AMS526: Numerical Analysis I (Numerical Linear Algebra for Computational and Data Sciences)

Lecture 2: Algorithmic Consideration; Orthogonality; Vector Norms

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Outline

Algorithms for Matrix-Vector Multiplication

- Suppose $A \in \mathbb{R}^{m \times n}$ and $x \in \mathbb{R}^n$
- MATLAB-style code for $b = Ax$:

Row oriented

```
for i = 1 : m
    b(i) = 0
    for j = 1 : n
        b(i) = b(i) + A(i, j) * x(j)
    end
end
```

Column oriented

```
b(:) = 0
for j = 1 : n
    for i = 1 : m
        b(i) = b(i) + A(i, j) * x(j)
    end
end
```

- Number of operations is $O(mn)$, but big-Oh notation is insufficient
- Number of operations is $2mn$: coefficient of leading-order term is important for comparison

Flop Count

- It is important to assess *efficiency* of algorithms. But how?
  - We could implement different algorithms and do direct comparison, but implementation details can affect true performance
  - We could estimate cost of all operations, but it is very tedious
  - Relatively simple and effective approach is to estimate amount of floating-point operations, or "flops", and focus on asymptotic analysis as sizes of matrices approach infinity
- Idealization
  - Count each operation $+$, $-$, $*$, $/$, and $\sqrt{\ }$ as one flop
  - This estimation is crude, as it omits data movement in memory, which is non-negligible on modern computer architectures (e.g., different loop orders can affect cache performance)
- Matrix-vector product requires about $2mn$ flops
- Suppose $m = n$, it takes quadratic time in n, or $O(n^2)$

Algorithms for Saxpy: Scalar a x plus y

- Saxpy computes $ax + y$ and updates y

$$y = ax + y \Rightarrow y_i = ax_i + y_i$$

- Suppose $x, y \in \mathbb{R}^n$ and $a \in \mathbb{R}$

MATLAB-style code

for $i = 1 : n$
  $y(i) = y(i) + a * x(i)$
end

Pseudo-code

for $i = 1 : n$
  $y_i \leftarrow y_i + a\, x_i$

- Number of flops is $2n$
- Pseudo-code cannot run on any computer, but are human readable and straightforward to convert into real codes in any programming language (e.g., C, FORTRAN, MATLAB, etc.)
- We use pseudo-code on slides for conciseness

Gaxpy: Generalized saxpy

- Computes $y = y + Ax$, where $A \in \mathbb{R}^{m \times n}$ and $x \in \mathbb{R}^n$

Row oriented	Column oriented

for $i = 1 : m$
    for $j = 1 : n$
        $y_i = y_i + a_{ij} x_j$
	for $j = 1 : n$
	    for $i = 1 : m$
	        $y_i = y_i + a_{ij} x_j$

- Inner loop of column-oriented algorithm can be converted to $y = y + x_j a_{:,j}$
- Number of flops is $2mn$

Matrix Multiplication Update

- Computes $C = C + AB$, where $A \in \mathbb{R}^{m\times r}$, $B \in \mathbb{R}^{r\times n}$, and $C \in \mathbb{R}^{m\times n}$

$$c_{ij} = c_{ij} + \sum_{k=1}^{r} a_{ik} b_{kj}$$

$$\boxed{\begin{array}{l} \textbf{for } i = 1 : m \\ \quad \textbf{for } j = 1 : n \\ \quad\quad \textbf{for } k = 1 : r \\ \quad\quad\quad c_{ij} = c_{ij} + a_{ik} b_{kj} \end{array}}$$

- Number of flops is $2mnr$
- In BLAS (Basic Linear Algebra Subroutines), functions are grouped into level-1, 2, and 3, depending on whether complexity is linear, quadratic, or cubic

