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Rank

Definition: The *rank*, r , of an $m \times n$ matrix A is the number of independent columns (or rows).

A has *full rank* if $r = \min\{m, n\}$.

Rank can be determined by Gaussian Elimination:

$$A = \begin{pmatrix} 1 & 2 \\ 2 & 4 \end{pmatrix} \mapsto \begin{pmatrix} 1 & 2 \\ 0 & 0 \end{pmatrix}$$

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But, *Rank is numerically unstable*.

$$B = \begin{pmatrix} 1 & 2 \\ 2 & 4.000001 \end{pmatrix}$$

B has rank 2. A random matrix has full rank.

Partial Differential Equations

Heat Equation:

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How is this related to RANK?

Products of Vectors

Dot Product: $\mathbf{u} \cdot \mathbf{v} = u_1 v_1 + u_2 v_2 + \dots + u_n v_n$ ($= |\mathbf{u}| |\mathbf{v}| \cos \theta$).

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The *Outer Product* is defined to be:

$$\mathbf{u} \otimes \mathbf{v} = \mathbf{u} \mathbf{v}^T = \begin{pmatrix} u_1 \\ u_2 \\ \vdots \\ u_n \end{pmatrix} \begin{pmatrix} v_1 & v_2 & \cdots & v_n \end{pmatrix}$$

Outer products are rank 1 matrices

Example:

$$\mathbf{uv}^T = \begin{pmatrix} 1 \\ 2 \\ 3 \end{pmatrix} (4 \ 5 \ 6) = \begin{pmatrix} 4 & 5 & 6 \\ 8 & 10 & 12 \\ 12 & 15 & 18 \end{pmatrix}$$

Each column is a multiple of \mathbf{u} and each row a multiple of \mathbf{v} .

\mathbf{uv}^T has rank 1.

Theorem: A matrix A has rank 1 iff $A = \mathbf{uv}^T$ for some \mathbf{u} , \mathbf{v} .

This representation is not unique since $\mathbf{uv}^T = (c\mathbf{u})(\frac{1}{c}\mathbf{v}^T)$.

$A = a\mathbf{uv}^T$ with $\|\mathbf{u}\| = \|\mathbf{v}\| = 1$ is unique, where $a = \|A\|_2$.

Heat Equation is Separable

Temperature $u(t, x)$ satisfies $\frac{\partial}{\partial t} u = c \frac{\partial^2}{\partial x^2} u$.

Assume an ansatz: $u(t, x) = T(t)X(x)$ - "separable".

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$$T' = CT \implies T(t) = T(0)e^{Ct}$$

$$X'' = CX \implies X(x) = A \sin(\sqrt{C}x) + B \cos(\sqrt{C}x)$$

$$u(t, x) = e^{Ct} \left(A \sin(\sqrt{C}x) + B \cos(\sqrt{C}x) \right)$$

$u = T(t)X(x)$ is an “outer product”.

Discretization of $u(t, x)$

In applications, solutions of differential equations are often approximated numerically rather than solved symbolically.

Numerical solutions are discrete. $t \mapsto \{t_j\}$, $x \mapsto \{x_i\}$.

$$u(t_j, x_i) \approx U_{ij}.$$

Think of (U_{ij}) as a matrix U . If u is separable,

$$u(t, x) = T(t)X(x) \implies U = (T(t_j))(X(x_i))^T = \overline{T} \overline{X}^T.$$

$\{u(t, x) \text{ is separable}\}$ corresponds to $\{U \text{ is an outer product}\}$.

Complexity and Storage

Suppose m grid points in x direction & n grid points in t direction.

U is a $m \times n$ matrix $\implies mn$ entries.

If U is an outer product of \bar{T} and \bar{X} , then you only really need to store $m + n$ numbers, i.e. the entires of \bar{T} and \bar{X}

Example: $m = 100$ and $n = 100$,

$mn = 10,000$ but $m + n = 200$.

