Performance Surfaces

Taylor Series Expansion

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

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

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

Example

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

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

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

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

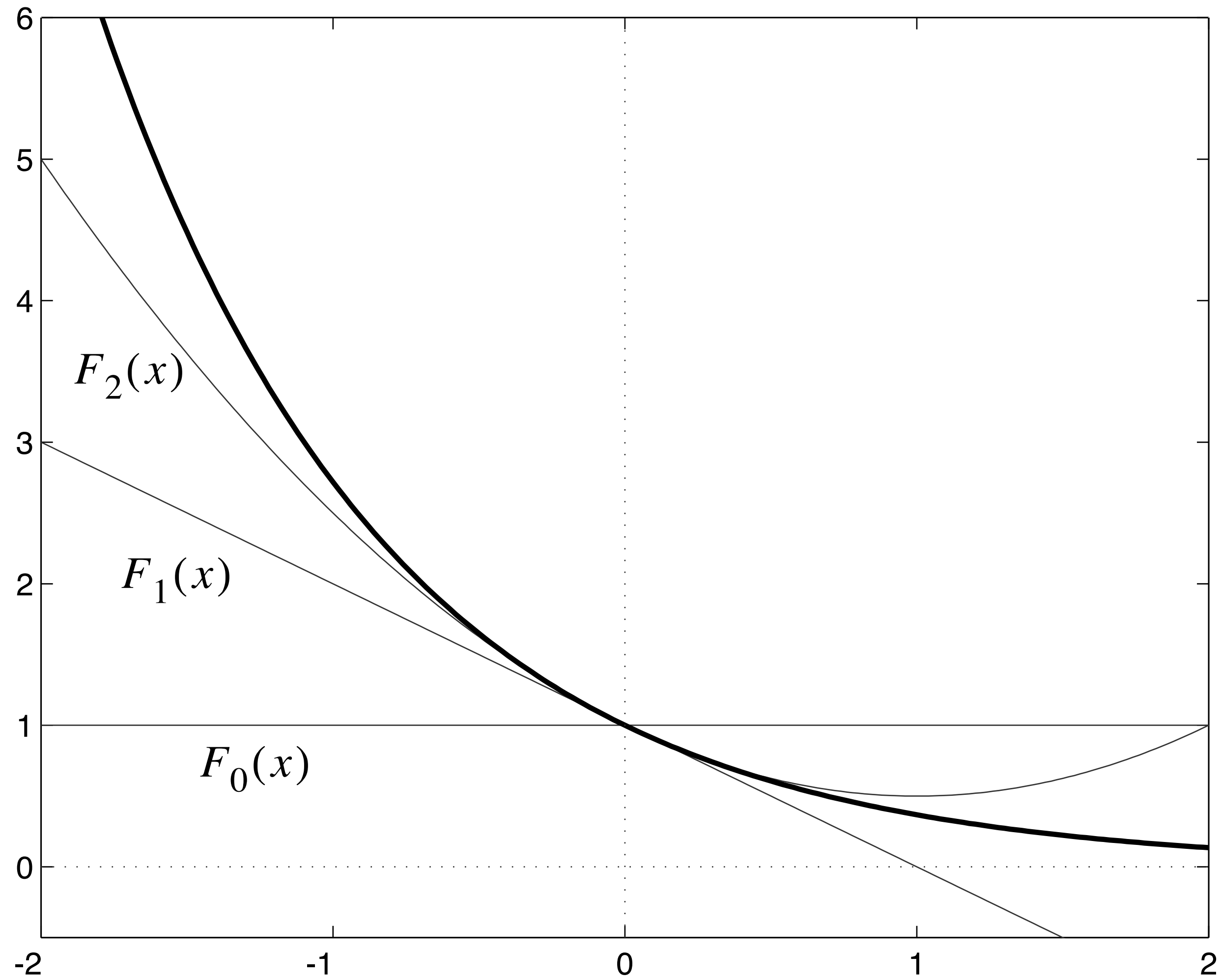
Taylor series approximations:

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

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

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

Plot of Approximations



Vector Case

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

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

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

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

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Matrix Form

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

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

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

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

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

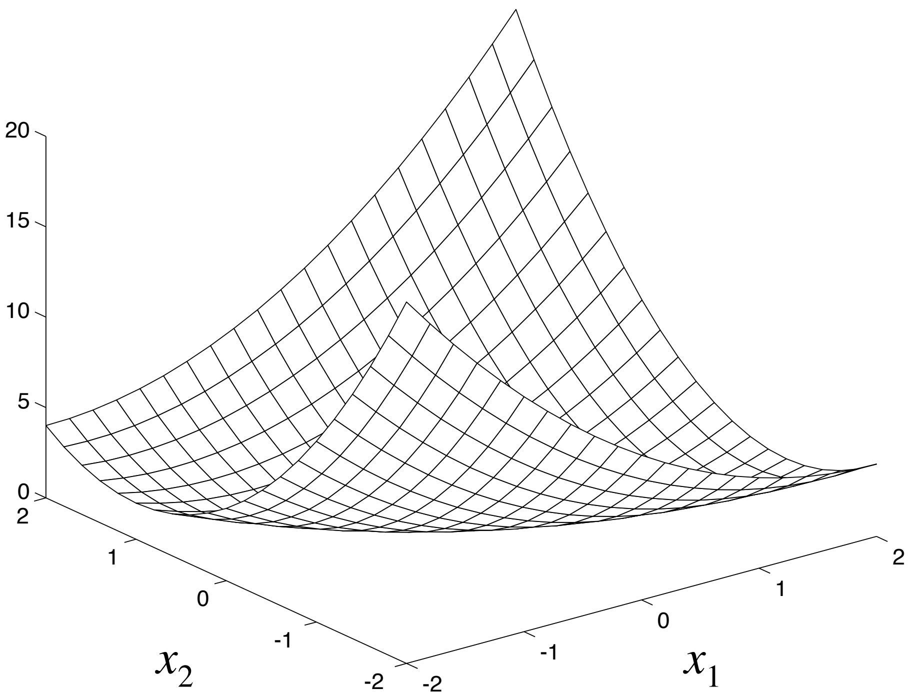
$$F(\mathbf{x}) = x_1^2 + 2x_1x_2 + 2x_2^2$$

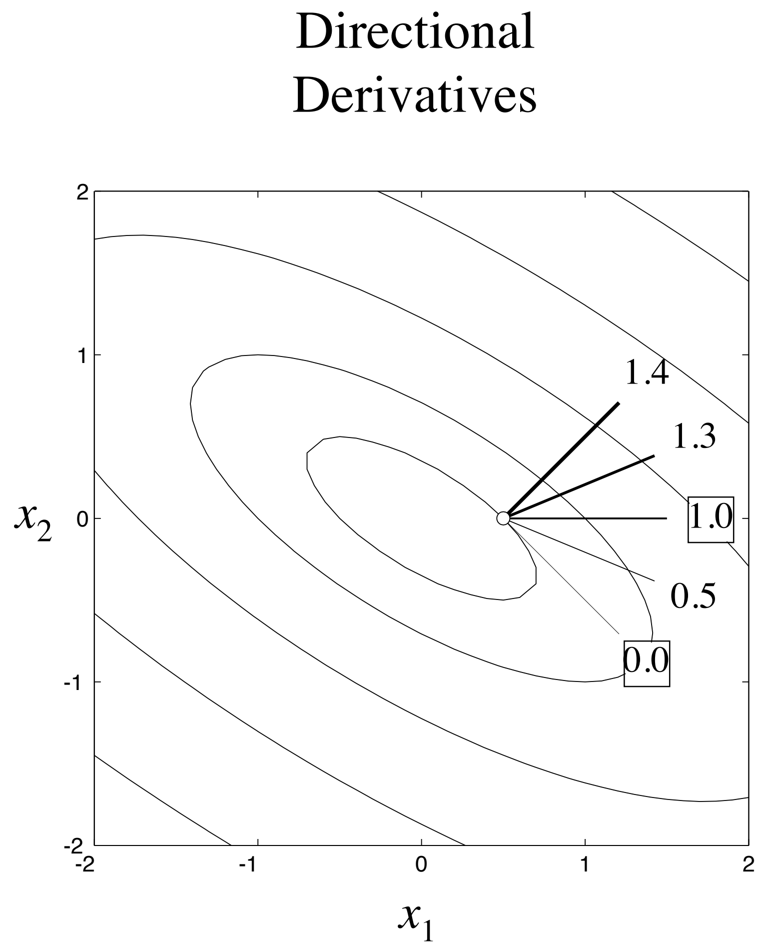
$$\mathbf{x}^* = \begin{bmatrix} 0.5 \\ 0 \end{bmatrix} \qquad \mathbf{p} = \begin{bmatrix} 1 \\ -1 \end{bmatrix}$$

