CME 307 / MS&E 311: Optimization

Least squares

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Management Science and Engineering
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February 28, 2024

Announcements

- 1:30pm Friday 4/14: team formation in Thornton 110
- homework 1 out, due Friday 4/21

Linear system

find $x \in \mathbf{R}^n$ such that

$$Ax = b$$

given **design matrix** $A \in \mathbf{R}^{m \times n}$, **righthand side** (rhs) $b \in \mathbf{R}^m$

how to solve?

- ▶ factor and solve
    - ▶ QR
    - ▶ singular value decomposition (SVD)
    - ▶ Cholesky (for symmetric A)
- ▶ iterative methods
    - ▶ conjugate gradient (CG) (for symmetric A)
    - ▶ iterative refinement

we will talk about QR, CG, and iterative refinement

The SVD and the pseudoinverse

if $r = \mathrm{Rank}(A)$ and $A = U\Sigma V^T$ is the SVD of A,

- $U \in \mathbf{R}^{m \times r}$ is orthogonal: $U^T U = I_r$
- $\Sigma \in \mathbf{R}_+^{r \times r}$ is diagonal and nonnegative
- $V \in \mathbf{R}^{n \times r}$ is orthogonal: $V^T V = I_r$

we can write the **pseudoinverse** $A^\dagger = V\Sigma^{-1}U^T$

- if $x \in \mathrm{span}(V)$, $A^\dagger A x = x$

Considerations in choosing a method

▶ sparse or dense A?

▶ symmetric A or rectangular problem?

▶ conditioning of A?

▶ one problem, or many righthand sides b with the same design matrix A?

	symmetric psd	**rectangular**
direct	Cholesky	QR
indirect	CG	LSQR

Table: Methods for solving linear systems

▶ direct methods get accurate solutions in $O(n^3)$ flops

▶ indirect methods get ok solution in a small number of matvecs

Optimality condition for least squares is a linear system

given $A \in \mathbf{R}^{m \times n}$, $y \in \mathbf{R}^m$. find x to solve

$$\text{minimize} \qquad \|Ax - b\|^2.$$

to solve, take gradient, set to 0. solution x satisfies **normal equations**

$$A^\top A x = A^\top b.$$

a linear system!

- ▶ $A^\top A$ symmetric positive semidefinite
- ▶ normal equations always have a solution (why?)

Outline

QR

Conjugate gradient

Preconditioned CG

Iterative refinement

How to solve a linear system?

never form the inverse explicitly: numerically unstable!

Corollary: never type `inv(A'*A)` or `pinv(A'*A)` to solve the normal equations.

How to solve a linear system?

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Corollary: never type `inv(A'*A)` or `pinv(A'*A)` to solve the normal equations.

Instead: compute the inverse using easier matrices to invert, like

- orthogonal matrix Q:

$$a = Qb \iff Q^\top a = b$$

- (upper) triangular matrix R:
  if $a = Rb$, can find b given R and a by solving sequence of simple, stable equations.

The QR factorization

every matrix A can be written using **QR decomposition** as
$A = QR$

- $Q \in \mathbf{R}^{m \times n}$ has orthogonal columns: $Q^\top Q = I_n$
- $R \in \mathbf{R}^{n \times n}$ is upper triangular: $R_{ij} = 0$ for $i > j$
- diagonal of $R \in \mathbf{R}^{n \times n}$ is positive: $R_{ii} > 0$ for $i = 1, \ldots, n$
- this factorization always exists and is unique
  (proof by Gram-Schmidt construction)

can compute QR factorization of X in $2mn^2$ flops

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can compute QR factorization of X in $2mn^2$ flops

use `LinearAlgebra.qr`:

$$Q, R = \mathbf{qr}(X)$$

advantage of QR: it's easy to invert R!

QR to solve linear system

use QR to solve linear system $Ax = b$: if $A = QR$,

$$
\begin{aligned}
Ax &= b \\
x &= R^{-1}Q^{\top}b
\end{aligned}
$$

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Q: What happens if we apply this method to solve an infeasible system with $m > n$?

