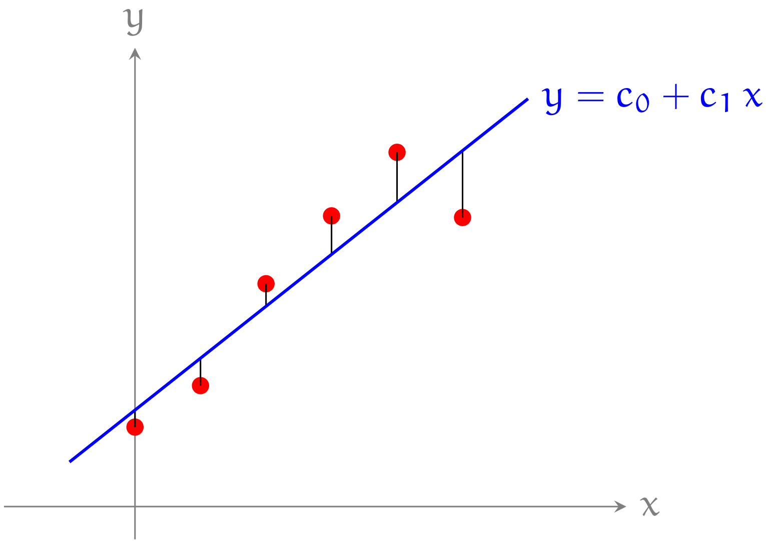
## Least Squares

that is, we try to minimize the length of the *residual* **r** whose components are given by

$$r_i = y_i - (c_0 + c_1\, x_i)\,.$$




Let **x** be the vector whose components are $x_i$ and **y** be the vector whose components are $y_i$. Furthermore let

## Least Squares

$$A = \begin{bmatrix} 1 & x_1 \\ 1 & x_2 \\ \vdots & \vdots \\ 1 & x_n \end{bmatrix} = \begin{bmatrix} \mathbf{1} & \mathbf{x} \end{bmatrix}$$

where **1** is a vector of ones (that is, in MATLAB, `ones(n,1)`). The equations

$$y_i = c_0 + c_1\, x_i$$

are given by the matrix equation

$$\begin{bmatrix} 1 & x_1 \\ 1 & x_2 \\ \vdots & \vdots \\ 1 & x_n \end{bmatrix} \begin{bmatrix} c_0 \\ c_1 \end{bmatrix} = \begin{bmatrix} y_1 \\ y_2 \\ \vdots \\ y_n \end{bmatrix};$$

## Least Squares

that is

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

where

$$\mathbf{c} = \begin{bmatrix} c_0 \\ c_1 \end{bmatrix}.$$

This is an overdetermined system ($n$ equations in $2$ variables).

### Example

Find the least squares fit for the data $(0,\ 0.485)$, $(0.4,\ 0.738)$, $(0.8,\ 1.360)$, $(1.2,\ 1.774)$, $(1.6,\ 2.162)$ and $(2.0,\ 1.764)$ (this is the data used to generate the above diagram).

**Solution:** Using MATLAB we have

## Least Squares

```
>> x=[0:0.4:2]'
x =
         0
    0.4000
    0.8000
    1.2000
    1.6000
    2.0000
>> A=[ones(6,1) x]
A =
    1.0000         0
    1.0000    0.4000
    1.0000    0.8000
    1.0000    1.2000
    1.0000    1.6000
    1.0000    2.0000
```

## LEAST SQUARES

```
>> y=[0.4846 0.7384 1.3595 1.7740 2.1620 1.7640]'
y =
    0.4846
    0.7384
    1.3595
    1.7740
    2.1620
    1.7640
>> c=A\y
c =
    0.5888
    0.7916
```

Thus the best fit is

$$y = 0.5888 + 0.7916\,x.$$

## LEAST SQUARES

Note that MATLAB'S backslash operator, \, will *automatically* compute the least squares solution for an overdetermined system. The residual for this fit is

```
>> r=y-A*c
r =
   -0.1042
   -0.1671
    0.1374
    0.2353
    0.3066
   -0.4080
>> norm(r)
ans =
    0.6111
```

