Introduction to Optimization II

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General Form

The General Form of Optimization Problem

$$\begin{aligned} \text{minimize} \quad & f(\mathbf{x}) \\ \text{subject to} \quad & g_i(\mathbf{x}) \leq 0, \quad i = 1, \ldots, m \\ & h_j(\mathbf{x}) = 0, \quad j = 1, \ldots, l \\ & \mathbf{x}^L \leq \mathbf{x} \leq \mathbf{x}^U \end{aligned}$$

- $\mathbf{x} \in \mathbb{R}^n$ is the optimization variable
- $f(\mathbf{x}) : \mathbb{R}^n \mapsto \mathbb{R}$ is the objective or cost function
- $g_i : \mathbb{R}^n \mapsto \mathbb{R}, i = 1, \ldots, m$, are the inequality constraint functions
- $h_i : \mathbb{R}^n \mapsto \mathbb{R}, i = 1, \ldots, l$, are the equality constraint functions.

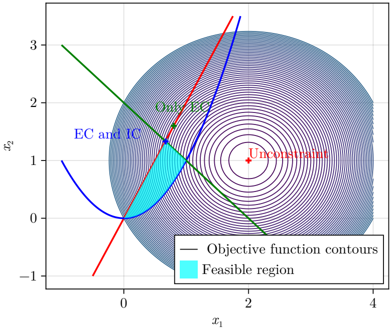
General Form

A Simple Problem:

$$\begin{aligned} \underset{\mathbf{x}}{\text{minimize}} \quad & f(\mathbf{x}) \\ \text{subject to} \quad & g_i(\mathbf{x}) \leq 0, \quad i = 1, \ldots, m \\ & h_j(\mathbf{x}) = 0, \quad j = 1, \ldots, l \end{aligned}$$

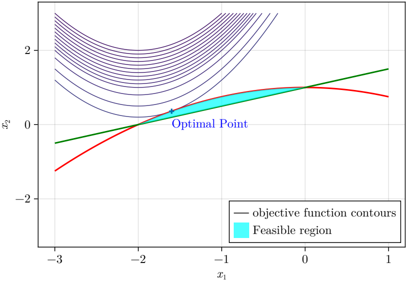
Example:

$$\begin{aligned} \underset{\mathbf{x}}{\text{minimize}} \quad & (x_1 - 2)^2 + (x_2 - 1)^2 \\ \text{subject to} \quad & x_2 - 2x_1 = 0 \\ & x_1^2 - x_2 \leq 0 \\ & x_1 + x_2 \leq 2 \end{aligned}$$



- Unconstrained Optimal Solution: $\mathbf{x} = \begin{bmatrix} 2 & 1 \end{bmatrix}$
- Solution with only equality con.: $\mathbf{x} = \begin{bmatrix} 0.8 & 1.6 \end{bmatrix}$
- Solution with both types of con.: $\mathbf{x} = \begin{bmatrix} 0.67 & 1.33 \end{bmatrix}$

For $n = 1$ or $n = 2$, we could plot the NLP problem to get the solution. The example shows the plotting of the feasible region Ω and objective function contours for the NLP problem with $n = 2$ as follow:



$$\begin{aligned} \underset{x_1, x_2}{\text{minimize}} \quad & (x_1 + 2)^2 - x_2 \\ \text{subject to} \quad & \frac{x_1^2}{4} + x_2 - 1 \leq 0 \\ & 2 + x_1 - 2x_2 \leq 0 \end{aligned}$$

Real optimal solution is

$$x_1^* = -1.6, \quad x_2^* = 0.36$$

Julia code: Graphical Method

Matlab code: Graphical Method

Existence of a Minimum and a Maximum: Weierstrass Theorem

Briefly details of important terms:

- **dom** f here means domain of the function.
- The set $\{x : |x| \leq 1\}$ is an example of a *closed* set while $\{x : |x| < 1\}$ is an *open* set.
- A set is *bounded* if it is contained within some sphere of finite radius, i.e. for any point $\mathbf{a}$ in the set, $\mathbf{a}^T\mathbf{a} < c$, where c is a finite number.
- For example, the set of all positive integers, $\{1, 2, \ldots\}$, is not bounded.
- A set that is both closed and bounded is called a *compact* set.