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Q: What happens if we apply this method to solve an infeasible system with $m > n$?

A: decompose $b = b^{\parallel} + b^{\perp}$ where $b^{\parallel} \in \mathrm{span}(A)$; QR solves $Ax = b^{\parallel}$

QR for least squares

use QR to solve least squares: if $A = QR$,

$$
\begin{aligned}
A^\top A x &= A^\top b \\
(QR)^\top QR x &= (QR)^\top b \\
R^\top Q^\top QR x &= R^\top Q^\top b \\
R^\top R x &= R^\top Q^\top b \\
R x &= Q^\top b \\
x &= R^{-1} Q^\top b
\end{aligned}
$$

Computational considerations

use QR factorization to solve $Ax = b$

▶ compute QR factorization of A ($2mn^2$ flops)

▶ to compute $x = R^{-1}Q^{\top}b$
  ▶ form $z = Q^{\top}b$ ($2mn$ flops)
  ▶ compute $x = R^{-1}z$ by back-substitution   (n^2 flops)

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in julia (or matlab), the **backslash operator** solves least-squares efficiently (usually, using QR)

x = A \ b

in python, use numpy.lstsq

Demo: QR

https: //github.com/stanford-cme-307/demos/blob/main/lsq.ipynb

Sparse QR

complexity of QR depends on the sparsity of Q and R:

- compute QR factorization of A (?? flops)
- to compute $x = R^{-1}Q^{\top}b$
    - form $z = Q^{\top}b$ (**nnz**(Q) flops)
    - compute $x = R^{-1}z$ by back-substitution   (**nnz**(R) flops)

Q-less QR

during QR, can compute $Q^\top b$ essentially for free!

▶ compute QR of $\begin{bmatrix} A & b \end{bmatrix}$.

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or compute it afterwards without forming Q:

$$\begin{aligned} A^\top b &= (QR)^\top b = R^\top Q^\top b \\ R^{-1} A^\top b &= Q^\top b \end{aligned}$$

Cholesky and QR

consider **Gram matrix** $G = A^\top A \succeq 0$. if $A = QR$,

$$G = R^\top Q^\top Q R = R^\top R$$

this construction gives **Cholesky factorization** of a spd matrix G

▶ factors spd matrix into triangular matrices
▶ Cholesky factors of $X^\top X$ have same structure as R

Sparse QR: exercise

- can you guess the sparsity of R given sparsity of A?
- can you change sparity of R by permuting columns of A?

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use 'colamd' in Matlab, equivalents in Python and julia

Chordal fill-in

to analyze fill-in

- ▶ consider spd matrix, for simplicity
- ▶ interpret matrix as directed graph
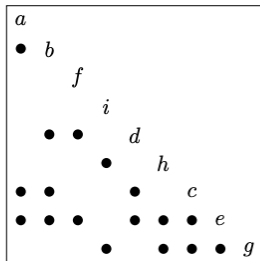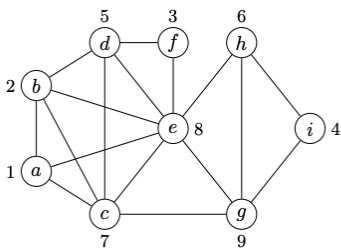- ▶ form clique tree
- ▶ identify fill-in

Figure 4.1: *Left.* Filled graph with 9 vertices. The number next to each vertex is the index $\sigma^{-1}(v)$. *Right.* Array representation of the same graph.

Outline

Conjugate gradients

symmetric positive semidefinite system of equations

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why use conjugate gradients?

