TANA15 Numerical Linear Algebra

Course Contents

- Standard Matrix Decompositions: LU, QR, SVD, FFT, Eigenvalue,...
- Basic Linear Algebra Operations: Projection, Rotation,...
- Computing and using the Standard Decompositions.
- Non-Linear Equations and Least Squares. The Newton and Gauss–Newton methods.
- Applications: Model fitting, Roots of Polynomials, Text models and Search Engines, Image processing,...

Examination

- Written Exam (4 hp)
- Computer Exercises (2 hp)

Lecturer

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Numerical Linear Algebra Objectives

Theory

- Define a **good** set of standard linear algebra operations and matrix decompositions.
- Show how application problems can be solved by using standard operations.
- Investigate stability properties, error estimates, etc.

Software

- Write efficient and reliable subroutines for computing decompositions.
- Modify existing software to take advantage of modern computer hardware.

TANA15/Lecture 1 - Contents

Basic Matrix Operations

- Matrix–Matrix multiplication. Operation counts
- Basic Linear Algebra Subroutines (BLAS,ATLAS)

Linear Spaces and Mappings

- Range and Null spaces. Rank. The Inverse.
- Scalar Products, Vector and Matrix Norms. The Transpose.

Example: Matrix–Matrix multiply

Compute $C = AB$ by

$$c_{ij} = \sum_{k=1}^{n} a_{ik} b_{kj}.$$

In Matlab

```
C=zeros(n,n);
for i=1:n
   for j=1:n
      for k=1:n
          C(i,j)=C(i,j)+A(i,k)*B(k,j);
      end
   end
end
```

Requires n^3 multiply/additions. Is this the best way?

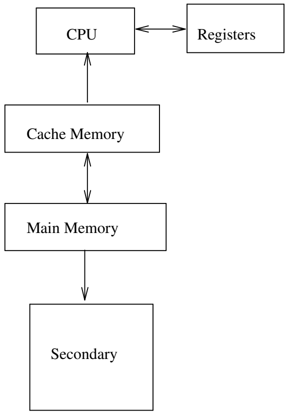
Memory Organization

Data storage and access

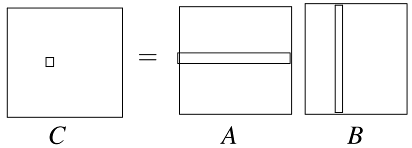
- CPU can **only** access Registers and Cache.
- Data is stored in *blocks*.
- A block can be moved between main and cache memory.

Memory Performance

- CPU and Registers are fast. Low storage capacity.
- Main memory is slow but has high storage capacity.



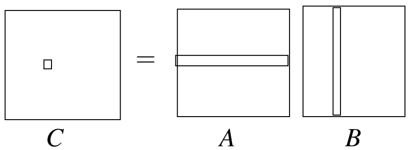
The structure of matrix-matrix multiply



Assumptions Matrices stored by column. One column/memory block. Three columns fit in the Cache memory.

Then the column `B(:,j)` is stored as one memory block and the elements in the row `A(i,:)` are stored in different blocks.

Conclusion Computing `A(i,:)`^{T}`B(:,j)` require one main memory access/multiply!



Alternative Store A by rows. Both `A(i,:)` and `B(:,j)` fit in Cache. Computing `A(i,:)`^{T}`B(:,j)` requires two Main memory access calls!

Conclusion Computing $C = AB$ requires n^3 multiply/additions and $2n^2$ main memory access calls.

Doesn't store A and B the same way!

$$\begin{pmatrix} C_{11} & \dots & C_{1p} \\ \vdots & & \vdots \\ C_{p1} & & C_{pp} \end{pmatrix} = \begin{pmatrix} A_{11} & \dots & A_{1p} \\ \vdots & & \vdots \\ A_{p1} & & A_{pp} \end{pmatrix} \begin{pmatrix} B_{11} & \dots & B_{1p} \\ \vdots & & \vdots \\ B_{p1} & & B_{pp} \end{pmatrix}$$

Alternative Block storage. Blocks are of size $\sqrt{n} \times \sqrt{n}$. Three blocks fit into cache.

Keep C_{ij} in Cache. Updating $C_{ij} = C_{ij} + A_{ik}B_{kj}$ needs two main memory calls and $(\sqrt{n})^3$ multiply/additions.

Conclusion Still need n^3 multiply/additions. But only $2(\sqrt{n})^3 = 2n^{1.5}$ main memory access calls.

Matrix-Matrix multiply

Compute $C = AB$ by

$$c_{ij} = \sum_{k=1}^{n} a_{ik} b_{kj}.$$

Remark This is not a *definition*. It is one possible algorithm for computing the matrix C representing the composite mapping $A \circ B$.