## LEAST SQUARES

If we were unhappy with this fit or we suspected that the relationship between the variables $x$ and $y$ was quadratic

$$y = c_0 + c_1\,x + c_2\,x^2$$

(for example, if the data came from projectile motion) then we would solve the matrix equation

$$\begin{bmatrix} 1 & x_1 & x_1^2 \\ 1 & x_2 & x_2^2 \\ \vdots & \vdots & \vdots \\ 1 & x_n & x_n^2 \end{bmatrix} \begin{bmatrix} c_0 \\ c_1 \\ c_2 \end{bmatrix} = \mathbf{y}.$$

Let

$$\mathbf{x}^2 = \begin{bmatrix} x_1^2 \\ x_2^2 \\ \vdots \\ x_n^2 \end{bmatrix}$$

## LEAST SQUARES

be the *component-wise* square of $\mathbf{x}$ (note that $\mathbf{x}^2$ is **not** defined as a matrix product). In MATLAB this is given by

```
x.*x
```

or

```
x.^2
```

Therefore the matrix system may be written as

$$\begin{bmatrix} \mathbf{1} & \mathbf{x} & \mathbf{x}^2 \end{bmatrix} \mathbf{c} = \mathbf{y}.$$

Using the above data, we have

```
>> A = [A x.*x]
A =
     1.0000         0         0
     1.0000    0.4000    0.1600
     1.0000    0.8000    0.6400
     1.0000    1.2000    1.4400
     1.0000    1.6000    2.5600
     1.0000    2.0000    4.0000
```

# Least Squares

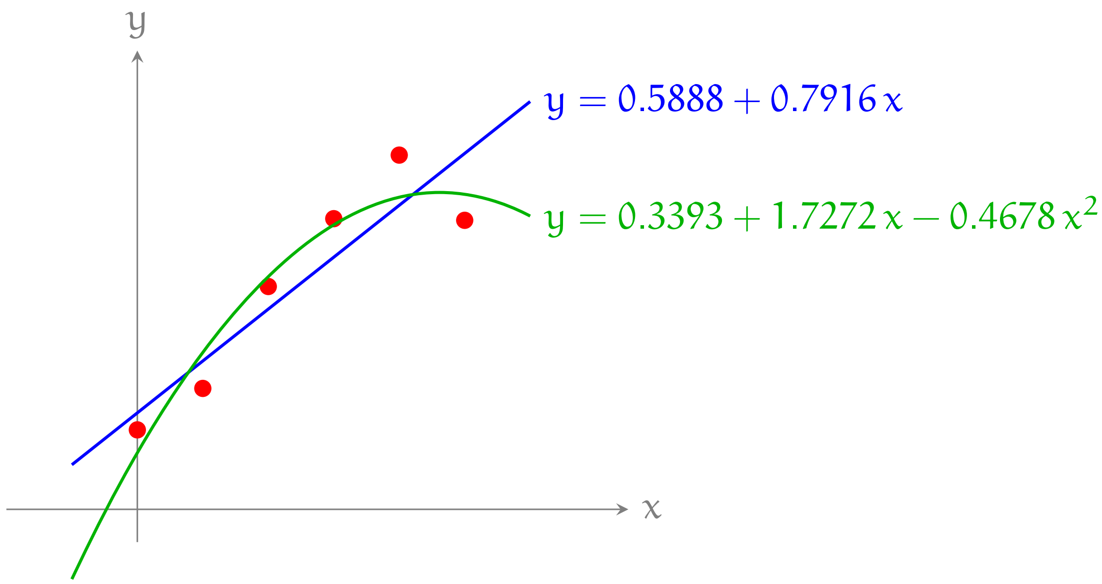
```
>> c=A\y
c =
    0.3393
    1.7272
   -0.4678
>> r=y-A*c
r =
    0.1453
   -0.2170
   -0.0622
    0.0357
    0.2567
   -0.1585
>> norm(r)
ans =
    0.4054
```

# Least Squares

The best quadratic fit is

$$y = 0.3393 + 1.7272\,x - 0.4678\,x^2$$

and the length of the residual has been reduced to $0.4054$.



## Least Squares

If we wish to fit a polynomial of degree $k$ to a data set then we solve

$$\begin{bmatrix}\mathbf{1} & \mathbf{x} & \mathbf{x}^2 & \cdots & \mathbf{x}^k\end{bmatrix} \mathbf{c} = \mathbf{y}.$$

Remember that the columns of the coefficient matrix are component-wise powers of the vector $\mathbf{x}$.

