Lay Chapter 6,
Orthogonality and Least Squares

Orthogonal Matrices

```
Clear[u];
```

$$u = \begin{pmatrix} -6 & -3 & 6 & 1 \\ -1 & 2 & 1 & -6 \\ 3 & 6 & 3 & -2 \\ 6 & -3 & 6 & -1 \\ 2 & -1 & 2 & 3 \\ -3 & 6 & 3 & 2 \\ -2 & -1 & 2 & -3 \\ 1 & 2 & 1 & 6 \end{pmatrix};$$

Note that the columns of u are orthogonal, and they are all of length 10.

```
Transpose[u].u;
% // MatrixForm
```

$$\begin{pmatrix} 100 & 0 & 0 & 0 \\ 0 & 100 & 0 & 0 \\ 0 & 0 & 100 & 0 \\ 0 & 0 & 0 & 100 \end{pmatrix}$$

Representation of Vectors in V == S ⊕ S^{Perp}

Let's find the projection of a vector y onto S = span(u1,u2,u3).

```
Clear[y, yHat, u1, u2, u3];

y  = {4, 3, 3, -1};

u1 = {1, 1, 0, 1};
u2 = {-1, 3, 1, -2};
u3 = {-1, 0, 1, 1};
```

Are the u's mutually orthogonal?

```
u = Transpose[{u1, u2, u3}];
% // MatrixForm
```

$$\begin{pmatrix} 1 & -1 & -1 \\ 1 & 3 & 0 \\ 0 & 1 & 1 \\ 1 & -2 & 1 \end{pmatrix}$$

```
Transpose[u].u;
% // MatrixForm
```

$$\begin{pmatrix} 3 & 0 & 0 \\ 0 & 15 & 0 \\ 0 & 0 & 3 \end{pmatrix}$$

Yes, the u's are mutually orthogonal

Find the projection of y onto span(u1,u2,u3).

$$\text{yHat} = \frac{\text{y.u1}}{\text{u1.u1}}\,\text{u1} + \frac{\text{y.u2}}{\text{u2.u2}}\,\text{u2} + \frac{\text{y.u3}}{\text{u3.u3}}\,\text{u3};$$

```
% // MatrixForm
```

$$\begin{pmatrix} 2 \\ 4 \\ 0 \\ 0 \end{pmatrix}$$

Then y - yHat is in U^{perp}

```
y - yHat;
% // MatrixForm
```

$$\begin{pmatrix} 2 \\ -1 \\ 3 \\ -1 \end{pmatrix}$$

... and the required decomposition is

```
Print["y = ", yHat, " + ", y - yHat]
```

```
y = {2, 4, 0, 0} + {2, -1, 3, -1}
```

Let's check that.
Is yHat in span(u1,u2,u3)?

```
RowReduce[{u1, u2, u3, yHat}];
% // MatrixForm
```

$$\begin{pmatrix} 1 & 0 & 0 & 2 \\ 0 & 1 & 0 & -1 \\ 0 & 0 & 1 & 3 \\ 0 & 0 & 0 & 0 \end{pmatrix}$$

Is y-yHat in (span(u1, u2, u3))^{perp} ?

```
Transpose[u].(y - yHat)
```

```
{0, 0, 0}
```

Is y == yHat + (y - yHat)?
This one should be easy.

```
y == yHat + (y - yHat)
```

```
True
```

Projection of a Vector onto the Column Space of an Orthogonal Matrix

```
Clear[u, y];
```

$$u = \begin{pmatrix} -6 & -3 & 6 & 1 \\ -1 & 2 & 1 & -6 \\ 3 & 6 & 3 & -2 \\ 6 & -3 & 6 & -1 \\ 2 & -1 & 2 & 3 \\ -3 & 6 & 3 & 2 \\ -2 & -1 & 2 & -3 \\ 1 & 2 & 1 & 6 \end{pmatrix};$$

```
y = {1, 1, 1, 1, 1, 1, 1, 1};
```

Note that the columns of u are orthogonal, and they are all of length 10.

```
Transpose[u].u;
% // MatrixForm
```

$$\begin{pmatrix} 100 & 0 & 0 & 0 \\ 0 & 100 & 0 & 0 \\ 0 & 0 & 100 & 0 \\ 0 & 0 & 0 & 100 \end{pmatrix}$$

Therefore, the closest point to y in the column space of u is yHat, where

```
(* yHat =
  1/100 ((y.u1) u1 + ... + (y.u4) u4) =  1/10 u.Transpose[u].y *)
```

Let's formalize that result. Let W be the column space of U.
See Lay 6.3, Theorem 10, p399.

```
projW[y_] := 1 / 100 u.Transpose[u].y

yHat = projW[y]
```

$$\left\{\frac{6}{5}, \frac{2}{5}, \frac{6}{5}, \frac{6}{5}, \frac{2}{5}, \frac{6}{5}, \frac{2}{5}, \frac{2}{5}\right\}$$

Check: Verify that yHat really is in the column space of u ...

```
Solve[u.{a1, a2, a3, a4} == yHat, {a1, a2, a3, a4}]
```

$$\left\{\left\{a1 \to 0,\ a2 \to \frac{2}{25},\ a3 \to \frac{6}{25},\ a4 \to 0\right\}\right\}$$

...and that y-yHat is orthogonal to each of the columns of u.

```
Transpose[u].(y - yHat)
```

{0, 0, 0, 0}

QR Decomposition

```
Clear[a, q, r];
```

$$a = \begin{pmatrix} 3 & 8 \\ 0 & 5 \\ -1 & -6 \end{pmatrix};$$

Mathematica has built-in support for QR factorization, but its definition of the matrices involved differs somewhat from that of Lay. Consult *Mathematica*'s Help Browser for the function QRDecomposition, and see that entry's "Further Examples."

```
{q, r} = QRDecomposition[a];

Map[MatrixForm, {q, r}]
```

$$\left\{\begin{pmatrix} \frac{3}{\sqrt{10}} & 0 & -\frac{1}{\sqrt{10}} \\ -\frac{1}{\sqrt{35}} & \sqrt{\frac{5}{7}} & -\frac{3}{\sqrt{35}} \end{pmatrix},\ \begin{pmatrix} \sqrt{10} & 3\sqrt{10} \\ 0 & \sqrt{35} \end{pmatrix}\right\}$$

Note that the matrix Q of Lay is the matrix Conjugate[Transpose[q]] of Mathematica.

```
Q = Conjugate[Transpose[q]];
% // MatrixForm
```

$$\begin{pmatrix} \frac{3}{\sqrt{10}} & -\frac{1}{\sqrt{35}} \\ 0 & \sqrt{\frac{5}{7}} \\ -\frac{1}{\sqrt{10}} & -\frac{3}{\sqrt{35}} \end{pmatrix}$$

Check.

```
a == Q.r

True
```

QR Decomposition

```
Clear[a, q, r];
```

$$a = \begin{pmatrix} -10 & 13 & 7 & -11 \\ 2 & 1 & -5 & 3 \\ -6 & 3 & 13 & -3 \\ 16 & -16 & -2 & 5 \\ 2 & 1 & -5 & -7 \end{pmatrix};$$

Mathematica has built-in support for QR factorization, but its definition of the matrices involved differs somewhat from that of Lay. Consult *Mathematica*'s Help Browser for the function QRDecomposition, and see that entry's "Further Examples."

```
{q, r} = QRDecomposition[a];

Map[MatrixForm, {q, r}]
```

$$\left\{ \begin{pmatrix} -\frac{1}{2} & \frac{1}{10} & -\frac{3}{10} & \frac{4}{5} & \frac{1}{10} \\ \frac{1}{2} & \frac{1}{2} & -\frac{1}{2} & 0 & \frac{1}{2} \\ \frac{1}{\sqrt{3}} & 0 & \frac{1}{\sqrt{3}} & \frac{1}{\sqrt{3}} & 0 \\ 0 & \frac{1}{\sqrt{2}} & 0 & 0 & -\frac{1}{\sqrt{2}} \end{pmatrix}, \begin{pmatrix} 20 & -20 & -10 & 10 \\ 0 & 6 & -8 & -6 \\ 0 & 0 & 6\sqrt{3} & -3\sqrt{3} \\ 0 & 0 & 0 & 5\sqrt{2} \end{pmatrix} \right\}$$

Note that the matrix Q of Lay is the matrix Conjugate[Transpose[q]] of Mathematica.

```
Q = Conjugate[Transpose[q]];
% // MatrixForm
```

$$\begin{pmatrix} -\frac{1}{2} & \frac{1}{2} & \frac{1}{\sqrt{3}} & 0 \\ \frac{1}{10} & \frac{1}{2} & 0 & \frac{1}{\sqrt{2}} \\ -\frac{3}{10} & -\frac{1}{2} & \frac{1}{\sqrt{3}} & 0 \\ \frac{4}{5} & 0 & \frac{1}{\sqrt{3}} & 0 \\ \frac{1}{10} & \frac{1}{2} & 0 & -\frac{1}{\sqrt{2}} \end{pmatrix}$$

Check.

```
a == Q.r

True
```

Least-Squares Solution of an Inconsistent System

Find a least-squares solution to the inconsistent system ax=b, where

```
Clear[a, b, x, x1, x2];
```

$$a = \begin{pmatrix} 4 & 0 \\ 0 & 2 \\ 1 & 1 \end{pmatrix};$$

```
b = {2, 0, 11};
```

Soln: Use the normal equations.

```
Transpose[a].a;
% // MatrixForm
```

$$\begin{pmatrix} 17 & 1 \\ 1 & 5 \end{pmatrix}$$

```
Transpose[a].b;
% // MatrixForm
```

$$\begin{pmatrix} 19 \\ 11 \end{pmatrix}$$

Now solve the system a^T ax = a^T b.

```
x = {x1, x2};
soln = Solve[Transpose[a].a.x == Transpose[a].b, {x1, x2}][[1]]
```

```
{x1 → 1, x2 → 2}
```

```
x /. soln
```

```
{1, 2}
```

Least-Squares Solution of an Inconsistent System

Find a least-squares solution to the inconsistent system ax=b, where

```
Clear[a, b, x, x1, x2, x3, x4];
```

$$a = \begin{pmatrix} 1 & 1 & 0 & 0 \\ 1 & 1 & 0 & 0 \\ 1 & 0 & 1 & 0 \\ 1 & 0 & 1 & 0 \\ 1 & 0 & 0 & 1 \\ 1 & 0 & 0 & 1 \end{pmatrix};$$

```
b = {-3, -1, 0, 2, 5, 1};
```

Soln: Use the normal equations.

```
Transpose[a].a;
% // MatrixForm
```

$$\begin{pmatrix} 6 & 2 & 2 & 2 \\ 2 & 2 & 0 & 0 \\ 2 & 0 & 2 & 0 \\ 2 & 0 & 0 & 2 \end{pmatrix}$$

```
Transpose[a].b;
% // MatrixForm
```

$$\begin{pmatrix} 4 \\ -4 \\ 2 \\ 6 \end{pmatrix}$$

Now solve the system a^T ax = a^T b.

```
x = {x1, x2, x3, x4};
soln = Solve[Transpose[a].a.x == Transpose[a].b, {x1, x2, x3, x4}]
```

```
Solve::svars : Equations may not give solutions for all "solve" variables. More…
```

```
{{x1 → 3 - x4, x2 → -5 + x4, x3 → -2 + x4}}
```

Here is a clearer view of the solution.

```
{x1, x2, x3, x4} /. soln
```

```
{{3 - x4, -5 + x4, -2 + x4, x4}}
```

and, better still, we have

```
(* x = {3,-5,-2,0} + x4 {-1,1,1,1} *)
```

Least-Squares Error

(1) Find a **least-squares solution** to the inconsistent system ax=b, where

```
Clear[a, b, x, x1, x2, xHat, soln, d];

a = (4  0
     0  2
     1  1);

b = {2, 0, 11};
```

Soln: Use the normal equations.

```
Transpose[a].a;
% // MatrixForm

(17  1
 1   5)
```

```
Transpose[a].b;
% // MatrixForm

(19
 11)
```

Now solve the system a^T ax = a^Tb.

```
x = {x1, x2};
soln = Solve[Transpose[a].a.x == Transpose[a].b, {x1, x2}]

{{x1 → 1, x2 → 2}}
```

xHat is the least-squares solution. In this case it is unique because a^T a is invertible: xHat = $(a^T\ a)^{-1} a^T$b.

```
xHat = x /. soln[[1]]

{1, 2}
```

(2) Find a **least-squares error** of this approximation.

```
d = Sqrt[(b - a.xHat).(b - a.xHat)]
```

$2\sqrt{21}$

Least-Squares Solution via QR Decomposition

Find a least-squares solution to the system ax=b, where

```
Clear[a, b, q, r, Q, xHat, x1, x2, x3, soln];

a = {{1, 3, 5}, {1, 1, 0}, {1, 1, 2}, {1, 3, 3}};

b = {3, 5, 7, -3};
```

$$a = \begin{pmatrix} 1 & 3 & 5 \\ 1 & 1 & 0 \\ 1 & 1 & 2 \\ 1 & 3 & 3 \end{pmatrix};$$

Let's use the QR Decomposition of a to find xHat, as in Lay Theorem 15, page 414.
(1) Calculate the QR Decomposition of a.

```
{q, r} = QRDecomposition[a];
Map[MatrixForm, {q, r}]
```

$$\left\{ \begin{pmatrix} \frac{1}{2} & \frac{1}{2} & \frac{1}{2} & \frac{1}{2} \\ \frac{1}{2} & -\frac{1}{2} & -\frac{1}{2} & \frac{1}{2} \\ \frac{1}{2} & -\frac{1}{2} & \frac{1}{2} & -\frac{1}{2} \end{pmatrix}, \begin{pmatrix} 2 & 4 & 5 \\ 0 & 2 & 3 \\ 0 & 0 & 2 \end{pmatrix} \right\}$$

Note that the matrix Q of Lay is the matrix Conjugate[Transpose[q]] of Mathematica.

```
Q = Conjugate[Transpose[q]];
% // MatrixForm
```

$$\begin{pmatrix} \frac{1}{2} & \frac{1}{2} & \frac{1}{2} \\ \frac{1}{2} & -\frac{1}{2} & -\frac{1}{2} \\ \frac{1}{2} & -\frac{1}{2} & \frac{1}{2} \\ \frac{1}{2} & \frac{1}{2} & -\frac{1}{2} \end{pmatrix}$$

Check.

```
a == Q.r

True
```

(2) Use the QR Decomposition of a to calculate xHat.

```
xHat = Inverse[r].Transpose[Q].b

{10, -6, 2}
```

Note that Lay suggests that, for numerical reasons, it is preferable to solve for xHat directly from the equation r.xHat==Transpose[Q].b.

```
Clear[x1, x2, x3, soln]

Print["r.{x1,x2,x3}^T == Q^T.b"]

Print[r // MatrixForm, ".", {x1, x2, x3} // MatrixForm,
 "==", Transpose[Q] // MatrixForm, ".", b // MatrixForm]
```

r.{x1,x2,x3}^{T} == Q^T.b

$$\begin{pmatrix} 2 & 4 & 5 \\ 0 & 2 & 3 \\ 0 & 0 & 2 \end{pmatrix} . \begin{pmatrix} x1 \\ x2 \\ x3 \end{pmatrix} == \begin{pmatrix} \frac{1}{2} & \frac{1}{2} & \frac{1}{2} & \frac{1}{2} \\ \frac{1}{2} & -\frac{1}{2} & -\frac{1}{2} & \frac{1}{2} \\ \frac{1}{2} & -\frac{1}{2} & \frac{1}{2} & -\frac{1}{2} \end{pmatrix} . \begin{pmatrix} 3 \\ 5 \\ 7 \\ -3 \end{pmatrix}$$

Let's try that.

```
soln = Solve[r.{x1, x2, x3} == Transpose[Q].b, {x1, x2, x3}][[1]];

{x1, x2, x3} = {x1, x2, x3} /. soln

{10, -6, 2}
```