Lecture 18: Preconditioned iterative methods

COMP5930M Scientific Computation

Today

Conjugate gradient examples

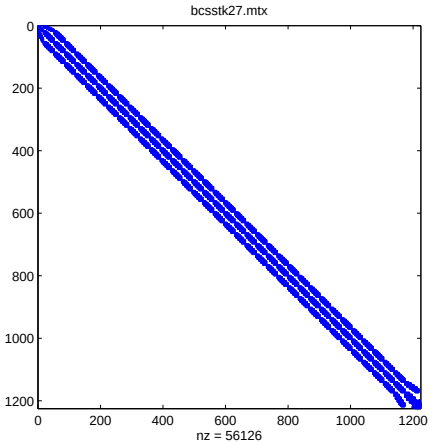
Preconditioning

Choosing a preconditioner

Matlab implementations

Preconditioned conjugate gradient examples

Conjugate gradient examples from MatrixMarket



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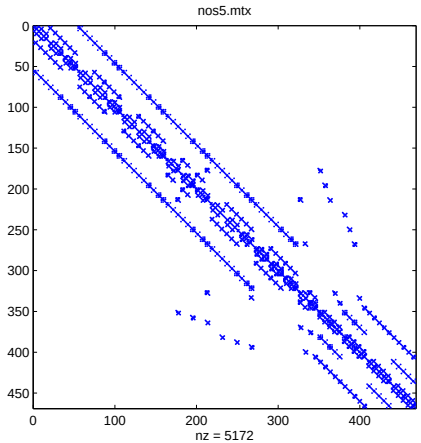

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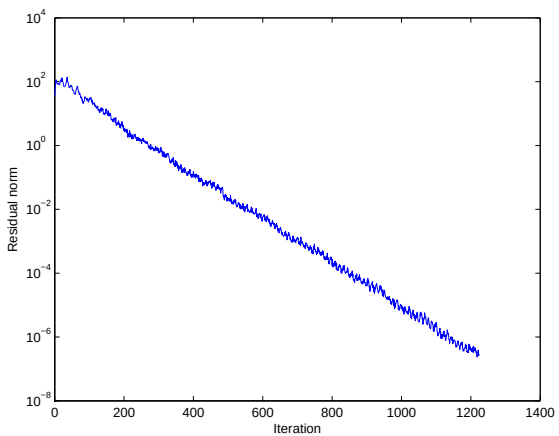
Sparsity pattern



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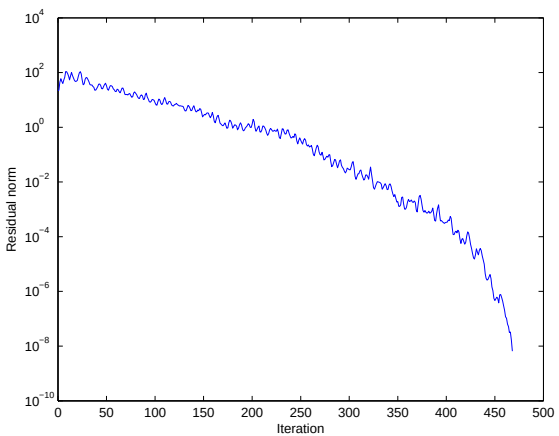

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CG convergence

Preconditioning

- The convergence of our iterative methods is governed by the distribution of eigenvalues of $\mathbf{A}$
  - Measured as the number of iterations required to achieve a certain reduction of the residual
- Recall the condition number $\kappa(\mathbf{A}) = \frac{\max_i |\lambda_i|}{\min_i |\lambda_i|}$
- We can attempt to transform our linear system $\mathbf{Ax} = \mathbf{b}$ into one with a better eigenvalue distribution through the use of a preconditioning matrix $\mathbf{M}$
  - We apply the iterative method to a modified linear system
  - The goal is to reduce: the number of iterations required, and the overall time taken

The preconditioned system

Given a linear system $\mathbf{Ax} = \mathbf{b}$ and preconditioning matrix $\mathbf{M}$ we can define a modified system in a number of ways