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

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

8 Plots


20
15
10
5
0
2
1
0
-1
-2
-2
-1
0
1
2
x_2
x_1


Directional
Derivatives
1.4
1.3
1.0
0.5
0.0
x_2
x_1
2
1
0
-1
-2
-2
-1
0
1
2

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

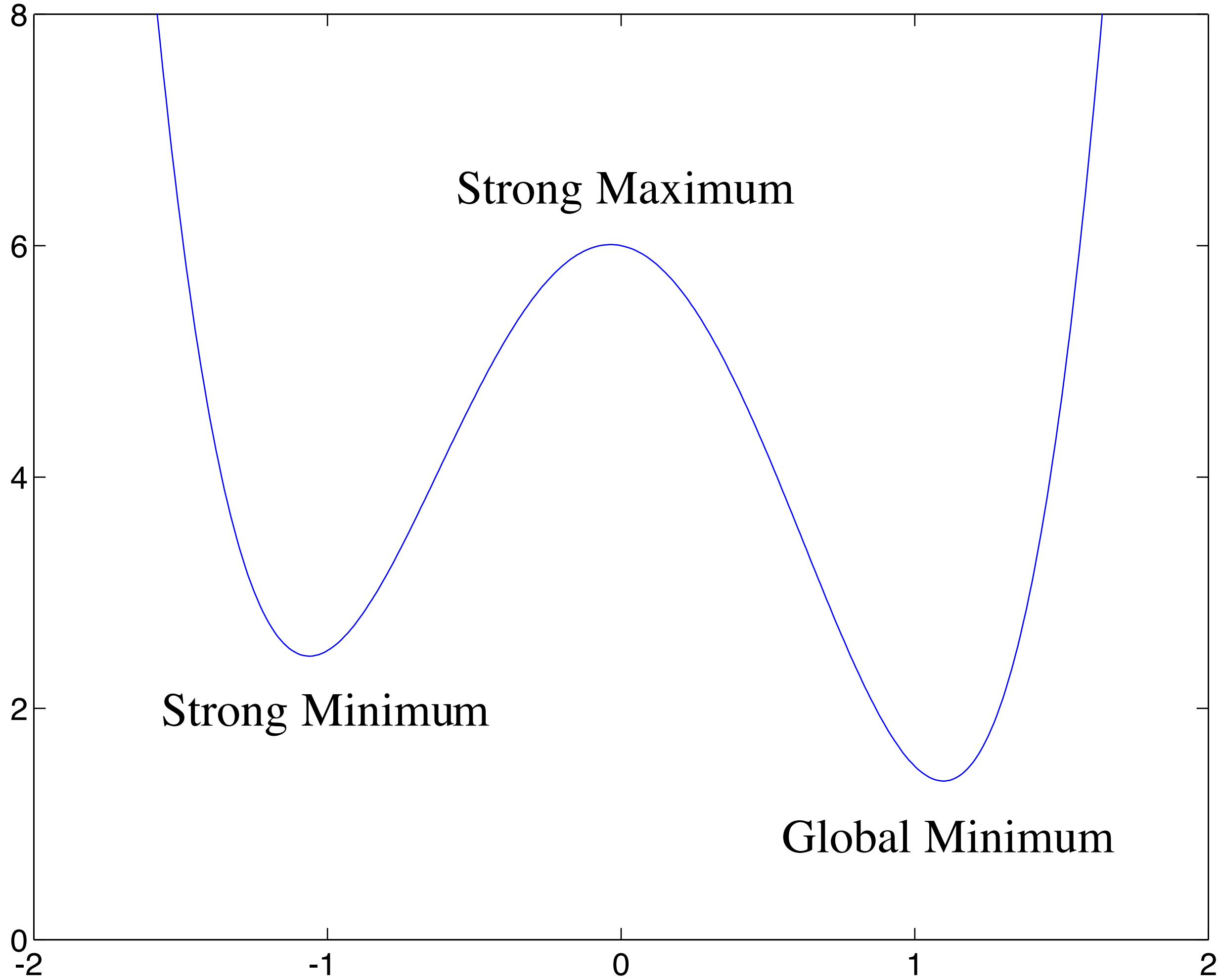
The point $\mathbf{x}^*$ is a unique global minimum of $F(\mathbf{x})$ if $F(\mathbf{x}^*) < F(\mathbf{x}^* + \Delta\mathbf{x})$ for all $\Delta\mathbf{x} \neq 0$.