Theorem

*Let $f(\mathbf{x})$ be a continuous function defined over a closed and bounded set $\Omega \subset$ **dom** f. Then, there exist points $\mathbf{x}^*$ and $\mathbf{x}^{**}$ in Ω where f attains its minimum and maximum, respectively. That is $f(\mathbf{x}^*)$ and $f(\mathbf{x}^{**})$ are the minimum and maximum values of f in the set.*

Existence of a Minimum and a Maximum: Weierstrass Theorem

Let $\mathbf{x}^*$ and $\mathbf{x}^{**}$ denote the solutions, if one exists, to the minimization, and maximization problems

$$\begin{aligned} \text{minimize} \quad & f(\mathbf{x}) \\ \text{subject to} \quad & \mathbf{x} \in \Omega \end{aligned} \qquad\qquad \begin{aligned} \text{maximize} \quad & f(\mathbf{x}) \\ \text{subject to} \quad & \mathbf{x} \in \Omega \end{aligned}$$

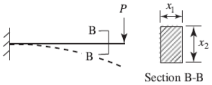
Consider a problem

$$\text{minimize} \quad x \qquad \text{subject to} \qquad 0 < x \leq 1$$

This simple problem does not have a solution. We observe that the constraint set Ω is not closed. Re-writing the constraint as $0 \leq x \leq 1$ results in $x = 0$ being the solution.

Existence of a Minimum and a Maximum: Weierstrass Theorem

Consider the cantilever beam in Fig. with a tip load P and tip deflection δ. The cross-section is rectangular with width and height equal to x_1, x_2, respectively. It is desired to minimize the tip deflection with given amount of material, or



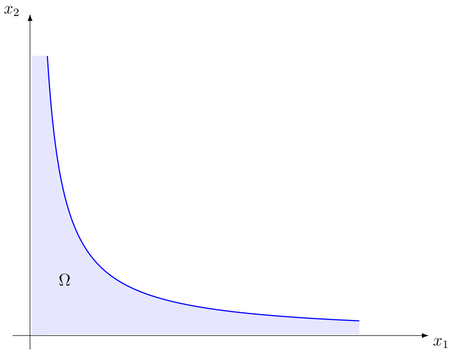
$$\begin{aligned} &\text{minimize} && \delta \\ &\text{subject to} && A \leq A_0 \end{aligned}$$

This problem does not have a solution. It is *ill-posed*. This can be seen by substituting the beam equation

$$\delta = \frac{PL^2}{3EI} = \frac{c}{x_1 x_2^3},$$

where c is a known scalar. Owing to the fact that x_2 is cubed in the denominator of the δ expression, with a given $A = x_1 x_2$ (the cross section area), the solution will tend to increase x_2 and reduce x_1. That is, the beam will tend to be infinitely slender with $x_1 \mapsto 0$, $x_2 \mapsto \infty$.

Existence of a Minimum and a Maximum: Weierstrass Theorem



Look at the feasible region Ω shown that it is unbounded, violating the simple conditions in Weierstrass theorem.

Quadratic Forms and Positive Definite matrices

Consider a function

$$f(x_1, x_2) = x_1^2 - 6x_1x_2 + 9x_2^2$$

We can write $f(x_1, x_2)$ in a matrix notation as:

$$\begin{aligned} f(x_1, x_2) &= \begin{bmatrix} x_1 & x_2 \end{bmatrix} \begin{bmatrix} 1 & -3 \\ -3 & 9 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \end{bmatrix} \\ &= \mathbf{x}^T \mathbf{A} \mathbf{x} \end{aligned}$$

The matrix $\mathbf{A}$ is symmetric since

$$\mathbf{x}^T \mathbf{A} \mathbf{x} = \mathbf{x}^T \left(\frac{\mathbf{A} + \mathbf{A}^T}{2} \right) \mathbf{x}$$

$$\mathbf{B} = \frac{\mathbf{A} + \mathbf{A}^T}{2} \text{ is a symmetric matrix.}$$

Quadratic Forms and Positive Definite matrices

Definition (positive definiteness)

- A symmetric matrix $\mathbf{A} \in \mathbb{R}^{n\times n}$ is called *positive semidefinite*, denoted by $\mathbf{A} \succeq 0$, if $\mathbf{x}^T\mathbf{A}\mathbf{x} \geq 0\ \forall \mathbf{x} \in \mathbb{R}^n$.
- A symmetric matrix $\mathbf{A} \in \mathbb{R}^{n\times n}$ is called *positive definite*, denoted by $\mathbf{A} \succ 0$, if $\mathbf{x}^T\mathbf{A}\mathbf{x} > 0\ \forall \mathbf{x} \in \mathbb{R}^n$ and $\mathbf{x} \neq 0$.

Example Let

$$\mathbf{A} = \begin{bmatrix} 2 & -1 \\ -1 & 1 \end{bmatrix}, \text{ for any } \mathbf{x} = \begin{bmatrix} x_1 & x_2 \end{bmatrix}^T \in \mathbb{R}^2$$

$$\mathbf{x}^T\mathbf{A}\mathbf{x} = \begin{bmatrix} x_1 & x_2 \end{bmatrix} \begin{bmatrix} 2 & -1 \\ -1 & 1 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \end{bmatrix} = 2x_1^2 - 2x_1x_2 + x_2^2 = x_1^2 + (x_1 - x_2)^2 \geq 0.$$

The matrix $\mathbf{A}$ is positive semidefinite. Since $x_1^2 + (x_1 - x_2)^2 = 0$ if and only if $x_1 = x_2 = 0$ it follows that $\mathbf{A}$ is positive definite. **Note:** the *negative (semi)definite* is just the opposite sign of the positive (semi)definite.

