

Eigenvalue Problems

Eigenvalue problems arise in many contexts in physics. In matrix form,

$$A\vec{x} = \lambda\vec{x}$$

This is somewhat different from our previous SLE, which had the form

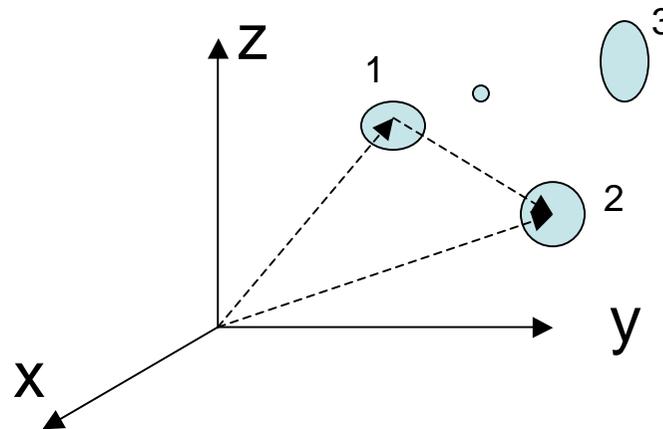
$$A\vec{x} = \vec{b}$$

where A , b were assumed known. In the eigenvalue problem we don't know x **or** λ . This makes the problem more difficult to solve.

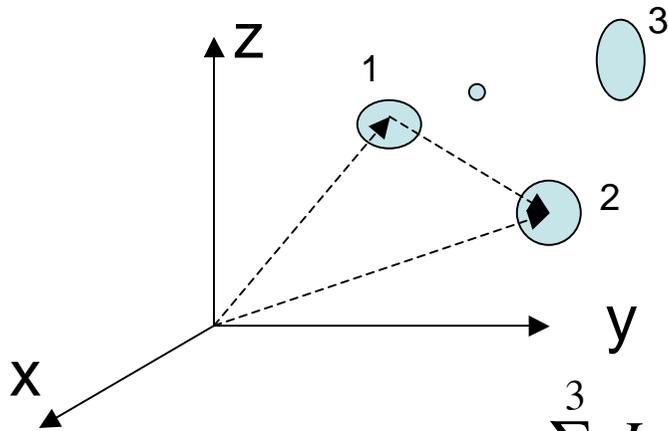
First example, moments of inertia

$$I_{m,n} = \sum_{i=1}^3 m_i r_i^2 \delta_{m,n} - m_i r_{i,m} r_{i,n}$$

Symmetric second rank tensor



Eigenvalue Problems



We can find the principal axes (orthonormal vectors) as follows:

$$\sum_{n=1}^3 I_{m,n} x_n^{(r)} = I^{(r)} x_m^{(r)} \quad \text{where } I^{(r)} \text{ is the } r^{\text{th}} \text{ eigenvalue}$$

or, in matrix notation $I \vec{x}^{(r)} = I^{(r)} \vec{x}^{(r)}, \quad r = 1, 2, 3$

The eigenvectors satisfy $\sum_{n=1}^3 x_n^{(r)} x_n^{(r')} = \delta_{r,r'}$

Therefore $\sum_{m,n=1}^3 x_m^{(r)} I_{m,n} x_n^{(r')} = \sum_{m=1}^3 x_m^{(r)} I^{(r')} x_m^{(r')} = I^{(r')} \delta_{r,r'}$

Matrix Diagonalization

If we can make our matrix diagonal, then the solution is easy (elements of a diagonal matrix are its eigenvalues). So, most numerical methods look for a similarity transformation which diagonalizes the matrix

$$A\vec{x} = \lambda\vec{x} \text{ is our starting equation}$$

$$P^{-1}AP = A' \text{ where } A' \text{ is diagonal}$$

Eigenvalues of A can be calculated in principle from the secular equation:

$$\det|A - \lambda E| = 0$$

Similarity transformations leave the eigenvalues unchanged:

$$\begin{aligned} \det|P^{-1}AP - \lambda E| &= \det|P^{-1}(A - \lambda E)P| \\ &= \det|P| \det|A - \lambda E| \det|P^{-1}| \\ &= \det|A - \lambda E| \end{aligned}$$

Matrix Diagonalization

Let $\vec{v} = P^{-1}\vec{x}$, then

$$A'\vec{v} = P^{-1}APP^{-1}\vec{x} = \lambda P^{-1}\vec{x} = \lambda\vec{v}$$

The elements of a diagonal matrix are its eigenvalues, so we can read off the eigenvalues of A from A' . The eigenvectors of the diagonal matrix A' are vectors with zeros everywhere except for one component, which we can take as 1. I.e.,

$$\vec{v}^{(i)} = \begin{pmatrix} 0 \\ \vdots \\ 0 \\ 1 \\ 0 \\ \vdots \\ 0 \end{pmatrix} \quad \text{for eigenvalue } \lambda_i$$

and so we get the eigenvectors of interest as follows:

$$\vec{x}^{(i)} = P\vec{v}^{(i)}$$

which is just the i^{th} column of P

Jacobi Method

Consider a symmetric 2x2 matrix. It can be diagonalized by a rotation of the coordinate system (Jacobi Method). Rotation by an angle φ corresponds to an orthogonal transformation with the rotation matrix:

$$R^{(12)} = \begin{pmatrix} \cos \varphi & \sin \varphi \\ -\sin \varphi & \cos \varphi \end{pmatrix}$$

