신경망 네트워크와 수학적 기반

Matrix inverses

Left inverses

- a number x that satisfies $xa = 1$ is called the inverse of a
- inverse (*i.e.*, $1/a$) exists if and only if $a \neq 0$, and is unique
- a matrix X that satisfies $XA = I$ is called a left inverse of A
- if a left inverse exists, we say that A is *left-invertible*
- example: the matrix

$$A = \begin{bmatrix} -3 & -4 \\ 4 & 6 \\ 1 & 1 \end{bmatrix}$$

has two different left inverses:

$$B = \frac{1}{9}\begin{bmatrix} -11 & -10 & 16 \\ 7 & 8 & -11 \end{bmatrix}, \qquad C = \frac{1}{2}\begin{bmatrix} 0 & -1 & 6 \\ 0 & 1 & -4 \end{bmatrix}$$

Left inverse and column independence

- if A has a left inverse C then the columns of A are linearly independent
- to see this: if $Ax = 0$ and $CA = I$ then

$$0 = C\,0 = C\,(Ax) = (CA)\,x = Ix = x$$

- the converse is also true, so

  a matrix is left-invertible if and only if its columns are linearly independent

- matrix generalization of

  a number is invertible if and only if it is nonzero

- so left-invertible matrices are tall or square

Solving linear equations with a left inverse

- suppose $Ax = b$, and A has a left inverse C
- then $C\,b = C\,(Ax) = (CA)\,x = I\,x = x$
- so multiplying the right-hand side by a left inverse yields the solution

Matrix inverses

Example

$$A = \begin{bmatrix} -3 & -4 \\ 4 & 6 \\ 1 & 1 \end{bmatrix}, \qquad b = \begin{bmatrix} 1 \\ -2 \\ 0 \end{bmatrix}$$

- over-determined equations $Ax = b$ have (unique) solution $x = (1, -1)$
- A has two different left inverses

$$B = \frac{1}{9}\begin{bmatrix} -11 & -10 & 16 \\ 7 & 8 & -11 \end{bmatrix}, \qquad C = \frac{1}{2}\begin{bmatrix} 0 & -1 & 6 \\ 0 & 1 & -4 \end{bmatrix}$$

- multiplying the right-hand side with the left inverse B we get

$$Bb = \begin{bmatrix} 1 \\ -1 \end{bmatrix}$$

- and also

$$Cb = \begin{bmatrix} 1 \\ -1 \end{bmatrix}$$

Right inverses

- a matrix X that satisfies $AX = I$ is a *right inverse* of A
- if a right inverse exists, we say that A is *right-invertible*
- A is right-invertible if and only if A^T is left-invertible:

$$AX = I \iff (AX)^T = I \iff X^T A^T = I$$

- so we conclude

  A is right-invertible if and only if its rows are linearly independent

- right-invertible matrices are wide or square

Solving linear equations with a right inverse

- suppose A has a right inverse B
- consider the (square or underdetermined) equations $Ax = b$
- $x = Bb$ is a solution:

$$Ax = A\,(Bb) = (AB)\,b = I\,b = b$$

- so $Ax = b$ has a solution for *any* b

Matrix inverses

Inverse

- if A has a left and a right inverse, they are unique and equal (and we say that A is *invertible*)
- so A must be square
- to see this: if $AX = I$, $YA = I$

$$X = IX = (YA)X = Y(AX) = YI = Y$$

- we denote them by A^{-1}:

$$A^{-1}A = AA^{-1} = I$$

- inverse of inverse: $(A^{-1})^{-1} = A$

Matrix inverses

Solving square systems of linear equations

- suppose A is invertible
- for any b, $Ax = b$ has the unique solution

$$x = A^{-1}b$$

- matrix generalization of simple scalar equation $ax = b$ having solution $x = (1/a)\, b$ (for $a \neq 0$)
- simple-looking formula $x = A^{-1}b$ is basis for many applications

Invertible matrices

- the following are equivalent for a square matrix A:
  - A is invertible
  - columns of A are linearly independent
  - rows of A are linearly independent
  - A has a left inverse
  - A has a right inverse

  if any of these hold, all others do

Matrix inverses
Examples

- $I^{-1} = I$
- if Q is orthogonal, *i.e.*, square with $Q^TQ = I$, then $Q^{-1} = Q^T$
- 2×2 matrix A is invertible if and only $A_{11}A_{22} \neq A_{12}A_{21}$

$$A^{-1} = \frac{1}{A_{11}A_{22} - A_{12}A_{21}} \begin{bmatrix} A_{22} & -A_{12} \\ -A_{21} & A_{11} \end{bmatrix}$$

  - there are similar but much more complicated formulas for larger matrices

Matrix inverses

Non-obvious example

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

- A is invertible, with inverse

$$A^{-1} = \frac{1}{30}\begin{bmatrix} 0 & -20 & -10 \\ -6 & 5 & -2 \\ 6 & 10 & 2 \end{bmatrix}$$

- verified by checking $AA^{-1} = I$ (or $A^{-1}A = I$)

Matrix inverses

Properties

- $(AB)^{-1} = B^{-1}A^{-1}$ (provided inverses exist)
- $(A^T)^{-1} = (A^{-1})^T$(sometimes denoted A^{-T})
- negative matrix powers: $(A^{-1})^k$ is denoted A^{-k}
- with $A^0 = I$, identity $A^kA^l = A^{k+l}$ holds for any integers k, l

Triangular matrices

- lower triangular L with nonzero diagonal entries is invertible
- so see this, write $Lx = 0$ as

$$\begin{array}{rcl} L_{11}x_1 & = & 0 \\ L_{21}x_1 + L_{22}x_2 & = & 0 \\ & \vdots & \\ L_{n1}x_1 + L_{n2}x_2 + \cdots + L_{n,n-1}x_{n-1} + L_{nn}x_n & = & 0 \end{array}$$

  - from first equation, $x_1 = 0$ (since $L_{11} \neq 0$)
  - second equation reduces to $L_{22}x_2 = 0$, so $x_2 = 0$ (since $L_{22} \neq 0$)
  - and so on

  this shows columns of L are linearly independent, so L is invertible

- upper triangular R with nonzero diagonal entries is invertible

Matrix inverses

Inverse via QR factorization

- suppose A is square and invertible
- so its columns are linearly independent
- so Gram–Schmidt gives QR factorization
  - $A = QR$
  - Q is orthogonal: $Q^TQ = I$
  - R is upper triangular with positive diagonal entries, hence invertible
- so we have

$$A^{-1} = (QR)^{-1} = R^{-1}Q^{-1} = R^{-1}Q^T$$

Matrix inverses

Back substitution

- suppose R is upper triangular with nonzero diagonal entries
- write out $Rx = b$ as

$$
\begin{aligned}
R_{11}x_1 + R_{12}x_2 + \cdots + R_{1,n-1}x_{n-1} + R_{1n}x_n &= b_1 \\
&\vdots \\
R_{n-1,n-1}x_{n-1} + R_{n-1,n}x_n &= b_{n-1} \\
R_{nn}x_n &= b_n
\end{aligned}
$$

- from last equation we get $x_n = b_n / R_{nn}$
- from 2nd to last equation we get

$$
x_{n-1} = (b_{n-1} - R_{n-1,n}x_n)/R_{n-1,n-1}
$$

- continue to get $x_{n-2}, x_{n-3}, \ldots, x_1$

Back substitution

- called *back substitution* since we find the variables in reverse order, substituting the already known values of x_i
- computes $x = R^{-1}b$

Solving linear equations via QR factorization

- assuming A is invertible, let's solve $Ax = b$, *i.e.*, compute $x = A^{-1}b$
- with QR factorization $A = QR$, we have

$$A^{-1} = (QR)^{-1} = R^{-1}Q^T$$

- compute $x = R^{-1}(Q^T b)$ by back substitution

Solving linear equations via QR factorization

- given an $n \times n$ invertible matrix A and an n-vector b

1. *QR factorization*: compute the QR factorization $A = QR$
2. compute $Q^T b$.
3. *Back substitution*: Solve the triangular equation $Rx = Q^T b$ using back substitution

Polynomial interpolation

- let's find coefficients of a cubic polynomial

$$p(x) = c_1 + c_2 x + c_3 x^2 + c_4 x^3$$

that satisfies

$$p(-1.1) = b_1, \qquad p(-0.4) = b_2, \qquad p(0.1) = b_3, \qquad p(0.8) = b_4$$

- write as $Ac = b$, with

$$A = \begin{bmatrix} 1 & -1.1 & (-1.1)^2 & (-1.1)^3 \\ 1 & -0.4 & (-0.4)^2 & (-0.4)^3 \\ 1 & 0.1 & (0.1)^2 & (0.1)^3 \\ 1 & 0.8 & (0.8)^2 & (0.8)^3 \end{bmatrix}$$

Matrix inverses

Polynomial interpolation

- (unique) coefficients given by $c = A^{-1}b$, with

$$A^{-1} = \begin{bmatrix} -0.0201 & 0.2095 & 0.8381 & -0.0276 \\ 0.1754 & -2.1667 & 1.8095 & 0.1817 \\ 0.3133 & 0.4762 & -1.6667 & 0.8772 \\ -0.6266 & 2.381 & -2.381 & 0.6266 \end{bmatrix}$$

- so, *e.g.*, c_1 is not very sensitive to b_1 or b_4

Matrix inverses

Invertibility of Gram matrix

- A has linearly independent columns if and only if A^TA is invertible
- to see this, we'll show that $Ax = 0 \Leftrightarrow A^TAx = 0$
- $\Rightarrow$: if $Ax = 0$ then $(A^TA)x = A^T(Ax) = A^T 0 = 0$
- $\Leftarrow$: if $(A^TA)x = 0$ then

$$0 = x^T(A^TA)x = (Ax)^T(Ax) = \|Ax\|^2 = 0$$

so $Ax = 0$. We have $x = 0$ since the columns of A are linear independent

Pseudo-inverse of tall matrix

- the *pseudo-inverse* of A with independent columns is

$$A^{\dagger} = (A^T A)^{-1} A^T$$

- it is a left inverse of A:

$$A^{\dagger} A = (A^T A)^{-1} A^T A = (A^T A)^{-1} (A^T A) = I$$

- reduces to A^{-1} when A is square:

$$A^{\dagger} = (A^T A)^{-1} A^T = A^{-1} A^{-T} A^T = A^{-1} I = A^{-1}$$

Matrix inverses

Pseudo-inverse of wide matrix

- if A is wide, with linearly independent rows, AA^T is invertible
- pseudo-inverse is defined as

$$A^\dagger = A^T(AA^T)^{-1}$$

- $A^\dagger$ is a right inverse of A:

$$AA^\dagger = AA^T(AA^T)^{-1} = I$$

- reduces to A^{-1} when A is square:

$$A^T(AA^T)^{-1} = A^T A^{-T} A^{-1} = A^{-1}$$

Pseudo-inverse via QR factorization

- suppose A has linearly independent columns, $A = QR$
- then $A^TA = (QR)^T (QR) = R^TQ^TQR = R^TR$
- so

$$A^\dagger = (A^TA)^{-1}A^T = (R^TR)^{-1}(QR)^T = R^{-1}R^{-T}R^TQ^T = R^{-1}Q^T$$

- can compute $A^\dagger$ using back substitution on columns of Q^T
- for A with linearly independent rows, $A^\dagger = QR^{-T}$