Department of Mathematics and Computer Science
University of Southern Denmark, Odense

March 6, 2025
Marco Chiarandini

# AI505 – Optimization

## Sheet 03, Spring 2025

---

**Solution:**

Included.

Exercises with the symbol $^+$ are to be done at home before the class. Exercises with the symbol $^*$ will be tackled in class. The remaining exercises are left for self training after the exercise class. Some exercises are from the text book and the number is reported. They have the solution at the end of the book.

### Exercise 1$^+$ (6.1)

What advantage does second-order information provide about the point of convergence that first-order information lacks?

**Solution:**

Second-order information can guarantee that one is at a local minimum, whereas a gradient of zero is necessary but insufficient to guarantee local optimality.

### Exercise 2$^+$ (6.2)

When would we use Newton's method instead of the bisection method for the task of finding roots in one dimension?

**Solution:**

We would prefer Newtons method if we start sufficiently close to the root and can compute derivatives analytically. Newton's method enjoys a better rate of convergence.

### Exercise 3$^*$ (6.4, 6.9)

Apply Newton's method to $f(\mathbf{x}) = \frac{1}{2}\mathbf{x}^T H\mathbf{x}$ starting from $\mathbf{x}_0 = [1, 1]$. What have you observed? Use $H$ as follows:

$$H = \begin{bmatrix} 1 & 0 \\ 0 & 1000 \end{bmatrix}$$

Next, apply gradient descent to the same optimization problem by stepping with the unnormalized gradient. Do two steps of the algorithm. What have you observed? Finally, apply the conjugate gradient method. How many steps do you need to converge?
Repeat the exercise for:

$$f(\mathbf{x}) = (x_1 + 1)^2 + (x_2 + 3)^2 + 4.$$

starting at the origin.

**Solution:**

*Newton's method* updates design points (solutions) as follows:

$$\mathbf{x}_{k+1} = \mathbf{x}_k - H_k^{-1}\nabla f(\mathbf{x}_k)$$

and substituting $\nabla f(\mathbf{x}_k) = H\mathbf{x}_k$ yields:

$$\mathbf{x}_{k+1} = \mathbf{x}_k - \mathbf{x}_k = \mathbf{0}$$

Hence

$$\mathbf{x}_1 = \mathbf{0}$$

and the search finishes in one step because the following ones would not yield any change.

*Gradient Descent* update rule is as follows for unnormalized case:

$$\mathbf{x}_{k+1} = \mathbf{x}_k - \alpha \nabla f(\mathbf{x}_k)$$

and subtituting $\nabla f(\mathbf{x}_k) = H\mathbf{x}_k$ for the specific case and setting $\alpha = 1$ yields:

$$\mathbf{x}_{k+1} = \mathbf{x}_k - H\mathbf{x}_k$$

$$\mathbf{x}_1 = \begin{bmatrix} 1 \\ 1 \end{bmatrix} - \begin{bmatrix} 1 & 0 \\ 0 & 1000 \end{bmatrix} \begin{bmatrix} 1 \\ 1 \end{bmatrix} = \begin{bmatrix} 1 \\ -999 \end{bmatrix}$$

$$\mathbf{x}_2 = \begin{bmatrix} 0 \\ -999 \end{bmatrix} - \begin{bmatrix} 1 & 0 \\ 0 & 1000 \end{bmatrix} \begin{bmatrix} 0 \\ -999 \end{bmatrix} = \begin{bmatrix} 0 \\ 998111 \end{bmatrix}$$

$$\mathbf{x}_3 = \begin{bmatrix} 0 \\ 998001 \end{bmatrix} - \begin{bmatrix} 1 & 0 \\ 0 & 1000 \end{bmatrix} \begin{bmatrix} 0 \\ 998001 \end{bmatrix} = \begin{bmatrix} 0 \\ -997002999 \end{bmatrix}$$

