MS-C2105 - Introduction to Optimization
Lecture 11

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Outline of this lecture

Newton's method for constrained problems

Newton's method for constrained problems

- Using Newton's method to solve KKT conditions

Barrier method

Primal-dual path following interior point method

Reading: Taha: Chapter 20; Winston: Chapter 11

Solving non-linear constrained optimisation problems

There are several methods available to solve nonlinear problems.

- **local solvers:** packages that employ methods that search for solutions satisfying first-order optimality conditions.
- **global solvers:** combine local solvers and specialised search methods (e.g., spatial branching).

For convex problems, local solvers can find global optimal solutions. This is a desirable feature, since local solvers are typically more efficient computationally.

We focus on a provenly efficient local solver method: barrier (or interior point) methods. They combine two central ideas:

1. The employment of Newton's method to solve optimality (KKT) conditions;
2. The use of barrier functions to eliminate inequalities.

Newton's method with equality constraints

Newton's method can (also) be used to solve systems of nonlinear equations.

- Relies on first-order approximations that are successively solved as systems of linear equations.
- Can be used as a root finding (Newton-Raphson) method to solve the system of equations arising from KKT conditions.

Newton-Raphson (NR) method: Let $f : \mathbb{R}^n \to \mathbb{R}^n$, with $f_i : \mathbb{R}^n \to \mathbb{R}$ differentiable. We wish to find x^* (a root) that solves

$$f(x) = \begin{bmatrix} f_1(x) \\ \vdots \\ f_n(x) \end{bmatrix} = \begin{bmatrix} 0 \\ \vdots \\ 0 \end{bmatrix}.$$

- NR starts from an initial guess x^k for x^* and iterates by finding the root x^{k+1} of a linear approximations of f at x^k.
- Under suitable conditions, the sequence $\left\{x^k\right\}$ converges to x^*.

Newton's method with equality constraints

At x^k, the first-order approximation of $f(x)$ is

$$f(x^k + d) = f(x^k) + \nabla f(x^k)^\top d,$$

where $\nabla f(x^k)$ is the Jacobian of $f(x)$ given by

$$\nabla f(x^k) = \begin{bmatrix} \nabla f_1(x^k)^\top \\ \vdots \\ \nabla f_n(x^k)^\top \end{bmatrix}.$$

We want to obtain d such that $f(x^k + d) = 0$. Therefore

$$\begin{aligned} f(x^k) + \nabla f(x^k)^\top d &= 0 \\ d &= -\nabla f(x^k)^{-1} f(x^k). \end{aligned}$$

The vector d is called Newton direction.

Newton's method with equality constraints

Algorithm Newton-Raphson method

initialise. tolerance $\epsilon > 0$, initial point x^0, iteration count $k = 0$.
while $||d|| > \epsilon$ **do**
    $d = -\nabla f(x^k)^{-1} f(x^k)$
    $x^{k+1} = x^k + d$
    $k = k + 1$
end while
return x^k

Remarks:

1. NR assumes that the Jacobian is invertible;
2. It is more efficient to solve $\nabla f(x^k)d = -f(x^k)$ using an appropriate operator than calculating inverses;
3. If x_0 is too far from optimal, NR might not converge;

Newton's method with equality constraints

Example: find the root of f with $x^0 = (1, 0, 1)$ and $\epsilon = 0.01$.

$$f(x) = \begin{bmatrix} f_1(x) \\ f_2(x) \\ f_3(x) \end{bmatrix} = \begin{bmatrix} x_1^2 + x_2^2 + x_3^2 - 3 \\ x_1^2 + x_2^2 - x_3 - 1 \\ x_1 + x_2 + x_3 - 3 \end{bmatrix}$$

The Jacobian is given by $\nabla f(x) = \begin{bmatrix} 2x_1 & 2x_2 & 2x_3 \\ 2x_1 & 2x_2 & -1 \\ 1 & 1 & 1 \end{bmatrix}$.