Similarity transformation

Note: $P=R^{-1}$

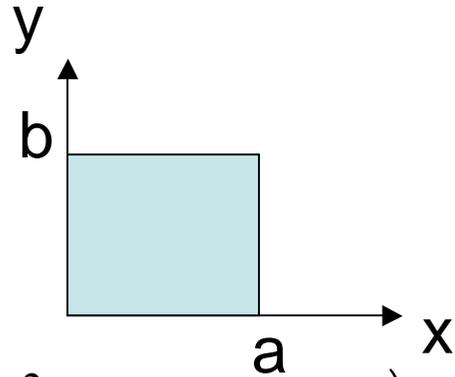
$$\begin{aligned} A \rightarrow RAR^{-1} &= \begin{pmatrix} \cos \varphi & \sin \varphi \\ -\sin \varphi & \cos \varphi \end{pmatrix} \begin{pmatrix} A_{11} & A_{12} \\ A_{12} & A_{22} \end{pmatrix} \begin{pmatrix} \cos \varphi & -\sin \varphi \\ \sin \varphi & \cos \varphi \end{pmatrix} \\ &= \begin{pmatrix} c^2 A_{11} + s^2 A_{22} - 2csA_{12} & cs(A_{11} - A_{22}) + (c^2 - s^2)A_{12} \\ cs(A_{11} - A_{22}) + (c^2 - s^2)A_{12} & s^2 A_{11} + c^2 A_{22} + 2csA_{12} \end{pmatrix} \end{aligned}$$

is diagonal if

$$cs(A_{11} - A_{22}) + (c^2 - s^2)A_{12} = 0 \quad \text{where } c = \cos \varphi, s = \sin \varphi$$

Example - square

As an example, consider the principal axes of a thin, square plate.



The plate is infinitely thin in the z direction.

$$I_{mn} = \sum_i (m_i r_i^2 \delta_{mn} - m_i r_{im} r_{in}) \rightarrow \int (r^2 \delta_{mn} - r_m r_n) dm$$

$dm = \sigma dx dy$ where σ is the mass density

$$I_{11} = \sigma \int_0^b \int_0^a ((x^2 + y^2) - x^2) dx dy = \sigma a \frac{b^3}{3} = \frac{mb^2}{3}$$

Similarly:
$$I_{22} = \frac{ma^2}{3}$$

$$I_{33} = \sigma \int_0^b \int_0^a (x^2 + y^2) dx dy = \sigma \left(b \frac{a^3}{3} + a \frac{b^3}{3} \right) = m \left(\frac{a^2}{3} + \frac{b^2}{3} \right)$$

Square Plate

The off-diagonal elements are:

$$I_{12} = I_{21} = -\sigma \int_0^a x dx \int_0^b y dy = -\sigma \frac{a^2 b^2}{4} = -\frac{mab}{4}$$

$$I_{13} = I_{23} = I_{31} = I_{32} = 0$$

Because no width in z

So, we have

$$I = \frac{m}{12} \begin{pmatrix} 4b^2 & -3ab & 0 \\ -3ab & 4a^2 & 0 \\ 0 & 0 & 4(a^2 + b^2) \end{pmatrix}$$

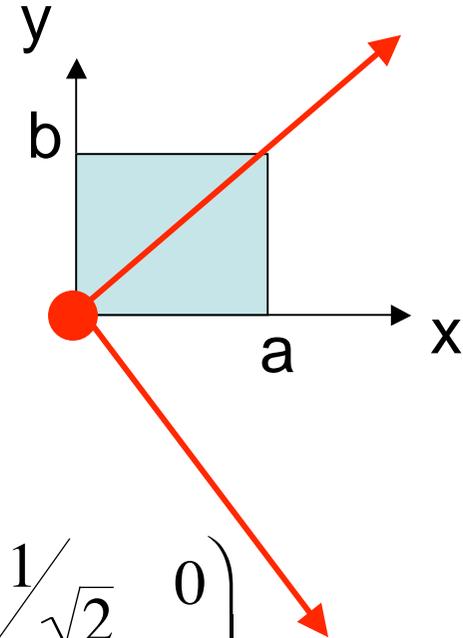
We will now find the rotation which produces a diagonal matrix.

$$\tan(2\phi) = \frac{2A_{12}}{A_{22} - A_{11}} = \frac{2(-3ab)}{(4a^2 - 4b^2)} = \frac{3ab}{2(b^2 - a^2)}$$