The Singular Value Decomposition

SVD theorem: Given any $m \times n$ matrix A ,

$$A = \sum_{i=1}^r \sigma_i \mathbf{u}_i \mathbf{v}_i^T = U \Sigma V^T$$

- $\{\mathbf{u}_i\}$, $\{\mathbf{v}_i\}$ are orthonormal sets of vectors,
- $\{\sigma_i\}$ are positive real numbers called *singular values*,
- $r \leq \min(m, n)$ is the rank of A .

May order: $\sigma_1 \geq \sigma_2 \geq \dots \geq \sigma_r > 0$.

The SVD Approximation Theorem

Principle: The larger singular values are more important.

For $k < r$ let

$$A_k \equiv \sum_{i=1}^k \sigma_i \mathbf{u}_i \mathbf{v}_i^T = \sigma_1 \mathbf{u}_1 \mathbf{v}_1^T + \sigma_2 \mathbf{u}_2 \mathbf{v}_2^T + \dots + \sigma_k \mathbf{u}_k \mathbf{v}_k^T$$

Theorem (Eckart-Young-Mirsky): A_k is the best rank- k approximation of A with respect to either the Frobenius norm or the 2-norm. Further,

$$\|A - A_k\|_2 = \sigma_{k+1}, \quad \|A - A_k\|_F = \sigma_{k+1} + \sigma_{k+2} + \dots + \sigma_r.$$

$$\|A - A_k\|_2 \equiv \max_{|\mathbf{x}|=1} |\mathbf{A}\mathbf{x}|, \quad \|A - A_k\|_F \equiv \sqrt{\sum_{i,j=1,1}^{m,n} a_{ij}^2}$$

Application to Image Compression

An image is recorded in an array of RGB values from 0 to 255.

Example: 500 by 500 pixel image is $500 \times 500 \times 3 = 750,000$.

Suppose R is the 500×500 matrix of red values and let

$R = \sum_{i=1}^r \sigma_i \mathbf{u}_i \mathbf{v}_i^T = U \Sigma V^T$ be the SVD of R .

Let $R_k = \sum_{i=1}^k \sigma_i \mathbf{u}_i \mathbf{v}_i^T$ the best rank- k approximation of R .

Storing R_k requires $k(m + n + 1)$ numbers. If $k < n/2$ then this is fewer numbers to store.

In the above example, with $k = 100$, then $3k(2n + 1) = 300,300$.

- Maybe R_k is good enough?

Back to Partial Differential Equations

$u(t, x) = T(t)X(x)$ being separable depended on the linearity of the PDE.

What if:

$$\frac{\partial}{\partial t} u = c \frac{\partial^2}{\partial x^2} u + g(u)$$

where $g(u)$ is a small nonlinearity.

Maybe $u(t, x) \approx T_1(t)X_1(x) + T_2(t)X_2(x)$?

Or at worst:

$$u(t, x) \approx T_1(t)X_1(x) + T_2(t)X_2(x) + \dots + T_k(t)X_k(x),$$

where k is small. Then storing an approximation U_{ij} would require $k(m + n + 1)$ numbers rather than mn .

Working efficiently with low rank representations is a subject of current research by Mohlenkamp and Young.

The Curse of dimensionality

Example: Electrons in an atom

Hydrogen - 1 electron \times 3 dim = 3 variables, linear equation - separable.

Helium - 2 electrons \times 3 dim = 6 variables, nonlinear - not separable.

Carbon - 6 electrons \times 3 dim = 18 variables, nonlinear - not separable.

Suppose we wish to represent the carbon “wave function.”

With 100 grid points in each variable then

$$100^{18} = 10^{24} \text{ Terabytes} \implies \mathbf{Intractable.}$$

With a rank 100 approximation instead:

$$100(18 \times 100) = 180,000 \text{ Numbers} \implies \text{No Problem.}$$

Conclusions

Thank you for your attention!

Study more Linear Algebra!