Quadratic Forms and Positive Definite matrices

The matrix, whose components are all positive, is note positive definite since for $\mathbf{x} = \begin{bmatrix} 1 & -1 \end{bmatrix}^T$, we have

$$\mathbf{A} = \begin{bmatrix} 1 & 2 \\ 2 & 1 \end{bmatrix}, \qquad \mathbf{x}^T\mathbf{A}\mathbf{x} = \begin{bmatrix} 1 & -1 \end{bmatrix} \begin{bmatrix} 1 & 2 \\ 2 & 1 \end{bmatrix} \begin{bmatrix} 1 \\ -1 \end{bmatrix} = -2$$

Definition (eigenvalue characterization (proof is omit.))

Let $\mathbf{A}$ be a symmetric $n \times n$ matrix. Then

- $\mathbf{A}$ is positive definite if and only if all its eigenvalues are positive,
- $\mathbf{A}$ is positive semidefinite if and only if all its eigenvalues are nonnegative,
- $\mathbf{A}$ is negative definite if and only if all its eigenvalues are negative,
- $\mathbf{A}$ is negative semidefinite if and only if all its eigenvalues are nonpositive,
- $\mathbf{A}$ is indefinite if and only if it has at least one positive eigenvalue and at lease one negative eigenvalue.

$$\mathbf{A} = \begin{bmatrix} 1 & 2 \\ 2 & 1 \end{bmatrix}, \qquad \det(\lambda\mathbf{I} - \mathbf{A}) = \begin{vmatrix} \lambda - 1 - 2 \\ -2\lambda - 1 \end{vmatrix} = 0, \qquad \lambda = -1, 3$$

It is obvious that the matrix $\mathbf{A}$ is not positive definite.

Definition (Sylvester's Test for a Positive definite Matrix)

Let $\mathbf{A}^i$ denote the submatrix formed by deleting the last $n - i$ rows and columns of $\mathbf{A}$, and let $\det(\mathbf{A}^i)$ is the determinant of $\mathbf{A}^i$. Then, $\mathbf{A}$ is positive definite if and only if $\det(\mathbf{A}^i) > 0$ for $i = 1, 2, \ldots, n$. This is, the determinants of all principal minors are positive.

- $\mathbf{A}$ is positive (semi-)definite if and only if all its leading principal minors are positive, i.e. , $\det \mathbf{A}^i > (\geq) 0$ for all i.
- $\mathbf{A}$ is negative (semi-)definite if and only if all the leading principal minors of $-\mathbf{A}$ are positive, i.e., $\det -\mathbf{A}^i > (\geq) 0$ for all i
- $\mathbf{A}$ is indefinite if neither positive or negative definite.

Quadratic Forms and Positive Definite matrices

Consider a matrix $\mathbf{A}$ below:

$$\mathbf{A} = \begin{bmatrix} 1 & 2 & 3 \\ 2 & 5 & -1 \\ 3 & -1 & 2 \end{bmatrix}$$

We have

$$\mathbf{A}^1 = 1 > 0, \quad \mathbf{A}^2 = \begin{vmatrix} 1 & 2 \\ 2 & 5 \end{vmatrix} = 5 - 4 = 1 > 0, \quad \mathbf{A}^3 = \begin{vmatrix} 1 & 2 & 3 \\ 2 & 5 & -1 \\ 3 & -1 & 2 \end{vmatrix} = -56 < 0$$

Thus , $\mathbf{A}$ is not positive definite.

Quadratic Forms and Positive Definite matrices

Check the characteristic of the following matrices:

$$\mathbf{A} = \begin{bmatrix} 1 & -2 & 4 \\ -2 & 2 & 0 \\ 4 & 0 & -7 \end{bmatrix}, \qquad \mathbf{B} = \begin{bmatrix} 4 & -2 & 0 \\ -2 & 3 & 0 \\ 0 & 0 & 50 \end{bmatrix}$$

$\mathbf{A}$ is indefinite,and $\mathbf{B}$ is positive definite.

$\mathbb{C}^n$ Continuity of a Function

The function f is $\mathbb{C}^0$ *continuous* at a point a if : given any sequence $\{x_k\}$ in **dom**(f) which converts to a, then $f(x_k)$ must converge to $f(a)$. Further, f is continuous over a set $\mathbb{S}$ implies that it is continuous at each pint in $\mathbb{S}$.