Jacobi Method

Let's try it on our example - assume a square plate ($a=b$):

$$\tan(2\phi) = \frac{3ab}{2(b^2 - a^2)} = \infty, \quad \phi = 45^\circ$$



$$R^{(12)} = \begin{pmatrix} 1/\sqrt{2} & 1/\sqrt{2} & 0 \\ -1/\sqrt{2} & 1/\sqrt{2} & 0 \\ 0 & 0 & 1 \end{pmatrix} \quad R^{(12)-1} = \begin{pmatrix} 1/\sqrt{2} & -1/\sqrt{2} & 0 \\ 1/\sqrt{2} & 1/\sqrt{2} & 0 \\ 0 & 0 & 1 \end{pmatrix}$$

Jacobi Method

Applying the similarity transformation:

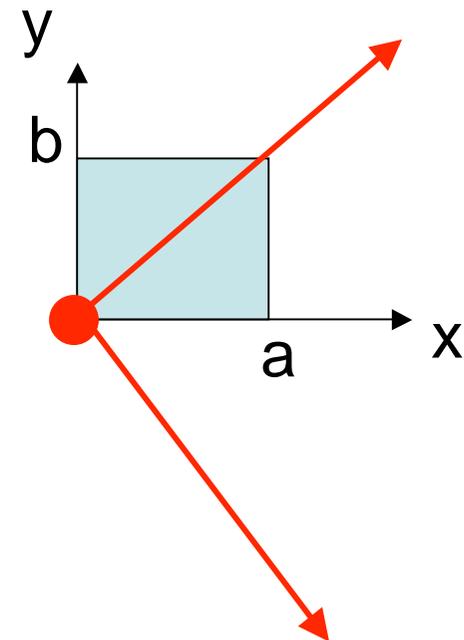
$$\begin{aligned} R^{(12)} I R^{(12)-1} &= \frac{ma^2}{12} \begin{pmatrix} 1/\sqrt{2} & 1/\sqrt{2} & 0 \\ -1/\sqrt{2} & 1/\sqrt{2} & 0 \\ 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} 4 & -3 & 0 \\ -3 & 4 & 0 \\ 0 & 0 & 8 \end{pmatrix} \begin{pmatrix} 1/\sqrt{2} & -1/\sqrt{2} & 0 \\ 1/\sqrt{2} & 1/\sqrt{2} & 0 \\ 0 & 0 & 1 \end{pmatrix} \\ &= \frac{ma^2}{12} \begin{pmatrix} 1/\sqrt{2} & 1/\sqrt{2} & 0 \\ -1/\sqrt{2} & 1/\sqrt{2} & 0 \\ 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} 1/\sqrt{2} & -7/\sqrt{2} & 0 \\ 1/\sqrt{2} & 7/\sqrt{2} & 0 \\ 0 & 0 & 8 \end{pmatrix} \\ &= \frac{ma^2}{12} \begin{pmatrix} 1 & 0 & 0 \\ 0 & 7 & 0 \\ 0 & 0 & 8 \end{pmatrix} \end{aligned}$$

Jacobi Method

The eigenvalues are therefore: $\frac{ma^2}{12}$, $\frac{7ma^2}{12}$, $\frac{8ma^2}{12}$,

The eigenvectors are the columns of $P=R^{-1}$:

$$R^{(12)^{-1}} = \begin{pmatrix} 1/\sqrt{2} & -1/\sqrt{2} & 0 \\ 1/\sqrt{2} & 1/\sqrt{2} & 0 \\ 0 & 0 & 1 \end{pmatrix} \quad \text{so,}$$
$$\vec{x}^{(1)} = \begin{pmatrix} 1/\sqrt{2} \\ 1/\sqrt{2} \\ 0 \end{pmatrix} \quad \vec{x}^{(2)} = \begin{pmatrix} -1/\sqrt{2} \\ 1/\sqrt{2} \\ 0 \end{pmatrix} \quad \vec{x}^{(3)} = \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix}$$



Square Plate

Let's go back to the square plate problem and look at other ways to solve these types of problems:

Recall, we have

$$I = \frac{m}{12} \begin{pmatrix} 4b^2 & -3ab & 0 \\ -3ab & 4a^2 & 0 \\ 0 & 0 & 4(a^2 + b^2) \end{pmatrix}$$

To find the eigenvalues, we can solve

$$\det|I - \lambda E| = 0 = \det \begin{pmatrix} 4b^2 - 12\lambda/m & -3ab & 0 \\ -3ab & 4a^2 - 12\lambda/m & 0 \\ 0 & 0 & 4(a^2 + b^2) - 12\lambda/m \end{pmatrix}$$

Square Plate

$$\begin{aligned} &= \left[(4b^2 - \kappa)(4a^2 - \kappa)(4(a^2 + b^2) - \kappa) + 3ab(-3ab)(4(a^2 + b^2) - \kappa) \right] \\ &= \left[-\kappa^3 + 8\kappa^2(a^2 + b^2) - \kappa(16a^4 + 39a^2b^2 + 16b^4) + 28a^2b^2(a^2 + b^2) \right] \end{aligned}$$

where $\kappa = \frac{12\lambda}{m}$

At this point, we can try to solve with a symbolic algebra solver (e.g., Mathematica, Maple)

Let's put in concrete values and solve numerically:

$$a = 1, b = 1$$

$$0 = \left[\kappa^3 - 16\kappa^2 + 71\kappa - 56 \right]$$

$$\kappa_1 = 8, \quad \kappa_2 = 1, \quad \kappa_3 = 7$$

$$\text{so, } \lambda_1 = 8m/12, \quad \lambda_2 = m/12, \quad \lambda_3 = 7m/12$$

Roots to Cubic Equation

C207: Roots of a Cubic Equation

Author(s): K.S. Kölbig Library: MATHLIB

Submitter: Submitted: 15.01.1988

Language: Fortran Revised: 01.12.1994

CERN Library

Subroutine subprograms RRTEQ3 and DRTEQ3 compute the three roots of
 $x^3+rx^2+sx+t=0$

for real coefficients r, s, t.