- ▶ uses only matrix-vector multiplies with A
  - ▶ useful for structured (from PDE or graph) or sparse matrices, easy to parallelize, . . .
- ▶ most useful for problems with $n > 10^5$ or more
- ▶ converges exactly in n iterations
- ▶ converges approximately much faster
- ▶ quick-and-dirty solve is appropriate **inside** inner loop of optimization algo

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other variants for indefinite (MINRES) or nonsymmetric matrices (GMRES)

Iterative methods for least squares

define

- ▶ (convex) objective $f(x) = (1/2)x^\top A x - x^\top b$
- ▶ gradient $\nabla f(x) = Ax - b$
- ▶ condition number $\kappa(A) = \lambda_1(A)/\lambda_n(A)$
- ▶ A-norm $\|x\|_A^2 = x^T A x$
- ▶ bound $R \geq \|x_\star\|$ on norm of solution $x_\star$
- ▶ goal: find apx solution within accuracy $f(x) - f(x_\star) \leq \epsilon$

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how many iterations (matvecs) required?

- ▶ conjugate gradient
  - ▶ $O\left(\sqrt{\kappa}\log(\frac{1}{\epsilon})\right)$
- ▶ gradient descent (GD)
  - ▶ $O\left(\kappa\log(1/\epsilon)\right)$
- ▶ accelerated gradient descent
  - ▶ $O\left(\sqrt{\kappa}\log(\frac{R^2}{\epsilon})\right)$ more generalizable, but more parameters to tune

source: Bubeck, 2014; Karimi, Nutini, and Schmidt, 2016

Residual

define **residual** $r = b - Ax$ at putative solution x

- $r = -\nabla f(x) = A(x_\star - x)$

Residual

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▶ $r = -\nabla f(x) = A(x_\star - x)$

measures of error:

▶ objective function $f(x) - f(x_\star)$
▶ norm of residual $\|r\|$
▶ norm of gradient $\|\nabla f(x)\|$
▶ in terms of r, can compute error in objective

$$\begin{aligned}
f(x) - f(x_\star) &= \|x - x_\star\|_A \\
&= \frac{1}{2}(x - x_\star)^\top A(x - x_\star) \\
&= \frac{1}{2}(r)^\top A^{-1}(r) \\
&= \|r\|_{A^{-1}}
\end{aligned}$$

Krylov subspace

the Krylov subspace of dimension k is

$$\mathcal{K}_k = \operatorname{span}\{b, Ab, \ldots, A^{k-1}b\} = \operatorname{span}\{p_k(A)b \mid degree(p) < k\}$$

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the iterates of the **Krylov sequence** $x^{(1)}, x^{(2)}, \ldots$, minimize objective over successive Krylov subspaces

$$x^{(k)} = \operatorname*{argmin}_{x \in \mathcal{K}_k} f(x) = \operatorname*{argmin}_{x \in \mathcal{K}_k} \|Ax - b\| = \operatorname*{argmin}_{x \in \mathcal{K}_k} \|x - x_\star\|_A$$

the CG algorithm generates the Krylov sequence

Properties of Krylov sequence

- $f(x^{(k+1)}) \leq f(x^{(k)})$ (but $\|r\|$ can increase)
- $x^{(n)} = x_\star$
- $x^{(k)} = p_k(A)b$, where p_k is a polynomial with degree $< k$
- less obvious: there is a two-term recurrence

$$x^{(k+1)} = x^{(k)} + \alpha_k p^{(k)} \qquad \text{where} \qquad p^{(k)} = -r^{(k)} + \beta_k p^{(k-1)}$$

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  - α_k and β_k are determined by the CG algorithm
  - can derive recurrence from optimality conditions:
    each new iterate $x^{(k+1)}$ must have gradient (residual)
    orthogonal to $\mathcal{K}_k$

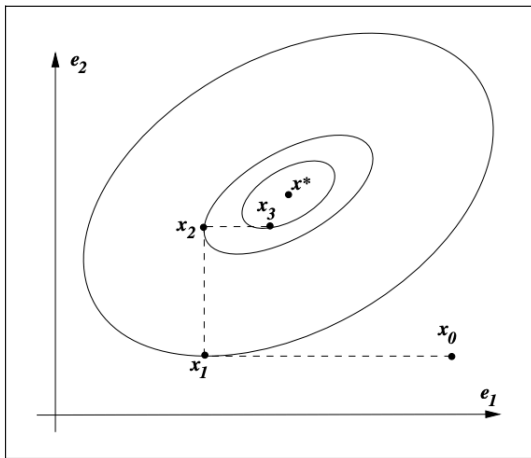# Coordinate descent does not solve in n iterations

