Contents

Part I

Introducing the SVD

Chapter 1

The Fundamental Theorem of Linear Algebra

The Fundamental Theorem of Linear Algebra and the singular value decompositionare cornerstones in the study of linear algebra.

1.1 Theorem Statement

Given a matrix of numbers $\mathbf{A}$ with m rows and n columns. Perhaps some entries are complex numbers. This matrix $\mathbf{A} \in \mathbb{C}^{m\times n}$

In spaces with finite dimension

$$\begin{array}{ccccc} \mathbb{C}^n & = & \mathcal{R}\left(\mathbf{A}^*\right) & \oplus & \mathcal{N}\left(\mathbf{A}\right) \\ \mathbb{C}^m & = & \mathcal{R}\left(\mathbf{A}\right) & \oplus & \mathcal{N}\left(\mathbf{A}^*\right) \end{array}$$

1.2 Sample resolutions

Gaussian elimination is a foundation topic in linear algebra and is treated with skill and detail in Meyer, Strang and Laub. The point of this section is to refresh the memory and to make the process less abstract and more definitive.

We examine three types of matrices through example. The first type has both row and column rank deficiencies. The second has full column rank and a row rank deficiency. (Notice that the transpose of this matrix has full row rank and column rank deficiency.) The third example is a square matrix with full rank. The examples typify the different types of subspace decompositions.

Table 1.1. *Range and null spacedecompositions of the sample matrices. Knowing the matrix dimensions and the rank we can state the forms of the decomposition in the four fundamental subspaces.*

	matrix	matrix rank	$\mathcal{R}(\mathbf{A})$	$\mathcal{N}(\mathbf{A}^*)$	$\mathcal{R}(\mathbf{A}^*)$	$\mathcal{N}(\mathbf{A})$
(a)	$\begin{bmatrix} 1 & -1 \\ -1 & 1 \\ 1 & -1 \end{bmatrix}$	$\rho = 1$	$\text{sp}\left\{ \begin{bmatrix} \star \\ \star \\ \star \end{bmatrix} \right\}$	$\text{sp}\left\{ \begin{bmatrix} \star \\ \star \\ \star \end{bmatrix}, \begin{bmatrix} \star \\ \star \\ \star \end{bmatrix} \right\}$	$\text{sp}\left\{ \begin{bmatrix} \star \\ \star \end{bmatrix} \right\}$	$\text{sp}\left\{ \begin{bmatrix} \star \\ \star \end{bmatrix} \right\}$
(b)	$\frac{1}{4}\begin{bmatrix} 0 & 1 \\ 3 & 2 \\ 0 & 2 \end{bmatrix}$	$\rho = 2$	$\text{sp}\left\{ \begin{bmatrix} \star \\ \star \\ \star \end{bmatrix}, \begin{bmatrix} \star \\ \star \\ \star \end{bmatrix} \right\}$	$\text{sp}\left\{ \begin{bmatrix} \star \\ \star \\ \star \end{bmatrix} \right\}$	$\text{sp}\left\{ \begin{bmatrix} \star \\ \star \end{bmatrix}, \begin{bmatrix} \star \\ \star \end{bmatrix} \right\}$	$\left\{ \begin{bmatrix} 0 \\ 0 \end{bmatrix} \right\}$
(c)	$\begin{bmatrix} 1 & 2 \\ -1 & 2 \end{bmatrix}$	$\rho = 2$	$\text{sp}\left\{ \begin{bmatrix} \star \\ \star \end{bmatrix}, \begin{bmatrix} \star \\ \star \end{bmatrix} \right\}$	$\left\{ \begin{bmatrix} 0 \\ 0 \end{bmatrix} \right\}$	$\text{sp}\left\{ \begin{bmatrix} \star \\ \star \end{bmatrix}, \begin{bmatrix} \star \\ \star \end{bmatrix} \right\}$	$\left\{ \begin{bmatrix} 0 \\ 0 \end{bmatrix} \right\}$

1.2.1 Example matrix (a) both null spaces are nontrivial

The initial example is a matrix which has both row and column rank deficiency. The first the column space is to reduce the matrix $\mathbf{A}$ to the row echelon form $\mathbf{E}$. The matrix is

$$\mathbf{A} = \left[\begin{array}{rr} 1 & -1 \\ -1 & 1 \\ 1 & -1 \end{array} \right]. \tag{1.1}$$

This matrix takes a $2-$vector and returns a $3-$vector. Notice that the second column is the negative of the first column. By inspection we see there is one linearly independent column and therefore this is a rank one matrix. The image of this matrix is the line through the origin and the point $(1, -1, 1)^{\mathrm{T}}$.

With one linearly independent column, the rank of the matrix is one. The rank plus nullity theorem tells us that the sum of the rank of the nullity is three, the dimension of the space $\mathbb{C}^3$.

$$\mathbb{C}^3 : \operatorname{rank}(\mathbf{A}) + \dim(\operatorname{nullity}(\mathbf{A})) = {\color{blue}1} + {\color{red}2} = 3. \tag{1.2}$$

This implies that the range will have dimension one and the null space will have have dimension two:

$$\mathbb{C}^3 = \underbrace{\operatorname{sp}\left\{ {\color{blue}\left[\begin{array}{c} \star \\ \star \\ \star \end{array} \right]} \right\}}_{\text{range}} \oplus \underbrace{\operatorname{sp}\left\{ {\color{red}\left[\begin{array}{c} \star \\ \star \\ \star \end{array} \right]}, {\color{red}\left[\begin{array}{c} \star \\ \star \\ \star \end{array} \right]} \right\}}_{\text{null space}}. \tag{1.3}$$

Similarly, for the transpose matrix, we see again that there is only one linearly independent column vector and the image of the transpose matrix is the line through the origin and the point $(1, -1)^{\mathrm{T}}$. Again the rank of the matrix is one. For the row space the range will have dimension one and the null space will have have dimension two:

$$\mathbb{C}^2 : \operatorname{rank}(\mathbf{A}) + \dim(\operatorname{nullity}(\mathbf{A})) = {\color{blue}1} + {\color{red}1} = 2. \tag{1.4}$$

$$\mathbb{C}^2 = \underbrace{\operatorname{sp}\left\{ {\color{blue}\left[\begin{array}{c} \star \\ \star \end{array} \right]} \right\}}_{\text{range}} \oplus \underbrace{\operatorname{sp}\left\{ {\color{red}\left[\begin{array}{c} \star \\ \star \end{array} \right]} \right\}}_{\text{null space}} \tag{1.5}$$

For instructional purpose, proceed with the reductions to row echelon form. The pivot elements are boxed. The matrix reduces to the following:

$$\mathbf{R} \left[\begin{array}{c|c} \mathbf{A} & \mathbf{I}_3 \end{array} \right] = \left[\begin{array}{c|c} \mathbf{E} & \mathbf{R} \end{array} \right]$$

$$\left[\begin{array}{rrr} 1 & 0 & 0 \\ 1 & 1 & 0 \\ -1 & 0 & 1 \end{array} \right] \left[\begin{array}{rr|rrr} 1 & -1 & 1 & 0 & 0 \\ -1 & 1 & 0 & 1 & 0 \\ 1 & -1 & 0 & 0 & 1 \end{array} \right] = \left[\begin{array}{rr|rrr} \boxed{1} & -1 & 1 & 0 & 0 \\ \hline 0 & 0 & {\color{red}1} & {\color{red}1} & {\color{red}0} \\ 0 & 0 & {\color{red}-1} & {\color{red}0} & {\color{red}1} \end{array} \right] \tag{1.6}$$

The range of the matrix $\mathbf{A}$ is given by the basic columns of $\mathbf{A}$. Since there is but one pivot there is but one basic column:

$$\mathcal{R}\left(\mathbf{A}\right) = \text{sp}\left\{ \left[\begin{array}{r} 1 \\ -1 \\ 1 \end{array} \right] \right\}. \tag{1.7}$$

The null space vectors are associated with the zero pivots in the reduced matrix $\mathbf{E}$. These and subsequent null space vectors are shaded red. The null space vectors span the null space:

$$\mathcal{N}\left(\mathbf{A}^{*}\right) = \text{sp}\left\{ \left[\begin{array}{r} 1 \\ 1 \\ 0 \end{array} \right], \left[\begin{array}{r} -1 \\ 0 \\ 1 \end{array} \right] \right\}. \tag{1.8}$$

Recall that these are the null space vectors for the transpose matrix. For example,

$$\left[\begin{array}{rrr} 1 & -1 & 1 \\ -1 & 1 & -1 \end{array} \right] \left[\begin{array}{r} 1 \\ 1 \\ 0 \end{array} \right] = \left[\begin{array}{r} 0 \\ 0 \end{array} \right] = \mathbf{0}. \tag{1.9}$$

The codomain, or range or image space or column space, then is resolved as

$$\begin{aligned} \mathbb{C}^{3} &= \mathcal{R}\left(\mathbf{A}\right) \oplus \mathcal{N}\left(\mathbf{A}^{*}\right) \\ &= \text{sp}\left\{ \left[\begin{array}{r} 1 \\ -1 \\ 1 \end{array} \right] \right\} \oplus \text{sp}\left\{ \left[\begin{array}{r} 1 \\ 1 \\ 0 \end{array} \right], \left[\begin{array}{r} -1 \\ 0 \\ 1 \end{array} \right] \right\}. \end{aligned} \tag{1.10}$$

To resolve the row space, resolve the column space of the transpose matrix.

$$\begin{gathered} \mathbf{R} \left[\begin{array}{c|c} \mathbf{A}^{*} & \mathbf{I}_{2} \end{array} \right] = \left[\begin{array}{c|c} \mathbf{E} & \mathbf{R} \end{array} \right] \\ \left[\begin{array}{rr} 1 & 0 \\ 1 & 1 \end{array} \right] \left[\begin{array}{rrr|rr} 1 & -1 & 1 & 1 & 0 \\ -1 & 1 & -1 & 0 & 1 \end{array} \right] = \left[\begin{array}{rrr|rr} \boxed{1} & -1 & 1 & 1 & 0 \\ \hline 0 & 0 & 0 & 1 & 1 \end{array} \right] \end{gathered} \tag{1.11}$$

The range of the matrix $\mathbf{A}^{*}$ is given by the basic columns of $\mathbf{A}^{*}$. Again there is a single pivot and one basic column:

$$\mathcal{R}\left(\mathbf{A}^{*}\right) = \text{sp}\left\{ \left[\begin{array}{r} 1 \\ -1 \end{array} \right] \right\}. \tag{1.12}$$

The null space vector is associated with the zero pivot in the reduced matrix $\mathbf{E}$, and is the shaded vector:

$$\mathcal{N}\left(\mathbf{A}\right) = \text{sp}\left\{ \left[\begin{array}{r} 1 \\ 1 \end{array} \right] \right\}. \tag{1.13}$$

The codomain, or range or image space or column space, then is resolved as

$$\begin{aligned}\mathbb{C}^2 &= \quad \mathcal{R}\left(\mathbf{A}\right) \quad \oplus \quad \mathcal{N}\left(\mathbf{A}^*\right) \\ &= \operatorname{sp}\left\{\left[\begin{array}{r} 1 \\ -1 \end{array}\right]\right\} \oplus \operatorname{sp}\left\{\left[\begin{array}{r} 1 \\ 1 \end{array}\right]\right\}.\end{aligned} \tag{1.14}$$

1.2.2 (b) Row rank deficiency: overdetermined systems

The next example matrix $\mathbf{A} \in \mathbb{R}^{3\times 2}$ has full column rank, but has a row rank deficiency. We know this matrix must have a column rank deficiency by inspecting the matrix dimensions: $m < n$. There are fewer columns than rows and we cannot have a case of full row rank. The matrix is given by

$$\mathbf{A} = \frac{1}{4}\left[\begin{array}{cc} 0 & 1 \\ 3 & 2 \\ 0 & 2 \end{array}\right]. \tag{1.15}$$

This matrix takes a $2-$vector and returns a $3-$vector.

The host space is $\mathbb{C}^3$. With two linearly independent columns the rank of the matrix is two. Using the rank plus nullity theorem we see that the nullity is one.

$$\mathbb{C}^3 : \operatorname{rank}\left(\mathbf{A}\right) + \dim\left(\operatorname{nullity}\left(\mathbf{A}\right)\right) = 2 + 1 = 3. \tag{1.16}$$

This implies that the range will have dimension two and the null space will have have dimension two:

$$\mathbb{C}^3 = \underbrace{\operatorname{sp}\left\{\left[\begin{array}{c} \star \\ \star \\ \star \end{array}\right], \left[\begin{array}{c} \star \\ \star \\ \star \end{array}\right]\right\}}_{\text{range}} \oplus \underbrace{\operatorname{sp}\left\{\left[\begin{array}{c} \star \\ \star \\ \star \end{array}\right]\right\}}_{\text{null space}}. \tag{1.17}$$

Similarly, for the transpose matrix, we see again that there is only one linearly independent column vector and the image of the transpose matrix is the line through the origin and the point $(1, -1)^{\mathrm{T}}$. Again the rank of the matrix is one. For the row space the range will have dimension one and the null space will have have dimension two:

$$\mathbb{C}^2 : \operatorname{rank}\left(\mathbf{A}\right) + \dim\left(\operatorname{nullity}\left(\mathbf{A}\right)\right) = 2 + 0 = 2. \tag{1.18}$$

$$\mathbb{C}^2 = \underbrace{\operatorname{sp}\left\{\left[\begin{array}{c} \star \\ \star \end{array}\right], \left[\begin{array}{c} \star \\ \star \end{array}\right]\right\}}_{\text{range}} \tag{1.19}$$

The first step in the reduction is to alter the order of the rows by interchanging the first and second rows:

$$\mathbf{P\,A} = \left[\begin{array}{ccc} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 1 \end{array}\right] \frac{1}{4}\left[\begin{array}{cc} 0 & 1 \\ 3 & 2 \\ 0 & 2 \end{array}\right] = \frac{1}{4}\left[\begin{array}{cc} 3 & 2 \\ 0 & 1 \\ 0 & 2 \end{array}\right] \tag{1.20}$$

The reduction is now immediate. By inspection we see that it is equivalent to a reduced form

$$
\begin{gathered}
\mathbf{R}\left[\begin{array}{c|c}\mathbf{PA} & \mathbf{PI}_3\end{array}\right] = \left[\begin{array}{c|c}\mathbf{E} & \mathbf{R}\end{array}\right] \\
\frac{1}{4}\left[\begin{array}{rrr} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & -2 & 1 \end{array}\right]\left[\begin{array}{cc|ccc} 3 & 2 & 0 & 1 & 0 \\ 0 & 1 & 1 & 0 & 0 \\ 0 & 2 & 0 & 0 & 1 \end{array}\right] = \frac{1}{4}\left[\begin{array}{cc|ccc} \boxed{3} & 2 & 1 & 0 & 0 \\ 0 & \boxed{1} & 0 & 1 & 0 \\ \hline 0 & 0 & -2 & 0 & 1 \end{array}\right]
\end{gathered} \tag{1.21}
$$

The codomain is resolved as

$$
\begin{aligned}
\mathbb{C}^3 &= \quad \mathcal{R}\left(\mathbf{A}\right) \quad \oplus \quad \mathcal{N}\left(\mathbf{A}^*\right) \\
&= \text{sp}\left\{ \frac{1}{4}\left[\begin{array}{c} 0 \\ 3 \\ 0 \end{array}\right], \frac{1}{4}\left[\begin{array}{c} 1 \\ 2 \\ 2 \end{array}\right] \right\} \oplus \text{sp}\left\{ \left[\begin{array}{r} -2 \\ 0 \\ 1 \end{array}\right] \right\}.
\end{aligned} \tag{1.22}
$$

Onto the row space. Again we resolve the column space of the Hermitian conjugate matrix. More specifically, the equivalent form in equation (1.23):

$$
\frac{1}{4}\left[\begin{array}{ccc} 0 & 3 & 0 \\ 1 & 2 & 2 \end{array}\right] \sim \frac{1}{4}\left[\begin{array}{ccc} \boxed{1} & 2 & 2 \\ 0 & \boxed{3} & 0 \end{array}\right]. \tag{1.23}
$$

There are two nonzero pivots and therefore the first two columns of the matrix $\mathbf{A}^*$ are basic. These columns define the span of the range of $\mathbf{A}^*$:

$$
\mathcal{R}\left(\mathbf{A}\right) = \text{sp}\left\{ \frac{1}{4}\left[\begin{array}{c} 0 \\ 1 \end{array}\right], \frac{1}{4}\left[\begin{array}{c} 3 \\ 2 \end{array}\right] \right\}. \tag{1.24}
$$

Using the rank plus nullity theorem, we see that the null space must be trivial. That is

$$
\mathcal{N}\left(\mathbf{A}^*\right) = \left\{ \left[\begin{array}{c} 0 \\ 0 \end{array}\right] \right\} = \{\mathbf{0}\}. \tag{1.25}
$$

The space $\mathbb{C}^2$ will be spanned by two linearly independent 2−vectors and the span of the $\mathcal{R}\left(\mathbf{A}^*\right)$ has two linearly independent vectors.

$$
\begin{aligned}
\mathbb{C}^2 &= \quad \mathcal{R}\left(\mathbf{A}\right) \quad \oplus \quad \mathcal{N}\left(\mathbf{A}^*\right) \\
&= \text{sp}\left\{ \frac{1}{4}\left[\begin{array}{c} 0 \\ 1 \end{array}\right], \frac{1}{4}\left[\begin{array}{c} 3 \\ 2 \end{array}\right] \right\}.
\end{aligned} \tag{1.26}
$$

All four fundamental spaces are resolved and we see that $\mathbf{A} \in \mathbb{C}_2^{2\times 3}$.

Table 1.2. *Composition of the fundamental subspaces of a matrix* $\boldsymbol{A} \in \mathbb{C}_{\rho}^{m \times n}$.

the span of ...	is comprised of ...	using ...
$\mathcal{R}(\mathbf{A})$	the basic columns of $\mathbf{A}$	$m-$vectors
$\mathcal{N}(\mathbf{A}^*)$	the last $m-\rho$ rows of $\mathbf{R}$	$m-$vectors
$\mathcal{R}(\mathbf{A}^*)$	the nonzero rows of $\mathbf{U}$	$n-$vectors
$\mathcal{N}(\mathbf{A})$	the solution vectors in $\mathbf{A}x=0$	$n-$vectors

Chapter 2

SVD *Ex Nihilo*

The previous chapter starts with the Fundamental Theorem of Linear Algebra and it's subspace decomposition. Then it explores how the domain and codomain are connected. This brings up the alignment of the spaces and scale factors. The goal of this chapter is to look at the singular value decompositions of the example matrices and show that they provide the missing alignment and scaling information. The issue of how to compute a singular value decomposition is deferred until the next chapter. Here, the SVDs appear *ex nihilo* and the focus is on how this takes us beyond the Fundamental Theorem of Linear Algebra.

2.1 SVD vs. FTOLA

2.1.1 Extending the Fundamental Theorem

The first order of business is to present the singular value decompositions in table (2.1). The decomposition takes the form

$$\begin{array}{ccccc} \mathbf{A} & = & \mathbf{U} & \Sigma & \mathbf{V}^{*} \\ [m \times n] & & [m \times m] & [m \times n] & [m \times n] \\ & & \text{column space} & \text{scale factors} & \text{row space} \end{array}$$

The domain matrices $\mathbf{U}$ and $\mathbf{V}$ are unitary and they serve to align the row and column spaces. The Σ matrix contains the factors which describe the relative scale of the row and column spaces. We can think of the domain matrices in terms of column vectors

$$\begin{aligned} \mathbf{U} &= \left[\begin{array}{ccc|ccc} {\color{blue}u_1} & {\color{blue}\dots} & {\color{blue}u_\rho} & {\color{red}u_{\rho+1}} & {\color{red}\dots} & {\color{red}u_m} \end{array} \right] \\ \mathbf{V} &= \left[\begin{array}{ccc|ccc} {\color{blue}v_1} & {\color{blue}\dots} & {\color{blue}v_\rho} & {\color{red}v_{\rho+1}} & {\color{red}\dots} & {\color{red}v_n} \end{array} \right] \end{aligned} \tag{2.1}$$

The connection to the Fundamental Theorem of Linear Algebra is direct. For the *column* space we have

$$
\begin{aligned}
\mathcal{R}\left(\mathbf{A}\right) &= \text{sp}\left\{u_1, \ldots, u_\rho\right\}, \\
\mathcal{N}\left(\mathbf{A}^*\right) &= \text{sp}\left\{u_{\rho+1}, \ldots, u_m\right\}.
\end{aligned}
\tag{2.2}
$$

The rank of the matrix $\mathbf{A}$ is ρ and the dimension of the nullity of $\mathbf{A}$ is $m - \rho$. For the *row* space we have

$$
\begin{aligned}
\mathcal{R}\left(\mathbf{A}^*\right) &= \text{sp}\left\{v_1, \ldots, v_\rho\right\}, \\
\mathcal{N}\left(\mathbf{A}\right) &= \text{sp}\left\{v_{\rho+1}, \ldots, v_n\right\}.
\end{aligned}
\tag{2.3}
$$

The rank of the matrix $\mathbf{A}^*$ is ρ and the dimension of the nullity of $\mathbf{A}^*$ is $n - \rho$.

We now have new information beyond the Fundamental Theorem of Linear Algebra with the alignment and scale factors. The Fundamental Theorem dictates that

1. Every vector in $\mathcal{R}\left(\mathbf{A}\right)$ is orthogonal to every vector in $\mathcal{N}\left(\mathbf{A}^*\right)$.
2. Every vector in $\mathcal{R}\left(\mathbf{A}^*\right)$ is orthogonal to every vector in $\mathcal{N}\left(\mathbf{A}\right)$.

But now have an orthonormal basis for the row and column spaces. In addition to the above two properties we gain the following

1. For $\mathcal{R}\left(\mathbf{A}\right)$, $u_j \cdot u_k = \delta_{jk}, \quad j, k \in 1, \ldots, \rho$
2. For $\mathcal{N}\left(\mathbf{A}^*\right)$, $u_j \cdot u_k = \delta_{jk}, \quad j, k \in \rho + 1, \ldots, m$
3. For $\mathcal{R}\left(\mathbf{A}^*\right)$, $v_j \cdot v_k = \delta_{jk}, \quad j, k \in 1, \ldots, \rho$
4. For $\mathcal{N}\left(\mathbf{A}\right)$, $v_j \cdot v_k = \delta_{jk}, \quad j, k \in \rho + 1, \ldots, n$

The resolution of the subspaces into orthonormal bases makes the SVD a very powerful numerical tool.

Taken together, tables (2.2) and (2.1) show the singular value decomposition and spans for the four fundamental subspaces in terms of the column vectors of the domain matrices.

Table 2.1. *Dimension, rank and subspace decomposition.*

$$
\begin{array}{cccccc}
 & \mathbf{A} & = & \mathbf{U} & \Sigma & \mathbf{V}^* \\
\hline
\mathbb{C}_1^{3\times 2} & \left[\begin{array}{rr} 1 & -1 \\ -1 & 1 \\ 1 & -1 \end{array}\right] & = & \left[\begin{array}{ccc} \frac{1}{\sqrt{3}} & 0 & \frac{2}{\sqrt{6}} \\ -\frac{1}{\sqrt{3}} & \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{6}} \\ \frac{1}{\sqrt{3}} & \frac{1}{\sqrt{2}} & -\frac{1}{\sqrt{6}} \end{array}\right] & \left[\begin{array}{c|c} \sqrt{6} & 0 \\ \hline 0 & 0 \\ 0 & 0 \end{array}\right] & \frac{1}{\sqrt{2}}\left[\begin{array}{rr} 1 & -1 \\ 1 & 1 \end{array}\right] \\
\mathbb{C}_2^{3\times 2} & \frac{1}{4}\left[\begin{array}{cc} 0 & 1 \\ 3 & 2 \\ 0 & 2 \end{array}\right] & = & \left[\begin{array}{ccc} \frac{1}{\sqrt{30}} & \frac{1}{\sqrt{6}} & -\frac{2}{\sqrt{5}} \\ \frac{5}{\sqrt{30}} & -\frac{1}{\sqrt{6}} & 0 \\ \frac{2}{\sqrt{30}} & \frac{2}{\sqrt{6}} & \frac{1}{\sqrt{5}} \end{array}\right] & \frac{1}{4}\left[\begin{array}{cc} \sqrt{15} & 0 \\ 0 & \sqrt{3} \\ \hline 0 & 0 \end{array}\right] & \frac{1}{\sqrt{2}}\left[\begin{array}{rr} 1 & 1 \\ -1 & 1 \end{array}\right] \\
\mathbb{C}_2^{2\times 2} & \left[\begin{array}{rr} 1 & 2 \\ -1 & 2 \end{array}\right] & = & \frac{1}{\sqrt{2}}\left[\begin{array}{rr} 1 & 1 \\ 1 & -1 \end{array}\right] & \sqrt{2}\left[\begin{array}{cc} 2 & 0 \\ 0 & 1 \end{array}\right] & \frac{1}{\sqrt{2}}\left[\begin{array}{cc} 0 & 1 \\ 1 & 0 \end{array}\right]
\end{array}
$$

Table 2.2. *The column vectors of the subspaces of the domain matrices* $\mathbf{U}$ *and* $\boldsymbol{V}$ *form an orthonormal span for the four fundamental subspaces.*

	matrix	$\mathcal{R}(\mathbf{A})$	$\mathcal{N}(\mathbf{A}^*)$	$\mathcal{R}(\mathbf{A}^*)$	$\mathcal{N}(\mathbf{A})$
$\mathbb{C}_1^{3\times 2}$	$\left[\begin{array}{rr} 1 & -1 \\ -1 & 1 \\ 1 & -1 \end{array}\right]$	$\text{sp}\left\{\frac{1}{\sqrt{3}}\left[\begin{array}{r} 1 \\ -1 \\ 1 \end{array}\right]\right\}$	$\text{sp}\left\{\frac{1}{\sqrt{2}}\left[\begin{array}{r} 0 \\ 1 \\ 1 \end{array}\right], \frac{1}{\sqrt{6}}\left[\begin{array}{r} 2 \\ 0 \\ -1 \end{array}\right]\right\}$	$\text{sp}\left\{\frac{1}{\sqrt{2}}\left[\begin{array}{r} 1 \\ -1 \end{array}\right]\right\}$	$\text{sp}\left\{\frac{1}{\sqrt{2}}\left[\begin{array}{r} 1 \\ 1 \end{array}\right]\right\}$
$\mathbb{C}_2^{3\times 2}$	$\frac{1}{4}\left[\begin{array}{rr} 0 & 1 \\ 3 & 2 \\ 0 & 2 \end{array}\right]$	$\text{sp}\left\{\frac{1}{\sqrt{30}}\left[\begin{array}{r} 0 \\ 3 \\ 0 \end{array}\right], \frac{1}{\sqrt{6}}\left[\begin{array}{r} 1 \\ 2 \\ 2 \end{array}\right]\right\}$	$\text{sp}\left\{\frac{1}{\sqrt{5}}\left[\begin{array}{r} -2 \\ 0 \\ 1 \end{array}\right]\right\}$	$\text{sp}\left\{\frac{1}{\sqrt{2}}\left[\begin{array}{r} 0 \\ 1 \end{array}\right], \frac{1}{\sqrt{2}}\left[\begin{array}{r} 3 \\ 2 \end{array}\right]\right\}$	$\left\{\left[\begin{array}{r} 0 \\ 0 \end{array}\right]\right\}$
$\mathbb{C}_2^{2\times 2}$	$\left[\begin{array}{rr} 1 & 2 \\ -1 & 2 \end{array}\right]$	$\text{sp}\left\{\frac{1}{\sqrt{2}}\left[\begin{array}{r} 1 \\ -1 \end{array}\right], \frac{1}{\sqrt{2}}\left[\begin{array}{r} 1 \\ 1 \end{array}\right]\right\}$	$\left\{\left[\begin{array}{r} 0 \\ 0 \end{array}\right]\right\}$	$\text{sp}\left\{\frac{1}{\sqrt{2}}\left[\begin{array}{r} 0 \\ 1 \end{array}\right], \frac{1}{\sqrt{2}}\left[\begin{array}{r} 1 \\ 0 \end{array}\right]\right\}$	$\left\{\left[\begin{array}{r} 0 \\ 0 \end{array}\right]\right\}$

2.1.2 Exemplars in block form

Explicitly separating the range and null space components in the decomposition products will prove helpful time and again.

Table 2.3. *Exemplars of the singular value decomposition of a matrix* $\boldsymbol{A} \in \mathbb{C}_{\rho}^{m\times n}$*. These four block structures describe every possible decomposition. The top row represents the most general case. Subsequent rows are special cases.*

rank and dimension			$\mathbf{U}$ codomain	Σ scale	$\mathbf{V}^{*}$ domain
$\rho \neq m \neq n$	$\mathbf{A}$	$=$	$\left[\begin{array}{c\|c} \mathbf{U}_{\mathcal{R}} & \mathbf{U}_{\mathcal{N}} \end{array}\right]$	$\left[\begin{array}{c\|c} \mathbf{S} & \mathbf{0} \\ \hline \mathbf{0} & \mathbf{0} \end{array}\right]$	$\left[\begin{array}{c} \mathbf{V}_{\mathcal{R}}^{*} \\ \hline \mathbf{V}_{\mathcal{N}}^{*} \end{array}\right]$
$\rho = m < n$	$\mathbf{A}$	$=$	$\mathbf{U}_{\mathcal{R}}$	$\left[\begin{array}{c\|c} \mathbf{S} & \mathbf{0} \end{array}\right]$	$\left[\begin{array}{c} \mathbf{V}_{\mathcal{R}}^{*} \\ \hline \mathbf{V}_{\mathcal{N}}^{*} \end{array}\right]$
$\rho = n < m$	$\mathbf{A}$	$=$	$\left[\begin{array}{c\|c} \mathbf{U}_{\mathcal{R}} & \mathbf{U}_{\mathcal{N}} \end{array}\right]$	$\left[\begin{array}{c} \mathbf{S} \\ \hline \mathbf{0} \end{array}\right]$	$\mathbf{V}_{\mathcal{R}}^{*}$
$\rho = n = m$	$\mathbf{A}$	$=$	$\mathbf{U}_{\mathcal{R}}$	$\mathbf{S}$	$\mathbf{V}_{\mathcal{R}}^{*}$

Equations (2.1), (2.3), (2.2) are precise mathematical statements which delineate the relationship between the column vectors of the domain matrices and the four fundamental subspaces. We summarize with an impressionistic view of the SVD. While in the guise of a mathematical equality it must be read a simple device reminding us of subspace representation of the vectors in the decomposition matrices:

$$\mathbf{A} = \left[\begin{array}{c|c} \mathcal{R}(\mathbf{A}) & \mathcal{N}(\mathbf{A}^{*}) \end{array}\right] \left[\begin{array}{c|c} \mathbf{S} & \mathbf{0}_{1} \\ \hline \mathbf{0}_{2} & \mathbf{0}_{3} \end{array}\right] \left[\begin{array}{c} \mathcal{R}(\mathbf{A}^{*})^{\mathrm{T}} \\ \hline \mathcal{N}(\mathbf{A})^{\mathrm{T}} \end{array}\right] \tag{2.4}$$

The column vectors $\mathbf{0}_2$ and $\mathbf{0}_3$ mask the vectors which span $\mathcal{N}(\mathbf{A}^{*})$; the row vectors in $\mathbf{0}_1$ and $\mathbf{0}_2$ mask the vectors which span $\mathcal{N}(\mathbf{A})$. In this manner the null space vectors are silenced.

Chapter 3

Computing the SVD

Chapter 4

Proofs

The noted explicator P.F. Embid remarks that ”a proof is worth an infinite number of exrcises.” The point is to motivate applied mathematicians to the value of a proof. Certainly there are proofs which provide meager insight. Yet there are many proofs which are revealing.

4.1 A constructive proof

The beauty of a constructive proof is that we ultimately end up with a method to construct the SVD.

Part II

Applications

Chapter 5

The Method of Least Squares

Consider the archetypal linear system

$$\mathbf{A}x = b \tag{5.1}$$

with $\mathbf{A} \in \mathbb{C}_m^{m\times m}$, $x \in \mathbb{C}^m$, $b \in \mathbb{C}^m$. Because the matrix is square and has full rank an inverse exists we can write the solution as

$$x = \mathbf{A}^{-1}b. \tag{5.2}$$

When the data vector b is in the range of the matrix $\mathbf{A}$ the linear system has a direct solution.

What do we do when the data vector b is not in the range of the matrix $\mathbf{A}$? In such cases there is no inverse matrix

The method of least squares is on of the most potent tools in linear algebra. There are three popular algorithms for finding the least squares solution:

1. SVD,
2. **QR** factorization,
3. normal equations.

To more fully understand the SVD solution we will also explore the the other two methods.

One delightful discovery is that the pseudoinverse arises naturally in the SVD solution.

s

5.1 The least squares problem

A crisp problem statement is a value tool when casting for solution methods. This section defines the least squares problem.

5.1.1 When least squares?

The method of least squares will provide a nontrivial solution as long as the data vector is not in the null space $\mathcal{N}\left(\mathbf{A}^*\right)$. This is the most robust and most general method to solve linear systems. There are also

Class I: Classic inverse exists

This class of linear equations is the most restrictive. The matrix $\mathbf{A}$ is square and has full rank. Therefore all data vectors lie in the range $\mathcal{R}\left(\mathbf{A}\right)$.

$$\begin{gathered}\mathbf{A}x = b \\ \left[\begin{array}{rr} 1 & 2 \\ -1 & 2 \end{array}\right]\left[\begin{array}{c} x_1 \\ x_2 \end{array}\right] = \left[\begin{array}{r} -1 \\ 1 \end{array}\right]\end{gathered} \tag{5.3}$$

Solution: Gaussian elimination.

$$\mathbf{R}\left[\begin{array}{c|c} \mathbf{A} & b \end{array}\right] = \left[\begin{array}{cc} 1 & 0 \\ 1 & 1 \end{array}\right]\left[\begin{array}{rr|r} 1 & 2 & -1 \\ -1 & 2 & 1 \end{array}\right] = \left[\begin{array}{cc|r} 1 & 2 & -1 \\ 0 & 4 & 0 \end{array}\right] \tag{5.4}$$

This implies the solution vector is

$$x = \left[\begin{array}{r} -1 \\ 0 \end{array}\right] \tag{5.5}$$

The solution using the matrix inverse is the same:

$$x = \mathbf{A}^{-1} b = \frac{1}{4}\left[\begin{array}{rr} 2 & -2 \\ 1 & 1 \end{array}\right]\left[\begin{array}{r} -1 \\ 1 \end{array}\right] = \left[\begin{array}{r} -1 \\ 0 \end{array}\right]. \tag{5.6}$$

Class II: No classic inverse, consistent system

This is the most general class of problem. The matrix is either not square or it has a rank deficit. But since it is consistent there is a solution.

$$\begin{gathered}\mathbf{A}x = b \\ \left[\begin{array}{rr} 1 & -1 \\ -1 & 1 \\ 1 & -1 \end{array}\right]\left[\begin{array}{c} x_1 \\ x_2 \end{array}\right] = \left[\begin{array}{r} 1 \\ -1 \\ 1 \end{array}\right]\end{gathered} \tag{5.7}$$

Solutions: $x = \left[\begin{array}{c} 1 \\ 0 \end{array}\right], \left[\begin{array}{r} 0 \\ -1 \end{array}\right].$

Class I: Trivial solution

$$\mathbf{A}x = b$$

$$\begin{bmatrix} 1 & -1 \\ -1 & 1 \\ 1 & -1 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \end{bmatrix} = \begin{bmatrix} 1 \\ 1 \\ 0 \end{bmatrix} \tag{5.8}$$

Solution: $x = \begin{bmatrix} 0 \\ 0 \end{bmatrix}$.

$$\mathbf{A} = \begin{bmatrix} \frac{1}{\sqrt{3}} & 0 & \frac{2}{\sqrt{6}} \\ -\frac{1}{\sqrt{3}} & \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{6}} \\ \frac{1}{\sqrt{3}} & \frac{1}{\sqrt{2}} & -\frac{1}{\sqrt{6}} \end{bmatrix} \left[\begin{array}{c|c} \sqrt{6} & 0 \\ \hline 0 & 0 \\ 0 & 0 \end{array} \right] \frac{1}{\sqrt{2}} \begin{bmatrix} 1 & -1 \\ 1 & 1 \end{bmatrix} \tag{5.9}$$

5.1.2 Forming the least squares problem

The least squares problem starts with a linear system

$$\mathbf{A}x = b \tag{5.10}$$

where the inputs are the matrix $\mathbf{A} \in \mathbb{C}_{\rho}^{m\times n}$ and the data vector $b \in \mathbb{C}^m$. The goal is to find the solution vector $x \in \mathbb{C}^n$ which solves the linear system.

$$\min_{x\in\mathbb{C}^n} \|\mathbf{A}x - b\|_2^2 \tag{5.11}$$

The focus of this work is on the *overdetermined* least squares problem where there are more measurement points than solution parameters. The system has full column rank

$$\mathbf{A} \in \mathbb{C}_n^{m\times n}, \quad m \geq n$$

$$\begin{bmatrix} \star & \star \\ \star & \star \\ \star & \star \\ \star & \star \end{bmatrix} \begin{bmatrix} \star \\ \star \end{bmatrix} = \begin{bmatrix} \star \\ \star \\ \star \\ \star \end{bmatrix} \tag{5.12}$$

5.1.3 Why least squares?

Why choose the 2−norm?

1. The norm is continuous and allows for differentiation.

2. Gauss-Markov theorem

3. The method is familiar, widely accepted and well documented.

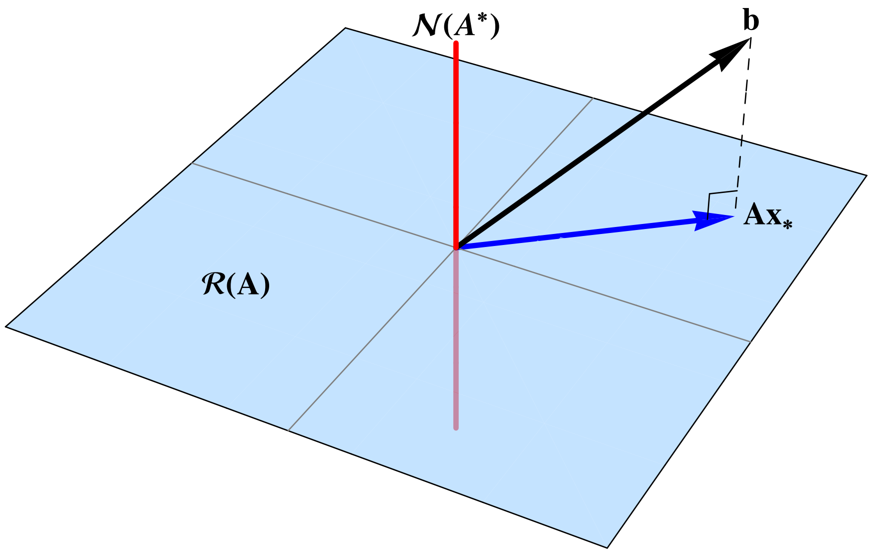

Figure 5.1. *The geometry of least squares. We see the column space resolved into a range (blue hyperplane) and an orthogonal null space (shown in red). The data vector b is not in the range space and there is no direct solution. The vector $\boldsymbol{A}x_*$ which minimizes the least squares criteria is the vector which is closest to b.*

5.2 Rudiments

Considerable insight into the method of least squares can be gleaned from toy problems. These are problems were the solution is at least discernible and perhaps manifest. In all cases the system matrix $\mathbf{A}$ does not posses an inverse. These exercises should clarify when one must turn to least squares and what the solution implies.

The first case involves a data vector b which is clearly in the column space of the matrix $\mathbf{A}$.

$$\begin{gathered}\mathbf{A}x = b\\ \left[\begin{array}{cc} 1 & 0\\ 0 & 1\\ 0 & 0\end{array}\right]\left[\begin{array}{c} x_1\\ x_2\end{array}\right] = \left[\begin{array}{c} b_1\\ b_2\\ 0\end{array}\right]\end{gathered} \tag{5.13}$$

We can use Gaussian elimination to find the answer

$$\left[\begin{array}{c} x_1\\ x_2\end{array}\right] = \left[\begin{array}{c} b_1\\ b_2\end{array}\right]. \tag{5.14}$$

This is also the least squares solution. The situation changes significantly when the data has a nonzero component in the x_3 direction.

$$\begin{gathered}\mathbf{A}x = b \\ \begin{bmatrix} 1 & 0 \\ 0 & 1 \\ 0 & 0 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \end{bmatrix} = \begin{bmatrix} b_1 \\ b_2 \\ b_3 \end{bmatrix}, \qquad b_3 \neq 0.\end{gathered} \tag{5.15}$$

There is no solution for this linear system. Yet instead of seeking an exact solution we look for the best solution x_*. How close can we get?

There are a few different ways to discern the answer. For instance, if the number b_3 was very small compared to the other two entries, then we would expect that the solution in equation (5.14) would be very close to the ideal answer. In fact, the solution (5.14) is the best that we can do in the Euclidean norm regardless of the size of b_3. That is, if we use the Pythagorean theorem to measure the distance between the data vector and the image of the solution vector

$$\|\mathbf{A}x - b\|_2^2 = \left\| \begin{bmatrix} b_1 \\ b_2 \\ 0 \end{bmatrix} - \begin{bmatrix} b_1 \\ b_2 \\ b_3 \end{bmatrix} \right\|_2^2 = b_3^2. \tag{5.16}$$

then the solution vector in (5.14) provides the least error.

$$\begin{gathered}\mathbf{A}x = b \\ \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} = \begin{bmatrix} b_1 \\ b_2 \end{bmatrix}, \qquad b_3 \neq 0.\end{gathered} \tag{5.17}$$

Now there is a null space vector.

$$\begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} = \begin{bmatrix} b_1 \\ b_2 \\ 0 \end{bmatrix} + \alpha \begin{bmatrix} 0 \\ 0 \\ 1 \end{bmatrix}, \qquad \alpha \in \mathbb{C} \tag{5.18}$$

There is an infinitude of solutions. Which one will least squares select? All solutions have the same error, and therefore are equivalent.

$$\begin{aligned}\|\mathbf{A}x - b\|_2^2 &= \left\| \mathbf{A} \left(\begin{bmatrix} b_1 \\ b_2 \\ 0 \end{bmatrix} + \alpha \begin{bmatrix} 0 \\ 0 \\ 1 \end{bmatrix} \right) - \begin{bmatrix} b_1 \\ b_2 \\ b_3 \end{bmatrix} \right\|_2^2 \\ &= \left\| \begin{bmatrix} b_1 \\ b_2 \\ 0 \end{bmatrix} - \begin{bmatrix} b_1 \\ b_2 \\ b_3 \end{bmatrix} \right\|_2^2 = b_3^2.\end{aligned} \tag{5.19}$$

The least squares algorithm will produce a particular answer, a point in parameter space, x.

5.3 Solution using SVD

The singular value decomposition is a powerful theoretical tool for studying the least squares problem. In addition to needing the decomposition products, we will need to exploit the unitary equivalence of the 2−norm, the norm of least squares.

5.3.1 Unitary transformation

The gift of unitary transformation allows us to take a difficult problem and convert into a more benign form.

Invariance of the $2-$norm

The importance of this class of transformations commands review. The 2−norm is preserved under unitary transformation. Let $\mathbf{A}$ be the obligatory rectangular matrix in $\mathbb{C}^{m\times n}$ and consider the unitary matrices $\mathbf{W} \in \mathbb{C}^{m\times m}$ and $\mathbf{Z} \in \mathbb{C}^{n\times n}$. The invariance of the 2−norm is expressed by

$$\begin{aligned} \left\|\mathbf{W}\mathbf{A}\right\|_2 &= \left\|\mathbf{A}\right\|_2 , \\ \left\|\mathbf{A}\mathbf{Z}\right\|_2 &= \left\|\mathbf{A}\right\|_2 . \end{aligned} \tag{5.20}$$

(This is also true for the Frobenius norm.)

The proof is painless. Start with the first case and use a definition for norm as the greatest dilation of vectors composing the unit ball:

$$\left\|\mathbf{W}\mathbf{A}\right\|_2^2 = \max_{\|x\|_2=1} \left\|\mathbf{W}\mathbf{A}x\right\|_2^2 . \tag{5.21}$$

Express the norm as an inner product:

$$\left\|\mathbf{W}\mathbf{A}x\right\|_2^2 = \left(\mathbf{W}\mathbf{A}x\right)^* \left(\mathbf{W}\mathbf{A}x\right) \tag{5.22}$$

In this form we can exploit the defining property of the unitary matrix:

$$\mathbf{W}^*\mathbf{W} = \mathbf{I}_m \tag{5.23}$$

because

$$\left(\mathbf{W}\mathbf{A}x\right)^* \left(\mathbf{W}\mathbf{A}x\right) = x^*\mathbf{A}^* \left(\mathbf{W}^*\mathbf{W}\right)\mathbf{A}x = \left(x^*\mathbf{A}^*\right)\left(\mathbf{A}x\right). \tag{5.24}$$

Now we go back to the norm structure

$$\left(x^*\mathbf{A}^*\right)\left(\mathbf{A}x\right) = \left\|\mathbf{A}x\right\|_2^2 \tag{5.25}$$

This demonstrates

$$\left\|\mathbf{W}\mathbf{A}\right\|_2^2 = \max_{\|x\|_2=1} \left\|\mathbf{W}\mathbf{A}x\right\|_2^2 = \max_{\|x\|_2=1} \left\|\mathbf{A}x\right\|_2^2 = \left\|\mathbf{A}\right\|_2^2 . \tag{5.26}$$

Because the norm is positive definite we can take the positive value for the square root and state

$$\left\|\mathbf{W}\mathbf{A}\right\|_2 = \left\|\mathbf{A}\right\|_2 . \tag{5.27}$$

To show the other equality

$$\left\| \mathbf{A}\,\mathbf{Z} \right\|_2 = \left\| \mathbf{A} \right\|_2 \tag{5.28}$$

the insight is to exploit the fact that

$$\left\| \mathbf{A}^* \right\|_2 = \left\| \mathbf{A} \right\|_2 \tag{5.29}$$

and work with the adjoint matrix $\left(\mathbf{A}\,\mathbf{Z}\right)^*$.

We have seen invariance of the 2−norm under unitary transformation of a matrix by premultiplication and by posmultiplication. This implies invariance under simultaneous transformation:

$$\left\| \mathbf{W}\,\mathbf{A}\,\mathbf{Z} \right\|_2 = \left\| \mathbf{W}\left(\mathbf{A}\,\mathbf{Z}\right) \right\|_2 = \left\| \mathbf{A}\,\mathbf{Z} \right\|_2 = \left\| \mathbf{A} \right\|_2 . \tag{5.30}$$

Transforming the least squares problem

For the overdetermined problem there is no null space $\color{red}{\mathcal{N}\left(\mathbf{A}\right)}$ for the domain. If $m = n$, then the there is no null space $\color{red}{\mathcal{N}\left(\mathbf{A}^*\right)}$ for the codomain either. When $m > n$, the first n columns of $\mathbf{V}$ span $\color{blue}{\mathcal{R}\left(\mathbf{A}\right)}$, the last $n - m$ columns span the null space $\color{red}{\mathcal{N}\left(\mathbf{A}^*\right)}$. The structure of the decomposition for the overdetermined system is this

$$\mathbf{A} = \left[\begin{array}{c|c} \color{blue}{\mathbf{U}_{\mathcal{R}}} & \color{red}{\mathbf{U}_{\mathcal{N}}} \end{array}\right] \left[\begin{array}{c} \mathbf{S} \\ \hline \mathbf{0} \end{array}\right] \color{blue}{\mathbf{V}_{\mathcal{R}}^*} \tag{5.31}$$

We use a unitary matrix to transform the problem into a simpler form

$$\left\| \mathbf{A}x - b \right\|_2^2 = \left\| \mathbf{U}^*\left(\mathbf{A}x - b\right) \right\|_2^2 . \tag{5.32}$$

Now we can apply the decomposition. The form of SVD that we need is this

$$\mathbf{U}^*\mathbf{A} = \Sigma\,\mathbf{V}^* . \tag{5.33}$$

The least squares problem becomes

$$\begin{aligned} \left\| \mathbf{A}x - b \right\|_2^2 = \left\| \Sigma\,\mathbf{V}^* x - \mathbf{U}^* b \right\|_2^2 &= \left\| \left[\begin{array}{c} \mathbf{S} \\ \hline \mathbf{0} \end{array}\right] \color{blue}{\mathbf{V}_{\mathcal{R}}^*} x - \left[\begin{array}{c} \color{blue}{\mathbf{U}_{\mathcal{R}}^*} \\ \hline \color{red}{\mathbf{U}_{\mathcal{N}}^*} \end{array}\right] b \right\|_2^2 \\ &= \left\| \left[\begin{array}{c} \mathbf{S}\color{blue}{\mathbf{V}_{\mathcal{R}}^*} x \\ \hline \mathbf{0} \end{array}\right] - \left[\begin{array}{c} \color{blue}{\mathbf{U}_{\mathcal{R}}^*} b \\ \hline \color{red}{\mathbf{U}_{\mathcal{N}}^*} b \end{array}\right] \right\|_2^2 \end{aligned} \tag{5.34}$$

We have now untangled the range spaces from the null space.

5.3.2 The SVD solution for least squares

We rely upon the Pythagorean theorem to separate the range and null space components of the total error for the least squares problem

$$\left\| \mathbf{A}x - b \right\|_2^2 = \underbrace{\left\| \mathbf{S}\color{blue}{\mathbf{V}_{\mathcal{R}}^*} x - \color{blue}{\mathbf{U}_{\mathcal{R}}^*} b \right\|_2^2}_{x \text{ dependence}} + \underbrace{\left\| \color{red}{\mathbf{U}_{\mathcal{N}}^*} b \right\|_2^2}_{\text{residual}} \tag{5.35}$$

There are now two terms; the first depends upon the solution vector x, the second does not. To minimize the total error we must drive the first terms to zero. Then the total error will be given by the residual term. The error term that is controlled by the solution vector x is this

$$\mathbf{S}\mathbf{V}_{\mathcal{R}}^{*}x - \mathbf{U}_{\mathcal{R}}^{*}b. \tag{5.36}$$

We choose x to force this term to zero. This leads to the SVD solution for the least squares problem:

$$x_{LS} = \mathbf{V}_{\mathcal{R}}\mathbf{S}^{-1}\mathbf{U}_{\mathcal{R}}^{*}b = \mathbf{A}^{\dagger}b. \tag{5.37}$$

This is the pseudoinverse solution where

$$\mathbf{A}^{\dagger} = \mathbf{V}_{\mathcal{R}}\mathbf{S}^{-1}\mathbf{U}_{\mathcal{R}}^{*}. \tag{5.38}$$

It is always a good idea to verify conformability by writing out the matrix dimensions:

$$\begin{array}{ccccc} x & = & \mathbf{V}_{\mathcal{R}} & \mathbf{S}^{-1} & \mathbf{U}_{\mathcal{R}}^{*} & b \\ [n \times 1] & = & [n \times \rho] & [\rho \times \rho] & [\rho \times m] & [m \times 1] \end{array}$$

What we shown is that the vector x which minimizes the least squares error in (5.11) is exactly the same vector given by the SVD solution in equation (5.37). Using a unitary transform we were able to convert the general least squares problem into a form amenable to solution using the singular value decomposition.

For the overdetermined case as we have here the usually silent null space term can be heard as it pronounces the value of the total error

$$r^2 = \|\mathbf{U}_{\mathcal{N}}^{*}b\|_2^2 = \left(\mathbf{U}_{\mathcal{N}}^{*}b\right)^{*}\left(\mathbf{U}_{\mathcal{N}}^{*}b\right) = b^{*}\left(\mathbf{U}_{\mathcal{N}}\mathbf{U}_{\mathcal{N}}^{*}\right)b \tag{5.39}$$

5.3.3 Example

Consider the linear system

$$\begin{gathered} \mathbf{A}x = b, \\ \frac{1}{4}\begin{bmatrix} 0 & 1 \\ 3 & 2 \\ 0 & 2 \end{bmatrix}\begin{bmatrix} x_1 \\ x_2 \end{bmatrix} = \begin{bmatrix} 2 \\ 1 \\ 0 \end{bmatrix}. \end{gathered} \tag{5.40}$$

The pseudoinverse is shown in equation (5.38) allowing us to compute the particular solution as

$$x_{LS} = \mathbf{A}^{\dagger}b = \frac{1}{15}\begin{bmatrix} -8 & 20 & -16 \\ 12 & 0 & 24 \end{bmatrix}\begin{bmatrix} 2 \\ 1 \\ 0 \end{bmatrix} = \frac{1}{15}\begin{bmatrix} 4 \\ 24 \end{bmatrix}. \tag{5.41}$$

Since the matrix $\mathbf{A}$ has full column rank the null space $\mathcal{N}(\mathbf{A})$ is trivial and there is no contribution from an inhomogeneous solution. Therefore we must have

$$x_{LS} \in \mathcal{R}(\mathbf{A}^*). \tag{5.42}$$

The residual error vector is given by

$$r = \mathbf{A}x - b = \frac{1}{5}\begin{bmatrix} 2 \\ 5 \\ 4 \end{bmatrix} - \begin{bmatrix} 2 \\ 1 \\ 0 \end{bmatrix} = \frac{1}{5}\begin{bmatrix} -8 \\ 0 \\ 4 \end{bmatrix}. \tag{5.43}$$

Here is an important point: the method of least squares resolves the data vector into a range component and a null space component.

$$\begin{array}{ccccc} b & = & \mathbf{A}x & - & r \\ \begin{bmatrix} 2 \\ 1 \\ 0 \end{bmatrix} & = & \underbrace{\frac{1}{5}\begin{bmatrix} 2 \\ 5 \\ 4 \end{bmatrix}}_{\mathcal{R}(\mathbf{A})} & - & \underbrace{\frac{1}{5}\begin{bmatrix} -8 \\ 0 \\ 4 \end{bmatrix}}_{\mathcal{N}(\mathbf{A}^*)} \end{array} \tag{5.44}$$

These vectors are coplanar and we will see shortly the importance of the angle between the data vector and the vector $\mathbf{A}x$ as shown in figure (5.2)

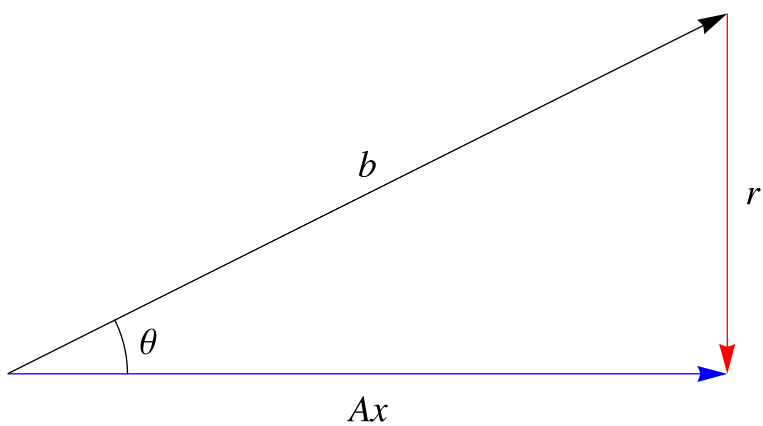

Figure 5.2. *The least squares solution is the projection of the data vector into $\mathcal{R}(\boldsymbol{A})$. The red arrow represents the residual error, the error which cannot be removed.*

The square of the norm of the residual error vector is the total error:

$$r^2 = r^{\mathrm{T}} r = \frac{16}{5}. \tag{5.45}$$

This agrees with the method of equation (5.39):

$$
\begin{aligned}
r^2 &= \|\mathbf{U}_{\mathcal{N}}^{*} b\|_2^2 = \left(b^{*}\mathbf{U}_{\mathcal{N}}\right)\left(\mathbf{U}_{\mathcal{N}}^{*} b\right) \\
&= \left(\left[\begin{array}{ccc} 2 & 1 & 0 \end{array}\right] \frac{1}{\sqrt{5}} \left[\begin{array}{r} -2 \\ 0 \\ 1 \end{array}\right]\right) \left(\frac{1}{\sqrt{5}} \left[\begin{array}{ccc} -2 & 0 & 1 \end{array}\right] \left[\begin{array}{c} 2 \\ 1 \\ 0 \end{array}\right]\right) \\
&= \frac{16}{5}.
\end{aligned}
\tag{5.46}
$$

5.4 Solution using QR factorization

The $\mathbf{QR}$ factorization is another powerful tool for solving the least squares problem. Like the SVD, the $\mathbf{QR}$ factorization resolves the column space into orthonormal basis for the range space $\mathcal{R}\left(\mathbf{A}\right)$ and orthonormal basis for the null space $\mathcal{N}\left(\mathbf{A}^{*}\right)$. However the row space is not resolved.

The QR factorization

Given a matrix $\mathbf{A} \in \mathbb{C}_{\rho}^{m\times n}$ the factorization has this form

$$
\mathbf{A} = \mathbf{Q}\,\mathbf{R} \tag{5.47}
$$

where the matrix $\mathbf{Q} \in \mathbb{C}^{m\times m}$ is unitary

$$
\mathbf{Q}^{*}\mathbf{Q} = \mathbf{I}_m \tag{5.48}
$$

and the upper triangular matrix $\mathbf{R} \in \mathbb{C}^{m\times n}$ has the same dimensions as the target matrix. We may think of the $\mathbf{Q}$ matrix as a domain matrix with the typical partition

$$
\mathbf{Q} = \left[\begin{array}{c|c} \mathbf{Q}_{\mathcal{R}} & \mathbf{Q}_{\mathcal{N}} \end{array}\right]. \tag{5.49}
$$

For $\mathbf{A} \in \mathbb{C}_2^{3\times 2}$ the factorization has the following form

$$
\left[\begin{array}{cc} \star & \star \\ \star & \star \\ \star & \star \end{array}\right] = \left[\begin{array}{cc|c} \star & \star & \star \\ \star & \star & \star \\ \star & \star & \star \end{array}\right] \left[\begin{array}{cc} \star & \star \\ 0 & \star \\ \hline 0 & 0 \end{array}\right] \tag{5.50}
$$

Transforming the least squares problem

The structure of the decomposition for the overdetermined system is this

$$
\mathbf{A} = \mathbf{Q}\,\mathbf{R} = \left[\begin{array}{c|c} \mathbf{Q}_{\mathcal{R}} & \mathbf{Q}_{\mathcal{N}} \end{array}\right] \left[\begin{array}{c} \mathsf{R} \\ \hline \mathbf{0} \end{array}\right] \tag{5.51}
$$

Again a unitary matrix transforms the problem into a simpler form

$$
\|\mathbf{A}y - b\|_2^2 = \|\mathbf{Q}^{*}\left(\mathbf{A}y - b\right)\|_2^2. \tag{5.52}
$$

with $y \in \mathbb{C}^n$. Now we can apply the factorization in the form of

$$\mathbf{Q}^* \mathbf{A} = \mathbf{R}. \tag{5.53}$$

The least squares problem becomes

$$\|\mathbf{A}y - b\|_2^2 = \|\mathbf{R}y - \mathbf{Q}^* b\|_2^2 = \left\| \begin{bmatrix} \mathsf{R}y \\ \hline \mathbf{0} \end{bmatrix} - \begin{bmatrix} \color{blue}{\mathbf{Q}^*_{\mathcal{R}}} b \\ \hline \color{red}{\mathbf{Q}^*_{\mathcal{N}}} b \end{bmatrix} \right\|_2^2 \tag{5.54}$$

The contributions of range space and the null space for the column space are now separated.

5.4.1 The QR factorization for least squares

The total error is expressed as a quadratic sum of terms using the range and null space components:

$$\|\mathbf{A}y - b\|_2^2 = \underbrace{\|\mathsf{R}y - \color{blue}{\mathbf{Q}^*_{\mathcal{R}}} b\|_2^2}_{y \text{ dependence}} + \underbrace{\|\color{red}{\mathbf{Q}^*_{\mathcal{N}}} b\|_2^2}_{\text{residual}} \tag{5.55}$$

The sole error term that is controlled by the solution vector x is this

$$\mathsf{R}y - \color{blue}{\mathbf{Q}^*_{\mathcal{R}}} b.$$

Choose y to force this term to zero. This leads to the **QR** solution for the least squares problem:

$$y_{LS} = \mathsf{R}^{-1} \color{blue}{\mathbf{Q}^*_{\mathcal{R}}} b. \tag{5.56}$$

The matrix dimensions of the components are these:

$$\begin{array}{ccccc} y & = & \mathsf{R}^{-1} & \color{blue}{\mathbf{Q}^*_{\mathcal{R}}} & b \\ [n \times 1] & = & [n \times n] & [n \times m] & [m \times 1] \end{array}$$

The vector y which minimizes the least squares error in (5.52) is exactly the same vector given by the QR solution in equation (5.56).

In the overdetermined case the null space term the total error is computed using the vectors which span the null space

$$r^2 = \|\color{red}{\mathbf{Q}^*_{\mathcal{N}}} b\|_2^2 \tag{5.57}$$

5.4.2 Example

Take the overdetermined linear system

$$\mathbf{A}y = b,$$

$$\frac{1}{4} \begin{bmatrix} 0 & 1 \\ 3 & 2 \\ 0 & 2 \end{bmatrix} \begin{bmatrix} y_1 \\ y_2 \end{bmatrix} = \begin{bmatrix} 2 \\ 1 \\ 0 \end{bmatrix}. \tag{5.58}$$

The $\mathbf{QR}$ decomposition of the system matrix is this

$$\mathbf{A} = \mathbf{Q}\,\mathbf{R}$$

$$\frac{1}{4}\left[\begin{array}{cc} 0 & 1 \\ 3 & 2 \\ 0 & 2 \end{array}\right] = \left[\begin{array}{cc|c} 0 & \frac{1}{\sqrt{5}} & -\frac{2}{\sqrt{5}} \\ 1 & 0 & 0 \\ 0 & \frac{2}{\sqrt{5}} & \frac{1}{\sqrt{5}} \end{array}\right] \frac{1}{4}\left[\begin{array}{cc} 3 & 2 \\ 0 & \sqrt{5} \\ \hline 0 & 0 \end{array}\right] \tag{5.59}$$

The solution is described in (5.56)

$$y_{LS} = \mathsf{R}^{-1}\mathbf{Q}^{*}_{\mathcal{R}} b = \left[\begin{array}{cc} \frac{4}{3} & 0 \\ \frac{1}{2} & \frac{4}{\sqrt{5}} \end{array}\right] \left[\begin{array}{ccc} 0 & \frac{1}{\sqrt{5}} & 0 \\ \frac{1}{\sqrt{5}} & 0 & \frac{2}{\sqrt{5}} \end{array}\right] \left[\begin{array}{c} 2 \\ 1 \\ 0 \end{array}\right] = \frac{1}{15}\left[\begin{array}{c} 4 \\ 24 \end{array}\right]. \tag{5.60}$$

This is the same solution as computed using the SVD. As before, the matrix $\mathbf{A}$ has full column rank the null space $\mathcal{N}(\mathbf{A})$ is trivial and there is no contribution from an inhomogeneous solution and

$$y_{LS} \in \mathcal{R}(\mathbf{A}^{*}). \tag{5.61}$$

The residual error vector is unchanged as we have

$$\mathbf{Q}^{*}_{\mathcal{N}} = \mathbf{U}^{*}_{\mathcal{N}}. \tag{5.62}$$

5.5 Solution using the normal equations

Typically, the method of the normal equations is the first tool introduced to solve the least squares problem.

5.6 Sensitivity of the least squares solution

A seminal result in the masterwork by Golub and Van Loan quantifies the sensitivity of the least squares solution. The beauty of this result is that it bounds the sensitivity of the *method* of least squares independent of the *algorithm* used. It answers the question "what is the best possible answer using least squares?" This allows one to evaluate the results from different algorithms in a meaningful way.

5.6.1 Example

Chapter 6

The Moore-Penrose pseudoinverse

6.1 The pseudoinverse

In the chapter on least squares we see that linear systems which do not have an inverse can still yield a solution if we relax the solution criteria. Instead of asking for the vector x which produces

$$\mathbf{A}x = b$$

we ask for the vector x which minimizes

$$\|\mathbf{A}x - b\|_2^2 \tag{6.1}$$

As we generalize the concept of solution we can also generalize the concept of a matrix inverse. In fact in §(5.3) we see how a generalized solution produces a generalized inverse. We call such a quantity a pseudoinverse.

6.2 Constructing the pseudoinverse

The pseudoinverse has a natural definition in terms of the SVD. Given the decomposition

$$\mathbf{A} = \mathbf{U}\,\Sigma\,\mathbf{V}^*,$$

the pseudoinverse is defined as

$$\mathbf{A}^{\dagger} = \mathbf{V}\,\Sigma^{(\dagger)}\,\mathbf{U}^*. \tag{6.2}$$

Notice this form is more general than that in equation (5.38) where the null space contributions are ignored. The two forms are equivalent in that they produce the exact same matrix $\mathbf{A}^{\dagger}$.

Table (6.1) shows the four different formats for the null space components of the pseudoinverse. Just as in the case for the singular value decomposition, the zero *columns* of the Σ matrix silence the null space contribution of $\mathcal{N}(\mathbf{A})$. The zero *rows* of the Σ matrix silence the null space contribution of $\mathcal{N}(\mathbf{A}^*)$. We can use the example matrices to construct each type.

Table 6.1. *Exemplars of the pseudoinverse of a matrix $\boldsymbol{A} \in \mathbb{C}_{\rho}^{m\times n}$. These four block structures describe every possible decomposition. Of course the null space components in red do not contribute to the pseudoinverse matrix. They are shown here to enable the reader to visualize more abstract manipulations of the pseudinverse.*

rank and dimension			$\mathbf{V}$	Σ	$\mathbf{U}^{*}$
$\rho \ne m \ne n$	$\mathbf{A}^{\dagger}$	$=$	$\begin{bmatrix} \mathbf{V}_{\mathcal{R}} & \mathbf{V}_{\mathcal{N}} \end{bmatrix}$	$\begin{bmatrix} \mathbf{S}^{-1} & \mathbf{0} \\ \mathbf{0} & \mathbf{0} \end{bmatrix}$	$\begin{bmatrix} \mathbf{U}_{\mathcal{R}}^{*} \\ \mathbf{U}_{\mathcal{N}}^{*} \end{bmatrix}$
$\rho = m < n$	$\mathbf{A}^{\dagger}$	$=$	$\mathbf{V}_{\mathcal{R}}$	$\begin{bmatrix} \mathbf{S}^{-1} & \mathbf{0} \end{bmatrix}$	$\begin{bmatrix} \mathbf{U}_{\mathcal{R}}^{*} \\ \mathbf{U}_{\mathcal{N}}^{*} \end{bmatrix}$
$\rho = n < m$	$\mathbf{A}^{\dagger}$	$=$	$\begin{bmatrix} \mathbf{V}_{\mathcal{R}} & \mathbf{V}_{\mathcal{N}} \end{bmatrix}$	$\begin{bmatrix} \mathbf{S}^{-1} \\ \mathbf{0} \end{bmatrix}$	$\mathbf{U}_{\mathcal{R}}^{*}$
$\rho = n = m$	$\mathbf{A}^{\dagger}$	$=$	$\mathbf{V}_{\mathcal{R}}$	$\mathbf{S}^{-1}$	$\mathbf{U}_{\mathcal{R}}^{*}$

Table 6.2. *Constructing the pseudoinverse from the singular value decomposition.*

$\rho \neq m \neq n$	$\mathbf{A}$	$= \begin{bmatrix} 1 & -1 \\ -1 & 1 \\ 1 & -1 \end{bmatrix} = \begin{bmatrix} \frac{1}{\sqrt{3}} & 0 & \frac{2}{\sqrt{6}} \\ -\frac{1}{\sqrt{3}} & \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{6}} \\ \frac{1}{\sqrt{3}} & \frac{1}{\sqrt{2}} & -\frac{1}{\sqrt{6}} \end{bmatrix} \left[\begin{array}{c\|c} \sqrt{6} & 0 \\ \hline 0 & 0 \\ 0 & 0 \end{array}\right] \frac{1}{\sqrt{2}} \begin{bmatrix} 1 & -1 \\ 1 & 1 \end{bmatrix}$
	$\mathbf{A}^{\dagger}$	$= \frac{1}{6} \begin{bmatrix} 1 & 1 & 1 \\ -1 & 1 & -1 \end{bmatrix} = \frac{1}{\sqrt{2}} \begin{bmatrix} 1 & 1 \\ -1 & 1 \end{bmatrix} \left[\begin{array}{c\|cc} \frac{1}{\sqrt{6}} & 0 & 0 \\ \hline 0 & 0 & 0 \end{array}\right] \begin{bmatrix} \frac{1}{\sqrt{3}} & -\frac{1}{\sqrt{3}} & \frac{1}{\sqrt{3}} \\ 0 & \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{6}} \\ \frac{2}{\sqrt{6}} & \frac{1}{\sqrt{2}} & -\frac{1}{\sqrt{6}} \end{bmatrix}$
$\rho = n < m$	$\mathbf{A}$	$= \frac{1}{4} \begin{bmatrix} 0 & 1 \\ 3 & 2 \\ 0 & 2 \end{bmatrix} = \begin{bmatrix} \frac{1}{\sqrt{30}} & \frac{1}{\sqrt{6}} & -\frac{2}{\sqrt{5}} \\ \frac{5}{\sqrt{30}} & -\frac{1}{\sqrt{6}} & 0 \\ \frac{2}{\sqrt{30}} & \frac{2}{\sqrt{6}} & \frac{1}{\sqrt{5}} \end{bmatrix} \frac{1}{4} \left[\begin{array}{cc} \sqrt{15} & 0 \\ 0 & \sqrt{3} \\ \hline 0 & 0 \end{array}\right] \frac{1}{\sqrt{2}} \begin{bmatrix} 1 & 1 \\ -1 & 1 \end{bmatrix}$
	$\mathbf{A}^{\dagger}$	$= \frac{1}{15} \begin{bmatrix} -8 & 20 & -16 \\ 12 & 0 & 24 \end{bmatrix} = \frac{1}{\sqrt{2}} \begin{bmatrix} 1 & -1 \\ 1 & 1 \end{bmatrix} \left[\begin{array}{cc\|c} \frac{4}{\sqrt{15}} & 0 & 0 \\ 0 & \frac{4}{\sqrt{3}} & 0 \end{array}\right] \begin{bmatrix} \frac{1}{\sqrt{30}} & \frac{5}{\sqrt{30}} & \frac{5}{\sqrt{30}} \\ \frac{1}{\sqrt{6}} & -\frac{1}{\sqrt{6}} & \frac{1}{\sqrt{6}} \\ -\frac{2}{\sqrt{5}} & 0 & \frac{1}{\sqrt{5}} \end{bmatrix}$
$\rho = m = n$	$\mathbf{A}$	$= \begin{bmatrix} 1 & 2 \\ -1 & 2 \end{bmatrix} = \frac{1}{\sqrt{2}} \begin{bmatrix} 1 & 1 \\ 1 & -1 \end{bmatrix} \sqrt{2} \begin{bmatrix} 2 & 0 \\ 0 & 1 \end{bmatrix} \frac{1}{\sqrt{2}} \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}$
	$\mathbf{A}^{\dagger}$	$= \frac{1}{4} \begin{bmatrix} 2 & -2 \\ 1 & 1 \end{bmatrix} = \frac{1}{\sqrt{2}} \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix} \frac{1}{\sqrt{2}} \begin{bmatrix} 1 & 0 \\ 0 & 2 \end{bmatrix} \frac{1}{\sqrt{2}} \begin{bmatrix} 1 & 1 \\ 1 & -1 \end{bmatrix}$

6.3 A Generalized Inverse for Matrices

[406]

A GENERALIZED INVERSE FOR MATRICES

By R. PENROSE

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This paper describes a generalization of the inverse of a non-singular matrix, as the unique solution of a certain set of equations. This generalized inverse exists for any (possibly rectangular) matrix whatsoever with complex elements‡. It is used here for solving linear matrix equations, and among other applications for finding an expression for the principal idempotent elements of a matrix. Also a new type of spectral decomposition is given.

Figure 6.1. *The Penrose paper. Mathematical Proceedings of the Cambridge Philosophical Society, Volume 51, Issue 03, July 1955, pp 406-413*

6.3.1 Defining the pseudoinverse

The matrix $\mathbf{X}$ is a pseudoinverse of the matrix $\mathbf{A}$ if and only if the following four equations are satisfied

$$\begin{aligned} \mathbf{AXA} &= \mathbf{A} \\ \mathbf{XAX} &= \mathbf{A} \end{aligned} \tag{6.3}$$

$$\begin{aligned} (\mathbf{AX})^* &= \mathbf{AX} \\ (\mathbf{XA})^* &= \mathbf{XA} \end{aligned} \tag{6.4}$$

Σ gymnastics

The singular value decomposition resolves a matrix into very basic components: two unitary matrices and a real diagonal-like matrix. Experience shows that many errors occur when manipulating the diagonal-like Σ matrices. Before investigating the Penrose criteria, we will devote a section to the manipulation of the Σ matrices.

This will cover product matrices like

$$\Sigma\,\Sigma^{(\dagger)},\ \Sigma^{(\dagger)}\Sigma,\ \Sigma\,\Sigma^{(\dagger)}\Sigma \text{ and } \Sigma^{(\dagger)}\Sigma\Sigma^{(\dagger)}.$$

Using the block structure of the SVD component matrices as done in the chapter on least squares. The Σ matrix (say "sigma matrix") is a diagonal matrix $\mathbf{S}$ in a matrix of zeros which acts as a sabot to provide the correct dimensionality. The Σ matrix has the same shape as the target matrix $\mathbf{A}$.

$$\Sigma = \left[\begin{array}{c|c} \mathbf{S} & \mathbf{0} \\ \hline \mathbf{0} & \mathbf{0} \end{array}\right] \tag{6.5}$$

This is a helpful representation but there is an inauspicious ambiguity. The block matrix of the Σ matrix has the same representation as the transpose matrix Σ^{T}. To be clear, we show the dimensions of the forms of the Σ matrices we will need. Given $\mathbf{A} \in \mathbb{C}_{\rho}^{m\times n}$,

$$\begin{aligned} \Sigma &= \left[\begin{array}{c|c} \mathbf{S} & \mathbf{0} \\ \hline \mathbf{0} & \mathbf{0} \end{array}\right]_{m\times n} \\ \Sigma^{\mathrm{T}} &= \left[\begin{array}{c|c} \mathbf{S}^{\mathrm{T}} & \mathbf{0} \\ \hline \mathbf{0} & \mathbf{0} \end{array}\right]_{n\times m} \\ \Sigma^{(\dagger)} &= \left[\begin{array}{c|c} \mathbf{S}^{-1} & \mathbf{0} \\ \hline \mathbf{0} & \mathbf{0} \end{array}\right]_{n\times m} \end{aligned} \tag{6.6}$$

where the singular values matrix $\mathbf{S}$ is square, real, and fully diagonal. To help the reader spot the transform of the sabot matrix we use light gray braces.

$$\mathbf{S} = \mathbf{S}^{\mathrm{T}} = \begin{bmatrix} \sigma_1 & & \\ & \ddots & \\ & & \sigma_\rho \end{bmatrix}, \quad \mathbf{S}^{-1} = \begin{bmatrix} \frac{1}{\sigma_1} & & \\ & \ddots & \\ & & \frac{1}{\sigma_\rho} \end{bmatrix} \tag{6.7}$$

The product of a Σ matrix and its pseudoinverse is a stencil matrix

$$\begin{aligned} \Sigma\,\Sigma^{(\dagger)} &= \mathbb{I}_{\rho,m} = \left[\begin{array}{c|c} \mathbf{I}_\rho & \mathbf{0} \\ \hline \mathbf{0} & \mathbf{0} \end{array}\right]_{m\times m}, \\ \Sigma^{(\dagger)}\Sigma &= \mathbb{I}_{\rho,n} = \left[\begin{array}{c|c} \mathbf{I}_\rho & \mathbf{0} \\ \hline \mathbf{0} & \mathbf{0} \end{array}\right]_{n\times n}. \end{aligned} \tag{6.8}$$

Two useful identities come from full rank conditions. For full column rank

$$\Sigma^{(\dagger)}\Sigma = \left[\begin{array}{c|c} \mathbf{S}^{-1} & \mathbf{0} \end{array}\right] \left[\begin{array}{c} \mathbf{S} \\ \hline \mathbf{0} \end{array}\right] = \mathbf{I}_n; \tag{6.9}$$

for full row rank

$$\Sigma\,\Sigma^{(\dagger)} = \left[\begin{array}{c|c} \mathbf{S} & \mathbf{0} \end{array}\right] \left[\begin{array}{c} \mathbf{S}^{-1} \\ \hline \mathbf{0} \end{array}\right] = \mathbf{I}_m. \tag{6.10}$$

Attention should be given to the dimensions of the stencil matrix. For example:

$$\mathbb{I}_{\rho,m} = \left[\begin{array}{c|c} \mathbf{I}_\rho & \mathbf{0}_{\rho\times(n-\rho)} \\ \hline \mathbf{0}_{(m-\rho)\times\rho} & \mathbf{0}_{(m-\rho)\times(n-\rho)} \end{array}\right] \tag{6.11}$$

The stencil matrix is named for its masking action under matrix multiplication. Consider a matrix $\mathbf{U} \in \mathbb{C}^{m\times m}$. Under postmultiplication the stencil matrix masks out the final $m-\rho$ columns:

$$\mathbf{U}\,\mathbb{I}_{\rho,m} = [u_1 \dots u_\rho | \mathbf{0}_1 \dots \mathbf{0}_{m-\rho}] = \left[\begin{array}{ccc|ccc} u_{1,1} & \dots & u_{1,\rho} & 0 & \dots & 0 \\ \vdots & & \vdots & \vdots & & \vdots \\ u_{m,1} & \dots & u_{m,\rho} & 0 & \dots & 0 \end{array}\right]. \tag{6.12}$$

Under premultiplication the stencil matrix masks out the final $m-\rho$ terms of each column vector:

$$\mathbb{I}_{\rho,m}\mathbf{U} = \left[\begin{array}{ccc} u_{1,1} & \dots & u_{1,m} \\ \vdots & & \vdots \\ u_{\rho,1} & \dots & u_{\rho,m} \\ \hline 0 & \dots & 0 \\ \vdots & & \vdots \\ 0 & \dots & 0 \end{array}\right] \tag{6.13}$$

The stencil matrices are square and named for their stencil action under multiplication. The first ρ rows (columns) of a target matrix are unchanged under premultiplication (postmultiplication). Of interest are the triple products:

$$\begin{aligned} \Sigma\,\Sigma^{(\dagger)}\Sigma &= \Sigma \\ \Sigma^{(\dagger)}\Sigma\Sigma^{(\dagger)} &= \Sigma^{(\dagger)} \end{aligned} \tag{6.14}$$

The stencil action is apparent in block form

$$\Sigma^{(\dagger)}\left(\Sigma\,\Sigma^{(\dagger)}\right) = \left[\begin{array}{c|c} \mathbf{S}^{-1} & \mathbf{0} \\ \hline \mathbf{0} & \mathbf{0} \end{array}\right] \left[\begin{array}{c|c} \mathbf{I}_\rho & \mathbf{0} \\ \hline \mathbf{0} & \mathbf{0} \end{array}\right] = \Sigma^{(\dagger)}. \tag{6.15}$$

yet the dimensions are ambiguous, a hazard with Σ matrices. One cannot emphasize enough the value of explicitly writing out the matrix dimensions to verify conformability:

For more practice, write out a triple product for the overdetermined linear system

$$\underset{[n\times m]}{\Sigma^{(\dagger)}} \quad \underset{[m\times n]}{\Sigma} \quad \underset{[n\times m]}{\Sigma^{(\dagger)}} \quad = \quad \underset{[n\times m]}{\Sigma^{(\dagger)}}$$

where $\rho = n \leq m$.

$$\begin{aligned}
\Sigma\,\Sigma^{(\dagger)}\Sigma &= \left[\begin{array}{c|c} \mathbf{S} & \mathbf{0} \end{array}\right] \left[\begin{array}{c} \mathbf{S}^{-1} \\ \hline \mathbf{0} \end{array}\right] \left[\begin{array}{c|c} \mathbf{S} & \mathbf{0} \end{array}\right] \\
&= \left[\begin{array}{c|c} \mathbf{S} & \mathbf{0} \end{array}\right] \mathbb{I}_{\rho,n} \\
&= \Sigma
\end{aligned} \tag{6.16}$$

Take the example (b) matrix in equation (??). The Σ matrix and its variants are

$$\begin{aligned}
\Sigma &= \frac{1}{4}\left[\begin{array}{cc} \sqrt{15} & 0 \\ 0 & \sqrt{3} \\ \hline 0 & 0 \end{array}\right] \\
\Sigma^{\mathrm{T}} &= \frac{1}{4}\left[\begin{array}{cc|c} \sqrt{15} & 0 & 0 \\ 0 & \sqrt{3} & 0 \end{array}\right] \\
\Sigma^{(\dagger)} &= \left[\begin{array}{cc|c} \frac{4}{\sqrt{15}} & 0 & 0 \\ 0 & \frac{4}{\sqrt{3}} & 0 \end{array}\right]
\end{aligned} \tag{6.17}$$

where the singular values matrices are

$$\mathbf{S} = \mathbf{S}^{\mathrm{T}} = \frac{1}{4}\left[\begin{array}{cc} \sqrt{15} & 0 \\ 0 & \sqrt{3} \end{array}\right], \quad \mathbf{S}^{-1} = \left[\begin{array}{cc} \frac{4}{\sqrt{15}} & 0 \\ 0 & \frac{4}{\sqrt{3}} \end{array}\right]. \tag{6.18}$$

The stencil matrices are these:

$$\begin{aligned}
\Sigma\,\Sigma^{(\dagger)} &= \mathbb{I}_{2,3} = \left[\begin{array}{cc|c} 1 & 0 & 0 \\ 0 & 1 & 0 \\ \hline 0 & 0 & 0 \end{array}\right] \\
\Sigma^{(\dagger)}\Sigma &= \mathbb{I}_{2,2} = \left[\begin{array}{cc} 1 & 0 \\ 0 & 1 \end{array}\right]
\end{aligned} \tag{6.19}$$

Checking the Penrose conditions with the SVD

The Penrose criteria are quickly verified using the SVD. However, this requires a firm grasp of the manipulation of the matrix of singular values.

Checking the Penrose conditions

Verification of the Penrose criteria in equations (6.3) and (6.4) is direct using the SVD. The exercise also provides insight into the SVD. Start with the decomposition forms

$$\begin{aligned}\mathbf{A} &= \mathbf{U}\,\Sigma\,\mathbf{V}^{*},\\ \mathbf{A}^{\dagger} &= \mathbf{V}\,\Sigma^{(\dagger)}\,\mathbf{U}^{*}.\end{aligned}$$

First we ponder the products $\mathbf{A}\mathbf{A}^{\dagger}$ and $\mathbf{A}^{\dagger}\mathbf{A}$. Start with

$$\mathbf{A}\mathbf{A}^{\dagger} = \mathbf{U}\Sigma\,\Sigma^{(\dagger)}\mathbf{U}^{*}. \tag{6.20}$$

We recognize the stencil matrix in the middle and write the product in block form:

$$\mathbf{A}\mathbf{A}^{\dagger} = \left[\begin{array}{c|c} \mathbf{U}_{\mathcal{R}} & \mathbf{U}_{\mathcal{N}} \end{array}\right] \left[\begin{array}{c|c} \mathbf{I}_{\rho} & \mathbf{0} \\ \hline \mathbf{0} & \mathbf{0} \end{array}\right] \left[\begin{array}{c} \mathbf{U}_{\mathcal{R}}^{*} \\ \hline \mathbf{U}_{\mathcal{N}}^{*} \end{array}\right] = \mathbf{U}_{\mathcal{R}}\mathbf{U}_{\mathcal{R}}^{*}. \tag{6.21}$$

The effect of the stencil matrix is to mask the null space contributions. The next matrix product is

$$\mathbf{A}^{\dagger}\mathbf{A} = \left[\begin{array}{c|c} \mathbf{V}_{\mathcal{R}} & \mathbf{V}_{\mathcal{N}} \end{array}\right] \left[\begin{array}{c|c} \mathbf{I}_{\rho} & \mathbf{0} \\ \hline \mathbf{0} & \mathbf{0} \end{array}\right] \left[\begin{array}{c} \mathbf{V}_{\mathcal{R}}^{*} \\ \hline \mathbf{V}_{\mathcal{N}}^{*} \end{array}\right] = \mathbf{V}_{\mathcal{R}}\mathbf{V}_{\mathcal{R}}^{*}. \tag{6.22}$$

The solutions The products satisfy the second set of Penrose criteria in equation (6.4). For example,

$$\left(\mathbf{U}_{\mathcal{R}}\mathbf{U}_{\mathcal{R}}^{*}\right)^{*} = \left(\mathbf{U}_{\mathcal{R}}^{*}\right)^{*}\mathbf{U}_{\mathcal{R}}^{*} = \mathbf{U}_{\mathcal{R}}\mathbf{U}_{\mathcal{R}}^{*}. \tag{6.23}$$

The Penrose criteria in equation (6.4) are quick to verify also. The first is shown here, the second is left as an exercise.

$$\begin{aligned}\left(\mathbf{A}\mathbf{A}^{\dagger}\right)\mathbf{A} &= \mathbf{U}\Sigma\,\Sigma^{(\dagger)}\Sigma\mathbf{V}^{*}\\ &= \mathbf{U}\mathbb{I}_{\rho,m}\Sigma\mathbf{V}^{*}\\ &= \mathbf{U}\,\Sigma\,\mathbf{V}^{*}\\ &= \mathbf{A}\end{aligned} \tag{6.24}$$

6.3.2 Properties of the pseudoinverse

The bulk of the paper lies in lemma 1 and its proof.

Lemma 1.1: pseudoinverse of the pseudoinverse

The pseudoinverse of the pseudoinverse is the original matrix:

$$\left(\mathbf{A}^{\dagger}\right)^{\dagger} = \mathbf{A}. \tag{6.25}$$

The critical observation point here is an exercise in Σ matrix gymnastics

$$\Sigma = \left[\begin{array}{c|c} \mathbf{S} & \mathbf{0} \\ \hline \mathbf{0} & \mathbf{0} \end{array}\right]_{m\times n} \quad \Rightarrow$$

$$\Sigma^{\dagger} = \left[\begin{array}{c|c} \mathbf{S}^{-1} & \mathbf{0} \\ \hline \mathbf{0} & \mathbf{0} \end{array}\right]_{n\times m} \quad \Rightarrow$$

$$\left(\Sigma^{\dagger}\right)^{\dagger} = \left[\begin{array}{c|c} \mathbf{S} & \mathbf{0} \\ \hline \mathbf{0} & \mathbf{0} \end{array}\right]_{m\times n}$$

Lemma 1.2: Hermitian conjugate of the pseudoinverse

The pseudoinverse of the Hermitian conjugate matrix is the Hermitian conjugate of the pseudoinverse matrix:

$$\left(\mathbf{A}^{*}\right)^{\dagger} = \left(\mathbf{A}^{\dagger}\right)^{*}. \tag{6.26}$$

The first half of the identity is this

$$\left(\mathbf{A}^{*}\right)^{\dagger} = \left(\mathbf{V}\,\Sigma^{\mathrm{T}}\,\mathbf{U}^{*}\right)^{\dagger} = \mathbf{U}\,\Sigma^{-\mathrm{T}}\,\mathbf{V}^{*} \tag{6.27}$$

where

$$\Sigma^{-\mathrm{T}} = \left[\begin{array}{c|c} \mathbf{S}^{-1} & \mathbf{0} \\ \hline \mathbf{0} & \mathbf{0} \end{array}\right]_{n\times m} \tag{6.28}$$

represents the inverse matrix $\mathbf{S}^{-1}$ in a transposed sabot matrix.

Lemma 1.3: pseudoinverse and standard inverse

If the matrix $\mathbf{A}$ is nonsingular then the pseudoinverse matrix is the standard matrix inverse:

$$\mathbf{A}^{-1} = \mathbf{A}^{\dagger}. \tag{6.29}$$

If $\mathbf{A}^{-1}$ exists, then $\rho = m = n$. Therefore the singular value decomposition is given as

$$\mathbf{A} = \mathbf{U}_{\mathcal{R}}\,\mathbf{S}\,\mathbf{V}_{\mathcal{R}}^{*}. \tag{6.30}$$

The pseudoinverse for this matrix is

$$\mathbf{A}^{\dagger} = \mathbf{V}_{\mathcal{R}}\,\mathbf{S}^{-1}\mathbf{U}_{\mathcal{R}}^{*}. \tag{6.31}$$

It should be apparent that this matrix acts as the standard inverse:

$$\mathbf{A}^{\dagger}\mathbf{A} = \mathbf{A}\,\mathbf{A}^{\dagger} = \mathbf{I}_{m}. \tag{6.32}$$

Lemma 1.4: pseudoinverse of matrix products

Given conformable matrices $\mathbf{A}$ and $\mathbf{B}$,

$$(\mathbf{AB})^{\dagger} = \mathbf{B}^{\dagger}\mathbf{A}^{\dagger}. \tag{6.33}$$

This proof relies upon the fact that the product of two unitary matrices is also unitary. To see this, let the matrices $\mathbf{C}$ and $\mathbf{D}$ be unitary. The Hermitian conjugate of the product matrix is this

$$(\mathbf{CD})^{*} = \mathbf{D}^{*}\mathbf{C}^{*}. \tag{6.34}$$

Therefore

$$(\mathbf{CD})^{*}(\mathbf{CD}) = \mathbf{I} \tag{6.35}$$

which establishes that the product matrix is also unitary.

Going back to the premise, we state the singular value decompositions for the target matrices

$$\begin{aligned} \mathbf{A} &= \mathbf{U}_A\,\Sigma_A\,\mathbf{V}_A^{*}, \\ \mathbf{B} &= \mathbf{U}_B\,\Sigma_B\,\mathbf{V}_B^{*}. \end{aligned} \tag{6.36}$$

Lemma 1.5: pseudoinverse and Hermitian conjugate

$$(\mathbf{A}^{*}\mathbf{A})^{\dagger} = \mathbf{A}^{\dagger}\left(\mathbf{A}^{\dagger}\right)^{*} \tag{6.37}$$

Lemma 1.6: unitary matrices

Given unitary matrices $\mathbf{C}$ and $\mathbf{D}$ the triple product has the following property

$$(\mathbf{CAD})^{\dagger} = \mathbf{D}^{*}\mathbf{A}^{\dagger}\mathbf{C}^{*} \tag{6.38}$$

Lemma 1.7: pseudoinverse of an unitary decomposition

Given a target matrix $\mathbf{A}$ with the following resolution

$$\mathbf{A} = \sum_i \mathbf{A}_i \tag{6.39}$$

with the constraint

$$\mathbf{A}_j\mathbf{A}_k^{*} = \mathbf{A}_j^{*}\mathbf{A}_k = 0, \qquad \text{for } j \neq k. \tag{6.40}$$

Then the pseudoinverse can be written as the sum of pseudoinverses

$$\mathbf{A}^{\dagger} = \sum_i \mathbf{A}_i^{\dagger} \tag{6.41}$$

Lemma 1.8: pseudoinverse of normal matrices

Given a normal matrix $\mathbf{A}$, that is a matrix where

$$\mathbf{A}^{*}\mathbf{A} = \mathbf{A}\,\mathbf{A}^{*}, \tag{6.42}$$

then we know that

$$\mathbf{A}^{\dagger}\mathbf{A} = \mathbf{A}\,\mathbf{A}^{\dagger}, \tag{6.43}$$

and that for $n \in \mathbb{Q}$

$$\left(\mathbf{A}^{n}\right)^{\dagger} = \left(\mathbf{A}^{\dagger}\right)^{n}. \tag{6.44}$$

Lemma 1.9: pseudoinverse and rank

The matrices $\mathbf{A}$, $\mathbf{A}^{*}$, $\mathbf{A}^{*}\mathbf{A}$, and $\mathbf{A}^{\dagger}\mathbf{A}$ all have a rank given by

$$\rho = \operatorname{tr}\left(\mathbf{A}^{\dagger}\mathbf{A}\right). \tag{6.45}$$

6.4 Chiral inverses

The pseudoinverse leads to the concept of a chiral inverse. We characterize the pseudoinverse according to its action on the right and left-hand side of the target matrix $\mathbf{A}$. For instance, if we have

$$\mathbf{A}^{\dagger}\mathbf{A} = \mathbf{I}_{n} \tag{6.46}$$

the pseudoinverse would be classified as a left-inverse [1] [example matrix b, (1.15)]. If the inverse if ampichiral then

$$\mathbf{A}\,\mathbf{A}^{\dagger} = \mathbf{A}^{\dagger}\mathbf{A} = \mathbf{I}_{m} \tag{6.47}$$

This property defines the standard inverse [example matrix c, (**??**)]. The pseudoinverse is ambichiral when

$$\begin{aligned} \mathbf{A}\,\mathbf{A}^{\dagger} &\ne \mathbf{I}_{m}, \\ \mathbf{A}^{\dagger}\mathbf{A} &\ne \mathbf{I}_{n}. \end{aligned} \tag{6.48}$$

[example matrix a, (**??**)].

[1] One may contend that a consistent nomenclature would call the left-handed inverse aristerochiral and the right-handed inverse dextrochiral. Here we defer to colloquialism.

Table 6.3. *default*

chirality	equivalence	definition	Σ condition	rank and dimension	null space condition
right-handed	$\mathbf{A}^{\dagger} = \mathbf{A}^{-\mathrm{R}}$	$\mathbf{A}^{\dagger}\mathbf{A} = \mathbf{I}_n$	$\Sigma^{(\dagger)}\Sigma = \mathbf{I}_n$	$\rho = n \leq m$	$\mathcal{N}\left(\mathbf{A}\right) = \{\mathbf{0}\}$
left-handed	$\mathbf{A}^{\dagger} = \mathbf{A}^{-\mathrm{L}}$	$\mathbf{A}\,\mathbf{A}^{\dagger} = \mathbf{I}_m$	$\Sigma\,\Sigma^{(\dagger)} = \mathbf{I}_m$	$\rho = m \leq n$	$\mathcal{N}\left(\mathbf{A}^{*}\right) = \{\mathbf{0}\}$
ambichiral	$\mathbf{A}^{\dagger} = \mathbf{A}^{-1}$	$\mathbf{A}^{\dagger}\mathbf{A} = \mathbf{I}_n$ and	$\Sigma^{(\dagger)}\Sigma = \mathbf{I}_n$ and	$\rho = m = n$	$\mathcal{N}\left(\mathbf{A}\right) = \{\mathbf{0}\}$ and
		$\mathbf{A}\,\mathbf{A}^{\dagger} = \mathbf{I}_m$	$\Sigma\,\Sigma^{(\dagger)} = \mathbf{I}_m$		$\mathcal{N}\left(\mathbf{A}^{*}\right) = \{\mathbf{0}\}$
ampichiral	$\mathbf{A}^{\dagger} \neq \mathbf{A}^{-\mathrm{R}}$ and	$\mathbf{A}^{\dagger}\mathbf{A} \neq \mathbf{I}_n$ and	$\Sigma^{(\dagger)}\Sigma \neq \mathbf{I}_n$ and	$\rho \neq m \neq n$	$\mathcal{N}\left(\mathbf{A}\right) \neq \{\mathbf{0}\}$ and
	$\mathbf{A}^{\dagger} \neq \mathbf{A}^{-\mathrm{L}}$	$\mathbf{A}\,\mathbf{A}^{\dagger} \neq \mathbf{I}_m$	$\Sigma\,\Sigma^{(\dagger)} \neq \mathbf{I}_m$		$\mathcal{N}\left(\mathbf{A}^{*}\right) \neq \{\mathbf{0}\}$

$$
\begin{aligned}
\left\| \mathbf{A}^{\dagger} \mathbf{A} - \mathbf{I}_n \right\|_2 &= 1, \\
\left\| \mathbf{A}\, \mathbf{A}^{\dagger} - \mathbf{I}_m \right\|_2 &= 1.
\end{aligned}
\tag{6.49}
$$

Part III

Visualizations

Part IV

Explorations

Chapter 7

The Pantheon of Matrix Factorizations

Where does the SVD reside in the pantheon of matrix factorizations?

Chapter 8

Examples

Where does the SVD reside in the pantheon of matrix factorizations?

8.1 Famous matrices

A survey of famous matrices.

8.1.1 The Pauli matrices

The Pauli spin matrices σ_k are a set of three 2×2 matrices which arise in quantum mechanics in the treatment of spin.

The singular value decompositions are

$$\begin{aligned}
\sigma_1 &= \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix} = \mathbf{I}_2 \ \mathbf{I}_2 \ \mathbf{K}_2, \\
\sigma_2 &= \begin{bmatrix} 0 & -i \\ i & 0 \end{bmatrix} = \begin{bmatrix} -i & 0 \\ 0 & i \end{bmatrix} \mathbf{I}_2 \ \mathbf{K}_2, \\
\sigma_3 &= \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix} = \begin{bmatrix} 0 & 1 \\ -1 & 0 \end{bmatrix} \mathbf{I}_2 \ \mathbf{K}_2.
\end{aligned} \tag{8.1}$$

Notice the incidental equality

$$\mathbf{K}_2 = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix} = \sigma_1. \tag{8.2}$$

Observations: The singular values are always one, therefore these matrices are unitary. The matrices are involutary

$$\sigma_k^2 = \mathbf{I}_2, \quad k = 1, 2, 3. \tag{8.3}$$

They satisfy the anticommutation relationship

$$\{\sigma_j, \sigma_k\} = \sigma_j \sigma_k + \sigma_k \sigma_j = 2\delta_{j,k}\mathbf{I}_2, \quad j,k = 1,2,3. \tag{8.4}$$

Mystery equation

$$\sigma_j \sigma_k = \delta_{j,k}\mathbf{I}_2 + \epsilon_{jkl}\sigma_l. \tag{8.5}$$

These matrices, along with the identity, form a basis for $\mathbb{C}^{2\times 2}$

$$A = \alpha_0 \mathbf{I}_2 + \sum_{k=1}^{3} \alpha_k \sigma_k. \tag{8.6}$$

For example,

$$\begin{bmatrix} 1+i & -1+i \\ -1-i & -1+i \end{bmatrix} = i\mathbf{I}_2 - \sigma_1 - \sigma_2 + \sigma_3 \tag{8.7}$$

8.1.2 The Dirac matrices

The matrices form a basis for $\mathbb{C}^3$

8.1.3 The Gell-Mann matrices

The matrices form a basis for $\mathbb{C}^3$

8.1.4 Rotation matrices

Part V

Machinations

Part VI

Appendices

Appendix A

Lexicon

Table A.1. *default*

row space	column space
domain	codomain
preimage	image

1. pseudoinverse
2. Moore-Penrose pseudoinverse
3. generalized matrix inverse

Table A.2. *default*

$m = n$	square	equal number of rows and columns
$m \geq n$	tall	more rows than columns
$n \geq m$	wide	more columns than rows

Table A.3. *default*

$\rho = m = n$	full rank	square	
$\rho = n \leq m$	full column rank	tall	overdetermined
$\rho = m \leq n$	full row rank	wide	underdetermined

Appendix B

$\mathbb{C}$ vs. $\mathbb{R}$

B.1 Life is complex

The salient observation is that the real line is embedded in the complex plane. Therefore we may view real numbers as a subset of the complex numbers. Even simple operations with purely real numbers cannot be restricted to the real number line. For example, the solutions to equations like

$$x^2 + 1 = 0 \tag{B.1}$$

force us into the complex plane. The function

$$y(x) = \frac{1}{\sqrt{x^2 + 1}} \tag{B.2}$$

has finite values for all derivatives for all orders over the entire real line; this function is very well-behaved. Yet why does the Taylor expansion about the origin have a radius of convergence of 1? The answer is because of the pole in the complex plane.

Finite binary representation of real numbers can generate complex numbers. For example, in the error propagation numbers are added quadratically. The final step is a square root operation. Sets of large numbers should almost completely cancel. While we know the result must be real, the digital representation will often have a very small imaginary component. While the difference between -10^{-16} and 10^{-16} is usually negligible in practice, the difference between $\sqrt{10^{-16}}$ and $\sqrt{-10^{-16}}$ is the difference between success and failure.

B.2 Life is complex

If we are in the field of complex numbers

$$\alpha = a + ib \tag{B.3}$$

where i is the imaginary unit. The complex conjugate

$$\overline{\alpha} = a - ib. \tag{B.4}$$

is the reflection of α through the real axis. The expression

$$\alpha = \overline{\alpha} \quad \Rightarrow \quad b = 0. \tag{B.5}$$

B.3 Spaces

Take a matrix with real entries such as

$$\mathbf{A} = \begin{bmatrix} a & b \\ c & d \end{bmatrix}. \tag{B.6}$$

This matrix is a member of the space of 2×2 matrices with real elements:

$$\mathbf{A} \in \mathbb{R}^{2\times 2} \tag{B.7}$$

Matrices in this class include $-\mathbf{A}$, $\frac{1}{2}\mathbf{A}$, $\pi\mathbf{A}$, $10^{23}\mathbf{A}$, ...

We use real numbers in any example where we want to plot vectors.

B.4 Conversion

Table B.1. *default*

unitary	$\Longrightarrow$	orthogonal
Hermitian conjugate	$\Longrightarrow$	transpose

B.5 Algorithms

Consider an early step in computing the singular value decomposition, forming the product matrix $\mathbf{W}_x$. The command

$$Wx = \mathbf{A}^* \mathbf{A} \tag{B.8}$$

always works. The command

$$Wx = \mathbf{A}^{\mathrm{T}} \mathbf{A} \tag{B.9}$$

will not work if there is a single complex number in the matrix $\mathbf{A}$. If the goal is to write a computer code for general application, then one can either use the economical statement or ...? Test each entry to see if any values are complex? (Slow.) Hope that all entries are real? (Overly optimistic.)

Part VII

Backmatter

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