Equality Constrained Optimization

- Problem Formulation
- Optimization Problems with Linear Equality Constraints
- Optimization Problems with Nonlinear Equality Constraints

Contents

Problem Formulation

Let $F : \mathbb{R}^n \to \mathbb{R}$ and $G : \mathbb{R}^n \to \mathbb{R}^m$ be given twice continuously differentiable functions. We are searching for solutions of the minimization problem

$$\min_x F(x) \qquad \text{s.t.} \qquad G(x) = 0$$

Simple examples:

- For $F(x) = x_1^2 + x_2^2$ and $G(x) = x_1 + x_2 - 1$ the solution is $x_1 = x_2 = \frac{1}{2}$.
- More generally, for $F(x) = \|x\|_2^2$ and $G(x) = Ax - b$ the aim is to find the solution x of the equation $Ax = b$ whose norm is minimal.
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Optimization Problems with Linear Equality Constraints

Let us first consider the special case that the equality constraints are linear,

$$\min_x F(x) \qquad \text{s.t.} \qquad Ax - b = 0 \; .$$

In the following, we assume that the matrix $A \in \mathbb{R}^{m \times n}$ has full rank (and $m \leq n$).

Elimination of Linear Equality Constraints

Since we assume that A has full rank we can compute a QR factorization as

$$A = Q[R_1 R_2]$$

with R_1 being an upper triangular and invertible matrix. (we permute the components of x if necessary)

This implies that the components $x = (y^T, z^T)^T$ of the vector x satisfy

$$y = R_1^{-1} \left[Q^T b - R_2 z \right] \ .$$

Now, we can eliminate y explicitly and solve

$$\min_z \ \tilde{F}(z) \qquad \text{with} \qquad \tilde{F}(z) = F\left(\begin{pmatrix} R_1^{-1} \left[Q^T b - R_2 z \right] \\ z \end{pmatrix} \right) \ ,$$

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A Closer Look at the Newton iterates

If we apply a Newton type method with $\tilde{M}(z) = \tilde{F}''(z)$ to the reduced optimization problem

$$\min_{z} \ \tilde{F}(z)$$

the step direction Δz_k is found by solving the quadratic optimization optimization problems

$$\min_{\Delta z} \ \tilde{F}(z) + \tilde{F}'(z)\Delta z + \frac{1}{2}\Delta z^T \tilde{M}(z)\Delta z$$

as long as $\tilde{F}''(z)$ is positive definite; the next iterate is $z^+ = z + \alpha\Delta z$.

This is the same as solving the quadratic optimization problem

$$\min_{\Delta x} \ F(x) + F'(x)\Delta x + \frac{1}{2}\Delta x^T M(x)\Delta x \qquad \text{s.t.} \qquad A(x + \Delta x) - b = 0$$

with $M(x) = \tilde{F}''(x)$ associating $\Delta x = \left(\Delta y^T \Delta z^T\right)^T$.

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A Closer Look at the Newton iterates

Proof:

The derivatives of the function

$$\tilde{F}(z) = F\left(Wz + w\right) \quad \text{with} \quad W = \begin{pmatrix} -R_1^{-1} R_2 \\ I \end{pmatrix}, \;\; w = \begin{pmatrix} R_1^{-1} Q^T b \\ 0 \end{pmatrix}$$

can be written in the form

$$\tilde{F}'(z) = F'(x)\, W \quad \text{and} \quad \tilde{F}''(z) = W^T F''(x)\, W$$

The statement from the previous slide follows then by substituting $\Delta x = W \Delta z$. (Also notice the relations $AW = 0$ and $Aw = b$.)

A Closer Look at the Newton iterates

The Newton iterates for the equality constrained problem also satisfy

$$\begin{pmatrix} M(x) & A^T \\ A & 0 \end{pmatrix} \begin{pmatrix} \Delta x \\ \lambda \end{pmatrix} = \begin{pmatrix} -F'(x)^T \\ b - Ax \end{pmatrix}$$

The auxiliary variable λ is called the dual iterate.