*Conjugate gradient*

$$\mathbf{x}_{k+1} = \mathbf{x}_k + \alpha_k \mathbf{d}_k \qquad \mathbf{d}_k = -\mathbf{r}_k + \beta_k \mathbf{d}_{k-1}$$

$$\mathbf{r}_k = \nabla f(\mathbf{x}_k) = H\mathbf{x}_k \qquad \beta_k = \frac{\mathbf{r}_k^T H \mathbf{d}_{k-1}}{\mathbf{d}_k^T H \mathbf{d}_{k-1}} \qquad \alpha_k = -\frac{\mathbf{r}_k \mathbf{d}_k}{\mathbf{d}_k^T H \mathbf{d}_k}$$

$$\mathbf{x}_1 = \mathbf{x}_0 + \alpha_0 \mathbf{d}_0$$

We choose the first search direction $\mathbf{d}_0$ to be the steepest descent direction at the initial point $\mathbf{x}_0$. Hence, $\mathbf{d}_0 = -\nabla f(\mathbf{x}_0) = -H\mathbf{x}_0$ and

$$\alpha_0 = -\frac{(H\mathbf{x}_0)^T(-H\mathbf{x}_0)}{(-H\mathbf{x}_0)^T H(-H\mathbf{x}_0)} = -\frac{10001}{1000001}$$

The first iteration then yields:

$$\mathbf{x}_1 = \mathbf{x}_0 + \alpha_0 \mathbf{d}_0 = \begin{bmatrix} 1 \\ 1 \end{bmatrix} + 0.010 \begin{bmatrix} 1 \\ 100 \end{bmatrix} = \begin{bmatrix} 1.010 \\ 2 \end{bmatrix}$$

The second iteration:

$$\mathbf{x}_2 = \mathbf{x}_1 + \alpha_1 \mathbf{d}_1$$

Setting $r_1 = H\mathbf{x}_1$:

$$\beta_1 = \frac{\mathbf{r}_1^T H \mathbf{d}_0}{\mathbf{d}_0^T H \mathbf{d}_0} = \frac{(H\mathbf{x}_1)^T H \mathbf{d}_0}{\mathbf{d}_0^T H \mathbf{d}_0} = \ldots$$

$$\mathbf{d}_1 = -\mathbf{r}_1 + \beta_1 \mathbf{d}_0 = \ldots$$

$$\alpha_1 = -\frac{(H\mathbf{x}_1)^T \mathbf{d}_0}{\mathbf{d}_0^T H \mathbf{d}_0} = \ldots$$

The matrix $H$ has eigenvalues 1 and 100 that are both positive, hence the matrix is positive definite (and hence symmetric). In this case, the conjugate gradient method needs $n$ iterations to find the local optimum.
The function:

$$f(\mathbf{x}) = (x_1 + 1)^2 + (x_2 + 3)^2 + 4 = x_1^2 + 2x_1 + 1 + x_2^2 + 6x_2 + 9 + 4$$

Can be obtained by

$$f(\mathbf{x}) = \mathbf{x}^T A \mathbf{x} + \mathbf{b}^T \mathbf{x} + c$$

where $\mathbf{x} = [x_1, x_2]^T$, $\mathbf{b} = [2, 6]$, $c = 14$ and

$$A = \begin{bmatrix} 1 & 0 \\ 0 & 3 \end{bmatrix}$$

The matrix $A$ is positive definite since its eigenvalues are positive. Hence, this is a quadratic function where the Netwon's method finds the optimal solution in one iteration.

$$\nabla f(\mathbf{x}) = [2(x_1+1), 2(x_2+3)]$$

$$H = \begin{bmatrix} 2 & 0 \\ 0 & 2 \end{bmatrix}$$

$$\mathbf{x}_1 = \mathbf{x}_0 - H^{-1}\nabla(\mathbf{x}_0) = \begin{bmatrix} 0 \\ 0 \end{bmatrix} - \begin{bmatrix} 2 & 0 \\ 0 & 2 \end{bmatrix}^{-1} \begin{bmatrix} 2 \\ 6 \end{bmatrix} = \begin{bmatrix} -1 \\ -3 \end{bmatrix}$$

## Exercise 4$^+$ (6.5)

Compare Newton's method and the secant method on $f(x) = x^2 + x^4$, with $x_1 = -3$ and $x_0 = -4$. Run each method for 10 iterations. Make two plots:

1. Plot $f$ vs. the iteration for each method.
2. Plot $f'$ vs. $x$. Overlay the progression of each method, drawing lines from $(x_i, f'(x_i))$ to $(x_{i+1}, 0)$ to $(x_{i+1}, f'(x_{i+1}))$ for each transition.

What can we conclude about this comparison?