$$d^0 = -[\nabla f(x^0)]^{-1} f(x^0) = -\begin{bmatrix} 2 & 0 & 2 \\ 2 & 0 & -1 \\ 1 & 1 & 1 \end{bmatrix}^{-1} \begin{bmatrix} -1 \\ -1 \\ -1 \end{bmatrix} = \begin{bmatrix} 1/2 \\ 1/2 \\ 0 \end{bmatrix}$$

Thus $x^1 = x^0 + d^0 = \begin{bmatrix} 3/2 & 1/2 & 1 \end{bmatrix}$. As $||x^1 - x^0|| = ||d^0|| \approx 0.7$, the method carries on until $||d^k|| < \epsilon$.

$x^* = (1, 1, 1)$ is reached after approx. 20 iterations.

Newton's method with equality constraints

NR can be employed to solve the KKT conditions of equality-constrained optimisation problems. Consider the problem

$$\begin{aligned} \text{min. } & f(x) \\ \text{s.t.: } & Ax = b \end{aligned}$$

First, consider the second-order Taylor approximation of f at x^k, where $Ax^k = b$.

$$f(x^k + \Delta x) = f(x^k) + \nabla f(x^k)^\top \Delta x + \frac{1}{2} \Delta x H(x^k) \Delta x,$$

where $H(x^k)$ is the Hessian of f at x^k and $\Delta x = x - x^k$.

The KKT conditions for the second-order approximation problem state that $x^k + \Delta x$ is optimal if exists μ such that

$$\nabla f(x^k) + H(x^k)\Delta x + A^\top \mu = 0 \tag{1}$$

$$A(x^k + \Delta x) = b \Rightarrow A\Delta x = 0 : \tag{2}$$

Using Newton's method to solve KKT conditions

These conditions are typically stated in the matrix form

$$\begin{bmatrix} H(x) & A^\top \\ A & 0 \end{bmatrix} \begin{bmatrix} \Delta x \\ \mu \end{bmatrix} = \begin{bmatrix} -\nabla f(x) \\ 0 \end{bmatrix},$$

which is known as the Newton system.

Remarks:

- the 2^{nd}-order approximation allows for solving nonlinear optimisation problems (with linear constraints) by successively solving linear systems.
- A linearisation approach can be applied to handle nonlinear equality constraints.
- Notice that the iteration index k is omitted in this matrix form.

Using Newton's method to solve KKT conditions

Example: min. $\left\{x_1^2 - 2x_1x_2 + 4x_2^2 : 0.1x_1 - x_2 = 1\right\}$ with $x^0 = [11, 0.1]^\top$.

$\nabla f(x) = \begin{bmatrix} 2x_1 - 2x_2 \\ -2x_1 + 8x_2 \end{bmatrix}$; $H(x) = \begin{bmatrix} 2 & -2 \\ -2 & 8 \end{bmatrix}$; $A = [0.1, -1]$.

The Newton system is given by:

$$\begin{bmatrix} H(x) & A^\top \\ A & 0 \end{bmatrix} \begin{bmatrix} \Delta x \\ \mu \end{bmatrix} = \begin{bmatrix} -\nabla f(x) \\ 0 \end{bmatrix} = \begin{bmatrix} 2 & -2 & 0.1 \\ -2 & 8 & -1 \\ 0.1 & -1 & 0 \end{bmatrix} \begin{bmatrix} \Delta x_1 \\ \Delta x_2 \\ \mu \end{bmatrix} = \begin{bmatrix} -2x_1 + 2x_2 \\ 2x_1 - 8x_2 \\ 0 \end{bmatrix}.$$

For x^0, we obtain $d^1 = [\Delta x^1, \mu^1]^\top = [-11.714, -1.171, -7.142]^\top$, making $x^1 = x^0 + [-11.714, -1.171]^\top = [-0.714, -1.071]^\top$.

Remarks:

- x^1 is optimal for the problem;
- one can test for optimality by checking the KKT conditions for x^k using (1) and (2).

