# Lecture Notes 17: Direct Methods for Linear Systems

## CPSC 302: Numerical Computation for Algebraic Problems

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# Chapter 4: Direct Methods for Linear Systems

- Gaussian Elimination and Backward Substitution
- LU Decomposition
- Pivoting Strategies
- Efficient Implementation

- Estimating Errors and Condition Number

- Cholesky Decomposition
- Sparse Matrices

# Outline

1. Estimating Errors and Condition Number
   - The Error in the Numerical Solution
   - Condition Number and a Relative Error Estimate
   - The Error when using a Direct Method
   - More on the Condition Number

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## Relative Error in the Solution

- Still consider
$$A\mathbf{x} = \mathbf{b}$$
but now assess quality of approximate solution obtained somehow.

- Denote exact solution $\mathbf{x}$, computed (or given) approximate solution $\hat{\mathbf{x}}$. Want to estimate
$$\frac{\|\mathbf{x} - \hat{\mathbf{x}}\|}{\|\mathbf{x}\|}$$
in some vector norm ($\infty$-, $2$-, or $1$-norm).

- Can compute the residual $\hat{\mathbf{r}} = \mathbf{b} - A\hat{\mathbf{x}}$ and so also $\frac{\|\hat{\mathbf{r}}\|}{\|\mathbf{b}\|}$.
Does a small relative residual imply small relative error in solution?

# Example

- For the problem

$$A = \begin{pmatrix} 1.2969 & 0.8648 \\ 0.2161 & 0.1441 \end{pmatrix}, \quad \mathbf{b} = \begin{pmatrix} 0.8642 \\ 0.1440 \end{pmatrix},$$

  consider the approximate solution

$$\hat{\mathbf{x}} = \begin{pmatrix} 0.9911 \\ -0.4870 \end{pmatrix}.$$

- Then

$$\hat{\mathbf{r}} = \mathbf{b} - A\hat{\mathbf{x}} = \begin{pmatrix} -10^{-8} \\ 10^{-8} \end{pmatrix},$$

  so $\|\hat{\mathbf{r}}\|_\infty = 10^{-8}$.

- However, the exact solution is

$$\mathbf{x} = \begin{pmatrix} 2 \\ -2 \end{pmatrix}, \quad \text{so} \quad \|\mathbf{x} - \hat{\mathbf{x}}\|_\infty = 1.513\,.$$

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# Conditioning of Problem

- Since $\hat{\mathbf{r}} = \mathbf{b} - A\hat{\mathbf{x}} = A\mathbf{x} - A\hat{\mathbf{x}} = A(\mathbf{x} - \hat{\mathbf{x}})$, get

$$\mathbf{x} - \hat{\mathbf{x}} = A^{-1}\hat{\mathbf{r}} \quad \text{and hence} \quad \|\mathbf{x} - \hat{\mathbf{x}}\| = \|A^{-1}\hat{\mathbf{r}}\| \le \|A^{-1}\|\|\hat{\mathbf{r}}\| \,.$$

- Since $\mathbf{b} = A\mathbf{x}$, get

$$\|\mathbf{b}\| = \|A\mathbf{x}\| \le \|A\|\|\mathbf{x}\| \quad \text{and hence} \quad \frac{1}{\|\mathbf{x}\|} \le \frac{\|A\|}{\|\mathbf{b}\|} \,.$$

- Hence

$$\begin{aligned}
\frac{\|\mathbf{x} - \hat{\mathbf{x}}\|}{\|\mathbf{x}\|} &\le \|A^{-1}\|\|\hat{\mathbf{r}}\|\frac{\|A\|}{\|\mathbf{b}\|} = \|A^{-1}\|\|A\|\frac{\|\hat{\mathbf{r}}\|}{\|\mathbf{b}\|} = \kappa(A)\frac{\|\hat{\mathbf{r}}\|}{\|\mathbf{b}\|}, \\
\kappa(A) &= \|A\|\|A^{-1}\|.
\end{aligned}$$

The scalar $\kappa(A)$ is the **condition number** of $A$.
For defining $\kappa(A)$ use the induced matrix norm corresponding to the vector norm employed in the above estimates.

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# Quality of Solution

- Backward error analysis: associate result of numerical algorithm (GEPP) with the **exact solution** of a **perturbed problem**

$$(A + \delta A)\hat{\mathbf{x}} = \mathbf{b} + \delta \mathbf{b}.$$

- Can rewrite

$$\frac{\|\mathbf{x} - \hat{\mathbf{x}}\|}{\|\mathbf{x}\|} \leq \kappa(A) \frac{\|\hat{\mathbf{r}}\|}{\|\mathbf{b}\|}$$

  to

$$\frac{\|\mathbf{x} - \hat{\mathbf{x}}\|}{\|\mathbf{x}\|} \leq \kappa(A)\, f(\delta A, \delta \mathbf{b}, \hat{\mathbf{x}})$$

- The job of GEPP is to make $\delta A$ and $\delta \mathbf{b}$ small.

- Obtain good quality solution (only) if in addition, $\kappa(A)$ is not too large.

# Example (cont.)

In our $2 \times 2$ example, we saw $\|\mathbf{x} - \hat{\mathbf{x}}\|_\infty \approx 10^8 \, \|\hat{\mathbf{r}}\|_\infty$.

- For the problem

$$A = \begin{pmatrix} 1.2969 & 0.8648 \\ 0.2161 & 0.1441 \end{pmatrix},$$

  we have

$$A^{-1} = 10^8 \begin{pmatrix} 0.1441 & -0.8648 \\ -0.2161 & 1.2969 \end{pmatrix}.$$

- Hence

$$\kappa_\infty(A) = \|A\|_\infty \, \|A^{-1}\|_\infty = 2.1617 \cdot 1.513 \times 10^8 \approx 3.27 \times 10^8$$

  and $\|\mathbf{x} - \hat{\mathbf{x}}\|_\infty \approx \kappa_\infty(A) \, \|\hat{\mathbf{r}}\|_\infty$

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# The Condition Number

- Always $\kappa(A) \geq 1$.
- For orthogonal matrices, $\kappa_2(Q) = 1$: ideally conditioned!
- $\kappa(A)$ indicates how close $A$ is to being singular, which $\det(A)$ does not.

# Example

Consider

$$A = \begin{pmatrix} 0.01 & & & \\ & 0.01 & & \\ & & \ddots & \\ & & & 0.01 \end{pmatrix} \in \mathbb{R}^{n \times n}.$$

- Remember: A matrix is singular if and only if its determinant is equal to zero.
- $\det(A) = 0.01^n$, and hence close to zero for large $n$
- **BUT: $A$ is well-conditioned!**, $\kappa(A) = 1$ for all $n$

# The Condition Number (cont.)

- If $A$ is symmetric positive definite with eigenvalues $\lambda_1 \geq \cdots \geq \lambda_n > 0$ then

$$\kappa_2(A) = \frac{\lambda_1}{\lambda_n}.$$

- If $A$ is nonsingular with singular values $\sigma_1 \geq \cdots \geq \sigma_n > 0$ then

$$\kappa_2(A) = \frac{\sigma_1}{\sigma_n}.$$

- The exact value of $\kappa(A)$ rarely (if ever) matters in practice: typically, only its order of magnitude is important.