Fundamental Concepts in Computational and Applied Mathematics

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Consider the following matrix

$$K_n = \begin{bmatrix} 2 & -1 & 0 & 0 & \dots & 0 \\ -1 & 2 & -1 & 0 & \dots & 0 \\ 0 & -1 & 2 & -1 & \dots & 0 \\ \dots & 0 & -1 & 2 & \ddots & 0 \\ 0 & \dots & 0 & \ddots & 2 & -1 \\ 0 & 0 & 0 & 0 & -1 & 2 \end{bmatrix}$$

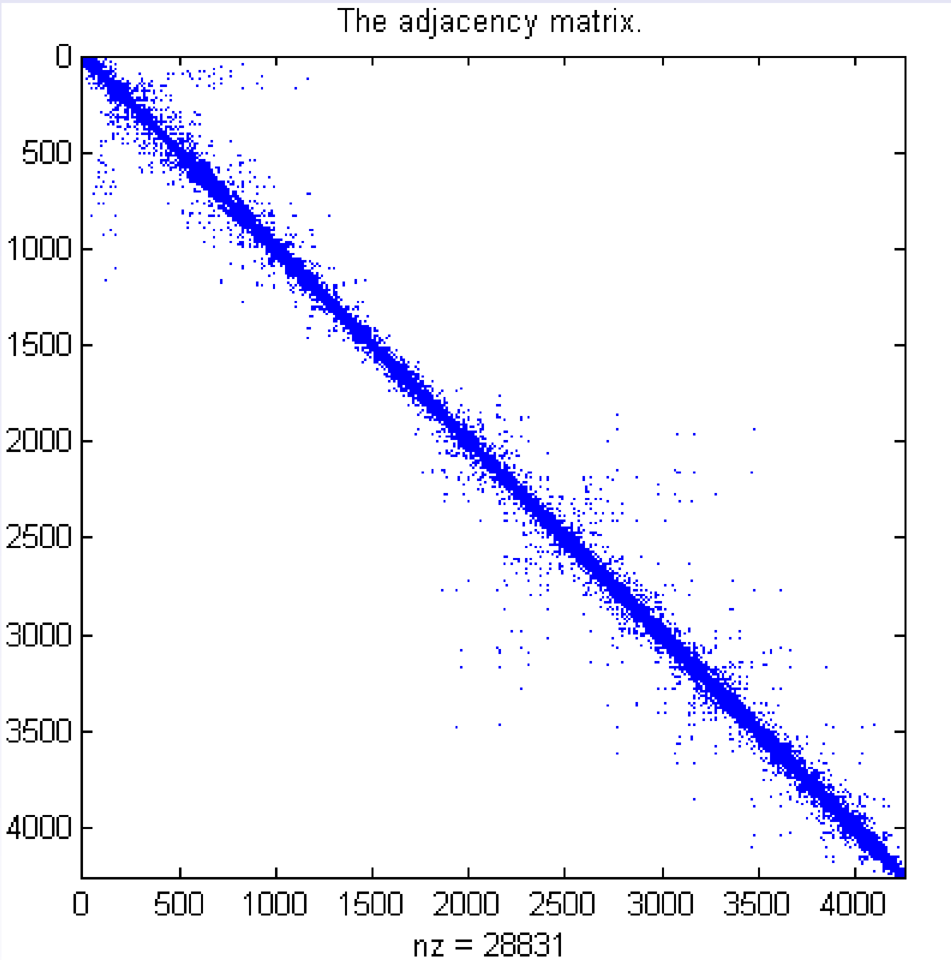
- We will encounter matrices of this form in future talks
- We can take advantage of the special structure to improve our algorithms
- This matrix is known as a Toeplitz matrix (constant diagonal)

Another interesting matrix

$$D = \begin{bmatrix} 0 & 1/2 & 0 & 0 & \dots & -1/2 \\ -1/2 & 0 & 1/2 & 0 & \dots & 0 \\ 0 & -1/2 & 0 & 1/2 & \dots & 0 \\ \dots & 0 & -1/2 & 0 & \ddots & 0 \\ 0 & \dots & 0 & \ddots & 0 & 1/2 \\ 1/2 & 0 & 0 & 0 & -1/2 & 0 \end{bmatrix}$$

- A second order method can be given by the following matrix
- This matrix is Toeplitz, skew-symmetrix, and circulant. All very nice properties.
- Does this structure remind you of anything?

More generally



Definition

Any matrix where the majority of entries are zero is referred to as a *sparse* matrix.

Discussion

So what does *majority* mean?