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 $F(\mathbf{x}^*) \leq F(\mathbf{x}^* + \Delta\mathbf{x})$ for all $\Delta\mathbf{x}$ such that $\delta > \|\Delta\mathbf{x}\| > 0$.

Scalar Example

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



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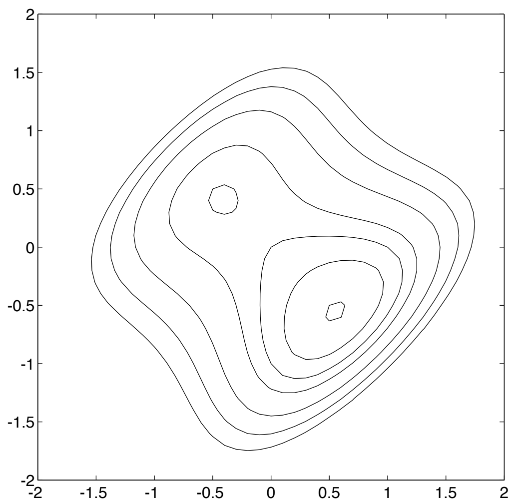
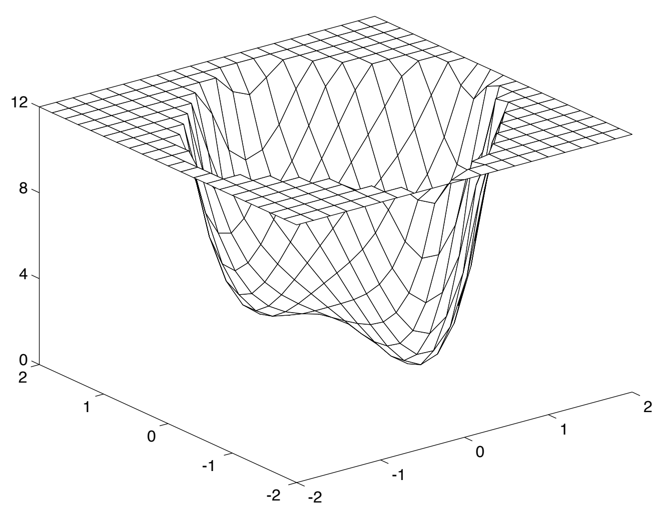
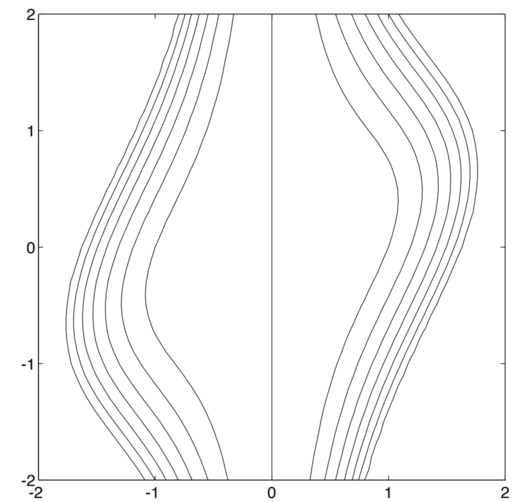
Vector Example