Structure:

SUBROUTINE subprograms

User Entry Names: RRTEQ3, DRTEQ3

We will look into root finding in 2 lectures from now.

Once we have the eigenvalues, we can find the eigenvectors:

Square Plate

$$\begin{pmatrix} 4b^2 - 12\lambda_i/m & -3ab & 0 \\ -3ab & 4a^2 - 12\lambda_i/m & 0 \\ 0 & 0 & 4(a^2 + b^2) - 12\lambda_i/m \end{pmatrix} \begin{pmatrix} x_1^{(i)} \\ x_2^{(i)} \\ x_3^{(i)} \end{pmatrix} = 0$$

Substituting our numerical values (starting with λ_1)

$$\begin{pmatrix} 4 - 8 & -3 & 0 \\ -3 & 4 - 8 & 0 \\ 0 & 0 & 8 - 8 \end{pmatrix} \begin{pmatrix} x_1^{(1)} \\ x_2^{(1)} \\ x_3^{(1)} \end{pmatrix} = 0$$

We now have a SLE which we need to solve to get $u^{(1)}$. *Note* that our matrix is singular, so we need a different technique than those described in the previous lecture.

Singular Value Decomposition

Singular Value Decomposition is based on following theorem: Any $M \times N$ matrix A whose number of rows, M , is greater than or equal to its number of columns, N , can be written as the product of an $M \times N$ column-orthogonal matrix U , and $N \times N$ diagonal matrix W with positive or zero elements, and the transpose of an $N \times N$ orthogonal matrix V . (recall, the transpose of an orthogonal matrix equals the inverse). By column orthogonal, we mean:

$$\sum_{i=1}^M U_{ik} U_{in} = \delta_{kn} \quad 1 \leq k, n \leq N$$

$$\sum_{j=1}^M V_{jk} V_{jn} = \delta_{kn} \quad 1 \leq k, n \leq N$$

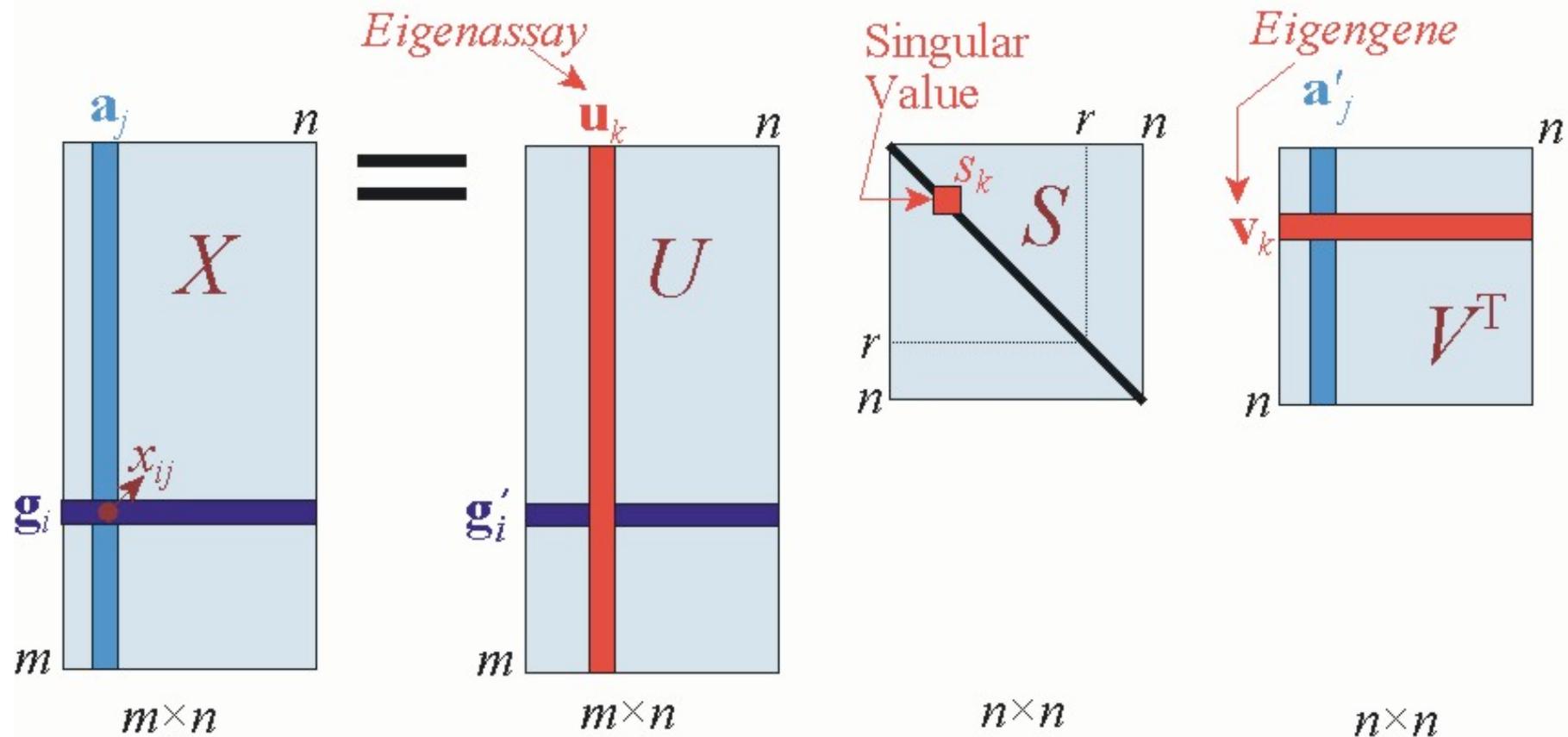
Usefulness: The columns of U whose same numbered elements W_{jj} are non-zero are an orthonormal set of basis vectors that span the range; the columns of V whose W_{jj} are zero are an orthonormal basis for the nullspace ($Ax=0$).

