VectorsMatrices

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0.1 STAT 207: Vectors and matrices

Zhe Fei (zhe.fei@ucr.edu) Many scientific computational problems involve vectors and matrices.

The distinction between the set of real numbers, \mathbb{R} , and the set of floating-point numbers, \mathbb{F} , that we use in the computer has important implications for numerical computations.

We will consider the floating-point representation of elements of vectors and matrices and the computations in \mathbb{F} .

- In multidimensional calculus, vector and matrix norms quantify notions of topology and convergence.
- Norms are also devices for deriving explicit bounds, theoretical developments in numerical analysis rely heavily on norms.
- They are particularly useful in establishing convergence and in estimating rates of convergence of iterative methods for solving linear and nonlinear equations.
- Norms also arise in almost every other branch of theoretical numerical analysis. Functional analysis, which deals with infinite-dimensional vector spaces, uses norms on functions.

0.1.1 Elementary Properties of Vector Norms

Euclidean vector norm:

$$||x||_2 = \sqrt{\sum_{i=1}^m x_i^2}$$

A norm on \mathbb{R}^m is formally defined by four properties:

- (a) $||x|| \ge 0$,
- (b) ||x|| = 0 if and only if x = 0,
- (c) $||cx|| = |c| \cdot ||x||$ for all real number c,
- (d) $||x + y|| \le ||x|| + ||y||$.

 ℓ -1 norm:

$$||x||_1 = \sum_{i=1}^m |x_i|,$$

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 ℓ - ∞ norm:

$$||x||_{\infty} = \max_{i} |x_i|.$$

For each of the norms $||x||_p$, p=1,2, and ∞ , a sequence of vectors x_n converges to a vector y if and only if each component sequence x_{ni} converges to y_i . Thus, all three norms give the same topology on \mathbb{R}^m .

NAS Proposition 6.2.1 Let ||x|| be any norm on R^m . Then there exist positive constants k_l and k_u such that $k_l||x||_1 \le ||x|| \le k_u||x||_1$ holds for all $x \in R^m$.

- $\sup_{x\neq 0}\|x\|/\|x\|^*$ is finite for any pair of norms $\|x\|$ and $\|x\|^*.$
- For p < q from $\{1, 2, \infty\}$,

$$||x||_q \le ||x||_p$$

$$||x||_p \le m^{1/p-1/q} ||x||_q$$

0.1.2 Elementary Properties of Matrix Norms

An $m \times m$ matrix $A = (a_{ij})$ is simply a vector in \mathbb{R}^{m^2} .

It is preferred that a matrix norm is compatible with matrix multiplication.

In addition to (a) - (d), we require

(e)
$$||AB|| \le ||A|| \cdot ||B||$$

for any product of $m \times m$ matrices A and B.

- Frobenius norm: $\|A\|_F = \sqrt{\sum_{i=1}^m \sum_{j=1}^m a_{ij}^2} = \sqrt{tr(AA^T)} = \sqrt{tr(A^TA)}$
- Matrix norm induced from any vector norm ||x|| on R^m :

$$||A|| = \sup_{x \neq 0} \frac{||Ax||}{||x||} = \sup_{||x|| = 1} ||Ax||.$$

• What is ||I|| and $||I||_F$?

In infinite-dimensional settings, induced matrix norms are called operator norms.

NAS Proposition 6.2.1 If $A = (a_{ij})$ is an $m \times m$ matrix, then

- (a) $||A||_1 = \max_j \sum_i |a_{ij}|$,
- (b) $||A||_2 = \sqrt{\rho(A^T A)}$, which reduces to $\rho(A)$ if A is symmetric,
- (c) $||A||_2 = \max_{||u||_2=1, ||v||_2=1} u^T A v$,
- (d) $||A||_{\infty} = \max_i \sum_j |a_{ij}|$.

0.1.3 Norm Preserving Linear Transformations

- Orthogonal matrix: $OO^T = I$;
- Orthonormal set of vectors S: every vector in S has magnitude 1 and the set of vectors are mutually orthogonal.

