Singular value decomposition and pseudo-inverses

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1 Gramian matrices

Given a set of vectors $a_1, a_2, \ldots, a_n \in \mathbb{R}^m$, the Gramian matrix is the traditionally matrix of inner products $\langle a_i, a_j \rangle$. If these vectors are collected into a $m \times n$ matrix A, this matrix can be expressed as $A^t A$. Here, we will use the term for any matrix in this form. By starting out with the transpose instead, this means that AA^t is also a Gramian, with dual results.

Theorem 1.1. *If $A \in \mathbb{R}^{m\times n}$, then A^tA is symmetric and positive semi-definite. Iff A has rank m, A^tA is positive definite.*

Proof. $(A^tA)^t = A^t(A^t)^t = A^tA$ shows symmetry. positive semi-definiteness, let $x \in \mathbb{R}^n$. Then:

$$x^tA^tAx = \langle Ax, Ax \rangle = ||Ax||^2 \tag{1.1}$$

As a norm, this is greater than or equal to zero. Hence A^tA is positive semi-definite. If A has rank m the map $x \mapsto Ax$ has a trivial kernel by the rank-kernel theorem. Which means only the zero vector is mapped to zero, and hence A^tA is positive definite. If the rank is less than m, the kernel is non-trivial and positive definiteness cannot be true. □

2 The rank-nullity theorem

2.1 For A and A^t

According to the rank-nullity theorem, for a matrix $A \in \mathbb{R}^{m\times n}$, the sum of the rank and nullity is n. So, if the rank of A is r, then $\text{null}A = n - r$. Applying the theorem to A^t, which also has rank r, we get $\text{null}A = m - r$.

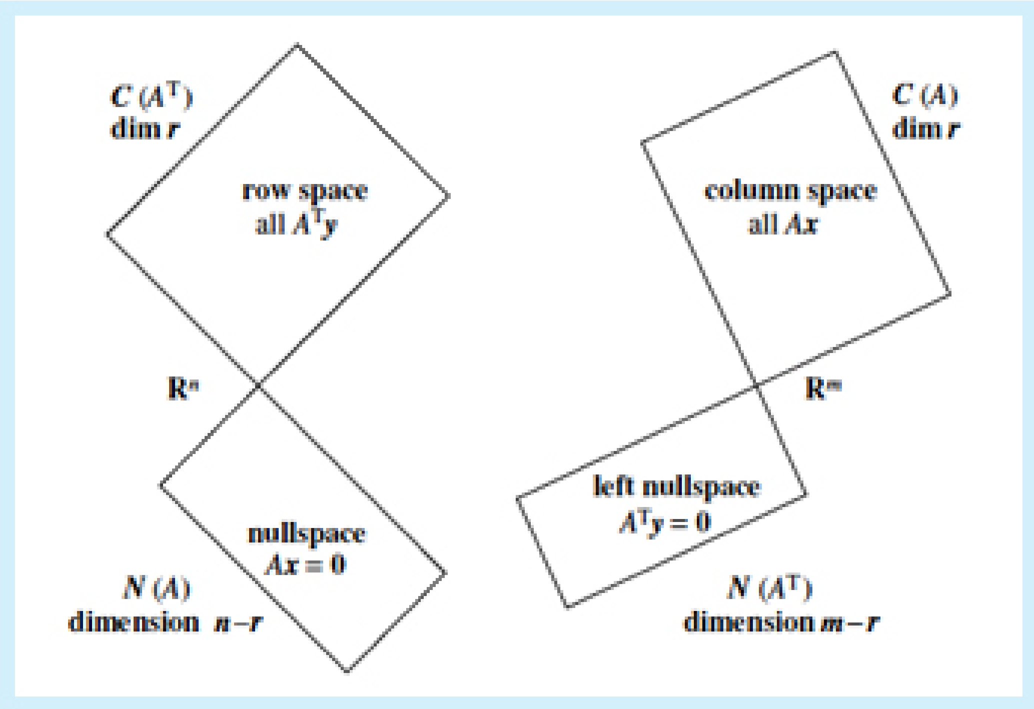

Figure 1: Visualization of dimensionality for the rank-nullity theorem

The image of A is also called the *column space* of A, denoted $C(A)$. The image of A^t is also called the *row space* of A, $C(A^t)$. The null space of A^t is often called the *left null space*.

