(5.71) ***Theorem*** (orthogonal projection). Let $\mathscr{V}$ be a vector space with an inner product. Let $\mathscr{V}_0$ be the subspace of $\mathscr{V}$ spanned by an orthogonal set

$$S = \{\mathbf{v}_1, \mathbf{v}_2, \ldots, \mathbf{v}_q\}$$

of *nonzero* vectors. Define the *orthogonal projection* P_0 *onto* $\mathscr{V}_0$ as follows: for any $\mathbf{v}$ in $\mathscr{V}$, set

$$P_0\mathbf{v} = \alpha_1\mathbf{v}_1 + \cdots + \alpha_q\mathbf{v}_q, \qquad \text{where } \alpha_i = \frac{(\mathbf{v}_i, \mathbf{v})}{(\mathbf{v}_i, \mathbf{v}_i)}.$$

Then:

(a) $\mathbf{v} - P_0\mathbf{v}$ is orthogonal to every vector $\mathbf{v}_0$ in $\mathscr{V}_0$.
(b) $P_0(\mathbf{u} + \mathbf{v}) = P_0\mathbf{u} + P_0\mathbf{v}$ for all $\mathbf{u}$, $\mathbf{v}$ in $\mathscr{V}$.
(c) $P_0(\alpha\mathbf{v}) = \alpha P_0\mathbf{v}$ for all scalars α and all $\mathbf{v}$ in $\mathscr{V}$.

PROOF

(a) Note first that $\mathbf{v} - P_0\mathbf{v}$ is orthogonal to each $\mathbf{v}_i$:

$$(\mathbf{v}_i, \mathbf{v} - P_0\mathbf{v}) = (\mathbf{v}_i, \mathbf{v}) - \alpha_1(\mathbf{v}_i, \mathbf{v}_1) - \cdots - \alpha_q(\mathbf{v}_i, \mathbf{v}_q) = (\mathbf{v}_i, \mathbf{v}) - \alpha_i(\mathbf{v}_i, \mathbf{v}_i) = 0.$$

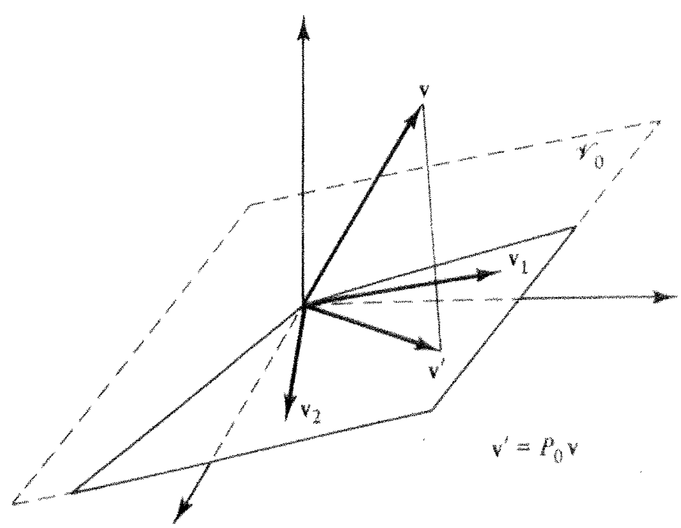
Since each $\mathbf{v}_0$ in $\mathscr{V}_0$ is a linear combination of the $\mathbf{v}_i$, each of which satisfies $(\mathbf{v}_i, \mathbf{v} - P_0\mathbf{v}) = 0$, we get $(\mathbf{v}_0, \mathbf{v} - P_0\mathbf{v}) = 0$ as claimed.

(b) and (c) follow immediately from the definition of the coefficients α_i. For example, the coefficient α_i in $P_0(\alpha\mathbf{v})$ is

$$(\mathbf{v}_i, \alpha\mathbf{v})/(\mathbf{v}_i, \mathbf{v}_i) = \alpha(\mathbf{v}_i, \mathbf{v})/(\mathbf{v}_i, \mathbf{v}_i),$$

which is just α times the coefficient α_i in $P_0\mathbf{v}$. ■

(5.72) ***Example.*** Suppose that $\mathscr{V}$ is $\mathbb{R}^3$ and that $q = 2$; then $\mathscr{V}_0$ is a plane. The geometric interpretation of $\mathbf{v}' = P_0\mathbf{v}$ is shown below:



Best Approximations

Section 2.6 on least squares showed that in determining parameters in mathematical models one often has to approximate a given vector as a linear combination of other given vectors. If the vectors from which one forms linear combinations are mutually *orthogonal*, then the solution of this problem is straightforward.

(5.73) ***Theorem*** (best approximation). Let $\mathscr{V}$ be a vector space with an inner product and with induced norm $\|\cdot\|$, and let $\mathscr{V}_0$ be the subspace spanned by the *orthogonal* set of nonzero vectors $\mathbf{v}_1, \ldots, \mathbf{v}_q$. Then, for any $\mathbf{v}$, $P_0\mathbf{v}$ is the unique *closest point* in $\mathscr{V}_0$ to $\mathbf{v}$ and $\|\mathbf{v} - P_0\mathbf{v}\|$ is the *distance from* $\mathbf{v}$ *to* $\mathscr{V}_0$, in the sense that $P_0\mathbf{v}$ is in $\mathscr{V}_0$ and

$$\|\mathbf{v} - P_0\mathbf{v}\| < \|\mathbf{v} - \mathbf{v}_0\| \qquad \text{for all } \mathbf{v}_0 \neq P_0\mathbf{v} \text{ in } \mathscr{V}_0.$$

PROOF. For convenience, let $\hat{\mathbf{v}}_0$ denote $P_0\mathbf{v}$, which is clearly in $\mathscr{V}_0$ by the definition of $P_0\mathbf{v}$; for any $\mathbf{v}_0$ in $\mathscr{V}_0$, calculate $\|\mathbf{v} - \mathbf{v}_0\|$ as follows:

$$\begin{aligned}\|\mathbf{v} - \mathbf{v}_0\|^2 &= (\mathbf{v} - \mathbf{v}_0, \mathbf{v} - \mathbf{v}_0)\\ &= (\mathbf{v} - \hat{\mathbf{v}}_0 + \hat{\mathbf{v}}_0 - \mathbf{v}_0, \mathbf{v} - \hat{\mathbf{v}}_0 + \hat{\mathbf{v}}_0 - \mathbf{v}_0)\\ &= (\mathbf{v} - \hat{\mathbf{v}}_0, \mathbf{v} - \hat{\mathbf{v}}_0) + (\mathbf{v} - \hat{\mathbf{v}}_0, \hat{\mathbf{v}}_0 - \mathbf{v}_0)\\ &\quad + (\hat{\mathbf{v}}_0 - \mathbf{v}_0, \mathbf{v} - \hat{\mathbf{v}}_0) + (\hat{\mathbf{v}}_0 - \mathbf{v}_0, \hat{\mathbf{v}}_0 - \mathbf{v}_0).\end{aligned}$$

By Theorem 5.71(a), $\mathbf{v} - \hat{\mathbf{v}}_0$ is orthogonal to all vectors in $\mathscr{V}_0$, including $\hat{\mathbf{v}}_0 - \mathbf{v}_0$; the two middle terms of the four terms on the right above therefore equal zero. That equality then becomes

$$\|\mathbf{v} - \mathbf{v}_0\|^2 = \|\mathbf{v} - \hat{\mathbf{v}}_0\|^2 + \|\hat{\mathbf{v}}_0 - \mathbf{v}_0\|^2.$$

Therefore, $\|\mathbf{v} - \mathbf{v}_0\|^2 > \|\mathbf{v} - \hat{\mathbf{v}}_0\|^2$ unless $\mathbf{v}_0 = \hat{\mathbf{v}}_0$. ■

According to Theorem 5.73, it is easy to find the best approximation in a given subspace $\mathscr{V}_0$ to a given vector $\mathbf{v}$ *as long as we have an orthogonal spanning set for* $\mathscr{V}_0$ *consisting of nonzero vectors.* Since this best-approximation problem arises so often in applications, we pursue this matter of orthogonal spanning sets.

Orthogonal and Orthonormal Bases

One important aspect of our main theorem on orthogonal projection is somewhat concealed by the notation: Every orthogonal set of nonzero vectors is linearly independent. To see this, suppose that $S = \{\mathbf{v}_1, \ldots, \mathbf{v}_q\}$ is such a set and that

$$c_1\mathbf{v}_1 + \cdots + c_q\mathbf{v}_q = \mathbf{0};$$

taking the inner product with each $\mathbf{v}_j$ gives

$$0 = (\mathbf{v}_j, \mathbf{0}) = (\mathbf{v}_j, c_1\mathbf{v}_1 + \cdots + c_q\mathbf{v}_q) = c_j(\mathbf{v}_j, \mathbf{v}_j),$$

which means that $c_j = 0$ since $(\mathbf{v}_j, \mathbf{v}_j) > 0$. Therefore, any orthogonal spanning set of nonzero vectors is an orthogonal linearly independent spanning set—that is, an *orthogonal basis* for $\mathscr{V}_0$. The orthogonal projection theorem says that orthogonal bases are extremely easy to use when we need to find a best approximation to a vector $\mathbf{v}$: We can immediately write it down as

$$\alpha_1\mathbf{v}_1 + \cdots + \alpha_q\mathbf{v}_q$$

with the α_i as defined in the theorem. If $\mathbf{v}$ happens itself to be in $\mathscr{V}_0$, then certainly $\mathbf{v}$ is the best approximation in $\mathscr{V}_0$ to itself and we have

$$\mathbf{v} = \alpha_1\mathbf{v}_1 + \cdots + \alpha_q\mathbf{v}_q$$

with the α_i as in the theorem. That is:

> We can express a vector $\mathbf{v}$ as a linear combination of vectors in an orthogonal basis without having to solve equations to determine the coefficients—we can simply evaluate some inner products to obtain the coefficients directly.

We summarize.

(5.74) ***Theorem*** (orthogonal bases). Let $B = \{\mathbf{v}_1, \mathbf{v}_2, \ldots, \mathbf{v}_q\}$ be an orthogonal (or orthonormal) basis. Then the representation of any vector $\mathbf{v}$ with respect to the orthogonal basis B can immediately be written down:

$$\mathbf{v} = \alpha_1\mathbf{v}_1 + \cdots + \alpha_q\mathbf{v}_q, \qquad \text{where } \alpha_i = \frac{(\mathbf{v}_i, \mathbf{v})}{(\mathbf{v}_i, \mathbf{v}_i)}.$$

We encountered a special case of this much earlier when we saw how easy it is to express any vector in $\mathbb{R}^p$ as a linear combination of $\mathbf{e}_1, \ldots, \mathbf{e}_p$: these vectors form an orthonormal basis for $\mathbb{R}^p$, so the coefficients in the representation of $\mathbf{v}$ are

$$\alpha_i = \frac{(\mathbf{e}_i, \mathbf{v})}{(\mathbf{e}_i, \mathbf{e}_i)} = \langle\mathbf{v}\rangle_i.$$

You should now be able to solve Problems 1 to 5.

Creating Orthogonal and Orthonormal Bases: Gram–Schmidt

Best-approximation problems are easy to solve *if we have an orthogonal basis for the approximating subspace*. This is not always the case in applications, however. Such a basis is so convenient that often we should attempt to *create* one for a space. This raises the following question:

> Given a basis or spanning set S for a vector space with an inner product, how can we find an orthogonal or orthonormal basis for the space?

13. Apply the modified Gram–Schmidt process of Problem 12 to the vectors in Example 5.77.

𝔐 14. Apply MATLAB or similar software to find an orthogonal or orthonormal basis for the space spanned by the vectors in Problem 11 (with ϵ chosen appropriately for your computer) to see how well that software performs on this challenging problem.

15. Another alternative to the traditional process for calculating the projections in **Key Theorem 5.75** makes use of *Householder matrices* (see Problems 13–17 of Section 5.9); a (real) Householder matrix is a $p \times p$ matrix $\mathbf{H}$ of the form $\mathbf{H} = \mathbf{I}_p - 2\mathbf{w}\mathbf{w}^T/\mathbf{w}^T\mathbf{w}$ for a real nonzero $p \times 1$ column matrix $\mathbf{w}$.
   (a) Show that every Householder matrix is symmetric.
   (b) Show that every Householder matrix is nonsingular and that $\mathbf{H}^{-1} = \mathbf{H} = \mathbf{H}^T$.
   (c) Use (b) to show that the columns of a Householder matrix form an orthonormal set.

▷ 16. Given two $p \times 1$ real matrices $\mathbf{x}$ and $\mathbf{y}$, with $\mathbf{x} \neq \mathbf{y}$, define

$$\mathbf{w}_{\pm} = \mathbf{x} \pm \mathbf{y}\|\mathbf{x}\|_2/\|\mathbf{y}\|_2$$

and let $\mathbf{H}_{\pm}$ be the Householder matrices of Problem 15 defined by $\mathbf{w}_{\pm}$. Show that $\mathbf{H}_{\pm}$ transforms $\mathbf{x}$ into a multiple of $\mathbf{y}$; more precisely, show that

$$\mathbf{H}_{\pm}\mathbf{x} = \mp\, \mathbf{y}\|\mathbf{x}\|_2/\|\mathbf{y}\|_2.$$

17. (a) Let $\mathbf{x} = [2 \quad 2 \quad 1]^T$ and $\mathbf{y} = [1 \quad 0 \quad 0]^T$. Find the matrices $\mathbf{H}_{\pm}$ of Problem 16 and verify that $\mathbf{H}_{\pm}\mathbf{x} = \mp 3\mathbf{y}$.
   (b) Show that for any $\mathbf{x}$ in $\mathbb{R}^p$ there is a Householder matrix $\mathbf{H}$ so that $\mathbf{H}\mathbf{x}$ equals either plus or minus $\|\mathbf{x}\|_2\mathbf{e}_1$, where $\mathbf{e}_1$ is the usual unit column matrix.

5.9 ORTHOGONAL PROJECTIONS AND BASES: $\mathbb{R}^p$, $\mathbb{C}^p$, QR, AND LEAST SQUARES

Many applications make crucial use of the techniques and concepts of orthogonal projections and bases introduced in Section 5.8 for general vector spaces. In the special case of $\mathbb{R}^p$ (or $\mathbb{C}^p$), these results—when couched in matrix terminology—provide powerful computational tools.

Orthogonal Projections

Our first results—Theorems 5.72 and 5.73—in the preceding section involved orthogonal projections is general vector spaces with inner products; we now reformulate these in $\mathbb{R}^p$ and $\mathbb{C}^p$ using matrix terminology. To be specific, we consider $\mathcal{V} = \mathbb{R}^p$ in the discussion below; we only need change transposes ^{T} to hermitian transposes ^{H} to make the argument apply in $\mathbb{C}^p$.

Suppose that $\mathscr{V}_0$ is a subspace of $\mathbb{R}^p$ spanned by the orthogonal set of vectors $S = \{\mathbf{v}_1, \mathbf{v}_2, \ldots, \mathbf{v}_q\}$ and that $\mathbf{v}$ is another $p \times 1$ matrix; we wish to calculate the orthogonal projection $P_0\mathbf{v}$ of Theorem 5.72. We specialize slightly by assuming that S is an *orthonormal* set—that $\|\mathbf{v}_i\|_2 = 1$ in addition to the orthogonality conditions $0 = (\mathbf{v}_i, \mathbf{v}_j) = \mathbf{v}_i^T\mathbf{v}_j$ for $i \neq j$. Define the $p \times q$ matrix $\mathbf{Q}$ by

$$\mathbf{Q} = [\mathbf{v}_1 \quad \mathbf{v}_2 \quad \cdots \quad \mathbf{v}_q].$$

If we compute $\mathbf{Q}^T\mathbf{Q}$, we find that

$$\mathbf{Q}^T\mathbf{Q} = [\mathbf{v}_1 \quad \mathbf{v}_2 \quad \cdots \quad \mathbf{v}_q]^T[\mathbf{v}_1 \quad \mathbf{v}_2 \quad \cdots \quad \mathbf{v}_q]$$

has as its (i, j)-entry just $\mathbf{v}_i^T\mathbf{v}_j$—which equals 1 if $i = j$ and 0 if $i \neq j$. That is: $\mathbf{Q}^T\mathbf{Q} = \mathbf{I}_q$; this is our matrix reformulation of the fact that S is orthonormal. Now to the computation of $P_0\mathbf{v}$. According to Theorem 5.72,

$$P_0\mathbf{v} = \alpha_1\mathbf{v}_1 + \cdots + \alpha_q\mathbf{v}_q$$

for appropriate α_i; in matrix notation, this says that $P_0\mathbf{v} = \mathbf{Q}\boldsymbol{\alpha}$, where $\mathbf{Q}$ is the matrix above and

$$\boldsymbol{\alpha} = [\alpha_1 \quad \alpha_2 \quad \cdots \quad \alpha_q]^T.$$

Again according to Theorem 5.72, α_i is computed as

$$\alpha_i = \frac{(\mathbf{v}_i, \mathbf{v})}{(\mathbf{v}_i, \mathbf{v}_i)} = \mathbf{v}_i^T\mathbf{v}$$

in the present case; in matrix notation, this says that $\boldsymbol{\alpha} = \mathbf{Q}^T\mathbf{v}$. Putting these two facts together gives

$$P_0\mathbf{v} = \mathbf{Q}\mathbf{Q}^T\mathbf{v}.$$

Note here that $\mathbf{Q}\mathbf{Q}^T \neq \mathbf{I}_p$ in general; $\mathbf{Q}^T$ is a left-inverse of $\mathbf{Q}$ since $\mathbf{Q}^T\mathbf{Q} = \mathbf{I}_q$, but it is not generally a right-inverse since we are not assuming $\mathbf{Q}$ to be square. This formula for P_0 shows that orthogonal projection is nothing more than multipli- cation by a special matrix $\mathbf{Q}\mathbf{Q}^T$, called a *projection matrix*. This completes our reformulation of Theorems 5.72 and 5.73 in matrix terminology.

(5.79) ***Theorem*** (projection matrices). Let $\mathbf{Q}$ be a $p \times q$ matrix having orthonormal columns in $\mathbb{R}^p$ (or $\mathbb{C}^p$)—that is, let

$$\mathbf{Q}^T\mathbf{Q} = \mathbf{I}_q \qquad (\text{or } \mathbf{Q}^H\mathbf{Q} = \mathbf{I}_q),$$

and let $\mathscr{V}_0$ be the subspace spanned by the orthonormal basis for $\mathscr{V}_0$ formed by the columns of $\mathbf{Q}$. Then:

(a) The orthogonal projection P_0 onto $\mathscr{V}_0$ as described in Theorems 5.72 and 5.73 is computed with the *projection matrix* $\mathbf{Q}\mathbf{Q}^T$ (or $\mathbf{Q}\mathbf{Q}^H$) as

$$P_0\mathbf{v} = \mathbf{P}_0\mathbf{v}$$

where $\mathbf{P}_0$ is the $p \times p$ matrix $\mathbf{P}_0 = \mathbf{Q}\mathbf{Q}^T$ (or $\mathbf{P}_0 = \mathbf{Q}\mathbf{Q}^H$).

(b) The projection matrix $\mathbf{P}_0$ satisfies:
1. $\mathbf{P}_0$ is symmetric (or hermitian).
2. $\mathbf{P}_0^2 = \mathbf{P}_0$.
3. $\mathbf{P}_0(\mathbf{I}_p - \mathbf{P}_0) = (\mathbf{I}_p - \mathbf{P}_0)\mathbf{P}_0 = \mathbf{0}$.
4. $(\mathbf{I}_p - \mathbf{P}_0)\mathbf{Q} = \mathbf{0}$.

PROOF

(a) We have already proved this.

(b) 1. $\mathbf{P}_0^T = (\mathbf{Q}\mathbf{Q}^T)^T = (\mathbf{Q}^T)^T\mathbf{Q}^T = \mathbf{Q}\mathbf{Q}^T = \mathbf{P}_0$ (and similarly for the complex case).
2. $\mathbf{P}_0^2 = \mathbf{Q}\mathbf{Q}^T\mathbf{Q}\mathbf{Q}^T = \mathbf{Q}\mathbf{I}_q\mathbf{Q}^T = \mathbf{Q}\mathbf{Q}^T = \mathbf{P}_0$ (and similarly for the complex case).
3. $\mathbf{P}_0(\mathbf{I}_p - \mathbf{P}_0) = \mathbf{P}_0 - \mathbf{P}_0^2 = \mathbf{0}$, and similarly for the others.
4. $(\mathbf{I}_p - \mathbf{P}_0)\mathbf{Q} = \mathbf{Q} - \mathbf{Q}\mathbf{Q}^T\mathbf{Q} = \mathbf{Q} - \mathbf{Q}\mathbf{I}_q = \mathbf{0}$ (and similarly for the complex case). ■

(5.80) ***Example.*** Let $\mathbf{Q}$ be 4×3 and let its columns be normalized versions of the nonzero orthogonal vectors $\mathbf{u}_1$, $\mathbf{u}_2$, $\mathbf{u}_4$ found in Example 5.77:

$$\mathbf{Q} = \begin{bmatrix} \frac{1}{2} & \frac{\sqrt{3}}{2} & 0 \\ \frac{1}{2} & -\frac{\sqrt{3}}{6} & \frac{\sqrt{6}}{6} \\ \frac{1}{2} & -\frac{\sqrt{3}}{6} & \frac{\sqrt{6}}{6} \\ -\frac{1}{2} & \frac{\sqrt{3}}{6} & \frac{\sqrt{6}}{3} \end{bmatrix}. \quad \text{Then} \quad \mathbf{P}_0 = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & \frac{1}{2} & \frac{1}{2} & 0 \\ 0 & \frac{1}{2} & \frac{1}{2} & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix}.$$

Therefore, the closest vector to $\mathbf{v} = [1 \quad 2 \quad 3 \quad 4]^T$ in the subspace $\mathscr{V}_0$ of $\mathbb{R}^4$ spanned by the columns of $\mathbf{Q}$ is

$$P_0\mathbf{v} = \mathbf{P}_0\mathbf{v} = [1 \quad 5/2 \quad 5/2 \quad 4]^T;$$

more generally, the closest point to $\mathbf{v} = [a \quad b \quad c \quad d]^T$ is

$$\mathbf{P}_0\mathbf{v} = \left[a \quad \frac{b+c}{2} \quad \frac{b+c}{2} \quad d\right]^T.$$

You should now be able to solve Problems 1 to 5.

QR-Decompositions

Our next task is to provide a matrix formulation for **Key Theorem 5.75** on how to compute an orthogonal spanning set from a general spanning set. Suppose that $\mathbf{v}_1, \mathbf{v}_2, \ldots, \mathbf{v}_q$ are $p \times 1$ column matrices and consider the traditional implementation (5.76) of the Gram–Schmidt process. From the definition of the column terms of least squares; see Section 2.6. This was one instance of a general phenomenon: One has a model depending on various parameters to be determined so as to model as accurately as possible how some system has actually behaved in the past. Problem 12 in Section 2.6 is of this type: It asks you to find the entries in the transition matrix for the dairy-competition model of Section 2.2 so that the model corresponds to data on how the market shares have actually changed. Problem 22 in Section 5.9 is also of this type.

More generally, the problem is to determine the parameters $\mathbf{x}$ so that the model's prediction $\mathbf{Ax}$ is close to the measured data $\mathbf{b}$. With least *squares*, we seek to find $\mathbf{x}$ to minimize $\|\mathbf{Ax} - \mathbf{b}\|_2$ over all possible $\mathbf{x}$, where $\mathbf{A}$ is $p \times q$ and given, $\mathbf{b}$ is $p \times 1$ and given, and $\mathbf{x}$ is $q \times 1$ and unknown. Problem 26 in Section 5.9 stated that $\mathbf{x}$ solves this if and only if $\mathbf{A}^H\mathbf{Ax} = \mathbf{A}^H\mathbf{b}$; as was shown in Problem 24 of Section 5.9, however, this can be a poor approach computationally. That section showed that a much better method can be based on the normalized QR-decomposition of $\mathbf{A}$: Write $p \times q$ $\mathbf{A}$ of rank k as $\mathbf{A} = \mathbf{QR}$ where $\mathbf{Q}$ is $p \times k$ and has orthonormal columns and $\mathbf{R}$ is $k \times q$ upper-triangular of rank k, and then $\mathbf{x}$ solves $\mathbf{Rx} = \mathbf{Q}^T\mathbf{b}$—which can be solved by simple back-substitution. We now consider another method for solving least-squares problems that is equally effective.

Singular Value Decompositions and Least Squares

Suppose that $\mathbf{A} = \mathbf{U\Sigma V}^H$ is the singular value decomposition from **Key Theorem 8.19** for the $p \times q$ matrix $\mathbf{A}$ of rank k. We consider the problem of minimizing $\|\mathbf{Ax} - \mathbf{b}\|_2$ with respect to $\mathbf{x}$. By Theorem 7.31 on unitary matrices, we can write

$$\|\mathbf{Ax} - \mathbf{b}\|_2 = \|\mathbf{U\Sigma V}^H\mathbf{x} - \mathbf{b}\|_2 = \|\mathbf{\Sigma y} - \mathbf{U}^H\mathbf{b}\|_2,$$

where $\mathbf{y} = \mathbf{V}^H\mathbf{x}$ is the new variable with respect to which we are minimizing. Thus $\mathbf{x}$ minimizes $\|\mathbf{Ax} - \mathbf{b}\|_2$ if and only if $\mathbf{y}$ $(= \mathbf{V}^H\mathbf{x})$ minimizes $\|\mathbf{\Sigma y} - \mathbf{b}'\|_2$, where we use $\mathbf{b}'$ to denote $\mathbf{U}^H\mathbf{b}$. But

$$\begin{aligned}\|\mathbf{\Sigma y} - \mathbf{b}'\|_2^2 = |\sigma_1 y_1 - b_1'|^2 + \cdots + |\sigma_k y_k - b_k'|^2 \\ + |b_{k+1}'|^2 + \cdots + |b_p'|^2,\end{aligned}$$

where $y_i = \langle\mathbf{y}\rangle_i$ and $b_i' = \langle\mathbf{b}'\rangle_i$. This expression is minimized by making as many terms zero as possible: $y_i = b_i'/\sigma_i$ for $1 \le i \le k$ and y_i arbitrary for $k + 1 \le i \le q$. Since $\|\mathbf{x}\|_2 = \|\mathbf{Vy}\|_2 = \|\mathbf{y}\|_2$, the $\mathbf{x}$ that has least norm from among all solutions to the least-squares problem comes from $y_i = 0$ for $k + 1 \le i \le q$; all other solutions can be obtained by adding to that $\mathbf{x}$ an arbitrary linear combination of $\mathbf{v}_{k+1}, \ldots, \mathbf{v}_q$, the last $q - k$ columns of $\mathbf{V}$.

This gives a method for solving least-squares problems:

(8.24) To find $\mathbf{x}$ minimizing $\|\mathbf{Ax} - \mathbf{b}\|_2$ with $\mathbf{A}$ having rank k:

1. Find the singular value decomposition $\mathbf{A} = \mathbf{U\Sigma V}^H$.
2. Compute $\mathbf{b}' = \mathbf{U}^H\mathbf{b}$.

3. Compute $\mathbf{y}$ with $y_i = b_i'/\sigma_i$ for $1 \le i \le k$, $y_i = 0$ otherwise.
4. Compute $\mathbf{x}_0 = \mathbf{V}\mathbf{y}$.
5. $\mathbf{x}_0$ solves the least-squares problem, and among all such solutions $\mathbf{x}_0$ has the smallest 2-norm; any other $\mathbf{x}'$ is a solution if and only if $\mathbf{x}'$ equals $\mathbf{x}_0$ plus a linear combination of the last $q - k$ columns of $\mathbf{V}$.

The process (8.24) can be more compactly described by the simple device of defining a matrix that handles step 3.

(8.25) ***Definition.*** Suppose that $\mathbf{\Sigma}$ is a $p \times q$ matrix with $\langle\mathbf{\Sigma}\rangle_{ij} = 0$ for $i \ne j$ and with $\langle\mathbf{\Sigma}\rangle_{ii} = \sigma_i$ for all i, with $\sigma_i \ne 0$ for $1 \le i \le k$ and $\sigma_i = 0$ for $k + 1 \le i \le \min\{p, q\}$. Then $\mathbf{\Sigma}^+$ is that $q \times p$ matrix (*note reversal of p and q*) whose only nonzero entries are $\langle\mathbf{\Sigma}^+\rangle_{ii} = 1/\sigma_i$ for $1 \le i \le k$.

In this notation, $\mathbf{x}_0$ in (8.24) is just $\mathbf{x}_0 = \mathbf{V}\mathbf{\Sigma}^+\mathbf{U}^H\mathbf{b}$; we have proved the following important result.

(8.26) **Key Theorem** (least squares and singular values). Suppose that $\mathbf{A} = \mathbf{U}\mathbf{\Sigma}\mathbf{V}^H$ is the singular value decomposition of the $p \times q$ matrix $\mathbf{A}$ of rank k, and that $\mathbf{A}^+ = \mathbf{V}\mathbf{\Sigma}^+\mathbf{U}^H$ is the so-called *pseudoinverse* of $\mathbf{A}$, where $\mathbf{\Sigma}^+$ is as in Definition 8.25. Then:
(a) $\mathbf{x}_0 = \mathbf{A}^+\mathbf{b}$ minimizes $\|\mathbf{A}\mathbf{x} - \mathbf{b}\|_2$ with respect to $\mathbf{x}$.
(b) Among all minimizers $\mathbf{x}'$ of $\|\mathbf{A}\mathbf{x} - \mathbf{b}\|_2$, $\mathbf{x}_0 = \mathbf{A}^+\mathbf{b}$ has least 2-norm.
(c) $\mathbf{x}'$ minimizes $\|\mathbf{A}\mathbf{x} - \mathbf{b}\|_2$ if and only if $\mathbf{x}' = \mathbf{x}_0 + \mathbf{v}$, where $\mathbf{v}$ is an arbitrary linear combination of the final $q - k$ columns of $\mathbf{V}$ and $\mathbf{x}_0 = \mathbf{A}^+\mathbf{b}$.

(8.27) ***Example.*** Consider the least-squares problem $\mathbf{A}\mathbf{x} \approx \mathbf{b}$:

$$\begin{bmatrix} 1 & 1 \\ 2 & 2 \\ 2 & 2 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \end{bmatrix} \approx \begin{bmatrix} 15 \\ 15 \\ -30 \end{bmatrix}.$$

The singular value decomposition of $\mathbf{A}$ was obtained in Example 8.17. Following the procedure in (8.24), we compute $\mathbf{b}' = \mathbf{U}^H\mathbf{b}$, $\mathbf{y} = \mathbf{\Sigma}^+\mathbf{b}'$, and then $\mathbf{x}_0 = \mathbf{V}\mathbf{y}$:

$$\mathbf{b}' = \begin{bmatrix} \frac{1}{3} & \frac{2}{3} & \frac{2}{3} \\ -\frac{2\sqrt{5}}{5} & \frac{\sqrt{5}}{5} & \frac{4\sqrt{5}}{15} \\ \frac{2\sqrt{5}}{15} & \frac{4\sqrt{5}}{15} & -\frac{\sqrt{5}}{3} \end{bmatrix} \begin{bmatrix} 15 \\ 15 \\ -30 \end{bmatrix} = \begin{bmatrix} -5 \\ -11\sqrt{5} \\ 16\sqrt{5} \end{bmatrix},$$

$$\mathbf{y} = \begin{bmatrix} \frac{1}{3\sqrt{2}} & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix} \begin{bmatrix} -5 \\ -11\sqrt{5} \\ 16\sqrt{5} \end{bmatrix} = \begin{bmatrix} -\frac{5\sqrt{2}}{6} \\ 0 \end{bmatrix},$$

$$\mathbf{x}_0 = \begin{bmatrix} \frac{\sqrt{2}}{2} & \frac{\sqrt{2}}{2} \\ \frac{\sqrt{2}}{2} & -\frac{\sqrt{2}}{2} \end{bmatrix} \begin{bmatrix} -\frac{5\sqrt{2}}{6} \\ 0 \end{bmatrix} = \begin{bmatrix} -\frac{5}{6} \\ -\frac{5}{6} \end{bmatrix}.$$

Alternatively, we can compute the pseudoinverse $\mathbf{A}^+ = \mathbf{V}\mathbf{\Sigma}^+\mathbf{U}^H$:

$$\mathbf{A}^+ = \begin{bmatrix} \frac{\sqrt{2}}{2} & \frac{\sqrt{2}}{2} \\ \frac{\sqrt{2}}{2} & -\frac{\sqrt{2}}{2} \end{bmatrix} \begin{bmatrix} \frac{1}{3\sqrt{2}} & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix} \begin{bmatrix} \frac{1}{3} & \frac{2}{3} & \frac{2}{3} \\ -\frac{2\sqrt{5}}{5} & \frac{\sqrt{5}}{5} & 0 \\ \frac{2\sqrt{5}}{15} & \frac{4\sqrt{5}}{15} & -\frac{\sqrt{5}}{15} \end{bmatrix}$$

$$= \begin{bmatrix} \frac{1}{18} & \frac{1}{9} & \frac{1}{9} \\ \frac{1}{18} & \frac{1}{9} & \frac{1}{9} \end{bmatrix}.$$

We then get $\mathbf{x}_0$ directly as $\mathbf{x}_0 = \mathbf{A}^+\mathbf{b}$:

$$\mathbf{x}_0 = \begin{bmatrix} \frac{1}{18} & \frac{1}{9} & \frac{1}{9} \\ \frac{1}{18} & \frac{1}{9} & \frac{1}{9} \end{bmatrix} \begin{bmatrix} 15 \\ 15 \\ -30 \end{bmatrix} = \begin{bmatrix} -\frac{5}{6} \\ -\frac{5}{6} \end{bmatrix},$$

as before. All other solutions $\mathbf{x}'$ are of the form $\mathbf{x}' = \mathbf{x}_0 + \alpha\mathbf{v}_2$:

$$\mathbf{x}' = \mathbf{x}_0 + \alpha\mathbf{v}_2 = \begin{bmatrix} -\frac{5}{6} \\ -\frac{5}{6} \end{bmatrix} + \alpha \begin{bmatrix} \frac{\sqrt{2}}{2} \\ -\frac{\sqrt{2}}{2} \end{bmatrix}.$$

When solving a least-squares problem in practice, it is often useful to modify the matrix $\mathbf{\Sigma}$ of singular values. Suppose, as is so often the case, that the entries in $\mathbf{A}$ are subject to measurement errors; then the smallest nonzero singular values computed for $\mathbf{A}$ may well have been zero if the measurements had been perfect. Using the reciprocal of such a singular value to solve a least-squares problem may well prove disastrous. It is often better to replace $\mathbf{\Sigma}$ by a matrix $\mathbf{\Sigma}_0$ obtained by replacing the smallest singular values in $\mathbf{\Sigma}$ by exact zeros, which is the effect of the construction in Theorem 8.21; those singular values that are of the magnitude of the errors inherent in the data should usually be treated this way. See Problem 6.

You should now be able to solve Problems 1 to 6.