- Left preconditioning

$$\left(\mathbf{M}^{-1}\mathbf{A}\right)\mathbf{x} \;=\; \mathbf{M}^{-1}\mathbf{b}$$

- Right preconditioning

$$\left(\mathbf{A}\mathbf{M}^{-1}\right)\left(\mathbf{M}\mathbf{x}\right) \;=\; \mathbf{b}$$

- Left and right preconditioning (assuming $\mathbf{M} = \mathbf{M}_1\mathbf{M}_2$)

$$\left(\mathbf{M}_1^{-1}\mathbf{A}\mathbf{M}_2^{-1}\right)\left(\mathbf{M}_2\mathbf{x}\right) \;=\; \mathbf{M}_1^{-1}\mathbf{b}$$

The preconditioned conjugate gradient (PCG) algorithm

Assume we applied left preconditioning, $\mathbf{M}^{-1}\mathbf{A}\mathbf{x} = \mathbf{M}^{-1}\mathbf{b}$. Then:

- $\mathbf{r}_0 = \mathbf{b} - \mathbf{A}\mathbf{x}_0$
- $\mathbf{M}\mathbf{z}_0 = \mathbf{r}_0$ (preconditioned residual)
- $\mathbf{d}_0 = \mathbf{z}_0$ (preconditioned search direction)
- $i = 0, 1, 2, \ldots$
  - $\alpha_i = \frac{\mathbf{r}_i^T \mathbf{z}_i}{\mathbf{d}_i^T \mathbf{A}\mathbf{d}_i}$
  - $\mathbf{x}_{i+1} = \mathbf{x}_i + \alpha_i \mathbf{d}_i$
  - $\mathbf{r}_{i+1} = \mathbf{r}_i - \alpha_i \mathbf{A}\mathbf{d}_i$
  - $\mathbf{M}\mathbf{z}_{i+1} = \mathbf{r}_{i+1}$ (preconditioned residual)
  - $\beta_{i+1} = \frac{\mathbf{r}_{i+1}^T \mathbf{z}_{i+1}}{\mathbf{r}_i^T \mathbf{z}_i}$
  - $\mathbf{d}_{i+1} = \mathbf{z}_{i+1} + \beta_{i+1} \mathbf{d}_i$

Notes on the PCG algorithm

- Largely unchanged (requires algebra to show this)
  - Although we apply the algorithm to the preconditioned system we can manipulate it back into the form $\mathbf{Ax} = \mathbf{b}$
- Only one matrix-multiply required per iteration: $\mathbf{Ad}_i$
- One linear system solution per iteration: $\mathbf{Mz}_{i+1} = \mathbf{r}_{i+1}$
  - Require this to be solved very efficiently
  - If possible in $\mathcal{O}(n^2)$ total cost per iteration does not increase

Remark on inverse matrices

- Here $\mathbf{M}$ approximates the matrix $\mathbf{A}$ so that $\mathbf{M}^{-1}\mathbf{A} \approx \mathbf{I}$
- We could also approximate the inverse matrix $\mathbf{A}^{-1}$, but:
  - We don't know anything about $\mathbf{A}^{-1}$ in general
  - For many sparse matrices, the inverse $\mathbf{A}^{-1}$ will be dense, e.g.

$$\mathbf{A} = \begin{bmatrix} 1 & 1 & 1 & 1 & 1 \\ 1 & 1 & 0 & 0 & 0 \\ 1 & 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 1 & 0 \\ 1 & 0 & 0 & 0 & 1 \end{bmatrix}, \quad \mathbf{A}^{-1} = \begin{bmatrix} -\frac{1}{3} & \frac{1}{3} & \frac{1}{3} & \frac{1}{3} & \frac{1}{3} \\ \frac{1}{3} & \frac{2}{3} & -\frac{1}{3} & -\frac{1}{3} & -\frac{1}{3} \\ \frac{1}{3} & -\frac{1}{3} & \frac{2}{3} & -\frac{1}{3} & -\frac{1}{3} \\ \frac{1}{3} & -\frac{1}{3} & -\frac{1}{3} & \frac{2}{3} & -\frac{1}{3} \\ \frac{1}{3} & -\frac{1}{3} & -\frac{1}{3} & -\frac{1}{3} & \frac{2}{3} \end{bmatrix}$$

