矩阵对角化与本征值问题

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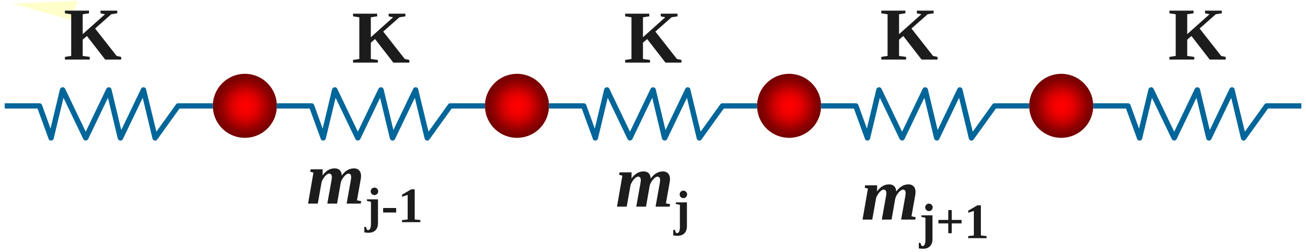
线性方程组：

$$AX = B$$

本征值问题：

$$AX = \lambda X$$



$$F_1 = m\frac{d^2x_1}{dt^2} = -Kx_1 + K(x_2 - x_1)$$

$$F_2 = m\frac{d^2x_2}{dt^2} = K(x_1 - x_2) + K(x_3 - x_2)$$

…

$$F_j = m\frac{d^2x_j}{dt^2} = K(x_{j-1} - x_j) + K(x_{j+1} - x_j)$$

…

$$F_N = m\frac{d^2x_N}{dt^2} = K(x_{N-1} - x_N) - Kx_N.$$

$$
\begin{aligned}
F_1 &= m\frac{d^2x_1}{dt^2} = -Kx_1 + K(x_2 - x_1) \\
F_2 &= m\frac{d^2x_2}{dt^2} = K(x_1 - x_2) + K(x_3 - x_2) \\
&\cdots \\
F_j &= m\frac{d^2x_j}{dt^2} = K(x_{j-1} - x_j) + K(x_{j+1} - x_j) \\
&\cdots \\
F_N &= m\frac{d^2x_N}{dt^2} = K(x_{N-1} - x_N) - Kx_N .
\end{aligned}
$$

$$x_j = A_j e^{-i\omega t}$$

$$
\frac{m\omega^2}{K}\begin{pmatrix} A_1 \\ A_2 \\ \cdots \\ A_j \\ \cdots \\ A_N \end{pmatrix} = \begin{pmatrix} 2 & -1 & 0 & 0 & \cdots & 0 \\ -1 & 2 & -1 & 0 & \cdots & 0 \\ 0 & -1 & 2 & -1 & \cdots & 0 \\ \cdots & & & & & \\ 0 & \cdots & 0 & 0 & -1 & 2 \end{pmatrix}\begin{pmatrix} A_1 \\ A_2 \\ \cdots \\ A_j \\ \cdots \\ A_N \end{pmatrix}
$$

$$\begin{pmatrix} a_{11} & a_{12} & \cdots & a_{1j} & \cdots & a_{1n} \\ a_{21} & a_{22} & \cdots & a_{2j} & \cdots & a_{2n} \\ \cdots & \cdots & \cdots & \cdots & \cdots & \cdots \\ a_{i1} & \cdots & \cdots & a_{ij} & \cdots & a_{in} \\ \cdots & \cdots & \cdots & \cdots & \cdots & \cdots \\ a_{n1} & a_{n2} & \cdots & a_{nj} & \cdots & a_{nn} \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \\ \vdots \\ x_i \\ \vdots \\ x_n \end{pmatrix} = \lambda \begin{pmatrix} x_1 \\ x_2 \\ \vdots \\ x_i \\ \vdots \\ x_n \end{pmatrix}$$

$$AX = \lambda X$$

$$\begin{pmatrix} a_{11}-\lambda & a_{12} & \cdots & a_{1j} & \cdots & a_{1n} \\ a_{21} & a_{22}-\lambda & \cdots & a_{2j} & \cdots & a_{2n} \\ \cdots & \cdots & \cdots & \cdots & \cdots & \cdots \\ a_{i1} & \cdots & \cdots & a_{ij}-\lambda & \cdots & a_{in} \\ \cdots & \cdots & \cdots & \cdots & \cdots & \cdots \\ a_{n1} & a_{n2} & \cdots & a_{nj} & \cdots & a_{nn}-\lambda \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \\ \vdots \\ x_i \\ \vdots \\ x_n \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \\ \vdots \\ 0 \\ \vdots \\ 0 \end{pmatrix}$$

$$\det(A-\lambda I)=0$$

求矩阵特征值与特征向量的方法

1. 乘幂法 （最大特征值）
2. 反幂法（最小特征值）
3. Jacobi方法（对称矩阵）
4. QR方法（更一般的算法）
5. SVD

……

Jacobi方法

（实对称矩阵的全部特征根与特征向量）

定理：P为n阶可逆阵，则A与$P^{-1}AP$相似，相似阵有相同的特征值；

若A对称，则存在正交矩阵$Q(Q^TQ=I)$，使得

$$Q^TAQ=\begin{pmatrix}\lambda_1 & & & \\ & \lambda_2 & & \\ & & \ddots & \\ & & & \lambda_n\end{pmatrix}$$

计算如下矩阵的特征值和相应的特征向量

$$A=\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \qquad B=\begin{pmatrix} \cos\theta & \sin\theta \\ -\sin\theta & \cos\theta \end{pmatrix}$$

计算如下矩阵的特征值和相应的特征向量

$$B^T AB = \begin{pmatrix} \cos\theta & -\sin\theta \\ \sin\theta & \cos\theta \end{pmatrix}\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}\begin{pmatrix} \cos\theta & \sin\theta \\ -\sin\theta & \cos\theta \end{pmatrix}$$

$$= \begin{pmatrix} -2\sin\theta\cos\theta & \cos^2\theta - \sin^2\theta \\ \cos^2\theta - \sin^2\theta & 2\sin\theta\cos\theta \end{pmatrix}$$

当θ=π/4时： $B^T AB = \begin{pmatrix} -1 & 0 \\ 0 & 1 \end{pmatrix}$ $B = \begin{pmatrix} \sqrt{2}/2 & \sqrt{2}/2 \\ -\sqrt{2}/2 & \sqrt{2}/2 \end{pmatrix}$

当θ=π/4时：
$$B^T AB = \begin{pmatrix} -1 & 0 \\ 0 & 1 \end{pmatrix} \qquad B = \begin{pmatrix} \sqrt{2}/2 & \sqrt{2}/2 \\ -\sqrt{2}/2 & \sqrt{2}/2 \end{pmatrix}$$

A的特征值为λ1=-1，λ2=1

A对应于λ1= -1的特征向量为： $v1 = \begin{pmatrix} \sqrt{2}/2 \\ -\sqrt{2}/2 \end{pmatrix}$

A对应于λ2= 1的特征向量为： $v2 = \begin{pmatrix} \sqrt{2}/2 \\ \sqrt{2}/2 \end{pmatrix}$

Jacobi法基本思路：

构造一系列特殊形式的正交阵$Q_1,\ldots,Q_n$

对A作正交变换使得对角元素比重逐次增加，非对角元变小。

当非对角元已经小得无足轻重时，可以近似认为对角元就是A的所有特征值。

*Givens*旋转变换：

$$Q(p,q,\theta)=\begin{array}{cc} \begin{pmatrix} 1 &&&&&& \\ &\ddots&&&&& \\ &&\cos\theta&&\sin\theta&& \\ &&&\ddots&&& \\ &&-\sin\theta&&\cos\theta&& \\ &&&&&\ddots& \\ &&&&&&1 \end{pmatrix} & \begin{matrix} \\ \\ \boldsymbol{p}\text{行} \\ \\ \boldsymbol{q}\text{行} \\ \\ \\ \end{matrix} \\ \begin{matrix} \qquad\qquad \boldsymbol{p}\text{列} & \qquad\qquad \boldsymbol{q}\text{列} \end{matrix} & \end{array}$$

记： $A=(a_{ij})$ ， $B=Q^T(p,q,\theta)AQ(p,q,\theta)=(b_{ij})$

则：
$$\begin{cases} b_{ip}=b_{pi}=a_{pi}\cos\theta-a_{qi}\sin\theta, i\neq p,q \\ b_{iq}=b_{qi}=a_{pi}\sin\theta+a_{qi}\cos\theta, i\neq p,q \\ b_{pp}=a_{pp}\cos^2\theta+a_{qq}\sin^2\theta-a_{pq}\sin 2\theta \\ b_{qq}=a_{pp}\sin^2\theta+a_{qq}\cos^2\theta+a_{pq}\sin 2\theta \\ b_{pq}=b_{qp}=a_{pq}\cos 2\theta+\dfrac{a_{pp}-a_{qq}}{2}\sin 2\theta \end{cases}$$

变换的目的是为了减少非对角元的分量，因此：

$$b_{pq}=b_{qp}=a_{pq}\cos 2\theta+\frac{a_{pp}-a_{qq}}{2}\sin 2\theta=0$$

$$
\begin{cases}
b_{ip} = b_{pi} = ca_{pi} - da_{qi}, i \neq p, q \\
b_{iq} = b_{qi} = da_{pi} + ca_{qi}, i \neq p, q \\
b_{pp} = a_{pp} - ta_{pq} \\
b_{pp} = a_{qq} + ta_{pq} \\
b_{pq} = b_{qp} = 0
\end{cases}
$$

其中

$$s = \frac{a_{qq} - a_{pp}}{2a_{pq}}$$

$$t^2 + 2ts - 1 = 0$$

$$t = \tan\theta$$

$$\mathrm{c} = \cos\theta = \frac{1}{\sqrt{1+t^2}}, d = \sin\theta = \frac{t}{\sqrt{1+t^2}}$$

Jacobi迭代法：

取***p*,*q***使 $\left|a_{pq}\right| = \max_{i \neq j}\left|a_{ij}\right|$，则

$$A^{(k+1)} = Q^T(p,q,\theta)A^{(k)}Q(p,q,\theta)$$

定理：若*A*对称，则

$$A^{(k+1)} \to diag\{\lambda_1,\cdots,\lambda_n\}$$

例：用Jacobi 方法计算对称矩阵的全部特征值

$$\mathbf{A} = \begin{pmatrix} 4 & 2 & 2 \\ 2 & 5 & 1 \\ 2 & 1 & 6 \end{pmatrix}$$

解 记 $A^{(0)}=A$, 取$p=1,q=2$, $a_{pq}^{(0)}=a_{12}^{(0)}=2$,于是有

$$s = \frac{a_{11}^{(0)} - a_{22}^{(0)}}{2a_{12}^{(0)}} = -0.25 \qquad t = -0.780776$$

$$\cos\theta = \frac{1}{\sqrt{1+t^2}} = 0.788206 \qquad \sin\theta = \frac{t}{\sqrt{1+t^2}} = -0.615412$$

$$\mathbf{R}_1 = \mathbf{R}_{pq}(\theta) = \begin{pmatrix} \cos\theta & -\sin\theta & 0 \\ \sin\theta & \cos\theta & 0 \\ 0 & 0 & 1 \end{pmatrix} = \begin{pmatrix} 0.788206 & 0.615412 & 0 \\ -0.615412 & 0.788206 & 0 \\ 0 & 0 & 1 \end{pmatrix}$$

所以 $\mathbf{A}^{(1)} = \mathbf{R}_1^T \mathbf{A}^{(0)} \mathbf{R}_1 = \begin{pmatrix} 2.438448 & 0 & 0.961 \\ 0 & 6.561552 & 2.020190 \\ 0.961 & 2.020190 & 6 \end{pmatrix}$

再取p=2, q=3, $a_{pq}^{(1)}=a_{23}^{(1)}=2.020190$, 类似地可得

$$\mathbf{A}^{(2)} = \begin{pmatrix} 2.438448 & 0.631026 & 0.724794 \\ 0.631026 & 8.320386 & 0 \\ 0.724794 & 0 & 4.241166 \end{pmatrix}$$

$$\mathbf{A}^{(3)} = \begin{pmatrix} 2.183185 & 0.595192 & 0 \\ 0.595192 & 8.320386 & 0.209614 \\ 0 & 0.209614 & 4.496424 \end{pmatrix}$$

$$\mathbf{A}^{(4)} = \begin{pmatrix} 2.125995 & 0 & -0.020048 \\ 0 & 8.377576 & 0.208653 \\ -0.020048 & 0.208653 & 4.496424 \end{pmatrix}$$

$$\mathbf{A}^{(5)} = \begin{pmatrix} 2.125995 & -0.001073 & -0.020019 \\ -0.001073 & 8.388761 & 0 \\ -0.020019 & 0 & 4.485239 \end{pmatrix}$$

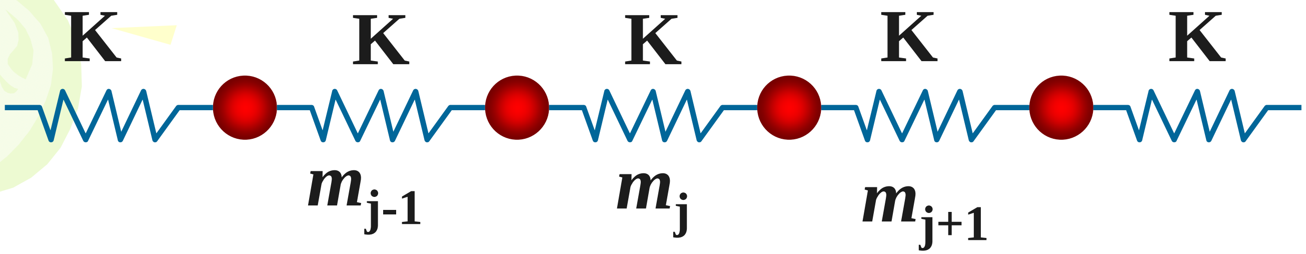
$$\mathbf{A}^{(6)} = \begin{pmatrix} 2.125825 & -0.001072 & 0 \\ 0 & 8.388761 & 0.000009 \\ -0.001072 & 0.000009 & 4.485401 \end{pmatrix}$$

$$\mathbf{A}^{(7)} = \begin{pmatrix} 2.125825 & 0 & 0 \\ 0 & 8.388761 & 0.000009 \\ 0 & 0.000009 & 4.485401 \end{pmatrix}$$

从而A的特征值可取为

$$\lambda_1 \approx 2.125825,\ \lambda_2 \approx 8.388761,\ \lambda_3 \approx 4.485401$$

特征向量为旋转矩阵$R=R_1R_2\ldots$的相应的各列矢量

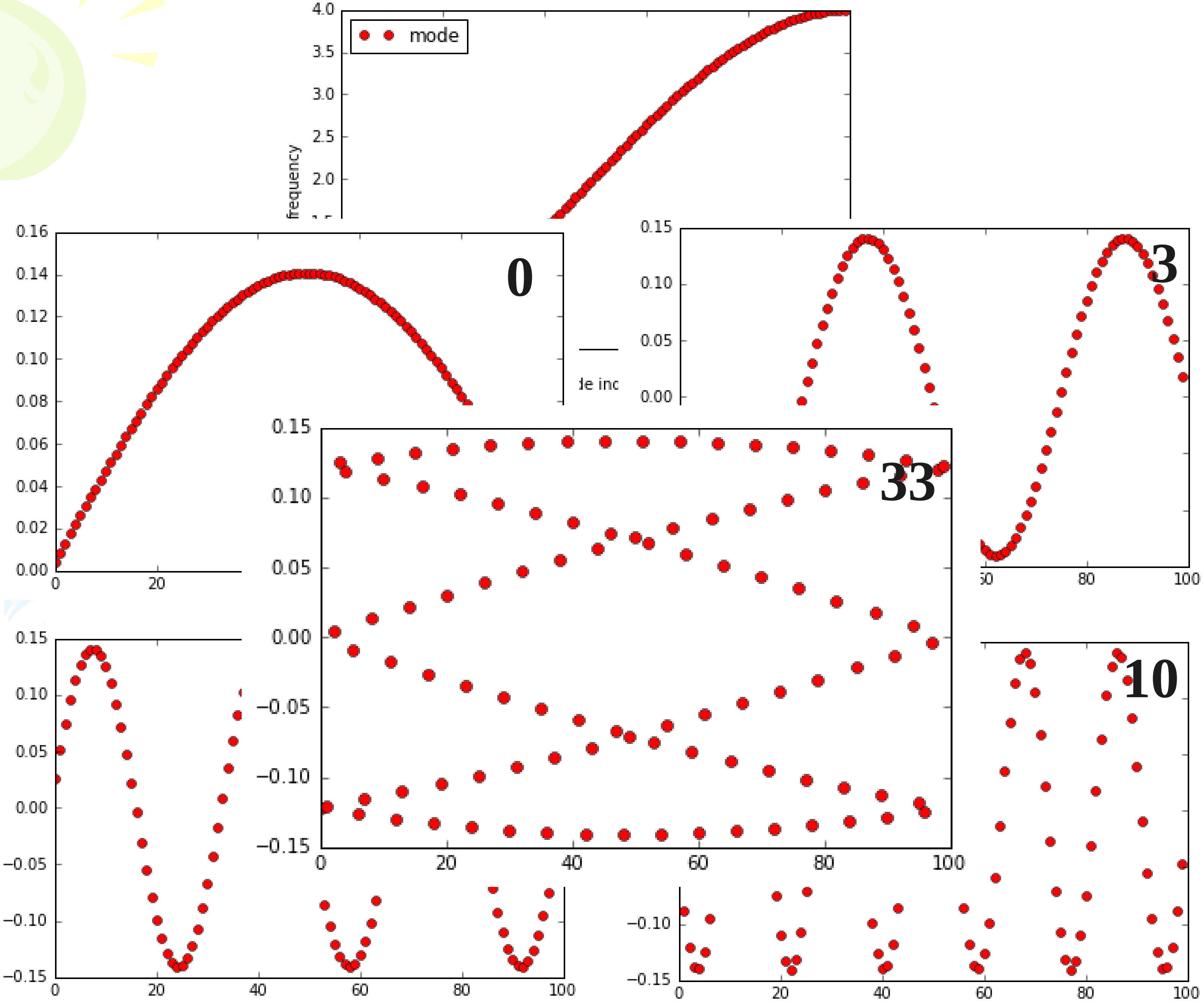


周期边界

$$m\frac{d^2}{dt^2}x_i = k(x_{i+1}-x_i) - k(x_i - x_{i-1}) \qquad x_i = A_i \exp(-i\omega t)$$

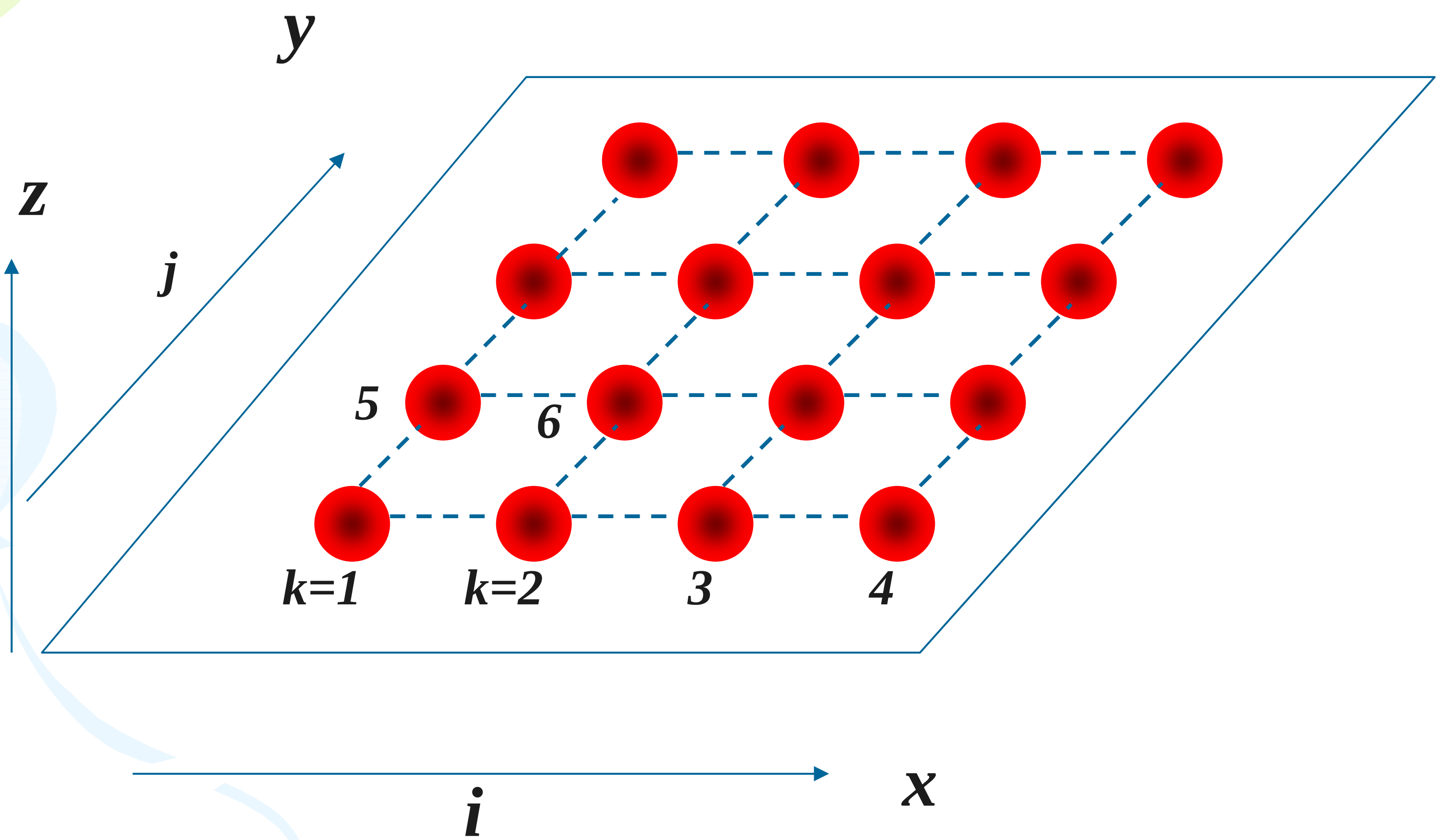
$$\frac{m\omega^2}{K}\begin{pmatrix} A_1 \\ A_2 \\ \dots \\ A_j \\ \dots \\ A_N \end{pmatrix} = \begin{pmatrix} 2 & -1 & 0 & 0 & \dots & 0 \\ -1 & 2 & -1 & 0 & \dots & 0 \\ 0 & -1 & 2 & -1 & \dots & 0 \\ \dots & & & & & \\ 0 & \dots & 0 & 0 & -1 & 2 \end{pmatrix}\begin{pmatrix} A_1 \\ A_2 \\ \dots \\ A_j \\ \dots \\ A_N \end{pmatrix}$$

N=100, K=1, m=1



mode
frequency
0
3
33
10

二维薄膜振动



$$\frac{\partial^2 z}{\partial t^2} = \frac{T}{\sigma}\left(\frac{\partial^2 z}{\partial x^2} + \frac{\partial^2 z}{\partial y^2}\right)$$

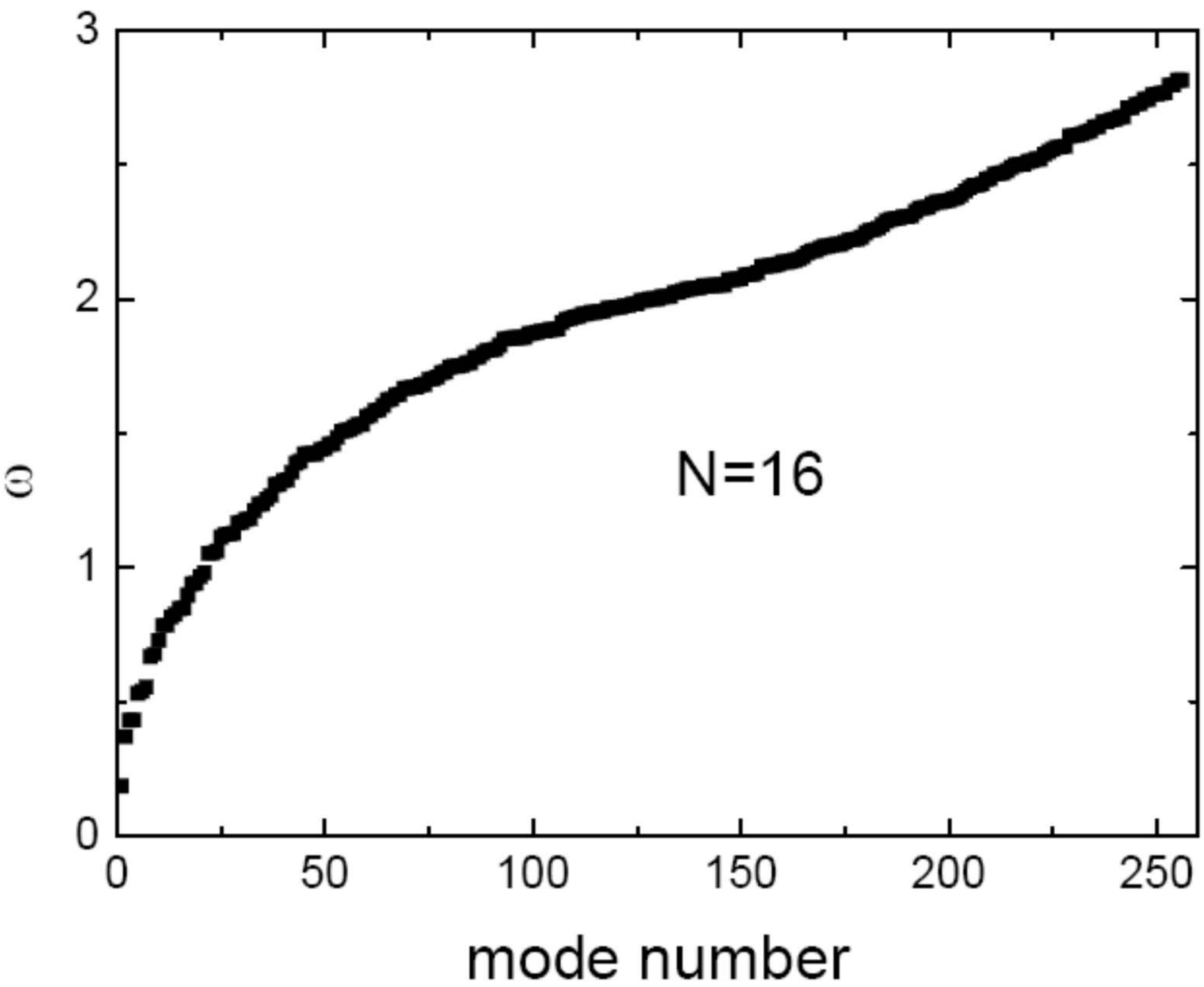
$$k = i + Nj$$

$$\left(\sigma \Delta x \Delta y\right)\frac{\partial^2 z_k}{\partial t^2} = T\left(z_{k+1} + z_{k-1} + z_{k+N} + z_{k-N} - 4z_k\right)$$

$$z_k = A_k e^{-i\omega t}$$

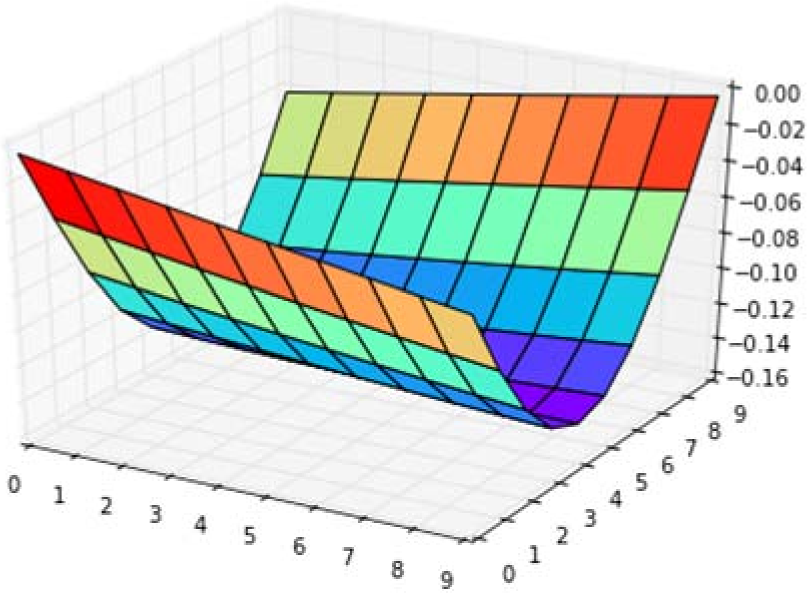
$$\frac{\sigma \Delta x \Delta y}{T}\omega^2 \vec{A} = D\vec{A}$$

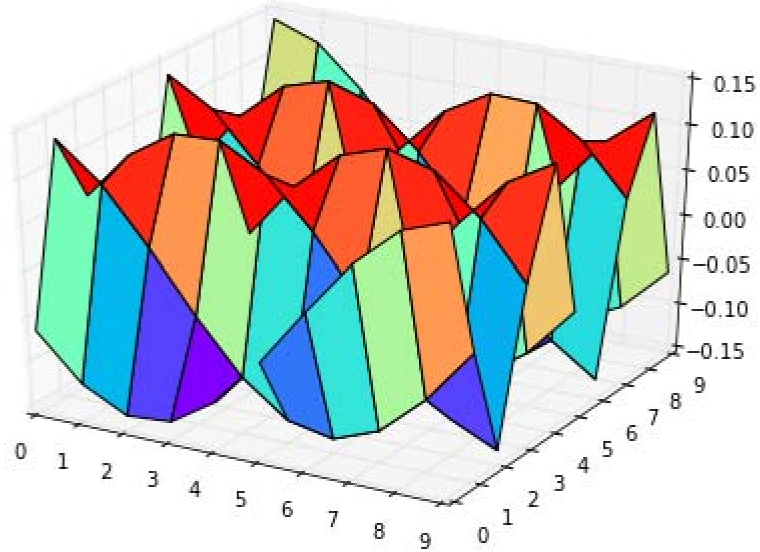
$$D=\begin{pmatrix} 4 & -1 & 0 & 0 & \cdots & 0 & 0 & 0 & 0 & 0 \\ -1 & 4 & -1 & 0 & \cdots & -1 & 0 & 0 & \cdots & 0 \\ 0 & -1 & 4 & -1 & \cdots & 0 & -1 & 0 & \cdots & 0 \\ \cdots & & & & & & & & & \\ 0 & \cdots & 0 & 0 & 0 & 0 & 0 & 0 & -1 & 4 \end{pmatrix}$$

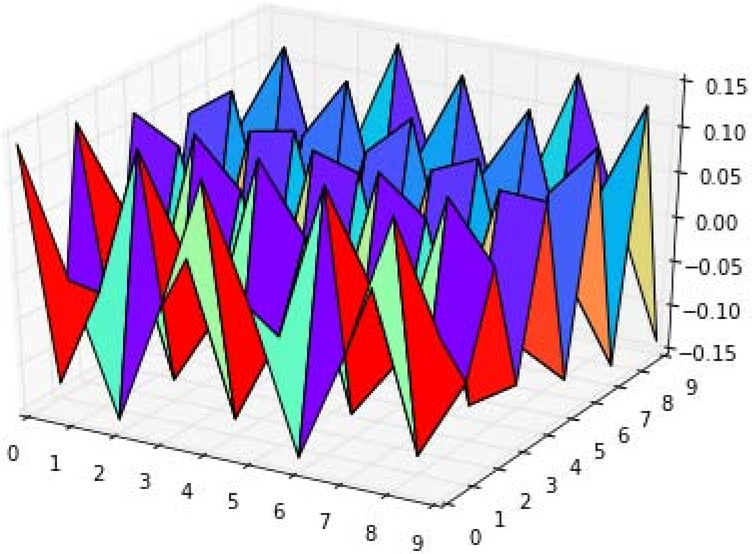


3
2
1
0
ω
N=16
0
50
100
150
200
250
mode number

N=10*10=100


0.00
−0.02
−0.04
−0.06
−0.08
−0.10
−0.12
−0.14
−0.16
0 1 2 3 4 5 6 7 8 9
0 1 2 3 4 5 6 7 8 9


0.15
0.10
0.05
0.00
−0.05
−0.10
−0.15
0 1 2 3 4 5 6 7 8 9
0 1 2 3 4 5 6 7 8 9


0.15
0.10
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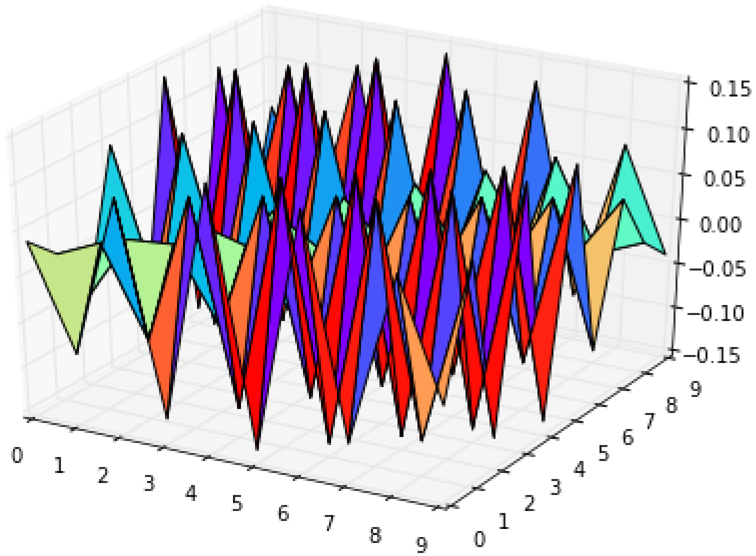
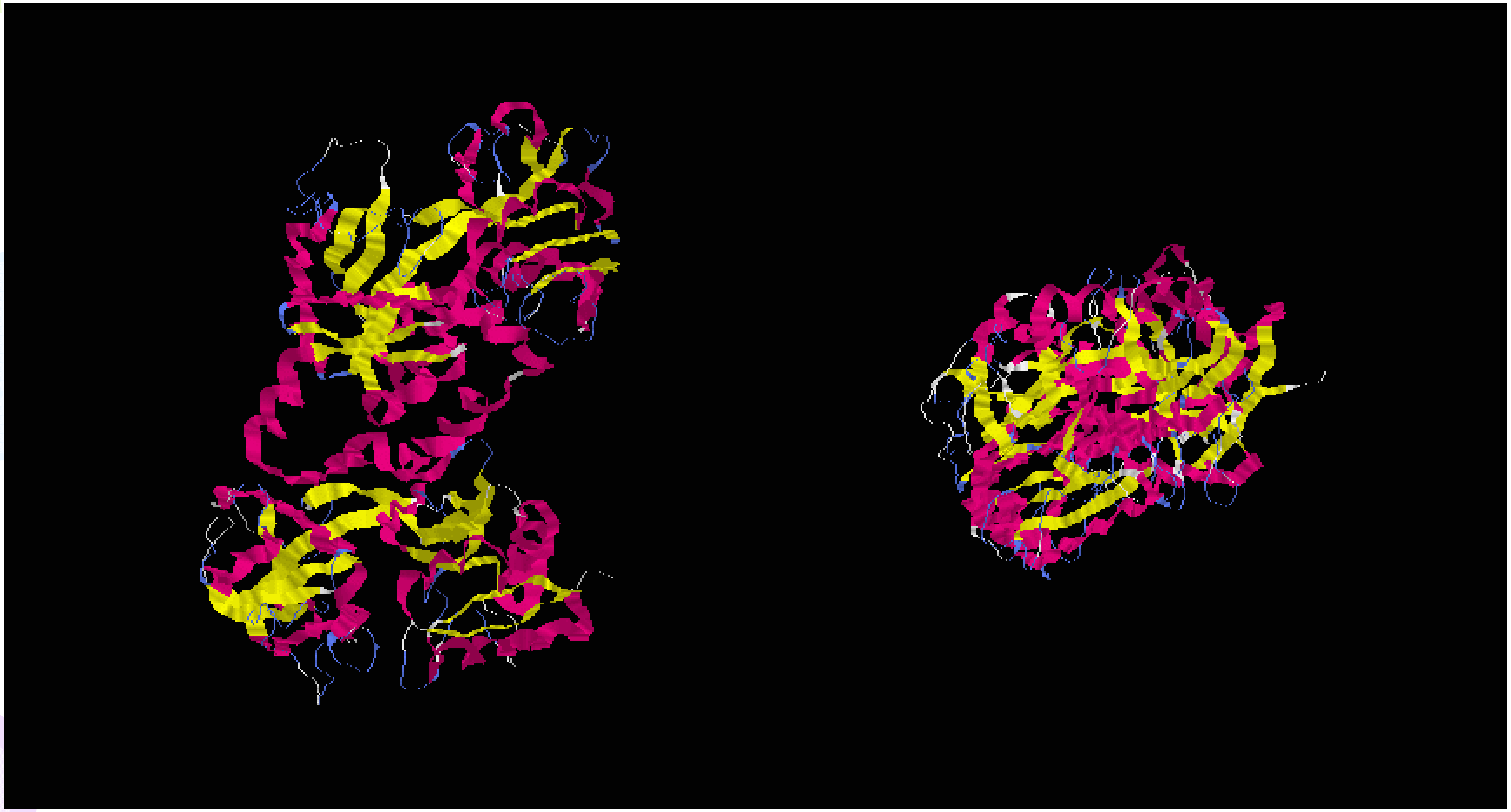
0 1 2 3 4 5 6 7 8 9
0 1 2 3 4 5 6 7 8 9


0.15
0.10
0.05
0.00
−0.05
−0.10
−0.15
0 1 2 3 4 5 6 7 8 9
0 1 2 3 4 5 6 7 8 9



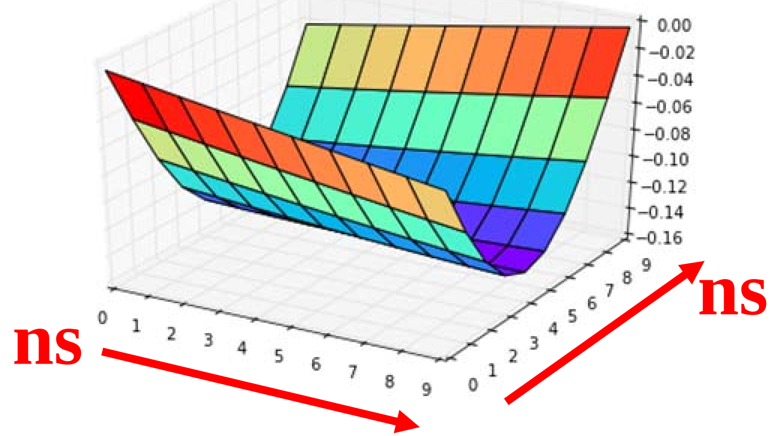
课堂练习

```
from numpy import array, arange, zeros, linalg
import pylab as pl

#在下面给A赋值
A = …
eigenValues, eigenVectors = linalg.eig(A)

print("eigenValues", eigenValues)
print("eigenVectors ", eigenVectors)
n=…
pl.plot(range(n),  eigenValues, ’ro’)
pl.show()
pl.plot(range(n),  eigenVectors[0,:], ’ro’)
pl.show()
```

$$\mathbf{A} = \begin{pmatrix} 4 & 2 & 2 \\ 2 & 5 & 1 \\ 2 & 1 & 6 \end{pmatrix}$$

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

```
from mpl_toolkits.mplot3d import Axes3D
eigenValues, eigenVectors
                    = linalg.eig(A)
ns = 4
N=ns*ns
x = arange(ns)
y = arange(ns)
x,y = meshgrid(x,y)
id=3  #画第三个本征矢
fig = pl.figure()
ax = Axes3D(fig)
ev = eigenVectors[:,id]
ev.shape = (ns,ns)
ax.plot_surface(x,y,ev, rstride=1, cstride=1,
                         cmap='rainbow')
```



ns为二维膜一个方向格点数即矩阵大小N的平方根。

$$D=\begin{pmatrix} 4 & -1 & 0 & 0 & \cdots & 0 & 0 & 0 & 0 & 0 \\ -1 & 4 & -1 & 0 & \cdots & -1 & 0 & 0 & \cdots & 0 \\ 0 & -1 & 4 & -1 & \cdots & 0 & -1 & 0 & \cdots & 0 \\ \cdots & & & & & & & & & \\ 0 & \cdots & 0 & 0 & 0 & 0 & 0 & 0 & -1 & 4 \end{pmatrix}$$

E N D