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Karush-Kuhn-Tucker (KKT) Matrix

The matrix

$$\begin{pmatrix} F''(x) & A^T \\ A & 0 \end{pmatrix}$$

is called Karush-Kuhn-Tucker (KKT) matrix.

- The KKT matrix is invertible if for all $x \neq 0$ with $Ax = 0$ the inequality $x^T F''(x) x > 0$ is satisfied. (i.e., if the Hessian matrix is positive definite on the null-space of the linear equality constraints)
- This is condition is equivalent to stating that the matrix $\tilde{F}''(z) = W^T F''(x) \, W$ is positive definite. (this is the case if z is a "regular" local minimizer of $\tilde{F}$.)

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Summary: Newton-type methods for Optimization Problems with Linear Equality Constraints

1. Choose an initial guess $x_0 \in \mathbb{R}^n$ and termination tolerance $\epsilon > 0$.
2. **Repeat:**
   - 2.1 Choose a positive definite Hessian approximation $M(x_k) \approx F''(x_k)$.
   - 2.2 Solve the KKT system

$$\begin{pmatrix} M(x_k) & A^T \\ A & 0 \end{pmatrix} \begin{pmatrix} \Delta x_k \\ \lambda \end{pmatrix} = \begin{pmatrix} -F'(x_k)^T \\ b - Ax_k \end{pmatrix}$$

   - 2.3 Terminate if $|F'(x_k)\Delta x_k| + \sum_{i=0}^{m} |\lambda_i||A_i x_k + b_i| < \epsilon$.
   - 2.4 Choose a line-search parameter $\alpha \in [0,1]$ and set $x_{k+1} = x_k + \alpha \Delta x_k$, $k \leftarrow k+1$.
3. Output $x^* \approx x_k$ and $\lambda^* \approx \lambda$ as an approximate optimal solution.

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First Order Optimality Conditions

Let us come back to the general nonlinear equality constrained optimization problem

$$\min_x F(x) \qquad \text{s.t.} \qquad G(x) = 0$$

First Order Optimality Conditions: If x^* is a minimizer at which the matrix $A^* = G'(x^*)$ has full rank, then there exists a multiplier $\lambda \in \mathbb{R}^m$ such that

$$\begin{aligned} 0 &= F'(x^*)^T + G'(x^*)^T \lambda^* \\ 0 &= G(x^*) \end{aligned}$$

This condition is called the first order necessary KKT (Karush-Kuhn-Tucker) condition.

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Example

Unlike in the linear case, if the linear linear independence constraint qualification is not satisfied, an opimization problem might violate the first order KKT conditions: the problem

$$\min x \quad \text{s.t.} \quad x^2 = 0$$

has a solution at $x^* = 0$, but we have $G'(x^*) = 0$.

In this example, we cannot find a multiplier λ since the equation

$$0 = F'(x^*) + G'(x^*)\lambda = 1$$

is wrong. In practice such degeneracies can often be avoided: in the above example, we could replace the constraint $x^2 = 0$ by the equivalent constraint $x = 0$.

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Notation

The first order optimality conditions is sometimes written in the more compact form

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\begin{aligned}
0 &= \nabla_x L(x^*, \lambda^*) \\
0 &= G(x^*)
\end{aligned}
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where L denotes the so-called Lagrange function,

$$L(x, \lambda) = F(x) + G(x)^T \lambda \ .$$

The condition that the matrix $G'(x^*)$ has full rank, is in the literature often called "linear independence constraint qualification" (LICQ).

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Newton's Method for Equality Constrained Optimization

An important algorithm for solving equality constrained optimization problems is obtained by applying Newton's method to the equation

$$R(y) = \begin{pmatrix} \nabla_x L(x, \lambda) \\ G(x) \end{pmatrix} = 0 \qquad \text{with} \qquad y = \begin{pmatrix} x \\ \lambda \end{pmatrix} .$$

Here, the iterates have the form

$$y^+ = y - \alpha M(y)^{-1} R(y) \qquad \text{with} \qquad M(y) = \begin{pmatrix} H(x) & A(x)^T \\ A(x) & 0 \end{pmatrix} ,$$

where $H(x) \approx \nabla_x^2 L(x, \lambda)$ and $A(x) \approx G'(x)$ are the Hessian and constraint Jacobian approximation, respectively.

