Optimization Lecture 10: Equality constrained minimization

Qingfu Zhang

Dept of CS , CityU

Outline

Equality constrained minimization

Newton's method with equality constraints

Infeasible start Newton method

Implementation

Equality constrained minimization

Equality constrained minimization

- equality constrained smooth minimization problem:

$$\begin{array}{ll} \text{minimize} & f(x) \\ \text{subject to} & Ax = b \end{array}$$

- we assume
  - f convex, twice continuously differentiable
  - $A \in \mathbf{R}^{p \times n}$ with $\mathbf{rank}\, A = p$
  - $p^\star$ is finite and attained
- **optimality conditions**: $x^\star$ is optimal if and only if there exists a $\mu^\star$ such that

$$\nabla f(x^\star) + A^T \mu^\star = 0, \quad Ax^\star = b$$

why? Slater's condition is met. KKT condition is sufficient and necessary.

Equality constrained quadratic minimization

- $f(x) = (1/2)x^T Px + q^T x + r, P \in \mathbf{S}^n_+$
- $\nabla f(x) = Px + q$
- optimality conditions are a **system of linear equations**

$$\begin{bmatrix} P & A^T \\ A & 0 \end{bmatrix} \begin{bmatrix} x^\star \\ \mu^\star \end{bmatrix} = \begin{bmatrix} -q \\ b \end{bmatrix}$$

- coefficient matrix is called KKT matrix
- KKT matrix is nonsingular if and only if

$$Ax = 0, \quad x \neq 0 \quad \Longrightarrow \quad x^T Px > 0$$

- equivalent condition for nonsingularity: $P + A^T A > 0$

Noting $P \in S^n_+$, $x^T Px > 0 \Leftrightarrow Px \neq 0$.

Eliminating equality constraints

- represent feasible set $\{x \mid Ax = b\}$ as $\{Fz + \hat{x} \mid z \in \mathbf{R}^{n-p}\}$
  - $\hat{x}$ is (any) **particular solution** of $Ax = b$
  - range of $F \in \mathbf{R}^{n\times(n-p)}$ is nullspace of A(**rank** $F = n - p$ and $AF = 0$)
- **reduced or eliminated problem**: minimize $f(Fz + \hat{x})$
- an unconstrained problem with variable $z \in \mathbf{R}^{n-p}$
- from solution $z^\star$, obtain $x^\star$ and $\mu^\star$ as

$$x^\star = Fz^\star + \hat{x}, \quad \mu^\star = -\left(AA^T\right)^{-1} A\nabla f\left(x^\star\right)$$

Example: Optimal resource allocation

- allocate resource amount $x_i \in \mathbf{R}$ to agent i
- agent i cost $= f_i(x_i)$
- resource budget is b, so $x_1 + \cdots + x_n = b$
- resource allocation problem is

$$\begin{array}{ll} \text{minimize} & f_1(x_1) + f_2(x_2) + \cdots + f_n(x_n) \\ \text{subject to} & x_1 + x_2 + \cdots + x_n = b \end{array}$$

- eliminate $x_n = b - x_1 - \cdots - x_{n-1}$, i.e., choose

$$\hat{x} = be_n, \quad F = \begin{bmatrix} \mathbf{I}_{(n-1)\times(n-1)} \\ -\mathbf{1}^T \end{bmatrix} \in \mathbf{R}^{n\times(n-1)}$$

- reduced problem: minimize
  $f_1(x_1) + \cdots + f_{n-1}(x_{n-1}) + f_n(b - x_1 - \cdots - x_{n-1})$

Newton's method with equality constraints

Newton step

- Newton step Δx_{nt} of f at feasible x is given by solution v of

$$\begin{bmatrix} \nabla^2 f(x) & A^T \\ A & 0 \end{bmatrix} \begin{bmatrix} v \\ w \end{bmatrix} = \begin{bmatrix} -\nabla f(x) \\ 0 \end{bmatrix}$$

- Δx_{nt} solves second order approximation (with variable v)

$$\begin{array}{ll} \text{minimize} & \widehat{f}(x+v) = f(x) + \nabla f(x)^T v + (1/2) v^T \nabla^2 f(x) v \\ \text{subject to} & A(x+v) = b \end{array}$$

- Δx_{nt} equations follow from linearizing optimality conditions

$$\nabla f(x+v) + A^T w \approx \nabla f(x) + \nabla^2 f(x) v + A^T w = 0, \quad A(x+v) = b$$

Newton decrement

- Newton decrement for equality constrained minimization is

$$\lambda(x) = \left(\Delta x_{\mathrm{nt}}^T \nabla^2 f(x) \Delta x_{\mathrm{nt}}\right)^{1/2}$$

- gives an estimate of $f(x) - p^\star$ using quadratic approximation $\widehat{f}$:

$$f(x) - \inf_{Ay=b} \widehat{f}(y) = \lambda(x)^2/2$$

- directional derivative in Newton direction:

$$\left.\frac{d}{dt} f\left(x + t\Delta x_{\mathrm{nt}}\right)\right|_{t=0} = -\lambda(x)^2$$

Pf: Noting that $\nabla f(x)^T \Delta x_{nt} = -\lambda(x)^2$.

