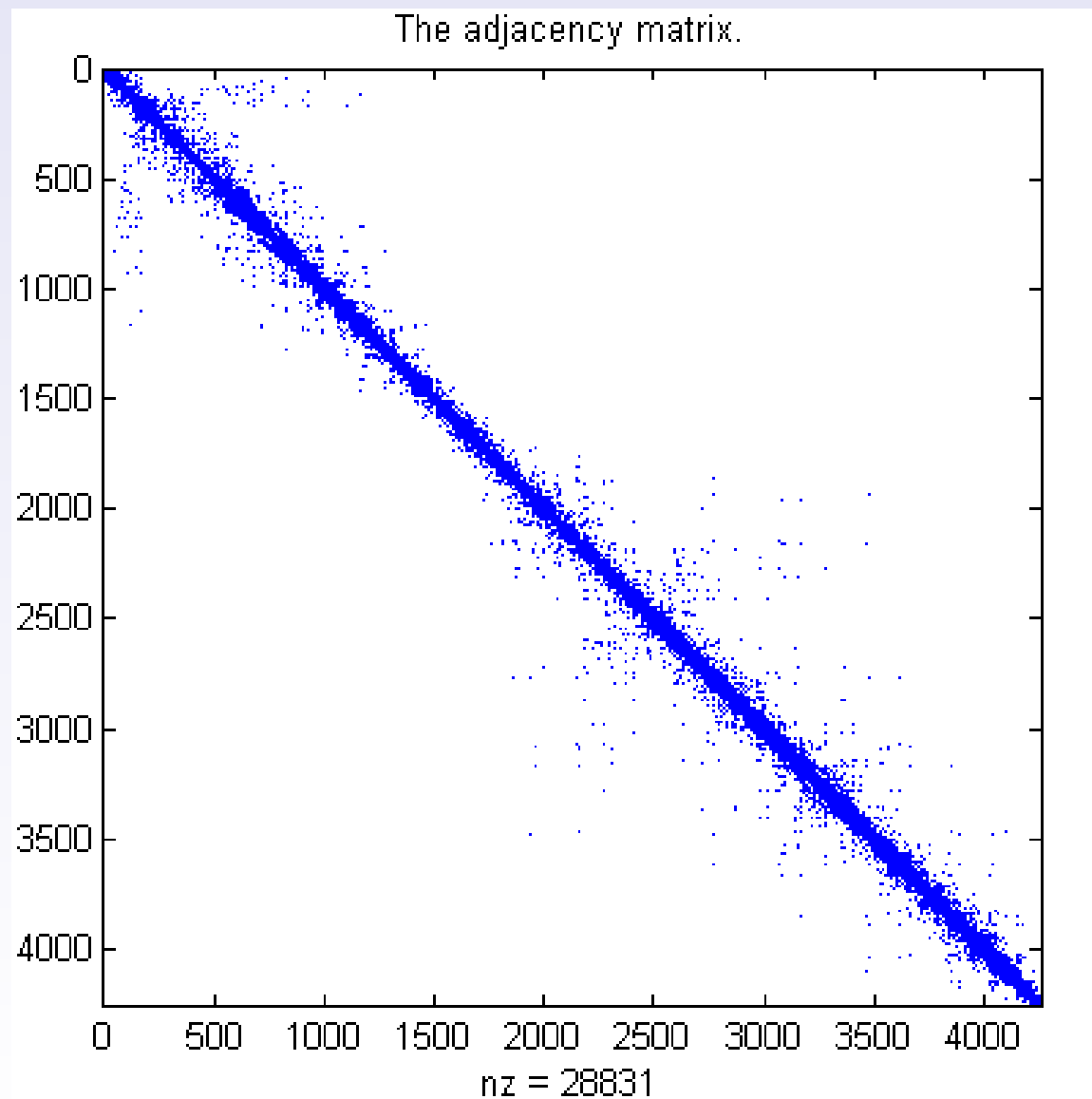# Fundamental Concepts in Computational and Applied Mathematics

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Fall 2014

Sparse Matrix Example

Consider the following matrix:

The adjacency matrix.
nz = 28831

Consider the following matrix

- We will encounter matrices of this form in future talks

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

Note: This matrix is Toeplitz (diagonal-constant).
We will encounter this matrix again when talking about derivatives

Another interesting matrix

- A second order method can be given by the following matrix

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

Note: This matrix is skew-symmetrix, Toeplitz (diagonal-constant), and circulant! All very nice properties.
The derivative is given by $w = \frac{1}{h} D \cdot u$

Sparse methods

- Sparse matrices arise in many science and engineering applications
- Almost all discretization methods you will encounter will have a special 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- Widely used in engineering, but have been superseded by more modern techniques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

Basic Method

Consider $Ax = b$

Let $A = L + D + U$ and then "split" the matrix A such that

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

or

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

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

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 it and $\hat{x}$

CG Convergence Rate

Can show that

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

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

Preconditioning Idea

Discussion

- Why precondition?
- What should the general idea be?
- How would you go about doing that?

Summary

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

References

- **Methods of Conjugate Gradients for Solving Linear Systems**, Magnus R. Hestenes and Eduard Stiefel, J. Res. of NBS, Vol. 49, No. 6, Dec. 1952.

- **Matrix Computations, 3rd Ed.**, Gene H. Golub and Charles F. Van Loan, Johns Hopkins, 1996.

- **Iterative Methods for Linear and Nonlinear Equations**, C.T. Kelley, SIAM, 1995.