We can extend this to fit any function to a data set. Suppose we wish to fit the data to a collection of functions $f_i(x)$; that is

$$y = c_1 f_1(x) + c_2 f_2(x) + \cdots + c_k f_k(x)$$

then we solve the system

$$\begin{bmatrix}f_1(\mathbf{x}) & f_2(\mathbf{x}) & \cdots & f_k(\mathbf{x})\end{bmatrix} \mathbf{c} = \mathbf{y}.$$

Again these columns are the function $f_i(x)$ applied to each component of $\mathbf{x}$. This is the default behaviour of MATLAB.

## Least Squares

In particular, if we wish to fit an exponential to a data set

$$y = a\,e^{bx}$$

we first take logarithms

$$\log y = \log a + b\,x$$

and then solve

$$\begin{bmatrix}\mathbf{1} & \mathbf{x}\end{bmatrix} \begin{bmatrix}\log a \\ b\end{bmatrix} = \log \mathbf{y}.$$

Similarly to fit a power law to a data set

$$y = a\,x^k,$$

we take logarithms

$$\log y = \log a + k \log x$$

and solve

$$\begin{bmatrix}\mathbf{1} & \log \mathbf{x}\end{bmatrix} \begin{bmatrix}\log a \\ k\end{bmatrix} = \log \mathbf{y}.$$

## Least Squares

We have seen that the residual from a least squares fit $A\mathbf{c} = \mathbf{y}$ is

$$\mathbf{r} = \mathbf{y} - A\mathbf{c} = \mathrm{perp}_{\mathrm{col}\,(A)}(\mathbf{y}) \in (\mathrm{col}\,(A))^{\perp}.$$

Therefore, for any column of $A$, $\mathbf{a}_i$, we have

$$0 = \mathbf{a}_i \cdot \mathbf{r} = \mathbf{a}_i^T \mathbf{r}.$$

Thus

$$\begin{bmatrix} \mathbf{a}_1^T \\ \mathbf{a}_2^T \\ \vdots \\ \mathbf{a}_n^T \end{bmatrix} \mathbf{r} = \mathbf{0};$$

in other words

$$A^T \mathbf{r} = \mathbf{0}.$$

This is equivalent to

$$A^T A\mathbf{c} = A^T \mathbf{y};$$

the so-called *normal equations* of the overdetermined system $A\mathbf{c} = \mathbf{y}$.

## Least Squares

If $A = QR$ then

$$A^T A = R^T Q^T Q R = R^T R$$

and so the normal equations become

$$R^T R\mathbf{c} = R^T Q^T \mathbf{y}.$$

If the columns of $A$ are linearly independent then $R$ is invertible and so we obtain

$$R\mathbf{c} = Q^T \mathbf{y}.$$

Hence

**Theorem 12.1 (Least Squares Theorem)**

*Let $A$ be an $n \times k$ matrix and $\mathbf{y} \in \mathbf{R}^n$. Then $A\mathbf{c} = \mathbf{y}$ always has a least squares solution $\bar{\mathbf{c}}$. Moreover $\bar{\mathbf{c}}$ is a least squares solution if and only if it is a solution of the normal equations*

$$A^T A\mathbf{c} = A^T \mathbf{y}.$$

*In addition, $A$ has linearly independent columns if and only if $A^T A$ is invertible. In this case the least squares solution is unique.*

## Normal Equations

For an overdetermined system $A\mathbf{x} = \mathbf{b}$ we have seen that the least squares solution is the solution of the normal equations

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

and that if $A$ has linearly independent columns then $A^T A$ is invertible. Thus, in this case, the solution is

$$\mathbf{x} = (A^T A)^{-1} A^T \mathbf{b}.$$

Note that $A$ is, in general, not a square matrix and so we can **not** simplify this expression by writing

$$(A^T A)^{-1} \overset{!}{=} A^{-1} A^{-T}.$$

Normally would not want to compute an inverse. However if the rank of $A$ is small (that is $A$ has a small number of columns) then $A^T A$ will be a small square matrix. For example, in the least squares fit for a straight line, $A$ has 2 columns and so $A^T A$ is a $2 \times 2$ matrix