The barrier method

The next step towards a comprehensive optimisation framework is to deal with inequality constraints in problems of the form

$$\begin{aligned}(P) : \text{min. } & f(x) \\ \text{s.t.: } & g_i(x) \leq 0, \ i = 1, \dots, m \\ & Ax = b.\end{aligned}$$

We rely on the framework of barrier functions to represent the feasibility conditions imposed by inequality constraints.

For that, we reformulate problem P using a feasibility indicator function I that reacts to infeasibility in $g_i(x) \leq 0$, $\forall i \in \{1, \dots, m\}$.

$$\begin{aligned}\text{min. } & f(x) + \sum_{i=1}^{m} I(g_i(x)) \\ \text{s.t.: } & Ax = b,\end{aligned}$$

with $I : \mathbb{R} \to \mathbb{R}$ given by

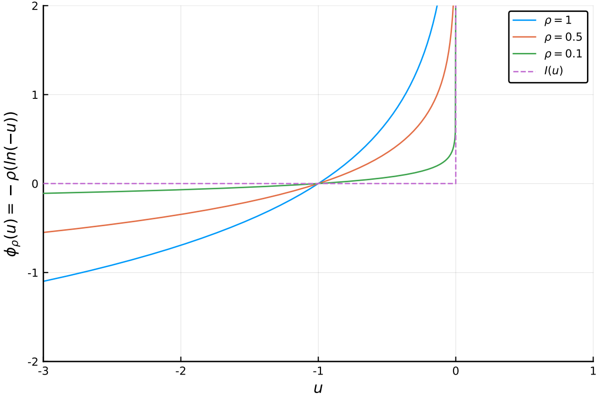
$$I(u) = \begin{cases} 0, & \text{if } u \leq 0 \\ \infty, & \text{if } u > 0 \end{cases}$$

The barrier method

To alleviate the numerical issues caused by the discontinuity of I, we approximate the indicator function using a logarithmic barrier.

$$\Phi_\rho(u) = -\rho \ln(-u)$$

where $\rho > 0$ sets the accuracy of the barrier term $\Phi_\rho(u)$.



The barrier method

Using Φ_ρ as the barrier function, the barrier problem B_ρ can be formulated as

$$(B_\rho) : \text{min. } f(x) - \rho \sum_{i=1}^{m} \ln(-g_i(x))$$
$$\text{s.t.: } Ax = b.$$

Remarks:

- Notice that the barrier problem can be solved employing NR method to its first-order optimality conditions.
- At each NR iteration, one can gradually decrease ρ by making $\rho^{k+1} = \beta\rho$ with $\beta \in (0, 1)$ (known as SUMT[1]).
- As $\rho \to 0$, $x^*(\rho) \to x^*$, where $x^*(\rho)$ and x^* are the optimal values for problems B_ρ and P, respectively.
- For small ρ, the barrier problem is challenging numerically.

[1] Sequential Unconstrained Minimisation Technique

The barrier method

Example: P : min. $\left\{f(x) = (x-3)^2 : x \geq 0\right\}$.

The barrier problem is given by

$$B_\rho : \text{min. } f(x) + \phi_\rho(x) = (x-3)^2 - \rho \ln(x)$$

The first order optimality condition for B_ρ is given by

$$\begin{aligned} & f'(x) + \phi'_\rho(x) = 0 \\ & 2(x-3) - \frac{\rho}{x} = 2x^2 - 6x - \rho = 0. \end{aligned}$$