$\mathbb{C}^1$ and $\mathbb{C}^2$ Continuity

Let A be an open set of $\mathbb{R}^n$ and $f : \mathbb{R}^n \mapsto \mathbb{R}^1$. if each of the functions $\frac{\partial f}{\partial x_i}, i = 1, \ldots, n$, is continuous on this set then we write $f \in \mathbb{C}^1$ or that f is $\mathbb{C}^1$ continuous or state that f is "smooth". If each of the functions $\frac{\partial f}{\partial x_i, \partial x_j}, 1 \le i, j \le n$, is continuous on the set, then we write $f \in \mathbb{C}^2$. **Example:** Consider the function f with

dom $f \in \mathbb{R}^1$:

$$f(x) = \begin{cases} 0, & x \le 0 \\ 1, & x > 0 \end{cases}$$

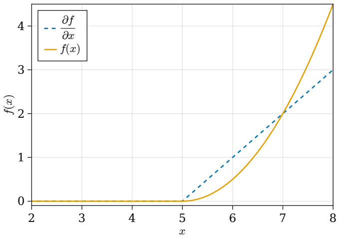
The sequence $x_k = 1/k, k = 1, 2, 3, \ldots$ converges (from the right) to $a = 0$ but the sequence $f(x_k) = 1$ for all k and does not converge to $f(a) = f(0) = 0$. Thus, f is discontinuous at $a = 0$.

Consider

$$f(x) = \frac{1}{2}\max(0, x-5)^2, \qquad x \in \mathbb{R}^1$$

$$\frac{\partial f}{\partial x} = \max(0, x-5)$$

$$\frac{\partial^2 f}{\partial x^2} = \begin{cases} 0 & \text{, for } x \le 5 \\ 1 & \text{, for } x > 5 \end{cases}$$



The first derivative is a continuous function, while the second derivative is not continuous at $x = 5$. Thus f is only $\mathbb{C}^1$ (and not $\mathbb{C}^2$) continuous on $\mathbb{R}^1$.

See ch1/positive_def.jl, $df/dx = \frac{1}{2}(2)\max(0, x-5)d(\max(0, x-5))/dx = \max(0, x-5)$

Derivatives and Gradient

We consider differentiable and continuous functions of n variables $\mathbf{x} = \begin{bmatrix} x_1 & x_2 & \cdots & x_n \end{bmatrix}^T$ denoted by $f(\mathbf{x})$ or $f(x_1, x_2, \ldots, x_3)$.

- **The derivative with respect to the ith parameter** is given by:

$$\frac{\partial f}{\partial x_i} = \lim_{\Delta x_i \to 0} \frac{f(x_1, x_2, \ldots, x_i + \Delta x_i, \ldots, x_n) - f(x_1, x_2, \ldots, x_i, \ldots, x_n)}{\Delta x_i}$$
$$\approx \frac{f(x_1, x_2, \ldots, x_i + \Delta x_i, \ldots, x_n) - f(x_1, x_2, \ldots, x_i, \ldots, x_n)}{\Delta x_i}$$

- **Gradient Vector:** Given a function $f(\mathbf{x}) \in \mathbb{C}^1$, we introduce the *gradient vector* ∇f, a column vector , as

$$\nabla f = \left[\frac{\partial f}{\partial x_1}, \frac{\partial f}{\partial x_2}, \ldots, \frac{\partial f}{\partial x_n} \right]^T$$

The gradient evaluated at a point $\mathbf{c}$ is denoted by $\nabla f(\mathbf{c})$.

Derivatives and Gradient

Example Consider the function:

$$f(\mathbf{x}) = (x_1 - 2)^2 + (x_2 - 1)^2 - x_1 x_2$$

Determine the gradient of the function at the point $\mathbf{x}_0 = \begin{bmatrix} 1.0 & 1.0 \end{bmatrix}^T$

Solution:

$$\nabla f = \begin{bmatrix} \frac{\partial f}{\partial x_1} \\ \frac{\partial f}{\partial x_2} \end{bmatrix} = \begin{bmatrix} 2(x_1 - 2) - x_2 \\ 2(x_2 - 1) - x_1 \end{bmatrix}$$

At the point $\mathbf{x}_0$

$$\nabla f = \begin{bmatrix} -3 \\ -1 \end{bmatrix}$$

Jacobian

Sometime we need to consider a number of functions at the same time, like the response of a circuit at a number of frequencies. In this case we have

$$\mathbf{f}(\mathbf{x}) = \begin{bmatrix} f_1 & f_2 & \cdots & f_m \end{bmatrix}^T$$

The Jacobian matrix is the matrix combining all these gradients together and is given by

$$\mathbf{J}(\mathbf{x}) = \begin{bmatrix} \nabla f_1^T \\ \nabla f_2^T \\ \vdots \\ \nabla f_m^T \end{bmatrix} = \begin{bmatrix} \frac{\partial f_1}{\partial x_1} & \frac{\partial f_1}{\partial x_2} & \cdots & \frac{\partial f_1}{\partial x_n} \\ \frac{\partial f_2}{\partial x_1} & \frac{\partial f_2}{\partial x_1} & \cdots & \frac{\partial f_2}{\partial x_n} \\ \vdots & \vdots & \ddots & \vdots \\ \frac{\partial f_m}{\partial x_1} & \frac{\partial f_m}{\partial x_1} & \cdots & \frac{\partial f_m}{\partial x_n} \end{bmatrix}$$