**Solution:**

Its first derivative is $f'(x) = 2x + 4x^3$.
Its second derivative is $f'(x) = 2 + 12x^2$.
Implement Newton's method:
Newton's method updates the estimate $x_k$ using the formula:

$$x_{k+1} = x_k - \frac{f'(x_k)}{f''(x_k)}$$

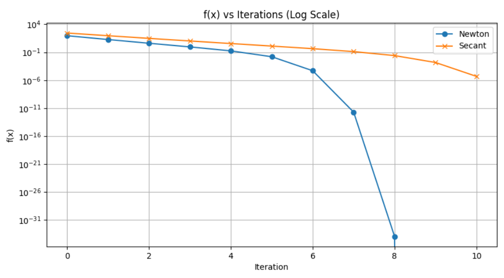
Implement the secant method:
The secant method updates the estimate $x_n$ using the formula:

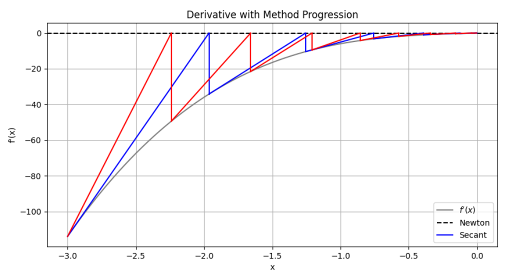
$$x_{k+1} = x_k - f'(x_k)\frac{x_k - x_{k-1}}{f(x_k) - f(x_{k-1}}$$

Note that the secant method requires two initial guesses, $x_0$ and $x_1$.
This plot illustrates how quickly each method converges to a local optimum.
This visualization shows how each method approaches the root in the context of the derivative's behavior.

```python
import numpy as np
import matplotlib.pyplot as plt

# Define the function and its derivative
def f(x):
    return x**2 + x**4

def df(x):
    return 2*x + 4*x**3

def ddf(x):
    return 2 + 12*x**2


# Newton's method
def newton_method(x0, iterations):
    xs = [x0]
    for _ in range(iterations):
        x0 = x0 - df(x0) / ddf(x0)
        xs.append(x0)
    return np.array(xs)

# Secant method
def secant_method(x0, x1, iterations):
    xs = [x0, x1]
    for _ in range(iterations - 1):
        x_new = xs[-1] - df(xs[-1]) * (xs[-1] - xs[-2]) / (df(xs[-1]) - df(xs[-2]))
        xs.append(x_new)
    return np.array(xs)

# Plot f(x) vs iteration
def plot_function_vs_iteration():
    iterations = 10
    x_newton = newton_method(-3, iterations)
    x_secant = secant_method(-4, -3, iterations)

    plt.figure(figsize=(10, 5))
    plt.plot(range(iterations + 1), f(x_newton), 'o-', label="Newton")
    plt.plot(range(iterations + 1), f(x_secant), 'x-', label="Secant")
    plt.yscale("log")
    plt.xlabel("Iteration")
    plt.ylabel("f(x)")
    plt.title("f(x) vs Iterations (Log Scale)")
    plt.legend()
    plt.grid()
    #plt.show()
    plt.savefig("secant_function.png")


# Plot f'(x) vs x with transitions
def plot_derivative_with_transitions():
    x_vals = np.linspace(-3, 0, 1000)
    plt.figure(figsize=(10, 5))
    plt.plot(x_vals, df(x_vals), label="$f'(x)$", color='grey')
    plt.axhline(0, color='black', linestyle='--')

    # Newton's method
    x_newton = newton_method(-3, 10)
    for i in range(len(x_newton) - 1):
        plt.plot([x_newton[i], x_newton[i+1]], [df(x_newton[i]), 0], 'b-')
        plt.plot([x_newton[i+1], x_newton[i+1]], [0, df(x_newton[i+1])], 'b-')

    # Secant method
    x_secant = secant_method(-4, -3, 10)
    for i in range(1,len(x_secant) - 1):
        plt.plot([x_secant[i], x_secant[i+1]], [df(x_secant[i]), 0], 'r-')
        plt.plot([x_secant[i+1], x_secant[i+1]], [0, df(x_secant[i+1])], 'r-')

    plt.xlabel("x")
    plt.ylabel("f'(x)")
    plt.title("Derivative with Method Progression")
    plt.legend(["$f'(x)$", "Newton", "Secant"])
    plt.grid()
    #plt.show()
    plt.savefig("secant_derivative.png")

# Run the plots
plot_function_vs_iteration()
```

