This set covers chapters 5–11 of the book *Numerical Optimization* by Nocedal and Wright, 2nd ed.

From the book, the following exercises: 5.1–5.3, 5.6, 5.8, 5.11, 6.1–6.4, 6.6, 7.1–7.3, 7.5–7.6, 8.1, 8.3, 9.2(a), 9.8–9.9, 10.1–10.2, 10.6, 11.1–11.3, 11.5, 11.8, 11.10. In addition, the exercises below. The Matlab programming exercises are 5.1, 5.8, 7.1 and **II.3–II.4**.

For exercise 5.8, try 2 different matrices **A** generated as follows:

```
% Matrix 1: uniform spectrum
n = 100; l = 1:n; U = gallery('orthog',n); A = U*diag(l)*U';
% Matrix 2: clustered spectrum; try s = 5, 1, 0.001, 0
n = 100; n1 = floor(n/4);
l = [ones(1,n1) n/5*ones(1,n1) n*ones(1,n-2*n1)]; rand('state',314); l = l + s*rand(1,n);
U = gallery('orthog',n); A = U*diag(l)*U';
```

and compare your results with figs. 5.4–5.5.

Hint for exercise 6.1(a): a function is strongly convex on a convex domain if at each point in the domain all the eigenvalues of the Hessian are positive and bounded away from zero.

II.1. Conjugate directions. Let **A** be a real, symmetric, positive definite, $n \times n$ matrix with eigenvectors $\mathbf{U} = (\mathbf{u}_1, \ldots, \mathbf{u}_n)$ and associated eigenvalues $\mathbf{\Lambda} = \mathrm{diag}(\lambda_1, \ldots, \lambda_n)$ (in matrix form). Show that: (i) If $\mathbf{R} = \mathbf{U}\mathbf{\Lambda}^{1/2}\mathbf{Q}$, where **Q** is any orthogonal matrix, then $\mathbf{A} = \mathbf{R}\mathbf{R}^T$. (ii) If $\{\mathbf{v}_1, \ldots, \mathbf{v}_n\}$ are nonzero orthogonal vectors then $\{\mathbf{p}_1, \ldots, \mathbf{p}_n\}$ where $\mathbf{p}_i = \mathbf{R}^{-T}\mathbf{v}_i$ are conjugate w.r.t. **A** (this shows there is an infinite number of conjugate direction sets). (iii) $\mathbf{p}_i = \mathbf{u}_i$ are conjugate w.r.t. **A** (this corresponds to the change of variables $\hat{\mathbf{x}} = \mathbf{S}^{-1}\mathbf{x}$ with $\mathbf{S} = \mathbf{U}$). Hint: use the spectral theorem.

II.2. Quasi-Newton methods. Verify that, in 1D, all 3 quasi-Newton methods BFGS, DFP and SR1 are equivalent to the secant method, where $B_{k+1} = \frac{f'_{k+1} - f'_k}{x_{k+1} - x_k}$ independent of B_k.

II.3. BFGS. Implement algorithm 6.1 (BFGS method) in Matlab with $\mathbf{H}_0 = \mathbf{I}$ and backtracking line search (with initial step length 1). Apply it to the Rosenbrock function (2.23) from two initial points $\mathbf{x}_0 = (1.2, 1.2)$ and $\mathbf{x}_0 = (-1.2, 1)$ (cf. exercise 3.1). Tabulate $\|\mathbf{x}_k - \mathbf{x}^*\|_2$, $\|\nabla f(\mathbf{x}_k)\|_2$ and $\|\mathbf{B}_k - \nabla^2 f(\mathbf{x}_k)\|_F$ where $\|\cdot\|_2$ is the Euclidean norm (for vectors) and $\|\cdot\|_F$ the Frobenius norm (for matrices). Use your `convseq` function to estimate the convergence rate.

