## 10. Equality constrained minimization

- equality constrained minimization
- eliminating equality constraints
- Newton's method with equality constraints
- infeasible start Newton method
- implementation


## Equality constrained minimization

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

- $f$ convex, twice continuously differentiable; hence, $\operatorname{dom} f$ is an open set
- $A \in \mathbf{R}^{p \times n}$ with $\mathbf{r a n k} A=p$
- we assume the optimal value $p^{\star}$ is finite and attained

Optimality conditions: $x$ is optimal if and only if

$$
\begin{equation*}
x \in \operatorname{dom} f, \quad A x=b, \quad \nabla f(x)+A^{T} v=0 \tag{1}
\end{equation*}
$$

for some $v \in \mathbf{R}^{p}$

## Equality constrained quadratic minimization

$$
\begin{array}{ll}
\text { minimize } & \frac{1}{2} x^{T} P x+q^{T} x+r \\
\text { subject to } & A x=b
\end{array}
$$

where $P \in \mathbf{S}_{+}^{n}$ and $\operatorname{rank}(A)=p$

- optimality conditions from previous page:

$$
P x+q+A^{T} v=0, \quad A x=b
$$

- this is a set of $n+p$ linear equations in $n+p$ variables

$$
\left[\begin{array}{cc}
P & A^{T} \\
A & 0
\end{array}\right]\left[\begin{array}{l}
x \\
v
\end{array}\right]=\left[\begin{array}{c}
-q \\
b
\end{array}\right]
$$

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

## Nonsingular KKT matrix

each of the following three conditions is equivalent to nonsingularity of

$$
\left[\begin{array}{cc}
P & A^{T} \\
A & 0
\end{array}\right]
$$

(assuming $P \geq 0$ and $\operatorname{rank}(A)=p$ )

1. the first block column has full column rank

$$
\operatorname{rank}\left(\left[\begin{array}{c}
P  \tag{2}\\
A
\end{array}\right]\right)=n
$$

2. $P$ is positive definite on the nullspace of $A$

$$
\begin{equation*}
A x=0, \quad x \neq 0 \quad \Longrightarrow \quad x^{T} P x>0 \tag{3}
\end{equation*}
$$

3. the matrix $P+A^{T} A$ is positive definite

## Exercise

show that the three conditions are equivalent to nonsingularity of the KKT matrix

## Solution (condition 1)

- clearly, (2) is necessary (first $n$ columns of KKT matrix must be independent)
- to show it is sufficient, we assume that (2) holds and show that

$$
\begin{equation*}
P x+A^{T} y=0, \quad A x=0 \tag{4}
\end{equation*}
$$

holds only if $x=0, y=0$

- inner product of $x$ and first equation of (4) gives $x^{T} P x=x^{T}\left(P x+A^{T} y\right)=0$
- $x^{T} P x=0$ if and only if $P x=0$ (for positive semidefinite $P$ )
- hence (4) is equivalent to $P x=0, A x=0, A^{T} y=0$
- by the rank property (2) and $\operatorname{rank}(A)=p$, this holds only if $x=0, y=0$


## Exercise

## Condition 2

- (3) means the same as

$$
x^{T} P x=0, \quad A x=0 \quad \Longrightarrow \quad x=0
$$

- for $P \geq 0$, can replace $x^{T} P x=0$ with $P x=0$, so (3) is the same as (2)


## Condition 3

- the matrix $P+A^{T} A$ is positive definite if

$$
x^{T}\left(P+A^{T} A\right) x=x^{T} P x+\|A x\|_{2}^{2}>0 \quad \text { for all } x \neq 0
$$

- for $P \geq 0$, this is the same as condition $2\left(x^{T} P x>0\right.$ for nonzero $x$ with $\left.A x=0\right)$


## Eliminating equality constraints

| minimize | $f(x)$ |
| :--- | :--- |
| subject to | $A x=b$ |$\longrightarrow$ minimize $f(F z+\hat{x})$

- the affine set defined by $A x=b$ is represented as translate of range of $F$

$$
\{x \mid A x=b\}=\left\{F z+\hat{x} \mid z \in \mathbf{R}^{n-p}\right\}
$$

- $\hat{x}$ is (any) particular solution of the linear equation $A x=b$
- $F \in \mathbf{R}^{n \times(n-p)}$ is a full-rank matrix with range equal to nullspace of $A$
- the reformulated problem is unconstrained with variable $z \in \mathbf{R}^{n-p}$
- from solution $z^{\star}$, solution of optimality conditions (1) is

$$
x^{\star}=F z^{\star}+\hat{x}, \quad v^{\star}=-\left(A A^{T}\right)^{-1} A \nabla f\left(x^{\star}\right)
$$