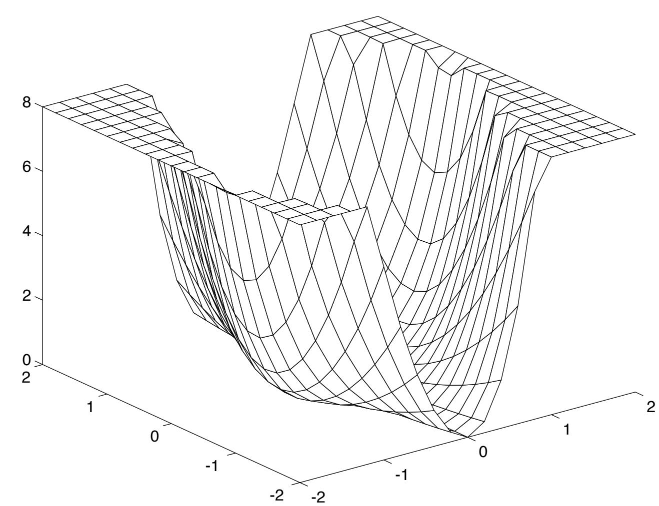
$$F(\mathbf{x}) = (x_2 - x_1)^4 + 8x_1x_2 - x_1 + x_2 + 3$$





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





8 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:

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

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:

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

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 **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 strong minimum.

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.

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

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

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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):

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

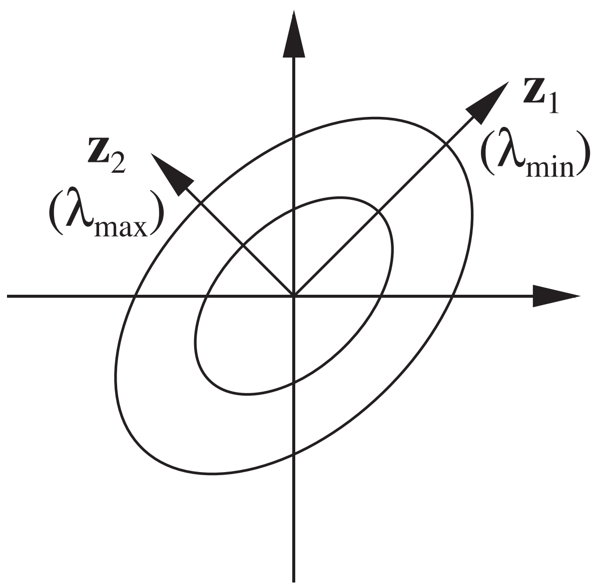
$$\frac{\mathbf{p}^T \mathbf{A} \mathbf{p}}{\|\mathbf{p}\|^2} = \frac{\mathbf{c}^T \mathbf{B}^T (\mathbf{B} \Lambda \mathbf{B}^T) \mathbf{B} \mathbf{c}}{\mathbf{c}^T \mathbf{B}^T \mathbf{B} \mathbf{c}} = \frac{\mathbf{c}^T \Lambda \mathbf{c}}{\mathbf{c}^T \mathbf{c}} = \frac{\sum_{i=1}^{n} \lambda_i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

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

Eigenvector (Largest Eigenvalue)