Newton's method with equality constraints

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given starting point $x \in \textbf{dom}\, f$ with $Ax = b$, tolerance $\epsilon > 0$.
repeat

1. Compute the Newton step and decrement $\Delta x_{\mathrm{nt}}, \lambda(x)$.
2. Stopping criterion. **quit** if $\lambda^2/2 \leq \epsilon$.
3. Line search. Choose step size t by backtracking line search.
4. Update. $x := x + t\Delta x_{\mathrm{nt}}$.

- a feasible descent method: $x^{(k)}$ feasible and $f\left(x^{(k+1)}\right) < f\left(x^{(k)}\right)$
- Δx_{nt} is feasible descent direction. (ex)
- affine invariant (ex).

Newton's method and elimination

- reduced problem: minimize $\tilde{f}(z) = f(Fz + \hat{x})$
  - variables $z \in \mathbf{R}^{n-p}$
  - $\hat{x}$ satisfies $A\hat{x} = b$; $\textbf{\textit{rank}}\, F = n - p$ and $AF = 0$
- (unconstrained) Newton's method for $\tilde{f}$, started at $z^{(0)}$, generates iterates $z^{(k)}$
- iterates of Newton's method with equality constraints, started at $x^{(0)} = Fz^{(0)} + \hat{x}$, are

$$x^{(k+1)} = Fz^{(k)} + \hat{x}$$

- hence, don't need separate convergence analysis

Infeasible start Newton method

Newton step at infeasible points

- with $y = (x, \mu)$, write optimality condition as $r(y) = 0$, where

$$r(y) = \left(\nabla f(x) + A^T \mu, Ax - b\right)$$

  is **primal-dual residual**

- consider $x \in \mathbf{dom}\, f$, $Ax \neq b$, i.e., x is infeasible
- linearizing $r(y) = 0$ gives $r(y + \Delta y) \approx r(y) + \mathrm{D}r(y)\Delta y = 0$
  $(\nabla f(x + \Delta x_{\mathrm{nt}}) \approx \nabla f(x) + \nabla^2 f(x) \Delta x_{\mathrm{nt}})$

$$\begin{bmatrix} \nabla^2 f(x) & A^T \\ A & 0 \end{bmatrix} \begin{bmatrix} \Delta x_{\mathrm{nt}} \\ \Delta \mu_{\mathrm{nt}} \end{bmatrix} = - \begin{bmatrix} \nabla f(x) + A^T \mu \\ Ax - b \end{bmatrix}$$

- $(\Delta x_{\mathrm{nt}}, \Delta \mu_{\mathrm{nt}})$ is called **infeasible** or **primal-dual** Newton step at x

Infeasible start Newton method

given starting point $x \in \textbf{dom}\, f, \mu$, tolerance $\epsilon > 0, \alpha \in (0, 1/2), \beta \in (0, 1)$.
repeat

1. Compute primal and dual Newton steps $\Delta x_{\rm nt}, \Delta \mu_{\rm nt}$.
2. *Backtracking line search* on $\|r\|_2$.
   $t := 1$.
   while $\left\|r\left(x + t\Delta x_{\rm nt}, \mu + t\Delta \mu_{\rm nt}\right)\right\|_2 > (1 - \alpha t)\|r(x, \mu)\|_2, \quad t := \beta t$.
3. *Update*. $x := x + t\Delta x_{\rm nt}, \mu := \mu + t\Delta \mu_{\rm nt}$.

until $Ax = b$ and $\|r(x, \mu)\|_2 \leq \epsilon$.

- not a descent method: $f\left(x^{(k+1)}\right) > f\left(x^{(k)}\right)$ is possible
- directional derivative of $\|r(y)\|_2$ in direction $\Delta y = (\Delta x_{\rm nt}, \Delta \mu_{\rm nt})$ is

$$\frac{d}{dt}\|r(y + t\Delta y)\|_2\bigg|_{t=0} = -\|r(y)\|_2$$

Implementation

Solving KKT systems

- feasible and infeasible Newton methods require solving KKT system

$$\begin{bmatrix} H & A^T \\ A & 0 \end{bmatrix} \begin{bmatrix} v \\ w \end{bmatrix} = - \begin{bmatrix} g \\ h \end{bmatrix}$$