Singular Value Decomposition

2. SVD analysis of gene expression data
Singular value decomposition and principal component analysis

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$$X = USV^T$$



Singular Value Decomposition

We use a standard code to perform the singular value decomposition.

See <http://www.bluebit.gr/matrix-calculator/>

$$U = \begin{pmatrix} -1/\sqrt{2} & -1/\sqrt{2} & 0 \\ -1/\sqrt{2} & 1/\sqrt{2} & 0 \\ 0 & 0 & 0 \end{pmatrix}$$

So, basis vector corresponding to λ_1

$$W = \begin{pmatrix} 7 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 0 \end{pmatrix}$$

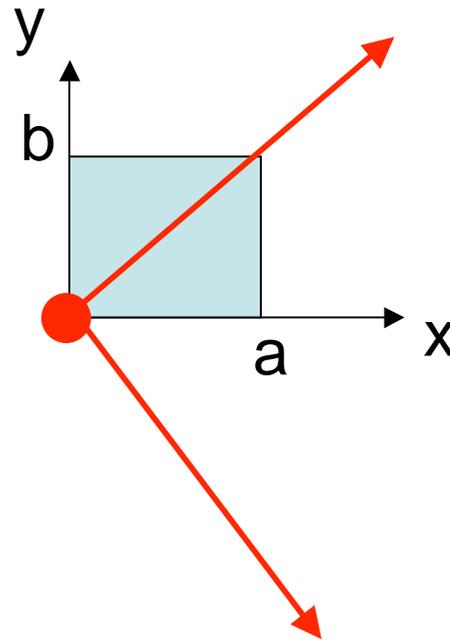
$$\vec{x}^{(1)} = \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix}$$

$$V^T = \begin{pmatrix} 1/\sqrt{2} & 1/\sqrt{2} & 0 \\ 1/\sqrt{2} & -1/\sqrt{2} & 0 \\ 0 & 0 & 1 \end{pmatrix} \quad V = \begin{pmatrix} 1/\sqrt{2} & 1/\sqrt{2} & 0 \\ 1/\sqrt{2} & -1/\sqrt{2} & 0 \\ 0 & 0 & 1 \end{pmatrix}$$

Singular Value Decomposition

The other two basis vectors are found in a similar way (see exercises):

$$\vec{x}^{(1)} = \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix} \quad \vec{x}^{(2)} = \begin{pmatrix} 1/\sqrt{2} \\ 1/\sqrt{2} \\ 0 \end{pmatrix} \quad \vec{x}^{(3)} = \begin{pmatrix} 1/\sqrt{2} \\ -1/\sqrt{2} \\ 0 \end{pmatrix}$$



Quantum Mechanics

Eigenvalue problems are natural in quantum mechanics. We start by considering a two dimensional problem:

$$-\frac{\hbar^2}{2m} \nabla^2 \psi(\vec{r}) + V(\vec{r})\psi(\vec{r}) = E\psi(\vec{r}) \quad \text{Schroedinger Eqn}$$

On a grid, we have

$$-\frac{\hbar^2}{2m} \left[\frac{\psi(m+1,n) + \psi(m-1,n) - 2\psi(m,n)}{(\Delta x)^2} + \frac{\psi(m,n+1) + \psi(m,n-1) - 2\psi(m,n)}{(\Delta y)^2} \right] + V(m,n)\psi(m,n) \approx E\psi(m,n)$$

Eigenvalue problem - only certain E will give solutions. Boundary values are specified. Have MxN unknown values of ψ and in principle also of E.