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

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



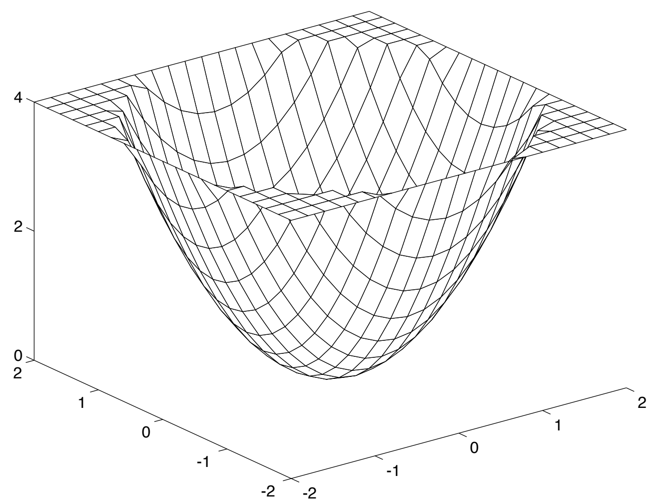
The eigenvalues represent curvature (second derivatives) along the eigenvectors (the principal axes).

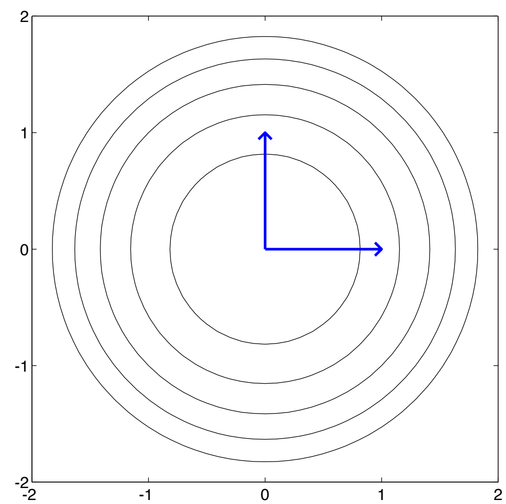
Circular Hollow

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

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

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

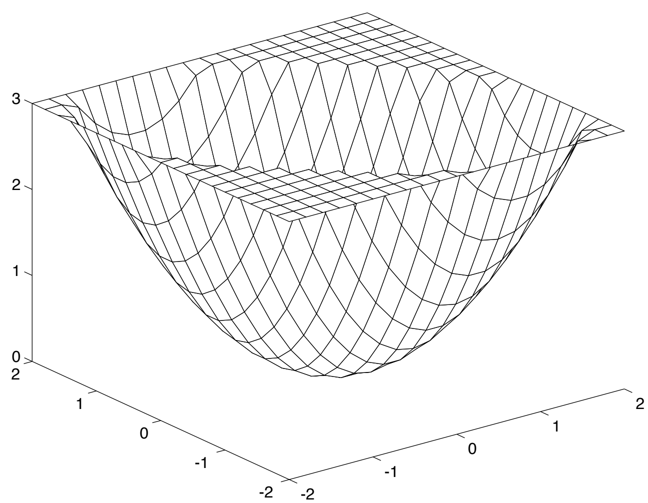


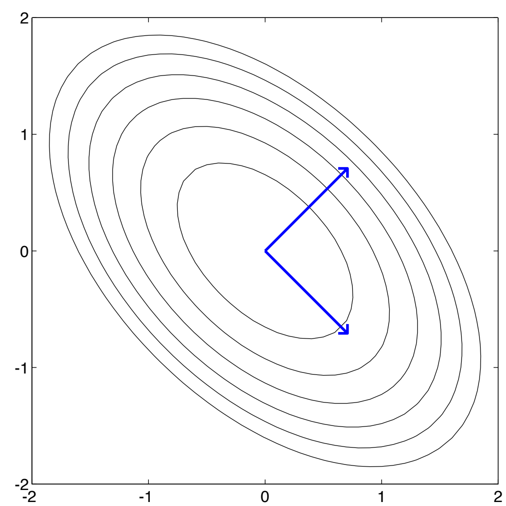


Elliptical Hollow

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

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

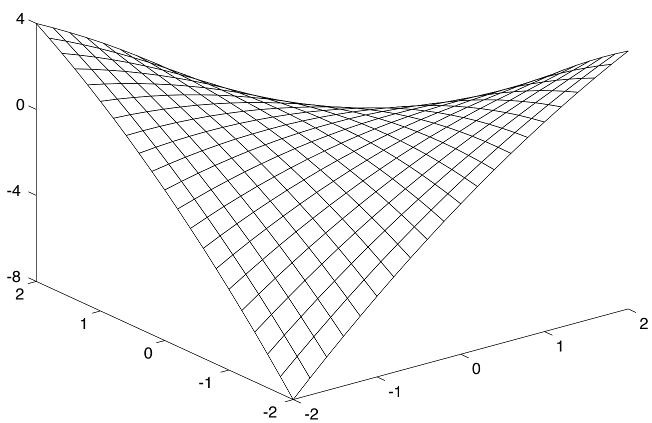


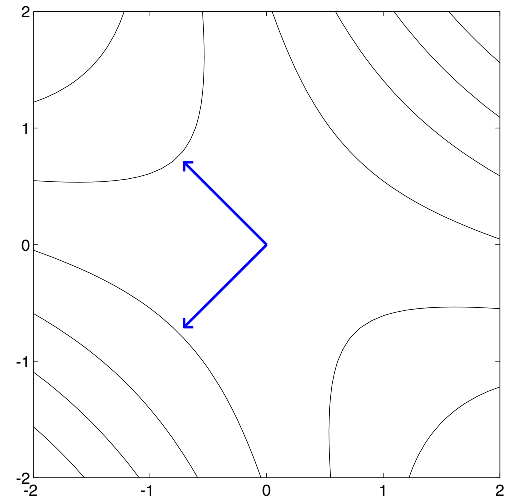


Elongated Saddle

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

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

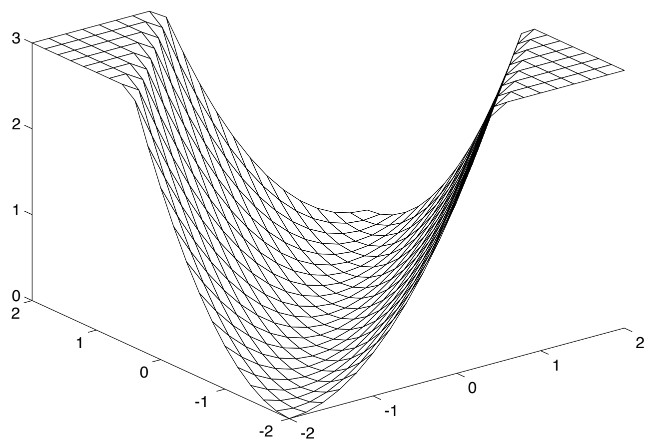


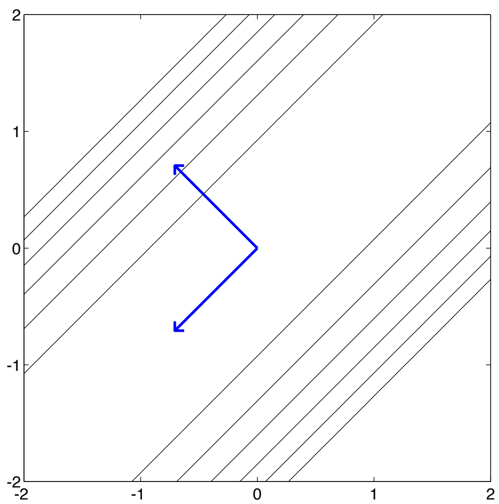


8 Stationary Valley

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

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





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