Using GMRES in a Constraint Optimization Algorithm

Nenna Giulio, Ornella Elena Grassi

Computational Linear Algebra For Large Scale Problems

The aim of this homework is to implement the GMRES algorithm (Generalized minimal residual method) for solving linear systems and test its effectiveness in a quadratic constraint optimization problem. In particular, we will introduce an Interior Point Method (IPM) for solving a quadratic constraint optimization problem which is an iterative method that requires to solve two sparse large scale linear systems at each iteration. We will use our implementation of the GMRES algorithm to solve those linear systems and measure both the accuracy and the speed of the method compared to other linear solvers.

1 Problem Setting

The prototype of constrained quadratic programming problem that we are dealing with is the following:

$$\begin{aligned} \min_{\boldsymbol{x}\in\mathbb{R}^n} \quad & \frac{1}{2}\boldsymbol{x}^{\mathrm{T}}\mathbf{Q}\boldsymbol{x} + \boldsymbol{c}^{\mathrm{T}}\boldsymbol{x} \\ \text{subject to} \quad & \mathbf{A}\boldsymbol{x} = \boldsymbol{b}, \\ & \boldsymbol{x} \geq \mathbf{0}, \end{aligned} \tag{1.1}$$

Where $\mathbf{Q} \in \mathbb{R}^{n\times n}$ is a symmetric positive semi-definite matrix, $\boldsymbol{c} \in \mathbb{R}^n$, $\mathbf{A} \in \mathbb{R}^{K\times n}$ and $\boldsymbol{b} \in \mathbb{R}^K$ define K equality constraints. Problem 1.1 can be reformulated without equality constraints if we consider that:

$$\mathbf{A}\boldsymbol{x} = \boldsymbol{b} \iff \begin{cases} \mathbf{A}\boldsymbol{x} \geq \boldsymbol{b}, \\ \mathbf{A}\boldsymbol{x} \leq \boldsymbol{b}. \end{cases} \tag{1.2}$$

Hence we can write a new problem, equivalent to 1.1, in which there are only inequality constraints:

$$\begin{aligned} \min_{\boldsymbol{x}\in\mathbb{R}^n} \quad & \frac{1}{2}\boldsymbol{x}^{\mathrm{T}}\mathbf{Q}\boldsymbol{x} + \boldsymbol{c}^{\mathrm{T}}\boldsymbol{x} \\ \text{subject to} \quad & \hat{\mathbf{A}}\boldsymbol{x} \geq \hat{\boldsymbol{b}}, \end{aligned} \tag{1.3}$$

where $\hat{\mathbf{A}} \in \mathbb{R}^{(2K+n)\times n}$ and $\hat{\boldsymbol{b}} \in \mathbb{R}^{2K+n}$ are defined as

$$\hat{\mathbf{A}} = \begin{bmatrix} \mathbf{A} \\ -\mathbf{A} \\ \mathbf{I}_{n\times n} \end{bmatrix}, \qquad \hat{\boldsymbol{b}} = \begin{bmatrix} \boldsymbol{b} \\ -\boldsymbol{b} \\ \mathbf{0}_n \end{bmatrix}. \tag{1.4}$$

We will solve the constraint quadratic programming problem as formulated in 1.3 since this formulation is valid both for problems with and without equality constraints.

We can now define the corresponding Lagrangian function as:

$$\mathcal{L}(\boldsymbol{x}, \boldsymbol{\lambda}) := \frac{1}{2}\boldsymbol{x}^{\mathrm{T}}\mathbf{Q}\boldsymbol{x} + \boldsymbol{c}^{\mathrm{T}}\boldsymbol{x} + \hat{\boldsymbol{\lambda}}^{\mathrm{T}}(\hat{\mathbf{A}}\boldsymbol{x} - \hat{\boldsymbol{b}}) \tag{1.5}$$

where $\hat{\boldsymbol{\lambda}} \in \mathbb{R}^{2K+n}$ is the vector of Lagrangian multipliers associated with the inequality constraints and we can also write the corresponding KKT conditions:

$$\begin{cases} \mathbf{Q}\boldsymbol{x} + \boldsymbol{c} - \hat{\mathbf{A}}^{\mathrm{T}}\hat{\boldsymbol{\lambda}} = \mathbf{0} & \text{Stationarity condition,} \\ \hat{\mathbf{A}}\boldsymbol{x} - \hat{\boldsymbol{b}} \geq \mathbf{0} & \text{Primal feasibility,} \\ \hat{\boldsymbol{\lambda}} \geq \mathbf{0} & \text{Dual feasibility,} \\ \hat{\boldsymbol{\lambda}}^{\mathrm{T}}\left(\hat{\mathbf{A}}\boldsymbol{x} - \hat{\boldsymbol{b}}\right) = \mathbf{0} & \text{Complementary slackness condition.} \end{cases} \tag{1.6}$$

We can manipulate the system (1.6) in order to simplify the system of equations. In particular, we define a *slack variable* $\boldsymbol{y} := \hat{\mathbf{A}}\boldsymbol{x} - \hat{\boldsymbol{b}} \in \mathbb{R}^{2K+n}$ such that the KKT conditions becomes

$$\begin{cases} \mathbf{Q}\boldsymbol{x} + \boldsymbol{c} - \hat{\mathbf{A}}^{\mathrm{T}}\hat{\boldsymbol{\lambda}} = \mathbf{0} & \text{Stationarity condition,} \\ \boldsymbol{y} \geq \mathbf{0} & \text{Primal feasibility,} \\ \hat{\boldsymbol{\lambda}} \geq \mathbf{0} & \text{Dual feasibility,} \\ \hat{\mathbf{A}}\boldsymbol{x} - \hat{\boldsymbol{b}} - \boldsymbol{y} = \mathbf{0} & \text{Slack variable constraint,} \\ \hat{\boldsymbol{\lambda}}^{\mathrm{T}}\boldsymbol{y} = \mathbf{0} & \text{Complementary slackness condition.} \end{cases} \tag{1.7}$$

2 Predictor-Corrector IPM

Let's implement a Predictor-Corrector Interior Point Method for finding the solutions of the system (1.7). We can rewrite the problem as finding the zeros of the function $F : \mathbb{R}^{4K+3n} \to \mathbb{R}^{4K+3n}$

$$F(\boldsymbol{x}, \boldsymbol{y}, \boldsymbol{\lambda}) = \begin{bmatrix} \mathbf{Q}\boldsymbol{x} + \boldsymbol{c} - \hat{\mathbf{A}}^{\mathrm{T}}\hat{\boldsymbol{\lambda}} \\ \hat{\mathbf{A}}\boldsymbol{x} - \hat{\boldsymbol{b}} - \boldsymbol{y} \\ \mathbf{Y}\hat{\mathbf{\Lambda}}e \end{bmatrix} = \mathbf{0} \tag{2.1}$$

with the inequality constraints $\boldsymbol{y} = \hat{\mathbf{A}}\boldsymbol{x} - \hat{\boldsymbol{b}} \geq \mathbf{0}$ and $\hat{\boldsymbol{\lambda}} \geq \mathbf{0}$, where we have defined

$$\mathbf{Y} = \begin{bmatrix} y_1 & & \mathbf{0} \\ & \ddots & \\ \mathbf{0} & & y_n \end{bmatrix} \in \mathbb{R}^{(2K+n)\times(2K+n)}, \quad \hat{\mathbf{\Lambda}} = \begin{bmatrix} \hat{\lambda}_1 & & \mathbf{0} \\ & \ddots & \\ \mathbf{0} & & \hat{\lambda}_n \end{bmatrix} \in \mathbb{R}^{(2K+n)\times(2K+n)},$$

and $\boldsymbol{e} = [1, \ldots, 1]^{\mathrm{T}} \in \mathbb{R}^{2K+n}$. Since we will solve Equation (2.1) with the Newton method, we will need the Jacobian of F, which is computed as

$$\mathbf{J}_F = \begin{bmatrix} \mathbf{Q} & \mathbf{0} & -\hat{\mathbf{A}}^{\mathrm{T}} \\ \hat{\mathbf{A}} & -\mathbf{I} & \mathbf{0} \\ \mathbf{0} & \hat{\mathbf{\Lambda}} & \mathbf{Y} \end{bmatrix}.$$