Sparse methods

- Sparse matrices arise in many science and engineering applications
- Almost all discretization methods you will encounter will have a sparse structure
- Sparse methods take advantage of special structure in matrices to improve computational efficiency

Stationary Iterative Methods

- Based on splitting techniques
- Widely used in engineering, but have been superseded by more modern techniques
- Still useful in certain contexts, e.g. preconditioners (more later)

Basic Stationary Iterative Method (SIM)

Consider $Ax = b$
First we'll "split" the matrix $A = M - N$, where $M = L + D$ and $N = -U$. Now I'll define an iteration for $k = 0, \ldots,$ s.t.

$$
\begin{aligned}
(L+D)x^{k+1} &= b - Ux^k, &(1)\\
Mx^{k+1} &= b + Nx^k, &(2)\\
x^{k+1} &= M^{-1}b + M^{-1}Nx^k, &(3)\\
x^{k+1} &= Gx^k + c, &(4)
\end{aligned}
$$

where $G = M^{-1}N, c = M^{-1}b$.

Note

This is one of several splittings one can use. Can you think of others?

Useful Facts

Fact 1

$e^{k+1} = Ge^k, \quad k = 0, \ldots.$

Fact 2

If we use the SIM in equation (4) $x^k \to \hat{x} \iff \rho(G) < 1.$

Fact 3

Many important matrices resulting from problems arising in CSE satisfy $\rho(G) < 1.$

Discussion: Hestenes and Stiefel

Finite Precision

- In exact arithmetic the CG method will converge to the solution of $Ax = b$ in at most n iterations for A spd.
- In finite precision, roundoff error will contaminate the solution.
- And even in the exact case, what does this mean for a system with dimension 1M or 1B?

CG Convergence Rate

Can show that

$$||x^k - \hat{x}||_A \leq 2 \left(\frac{\sqrt{\kappa(A)} - 1}{\sqrt{\kappa(A)} + 1} \right)^k ||x^0 - \hat{x}||_A \tag{5}$$

Table: Number of iterations to reduce error by 10^{-3}.

$\kappa(A)$	Value	iter
1	0.0	1
10^2	0.82	38
10^4	0.98	376
10^8	0.9998	38,000

Advanced Topic: Krylov subspace methods

CG is an example of what we now call a Krylov space method.

Definition

A *Krylov* space is defined by:

$$\mathcal{K}_k(A, b) = span\{b, Ab, A^2b, A^3b, \ldots, A^{k-1}b\}.$$

Idea

Choose your iterate, x^k, such that it belongs to the Krylov space and it minimizes the distance between x^k and $\hat{x}$.

Advanced Topic – Preconditioning

Fundamental Idea

If you don't like the problem you're given to solve, then change it into something that is easier to work with!

- If the error bound is dependent on the condition number can we do something about it?
- Ideally what would we want the condition number of the problem to be?
- Can we alter the problem to make it better conditioned, without changing the solution of the problem

Advanced Topic – Preconditioning

Consider $Ax = b$, where $\kappa(A)$ is large. Let M be a symmetric positive definite (spd) matrix. Then I can use CG to solve the equivalent problem:

$$M^{-1}Ax^{k+1} = M^{-1}b, \quad k = 0, \ldots \tag{6}$$

and if $\kappa(M^{-1}A) < \kappa(A)$, I should be able to reduce the number of iterations.

Preconditioning

Choose M^{-1} wisely and you will reduce the number of iterations significantly. Choose poorly and all you've done is create more work for yourself!

Exercise

Note that in general $M^{-1}A$ may not be symmetric. How then would you apply CG to this system?

Summary

- Sparse methods can be used to take advantage of special structure.
- Iterative methods are the dominant form of solving large-scale systems of linear equations in modern day applications.
- Most iterative methods must be preconditioned to be effective.

References I

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C. Tim Kelley.
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Appendix: Basic CG Method

Consider $Ax = b$, where A is spd. Let $x_0 = 0, r_0 = b, p_0 = r_0$.

for $k = 1, 2, 3, \ldots$

$$\begin{aligned}
\alpha_k &= (r_{k-1}^T r_{k-1})/(p_{k-1}^T A p_{k-1}) \\
x_k &= x_{k-1} + \alpha_k p_{k-1} \\
r_k &= r_{k-1} - \alpha_k A p_{k-1} \\
\beta_k &= (r_k^T r_k)/(r_{k-1}^T r_{k-1}) \\
p_k &= r_k + \beta_k p_{k-1}
\end{aligned}$$