- elimination step can be expensive, obscure structure in $A$ (e.g., sparsity)


## Newton step

we extend the definition of Newton step (p.9.18) to equality-constrained problems

- assume $x$ is feasible ( $x \in \operatorname{dom} f$ and $A x=b$ )
- define Newton step $\Delta x_{\mathrm{nt}}$ at $x$ as the solution $v$ of

$$
\left[\begin{array}{cc}
\nabla^{2} f(x) & A^{T} \\
A & 0
\end{array}\right]\left[\begin{array}{c}
v \\
w
\end{array}\right]=\left[\begin{array}{c}
-\nabla f(x) \\
0
\end{array}\right]
$$

- $x+\Delta x_{\text {nt }}$ solves problem if $f$ is replaced with 2nd order approximation $\hat{f}$ at $x$

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

- $x+\Delta x_{\mathrm{nt}}$ solves optimality conditions (1), linearized at $x$ :

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

## Newton decrement

for the equality-constrained problem, we define the Newton decrement as

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

- $\lambda(x)^{2}$ is directional derivative of $f$ at $x$ in Newton direction $\Delta x_{\mathrm{nt}}$ :

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

- $\lambda(x)$ is norm of Newton step in quadratic Hessian norm
- $\lambda(x)$ gives estimate of $f(x)-p^{\star}$, estimated using quadratic approximation $\hat{f}$ :

$$
f(x)-\inf _{A y=b} \hat{f}(y)=\frac{1}{2} \lambda(x)^{2}
$$

- in general,

$$
\lambda(x) \neq\left(\nabla f(x)^{T} \nabla^{2} f(x)^{-1} \nabla f(x)\right)^{1 / 2}
$$

## Newton's method with equality constraints

given: a starting point $x \in \operatorname{dom} f$ with $A x=b$, tolerance $\epsilon>0$
repeat

1. Newton step: compute Newton step $\Delta x_{\mathrm{nt}}$ and Newton decrement $\lambda(x)$
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: iterates $x^{(k)}$ are feasible and $f\left(x^{(k+1)}\right)<f\left(x^{(k)}\right)$
- affine-invariant


## Newton's method and elimination

Newton's method for unconstrained optimization (after eliminating $A x=b$ )

$$
\text { minimize } g(z)=f(F z+\hat{x})
$$

suppose Newton method for $g$, started at $z^{(0)}$, generates iterates $z^{(k)}$

Newton's method with equality constraints (method on page 10.10)
when started at $x^{(0)}=F z^{(0)}+\hat{x}$, iterates are

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

hence, we don't need separate convergence analysis for the method on p . 10.10

## Newton step at infeasible points

2nd interpretation of page 10.8 extends to infeasible $x$ (i.e., with $A x \neq b$ )
linearizing optimality conditions at infeasible $x$ (with $x \in \operatorname{dom} f$ ) gives

$$
\left[\begin{array}{cc}
\nabla^{2} f(x) & A^{T}  \tag{5}\\
A & 0
\end{array}\right]\left[\begin{array}{c}
\Delta x_{\mathrm{nt}} \\
w
\end{array}\right]=-\left[\begin{array}{c}
\nabla f(x) \\
A x-b
\end{array}\right]
$$

## Interpretation

- optimality condition (1) is nonlinear equation $r(x, v)=0$, where

$$
r(x, v)=\left[\begin{array}{c}
\nabla f(x)+A^{T} v \\
A x-b
\end{array}\right]
$$

- linearizing $r(y)=0$ gives

$$
\left[\begin{array}{cc}
\nabla^{2} f(x) & A^{T} \\
A & 0
\end{array}\right]\left[\begin{array}{c}
\Delta x_{\mathrm{nt}} \\
\Delta v_{\mathrm{nt}}
\end{array}\right]=-\left[\begin{array}{c}
\nabla f(x)+A^{T} v \\
A x-b
\end{array}\right]
$$

this is the same as (5) with $w=v+\Delta v_{\mathrm{nt}}$

## Infeasible start Newton method

given: a starting point $x \in \operatorname{dom} f, v$, tolerance $\epsilon>0, \alpha \in(0,1 / 2), \beta \in(0,1)$ repeat

