신경망 네트워크와 수학적 기반

Matrices

- a *matrix* is a rectangular array of numbers, *e.g.*,

$$\begin{bmatrix} 0 & 1 & -2.3 & 0.1 \\ 1.3 & 4 & -0.1 & 0 \\ 4.1 & -1 & 0 & 1.7 \end{bmatrix}$$

- its *size* is given by (row dimension) × (column dimension)
  e.g., matrix above is 3 × 4
- *elements* also called *entries* or *coefficients*
- B_{ij} is i,j element of matrix B
- i is the *row index*, j is the *column index*; indexes start at 1
- two matrices are *equal* (denoted with =) if they are the same size and corresponding entries are equal

Matrix shapes

an $m \times n$ matrix A is

- *tall* if $m > n$
- *wide* if $m < n$
- *square* if $m = n$

Column and row vectors

- we consider an $n \times 1$ matrix to be an n-vector
- we consider a 1×1 matrix to be a number
- a $1 \times n$ matrix is called a *row vector*, *e.g.*,

$$\begin{bmatrix} 1.2 & -0.3 & 1.4 & 2.6 \end{bmatrix}$$

which is *not* the same as the (column) vector

$$\begin{bmatrix} 1.2 \\ -0.3 \\ 1.4 \\ 2.6 \end{bmatrix}$$

Columns and rows of a matrix

- suppose A is an $m \times n$ matrix with entries A_{ij} for $i = 1,..., m, j = 1,..., n$
- its j-th *column* is (the m-vector)

$$\begin{bmatrix} A_{1j} \\ \vdots \\ A_{mj} \end{bmatrix}$$

- its i-th *row* is (the n-row-vector)

$$\begin{bmatrix} A_{i1} & \cdots & A_{in} \end{bmatrix}$$

- *slice* of matrix: $A_{p:q,r:s}$ is the $(q - p + 1) \times (s - r + 1)$ matrix

$$A_{p:q,r:s} = \begin{bmatrix} A_{pr} & A_{p,r+1} & \cdots & A_{ps} \\ A_{p+1,r} & A_{p+1,r+1} & \cdots & A_{p+1,s} \\ \vdots & \vdots & & \vdots \\ A_{qr} & A_{q,r+1} & \cdots & A_{qs} \end{bmatrix}$$

Matrices

Block matrices

- we can form *block matrices*, whose entries are matrices, such as

$$A = \begin{bmatrix} B & C \\ D & E \end{bmatrix}$$

where B, C, D, and E are matrices (called *submatrices* or *blocks* of A)

- matrices in each block row must have same height (row dimension)
- matrices in each block column must have same width (column dimension)
- example: if

$$B = \begin{bmatrix} 0 & 2 & 3 \end{bmatrix}, \quad C = \begin{bmatrix} -1 \end{bmatrix}, \quad D = \begin{bmatrix} 2 & 2 & 1 \\ 1 & 3 & 5 \end{bmatrix}, \quad E = \begin{bmatrix} 4 \\ 4 \end{bmatrix}$$

then

$$\begin{bmatrix} B & C \\ D & E \end{bmatrix} = \begin{bmatrix} 0 & 2 & 3 & -1 \\ 2 & 2 & 1 & 4 \\ 1 & 3 & 5 & 4 \end{bmatrix}$$

Column and row representation of matrix

- A is an $m \times n$ matrix
- can express as block matrix with its (m-vector) columns $a_1, \ldots, a_n$

$$A = \begin{bmatrix} a_1 & a_2 & \cdots & a_n \end{bmatrix}$$

- or as block matrix with its (n-row-vector) rows $b_1, \ldots, b_m$

$$A = \begin{bmatrix} b_1 \\ b_2 \\ \vdots \\ b_m \end{bmatrix}$$

Matrices

Examples

- *image:* X_{ij} is i, j pixel value in a monochrome image
- *feature matrix*: X_{ij} is value of feature i for entity j

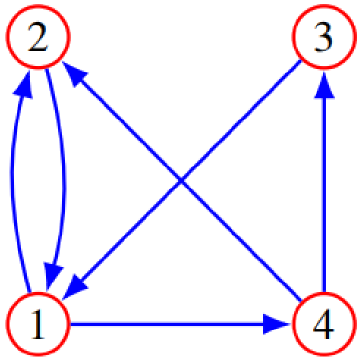
Matrices

Graph or relation

- a *relation* is a set of pairs of *objects*, labeled 1,..., *n*, such as

$$R = \{(1, 2), (1, 3), (2, 1), (2, 4), (3, 4), (4, 1)\}$$

- same as *directed graph*



- can be represented as $n \times n$ matrix with $A_{ij} = 1$ if $(i, j) \in R$

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

Special matrices

- $m \times n$ *zero matrix* has all entries zero, written as $0_{m \times n}$ or just 0
- *identity matrix* is square matrix with $I_{ii} = 1$ and $I_{ij} = 0$ for $i \neq j$, *e.g.*,

$$\begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}, \qquad \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix}$$