Quantum Mechanics

In matrix form:

$$\vec{\psi} = \begin{pmatrix} \psi(0,0) \\ \psi(0,1) \\ \vdots \end{pmatrix} \quad H \equiv -\frac{\hbar^2}{2m} \nabla^2 + V(\vec{r})$$
$$H\vec{\psi} = E\vec{\psi}$$

Setting $\Delta x = \Delta y = 1$ we have

$$H = \frac{\hbar^2}{2m} \begin{pmatrix} 4 + V(0,0) & -1 & 0 & \dots \\ -1 & 4 + V(0,1) & -1 & \dots \\ \dots & \dots & \dots & \dots \end{pmatrix}$$

Note that the matrix has $(MN)^2$ elements ! Solving this is an interesting computing problem

Note that there are other non-diagonal terms which are not 0 because we need also $m+1, m-1$. Also, need some prescription for the boundaries.

Power Method

It is usually not possible to find all eigenvalues and eigenvectors. Focus on finding the dominant ones (minimum energy states, e.g.) The matrix is typically sparse (mostly 0's), and special techniques exist for solving this. One example is the 'power method'.

Assume $|\lambda_1| > |\lambda_2| \geq |\lambda_3| \geq \dots \geq |\lambda_n|$

Also assume $\vec{x} = \sum_{i=1}^n a_i \vec{x}^{(i)}$ with $a_1 \neq 0$, $\vec{x}^{(i)}$ are eigenvectors with eigenvalues λ_i so that

$$H\vec{x}^{(i)} = \lambda_i \vec{x}^{(i)}$$

Now apply H repeatedly:

$$H\vec{x} = \sum_{i=1}^n a_i \lambda_i \vec{x}^{(i)}, \quad H^k \vec{x} = \sum_{i=1}^n a_i \lambda_i^k \vec{x}^{(i)} \xrightarrow{k \rightarrow \infty} \lambda_1^k a_1 \vec{x}^{(1)}$$

Get $\vec{x}^{(1)}$ by normalizing $H^k \vec{x}$

Power Method

Try it out on our thin square example.

$$\vec{x} = \begin{pmatrix} 1 \\ 1 \\ 1 \end{pmatrix}$$

$$I\vec{x} = \begin{pmatrix} 1 \\ 1 \\ 8 \end{pmatrix}$$

$$\vec{x}^{(1)} \approx \begin{pmatrix} 0.12 \\ 0.12 \\ 0.98 \end{pmatrix}$$

$$I^5\vec{x} = \begin{pmatrix} 1 \\ 1 \\ 32768 \end{pmatrix}$$

$$\vec{x}^{(1)} \approx \begin{pmatrix} 3.05 \cdot 10^{-5} \\ 3.05 \cdot 10^{-5} \\ 1 \end{pmatrix}$$

$$I^{10}\vec{x} = \begin{pmatrix} 1 \\ 1 \\ 1.07 \cdot 10^9 \end{pmatrix}$$

$$\vec{x}^{(1)} \approx \begin{pmatrix} 9.3 \cdot 10^{-10} \\ 9.3 \cdot 10^{-10} \\ 1 \end{pmatrix}$$

Power Method

It is also possible to get eigenvectors other than the one corresponding to the biggest eigenvalue by modifying the starting matrix. For example, we can shift the matrix

$$I' = \Lambda^2 E - I^2$$

where Λ is the largest eigenvalue. This then gives the eigenvector corresponding to the smallest eigenvalue. In our example, take $\Lambda=8$. We then find

$$\vec{x} = \begin{pmatrix} 1 \\ 1 \\ 1 \end{pmatrix} \quad I'\vec{x} = \begin{pmatrix} 63 \\ 63 \\ 0 \end{pmatrix} \quad \vec{x}^{(2)} \approx \begin{pmatrix} 0.7071 \\ 0.7071 \\ 0 \end{pmatrix}$$

With further manipulation of I , we can find the remaining eigenvector (see exercises).

Variational Technique

The methods discussed so far only work in some circumstances, and, since eigenvalue problems are so common, many other techniques have been developed. One further important example is the ‘variational technique’, which allows the determination of the ground state. This technique relies on the variational principle, which says that the energy of any wavefunction is at least as large as the energy of the ground state.

$$E^* \equiv \frac{\int \varphi^* H \varphi d\vec{r}}{\int \varphi^* \varphi d\vec{r}} \quad \text{where } \varphi \text{ is a trial wavefunction}$$

$$E^* \geq E_0$$

Technique: make repeated guesses for φ ; the one which gives the lowest energy is closest to the ground state wavefunction.

Variational Technique

As an example, we consider the 2-D harmonic oscillator potential:

$$V(x, y) = \frac{1}{2}k_x x^2 + \frac{1}{2}k_y y^2$$

Take a square grid, with equal spacing in x,y:

$$-N\Delta \leq x \leq N\Delta, \quad -N\Delta \leq y \leq N\Delta,$$

So we have a total of $(2N+1)^2$ bins.