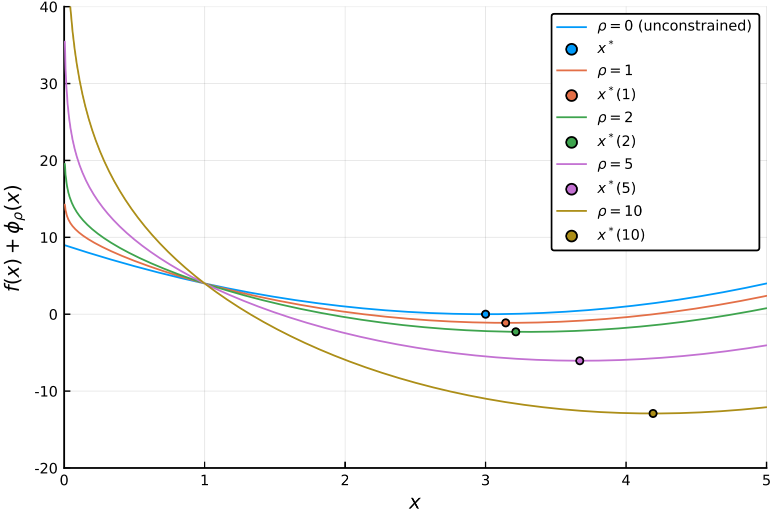
The positive solution (since $x \geq 0$) of $2x^2 - 6x - \rho = 0$ is given by

$$x^*(\rho) = \frac{6 + \sqrt{36 + 8\rho}}{4}.$$

Also, notice that $\lim_{\rho \to 0} x^*(\rho) = 3$, which is the optimal x^* for P.

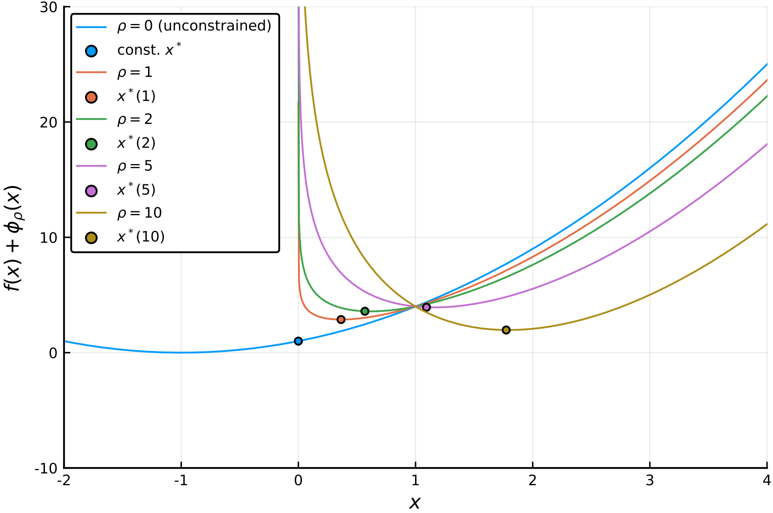
The barrier method

Example: min. $\left\{ f(x) = (x-3)^2 : x \geq 0 \right\}$



The barrier method

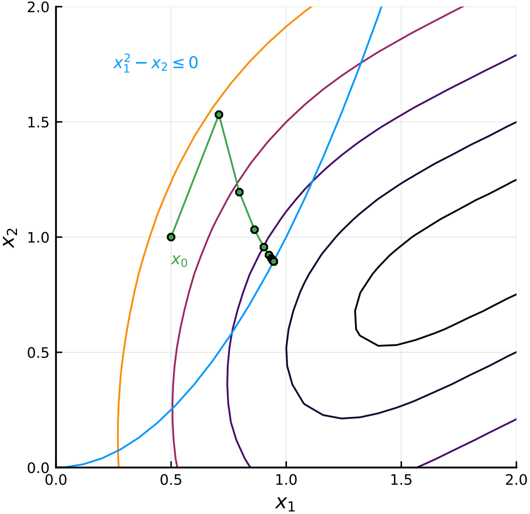
Example: min. $\left\{ f(x) = (x+1)^2 : x \geq 0 \right\}$.



The barrier method

Example:

min. $\left\{f(x) = (x_1 - 2)^4 + (x_1 - 2x_2)^2 : x_1^2 - x_2 \leq 0\right\}$.



The primal-dual interior point (IP) method

The barrier framework is remarkably efficient for solving linear (or quadratic with linear constraints) optimisation problems

- differently from simplex method, it can be shown to have polynomial complexity.
- practice has shown great performance for large-scale optimisation problems.
- can be generalised of other classes of nonlinear problems.