## Pseudoinverse

$$A^T A = \begin{bmatrix} \mathbf{1}^T \\ \mathbf{x}^T \end{bmatrix} \begin{bmatrix} \mathbf{1} & \mathbf{x} \end{bmatrix} = \begin{bmatrix} \mathbf{1}^T \mathbf{1} & \mathbf{1}^T \mathbf{x} \\ \mathbf{x}^T \mathbf{1} & \mathbf{x}^T \mathbf{x} \end{bmatrix} = \begin{bmatrix} n & \sum x_i \\ \sum x_i & \|\mathbf{x}\|^2 \end{bmatrix}$$

which can be easily inverted. Motivated by this we have

**Definition 12.2 (Pseudoinverse)**

*Let $A$ be a matrix with linearly independent columns. Then the pseudoinverse of $A$ is the matrix $A^+$ given by*

$$A^+ = (A^T A)^{-1} A^T.$$

Note that if $A$ is square then $A^+ = A^{-1}$. If $Q$ has orthonormal columns then $Q^T Q = I$ and so

$$Q^+ = Q^T.$$

## Pseudoinverse

### Example

Find the pseudoinverse of a (column) vector $\mathbf{v}$.
**Solution:** We have

$$\mathbf{v}^+ = \left(\mathbf{v}^T \mathbf{v}\right)^{-1} \mathbf{v}^T = \frac{\mathbf{v}^T}{\|\mathbf{v}\|^2}.$$

The solution to an overdetermined system $A\,\mathbf{x} = \mathbf{b}$ is

$$\mathbf{x} = A^+ \mathbf{b}.$$

We can also write the projection matrix in terms of the pseudoinverse. We have

## Pseudoinverse

### Theorem 12.3

*Let $W$ be a subspace of $\mathbf{R}^n$ and $A$ be a $n \times m$ matrix whose columns are linearly independent and form a basis for $W$. For any $\mathbf{x} \in \mathbf{R}^n$*

$$\mathrm{proj}_W(\mathbf{x}) = A\,A^+ \mathbf{x}.$$

*In particular, the projection matrix that projects $\mathbf{R}^n$ onto $W$ is given by*

$$P = A\,A^+.$$

This theorem allows us to find a projection *without* computing an orthonormal basis. However the price to pay is that we must invert the matrix $A^T A$. For a projection onto a 1-dimensional subspace spanned by $\mathbf{v}$ we have

$$P = \mathbf{v}\,\mathbf{v}^+ = \frac{1}{\|\mathbf{v}\|^2}\mathbf{v}\,\mathbf{v}^T = \mathbf{u}\,\mathbf{u}^T$$

where

# Pseudoinverse

$$\mathbf{u} = \frac{\mathbf{v}}{\|\mathbf{v}\|}$$

is a unit vector parallel to $\mathbf{v}$.

### Theorem 12.4

*Let $A$ be a matrix with linearly independent columns. Then the pseudoinverse $A^+$ of $A$ satisfies the Penrose conditions for $A$; that is*

(a) $A\,A^+\,A = A$

(b) $A^+\,A\,A^+ = A^+$

(c) $A\,A^+$ *and* $A^+\,A$ *are symmetric.*

Pseudoinverses can be generalised to matrices whose columns are not linearly independent.

# Symmetric Matrices

We have seen symmetric matrices (matrices that satisfy $A^T = A$) have featured in the discussion above. In fact symmetric matrices have some *very* nice properties. Consider the symmetric matrix

$$A = \begin{bmatrix} 1 & 2 \\ 2 & -2 \end{bmatrix}.$$

It is easily seen that the eigenvalues are $-3$ and $2$ with corresponding eigenvectors

$$\mathbf{x}_1 = \begin{bmatrix} 1 \\ -2 \end{bmatrix}, \qquad \mathbf{x}_2 = \begin{bmatrix} 2 \\ 1 \end{bmatrix}.$$

Thus $A$ is diagonalizable with $P = \begin{bmatrix} \mathbf{x}_1 & \mathbf{x}_2 \end{bmatrix}$ and

$$P^{-1}\,A\,P = \begin{bmatrix} -3 & 0 \\ 0 & 2 \end{bmatrix} = D.$$

However, note that

$$\mathbf{x}_1 \cdot \mathbf{x}_2 = 0;$$

the eigenvectors are *orthogonal*.