Jacobian

Consider the vector of functions $\mathbf{f}(\mathbf{x}) = \begin{bmatrix} 3x_1^2 + x_2^3 & x_1^3 - 2x_3 \end{bmatrix}^T$. Determine the Jacobian at the point $\mathbf{x}_0 = \begin{bmatrix} 2.0 & 1.0 & 1.0 \end{bmatrix}^T$

$$\mathbf{J}(\mathbf{x}) = \begin{bmatrix} \nabla f_1^T \\ \nabla f_2^T \end{bmatrix} = \begin{bmatrix} 6x_1 & 3x_2^2 & 0 \\ 3x_1^2 & 0 & -2 \end{bmatrix}$$

At the point $\mathbf{x}_0$, the Jacobian is given by:

$$\mathbf{J}(\mathbf{x}_0) = \begin{bmatrix} \nabla f_1^T \\ \nabla f_2^T \end{bmatrix} = \begin{bmatrix} 12 & 3 & 0 \\ 12 & 0 & -2 \end{bmatrix}$$

Second-order derivatives, Hessian Matrix

The mixed second-order derivativewith respect to the ith and jth parameters is given by:

$$\frac{\partial^2 f}{\partial x_i \partial x_j} = \lim_{\Delta x_j \to 0} \frac{\frac{\partial f(x_1, x_2, \ldots, x_j + \Delta x_j, \ldots, x_n}{\partial x_i} - \frac{\partial f(x_1, x_2, \ldots, x_i, \ldots, x_n)}{\partial x_i}}{\Delta x_j}$$

The gradient of a vector of m-function, $\mathbf{H} = \nabla \mathbf{g}$ is defined to be a matrix of dimension $(n \times m)$ as

$$\mathbf{H} = \nabla \mathbf{g} = \begin{bmatrix} \frac{\partial g_1}{\partial x_1} & \frac{\partial g_2}{\partial x_1} & \cdots & \frac{\partial g_m}{\partial x_1} \\ \frac{\partial g_1}{\partial x_2} & \frac{\partial g_2}{\partial x_2} & \cdots & \frac{\partial g_m}{\partial x_2} \\ \vdots & \vdots & \ddots & \vdots \\ \frac{\partial g_1}{\partial x_n} & \frac{\partial g_2}{\partial x_n} & \cdots & \frac{\partial g_m}{\partial x_n} \end{bmatrix} = \begin{bmatrix} \frac{\partial^2 f}{\partial x_1^2} & \frac{\partial^2 f}{\partial x_1 \partial x_2} & \cdots & \frac{\partial^2 f}{\partial x_1 \partial x_n} \\ \frac{\partial^2 f}{\partial x_2 \partial x_1} & \frac{\partial^2 f}{\partial x_2^2} & \cdots & \frac{\partial^2 f}{\partial x_2 \partial x_n} \\ \vdots & \vdots & \ddots & \vdots \\ \frac{\partial^2 f}{\partial x_n \partial x_1} & \frac{\partial^2 f}{\partial x_n \partial x_2} & \cdots & \frac{\partial^2 f}{\partial x_n^2} \end{bmatrix}$$

The Hessian matrix is a symmetric matrix because the order of differentiation does not make a difference.

Second-order derivatives, Hessian Matrix

Evaluate the gradient and the Hessian of the function
$f(\mathbf{x}) = 3x_1^2 + 2x_1x_2 + x_1x_3 + 2.5x_2^2 + 2x_2x_3 + 2x_3^2 - 8x_1 - 3x_2 - 3x_3$ at the point
$\mathbf{x}_0 = \begin{bmatrix} 1.0 & -1.0 & 1.0 \end{bmatrix}^T$

$$\nabla f(\mathbf{x}) = \mathbf{g}(\mathbf{x}) = \begin{bmatrix} 6x_1 + 2x_2 + x_3 - 8 \\ 2x_1 + 5x_2 + 2x_3 - 3 \\ x_1 + 2x_2 + 4x_3 - 3 \end{bmatrix} \quad \Rightarrow \quad \nabla f(\mathbf{x}_0) = \begin{bmatrix} -3 \\ -4 \\ 0 \end{bmatrix}$$

$$\mathbf{H} = \frac{\partial \mathbf{g}(\mathbf{x})^T}{\partial \mathbf{x}} = \begin{bmatrix} 6 & 2 & 1 \\ 2 & 5 & 2 \\ 1 & 2 & 4 \end{bmatrix}$$

