Lecture slides for

Introduction to Applied Linear Algebra: Vectors, Matrices, and Least Squares

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10. Matrix multiplication

Outline

Matrix multiplication

Composition of linear functions

Matrix powers

QR factorization

Householder transformations

Matrix multiplication

- can multiply $m \times p$ matrix A and $p \times n$ matrix B to get $C = AB$:

$$C_{ij} = \sum_{k=1}^{p} A_{ik}B_{kj} = A_{i1}B_{1j} + \cdots + A_{ip}B_{pj}$$

  for $i = 1, \ldots, m$, $j = 1, \ldots, n$

- to get C_{ij}: move along ith row of A, jth column of B
- example:

$$\begin{bmatrix} -1.5 & 3 & 2 \\ 1 & -1 & 0 \end{bmatrix} \begin{bmatrix} -1 & -1 \\ 0 & -2 \\ 1 & 0 \end{bmatrix} = \begin{bmatrix} 3.5 & -4.5 \\ -1 & 1 \end{bmatrix}$$

Special cases of matrix multiplication

- scalar-vector product (with scalar on right!) $x\alpha$
- inner product $a^T b$
- matrix-vector multiplication Ax
- *outer product* of m-vector a and n-vector b

$$ab^T = \begin{bmatrix} a_1b_1 & a_1b_2 & \cdots & a_1b_n \\ a_2b_1 & a_2b_2 & \cdots & a_2b_n \\ \vdots & \vdots & & \vdots \\ a_mb_1 & a_mb_2 & \cdots & a_mb_n \end{bmatrix}$$

Properties

- $(AB)C = A(BC)$, so both can be written ABC
- $A(B + C) = AB + AC$
- $(AB)^T = B^T A^T$
- $AI = A$ and $IA = A$
- $AB = BA$ *does not hold in general*

Block matrices

block matrices can be multiplied using the same formula, *e.g.*,

$$\begin{bmatrix} A & B \\ C & D \end{bmatrix} \begin{bmatrix} E & F \\ G & H \end{bmatrix} = \begin{bmatrix} AE+BG & AF+BH \\ CE+DG & CF+DH \end{bmatrix}$$

(provided the products all make sense)

Column interpretation

- denote columns of B by b_i:
$$B = \begin{bmatrix} b_1 & b_2 & \cdots & b_n \end{bmatrix}$$
- then we have
$$\begin{aligned} AB &= A \begin{bmatrix} b_1 & b_2 & \cdots & b_n \end{bmatrix} \\ &= \begin{bmatrix} Ab_1 & Ab_2 & \cdots & Ab_n \end{bmatrix} \end{aligned}$$
- so AB is 'batch' multiply of A times columns of B

Multiple sets of linear equations

- given k systems of linear equations, with same $m \times n$ coefficient matrix

$$Ax_i = b_i, \quad i = 1, \ldots, k$$

- write in compact matrix form as $AX = B$
- $X = [x_1 \ \cdots \ x_k]$, $B = [b_1 \ \cdots \ b_k]$

Inner product interpretation

- with a_i^T the rows of A, b_j the columns of B, we have

$$AB = \begin{bmatrix} a_1^T b_1 & a_1^T b_2 & \cdots & a_1^T b_n \\ a_2^T b_1 & a_2^T b_2 & \cdots & a_2^T b_n \\ \vdots & \vdots & & \vdots \\ a_m^T b_1 & a_m^T b_2 & \cdots & a_m^T b_n \end{bmatrix}$$

- so matrix product is all inner products of rows of A and columns of B, arranged in a matrix

Gram matrix

- let A be an $m \times n$ matrix with columns $a_1, \ldots, a_n$
- the *Gram matrix* of A is

$$G = A^T A = \begin{bmatrix} a_1^T a_1 & a_1^T a_2 & \cdots & a_1^T a_n \\ a_2^T a_1 & a_2^T a_2 & \cdots & a_2^T a_n \\ \vdots & \vdots & \ddots & \vdots \\ a_n^T a_1 & a_n^T a_2 & \cdots & a_n^T a_n \end{bmatrix}$$

- Gram matrix gives all inner products of columns of A
- example: $G = A^T A = I$ means columns of A are orthonormal

Complexity

- to compute $C_{ij} = (AB)_{ij}$ is inner product of p-vectors
- so total required flops is $(mn)(2p) = 2mnp$ flops
- multiplying two 1000×1000 matrices requires 2 billion flops
- ...and can be done in well under a second on current computers

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Composition of linear functions

- A is an $m \times p$ matrix, B is $p \times n$
- define $f : \mathbf{R}^p \to \mathbf{R}^m$ and $g : \mathbf{R}^n \to \mathbf{R}^p$ as

$$f(u) = Au, \qquad g(v) = Bv$$

- f and g are linear functions
- *composition* of f and g is $h : \mathbf{R}^n \to \mathbf{R}^m$ with $h(x) = f(g(x))$
- we have

$$h(x) = f(g(x)) = A(Bx) = (AB)x$$

- composition of linear functions is linear
- associated matrix is product of matrices of the functions

