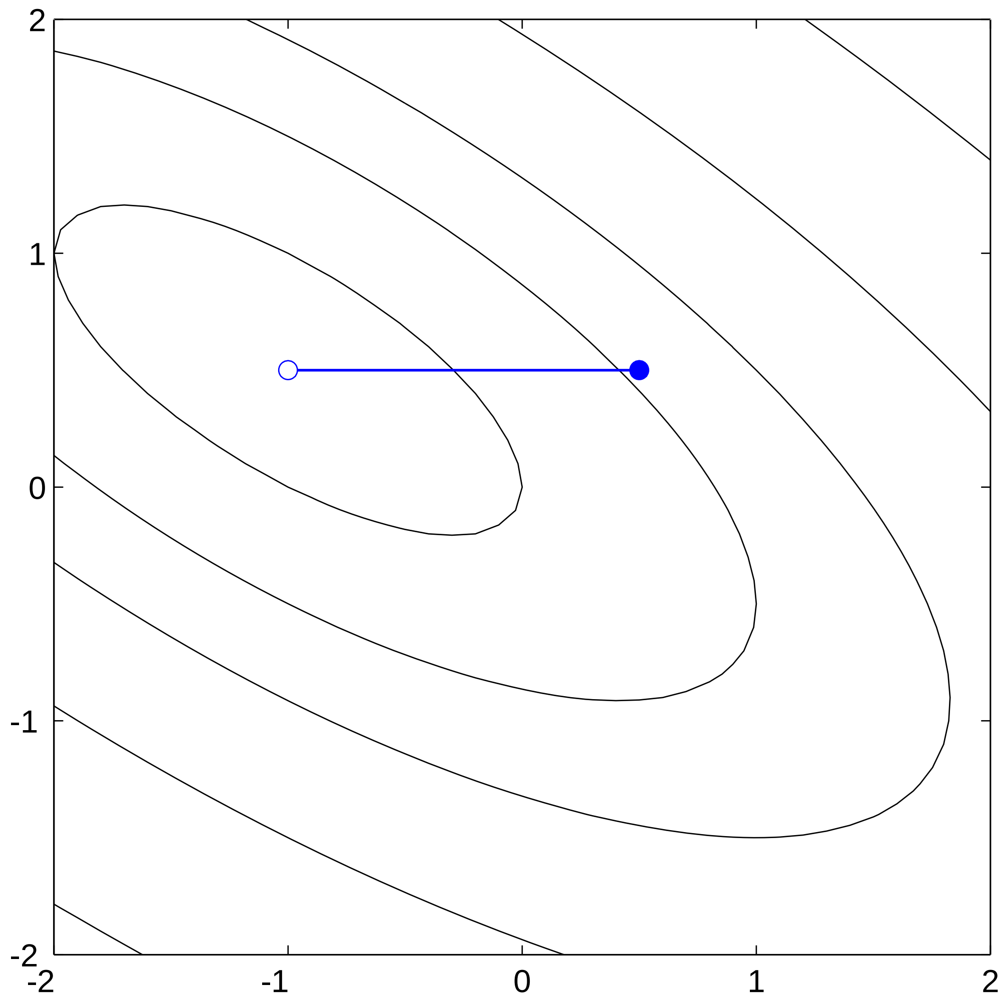
$$\nabla F(\mathbf{x}) = \begin{bmatrix} \frac{\partial}{\partial x_1}F(\mathbf{x}) \\ \frac{\partial}{\partial x_2}F(\mathbf{x}) \end{bmatrix} = \begin{bmatrix} 2x_1 + 2x_2 + 1 \\ 2x_1 + 4x_2 \end{bmatrix}$$