Note:

$$f(\mathbf{x}) = \begin{bmatrix} x_1 & x_2 & x_3 \end{bmatrix} \begin{bmatrix} 3 & 1 & 0.5 \\ 1 & 2.5 & 1 \\ 0.5 & 1 & 2 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} + \begin{bmatrix} -8 & -3 & -3 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix}$$

$$= \mathbf{x}^T \mathbf{Q} \mathbf{x} + \mathbf{b}^T \mathbf{x} = \frac{1}{2} \mathbf{x}^T \mathbf{H} \mathbf{x} + \mathbf{b}^T \mathbf{x}$$

Gradient and Hessian with Matlab

```
syms x1 x2 x3

f = 3*x1^2 + 2*x1*x2 + x1*x3 + 2.5*x2^2 + 2*x2*x3 ...
    + 2*x3^2 - 8*x1 - 3*x2 - 3*x3

g = gradient(f,[x1, x2, x3])
h = hessian(f,[x1, x2, x3])
g1 = subs(g, [x1, x2, x3], [1, -1, 1])
```

ans = $\begin{pmatrix} 6\,x_1 + 2\,x_2 + x_3 - 8 \\ 2\,x_1 + 5\,x_2 + 2\,x_3 - 3 \\ x_1 + 2\,x_2 + 4\,x_3 - 3 \end{pmatrix}$ ans = $\begin{pmatrix} 6 & 2 & 1 \\ 2 & 5 & 2 \\ 1 & 2 & 4 \end{pmatrix}$

ans = $\begin{pmatrix} -3 \\ -4 \\ 0 \end{pmatrix}$

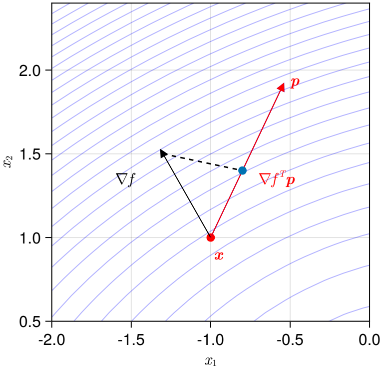
Gradient and Hessian with Julia

```julia
using Symbolics, ForwardDiff

@variables x1 x2 x3

f(x) = 3x[1]^2 + 2x[1]x[2] + x[1]x[3] + 2.5x[2]^2 + 2x[2]x[3] +
                        2x[3]^2 - 8x[1] - 3x[2] - 3x[3]

gf(x) = ForwardDiff.gradient(f,x)
Hf(x) = ForwardDiff.hessian(f,x)

g = gf([x1, x2, x3])
h = Hf([x1, x2, x3])
g1 = gf([1, -1, 1])
```

Directional Derivative

Directional Derivative: The rate of change in a direction $\mathbf{p}$ is quantified by a *directional derivative*, defined as

$$\nabla_{\mathbf{p}} f(\mathbf{x}) = \lim_{\tau \to 0} \frac{f(\mathbf{x} + \tau \mathbf{p}) - f(\mathbf{x})}{\tau} = \nabla f^T \mathbf{p} = \|\nabla f\| \|\mathbf{p}\| \cos\theta$$



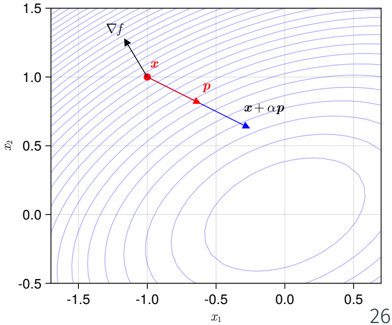
Directional Derivative

Consider the following function of two variables: $f(x_1, x_2) = x_1^2 + 2x_2^2 - x_1 x_2$. The gradient can be obtained using symbolic differentiation, yielding

$$\nabla f(x_1, x_2) = \begin{bmatrix} 2x_1 - x_2 \\ 4x_2 - x_1 \end{bmatrix}, \qquad \nabla f(-1, 1) = \begin{bmatrix} -3 \\ 5 \end{bmatrix}.$$

Taking the derivative in the normalized direction $\mathbf{p} = \begin{bmatrix} \frac{2}{\sqrt{5}} & -\frac{1}{\sqrt{5}} \end{bmatrix}$, we obtain

$$\nabla f^T \mathbf{p} = \begin{bmatrix} -3 & 5 \end{bmatrix} \begin{bmatrix} 2/\sqrt{5} \\ -1/\sqrt{5} \end{bmatrix} = -\frac{11}{\sqrt{5}}$$



Directional Derivative

We wish to compute the directional derivative of $f(\mathbf{x}) = x_1 x_2$ at $x = [1,\ 0]$ in the direction $\mathbf{p} = [-1,\ -1]$:

$$\nabla f(\mathbf{x}) = \begin{bmatrix} x_2 & x_1 \end{bmatrix}^T, \qquad \nabla_{\mathbf{p}} f(\mathbf{x}) = \nabla f(\mathbf{x})^T \mathbf{p} = \begin{bmatrix} 0 & 1 \end{bmatrix} \begin{bmatrix} -1 \\ -1 \end{bmatrix} = -1$$

We can also compute the directional derivative as follows:

- Introduce a scalar variable α and denote points along the vector $\mathbf{p}$ emanating from $\mathbf{x}$ as $g(\alpha) = \mathbf{x} + \alpha\mathbf{p}$
- Denote the function $f(\alpha) = f(g(\alpha)) = f(\mathbf{x} + \alpha\mathbf{p})$. We have

$$\nabla_{\mathbf{p}} f(\mathbf{x}) = \left.\frac{df}{d\alpha}\right|_{\alpha=0} = \left.\frac{\partial f}{\partial g}\right|_{\alpha=0} \frac{\partial g}{\partial \alpha} = \left(\frac{\partial f}{\partial \mathbf{x}}\right)^T \mathbf{p} = \nabla f(\mathbf{x})^T \mathbf{p}$$

- from above example, we have

$$g(\alpha) = f(\mathbf{x} + \alpha\mathbf{p}) = (1 - \alpha)(-\alpha) = \alpha^2 - \alpha$$
$$g'(\alpha) = 2\alpha - 1, \quad g'(0) = -1$$

Curvature and Hessian

The rate of change of the gradient–the *curvature*–is also useful information because it tells us if a function's slope is increasing (positive curvature), decreasing (negative curvature), or stationary (zero curvature). Given a function $f(x_1, \dots, x_n) \in \mathbb{C}^2$, we define the matrix of second partial derivatives

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

The Hessian is a symmetric matrix with $n(n+1)/2$ independent elements.

Curvature and Hessian

We can find the rate of change of the gradient in an arbitrary normalized direction $\mathbf{p}$ by taking the product $\mathbf{H}_\mathbf{p}$.

$$\mathbf{H}_\mathbf{p} = \nabla_\mathbf{p}(\nabla f(\mathbf{x})) = \lim_{\tau \to 0} \frac{\nabla f(\mathbf{x} + \tau\mathbf{p}) - \nabla f(\mathbf{x})}{\tau}$$

To find the curvature of the one-dimensional function along a direction $\mathbf{p}$, we need to project $\mathbf{H}_\mathbf{p}$ onto direction $\mathbf{p}$ as

$$\nabla_\mathbf{p}(\nabla_\mathbf{p} f(\mathbf{x})) = \mathbf{p}^T\mathbf{H}\mathbf{p}$$

which yields a scalar quantity. If we want to get the curvature in the original units of $\mathbf{x}$, $\mathbf{p}$ should be normalized.

Curvature and Hessian

Consider $f(x_1, x_2) = x_1^2 + 2x_2^2 - x_1 x_2$. The Hessian of this quadratic is

$$\mathbf{H} = \nabla(\nabla f(x)) = \nabla \left(\begin{bmatrix} 2x_1 - x_2 \\ 4x_2 - x_1 \end{bmatrix} \right) = \begin{bmatrix} 2 & -1 \\ -1 & 4 \end{bmatrix}$$

To find the curvature in the direction $\mathbf{p} = \begin{bmatrix} -1/2 & -\sqrt{3}/2 \end{bmatrix}^T$, we compute

$$\mathbf{p}^T \mathbf{H} \mathbf{p} = \begin{bmatrix} -\frac{1}{2} & -\frac{\sqrt{3}}{2} \end{bmatrix} \begin{bmatrix} 2 & -1 \\ -1 & 4 \end{bmatrix} \begin{bmatrix} -\frac{1}{2} \\ -\frac{\sqrt{3}}{2} \end{bmatrix} = \frac{7 - \sqrt{3}}{2}$$

Taylor's Theorem, Linear and Quadratic Approximations

Suppose that $f(x) \in \mathbb{C}^p$ on an interval $\mathbf{J} = [a, b]$. If x_0, x belong to $\mathbf{J}$, then there exists a number γ between x_0 and x such that

$$f(x) \approx f(x_0) + \frac{f'(x_0)}{1!}(x - x_0) + \frac{f''(x_0)}{2!}(x - x_0)^2 + \cdots + \frac{f^{(p-1)}(x_0)}{(p-1)!}(x - x_0)^{(p-1)} + \frac{f^{(p)}(x_0)}{p!}(x - x_0)^p$$

- Linear approximation: $f_l(x) \approx f(x_0) + f'(x_0)(x - x_0)$
- Quadratic approximation: $f_q(x) \approx f(x_0) + f'(x_0)(x - x_0) + \frac{1}{2} f''(x_0)(x - x_0)^2$