- Idea: Look for sparse preconditioner $\mathbf{M}$ such that

$$\min_{\mathbf{M} \in \mathcal{G}_S} \|\mathbf{AM} - \mathbf{I}\|^2$$

where $\mathcal{G}_S$ is the set of matrices with fixed sparsity pattern S.
This strategy is called an approximate inverse preconditioner.

Properties of a good preconditioner

The choice of preconditioner is determined by several factors:

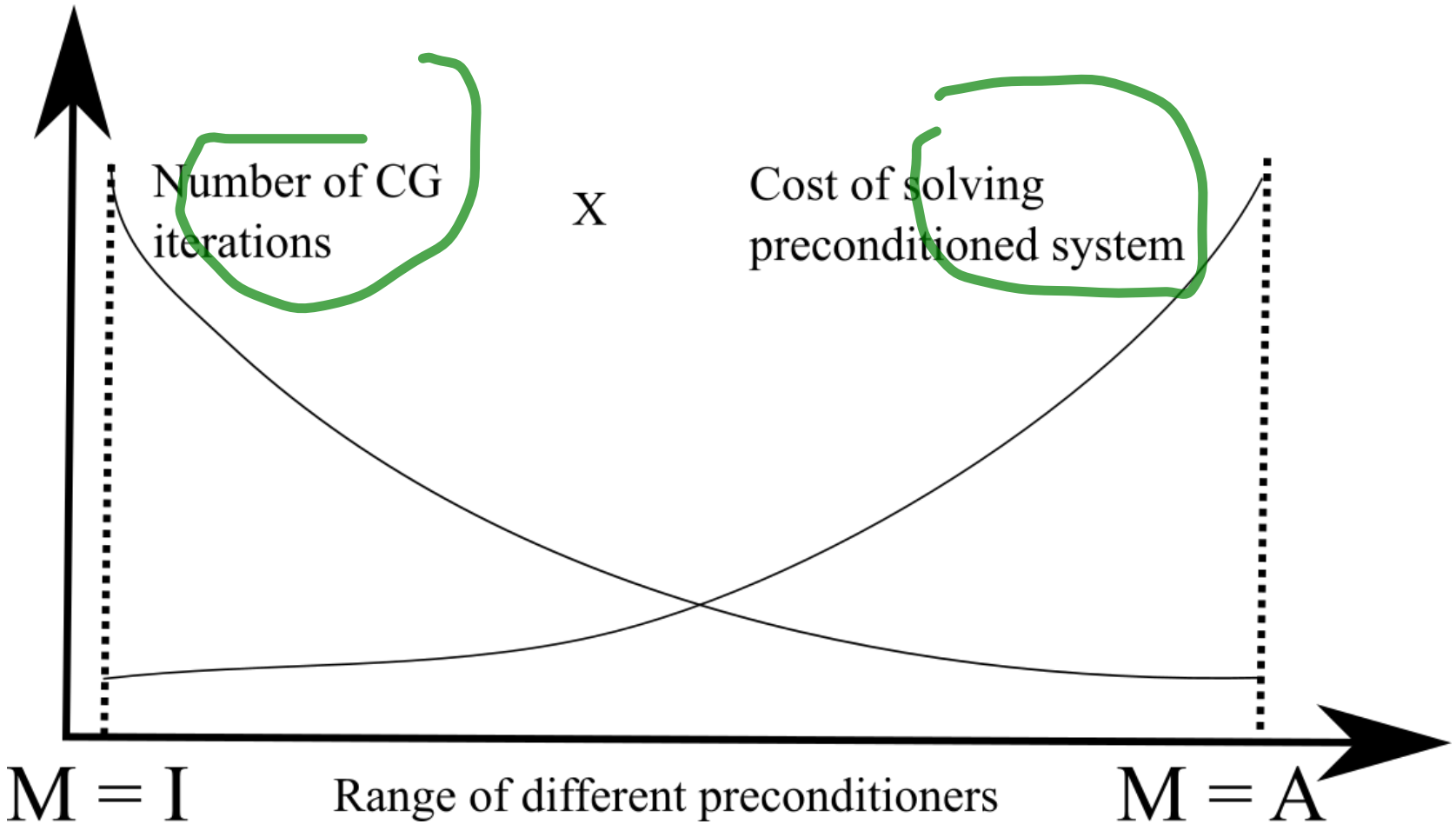
- Properties of the original system, eg. symmetry, pos.def.
- $\mathbf{M}$ should be cheap to build
- $\mathbf{Mz} = \mathbf{r}$ should be cheap to solve
- Trade-off: the fewer iterations the more expensive $\mathbf{M}$ is