Conclusions from the comparison:
Convergence Rate: Newton's method typically exhibits quadratic convergence, meaning the error de-





creases exponentially with each iteration when close to the root. The secant method generally has a convergence rate of approximately 1.618 (the golden ratio), which is superlinear but slower than Newton's method.
Initial Guess Sensitivity: Newton's method requires a good initial guess to ensure convergence, as poor initial guesses can lead to divergence or convergence to an unintended root. The secant method, while generally more robust to initial guesses, can still fail to converge if the initial guesses are not chosen appropriately.
Computational Efficiency: If derivative computation is costly or impractical, the secant method may be preferred despite its slower convergence rate. However, if the derivative is readily available and computationally inexpensive, Newton's method's faster convergence can lead to quicker results.

## Exercise 5$^+$ (7.1)

Direct methods are able to use only zero-order information—evaluations of $f$. How many evaluations are needed to approximate the derivative and the Hessian of an $n$-dimensional objective function using finite difference methods? Why do you think it is important to have zero-order methods?

**Solution:**
The derivative has $n$ terms whereas the Hessian has $n^2$ terms. Each derivative term requires two evaluations when using finite difference methods: $f(\mathbf{x})$ and $f(\mathbf{x} + h\mathbf{e}_i)$. Each Hessian term requires an additional evaluation when using finite difference methods:

$$\frac{\partial^2 f}{\partial x_i \partial x_j} \approx f(\mathbf{x} + h\mathbf{e}(i) + h\mathbf{e}(j)) - f(\mathbf{x} + h\mathbf{e}(i)) - f(\mathbf{x} + h\mathbf{e}(j)) + f(\mathbf{x})$$

Thus, to approximate the gradient, you need $n + 1$ evaluations, and to approximate the Hessian you need on the order of $n^2$ evaluations. Approximating the Hessian is prohibitively expensive for large $n$. Direct methods can take comparatively more steps using $n^2$ function evaluations, as direct methods need not estimate the derivative or Hessian at each step.

## Exercise 6$^*$

Implement the extended Rosenbrock function

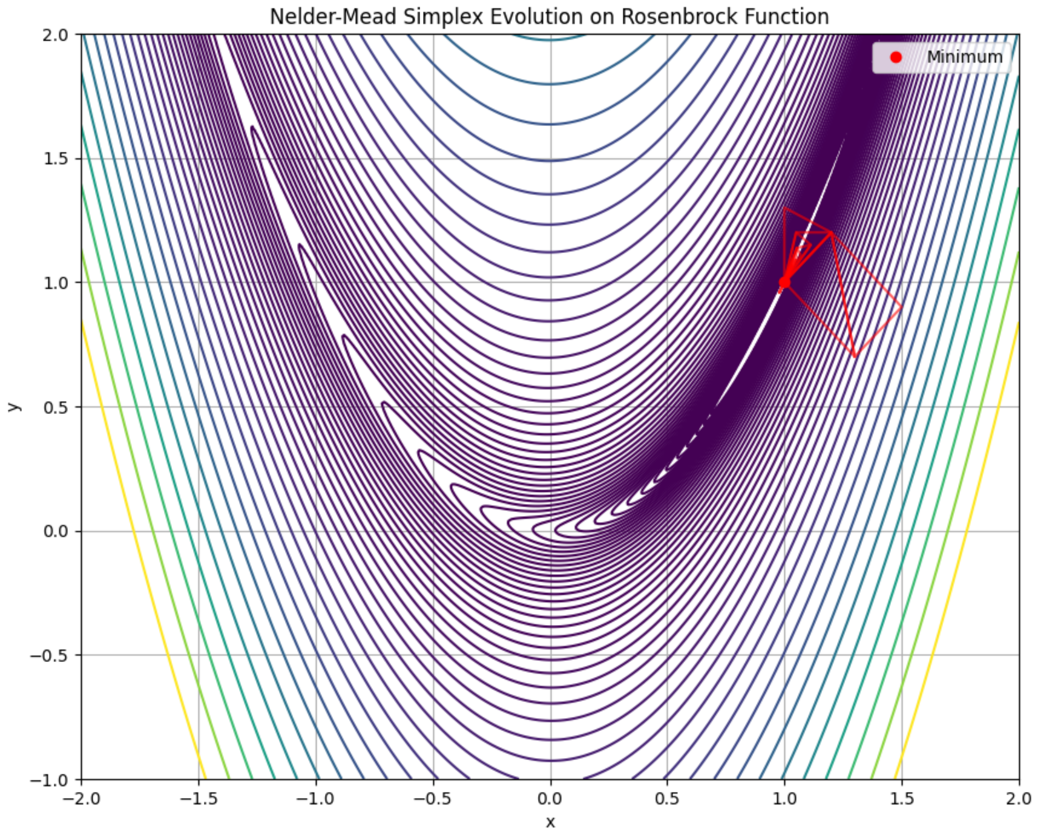
$$f(x) = \sum_{n/2}^{i=1} \left[a(x_{2i} - x_{2i-1}^2)^2 + (1 - x_{2i-1})^2\right]$$