## Symmetric Matrices

If we normalize the eigenvectors

$$\mathbf{u}_1 = \frac{\sqrt{5}}{5}\begin{bmatrix}1\\-2\end{bmatrix}, \qquad \mathbf{u}_2 = \frac{\sqrt{5}}{5}\begin{bmatrix}2\\1\end{bmatrix}.$$

we obtain an *orthogonal* matrix

$$Q = \begin{bmatrix}\mathbf{u}_1 & \mathbf{u}_2\end{bmatrix}$$

that diagonalizes $A$. Thus

$$A = Q\,D\,Q^T$$

since $Q^{-1} = Q^T$. Thus we make the definition

**Definition 13.1**

*A square matrix $A$ is orthogonally diagonalizable if there exists an orthogonal matrix $Q$ such that $Q^T A\,Q = D$, a diagonal matrix.*

## Symmetric Matrices

**Theorem 13.2**

*If $A$ is orthogonally diagonalizable then $A$ is symmetric.*

Proof: If $A$ is orthogonally diagonalizable then there exists an orthogonal matrix $Q$ such that $A = Q\,D\,Q^T$. Now

$$A^T = \left(Q\,D\,Q^T\right)^T = Q\,D^T\,Q^T = Q\,D\,Q^T = A$$

since $D$ is diagonal. Therefore $A$ is symmetric. $\square$

This result does not show that all symmetric matrices are orthogonally diagonalizable (we are coming to that). Symmetric matrices have several nice properties.

**Theorem 13.3**

*Let $A$ be a real symmetric matrix. The eigenvalues of $A$ are real.*

# Symmetric Matrices

Proof: Let $\lambda$ be an eigenvalue of $A$ with corresponding eigenvector $\mathbf{x}$. Therefore $A\,\mathbf{x} = \lambda\,\mathbf{x}$. Taking complex conjugates, we have

$$\overline{A}\,\overline{\mathbf{x}} = A\,\overline{\mathbf{x}} = \overline{\lambda}\,\overline{\mathbf{x}}$$

since $A$ is real. Thus

$$\overline{\mathbf{x}}^{T} A^{T} = \overline{\mathbf{x}}^{T} A = \overline{\lambda}\,\overline{\mathbf{x}}^{T}$$

since $A$ is symmetric. Now

$$\lambda\left(\overline{\mathbf{x}}^{T}\,\mathbf{x}\right) = \overline{\mathbf{x}}^{T}\,\lambda\,\mathbf{x} = \overline{\mathbf{x}}^{T}\,A\,\mathbf{x} = \overline{\lambda}\left(\overline{\mathbf{x}}^{T}\,\mathbf{x}\right)$$

and so

$$\left(\lambda - \overline{\lambda}\right)\overline{\mathbf{x}}^{T}\,\mathbf{x} = 0.$$

Let $\mathbf{x} = \mathbf{a} + i\,\mathbf{b}$ with $\mathbf{a}$ and $\mathbf{b}$ are real. Now $\overline{\mathbf{x}} = \mathbf{a} - i\,\mathbf{b}$

$$\overline{\mathbf{x}}^{T}\,\mathbf{x} = \left(\mathbf{a}^{T} - i\,\mathbf{b}^{T}\right)\left(\mathbf{a} + i\,\mathbf{b}\right) = \mathbf{a}^{T}\,\mathbf{a} + \mathbf{b}^{T}\mathbf{b} + i\left(\mathbf{a}^{T}\,\mathbf{b} - \mathbf{b}^{T}\,\mathbf{a}\right).$$

However $\mathbf{b}^{T}\,\mathbf{a} = \left(\mathbf{a}^{T}\,\mathbf{b}\right)^{T} = \mathbf{a}^{T}\,\mathbf{b}$ since $\mathbf{a}^{T}\,\mathbf{b}$ is a scalar and so



$$\overline{\mathbf{x}}^{T}\,\mathbf{x} = \mathbf{a}^{T}\,\mathbf{a} + \mathbf{b}^{T}\mathbf{b} \neq 0.$$

Therefore we conclude

$$\lambda - \overline{\lambda} = 0$$

and so $\lambda$ is real. □

**Theorem 13.4**

*Let $A$ be a symmetric matrix. Then any two eigenvectors corresponding to distinct eigenvalues are orthogonal.*

Proof: Suppose

$$A\,\mathbf{x}_1 = \lambda_1\,\mathbf{x}_1, \qquad A\,\mathbf{x}_2 = \lambda_2\,\mathbf{x}_2$$

with $\lambda_1 \neq \lambda_2$. Now

$$\lambda_1\left(\mathbf{x}_1 \cdot \mathbf{x}_2\right) = \left(A\,\mathbf{x}_1\right)^{T}\mathbf{x}_2 = \mathbf{x}_1^{T}\,A^{T}\,\mathbf{x}_2 = \mathbf{x}_1^{T}\,A\,\mathbf{x}_2$$

since $A$ is symmetric.