For n-dimension we have

$$f_q(\mathbf{x}) \approx f(\mathbf{x}_0) + \nabla f(\mathbf{x}_0)^T(\mathbf{x} - \mathbf{x}_0) + \frac{1}{2}(\mathbf{x} - \mathbf{x}_0)^T \mathbf{H}(\mathbf{x}_0)(\mathbf{x} - \mathbf{x}_0) + \text{ H.O.T.}$$

Taylor's Theorem, Linear and Quadratic Approximations

Given $f(\mathbf{x}) = 2x_1 + \frac{x_2}{x_1}$. Construct linear and quadratic approximations to the original function $f(\mathbf{x})$ at $\mathbf{x}_0 = [1\ 0.5]^T$

$$\nabla f(\mathbf{x}) = \begin{bmatrix} 2 - \frac{x_2}{x_1^2} \\ \frac{1}{x_1} \end{bmatrix}, \qquad \mathbf{H}(\mathbf{x}) = \begin{bmatrix} \frac{x_2}{x_1^3} & -\frac{1}{x_1^2} \\ -\frac{1}{x_1^2} & 0 \end{bmatrix}$$

The linear approximation is

$$f_l(\mathbf{x}) \approx f(\mathbf{x}_0) + \nabla f(\mathbf{x}_0)^T(\mathbf{x} - \mathbf{x}_0) = 2.5 + \begin{bmatrix} 1.5 & 1 \end{bmatrix}^T \begin{bmatrix} x_1 - 1 \\ x_2 - 0.5 \end{bmatrix}$$

$$= 0.5 + 1.5x_1 + x_2$$

The quadratic approximation is

$$f_q(\mathbf{x}) \approx f(\mathbf{x}_0) + \nabla f(\mathbf{x}_0)^T(\mathbf{x} - \mathbf{x}_0) + \frac{1}{2}(\mathbf{x} - \mathbf{x}_0)^T \mathbf{H}(\mathbf{x}_0)(\mathbf{x} - \mathbf{x}_0)$$

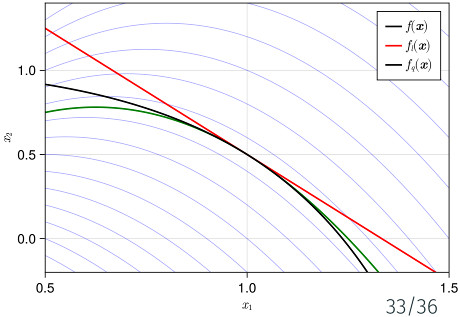
Taylor's Theorem, Linear and Quadratic Approximations

$$f_q(\mathbf{x}) \approx 0.5 + 1.5x_1 + x_2 + \frac{1}{2}\begin{bmatrix}(x_1-1) & (x_2-0.5)\end{bmatrix}\begin{bmatrix}1 & -1\\ -1 & 0\end{bmatrix}\begin{bmatrix}x_1-1\\ x_2-0.5\end{bmatrix}$$
$$= 0.5 + x_1 + 2x_2 - x_1x_2 + \frac{1}{2}x_1^2$$

Plotting: We need to plot, in variable-space or x-space, the contours

$$f(\mathbf{x}) = c, f_l(\mathbf{x}) = c, f_q(\mathbf{x}) = c,$$

where $c = f(\mathbf{x}_0) = 2.5$



Taylor's Theorem, Linear and Quadratic Approximations using Julia

```
using Symbolics, ForwardDiff, LinearAlgebra

@variables x1 x2
f(x) = 2x[1] + x[2]/x[1]
g(x) = ForwardDiff.gradient(f,x)
H(x) = ForwardDiff.hessian(f,x)

x0 = [1, 0.5]
fl(x) = f(x0) + g(x0)'*(x - x0)
fq(x) = f(x0) + g(x0)'*(x - x0) + (1/2)*(x - x0)'*H(x0)*(x - x0)
println(expand(fl([x1, x2])))
println(expand(fq([x1, x2])))
```

Taylor’s Theorem, Linear and Quadratic Approximations using Matlab

```
syms x1 x2 real

f = 2*x1 + x2/x1

x0 = [1 ,0.5];
g = gradient(f, [x1, x2])
H = hessian(f, [x1, x2 ])

f0 = subs(f,[x1, x2], x0)
g0 = subs(g,[x1, x2], x0)
H0 = subs(H, [x1, x2], x0)
dx = [x1; x2] - x0';

fl = f0 + g0'*dx
fq = expand(f0 + g0'*dx + (0.5)*dx'*H0*dx)
```

Reference

1. Joaquim R. R. A. Martins, Andrew Ning, ”*Engineering Design Optimization*,” Cambridge University Press, 2021
2. Alexander Mitsos, ”*Applied Numerical Optimization*,” Lecture Note RWTH AACHEN University
3. Ashok D. Belegundu, Tirupathi R. Chandrupatla, ”Optimization Concepts and Applications in Engineering,” Cambridge University Press, 2019