A heuristic argument

M should approximate **A**

- If $\mathbf{M} = \mathbf{A}$ our preconditioned system will be the identity matrix $\mathbf{I}$ and only 1 iteration is required
  - Not practical: inverting $\mathbf{M}$ now has the same expense as inverting $\mathbf{A}$
- There are roughly two general approaches
  - Approximate factorisation of $\mathbf{A}$
  - Approximate inverse of $\mathbf{A}$
- Finding problem-specific preconditioners an art in itself

Finding an optimal preconditioner as a trade-off



Symmetric linear systems

- CG requires a SPD matrix **A**
- Preconditioning must maintain the SPD property
- Left or right preconditioning are not guaranteed to maintain symmetry
  - Use left and right with $\mathbf{M1} = \mathbf{M2}^T$

Preconditioning SPD systems

- We can factorise a SPD matrix $\mathbf{A}$ in the form

$$\mathbf{A} = \mathbf{L}\mathbf{L}^T$$

- This is known as Cholesky decomposition a specialised form of LU decomposition

- For preconditioning we use a cheaper approximate process
  - Incomplete Cholesky decomposition

$$\mathbf{M} = \bar{\mathbf{L}}\bar{\mathbf{L}}^T$$

Incomplete factorisation

- Recall: The full factorisation process introduces fill-in
  - Sparse matrices can have non-sparse factorisations
  - Reordering algorithms help here too
- Incomplete factorisation ignores some of the fill-in
- Two approaches are adopted in practice
  - Structural - based on sparsity pattern of **A**
  - Numerical - based on size of matrix entries

(i) Structural incomplete factorisation

- We know the sparsity pattern of $\mathbf{A}$
- We pre-define the sparsity pattern of $\bar{\mathbf{L}}$ and ignore terms that do not fit this pattern
- The simplest scheme assumes that $\bar{\mathbf{L}}$ has the same sparsity pattern as $\mathbf{A}$
  - Our factorisation produces no fill-in
  - It approximates the true factorisation $\mathbf{L}$
- We can define approximations with larger amounts of fill-in to achieve greater accuracy
  - at greater expense

(ii) Numerical incomplete factorisation

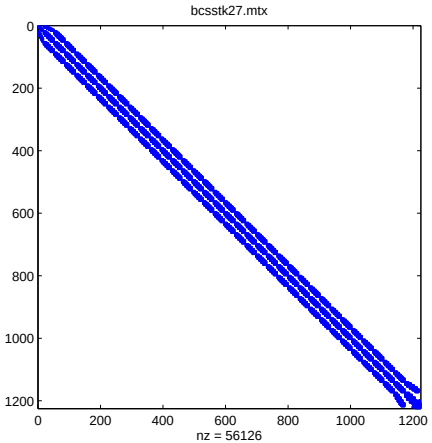
- We modify the algorithm such that only "large" entries of $\bar{\mathbf{L}}$ are stored
  - Cannot be pre-defined, must be computed
- Controlled by a drop-tolerance d_{tol} that specifies the minimum acceptable size
  - Often also a parameter l_{max} that restricts storage
- Accuracy of $\bar{\mathbf{L}}$ is determined by d_{tol} and l_{max}
- If d_{tol} too large, the approximate factor $\bar{\mathbf{L}}$ will be singular and solving $\bar{\mathbf{L}}\mathbf{z} = \mathbf{r}$ will fail