## Symmetric Matrices

However

$$\mathbf{x}_1^T A\,\mathbf{x}_2 = \mathbf{x}_1^T\,(\lambda_2\,\mathbf{x}_2) = \lambda_2\,(\mathbf{x}_1 \cdot \mathbf{x}_2)$$

and so

$$(\lambda_1 - \lambda_2)\,\mathbf{x}_1 \cdot \mathbf{x}_2 = 0.$$

Since $\lambda_1 \neq \lambda_2$, we have

$$\mathbf{x}_1 \cdot \mathbf{x}_2 = 0$$

and so $\mathbf{x}_1$ and $\mathbf{x}_2$ are orthogonal. $\square$

**THEOREM 13.5 (Spectral Theorem)**

*Let $A$ be a real $n \times n$ matrix. Then $A$ is symmetric if and only if it is orthogonally diagonalizable.*

Proof: See Poole Theorem 5.20.
This theorem shows that every real symmetric matrix is not defective (that is the geometric multiplicity is always equal to the algebraic multiplicity for each of its eigenvalues).

## Symmetric Matrices

**Example**

Orthogonally diagonalize the matrix

$$A = \begin{bmatrix} 2 & 1 & 1 \\ 1 & 2 & 1 \\ 1 & 1 & 2 \end{bmatrix}.$$

**Solution:** The eigenvalues of $A$ are 4, 1, 1 (check). The eigenspace associated with 4 is

$$[A - 4\,I] = \begin{bmatrix} -2 & 1 & 1 \\ 1 & -2 & 1 \\ 1 & 1 & -2 \end{bmatrix} \to \begin{bmatrix} -2 & 1 & 1 \\ 0 & -3 & 3 \\ 0 & 0 & 0 \end{bmatrix}$$

and so

$$E_4 = \text{span}\left(\begin{bmatrix} 1 \\ 1 \\ 1 \end{bmatrix}\right).$$

## Symmetric Matrices

For the repeated eigenvalue 1 we have

$$[A - I] = \begin{bmatrix} 1 & 1 & 1 \\ 1 & 1 & 1 \\ 1 & 1 & 1 \end{bmatrix} \to \begin{bmatrix} 1 & 1 & 1 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix}$$

and so

$$E_1 = \operatorname{span}\left( \begin{bmatrix} -1 \\ 0 \\ 1 \end{bmatrix}, \begin{bmatrix} 0 \\ -1 \\ 1 \end{bmatrix} \right).$$

An orthonormal basis for $E_4$ is given by

$$\mathbf{q}_1 = \frac{\sqrt{3}}{3} \begin{bmatrix} 1 \\ 1 \\ 1 \end{bmatrix}.$$

## Symmetric Matrices

We need to use Gram Schmidt to compute an orthonormal basis for $E_1$. We have

$$\mathbf{q}_2 = \frac{\sqrt{2}}{2} \begin{bmatrix} -1 \\ 0 \\ 1 \end{bmatrix}$$

and

$$\mathbf{v}_3 = \begin{bmatrix} 0 \\ -1 \\ 1 \end{bmatrix} - \left( \begin{bmatrix} 0 \\ -1 \\ 1 \end{bmatrix} \cdot \mathbf{q}_2 \right) \mathbf{q}_2 = \begin{bmatrix} 0 \\ -1 \\ 1 \end{bmatrix} - \frac{1}{2} \begin{bmatrix} -1 \\ 0 \\ 1 \end{bmatrix} = \begin{bmatrix} \frac{1}{2} \\ -1 \\ \frac{1}{2} \end{bmatrix}.$$

Therefore

$$\mathbf{q}_3 = \frac{\sqrt{6}}{6} \begin{bmatrix} 1 \\ -2 \\ 1 \end{bmatrix}.$$

# Symmetric Matrices

Finally

$$Q = \begin{bmatrix} \mathbf{q}_1 & \mathbf{q}_2 & \mathbf{q}_3 \end{bmatrix} = \begin{bmatrix} \frac{\sqrt{3}}{3} & -\frac{\sqrt{2}}{2} & \frac{\sqrt{6}}{6} \\ \frac{\sqrt{3}}{3} & 0 & -\frac{\sqrt{6}}{3} \\ \frac{\sqrt{3}}{3} & \frac{\sqrt{2}}{2} & \frac{\sqrt{6}}{6} \end{bmatrix}.$$

