

# Fundamental Concepts in Computational and Applied Mathematics

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## Consider the following matrix

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

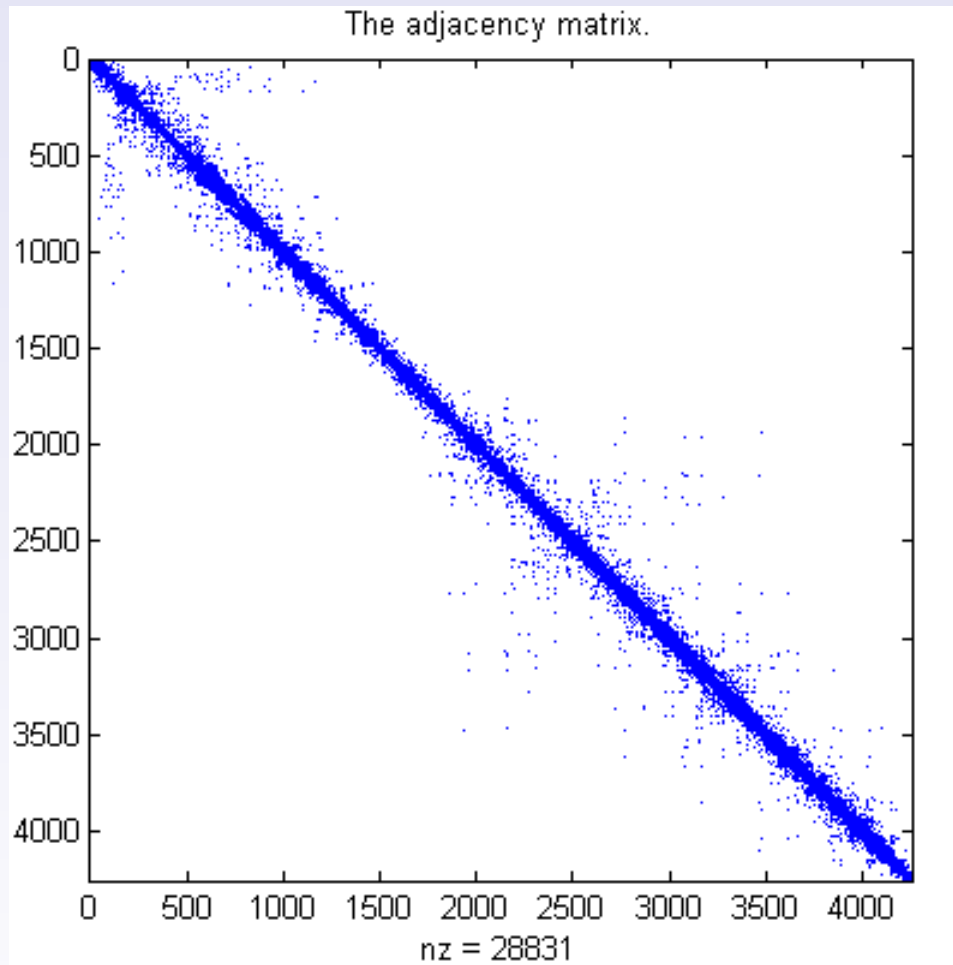
- We will encounter matrices of this form in future talks
- We can take advantage of the special structure to improve our algorithms
- This matrix is known as a Toeplitz matrix (constant diagonal)

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- Widely used in engineering, but have been superseded by more modern techniques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

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

or

$$Mx^{k+1} = b + Nx^k, \quad k = 0, \dots \quad (1)$$

$$x^{k+1} = M^{-1}b + M^{-1}Nx^k, \quad (2)$$

$$x^{k+1} = Gx^k + c, \quad (3)$$

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

# Useful Facts

## Fact 1

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

## 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  $Ax = b$  in  $n$  iterations.
- 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

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

**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:

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

## 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:

$$M^{-1}Ax^{k+1} = M^{-1}b, \quad k = 0, \dots \quad (5)$$

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

-  Gene H. Golub and Charles F. Van Loan.  
*Matrix Computations, 3rd Ed.*  
Johns Hopkins, 1996.
-  C. Tim Kelley.  
*Iterative Methods for Linear and Nonlinear Equations.*  
SIAM, 1995.
-  Magnus R. Hestenes and Eduard Stiefel.  
Methods of Conjugate Gradients for Solving Linear Systems  
J. Res. of NBS, Vol. 49, No. 6, Dec. 1952.