Using Matlab

- The Matlab function `ichol()` computes the incomplete Cholesky factorisation
  - `L = ichol(A,struct('type','nofill'))`
    computes the structural factorisation with no fill-in
  - `L = ichol(A,struct('type','ict','droptol',0.01))`
    computes the numerical factorisation with drop-tolerance d_{tol}

- The following symmetric examples demonstrate the benefits for the CG algorithm
  - The modified CG algorithm is covered next lecture

PCG examples - MatrixMarket



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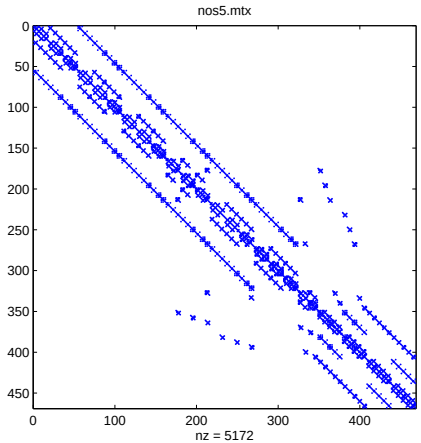

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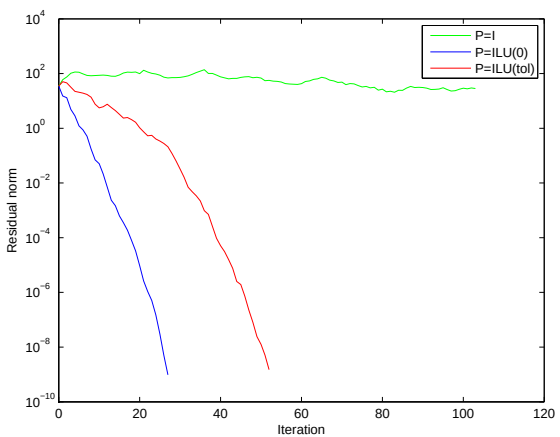

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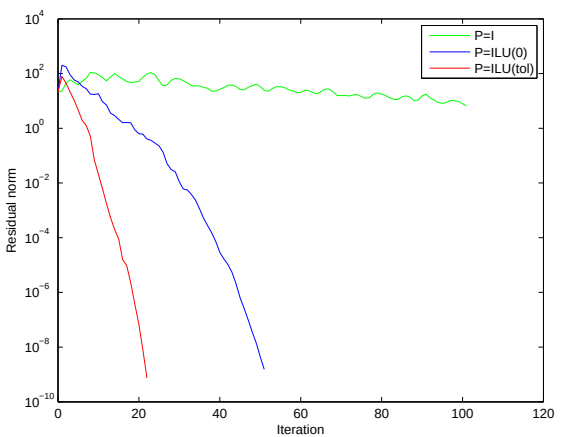

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General observations

- For a given amount of storage the numerical approach is almost always more effective than structural
  - The structural approach may store very small values and ignore much larger ones
  - The numerical approach will include fill-in but only if it is of significant size
  - The numerical approach requires *hand-tuning*
- The numerical approach is a more complex and costly algorithm but the reduction in iterations usually outweighs this cost

Non-symmetric linear systems

- GMRES is designed for non-symmetric, non-PD systems
  - The most general of the Krylov-subspace iterative methods
- There is no restriction on the preconditioner
- Can consider genuine left or right preconditioning
  - Incomplete LU algorithms for general non-symmetric linear systems

References

Templates for the Solution of Linear Systems
Richard Barrett *et al.*
http://www.netlib.org/linalg/html_templates/Templates.html

Iterative methods for sparse linear systems
Yousef Saad
http://www-users.cs.umn.edu/~saad/books.html