It is straightforward to verify

$$Q^T A Q = \begin{bmatrix} 4 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix}.$$

# Symmetric Matrices

Note that the spectral theorem implies

$$A = Q D Q^T = \begin{bmatrix} \mathbf{q}_1 & \mathbf{q}_2 & \cdots & \mathbf{q}_n \end{bmatrix} \begin{bmatrix} \lambda_1 & 0 & \cdots & 0 \\ 0 & \lambda_2 & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \vdots & \lambda_n \end{bmatrix} \begin{bmatrix} \mathbf{q}_1^T \\ \mathbf{q}_2^T \\ \vdots \\ \mathbf{q}_n^T \end{bmatrix}$$

$$= \begin{bmatrix} \lambda_1 \mathbf{q}_1 & \lambda_2 \mathbf{q}_2 & \cdots & \lambda_n \mathbf{q}_n \end{bmatrix} \begin{bmatrix} \mathbf{q}_1^T \\ \mathbf{q}_2^T \\ \vdots \\ \mathbf{q}_n^T \end{bmatrix}$$

$$= \lambda_1 \mathbf{q}_1 \mathbf{q}_1^T + \lambda_2 \mathbf{q}_2 \mathbf{q}_2^T + \cdots + \lambda_n \mathbf{q}_n \mathbf{q}_n^T.$$

This is called the *spectral decomposition* of $A$. Each of the terms $\lambda_i \mathbf{q}_i \mathbf{q}_i^T$ is a rank 1 matrix and $\mathbf{q}_i \mathbf{q}_i^T$ is the projection onto the subspace spanned by $\mathbf{q}_i$.

## Symmetric Matrices

### Example

Find the spectral decomposition for the matrix in the above example
**Solution:** We have $\lambda_1 = 4$ with

$$\mathbf{q}_1 = \frac{\sqrt{3}}{3}\begin{bmatrix}1\\1\\1\end{bmatrix}.$$

Therefore

$$\mathbf{q}_1\,\mathbf{q}_1^T = \frac{1}{3}\begin{bmatrix}1\\1\\1\end{bmatrix}\begin{bmatrix}1 & 1 & 1\end{bmatrix} = \frac{1}{3}\begin{bmatrix}1 & 1 & 1\\1 & 1 & 1\\1 & 1 & 1\end{bmatrix}.$$

$\lambda_2 = 1$ with

$$\mathbf{q}_2 = \frac{\sqrt{2}}{2}\begin{bmatrix}-1\\0\\1\end{bmatrix}$$

## Symmetric Matrices

and so

$$\mathbf{q}_2\,\mathbf{q}_2^T = \frac{1}{2}\begin{bmatrix}-1\\0\\1\end{bmatrix}\begin{bmatrix}-1 & 0 & 1\end{bmatrix} = \frac{1}{2}\begin{bmatrix}1 & 0 & -1\\0 & 0 & 0\\-1 & 0 & 1\end{bmatrix}.$$

Finally $\lambda_3 = 1$ with

$$\mathbf{q}_3 = \frac{\sqrt{6}}{6}\begin{bmatrix}1\\-2\\1\end{bmatrix}$$

and so

$$\mathbf{q}_3\,\mathbf{q}_3^T = \frac{1}{6}\begin{bmatrix}1\\-2\\1\end{bmatrix}\begin{bmatrix}1 & -2 & 1\end{bmatrix} = \frac{1}{6}\begin{bmatrix}1 & -2 & 1\\-2 & 4 & -2\\1 & -2 & 1\end{bmatrix}.$$

# Symmetric Matrices

Therefore

$$\begin{aligned} A &= \lambda_1 \mathbf{q}_1 \mathbf{q}_1^T + \lambda_2 \mathbf{q}_2 \mathbf{q}_2^T + \lambda_3 \mathbf{q}_3 \mathbf{q}_3^T \\ &= 4 \begin{bmatrix} \frac{1}{3} & \frac{1}{3} & \frac{1}{3} \\ \frac{1}{3} & \frac{1}{3} & \frac{1}{3} \\ \frac{1}{3} & \frac{1}{3} & \frac{1}{3} \end{bmatrix} + \begin{bmatrix} \frac{1}{2} & 0 & -\frac{1}{2} \\ 0 & 0 & 0 \\ -\frac{1}{2} & 0 & \frac{1}{2} \end{bmatrix} + \begin{bmatrix} \frac{1}{6} & -\frac{1}{3} & \frac{1}{6} \\ -\frac{1}{3} & \frac{2}{3} & -\frac{1}{3} \\ \frac{1}{6} & -\frac{1}{3} & \frac{1}{6} \end{bmatrix} \end{aligned}$$