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

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

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

Plot

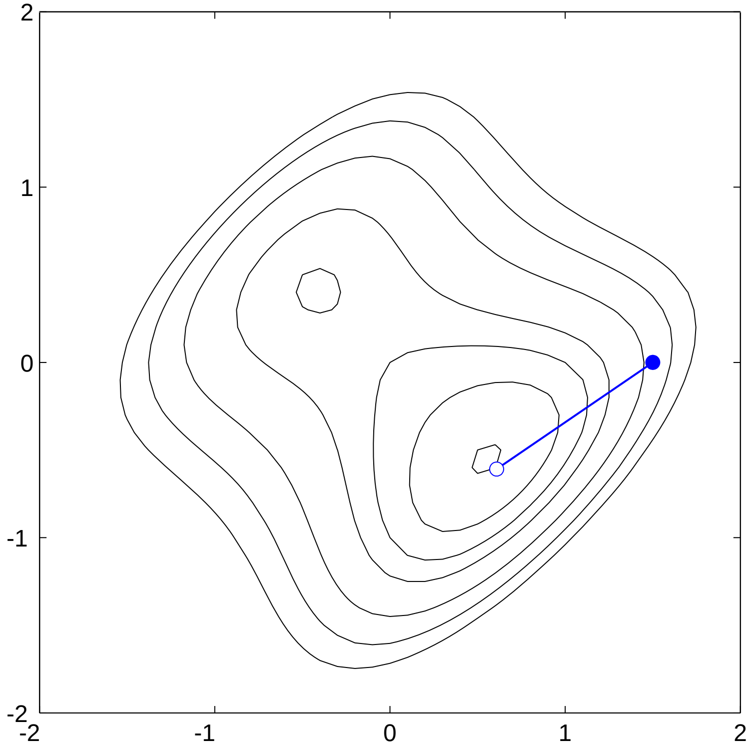


Non-Quadratic Example

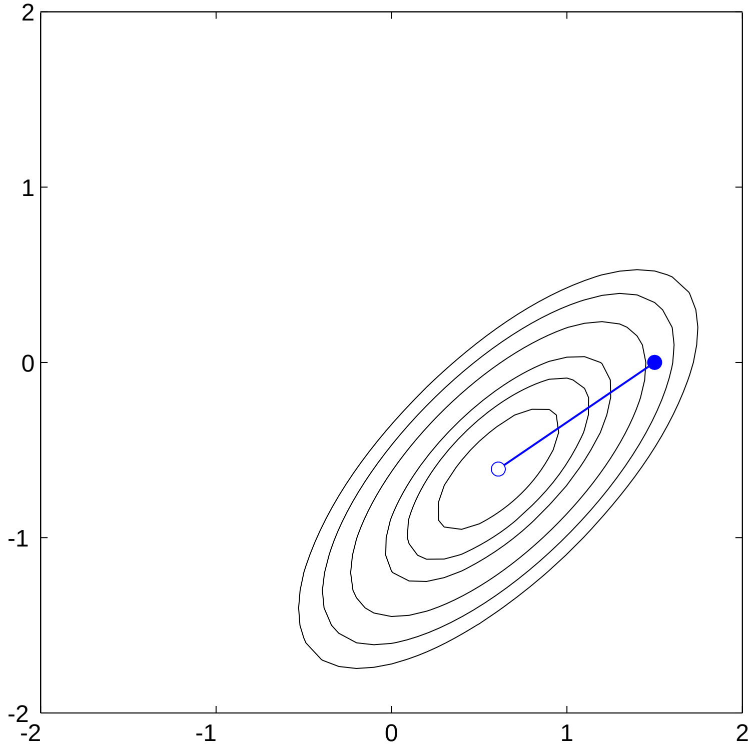
$$F(\mathbf{x}) = (x_2 - x_1)^4 + 8x_1x_2 - x_1 + x_2 + 3$$