where $a$ is a parameter that you can vary (for example, 1 or 100). The minimum is $\mathbf{x}^* = [1, 1, \ldots, 1]$, $f(\mathbf{x}^*) = 0$. Consider as starting point $[-1, -1, ..., -1]$.
Solve the minimization problem with scipy.optimize using all methods seen in class that are suitable for this task. Observe the behavior of the calls for various values of parameters, for example, for the L-BFGS algorithm the memory parameter $m$.

## Exercise 7

Below you find an implementation of Nelder-Mead algorithm in Python. Analyze it and use it to solve the Rosenbrock function in 2D. Plot the evolution of the simplex throughout the search (you can get help from chatGPT to code the plottig facilities).

```
import numpy as np
import matplotlib.pyplot as plt

def nelder_mead(f, S, eps, alpha=1.0, beta=2.0, gamma=0.5):
    delta = float("inf")
    y_arr = np.array([f(x) for x in S])
    simplex_history = [S.copy()]

    while delta > eps:
        # Sort by objective values (lowest to highest)
        p = np.argsort(y_arr)
        S, y_arr = S[p], y_arr[p]
        xl, yl = S[0], y_arr[0] # Lowest
        xh, yh = S[-1], y_arr[-1] # Highest
        xs, ys = S[-2], y_arr[-2] # Second-highest
        xm = np.mean(S[:-1], axis=0) # Centroid

        # Reflection
        xr = xm + alpha * (xm - xh)
        yr = f(xr)

        if yr < yl:
            # Expansion
            xe = xm + beta * (xr - xm)
            ye = f(xe)
            S[-1], y_arr[-1] = (xe, ye) if ye < yr else (xr, yr)
        elif yr >= ys:
            if yr < yh:
                xh, yh = xr, yr
                S[-1], y_arr[-1] = xr, yr
            # Contraction
            xc = xm + gamma * (xh - xm)
            yc = f(xc)
            if yc > yh:
                # Shrink
                for i in range(1, len(S)):
                    S[i] = (S[i] + xl) / 2
                    y_arr[i] = f(S[i])
            else:
                S[-1], y_arr[-1] = xc, yc
        else:
            S[-1], y_arr[-1] = xr, yr

        simplex_history.append(S.copy())
        delta = np.std(y_arr, ddof=0)

    return S[np.argmin(y_arr)], simplex_history

if __name__ == "__main__":
    # Test function: Rosenbrock function
    def rosenbrock(x):
        return (1 - x[0])**2 + 100 * (x[1] - x[0]**2)**2

    # Initial simplex
    S = np.array([[1.3, 0.7], [1.5, 0.9], [1.2, 1.2]])
    epsilon = 1e-6

    result, simplex_history = nelder_mead(rosenbrock, S, epsilon)
    print("Minimum found at:", result)
    print("Function value at minimum:", rosenbrock(result))

    # Plotting
    x = np.linspace(-2, 2, 400)
```



```
    y = np.linspace(-1, 2, 400)
    X, Y = np.meshgrid(x, y)
    Z = (1 - X)**2 + 100 * (Y - X**2)**2

    plt.figure(figsize=(10, 8))
    plt.contour(X, Y, Z, levels=np.logspace(-1, 3, 50), cmap="viridis")

    for simplex in simplex_history:
        plt.plotzip(*np.vstack([simplex, simplex[0]])), "r-", alpha=0.6)plt.plot(result[0],
            result[1], "ro", label="Minimum")plt.title("Nelder-Mead Simplex Evolution on
            Rosenbrock
            Function")plt.xlabel("x")plt.ylabel("y")plt.legend()plt.grid(True)plt.savefig("nelder.png")
```