Question The algorithm requires n^3 multiplications and $n^2(n-1)$ additions. Is it possible to do better?

Strassen's Matrix-Matrix multiply

Regular matrix-matrix multiply is

$$\begin{pmatrix} c_{11} & c_{12} \\ c_{21} & c_{22} \end{pmatrix} = \begin{pmatrix} a_{11} & a_{12} \\ a_{21} & a_{22} \end{pmatrix} \begin{pmatrix} b_{11} & b_{12} \\ b_{21} & b_{22} \end{pmatrix} = \begin{pmatrix} a_{11}b_{11}+a_{12}b_{21} & a_{11}b_{12}+a_{12}b_{22} \\ a_{21}b_{11}+a_{22}b_{21} & a_{21}b_{12}+a_{22}b_{22} \end{pmatrix}.$$

This requires 8 multiplications (and 4 additions). An equivalent formula is

$$\begin{pmatrix} c_{11} & c_{12} \\ c_{21} & c_{22} \end{pmatrix} = \begin{pmatrix} p_1+p_4-p_5+p_7 & p_3+p_5 \\ p_2+p_4 & p_1+p_3-p_2+p_6 \end{pmatrix},$$

where

$p_1 = (a_{11}+a_{22})(b_{11}+b_{22})$, $p_2 = (a_{21}+a_{22})b_{11}$, $p_3 = a_{11}(b_{12}-b_{22})$,
$p_4 = a_{22}(b_{21}-b_{11})$, $p_5 = (a_{11}+a_{12})b_{22}$, $p_6 = (a_{21}-a_{11})(b_{11}+b_{12})$,
och $p_7 = (a_{12}-a_{22})(b_{21}+b_{22})$.

Only 7 multiplications (and 18 additions). Volker Strassen, 1969.

Lemma Computing the product $C = AB$ requires *at least* $\mathcal{O}(n^2)$ arithmetic operations. □

This is the only result that exists!

Strassens method requires $\mathcal{O}(n^{2.807})$ operations. The currently best algorithm requires $\mathcal{O}(n^{2.3727})$. By Virginia Vassilevska Williams.

Remark Very large matrices are often *sparse*, i.e. most elements a_{ij} are zero, and other algorithms are much more efficient.

Operation counts

Lemma A matrix-matrix multiply $C = AB$ requires $\mathcal{O}(n^3)$ operations.

Lemma A matrix-vector multiply $y = Ax$ requires $\mathcal{O}(n^2)$ operations.

Example Suppose $A, B \in \mathbb{R}^{n\times n}$. How much computational work is needed to evaluate the product

$$y = ABx.$$

> **Lemma** Computing an *outer product* $A = uv^T$ requires $\mathcal{O}(n^2)$ operations.

Example How should we compute the matrix-vector product

$$y = Ax, \quad \text{where } A = uv^T, \quad u, v \in \mathbb{R}^n,$$

and how many arithmetic operations and memory slots are needed?

Remark Estimating the amount of work is important. The difference between $\mathcal{O}(n^2)$ and $\mathcal{O}(n^4)$ is huge for large n.

Basic Linear Algebra Subroutines (BLAS)

Standard set of basic linear algebra operations

- Level 1: Scalar–Vector.
- Level 2: Matrix–Vector.
- Level 3: Matrix–Matrix.

Software (C/C++, Fortran, Matlab)

- Efficient implementations available for most computers.
- Takes advantage of complex memory systems.
- Reference implementation available on `www.netlib.org`.
- Level 3 operations gains the most from code optimization!

Example A `SAXPY` call computes $z = \alpha x + y$ where α is a scalar and x, y are vectors. The `S` means single precison or 32 bit floating point numbers. A `DGEMM` call computes $C := \alpha AB + \beta C$, in 64 bit arithmetic.

Automatically Tuned Linear Algebra Subroutines (ATLAS)

- Implements most of the routines from BLAS and much more.
- Available from

  `http://math-atlas.sourceforge.net/`

  or package managers in Linux. Try

  ```
  >> yum info atlas
  >> man dgemm
  ```

  in the computer laboratory.
- Download the source and compile. Automatically detects cache size, memory read/write speed, etc, and produce close to the best available code.

Basic concepts

> A matrix $A \in \mathbb{R}^{m\times n}$ represents a *linear mapping* from $\mathbb{R}^n$ to $\mathbb{R}^m$.

> The *range* of the matrix A is the linear subspace
>
> $\text{Range}(A) = \{y \in \mathbb{R}^m \text{ such that } y = Ax \text{ for some } x \in \mathbb{R}^n\}.$

Remark Similarly the *domain* is the set $x \in \mathbb{R}^n$ such that $y = Ax$ is defined. This is not as often used since typically $\text{Domain}(A) = \mathbb{R}^n$.

