Fundamental Concepts in Computational and Applied Mathematics

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Consider the following matrix

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

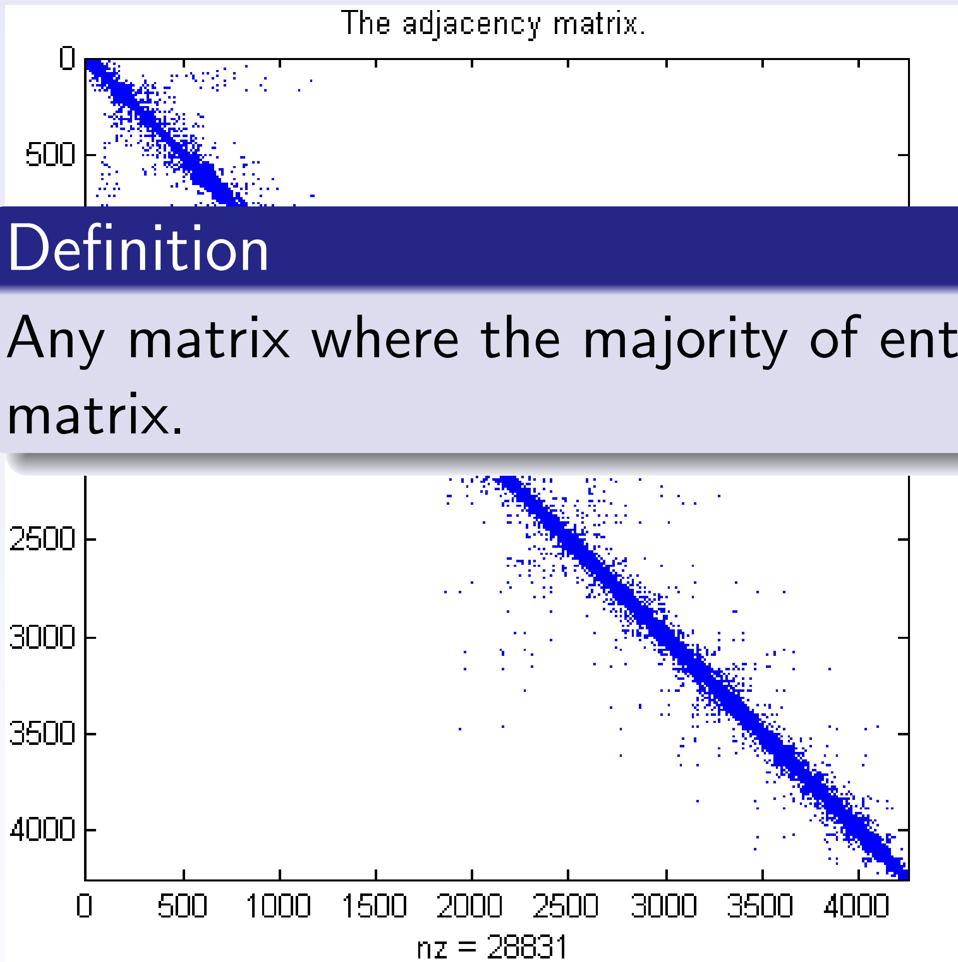
- We will encounter matrices of this form in future talks
- We can take advantage of the special structure to improve our algorithms
- This matrix is known as a Toeplitz matrix (constant diagonal)

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.

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- Widely used in engineering, but have been superseded by more modern techniques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 $A = L + D + U$, such that

$$(L + D)x^{k+1} = b - Ux^k, \quad k = 0, \ldots$$

or

$$\begin{aligned} Mx^{k+1} &= b + Nx^k, \quad k = 0, \ldots && (1) \\ x^{k+1} &= M^{-1}b + M^{-1}Nx^k, && (2) \\ x^{k+1} &= Gx^k + c, && (3) \end{aligned}$$

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

Useful Facts

Fact 1

If we use the SIM in equation (3) $x^k \to \hat{x} \iff \rho(G) < 1$.

Fact 2

$e^{k+1} = Ge^k$.

Fact 3

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

Discussion: Hestenes and Stiefel

Finite Precision

- In exact arithmetic the CG method will converge to the solution of $Ax = b$.
- Sadly, 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?

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 $\hat{x}$.

CG Convergence Rate

Can show that

$$||x^k - \hat{x}||_A \leq 2 \left(\frac{\sqrt{\kappa(A)} - 1}{\sqrt{\kappa(A)} + 1} \right)^k ||x^0 - \hat{x}||_A \tag{4}$$

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

$\kappa(A)$	Value	iter
1	0.0	1
10^2	0.82	15
10^4	0.98	150
10^8	0.9998	15,000

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:

$$\begin{aligned} M^{-1}Ax^{k+1} &= M^{-1}b, \quad k = 0, \ldots && (5) \\ \tilde{M}x^{k+1} &= \tilde{b}. && (6) \end{aligned}$$

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

Preconditioning

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

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.

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