- in general, can use $\mathrm{LDL}^\top$ factorization
- or elimination (if H nonsingular and easily inverted):
  - solve $AH^{-1}A^T w = h - AH^{-1} g$ for w
  - $v = -H^{-1}\left(g + A^T w\right)$

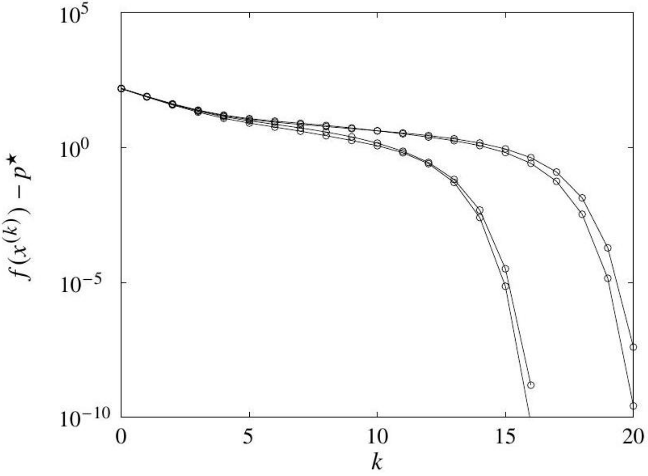
Example: Equality constrained analytic centering

- **primal problem**: minimize $-\sum_{i=1}^{n} \log x_i$ subject to $Ax = b$
- **dual problem**: maximize $-b^T v + \sum_{i=1}^{n} \log \left(A^T v\right)_i + n$
    - recover $x^\star$ as $x_i^\star = 1/\left(A^T v\right)_i$
- three methods to solve:
    - Newton method with equality constraints
    - Newton method applied to dual problem
    - infeasible start Newton method

  these have **different requirements for initialization**
- we'll look at an example with $A \in \mathbf{R}^{100 \times 500}$, different starting points

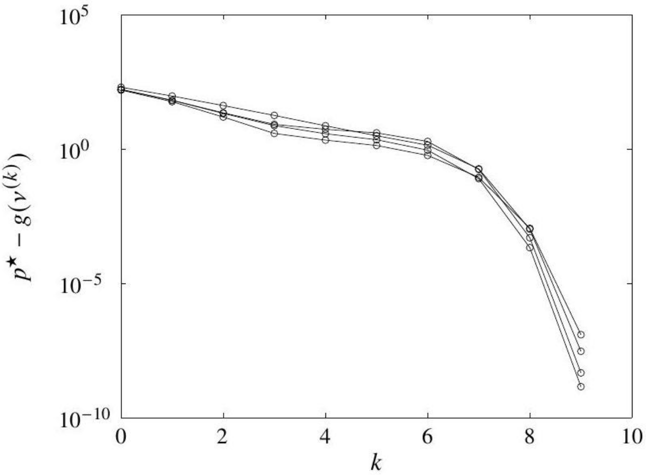
Newton's method with equality constraints

- requires $x^{(0)} > 0, Ax^{(0)} = b$



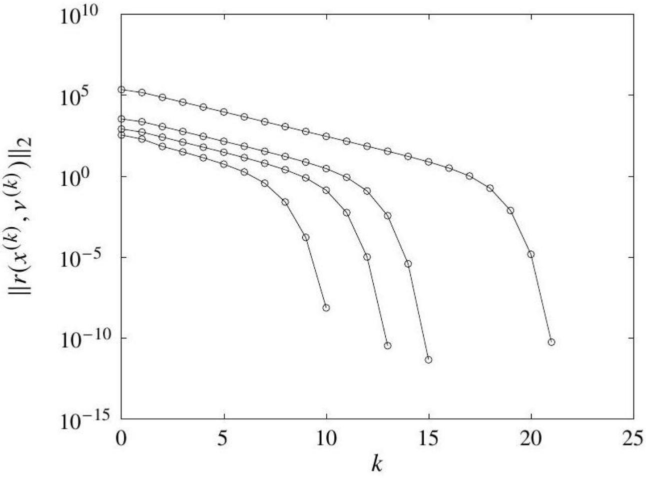
Newton method applied to dual problem

- requires $A^T v^{(0)} > 0$



Infeasible start Newton method

- requires $x^{(0)} > 0$



Complexity per iteration of three methods is identical

- for feasible Newton method, use block elimination to solve KKT system

$$\begin{bmatrix} \operatorname{diag}(x)^{-2} & A^T \\ A & 0 \end{bmatrix} \begin{bmatrix} \Delta x \\ w \end{bmatrix} = \begin{bmatrix} \operatorname{diag}(x)^{-1}\mathbf{1} \\ 0 \end{bmatrix}$$

  reduces to solving $A\operatorname{diag}(x)^2 A^T w = b$ (and then one can easily obtain Δx.