Figure 5.2 Successive minimization along coordinate axes does not find the solution in n iterations, for a general convex quadratic.

source: NW04

CG converges in $\mathrm{Rank}(A)$ iterations

write (don't compute!) SVD of $A = V \Lambda V^\top$ with

- $r = \mathrm{Rank}(A)$
- $\Lambda \in \mathbf{R}^r \times r$ diagonal and positive
- $V \in \mathbf{R}^{n \times r}$: orthonormal: $V^\top V = I_r$

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characteristic polynomial of Λ:

$$\xi(s) = \det(sI_r - \Lambda) = (s - \lambda_1) \cdots (s - \lambda_r) = s^r + \alpha s^{r-1} + \cdots + \alpha_r$$

Cayley-Hamilton theorem

$$
\begin{aligned}
\xi(\Lambda) = 0 &= \Lambda^r + \alpha_1 \Lambda^{r-1} + \cdots + \alpha_r I_r \\
\Lambda^{-1} &= -(1/\alpha_r)(\Lambda^{r-1} + \alpha_1 \Lambda^{r-2} + \cdots + \alpha_{r-1} I_r)
\end{aligned}
$$

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\end{aligned}$$

write $A^{-1} = V\Lambda^{-1}V^\top$ in terms of this decomposition:

$$\begin{aligned}
A^{-1} = V\Lambda^{-1}V^\top &= = -(1/\alpha_r)(V\Lambda^{r-1}V^\top + \alpha_1 V\Lambda^{r-2}V^\top + \cdots + \alpha_r \\
&= -(1/\alpha_r)(A^{r-1} + \alpha_1 A^{r-2} + \cdots + \alpha_{r-1} I)
\end{aligned}$$

in particular, $x_\star = A^{-1}b \in \mathcal{K}_r$

Outline

QR

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Matrix square root

$A \in \mathbf{S}_+^n$ has a square root $A^{1/2} \in \mathbf{S}_+^n$:

- if $A = U\Lambda U^\top$ is the eigendecomposition of A,
- then $A^{1/2} = U\Lambda^{1/2}U^\top$

so $A = A^{1/2}A^{1/2}$.

Preconditioning CG

for any $P \succ 0$,

$$Ax = b \iff P^{-1/2}Ax = P^{-1/2}b$$
$$P^{-1/2}AP^{-1/2}z = P^{-1/2}b$$

where $x = P^{-1/2}z$.

Preconditioning CG

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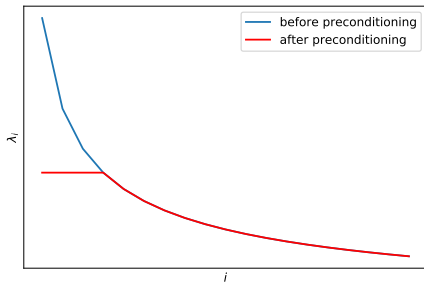▶ preconditioning works well when $\kappa(P^{-1/2}AP^{-1/2}) \ll \kappa(A)$

how to precondition?

▶ common heuristic: Jacobi preconditioning $P = \textbf{diag}(A)$
▶ incomplete Cholesky (best for structured sparsity)

An optimal low-rank preconditioner

▶ suppose $\lfloor A \rfloor_s = V_s \Lambda_s V_s^T$ is a best rank-s apx to $A \in \mathbf{S}_+^n$.

▶ the best preconditioner using this information is

$$P_\star = \frac{1}{\lambda_{s+1}} V_s(\Lambda_s) V_s^T + (I - V_s V_s^T)$$

Outline

Iterative refinement

want to solve $Ax = b$.

given approximate solution $Ax^{(0)} \approx b$, for $k = 1, \ldots,$

- ▶ compute residual $r^{(k)} = b - Ax^{(k)}$
- ▶ use any method to solve $A\delta^{(k)} = r^{(k)}$
- ▶ $x^{(k+1)} = x^{(k)} + \delta^{(k)}$