Following $(\det O)^2 = 1$, we can divide the orthogonal matrices into *rotations* with $\det O = 1$ and reflections with $\det O = -1$. Take 2×2 matrices for example,

• Rotation of angle θ can be presented as:

$$O = \begin{pmatrix} \cos \theta & -\sin \theta \\ \sin \theta & \cos \theta \end{pmatrix}$$

• Reflection of a point across the line at angle $\theta/2$ with the x axis:

$$O = \begin{pmatrix} \cos \theta & \sin \theta \\ \sin \theta & -\cos \theta \end{pmatrix}$$

Remarks

- The set of orthogonal matrices forms a group under matrix multiplication.
- The identity matrix is the unit of the group.
- The rotations constitute a subgroup of the orthogonal group, but the reflections do not since the product of two reflections is a rotation.

Orthogonal transformations preserve inner products and Euclidean norms: $(Ou)^T Ov = u^T O^T Ov = u^T v$.

As a result, all eigenvalues of O lie on the boundary of the unit circle.

Norm invariance for vectors also leads to norm invariance for matrices.

- $||OA||_2^2 = ||A||_2^2$
- $||AO||_2^2 = ||A||_2^2$
- $||OA||_F^2 = ||A||_F^2$
- $||AO||_F^2 = ||A||_F^2$

Householder matrices Given a unit vector u, the Householder matrix $H = I - 2uu^T$ represents a reflection across the plane perpendicular to u.

H is orthogonal and symmetric,

$$HH^T = I - 4uu^T + 4u\|u\|_2^2 u^T = I.$$

- Hv = v whenever v lies in the plane perpendicular to u.
- Hu = -u.
- H has one eigenvalue equal to -1 and all others equal to 1.

0.1.4 Iterative Solution of Linear Equations

Many numerical problems involve iterative schemes of the form

$$x_n = Bx_{n-1} + w \tag{1}$$

for solving the vector-matrix equation (I - B)x = w. The map f(x) = Bx + w satisfies

$$\|f(y) - f(x)\| = \|B(y - x)\| \le \|B\| \cdot \|y - x\|$$

and is contractive for a vector norm ||x|| if ||B|| < 1.

NAS Proposition 6.5.1 Let B be an arbitrary matrix with spectral radius $\rho(B)$. Then $\rho(B) < 1$ if and only if ||B|| < 1 for some induced matrix norm. The inequality ||B|| < 1 implies:

- (a) $\lim_{n\to\infty} |B^n| = 0$,
- (b) $(I B)^{-1} = \sum_{n=0}^{\infty} B^n$,
- (c) $\frac{1}{1+\|B\|} \le \|(I-B)^{-1}\| \le \frac{1}{1-\|B\|}$.

Linear iteration is especially useful in solving the equation Ax = b for x when an approximation C to A^{-1} is known, let B = I - CA and w = Cb and iterate equation (1).

Jacobi's Method Suppose $A=(a_{ij})$ is strictly diagonally dominant, let $D=\mathrm{diag}(a_{ii})$ be the diagonal matrix. Then $C=D^{-1}$ is an approximate inverse of A, and B=I-CA satisfies $\|B\|_{\infty}<1$.

```
[1]: import numpy as np
     def jacobi(A, b, x0, tol=1e-6, max_iter=1000):
         Solves the system of linear equations Ax = b using Jacobi's method.
         n = len(A)
         C = np.diag(1/np.diag(A))
         B = np.identity(n) - COA
         w = C@b
         x = B@x0 + w
         k = 1
         while max(abs(x-x0)) > tol:
             x = 0x
             x = B@x0 + w
             k += 1
         if k<max iter:
             print(f'Converged in {k} iterations.')
             return x
         else:
             print(f'Maximum iterations reached.')
             return x
```

```
[2]: # Example usage
A = np.array([[4, 1, 1], [2, 5, 1], [1, 2, 4]])
b = np.array([4, 1, 2])
x0 = np.array([0, 0, 0])

x = jacobi(A, b, x0)
print(f'Solution: {x}')

print(A@x)
```

Converged in 28 iterations.