- *sparse matrix*: most entries are zero
  - examples: 0 and I
  - can be stored and manipulated efficiently
  - nnz(A) is number of nonzero entries

Matrices

Diagonal and triangular matrices

- ***diagonal matrix***: square matrix with $A_{ij} = 0$ when $i \neq j$
- diag($a_1,\ldots, a_n$) denotes the diagonal matrix with $A_{ii} = a_i$ for $i = 1,\ldots, n$
- example:

$$\mathbf{diag}(0.2, -3, 1.2) = \begin{bmatrix} 0.2 & 0 & 0 \\ 0 & -3 & 0 \\ 0 & 0 & 1.2 \end{bmatrix}$$

- ***lower triangular matrix***: $A_{ij} = 0$ for $i < j$
- ***upper triangular matrix***: $A_{ij} = 0$ for $i > j$
- examples:

$$\begin{bmatrix} 1 & -1 & 0.7 \\ 0 & 1.2 & -1.1 \\ 0 & 0 & 3.2 \end{bmatrix} \text{(upper triangular)}, \qquad \begin{bmatrix} -0.6 & 0 \\ -0.3 & 3.5 \end{bmatrix} \text{(lower triangular)}$$

Transpose

- the *transpose* of an $m \times n$ matrix A is denoted A^T, and defined by

$$(A^T)_{ij} = A_{ji}, \quad i = 1, \ldots, n, \quad j = 1, \ldots, m$$

- for example,

$$\begin{bmatrix} 0 & 4 \\ 7 & 0 \\ 3 & 1 \end{bmatrix}^T = \begin{bmatrix} 0 & 7 & 3 \\ 4 & 0 & 1 \end{bmatrix}$$

- transpose converts column to row vectors (and vice versa)
- $(A^T)^T = A$

Addition, subtraction, and scalar multiplication

- (just like vectors) we can add or subtract matrices of the same size:

$$(A + B)_{ij} = A_{ij} + B_{ij}, \quad i = 1, \ldots, m, \quad j = 1, \ldots, n$$

(subtraction is similar)

- scalar multiplication:

$$(\alpha A)_{ij} = \alpha A_{ij}, \quad i = 1, \ldots, m, \quad j = 1, \ldots, n$$

- many obvious properties, *e.g.*,

$$A + B = B + A, \qquad \alpha(A + B) = \alpha A + \alpha B, \qquad (A + B)^T = A^T + B^T$$

Matrix norm

- for $m \times n$ matrix A, we define

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

- agrees with vector norm when $n = 1$
- satisfies norm properties:

$$\|\alpha A\| = |\alpha| \|A\|$$

$$\|A + B\| \leq \|A\| + \|B\|$$

$$\|A\| \geq 0$$

$$\|A\| = 0 \text{ only if } A = 0$$

- distance between two matrices: ||A - B||

Matrix-vector product

- ***matrix-vector product*** **of** $m \times n$ **matrix** A, n**-vector** x, **denoted** $y = Ax$, **with**

$$y_i = A_{i1}x_1 + \cdots + A_{in}x_n, \quad i = 1, \ldots, m$$

- **for example,**

$$\begin{bmatrix} 0 & 2 & -1 \\ -2 & 1 & 1 \end{bmatrix} \begin{bmatrix} 2 \\ 1 \\ -1 \end{bmatrix} = \begin{bmatrix} 3 \\ -4 \end{bmatrix}$$

Row interpretation

- y = Ax can be expressed as

$$y_i = b_i^T x, \quad i = 1, \ldots, m$$

where $b_1^T, \ldots, b_m^T$ are rows of A

- so $y = Ax$ is a 'batch' inner product of all rows of A with x
- example: $A1$ is vector of row sums of matrix A

Column interpretation

- $y = Ax$ can be expressed as

$$y = x_1 a_1 + x_2 a_2 + \cdots + x_n a_n$$

  where $a_1, \ldots, a_n$ are columns of A

- so $y = Ax$ is linear combination of columns of A, with coefficients $x_1, \ldots, x_n$
- important example: $A e_j = a_j$
- columns of A are linearly independent if $Ax = 0$ implies $x = 0$

General examples

- $0x = 0$, *i.e.*, multiplying by zero matrix gives zero
- $Ix = x$, *i.e.*, multiplying by identity matrix does nothing
- inner product $a^T b$ is matrix-vector product of $1 \times n$ matrix a^T and n-vector b
- $\tilde{x} = Ax$ is de-meaned version of x, with

$$A = \begin{bmatrix} 1 - 1/n & -1/n & \cdots & -1/n \\ -1/n & 1 - 1/n & \cdots & -1/n \\ \vdots & & \ddots & \vdots \\ -1/n & -1/n & \cdots & 1 - 1/n \end{bmatrix}$$

Difference matrix

- $(n - 1) \times n$ *difference matrix* is

$$D = \begin{bmatrix} -1 & 1 & 0 & \cdots & 0 & 0 & 0 \\ 0 & -1 & 1 & \cdots & 0 & 0 & 0 \\ & & \ddots & \ddots & & & \\ & & & \ddots & \ddots & & \\ 0 & 0 & 0 & \cdots & -1 & 1 & 0 \\ 0 & 0 & 0 & \cdots & 0 & -1 & 1 \end{bmatrix}$$

$y = Dx$ is $(n - 1)$-vector of differences of consecutive entries of x:

$$Dx = \begin{bmatrix} x_2 - x_1 \\ x_3 - x_2 \\ \vdots \\ x_n - x_{n-1} \end{bmatrix}$$

- *Dirichlet energy*: $\|Dx\|^2$ is measure of fluctuation for x a time series

Feature matrix – weight vector

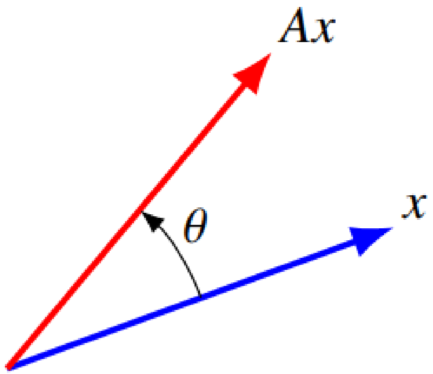
- $X = [x_1 \cdots x_N]$ is $n \times N$ *feature matrix*
- column x_j is feature n-vector for object or example j
- X_{ij} is value of feature i for example j
- n-vector w is weight vector
- $s = X^T w$ is vector of scores for each example; $s_j = x_j^T w$

Matrices

Geometric transformations

- many geometric transformations and mappings of 2-D and 3-D vectors can be represented via matrix multiplication $y = Ax$
- for example, rotation by θ :

$$y = \begin{bmatrix} \cos\theta & -\sin\theta \\ \sin\theta & \cos\theta \end{bmatrix} x$$



Matrices

Selectors

- an $m \times n$ *selector matrix*: each row is a unit vector (transposed)

$$A = \begin{bmatrix} e_{k_1}^T \\ \vdots \\ e_{k_m}^T \end{bmatrix}$$

- multiplying by A selects entries of x:

$$Ax = (x_{k_1}, x_{k_2}, \ldots, x_{k_m})$$

- example: the $m \times 2m$ matrix

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

'down-samples' by 2: if x is a $2m$-vector then $y = Ax = (x_1, x_3, \ldots, x_{2m-1})$

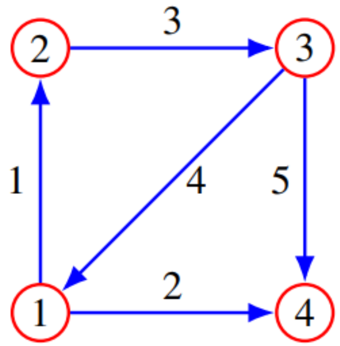
Matrices

Incidence matrix

- graph with n vertices or nodes, m (directed) edges or links
- incidence matrix is $n \times m$ matrix

$$A_{ij} = \begin{cases} 1 & \text{edge } j \text{ points to node } i \\ -1 & \text{edge } j \text{ points from node } i \\ 0 & \text{otherwise} \end{cases}$$

- example with $n = 4$, $m = 5$:



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

Convolution

- for n-vector a, m-vector b, the *convolution* $c = a \times b$ is the $(n + m - 1)$-vector

$$c_k = \sum_{i+j=k+1} a_i b_j, \quad k = 1, \ldots, n+m-1$$

- for example with $n = 4$, $m = 3$, we have

$$\begin{aligned}
c_1 &= a_1 b_1 \\
c_2 &= a_1 b_2 + a_2 b_1 \\
c_3 &= a_1 b_3 + a_2 b_2 + a_3 b_1 \\
c_4 &= a_2 b_3 + a_3 b_2 + a_4 b_1 \\
c_5 &= a_3 b_3 + a_4 b_2 \\
c_6 &= a_4 b_3
\end{aligned}$$