Take the following values: $k_x = 10$, $k_y = 40$, $\Delta = 0.2$, $N = 10$

Starting wavefunction: $\varphi(i, j) = 0$. for $i, j = 0, 2N$

$\varphi(i, j) = 1$. for all other i, j

$x = -2. + i\Delta$ $y = -2. + j\Delta$

Harmonic Oscillator

- * Calculate the energy of this configuration. First, we create the new wavefunction by operating on it with the Hamiltonian (units with $\hbar=m=1$):

```

Do i=1,19
  Do j=1,19
    x=-2.+i*step
    y=-2.+j*step
    phi1(i,j)=-0.5*(phi(i+1,j)+phi(i-1,j)+phi(i,j+1)+phi(i,j-1)
&          -4.*phi(i,j))/step**2+
&          0.5*(kx*x**2+ky*y**2)*phi(i,j)
  Enddo
Enddo

```

$$H\varphi(m,n) = -\frac{1}{2} \left[\frac{\varphi(m+1,n) + \varphi(m-1,n) - 2\varphi(m,n)}{(\Delta x)^2} + \frac{\varphi(m,n+1) + \varphi(m,n-1) - 2\varphi(m,n)}{(\Delta y)^2} \right] + V(m,n)\varphi(m,n)$$

$$= \varphi_1(m,n)$$

- * Now calculate the energy by integrating $\psi^*\psi_1$. Divide by $\psi^*\psi$ for normalization

```

top=0.
bottom=0.
Do i=1,19
  Do j=1,19
    top=top+phi(i,j)*phi1(i,j)
    bottom=bottom+phi(i,j)*phi(i,j)
  Enddo
Enddo

```

$$E^* \equiv \frac{\int \varphi^* H \varphi d\vec{r}}{\int \varphi^* \varphi d\vec{r}}$$

Note: don't need volume element since it cancels in the ratio. More on integration next time.

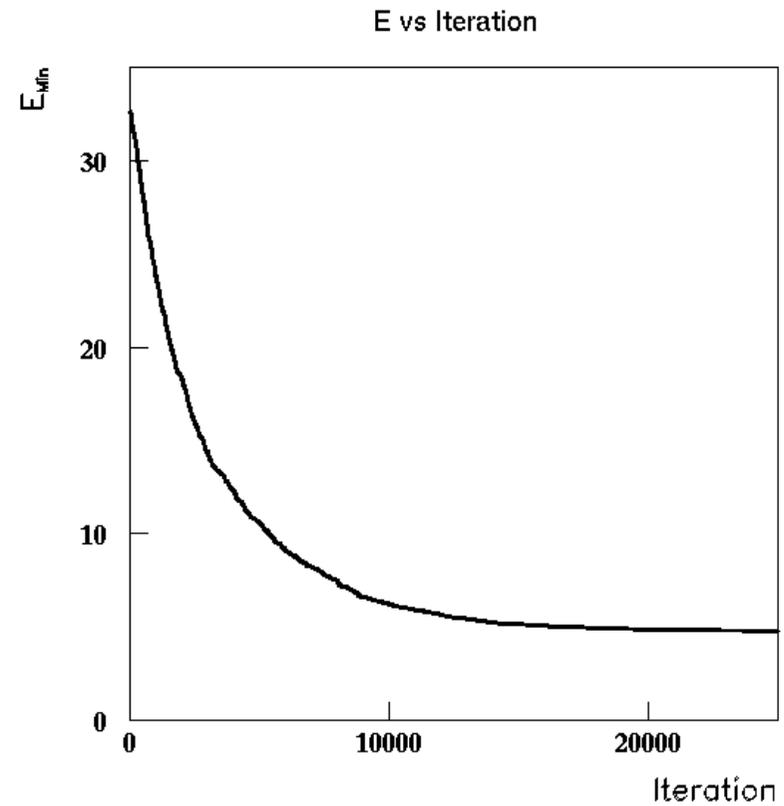
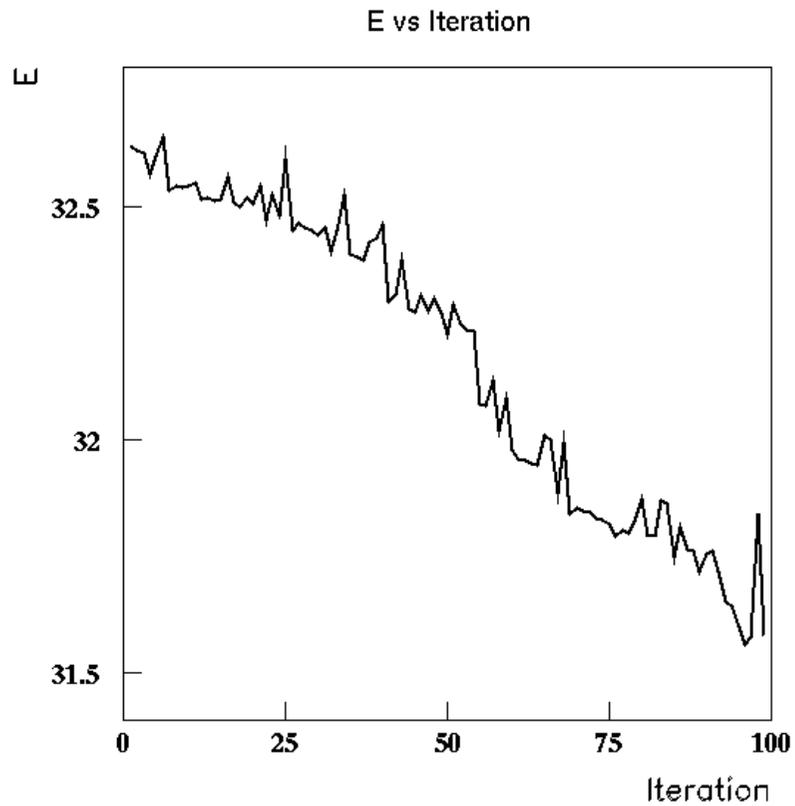
Energy=top/bottom