Six Variants of Algorithms

- There are six variants depending on permutation of i, j, and k:

$$ijk, \quad jik, \quad ikj, \quad jki, \quad kij, \quad kji$$

- Inner product: $c_{ij} = c_{ij} + a_{i,:} b_j$

$$\boxed{\begin{array}{l} \textbf{for } i = 1 : m \\ \quad \textbf{for } j = 1 : n \\ \quad\quad c_{ij} = c_{ij} + a_{i,:} b_j \end{array}}$$

- Saxpy: computes as $c_j = c_j + Ab_j$

$$\boxed{\begin{array}{l} \textbf{for } j = 1 : n \\ \quad c_j = c_j + Ab_j \end{array}}$$

- Outer product: computes as $C = C + \sum_{k=1}^{r} a_k b_{:,k}$

$$\boxed{\begin{array}{l} \textbf{for } k = 1 : r \\ \quad C = C + a_k b_{:,k} \end{array}}$$

Outline

Inner Product

- *Euclidean length* of u is square root of inner product of u with itself, i.e., $\sqrt{u^T u}$
- Inner product of two **unit** vectors u and v is cosine of angle α between u and v, i.e., $\cos\alpha = u^T v$
- Inner product is *bilinear*, in the sense that it is linear in each vertex separately:

$$\begin{aligned}(u_1 + u_2)^T v &= u_1^T v + u_2^T v\\ u^T(v_1 + v_2) &= u^T v_1 + u^T v_2\\ (\alpha u)^T(\beta v) &= \alpha\beta u^T v\end{aligned}$$

Orthogonal Vectors

Definition

A pair of vectors are *orthogonal* if $x^T y = 0$.

In other words, angle between them is 90 degrees

Definition

Two sets of vectors X and Y are orthogonal if every $x \in X$ is orthogonal to every $y \in Y$.

- Subspaces $S^\perp$ is *orthogonal complement* of S if they are orthogonal and complementary subspaces
- For $A \in \mathbb{R}^{m\times n}$, null($A$) is *orthogonal complement* of range(A^T)

Definition

A set of nonzero vectors S is *orthogonal* if they are pairwise orthogonal. They are *orthonormal* if it is orthogonal and in addition each vector has unit Euclidean length.

Orthogonal Vectors

Theorem

The vectors in an orthogonal set S are linearly independent.

Proof.

Prove by contradiction. If a vector can be expressed as linear combination of the other vectors in the set, then it is orthogonal to itself. $\square$

Question: If the column vectors of an $m \times n$ matrix A are orthogonal, what is the rank of A?

Orthogonal Vectors

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Question: If the column vectors of an $m \times n$ matrix A are orthogonal, what is the rank of A?

Answer: $n = \min\{m, n\}$. In other words, A has full rank.

Components of Vector

- Given an orthonormal set $\{q_1, q_2, \ldots, q_m\}$ forming a basis of $\mathbb{R}^m$, vector v can be decomposed into orthogonal components as $v = \sum_{i=1}^{m} (q_i^T v) q_i$
- Another way to express the decomposition is $v = \sum_{i=1}^{m} (q_i q_i^T) v$
- $q_i q_i^T$ is an *orthogonal projection matrix*
- More generally, given an orthonormal set $\{q_1, q_2, \ldots, q_n\}$ with $n \leq m$, we have

$$v = r + \sum_{i=1}^{n} (q_i^T v) q_i = r + \sum_{i=1}^{n} (q_i q_i^T) v \text{ and } r^T q_i = 0, 1 \leq i \leq n$$

- Let Q be composed of column vectors $\{q_1, q_2, \ldots, q_n\}$. $QQ^T = \sum_{i=1}^{n} (q_i q_i^T)$ is an orthogonal projection matrix (more in Lecture 4)

Orthogonal Matrices

Definition

A matrix is *orthogonal* if $Q^T = Q^{-1}$, i.e., if $Q^T Q = QQ^T = I$.

- Its column vectors are *orthonormal*. In other words, $q_i^T q_j = \delta_{ij}$, the *Kronecker delta*.
- For complex matrices, we say the matrix is *unitary* if $Q^H = Q^{-1}$.