Second difference matrix

- D_n is $(n-1) \times n$ difference matrix:

$$D_n x = (x_2 - x_1, \ldots, x_n - x_{n-1})$$

- D_{n-1} is $(n-2) \times (n-1)$ difference matrix:

$$D_{n-1} y = (y_2 - y_1, \ldots, y_{n-1} - y_{n-2})$$

- $\Delta = D_{n-1} D_n$ is $(n-2) \times n$ second difference matrix:

$$\Delta x = (x_1 - 2x_2 + x_3, x_2 - 2x_3 + x_4, \ldots, x_{n-2} - 2x_{n-1} + x_n)$$

- for $n = 5$, $\Delta = D_{n-1} D_n$ is

$$\begin{bmatrix} 1 & -2 & 1 & 0 & 0 \\ 0 & 1 & -2 & 1 & 0 \\ 0 & 0 & 1 & -2 & 1 \end{bmatrix} = \begin{bmatrix} -1 & 1 & 0 & 0 \\ 0 & -1 & 1 & 0 \\ 0 & 0 & -1 & 1 \end{bmatrix} \begin{bmatrix} -1 & 1 & 0 & 0 & 0 \\ 0 & -1 & 1 & 0 & 0 \\ 0 & 0 & -1 & 1 & 0 \\ 0 & 0 & 0 & -1 & 1 \end{bmatrix}$$

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Matrix powers

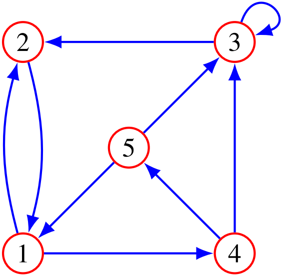
- for A square, A^2 means AA, and same for higher powers
- with convention $A^0 = I$ we have $A^k A^l = A^{k+l}$
- negative powers later; fractional powers in other courses

Directed graph

- $n \times n$ matrix A is adjacency matrix of directed graph:

$$A_{ij} = \begin{cases} 1 & \text{there is a edge from vertex } j \text{ to vertex } i \\ 0 & \text{otherwise} \end{cases}$$

- example:



$$A = \begin{bmatrix} 0 & 1 & 0 & 0 & 1 \\ 1 & 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 1 & 1 \\ 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 \end{bmatrix}$$

Paths in directed graph

- square of adjacency matrix:

$$(A^2)_{ij} = \sum_{k=1}^{n} A_{ik}A_{kj}$$

- $(A^2)_{ij}$ is number of paths of length 2 from j to i
- for the example,

$$A^2 = \begin{bmatrix} 1 & 0 & 1 & 1 & 0 \\ 0 & 1 & 1 & 1 & 2 \\ 1 & 0 & 1 & 2 & 1 \\ 0 & 1 & 0 & 0 & 1 \\ 1 & 0 & 0 & 0 & 0 \end{bmatrix}$$

  e.g., there are two paths from 4 to 3 (via 3 and 5)
- more generally, $(A^\ell)_{ij}$ = number of paths of length ℓ from j to i

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Gram–Schmidt in matrix notation

- run Gram–Schmidt on columns $a_1, \ldots, a_k$ of $n \times k$ matrix A
- if columns are linearly independent, get orthonormal $q_1, \ldots, q_k$
- define $n \times k$ matrix Q with columns $q_1, \ldots, q_k$
- $Q^T Q = I$
- from Gram–Schmidt algorithm

$$
\begin{aligned}
a_i &= (q_1^T a_i) q_1 + \cdots + (q_{i-1}^T a_i) q_{i-1} + \|\tilde{q}_i\| q_i \\
&= R_{1i} q_1 + \cdots + R_{ii} q_i
\end{aligned}
$$

  with $R_{ij} = q_i^T a_j$ for $i < j$ and $R_{ii} = \|\tilde{q}_i\|$
- defining $R_{ij} = 0$ for $i > j$ we have $A = QR$
- R is upper triangular, with positive diagonal entries

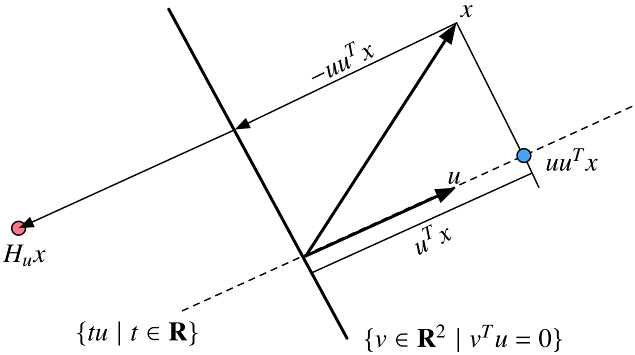
QR factorization

- $A = QR$ is called *QR factorization* of A
- factors satisfy $Q^T Q = I$, R upper triangular with positive diagonal entries
- can be computed using Gram–Schmidt algorithm (or some variations)
- has a *huge* number of uses, which we'll see soon

Outline

Householder transforms for QR factorization

- matrix multiplication to *compute* QR factorization
- Householder transform: for unit vector u, $H_u = I - 2uu^T$



Properties of Householder transforms

- symmetric and orthogonal:

$$H_u^T = (I - 2uu^T)^T = I - 2(uu^T)^T = I - 2uu^T$$

  and

$$H_u^T H_u = H_u^2 = I - 4uu^T uu^T + 4uu^T uu^T uu^T = I$$

- product of any number is orthogonal: for unit norm vectors $u_1, u_2, \ldots, u_k$

$$Q = H_{u_1} H_{u_2} \cdots H_{u_k}$$

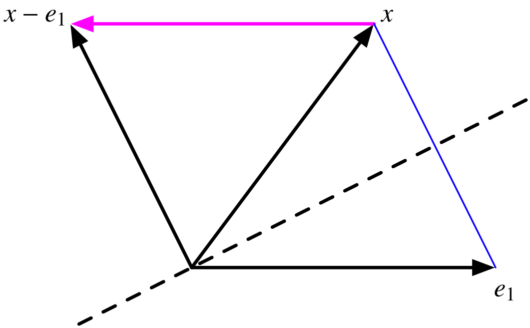
  satisfies

$$\begin{aligned} Q^T Q &= H_{u_k} H_{u_{k-1}} \cdots H_{u_2} H_{u_1} H_{u_1} H_{u_2} \cdots H_{u_k} \\ &= H_{u_k} H_{u_{k-1}} \cdots H_{u_2} H_{u_2} \cdots H_{u_{k-1}} H_{u_k} = \cdots = I. \end{aligned}$$

Annihilation with Householders

- for unit-norm n-vector $x \in \mathbf{R}^n$, find u so that

$$H_u x = e_1$$



- take $u = (x - e_1)/\|x - e_1\|$, verify $H_u x = e_1$

Annihilating below diagonals

- start with $n \times k$ matrix A with columns $a_1, a_2, \ldots, a_k$
- annihilate below diagonal for first column: if $a_1 \neq 0$, set $v = a_1/\|a_1\|$

$$H_u = I - 2uu^T \quad \text{for} \quad u = \frac{v - e_1}{\|v - e_1\|}$$

- then

$$H_u A = \begin{bmatrix} H_u a_1 & H_u a_2 & \cdots & H_u a_k \end{bmatrix} = \begin{bmatrix} \|a_1\| & * \\ 0 & \tilde{A}_1 \end{bmatrix}$$

- recurse: for block matrix with R_i an $i \times i$ upper triangular matrix

$$\begin{bmatrix} R_i & * \\ 0 & \tilde{A}_{i-1} \end{bmatrix}$$

then for $\tilde{A}_{i-1} = [\tilde{a}_1 \ \cdots \ \tilde{a}_{k-i}]$, choosing unit $\tilde{u}$ as above for $\tilde{a}_1$:

$$\begin{bmatrix} I & 0 \\ 0 & H_{\tilde{u}} \end{bmatrix} \begin{bmatrix} R_i & * \\ 0 & \tilde{A}_{i-1} \end{bmatrix} = \begin{bmatrix} R_i & * \\ 0 & \begin{pmatrix} \|\tilde{a}_1\| & * \\ 0 & \tilde{A}_i \end{pmatrix} \end{bmatrix}$$

Householder algorithm for QR factorization

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given $n \times k$ matrix A with columns $a_1, \ldots, a_k$
initialize $\tilde{A}_0 = A$
for $i = 0, \ldots, \min\{k, n-2\}$

1. *find first column* $\tilde{a} \in \mathbf{R}^{n-i}$ of $\tilde{A}_i$
2. *test for linear dependence*: if $\tilde{a} = 0$, recurse on $\tilde{A}_{i+1}$
   (the lower right $(n-i-1) \times (n-i-1)$ block of $\tilde{A}_i$)
3. *normalize:* $v = \tilde{a}/\|\tilde{a}\|$
4. *find projector:* $u = (v - e_1)/\|v - e_1\| \in \mathbf{R}^{n-i}$
5. *construct* $(n-i) \times (n-i)$ Householder matrix $H_i = I - 2uu^T$
6. *apply* H_i to obtain

$$\begin{bmatrix} r_{ii} & * \\ 0 & \tilde{A}_i \end{bmatrix} = H_i \tilde{A}_{i-1}$$

- final output: $A = QR$, where for $m = \min\{n-2, k\}$

$$Q = H_0 \begin{bmatrix} 1 & 0 \\ 0 & H_1 \end{bmatrix} \begin{bmatrix} I_2 & 0 \\ 0 & H_2 \end{bmatrix} \cdots \begin{bmatrix} I_m & 0 \\ 0 & H_m \end{bmatrix} \quad \text{and} \quad R = Q^T A$$