- for Newton system applied to dual, solve
  $A\operatorname{diag}\left(A^T v\right)^{-2} A^T \Delta v = -b + A\operatorname{diag}\left(A^T v\right)^{-1}\mathbf{1}$

- for infeasible start Newton method, use block elimination to solve KKT system

$$\begin{bmatrix} \operatorname{diag}(x)^{-2} & A^T \\ A & 0 \end{bmatrix} \begin{bmatrix} \Delta x \\ \Delta v \end{bmatrix} = \begin{bmatrix} \operatorname{diag}(x)^{-1}\mathbf{1} - A^T v \\ b - Ax \end{bmatrix}$$

  reduces to solving $A\operatorname{diag}(x)^2 A^T w = 2Ax - b$

- conclusion: in each case, solve $ADA^T w = h$ with D positive diagonal

Example: Network flow optimization

- directed graph with n arcs, $p+1$ nodes
- x_i : flow through arc i; ϕ_i : strictly convex flow cost function for arc i
- **incidence matrix** $\tilde{A} \in \mathbf{R}^{(p+1)\times n}$ defined as

$$\tilde{A}_{ij} = \begin{cases} 1 & \text{arc } j \text{ leaves node } i \\ -1 & \text{arc } j \text{ enters node } i \\ 0 & \text{otherwise} \end{cases}$$

- **reduced incidence matrix** $A \in \mathbf{R}^{p\times n}$ is $\tilde{A}$ with last row removed
- $\operatorname{rank} A = p$ if graph is connected
- flow conservation is $Ax = b$, $b \in \mathbf{R}^p$ is (reduced) source vector
- **network flow optimization problem**: minimize $\sum_{i=1}^n \phi_i(x_i)$ subject to $Ax = b$

KKT system

- KKT system is

$$\begin{bmatrix} H & A^T \\ A & 0 \end{bmatrix} \begin{bmatrix} v \\ w \end{bmatrix} = -\begin{bmatrix} g \\ h \end{bmatrix}$$

- $H = \mathbf{diag}\left(\phi_1''(x_1), \ldots, \phi_n''(x_n)\right)$, positive diagonal
- solve via elimination:

$$AH^{-1}A^T w = h - AH^{-1}g, \quad v = -H^{-1}\left(g + A^T w\right)$$

- sparsity pattern of $AH^{-1}A^T$ is given by graph connectivity

$$\begin{aligned} \left(AH^{-1}A^T\right)_{ij} \neq 0 &\iff \left(AA^T\right)_{ij} \neq 0 \\ &\iff \text{nodes } i \text{ and } j \text{ are connected by an arc} \end{aligned}$$

Analytic center of linear matrix inequality

- minimize $-\log\det X$ subject to $\mathbf{tr}(A_i X) = b_i,\ i = 1, \ldots, p$
- optimality conditions

$$X^\star \succ 0, \quad -(X^\star)^{-1} + \sum_{j=1}^{p} v_j^\star A_i = 0, \quad \mathbf{tr}(A_i X^\star) = b_i, \quad i = 1, \ldots, p$$

- Newton step ΔX at feasible X is defined by

$$X^{-1}(\Delta X)X^{-1} + \sum_{j=1}^{p} w_j A_i = X^{-1}, \quad \mathbf{tr}(A_i \Delta X) = 0, \quad i = 1, \ldots, p$$

- follows from linear approximation $(X + \Delta X)^{-1} \approx X^{-1} - X^{-1}(\Delta X)X^{-1}$
- $n(n+1)/2 + p$ variables $\Delta X, w$

Solution by block elimination

- eliminate ΔX from first equation to get $\Delta X = X - \sum_{j=1}^{p} w_j X A_j X$
- substitute ΔX in second equation to get

$$\sum_{j=1}^{p} \mathbf{tr}\,(A_i X A_j X)\, w_j = b_i, \quad i = 1, \ldots, p$$

- a dense positive definite set of linear equations with variable $w \in \mathbf{R}^p$
- form and solve this set of equations to get w, then get ΔX from equation above

Flop count

- find Cholesky factor L of X $\quad (1/3)n^3$
- form p products $L^T A_j L$ $\quad (3/2)pn^3$
- form $p(p+1)/2$ inner products $\mathrm{tr}\left(\left(L^T A_i L\right)\left(L^T A_j L\right)\right)$ to get coefficent matrix $\quad (1/2)p^2 n^2$
- solve $p \times p$ system of equations via Cholesky factorization $(1/3)\ p^3$
- flop count dominated by $pn^3 + p^2 n^2$
- cf. naïve method, $\left(n^2 + p\right)^3$