Note that, since $\lambda_2 = \lambda_3$ we could combine the last two terms to give the rank 2 matrix

$$\begin{bmatrix} \frac{2}{3} & -\frac{1}{3} & -\frac{1}{3} \\ -\frac{1}{3} & \frac{2}{3} & -\frac{1}{3} \\ -\frac{1}{3} & -\frac{1}{3} & \frac{2}{3} \end{bmatrix}.$$

This matrix is the projection onto the 2-dimensional subspace spanned by $\mathbf{q}_2$, $\mathbf{q}_3$; that is, the eigenspace $E_1$.

# Symmetric Matrices

Observe that the spectral decomposition expresses a real symmetric matrix in terms of its eigenvalues and eigenvectors. We can use this to construct a symmetric matrix with given eigenvalues and (orthonormal) eigenvectors.

## Example

Find a $2 \times 2$ matrix with eigenvalues $\lambda_1 = 13$ and $\lambda_2 = -13$ with corresponding eigenvectors

$$\mathbf{x}_1 = \begin{bmatrix} 12 \\ 5 \end{bmatrix}, \qquad \mathbf{x}_2 = \begin{bmatrix} -5 \\ 12 \end{bmatrix}.$$

**Solution:** Note that $\mathbf{x}_1$ and $\mathbf{x}_2$ are orthogonal. Normalizing these eigenvectors we have

$$\mathbf{q}_1 = \frac{1}{13} \begin{bmatrix} 12 \\ 5 \end{bmatrix}, \qquad \mathbf{q}_2 = \frac{1}{13} \begin{bmatrix} -5 \\ 12 \end{bmatrix}.$$

## Symmetric Matrices

Therefore a matrix with the required properties will be

$$\begin{aligned} A &= \lambda_1 \mathbf{q}_1 \mathbf{q}_1^T + \lambda_2 \mathbf{q}_2 \mathbf{q}_2^T \\ &= \frac{1}{13}\begin{bmatrix} 12 \\ 5 \end{bmatrix}\begin{bmatrix} 12 & 5 \end{bmatrix} - \frac{1}{13}\begin{bmatrix} -5 \\ 12 \end{bmatrix}\begin{bmatrix} -5 & 12 \end{bmatrix} \\ &= \frac{1}{13}\left(\begin{bmatrix} 144 & 60 \\ 60 & 25 \end{bmatrix} - \begin{bmatrix} 25 & -60 \\ -60 & 144 \end{bmatrix}\right) \\ &= \frac{1}{13}\begin{bmatrix} 119 & 120 \\ 120 & -119 \end{bmatrix}. \end{aligned}$$

## Singular Values

We have seen that real symmetric matrices, $A$, have a (very) nice representation via the spectral theorem

$$A = \lambda_1 \mathbf{q}_1 \mathbf{q}_1^T + \lambda_2 \mathbf{q}_2 \mathbf{q}_2^T + \cdots + \lambda_n \mathbf{q}_n \mathbf{q}_n^T.$$

Is there any similar form for a non-symmetric or non-square matrices? For *any* $k \times n$ matrix $A$, the $n \times n$ matrix $A^T A$ is symmetric. Suppose $\mu$ is an eigenvalue of $A^T A$ and $\mathbf{v}$ is an associated *unit* eigenvector; that is

$$A^T A \mathbf{v} = \mu \mathbf{v}.$$

Now

$$0 \leqslant \|A \mathbf{v}\|^2 = (A \mathbf{v})^T A \mathbf{v} = \mathbf{v}^T A^T A \mathbf{v} = \mu \mathbf{v}^T \mathbf{v} = \mu \|\mathbf{v}\|^2 = \mu$$

since $\mathbf{v}$ is a unit vector. Therefore all the eigenvalues of $A^T A$ are not only real but also *non-negative*. It therefore makes sense to take the positive square root of this eigenvalues.