These relationships are visualized in figure 1.

3 Singular value decomposition

3.1 Construction and intuition

We know that the dimensions of the row and column spaces of a matrix $A \in \mathbb{R}^{m \times n}$ are the same, r. We now seek out orthonormal bases of each of these spaces - $u_1, u_2, \ldots, u_r$ for column space and $v_1, v_2, \ldots, v_r$ for row space, such that

$$Av_i = \sigma_i u_i \tag{3.1}$$

The sigmas are known as *singular values* for A. Now, expand the orthonormal bases to include the null spaces. This means that $Av_i = 0$ for $r < i \leq n$. In matrix form this means:

$$AV = U\Sigma \tag{3.2}$$

Here, the columns of U and V are made from the respective bases, so $U \in \mathbb{R}^{m\times m}, V \in \mathbb{R}^{n\times n}$, and $\Sigma \in \mathbb{R}^{m\times n}$ is a diagonal $n \times n$ matrix with the σ_i's in the first r places of the diagonal and zeroes in the rest. Solving for A we get:

$$A = U\Sigma V^t \tag{3.3}$$

Here we have used that orthogonal matrices are invertible with their transpose as the inverse. This is the famous *singular value decomposition* of A.

3.2 Finding U and V

The question is how to find U and V? To do so, consider the Gramian matrix of A:

$$A^tA = (U\Sigma V^t)^tU\Sigma V^t = V\Sigma^tU^tU\Sigma V^t = V(\Sigma^t\Sigma)V^t \tag{3.4}$$

But since Σ is diagonal, $(\Sigma^t\Sigma)$ is simply a square, diagonal matrix with $\sigma_1^2, \sigma_2^2, \ldots, \sigma_r^2$ in the first r entries of the diagonal and zeroes for the rest. We know that A^tA is symmetric and hence diagonalizable. It is also positive semidefinite and so has non-negative eigenvalues. So we can find use normalized eigenvectors as columns of V and determine the singular values as the square roots of the non-zero eigenvalues.

Similarly, consider AA^t:

$$AA^t = U\Sigma V^t(U\Sigma V^t)^t = U\Sigma V^tV\Sigma^tU^t = U(\Sigma\Sigma^t)U^t \tag{3.5}$$

This is also symmetric and positive semi-definite. Again, $\Sigma\Sigma^t$ is square, this time $m \times m$. It still has the squares of singular values in the diagonal and zeroes for the rest. Now normalized eigenvectors can be used as columns of U.

4 Orthogonal projection

Let U be a subspace of $\mathbb{R}^n$ spanned by the linearly independent set of vectors $a_1, a_2, \ldots, a_m$. Given a $x \in \mathbb{R}^n$, we wish to find a vector u in U, such that $e = x - u$ is orthogonal to U. That means it should be orthogonal to all a_i's:

$$\forall i: \; a_i^t(x-u) = 0 \tag{4.1}$$

This can be expressed in matrix form by collecting all the a_i's into a $n \times m$ matrix A:

$$A = \begin{pmatrix} | & | & \cdots & | \\ a_1 & a_2 & \cdots & a_m \\ | & | & \cdots & | \end{pmatrix} \tag{4.2}$$

Then we may write:

$$A^t(x - u) = 0 \tag{4.3}$$

Since $u \in U$, it can be written as a linear combination of a_i's, so $u = A\beta$. We want to solve for the coefficient vector β:

$$A^t(x - A\beta) = 0 \Leftrightarrow A^t x = A^t A\beta \tag{4.4}$$

Since the a_i's are linearly independent, $A^t A$ is invertible, so:

$$\beta = (A^t A)^{-1} A^t x \tag{4.5}$$

The actual vector is then $A\beta = A(A^t A)^{-1} A^t x$. Which means that the projection operator $p_U : \mathbb{R}^n \to U$ is linear with the corresponding matrix being $P_U = A(A^t A)^{-1} A^t$.

Theorem 4.1. *The matrix P_U is symmetric and idempotent.*

Proof. Both follow directly from the formula $P_U = A(A^t A)^{-1} A^t$:

- Symmetry: $P_U^t = (A(A^t A)^{-1} A^t)^t = A\left[(A^t A)^{-1}\right]^t A^t$. But since the transpose of an inverse is the inverse of a transpose, and $A^t A$ is symmetric by theorem 1.1 we have $\left[(A^t A)^{-1}\right]^t = \left[(A^t A)^t\right]^{-1} = (A^t A)^{-1}$. Hence $P_U^t = A(A^t A)^{-1} A^t = P_U$.

- Idempotency: $P_U^2 = (A(A^t A)^{-1} A^t)^2 = A(A^t A)^{-1} A^t A(A^t A)^{-1} A^t = A(A^t A)^{-1} A^t = P_U$.

$\square$

5 Generalized inverses

For an invertible matrix A, it's obviously true that:

$$AA^{-1}A = A \tag{5.1}$$

If A is not invertible, we may still define a *generalized inverse* A^g as a matrix that satisfies the same equation:

$$AA^g A = A \tag{5.2}$$

If A^g further satisfies:

$$A^g A A^g = A^g, \tag{5.3}$$

it is called a *reflexive generalized inverse*.

5.1 Left inverses

If $A \in \mathbb{R}^{m\times n}$ has rank n, then the null space is trivial, and hence the corresponding linear transformation is injective. This means that the equation $Ax = b$ may or may not have a solution, but if it exists, it's unique. The matrix A^tA has rank n as well, and hence is invertible. This can be used to construct a left inverse:

$$A_L^{-1} = (A^tA)^{-1}A^t, \qquad A_L^{-1}A = (A^tA)^{-1}A^tA = I_n \tag{5.4}$$

But we already know from the last section that A_L^{-1} is the projection operator unto the image space of A. This means that $A^{-1}b$ is the vector in the image space that is closest to b.

5.1.1 Example

Consider the equation:

$$\begin{pmatrix}3\\4\end{pmatrix} x = \begin{pmatrix}7\\1\end{pmatrix} \tag{5.5}$$

Here x is a 1 by 1 matrix (or simply a real number). It is immediately clear, that this equation has no solutions. The situation is visualized in figure 2: The point $\begin{pmatrix}7\\1\end{pmatrix}$ clearly does not lie on the line traced by $\begin{pmatrix}3\\4\end{pmatrix}$

Using the general notation, here $A = \begin{pmatrix}3\\4\end{pmatrix} \in \mathbb{R}^{2\times 1}$ has rank 1, and so a left inverse can be found:

$$A_L^{-1} = (A^tA)^{-1}A^t = \left(\begin{pmatrix}3 & 4\end{pmatrix}\begin{pmatrix}3\\4\end{pmatrix}\right)^{-1}\begin{pmatrix}3 & 4\end{pmatrix} = \frac{1}{25}\begin{pmatrix}3 & 4\end{pmatrix} \tag{5.6}$$

The best approximation to a solution is then:

$$x = A_L^{-1}b = \frac{1}{25}\begin{pmatrix}3 & 4\end{pmatrix}\begin{pmatrix}7\\1\end{pmatrix} = \frac{21+4}{25} = 1 \tag{5.7}$$

5.2 Right inverses

Similarly, if $A \in \mathbb{R}^{m\times n}$ has rank m, then the image space is all of $\mathbb{R}^m$, and hence the corresponding linear transformation is surjective. This means that the equation $Ax = b$ always has a solution, and it may have infinitely many. The matrix AA^t has rank m as well, and hence is invertible. Analogously, we can use this to construct a right inverse:

$$A_R^{-1} = A^t(AA^t)^{-1}, \qquad AA_R^{-1} = AA^t(AA^t)^{-1} = I_m \tag{5.8}$$

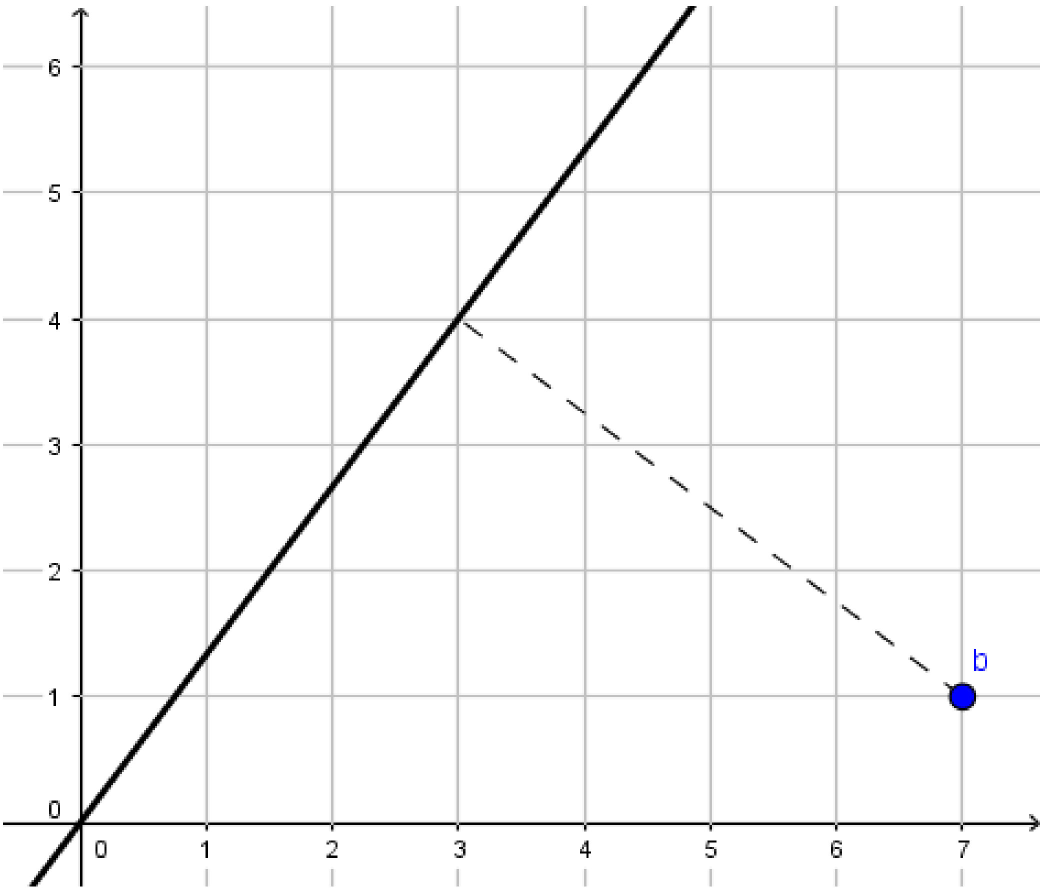

Figure 2: The geometry of equation 5.5

Both of of these inverses (when they exist) satisfies equation 5.2. They also satisfy 5.3. For instance:

$$A_L^{-1}AA_L^{-1} = (A^tA)^{-1}A^tA(A^tA)^{-1}A^t = (A^tA)^{-1}A^t = A_L^{-1} \tag{5.9}$$

So both are reflexive, generalized inverses.

6 The Moore-Penrose pseudoinverse

The *Moore-Penrose pseudoinverse* or simply the pseudoinverse of a real matrix A is the reflexive, generalized inverse A^+ which also satisfies:

$$(AA^+)^t = AA^+, \qquad (A^+A)^t = A^+A \tag{6.1}$$

In other words, for which AA^+ and A^+A are symmetrical.

6.1 Uniqueness

If such a pseudoinverse exists, it is unique (hence our use of definite article above). To show this, let B_1 and B_2 be pseudoinverses of A. Then:

$$AB_1 = (AB_1)^t = B_1^tA^t = B_1^t(AB_2A)^t = B_1^tA^tB_2^tA^t = \tag{6.2}$$

$$(AB_1)^t(AB_2)^t = AB_1AB_2 = AB_2 \tag{6.3}$$

Similarly:

$$B_1A = (B_1A)^t = A^tB_1^t = (AB_2A)^tB_1^t = A^tB_2^tA^tB_1^t = \tag{6.4}$$

$$(B_2A)^t(B_1A)^t = B_2AB_1A = B_2A \tag{6.5}$$

But then:

$$B_1 = B_1AB_1 = B_2AB_1 = B_2AB_2 = B_2 \tag{6.6}$$

6.2 Intuition behind the pseudoinverse

The idea behind the pseudoinverse is similar to the one used in singular value decomposition: The dimension of the column and row spaces of a matrix $A \in \mathbb{R}^{m\times n}$ have the same dimension, r. So if $y \in \mathbb{R}^m$ is in the column space, there is exactly one vector $x \in \mathbb{R}^n$ so that $Ax = y$. However, for y in the left null space, we're in trouble. But what if we just send these these vectors to the zero vector? This corresponds to projecting onto the column space.