Solution: [0.96874976 -0.26562527 0.39062468] [3.99999845 0.99999787 1.99999795]

Landweber's Iteration Scheme In practice, the approximate inverse C can be rather crude. $C = \epsilon A^T$ for ϵ small.

- A^TA is positive definite with eigenvalues $0 < \lambda_1 \le ... \le \lambda_m$.
- $I \epsilon A^T A$ has eigenvalues $1 \epsilon \lambda_1, ... 1 \epsilon \lambda_m$.
- Need $1 \epsilon \lambda_m > -1$, so that $||I \epsilon A^T A||_2 < 1$.

Equilibrium Distribution of a Markov Chain Movement among the m states of a Markov chain is governed by its $m \times m$ transition matrix $P = (p_{ij})$, whose entries are nonnegative and satisfy $\sum_i p_{ij} = 1$ for all i.

A column vector x with nonnegative entries and norm $||x||_1 = \sum_i x_i = 1$ is said to be an equilibrium (stationary) distribution for P provided $x^T P = x^T$, or equivalently Qx = x for $Q = P^T$.

Let $S = \{x : x_i \ge 0, i = 1, 2, ..m, \sum_i x_i = 1\}$. Assume for some power k, Q^k has all positive entries, then consider the matrix $R = Q^k - c\mathbf{1}\mathbf{1}^T$.

- We have the map $x \to Q^k x$ is contractive on S with unique fixed point x_{∞} .
- $Qx_{\infty} = x_{\infty}$.
- $\bullet \ \lim\nolimits_{n\to\infty}Q^nx=x_{\infty} \text{ for all } x\in S.$

This power method is also used in PageRank:

- Eldén L (2007) Matrix Methods in Data Mining and Pattern Recognition. SIAM, Philadelphia
- Langville AN, Meyer CD (2006) Google's PageRank and Beyond: The Science of Search Engine Rankings. Princeton University Press, Princeton NJ

0.1.5 Condition Number of a Matrix

Consider the matrix

$$A = \begin{pmatrix} 10 & 7 & 8 & 7 \\ 7 & 5 & 6 & 5 \\ 8 & 6 & 10 & 9 \\ 7 & 5 & 9 & 10 \end{pmatrix}$$

that is symmetric and positive definite, and Ax = b.

- for $b = (32, 23, 33, 31)^T$, we find $x = (1, 1, 1, 1)^T$,
- for $b + \Delta b = (32.1, 22.9, 33.1, 30.9)^T$, the solution is violently perturbed $x + \Delta x = (9.2, -12.6, 4.5, -1.1)^T$,
- for $b = (4, 3, 3, 1)^T$, $x = (1, -1, 1, -1)^T$,
- if we perturb A to A+0.01I, the solution is $x+\Delta x=(.59,-.32,.82,-.89)^T$.

How to explain these patterns? Define the condition number

$$cond(A) = ||A|| \cdot ||A^{-1}||$$

of matrix A relative to the given norm. We can have

 $\frac{\|\Delta x\|}{\|x\|} \le \operatorname{cond}(A) \frac{\|\Delta b\|}{\|b\|},$

if Ax = b and $A(x + \Delta x) = b + \Delta b$.

 $\frac{\|\Delta x\|}{\|x + \Delta x\|} \le \operatorname{cond}(A) \frac{\|\Delta A\|}{\|A\|},$

if Ax = b and $(A + \Delta A)(x + \Delta x) = b$.

The condition number $\operatorname{cond}_2(A)$ relative to the matrix norm $\|A\|_2$ is the ratio of the largest and smallest eigenvalues of A, which are $\lambda_1=0.01015, \lambda_4=30.2887$. Therefore, $\operatorname{cond}_2(A)=2984$.

[]: