Outline

Left and right inverses

Inverse

Solving linear equations

Examples

Pseudo-inverse

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 $(A^TA)x = A^T(Ax) = A^T0 = 0$
- $\Leftarrow$: if $(A^TA)x = 0$ then

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

so $Ax = 0$

Pseudo-inverse of tall matrix

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

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

- it is a left inverse of A:

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

  (we'll soon see that it's a very important left inverse of A)

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

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

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:

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

  (we'll see later it is an important right inverse)
- reduces to A^{-1} when A is square:

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

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, $A^\dagger = QR^{-T}$

12. Least squares

Outline

Least squares problem

Solution of least squares problem

Examples

Least squares problem

- suppose $m \times n$ matrix A is tall, so $Ax = b$ is over-determined
- for most choices of b, there is no x that satisfies $Ax = b$
- *residual* is $r = Ax - b$
- *least squares problem*: choose x to minimize $\|Ax - b\|^2$
- $\|Ax - b\|^2$ is the *objective function*
- $\hat{x}$ is a *solution* of least squares problem if

$$\|A\hat{x} - b\|^2 \leq \|Ax - b\|^2$$

  for any n-vector x
- idea: $\hat{x}$ makes residual as small as possible, if not 0
- also called *regression* (in data fitting context)

Least squares problem

- $\hat{x}$ called *least squares approximate solution* of $Ax = b$
- $\hat{x}$ is sometimes called 'solution of $Ax = b$ in the least squares sense'
  - this is very confusing
  - never say this
  - do not associate with people who say this

- $\hat{x}$ need not (and usually does not) satisfy $A\hat{x} = b$
- but if $\hat{x}$ does satisfy $A\hat{x} = b$, then it solves least squares problem

Column interpretation

- suppose $a_1, \ldots, a_n$ are columns of A
- then
$$\|Ax - b\|^2 = \|(x_1 a_1 + \cdots + x_n a_n) - b\|^2$$
- so least squares problem is to find a linear combination of columns of A that is closest to b
- if $\hat{x}$ is a solution of least squares problem, the m-vector
$$A\hat{x} = \hat{x}_1 a_1 + \cdots + \hat{x}_n a_n$$
is closest to b among all linear combinations of columns of A

Row interpretation

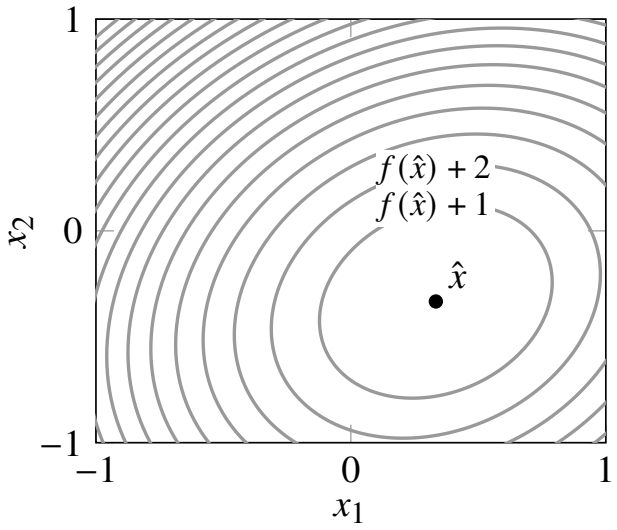
- suppose $\tilde{a}_1^T, \ldots, \tilde{a}_m^T$ are rows of A
- residual components are $r_i = \tilde{a}_i^T x - b_i$
- least squares objective is

$$\|Ax - b\|^2 = (\tilde{a}_1^T x - b_1)^2 + \cdots + (\tilde{a}_m^T x - b_m)^2$$

  the sum of squares of the residuals
- so least squares minimizes sum of squares of residuals
  - solving $Ax = b$ is making all residuals zero
  - least squares attempts to make them all small

Example

$$A = \begin{bmatrix} 2 & 0 \\ -1 & 1 \\ 0 & 2 \end{bmatrix}, \quad b = \begin{bmatrix} 1 \\ 0 \\ -1 \end{bmatrix}$$



- $Ax = b$ has no solution
- least squares problem is to choose x to minimize

$$\|Ax - b\|^2 = (2x_1 - 1)^2 + (-x_1 + x_2)^2 + (2x_2 + 1)^2$$

- least squares approximate solution is $\hat{x} = (1/3, -1/3)$ (say, via calculus)
- $\|A\hat{x} - b\|^2 = 2/3$ is smallest posible value of $\|Ax - b\|^2$
- $A\hat{x} = (2/3, -2/3, -2/3)$ is linear combination of columns of A closest to b