1. Newton step: compute primal and dual Newton steps $\Delta x_{\mathrm{nt}}, \Delta v_{\mathrm{nt}}$
2. backtracking line search:

$$
\begin{aligned}
& t:=1 \\
& \text { while }\left\|r\left(x+t \Delta x_{\mathrm{nt}}, v+t \Delta v_{\mathrm{nt}}\right)\right\|_{2}>(1-\alpha t)\|r(x, v)\|_{2} \\
& \quad t:=\beta t
\end{aligned}
$$

3. update: $x:=x+t \Delta x_{\mathrm{nt}}, v:=v+t \Delta v_{\mathrm{nt}}$
until $A x=b$ and $\|r(x, v)\|_{2} \leq \epsilon$

- not a descent method: $f\left(x^{(k+1)}\right)>f\left(x^{(k)}\right)$ is possible
- therefore we use norm of $r$ as merit function in line search
- directional derivative of norm of $r$, at $y=(x, v)$, in direction $\Delta y=\left(\Delta x_{\mathrm{nt}}, \Delta v_{\mathrm{nt}}\right)$ is

$$
\left.\frac{d}{d t}\|r(y+t \Delta y)\|_{2}\right|_{t=0}=-\|r(y)\|_{2}
$$

## Solving KKT systems

$$
\left[\begin{array}{cc}
H & A^{T} \\
A & 0
\end{array}\right]\left[\begin{array}{c}
v \\
w
\end{array}\right]=-\left[\begin{array}{l}
g \\
h
\end{array}\right]
$$

## Solution methods

- use matrix factorization for symmetric indefinite matrices $\left(\mathrm{LDL}^{\top}\right.$ factorization)
- if $H$ is positive definite, solve by block elimination: two equations

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

- if $H$ is not positive definite, first write KKT system as

$$
\left[\begin{array}{cc}
H+A^{T} Q A & A^{T} \\
A & 0
\end{array}\right]\left[\begin{array}{c}
v \\
w
\end{array}\right]=-\left[\begin{array}{c}
g+A^{T} Q h \\
h
\end{array}\right]
$$

with $Q \geq 0$ chosen so that $H+A^{T} Q A>0$; then apply block elimination

## Equality constrained analytic centering

## Primal and dual problems

$$
\begin{aligned}
& \text { minimize } \quad-\sum_{i=1}^{n} \log x_{i} \quad \text { maximize } \quad-b^{T} v+\sum_{i=1}^{n} \log \left(A^{T} v\right)_{i}+n \\
& \text { subject to } A x=b
\end{aligned}
$$

## Algorithms

- we compare three versions of Newton's method
- $A \in \mathbf{R}^{100 \times 500}$
- starting points are different for the three methods


## Equality constrained analytic centering

1. Newton method with equality constraints (requires $x^{(0)}>0, A x^{(0)}=b$ )

2. (unconstrained) Newton method applied to dual problem (requires $A^{T} v^{(0)}>0$ )


## Equality constrained analytic centering

3. infeasible start Newton method (requires $x^{(0)}>0$ )


## Equality constrained analytic centering

complexity per iteration of the three methods is identical

1. use block elimination to solve KKT system

$$
\left[\begin{array}{cc}
\boldsymbol{\operatorname { d i a g }}(x)^{-2} & A^{T} \\
A & 0
\end{array}\right]\left[\begin{array}{c}
\Delta x \\
w
\end{array}\right]=\left[\begin{array}{c}
\operatorname{diag}(x)^{-1} \mathbf{1} \\
0
\end{array}\right]
$$

reduces to solving $A \boldsymbol{\operatorname { d i a g }}(x)^{2} A^{T} w=b$
2. solve Newton system $A \boldsymbol{\operatorname { d i a g }}\left(A^{T} v\right)^{-2} A^{T} \Delta v=-b+A \boldsymbol{\operatorname { d i a g }}\left(A^{T} v\right)^{-1} \mathbf{1}$
3. use block elimination to solve KKT system

$$
\left[\begin{array}{cc}
\boldsymbol{\operatorname { d i a g }}(x)^{-2} & A^{T} \\
A & 0
\end{array}\right]\left[\begin{array}{c}
\Delta x \\
\Delta v
\end{array}\right]=\left[\begin{array}{c}
\operatorname{diag}(x)^{-1} \mathbf{1} \\
A x-b
\end{array}\right]
$$

reduces to solving $A \boldsymbol{\operatorname { d i a g }}(x)^{2} A^{T} w=2 A x-b$
conclusion: in each case, solve $A D A^{T} w=h$ with $D$ positive diagonal

## Network flow optimization

$$
\begin{array}{ll}
\operatorname{minimize} & \sum_{i=1}^{n} \phi_{i}\left(x_{i}\right) \\
\text { subject to } & A x=b
\end{array}
$$

- directed graph with $n$ arcs, $p+1$ nodes
- $x_{i}$ is flow through arc $i ; \phi_{i}$ is cost flow function for $\operatorname{arc} i$ (with $\left.\phi_{i}^{\prime \prime}(x)>0\right)$
- node-incidence matrix $\tilde{A} \in \mathbf{R}^{(p+1) \times n}$ defined as

$$
\tilde{A}_{i j}=\left\{\begin{aligned}
1 & \text { arc } j \text { leaves node } i \\
-1 & \text { arc } j \text { enters node } i \\
0 & \text { otherwise }
\end{aligned}\right.
$$

reduced node-incidence matrix $A \in \mathbf{R}^{p \times n}$ is $\tilde{A}$ with last row removed

- $b \in \mathbf{R}^{p}$ is (reduced) source vector
- $\operatorname{rank} A=p$ if graph is connected


## KKT system for network flow problem

$$
\left[\begin{array}{cc}
H & A^{T} \\
A & 0
\end{array}\right]\left[\begin{array}{c}
v \\
w
\end{array}\right]=-\left[\begin{array}{l}
g \\
h
\end{array}\right]
$$

- $H=\boldsymbol{\operatorname { d i a g }}\left(\phi_{1}^{\prime \prime}\left(x_{1}\right), \ldots, \phi_{n}^{\prime \prime}\left(x_{n}\right)\right)$, positive diagonal
- can be solved by block elimination:

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

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

$$
\begin{aligned}
\left(A H^{-1} A^{T}\right)_{i j} \neq 0 & \Longleftrightarrow\left(A A^{T}\right)_{i j} \neq 0 \\
& \Longleftrightarrow \text { nodes } i \text { and } j \text { are adjacent }
\end{aligned}
$$

## Analytic center of linear matrix inequality

$$
\begin{array}{ll}
\operatorname{minimize} & -\log \operatorname{det} X \\
\text { subject to } & \operatorname{tr}\left(A_{i} X\right)=b_{i}, \quad i=1, \ldots, p
\end{array}
$$

- variable is $X \in \mathbf{S}^{n}$
- includes an implicit constraint $X>0$


## Optimality conditions

$$
X>0, \quad-X^{-1}+\sum_{j=1}^{p} v_{j} A_{i}=0, \quad \operatorname{tr}\left(A_{i} X\right)=b_{i}, \quad i=1, \ldots, p
$$

## Newton equation at feasible $X$

$$
X^{-1} \Delta X X^{-1}+\sum_{j=1}^{p} w_{j} A_{j}=X^{-1}, \quad \operatorname{tr}\left(A_{i} \Delta X\right)=0, \quad i=1, \ldots, p
$$

- follows from linear approximation $(X+\Delta X)^{-1} \approx X^{-1}-X^{-1} \Delta X X^{-1}$
- a set of $\frac{1}{2} n(n+1)+p$ linear equations in $\frac{1}{2} n(n+1)+p$ variables $\Delta X, w$


## Solution by block elimination

- eliminate $\Delta X$ from first equation:

$$
\begin{equation*}
\Delta X=X-\sum_{j=1}^{p} w_{j} X A_{j} X \tag{6}
\end{equation*}
$$

- substitute expression for $\Delta X$ in second equation

$$
\begin{equation*}
\sum_{j=1}^{p} \operatorname{tr}\left(A_{i} X A_{j} X\right) w_{j}=b_{i}, \quad i=1, \ldots, p \tag{7}
\end{equation*}
$$

this is a dense positive definite set of linear equations $G w=b$ with

$$
G_{i j}=\operatorname{tr}\left(A_{i} X A_{j} X\right), \quad i, j=1, \ldots, p
$$

- first solve (7) by Cholesky factorization of $G$; then substitute $w$ in (6) to get $\Delta X$


## Complexity of block elimination method

the dominant terms in a flop count:

- Cholesky factorization $X=L L^{T}\left((1 / 3) n^{3}\right.$ flops)
- form $p$ products $L^{T} A_{j} L$ ((3/2)pn ${ }^{3}$ flops)
- compute $p(p+1) / 2$ elements of $G$

$$
G_{i j}=\operatorname{tr}\left(\left(L^{T} A_{i} L\right)\left(L^{T} A_{j} L\right)\right)
$$

((1/2) $p^{2} n^{2}$ flops)

- solve (7) via Cholesky factorization ((1/3) $p^{3}$ flops)
complexity is cubic in $n$ (although KKT system has $\frac{1}{2} n(n+1)+p$ variables)