Definition The *rank* of a matrix is

$$\mathrm{Rank}(A) = \dim(\mathrm{Range}(A))$$

Remark If $A \in \mathbb{R}^{n\times m}$ then $\mathrm{Rank}(A) \le \min(n,m)$.

Lemma Let $A \in \mathbb{R}^{n\times n}$. If $\mathrm{Rank}(A) = n$ then there exists an *inverse* A^{-1} such that $x = A^{-1}y$ for every x, y such that $y = Ax$.

Example Prove that $(AB)^{-1} = B^{-1}A^{-1}$.

Example Consider a linear system $Ax = b$. Existence of a solution?

Definition Let $A \in \mathbb{R}^{n\times m}$. The *null space* is

$$\mathrm{Null}(A) = \{x \in \mathbb{R}^n \text{ such that } Ax = 0\}.$$

Definition The identity mapping I is defined by $Ix = x$ for every $x \in \mathbb{R}^n$.

Remark If the inverse of A exists then $A^{-1}A = I$.

Norms and Scalar products

Definition Let $x \in \mathbb{R}^n$. The *norm* $\|x\|$ is a measure of the *size* of x.

Example The most commonly used norms are

$$\|x\|_2 = (\sum_{i=1}^{n} x_i^2)^{\frac{1}{2}} \quad \text{and} \quad \|x\|_\infty = \max_{1\le i\le n} |x_i|.$$

They satisfy the relation

$$\|x\|_\infty \le \|x\|_2 \le \sqrt{n}\|x\|_\infty.$$

Remark There are many different norms that are used.

Definition The *Scalar product* (x,y) measures the angle between x and y. If $(x,y) = 0$ then x and y are *orthogonal*.

Example The space $\mathbb{R}^n$ is a Hilbert space with the scalar product $(x,y) = x^T y$. We have $\|x\|_2^2 = (x,x)$.

Lemma The *Cauchy-Schwarz* inequality $(x,y) \le \|x\|\|y\|$ holds.

Definition Let $||\cdot||$ be a vector norm. A matrix norm is

$$||A|| = \max_{x\neq 0} \frac{||Ax||}{||x||}.$$

Remark The matrix norm is *induced* from a vector norm.

Lemma Suppose A is a matrix. Then

$$||A||_\infty = \max_{1\leq i\leq n} \sum_{j=1}^{n} |A_{ij}|.$$

Lemma Suppose A and B are matrices and $||\cdot||$ is a matrix norm *induced* from a vector norm. Then the *submultiplicative property* $||AB|| \leq ||A||||B||$ holds.

Example Prove that $||A||||A^{-1}|| \geq 1$ for *any* matrix norm induced by a vector norm.

Definition The *Frobenius* norm of a matrix A is

$$||A||_F = \left(\sum_{i=1}^{n}\sum_{j=1}^{m} |a_{ij}|^2\right)^{1/2}.$$

Remark The norm $||\cdot||_F$ is *not* induced by a vector norm.

Matlab

In order to compute the *rank* or the *nullspace* of a matrix we use

```
>> k = rank( A );
>> V = null( A );
```

The columns of V are an orthogonal basis for Null(A).

In order to compute norms there is a function

```
>> norm( x , 2 )
>> norm( A , 'fro' )
```

that computes most different norms. The inverse is computed using

```
>> inv(A)
```

The Transpose

Definition The *transpose* of a matrix $A \in \mathbb{R}^{n\times m}$ is a matrix $A^T \in \mathbb{R}^{m\times n}$ defined by $(A^T)_{ij} = (A)_{ji}$.

Lemma $(AB)^T = B^T A^T$

Proof Look at a component of the matrix $(AB)^T$

$$((AB)^T)_{ij} = (AB)_{ji} = \sum_{k=1}^{p} a_{jk} b_{ki} = \sum_{k=1}^{p} (A^T)_{kj} (B^T)_{ik} =$$

$$\sum_{k=1}^{p} (B^T)_{ik} (A^T)_{kj} = (B^T A^T)_{ij}.$$

Definition The *transpose* of A is the matrix A^T that satisfies $(Ax, y) = (x, A^T y)$ for every pair of vectors x, y.

Lemma If A maps $\mathbb{R}^n$ into $\mathbb{R}^m$ then $(A)_{ij} = (A^T)_{ji}$.

Proof Use the standard basis $\{e_i\}$ and the scalar product $(x, y) = x^T y$.

Corollary $(AB)^T = B^T A^T$.

Remark Compare with the *adjoint* from functional analysis. The proof gives more insight!