- example: $(1, 0, -1) \times (2, 1, -1) = (2, 1, -3, -1, 1)$

Matrices

Polynomial multiplication

- a and b are coefficients of two polynomials:

$$p(x) = a_1 + a_2 x + \cdots + a_n x^{n-1}, \qquad q(x) = b_1 + b_2 x + \cdots + b_m x^{m-1}$$

- convolution $c = a \times b$ gives the coefficients of the product $p(x)q(x)$:

$$p(x)q(x) = c_1 + c_2 x + \cdots + c_{n+m-1} x^{n+m-2}$$

- this gives simple proofs of many properties of convolution; for example,

$$a * b = b * a$$

$$(a * b) * c = a * (b * c)$$

$$a * b = 0 \text{ only if } a = 0 \text{ or } b = 0$$

Matrices

Toeplitz matrices

- function $f(b) = a * b$ is linear; in fact $c = T(b)\,a$ with

$$T(b) = \begin{bmatrix} b_1 & 0 & 0 & 0 \\ b_2 & b_1 & 0 & 0 \\ b_3 & b_2 & b_1 & 0 \\ 0 & b_3 & b_2 & b_1 \\ 0 & 0 & b_3 & b_2 \\ 0 & 0 & 0 & b_3 \end{bmatrix}$$

- $T(b)$ is a Toeplitz matrix (values on diagonals are equal)

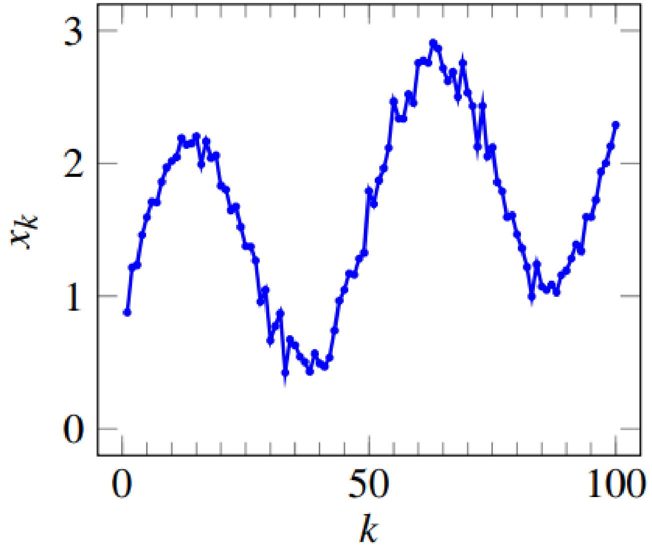
Matrices

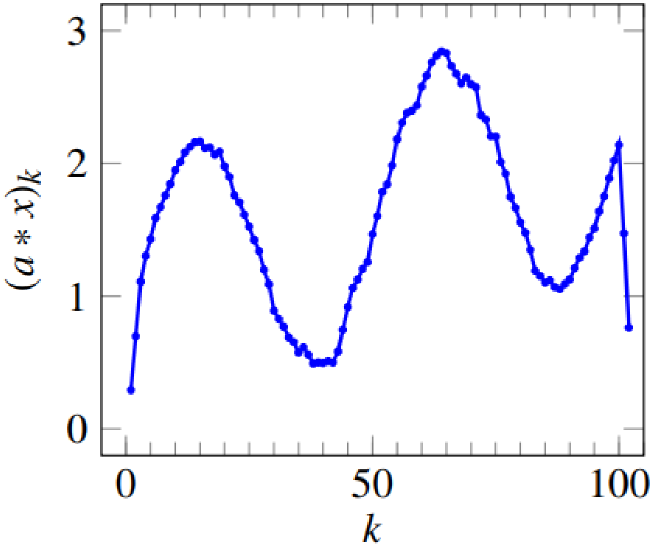
Moving average of time series

- n-vector x represents a time series
- convolution $y = a * x$ with $a = (1/3, 1/3, 1/3)$ is 3-period *moving average*:

$$y_k = \frac{1}{3}(x_k + x_{k-1} + x_{k-2}), \quad k = 1, 2, \ldots, n+2$$

(with x_k interpreted as zero for $k < 1$ and $k > n$)





Input-output convolution system

- m-vector u represents a time series *input*
- $m + n - 1$ vector y represents a time series *output*
- $y = h * u$ is a *convolution model*
- n-vector h is called the *system impulse response*
- we have

$$y_i = \sum_{j=1}^{n} u_{i-j+1} h_j$$

(interpreting u_k as zero for $k < n$ or $k > n$)

- interpretation: y_i, output at time i is a linear combination of $u_i, \ldots, u_{i-n+1}$