Harmonic Oscillator

```
*
* Compare this energy with previous
*
  If (Energy.lt.Energy0) then
*
* New minimum
*
  Energy0=Energy
  Print *, 'Iteration ', lter, ' New Energy ', Energy
  Do i=0,20
    Do j=0,20
      psi2(i,j)=psi(i,j)      !Save lowest energy configuration in psi2
    Enddo
  Enddo
Else
*
* Try a modified test function
*
  2  rn=rndm()
     lx=rn*4./step+1
     If (lx.le.0.or. lx.ge.20) goto 2
  3  rn=rndm()
     ly=rn*4./step+1
     If (ly.le.0.or. ly.ge.20) goto 3
     call RNORML(vec,1)
     psi(lx,ly)=psi(lx,ly)+vec*var
     goto 1
Endif
*
* reset psi and try new variation
*
  Do i=1,19
    Do j=1,19
      psi(i,j)=psi2(i,j)
    Enddo
  Enddo
Endif
*
```

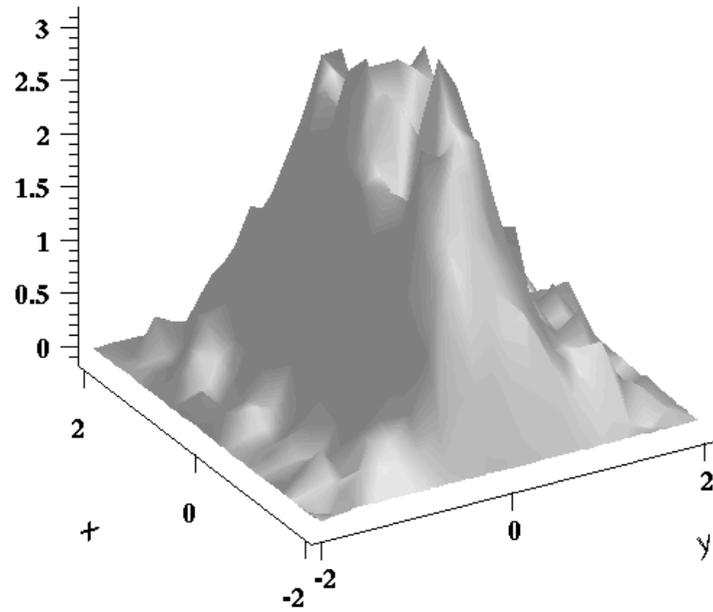
Gaussian distributed
random number

Harmonic Oscillator

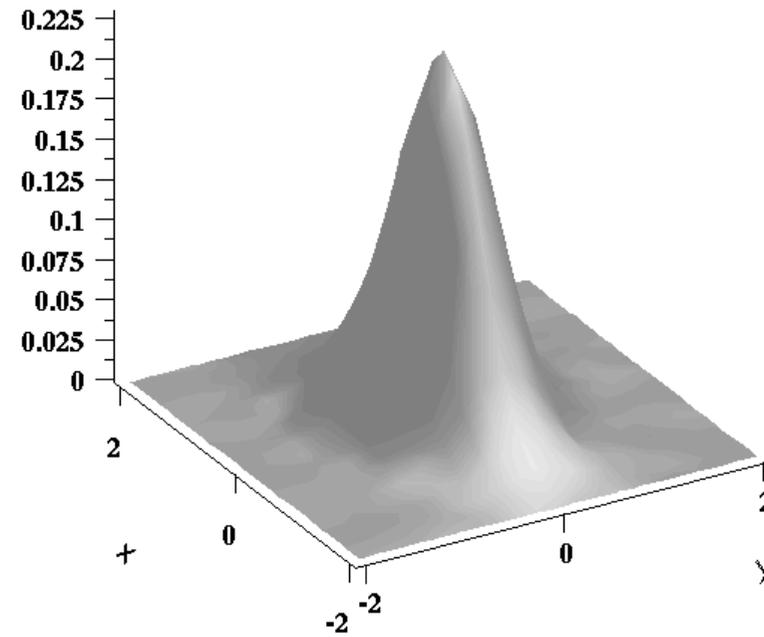


Harmonic Oscillator

Wavefunction after 5000 Iterations



Normalized Wavefunction after 25000 Iterations



Exercizes

1. Use the second and third eigenvalues found for the principal axes of a square example and find the basis vectors using the singular value decomposition technique.
2. Find the third eigenvector for the thin square plate problem using the power method with shifted matrix.