We start with a linear problem in the standard form and formulate the barrier problem as follows.

$$(P): \text{min. } c^\top x \quad \text{s.t.: } Ax = b, \quad x \geq 0$$

$$(B_\rho): \text{min. } c^\top x - \rho \sum_{i=1}^{n} \ln(x_i) \quad \text{s.t.: } Ax = b$$

The primal-dual interior point (IP) method

Let $X = \mathbf{diag}(x)$, and e be a vector of 1's of adequate size. Thus $X^{-1} = \mathbf{diag}\left(\frac{1}{x}\right)$ and $X^{-1}e = \left(\dots \frac{1}{x_i} \dots\right)^\top$.

The KKT conditions for B_ρ can be stated as follows. First, we define the Lagrangian function

$$L(x, \mu) = c^\top x - \rho \sum_{i=1}^{n} \ln(x_i) - \mu^\top (b - Ax)$$

which leads to the following KKT (optimality) conditions:

$$\begin{aligned} \frac{\partial L(x,\mu)}{\partial x} &= c - \rho X^{-1}e - A^\top \mu = 0 \\ \frac{\partial L(x,\mu)}{\partial \mu} &= b - Ax = 0. \end{aligned}$$

Remark: notice that KKT are also sufficient for global optimality.

The primal-dual interior point (IP) method

Let $z = \rho X^{-1} e$. Then $Xz = \rho e$ or $XZe = \rho e$, with $Z = \mathbf{diag}(z)$. The KKT optimality conditions can be rewritten as

$$\begin{aligned} A^\top \mu + z &= c \\ Ax &= b \\ XZe &= \rho e. \end{aligned} \tag{3}$$

The Newton system for solving (3) using RN can be stated as

$$\begin{bmatrix} 0 & A^\top & I \\ A & 0 & 0 \\ Z & 0 & X \end{bmatrix} \begin{bmatrix} \Delta x \\ \Delta \mu \\ \Delta z \end{bmatrix} = - \begin{bmatrix} A^\top \mu + z - c \\ Ax - b \\ XZe - \rho e \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \\ -XZe + \rho e \end{bmatrix}. \tag{4}$$

Remark: the second equality in (4) is due to primal $(Ax = b)$ and dual $(A^\top \mu + z = c)$ feasibility.

The primal-dual interior point (IP) method

Algorithm Primal-dual interior point method for LP

1: **initialise.** primal-dual feasible $w^k = (x^k, \mu^k, z^k)$, $\epsilon > 0$, ρ^k, $\beta \in (0,1)$, $k = 0$.
2: **while** $|Ax - b| > \epsilon$ and $|A^\top \mu + z - c| > \epsilon$ **do**
3: compute $\Delta w^{k+1} = (\Delta x^{k+1}, \Delta \mu^{k+1}, \Delta z^{k+1})$ using (4) and w^k.
4: $w^{k+1} = w^k + \Delta w^{k+1}$
5: $\rho^{k+1} = \beta \rho^k$, $k = k + 1$
6: **end while**
7: **return** w^k.

Remarks:

- Notice that, as $\rho \to 0$, (3) become closer to the optimality conditions for LP.
- Instead of finding optimal $x^*(\rho)$ for each ρ, the method takes a single Newton step before reducing ρ.
- Interior point methods have polynomial complexity $(O(\sqrt{n} \log \frac{1}{\epsilon}))$.

The primal-dual interior point (IP) method

Example:

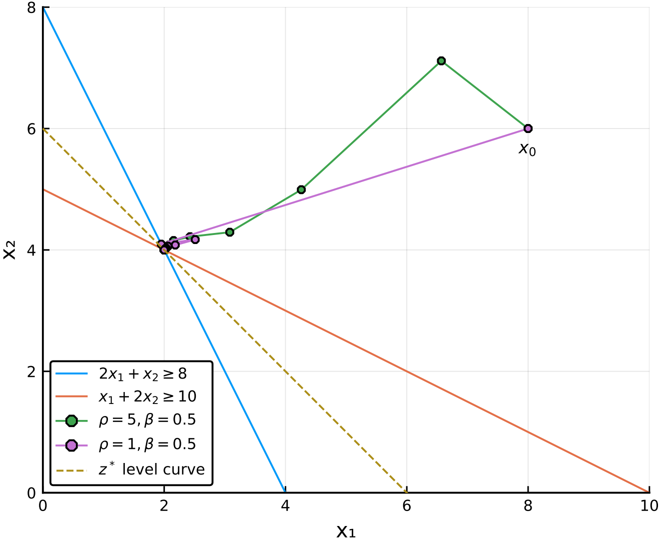
min. $\{f(x) = x_1 + x_2 : 2x_1 + x_2 \geq 8,\ x_1 + 2x_2 \geq 10,\ x_1, x_2 \geq 0\}$.

In the standard from, $A = \begin{bmatrix} 2 & 1 & -1 & 0 \\ 1 & 2 & 0 & -1 \end{bmatrix}$.

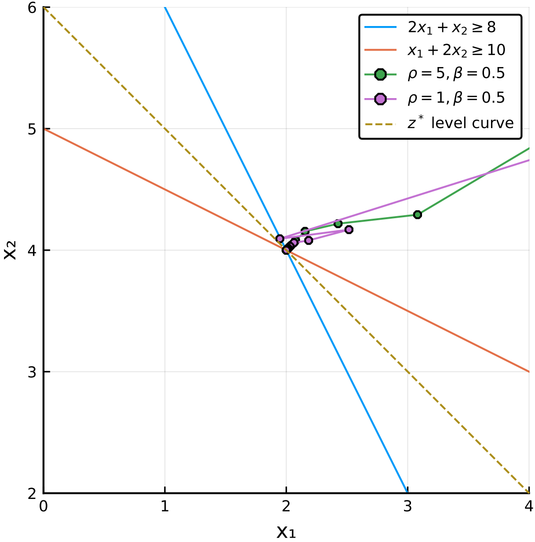
The Newton system is given by

$$\begin{bmatrix}
0 & 0 & 0 & 0 & 2 & 1 & 1 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 1 & 2 & 0 & 1 & 0 & 0 \\
0 & 0 & 0 & 0 & -1 & 0 & 0 & 0 & 1 & 0 \\
0 & 0 & 0 & 0 & 0 & -1 & 0 & 0 & 0 & 1 \\
2 & 1 & -1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
1 & 2 & 0 & -1 & 0 & 0 & 0 & 0 & 0 & 0 \\
z_1^k & 0 & 0 & 0 & 0 & 0 & x_1^k & 0 & 0 & 0 \\
0 & z_2^k & 0 & 0 & 0 & 0 & 0 & x_2^k & 0 & 0 \\
0 & 0 & z_3^k & 0 & 0 & 0 & 0 & 0 & x_3^k & 0 \\
0 & 0 & 0 & z_4^k & 0 & 0 & 0 & 0 & 0 & x_4^k
\end{bmatrix}
\begin{bmatrix} \Delta x_1 \\ \Delta x_2 \\ \Delta x_3 \\ \Delta x_4 \\ \Delta \mu_1 \\ \Delta \mu_2 \\ \Delta z_1 \\ \Delta z_2 \\ \Delta z_3 \\ \Delta z_4 \end{bmatrix}
=
\begin{bmatrix} 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ -x_1^k z_1^k + \rho^{k+1} \\ -x_2^k z_2^k + \rho^{k+1} \\ -x_3^k z_3^k + \rho^{k+1} \\ -x_4^k z_4^k + \rho^{k+1} \end{bmatrix}$$

The primal-dual interior point (IP) method



The barrier method



The primal-dual interior point (IP) method

Example: max. $z = x_1 + x_2 : \frac{1}{3}x_1 + x_2 \leq 5,\ \frac{1}{5}x_1 - x_2 \leq -1,$
$-\frac{8}{3}x_1 - x_2 \leq -8,\ \ \frac{1}{2}x_1 + x_2 \leq 9,\ x_1 - x_2 \leq 4, x_1, x_2 \geq 0$