II.4. Newton-CG. Program a pure Newton iteration without line searches, where the search direction is computed by the CG method. Select stopping criteria such that the rate of convergence is linear, superlinear, and quadratic. Try your program on the following quartic function:

$$f(\mathbf{x}) = \frac{1}{2}\mathbf{x}^T\mathbf{x} + \frac{1}{4}\sigma(\mathbf{x}^T\mathbf{A}\mathbf{x})^2, \ \mathbf{x} \in \mathbb{R}^n$$

where **A** is symmetric pd of $n \times n$ and $\sigma \geq 0$ is a parameter that allows us to control the deviation from a quadratic. Use a random starting point $\mathbf{x}_0 \in \mathbb{R}^n$. Try $\sigma = 1$ or larger values (e.g. 100, 1 000) and observe the rate of convergence of the iteration. For example:

```
sigma = 1000; A = rand(n,n); A = sqrt(sigma)*A*A'; x0 = 10*randn(n,1);
```

Use the `convseq` function you wrote in exercise **I.4** to estimate the convergence rate. To see differences in convergence rate, you may have to use a relatively large n (e.g. 1 000).

Also:

1. Prove that f is a strictly convex function (hint: prove that its Hessian is pd everywhere). Find all the stationary points of f and classify them into minima, maxima and saddle points.

2. Compute the cost in multiplications in $\mathcal{O}$–notation of computing $f(\mathbf{x})$, $\nabla f(\mathbf{x})$ and $\nabla^2 f(\mathbf{x})$ at a point $\mathbf{x}$.

3. What would be the cost of computing $\nabla f(\mathbf{x})$ and $\nabla^2 f(\mathbf{x})$ approximately with finite differences if only function evaluations are allowed?

II.5. Finite differences. Using Matlab, compare numerically the true value of the derivative of a function with the value of a finite-difference approximation. That is, do a log-log plot of the absolute error $E = |f'(x) - \Delta_\epsilon f(x)|$ for different values of ϵ, where $\Delta_\epsilon f(x) = \frac{f(x+\epsilon)-f(x)}{\epsilon}$ for the forward difference and $\Delta_\epsilon f(x) = \frac{f(x+\epsilon)-f(x-\epsilon)}{2\epsilon}$ for the central difference. Apply it to the function $f(x) = x^3$ evaluated at $x = 1$ with $\epsilon \in \{10^{-16}, 10^{-15}, \ldots, 10^1\}$. Compare it with the rule of thumb for the value of ϵ.

II.6. Continuation method. Consider a nonlinear system of equations $\mathbf{r}(\mathbf{x}) = \mathbf{0}$, $\mathbf{x} \in \mathbb{R}^n$.

1. Write the homotopy function $H(\mathbf{x}, \lambda)$.

2. Write the equation that defines the tangent vector $(\dot{\mathbf{x}}, \dot{\lambda}) = \left(\frac{d\mathbf{x}}{ds}, \frac{d\lambda}{ds}\right)$ to the homotopy path $(\mathbf{x}(s), \lambda(s))$ (where s is the arc length).

3. Concisely describe how a homotopy method works in finding a root $\mathbf{x}^*$ of $\mathbf{r}(\mathbf{x})$.

4. Consider the case $r(x) = kx$, $x \in \mathbb{R}$.

   (a) Write the homotopy function $H(x, \lambda)$.

   (b) For fixed λ, find its root(s) $x^*(\lambda)$.

   (c) Compute the path tangent direction (no need to find its length) using your equation from point 2. Verify it is correct by direct calculation of $dx^*(\lambda)/d\lambda$.

   (d) Sketch the homotopy path $x^*(\lambda)$ for $k = 2$ and $k = -2$.

   (e) Plot the homotopy function $H(x, \lambda)$ as a function of x for a few values of $\lambda \in [0, 1]$, for $k = 2$ and $k = -2$.

   (f) Give a condition on k for which a continuous path exists from $(x, \lambda) = (x_0, 0)$ to $(0, 1)$. Intuitively explain this condition based on the previous plots.