Question: What is the geometric meaning of multiplication by an orthogonal matrix?

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Question: What is the geometric meaning of multiplication by an orthogonal matrix?

Answer: It preserves angles and Euclidean length. In the real case, multiplication by an orthogonal matrix Q is a rotation (if $\det(Q) = 1$) or reflection (if $\det(Q) = -1$).

Outline

Definition of Norms

- Norm captures "size" of vector or "distance" between vectors
- There are many different measures for "sizes" but a norm must satisfy some requirements:

Definition

A *norm* is a function $\|\cdot\| : \mathbb{R}^n \to \mathbb{R}$ that assigns a real-valued length to each vector. It must satisfy the following conditions:

$$\begin{aligned}
&(1)\|x\| \geq 0, \text{ and } \|x\| = 0 \text{ only if } x = 0,\\
&(2)\|x+y\| \leq \|x\| + \|y\|,\\
&(3)\|\alpha x\| = |\alpha|\|x\|.
\end{aligned}$$

- An example is Euclidean length (i.e, $\|x\| = \sqrt{\sum_{i=1}^n |x_i|^2}$)

p-norms

- Euclidean length is a special case of p-norms, defined as

$$\|x\|_p = \left(\sum_{i=1}^{n} |x_i|^p \right)^{1/p}$$

  for $1 \le p \le \infty$
- Euclidean norm is 2-norm $\|x\|_2$ (i.e., $p = 2$)
- 1-norm: $\|x\|_1 = \sum_{i=1}^{n} |x_i|$
- ∞-norm: $\|x\|_\infty$. What is its value?

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- 1-norm: $\|x\|_1 = \sum_{i=1}^{n} |x_i|$
- ∞-norm: $\|x\|_\infty$. What is its value?
  - Answer: $\|x\|_\infty = \max_{1\leq i\leq n} |x_i|$
- Why we require $p \geq 1$? What happens if $0 \leq p < 1$?

Some Properties of Vector Norms

- Hölder inequality: $|x^T y| \leq \|x\|_p \|y\|_q, \quad \frac{1}{p} + \frac{1}{q} = 1$
- In particular when $p = q = 2$: $|x^T y| \leq \|x\|_2 \|y\|_2$ (Cauchy-Schwarz inequality)
- All norms are *equivalent*, in that there exists c_1 and c_2 s.t.

$$c_1 \|x\|_\alpha \leq \|x\|_\beta \leq c_2 \|x\|_\alpha$$

  where c_1 and c_2 are constants and may depend on n. e.g.,

$$\|x\|_2 \leq \|x\|_1 \leq \sqrt{n} \|x\|_2$$

- 2-norm is preserved under orthogonal transformation Qx

$$\|Qx\|_2 = \|x\|_2$$

Weighted p-norms

- A generalization of p-norm is *weighted p-norm*, which assigns different weights (priorities) to different components.
  - It is anisotropic instead of isotropic
- Algebraically, $\|x\|_W = \|Wx\|$, where W is diagonal matrix with ith diagonal entry $w_i \neq 0$ being weight for ith component
- In other words,

$$\|x\|_W = \left(\sum_{i=1}^{n} |w_i x_i|^p \right)^{1/p}$$

- What happens if we allow $w_i = 0$?

Weighted p-norms

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- What happens if we allow $w_i = 0$?
- Can we further generalize it to allow W being arbitrary matrix?
  - No. But we can allow W to be arbitrary nonsingular matrix.

A-norm of Vectors

- Given a positive definite matrix $A \in \mathbb{R}^{n \times n}$, the A-norm on $\mathbb{R}^n$ is

$$\|x\|_A = \sqrt{x^T A x}$$

- Note: Weighted p-norm with W is A-norm with $A = W^2$.
- These conventions are somewhat inconsistent, but they are both commonly used in the literature