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is called the KKT-residuum. If we apply Newton's method,

$$y^+ = y - \alpha M(y)^{-1} R(y)$$

we need to compute $R(y)$ at every step.

Since we have to compute $G'(x)$ anyhow, we usually choose $A(x) = G'(x)$, i.e., the first order derivative of the function G is evaluated with high accuracy. (Expceptions are the so-called inexact sequential quadratic programming methods; not discussed in this lecture)

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Globalization

How do we measure progress towards a solution?

Recall: in unconstrained minimization, the main idea was to accept the next iterate "x^+" if $F(x^+)$ is sufficiently smaller than $F(x)$.

In equality constrained optimization we need to measure two things:

1. The objective value $F(x)$ and
2. the constraint violation $\|G(x)\|$.

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L1-penalty functions

One way to measure progress towards a solution is to introduce the L1-penalty function

$$\Phi(x) = F(x) + \sum_{i=1}^{m} \overline{\lambda}_i |G_i(x)| \ .$$

with $\overline{\lambda}_i$ being sufficiently large constants.

An important property of the function $\Phi(x)$ is that (under mild conditions) we have

$$F(x^*) = \Phi(x^*) \qquad \text{but also} \qquad \Phi(x) \geq F(x)$$

for all $x \in C$ for a compact domain $C \subseteq \mathbb{R}^n$ as long as the coefficients $\overline{\lambda}_i$ are sufficiently large.

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Armijo Line Search

Similar to unconstrained optimization, the line search parameter α can be found by using back-tracking until the Armijo condition

$$\Phi(x_k + \alpha_k \Delta x_k) \leq \Phi(x_k) + c\alpha_k D(\Phi(x_k), \Delta x_k)$$

for a constant $c \ll 1$ is satisfied. (This condition ensures that the line search parameter is not excessively large, although it is not sufficient to prove convergence in general.) Here, $D(\Phi(x_k), \Delta x_k)$ denotes the directional derivative

$$D(\Phi(x_k), \Delta x_k) = \lim_{\alpha \to 0^+} \frac{\Phi(x_k + \alpha \Delta x_k) - \Phi(x_k)}{\alpha}.$$

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Summary: Newton-type methods for Optimization Problems with Equality Constraints

1. Choose initial guesses $x_0 \in \mathbb{R}^n$ and $\lambda_0 \in \mathbb{R}^m$, tolerance $\epsilon > 0$.
2. **Repeat:**

   2.1 Choose a positive definite Hessian approximation $M(x_k) \approx F''(x_k) + \lambda_k^T G''(x_k)$ and set $A(x) = G'(x)$.

   2.2 Solve the KKT system

   $$\begin{pmatrix} M(x_k) & A(x_k)^T \\ A(x_k) & 0 \end{pmatrix} \begin{pmatrix} \Delta x_k \\ \tilde{\lambda}_{k+1} \end{pmatrix} = \begin{pmatrix} -\nabla_x L(x_k, \lambda_k) \\ -G(x_k) \end{pmatrix}$$

   2.3 Terminate if $|F'(x_k)\Delta x_k| + \sum_{i=0}^{m} |\lambda_i||G_i(x_k)| < \epsilon$.

   2.4 Choose a line-search parameter $\alpha \in [0, 1]$ and set $x_{k+1} = x_k + \alpha \Delta x_k$ as well as $\lambda_{k+1} = \lambda_k + \alpha(\lambda_{k+1} - \lambda_k)$, $k \leftarrow k + 1$.

3. Output $x^* \approx x_k$ and $\lambda^* \approx \lambda_k$ as an approximate optimal solution.

Summary: Newton-type methods for Optimization Problems with Equality Constraints

1. Choose initial guesses $x_0 \in \mathbb{R}^n$ and $\lambda_0 \in \mathbb{R}^m$, tolerance $\epsilon > 0$.
2. **Repeat:**
   2.1 Choose a positive definite Hessian approximation
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