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

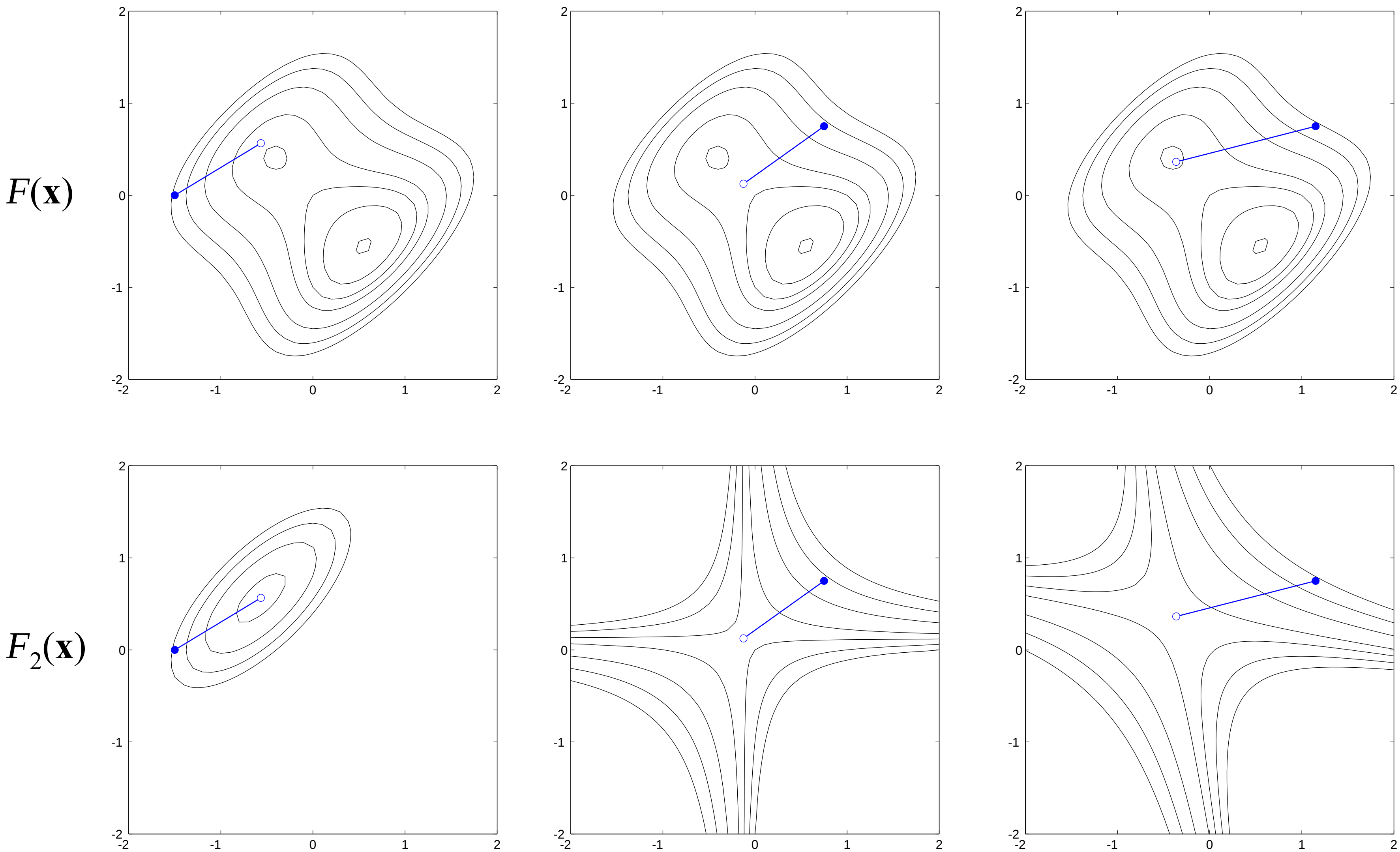
$F(\mathbf{x})$



$F_2(\mathbf{x})$



Different Initial Conditions



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.)

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.

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

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

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

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

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

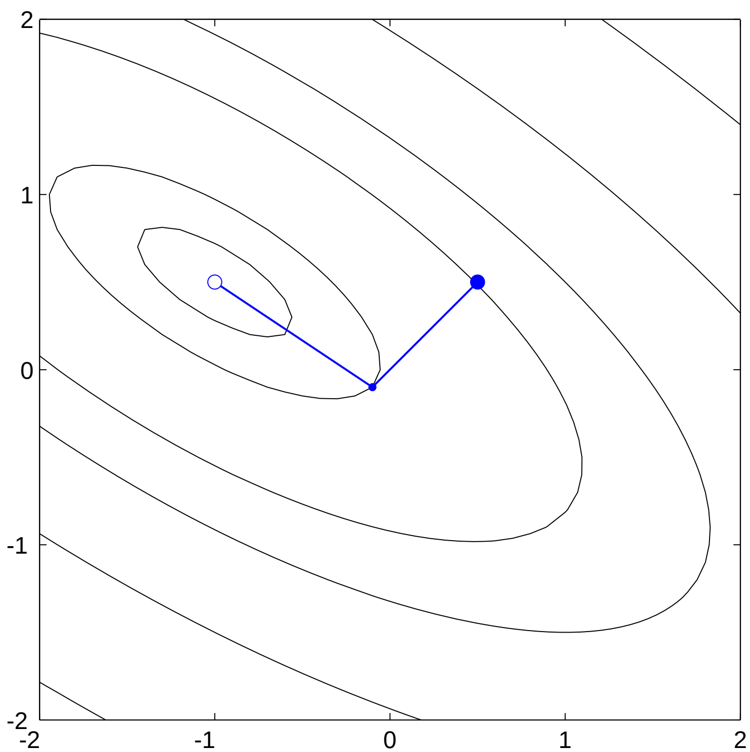
$$\mathbf{p}_1 = -\mathbf{g}_1 + \beta_1 \mathbf{p}_0 = \begin{bmatrix} -0.6 \\ 0.6 \end{bmatrix} + 0.04\begin{bmatrix} -3 \\ -3 \end{bmatrix} = \begin{bmatrix} -0.72 \\ 0.48 \end{bmatrix}$$

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

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