CS 2601 Linear and Convex Optimization 12. Newton's method for equality constrained problems

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Outline

Equality constrained convex QP

Newton's method

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Equality constrained convex QP

$$\min_{\mathbf{x}} f(\mathbf{x}) = \frac{1}{2} \mathbf{x}^T \mathbf{Q} \mathbf{x} + \mathbf{g}^T \mathbf{x} + c$$
s.t. $A\mathbf{x} = \mathbf{b}$ (QP)

where $Q \in \mathbb{R}^n$, $Q \succeq O$, $A \in \mathbb{R}^{k \times n}$, rank A = k.

• The Lagrange/KKT conditions $\nabla \mathcal{L}(x^*, \lambda^*) = \mathbf{0}$ gives the KKT system of the problem,

$$\begin{cases} \nabla_{x} \mathcal{L}(x^{*}, \boldsymbol{\lambda}^{*}) = \boldsymbol{Q} x^{*} + \boldsymbol{g} + \boldsymbol{A}^{T} \boldsymbol{\lambda}^{*} = \boldsymbol{0} \\ \nabla_{\lambda} \mathcal{L}(x^{*}, \boldsymbol{\lambda}^{*}) = \boldsymbol{A} x^{*} - \boldsymbol{b} = \boldsymbol{0} \end{cases} \quad \text{or} \quad \begin{bmatrix} \boldsymbol{Q} & \boldsymbol{A}^{T} \\ \boldsymbol{A} & \boldsymbol{O} \end{bmatrix} \begin{bmatrix} \boldsymbol{x}^{*} \\ \boldsymbol{\lambda}^{*} \end{bmatrix} = \begin{bmatrix} -\boldsymbol{g} \\ \boldsymbol{b} \end{bmatrix}$$

The coefficient matrix $\mathbf{K} = \begin{bmatrix} \mathbf{Q} & \mathbf{A}^T \\ \mathbf{A} & \mathbf{O} \end{bmatrix}$ is called the KKT matrix.

• Any solution to the KKT system gives an optimal solution x^* with corresponding Lagrange multiplier λ^* .

Question. When is the KKT system solvable?

Lemma.

$$\operatorname{Null}(\textit{\textbf{K}}) = \left\{ egin{bmatrix} \textit{\textbf{d}} \\ \textit{\textbf{0}} \end{bmatrix} : \textit{\textbf{d}} \in \operatorname{Null}(\textit{\textbf{A}}) \cap \operatorname{Null}(\textit{\textbf{Q}})
ight\}$$

Proof. Denote the RHS by S. It is trivial that $S \subset \operatorname{Null}(K)$. To show $\operatorname{Null}(K) \subset S$. Let $\begin{bmatrix} d \\ \lambda \end{bmatrix} \in \operatorname{Null}(K)$, i.e. $Qd + A^T\lambda = 0$, Ad = 0. Then

$$d^{T}Qd = d^{T}(-A^{T}\lambda) = -(Ad)^{T}\lambda = -\mathbf{0}^{T}\lambda = 0$$

Since $Q \succeq O$, Qd = 0¹, so $d \in \text{Null}(A) \cap \text{Null}(Q)$ and $A^T \lambda = 0$. Since A^T has full column rank, $\lambda = 0$. Thus $\text{Null}(K) \subset S$.

$$0 = \mathbf{d}^T \mathbf{Q} \mathbf{d} = \mathbf{d}^T \left(\sum_{i=1}^n \alpha_i \beta_i \mathbf{v}_i \right) = \sum_{i=1}^n \alpha_i \beta_i \mathbf{d}^T \mathbf{v}_i = \sum_{i=1}^{n-1} \alpha_i \beta_i^2 \implies \alpha_i \beta_i^2 = 0, \forall i$$

so $\alpha_i \beta_i = 0$ for all i, and $\mathbf{Qd} = \sum_{i=1}^n \alpha_i \beta_i \mathbf{v}_i = \mathbf{0}$.

¹Proof. Let v_1, \ldots, v_n be an orthonormal eigenbasis of Q and $Qv_i = \alpha_i v_i$. Note $\alpha_i \geq 0$, since $Q \succeq O$. Expand d in the eigenbasis, $d = \sum_{i=1}^n \beta_i v_i$. Then $Qd = \sum_{i=1}^n \beta_i \alpha_i v_i$.

Solution of KKT system

Let $Ax_0 = b$ and $x = x_0 + d$. The problem QP is equivalent to

$$\min_{\boldsymbol{d}} f(\boldsymbol{x}_0 + \boldsymbol{d}) = f(\boldsymbol{x}_0) + \boldsymbol{g}^T \boldsymbol{d} + \boldsymbol{x}_0^T \boldsymbol{Q} \boldsymbol{d} + \frac{1}{2} \boldsymbol{d}^T \boldsymbol{Q} \boldsymbol{d}$$

s.t. $A\boldsymbol{d} = \boldsymbol{0}$

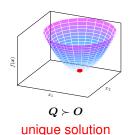
If $d_0 \in \text{Null}(A) \cap \text{Null}(Q)$, then d_0 is a feasible direction along which f reduces to an affine function

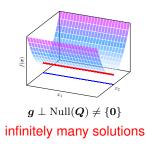
$$f(\boldsymbol{x}_0 + t\boldsymbol{d}_0) = f(\boldsymbol{x}_0) + t\boldsymbol{g}^T \boldsymbol{d}_0$$

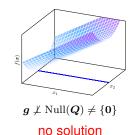
- 1. $Null(A) \cap Null(Q) = \{0\} \implies K$ nonsingular & unique solution.
- 2. $Null(A) \cap Null(Q) \neq \{0\} \implies K \text{ singular.}$
 - 2.1 $g \perp \text{Null}(A) \cap \text{Null}(Q) \implies \text{infinitely many solutions.}$
 - **2.2** $g \not\perp \text{Null}(A) \cap \text{Null}(Q) \implies \text{no solution and } f^* = -\infty.$

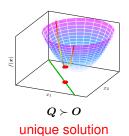
Note. When A = O, this reduces to the unconstrained case (cf. slide 10 of $\S 5$ part 2).

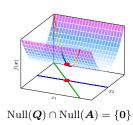
Unconstrained vs constrained problems



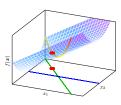








unique solution



 $Null(Q) \cap Null(A) = \{0\}$ unique solution

Unsolvable KKT system (case 2.2)

Example.

$$\min_{x_1, x_2} f(x_1, x_2) = \frac{1}{2}x_2^2 + x_1$$
s.t. $x_2 = 0$

The KKT system is

$$Q = diag\{0,1\}, g = (1,0)^T, A = (0,1), b = 0$$

This is a convex QP with

$$\begin{bmatrix} 0 & 0 & 0 \\ 0 & 1 & 1 \\ 0 & 1 & 0 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ \lambda \end{bmatrix} = \begin{bmatrix} -1 \\ 0 \\ 0 \end{bmatrix}$$

which has no solution, since $0 \cdot x_1 + 0 \cdot x_2 + 0 \cdot \lambda \neq -1$.

Note $f^* = -\infty$, and $e_1 = (1,0)^T \in \text{Null}(A) \cap \text{Null}(Q)$ and $g^T e_1 \neq 0$, i.e. there is a feasible direction along which the linear term dominates.

Unsolvable KKT system (cont'd)

If the KKT system has no solution, then the problem (QP) is either infeasible (impossible when rank A = k) or unbounded below.

KKT system has no solution iff

$$\begin{bmatrix} -\mathbf{g} \\ \mathbf{b} \end{bmatrix} \notin \operatorname{Range}(\mathbf{K}) = \operatorname{Range}(\mathbf{K}^T) = \operatorname{Null}(\mathbf{K})^{\perp}$$

- There exists $\begin{bmatrix} \mathbf{v} \\ \mathbf{\lambda} \end{bmatrix} \in \text{Null}(\mathbf{K}) \text{ s.t. } \begin{bmatrix} -\mathbf{g} \\ \mathbf{b} \end{bmatrix}^T \begin{bmatrix} \mathbf{v} \\ \mathbf{\lambda} \end{bmatrix} \neq 0, \text{ i.e. } \mathbf{g}^T \mathbf{v} \neq \mathbf{b}^T \mathbf{\lambda}.$
- By the previous lemma, Av = 0, Qv = 0, $\lambda = 0$. So $g^Tv \neq 0$.
- If x_0 is feasible, then $x_0 + tv$ is feasible for any $t \in \mathbb{R}$, since Av = 0. Since Qv = 0,

$$f(\mathbf{x}_0 + t\mathbf{v}) = f(\mathbf{x}_0) + t(\mathbf{Q}\mathbf{x}_0 + \mathbf{g})^T\mathbf{v} + \frac{1}{2}t^2\mathbf{v}^T\mathbf{Q}\mathbf{v} = f(\mathbf{x}_0) + t(\mathbf{g}^T\mathbf{v})$$

which goes to $-\infty$, as $t \to -\operatorname{sgn}(\mathbf{g}^T \mathbf{v}) \cdot \infty$.

Note. Similar to slide 6, $v \in \text{Null}(A) \cap \text{Null}(Q)$ and $g^T v \neq 0$.

Nonsingularity of KKT matrix (case 1)

If the KKT matrix \mathbf{K} is nonsingular, then the KKT system has a unique solution, which is optimal.

Recall $Q \succeq O$ and rank A = k. The following conditions are equivalent

- 1. K is nonsingular
- 2. $\text{Null}(Q) \cap \text{Null}(A) = \{0\}$, i.e. Q and A have no nontrivial common nullspace, i.e. Ax = 0, Qx = 0 only have the trivial solution x = 0.
- 3. $Ax = \mathbf{0}, x \neq \mathbf{0} \implies x^T Qx > 0$, i.e. Q is positive definite on the nullspace of A.
- 4. $F^TQF \succ O$ for any $F \in \mathbb{R}^{n \times (n-k)}$ s.t. Range(F) = Null(A), i.e. the columns of F are linearly independent solutions of Ax = 0.

In particular, if $Q \succ O$, then K is nonsingular (by 3).

Proof

We show $1 \iff 2 \iff 3 \iff 4$.

• $(1 \Leftrightarrow 2)$. By the lemma on slide 4,

$$extbf{ extit{K}} ext{ nonsingular } \iff \operatorname{Null}(extbf{ extit{K}}) = \{ extbf{0} \} \iff \operatorname{Null}(extbf{A}) \cap \operatorname{Null}(extbf{ extit{Q}}) = \{ extbf{0} \}$$

• $(2 \Leftrightarrow 3.)$ Since $Q \succeq O$, $x^TQx = 0$ iff Qx = 0 (footnote on slide 4).

$$2 \iff Ax = \mathbf{0} \text{ and } Qx = \mathbf{0} \text{ implies } x = \mathbf{0}$$

 $\iff Ax = \mathbf{0} \text{ and } x^T Qx = 0 \text{ implies } x = \mathbf{0} \iff 3$

• $(3 \Leftrightarrow 4.)$ Note $x \in \text{Null}(A)$ iff x = Fz, and $Fz \neq 0$ iff $z \neq 0$,

$$3 \iff x^{T}Qx > 0 \text{ if } Ax = 0, x \neq 0$$

$$\iff x^{T}Qx > 0 \text{ if } x = Fz, z \neq 0$$

$$\iff z^{T}F^{T}QFz > 0 \text{ if } z \neq 0$$

$$\iff F^{T}QF \succ O$$

Example

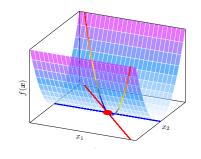
$$\min_{x_1, x_2} f(x_1, x_2) = \frac{1}{2} x_2^2$$

s.t.
$$x_1 + 2x_2 = b$$

Trivial with solution $x_1^* = b, x_2^* = 0$.

But let's check the condition on slide 8.

$$Q = diag\{0,1\}, \quad A = (1,2)$$



Let
$$F = (2, -1)^T$$
. Then Range(F) = Null(A), and

$$F^TQF = [1] \succ O$$

By 4 of slide 8, the KKT matrix in nonsingular, so \exists a unique solution.

Note. The unconstrained problem $\min_{x} f(x)$ has infinitely many solutions. But this does not prevent the constrained problem from having a unique solution, as $Q \succ O$ on Null(A) (see 3 on slide 8).

Outline

Equality constrained convex QP

Newton's method

Newton direction for equality constrained problem

Consider the second-order Taylor approximation for f at a feasible x_k ,

$$\min_{\boldsymbol{d}} h(\boldsymbol{d}) \triangleq \hat{f}(\boldsymbol{x}_k + \boldsymbol{d}) = f(\boldsymbol{x}_k) + \nabla f(\boldsymbol{x}_k)^T \boldsymbol{d} + \frac{1}{2} \boldsymbol{d}^T \nabla^2 f(\boldsymbol{x}_k) \boldsymbol{d}$$

s.t. $A(\boldsymbol{x}_k + \boldsymbol{d}) = \boldsymbol{b}$

Using $Ax_k = b$,

$$\min_{\mathbf{d}} h(\mathbf{d}) = f(\mathbf{x}_k) + \nabla f(\mathbf{x}_k)^T \mathbf{d} + \frac{1}{2} \mathbf{d}^T \nabla^2 f(\mathbf{x}_k) \mathbf{d}$$

s.t. $A\mathbf{d} = \mathbf{0}$

KKT system for this quadratic problem is

$$\begin{bmatrix} \nabla^2 f(\mathbf{x}_k) & \mathbf{A}^T \\ \mathbf{A} & \mathbf{O} \end{bmatrix} \begin{bmatrix} \mathbf{d} \\ \boldsymbol{\lambda} \end{bmatrix} = \begin{bmatrix} -\nabla f(\mathbf{x}_k) \\ \mathbf{0} \end{bmatrix}$$

The Newton direction d_k is given by the solution to the KKT system. We will assume the KKT matrix is always nonsingular (cf. slides 4 & 8),

Newton's method for equality constrained problem

- 1: initialization $x \leftarrow x_0 \in X$ $\triangleright x_0$ is feasible, i.e. $Ax_0 = b$
- 2: repeat
- 3: Compute Newton's direction *d* by solving

$$\begin{bmatrix} \nabla^2 f(\mathbf{x}) & \mathbf{A}^T \\ \mathbf{A} & \mathbf{O} \end{bmatrix} \begin{bmatrix} \mathbf{d} \\ \boldsymbol{\lambda} \end{bmatrix} = \begin{bmatrix} -\nabla f(\mathbf{x}) \\ \mathbf{0} \end{bmatrix}$$

- 4: $t \leftarrow 1$ \Rightarrow backtracking line search on lines 4-7
- 5: **while** $f(\mathbf{x} + t\mathbf{d}) > f(\mathbf{x}) + \alpha t \nabla f(\mathbf{x})^T \mathbf{d}$ **do** 6: $t \leftarrow \beta t$
- 7: end while
- 8: $x \leftarrow x + td$
- 9: **until** $||d|| \le \delta$
- 10: **return** *x*

Note. We cannot use $\|\nabla f(x)\| \le \delta$ as stopping criterion now, as $\nabla f(x^*) = \mathbf{0}$ no longer holds in general. [BV] uses $\sqrt{d^T \nabla^2 f(x)} d \le \delta$.

Note. This is called a feasible descent method, since all x_k are feasible and $f(x_{k+1}) < f(x_k)$ unless x_k is optimal.

Newton's method and constraint elimination

Let $F \in \mathbb{R}^{n \times (n-k)}$ be a matrix whose columns are linearly independent solutions to $Ax = \mathbf{0}$. Fix a feasible $\tilde{x} \in X$. Every $x \in X$ has a unique representation of the form $x = \tilde{x} + Fz$,

$$X = \{x : Ax = b\} = \{\tilde{x} + Fz : z \in \mathbb{R}^{n-k}\}\$$

Constrained problem reduces to unconstrained problem by $x = \tilde{x} + Fz$,

$$(C): \begin{cases} \min_{\mathbf{x}} & f(\mathbf{x}) \\ \text{s.t.} & A\mathbf{x} = \mathbf{b} \end{cases} \iff (U): \min_{\mathbf{z}} g(\mathbf{z}) = f(\tilde{\mathbf{x}} + \mathbf{F}\mathbf{z})$$

Applying Newton's method to (C) with initial point $x_0 = \tilde{x} + Fz_0$ is equivalent to applying Newton's method to (U) with initial point z_0 :

If $\{x_k\}$ and $\{z_k\}$ are the iterates for (C) and (U), respectively, then

$$x_k = \tilde{x} + Fz_k, \quad \forall k$$

Newton's method has same convergence properties for (C) and (U).

Proof

We only need to show $x_1 = \tilde{x} + Fz_1$ and then use induction.

Let Δx_0 and Δz_0 denote the Newton directions for (C) and (U), i.e. Δx_0 satisfies

$$\begin{bmatrix} \nabla^2 f(\boldsymbol{x}_0) & \boldsymbol{A}^T \\ \boldsymbol{A} & \boldsymbol{O} \end{bmatrix} \begin{bmatrix} \Delta \boldsymbol{x}_0 \\ \boldsymbol{\lambda}_0 \end{bmatrix} = \begin{bmatrix} -\nabla f(\boldsymbol{x}_0) \\ \boldsymbol{0} \end{bmatrix}$$

and Δz_0 satisfies

$$\nabla^2 g(z_0) \Delta z_0 = -\nabla g(z_0)$$

- 1. Both Δx_0 and Δz_0 are well-defined
- 2. $\Delta x_0 = F \Delta z_0$. This also shows $\Delta x_0 = \mathbf{0}$ iff $\Delta z_0 = \mathbf{0}$.
- 3. Backtracking line search gives the same step size t_0 in both cases
- 4. By 2 and 3,

$$x_1 = x_0 + t_0 \Delta x_0 = \tilde{x} + F z_0 + t_0 F \Delta z_0 = \tilde{x} + F (z_0 + t_0 \Delta z_0) = \tilde{x} + F z_1$$

Proof (cont'd)

More details.

1. Both Δx_0 and Δz_0 are well-defined. By the chain rule,

$$\nabla^2 g(\mathbf{z}_0) = \mathbf{F}^T \nabla^2 f(\mathbf{x}_0) \mathbf{F}, \quad \nabla g(\mathbf{z}_0) = \mathbf{F}^T \nabla f(\mathbf{x}_0)$$

Since we assume the KKT matrix of (C) is nonsingular, by 4 on slide 8, $\nabla^2 g(z_0) \succ \mathbf{O}$. Hence both Δx_0 and Δz_0 are well-defined.

- 2. $\Delta x_0 = \mathbf{F} \Delta z_0$.
 - ightharpoonup Pre-multiplying the first KKT equation by F^T ,

$$\mathbf{F}^T \nabla^2 f(\mathbf{x}_0) \Delta \mathbf{x}_0 + (\mathbf{A}\mathbf{F})^T \lambda_0 = -\mathbf{F}^T \nabla f(\mathbf{x}_0)$$

Since the columns of *F* are solutions to Ax = 0, AF = 0. Thus

$$\mathbf{F}^T \nabla^2 f(\mathbf{x}_0) \Delta \mathbf{x}_0 = -\mathbf{F}^T \nabla f(\mathbf{x}_0)$$

► $A\Delta x_0 = \mathbf{0}$ by the second KKT equation, so $\Delta x_0 = Fu$ for some u.

$$\mathbf{F}^T \nabla^2 f(\mathbf{x}_0) \mathbf{F} \mathbf{u} = -\mathbf{F}^T \nabla f(\mathbf{x}_0) \iff \nabla^2 g(\mathbf{z}_0) \mathbf{u} = -\nabla g(\mathbf{z}_0)$$

Thus
$$u = \Delta z_0$$
 and $\Delta x_0 = Fu = F\Delta z_0$

Proof (cont'd)

3. Backtracking line search gives the same step size t_0 .

Note

$$f(\mathbf{x}_0) = f(\tilde{\mathbf{x}} + \mathbf{F} z_0) = g(z_0)$$

$$f(\mathbf{x}_0 + t\Delta \mathbf{x}_0) = f(\tilde{\mathbf{x}} + \mathbf{F} (z_0 + t\Delta z_0)) = g(z_0 + t\Delta z_0)$$

$$\nabla f(\mathbf{x}_0)^T \Delta \mathbf{x}_0 = \nabla f(\mathbf{x}_0)^T \mathbf{F} \Delta z_0 = \nabla g(z_0)^T \Delta z_0$$

Thus the test condition in backtracking line search for f

$$f(\mathbf{x}_0 + t\Delta\mathbf{x}_0) > f(\mathbf{x}_0) + \alpha t \nabla f(\mathbf{x}_0)^T \Delta\mathbf{x}_0$$

is exactly the same as that for g,

$$g(\mathbf{z}_0 + t\Delta\mathbf{z}_0) > g(\mathbf{z}_0) + \alpha t \nabla g(\mathbf{x}_0)^T \Delta \mathbf{z}_0$$