Chapter 9 Eigenvalues and Pseudospectra

Example 1: Mathieu equation

(Eq. 1) $-u_{xx} + 2q\cos(2x)u = \lambda u$ on $x \in [0, 2\pi]$ with periodic boundary condition $u(0) = u(2\pi)$ and $u_x(0) = u_x(2\pi)$.

We use Fourier basis on discrete grid $x_0 = 0, x_1, x_2, \dots x_N$ where $x_j = jh$, $h = \frac{2\pi}{N}$ and N is even. Under such basis, boundary condition is automatically satisfied.

(Eq. 2)
$$p(x) = \frac{1}{2\pi} P \sum_{k=-m}^{m} e^{ikx} \hat{v}_k = \sum_{k=1}^{N} v_k S_N(x - x_k)$$
 and

the derivative is according to

(Eq. 3)
$$w_j = p''(x_j) = \sum_{k=1}^N v_k S''_N(x_j - x_k)$$
 for $j = 1, 2, \dots, N$

Prop 1: direct compute 2nd directive of $S_N(x) = \frac{\sin(\pi x/h)}{(2\pi/h)\tan(x/2)}$ on $[0, 2\pi]$

(Eq. 4)
$$S_N''(x_j) = \begin{cases} -\frac{1}{6} - \frac{\pi^2}{3h^2}, \quad j = 0 \pmod{N} \\ -\frac{(-1)^j}{2\sin^2(jh/2)}, \quad j \neq 0 \pmod{N} \end{cases}$$

Since N is even, second order differentiation matrix is symmetry

$$(\text{Eq. 5}) \quad D_{N}^{(2)} = \begin{pmatrix} \ddots & \ddots & \ddots & \ddots \\ \ddots & -\frac{1}{2}\csc^{2}(2h/2) & \ddots \\ \ddots & \frac{1}{2}\csc^{2}(h/2) & \ddots \\ \ddots & -\frac{1}{6}-\frac{\pi^{2}}{3h^{2}} & \frac{1}{2}\csc^{2}(h/2) & \ddots \\ & \frac{1}{2}\csc^{2}(2h/2) & \ddots \\ & \ddots & \ddots \end{pmatrix}$$

we use MATLAB build-in function "TOEPLITZ(R) is a symmetric (or Hermitian) Toeplitz matrix." To create such Toeplitz matrix $D2 = toeplitz \left(-\frac{1}{6} - \frac{\pi^2}{3h^2}, -\frac{(-1)^{1:N-1}}{2\sin^2((1:N-1)h/2)} \right)$.

Under (Eq. 4), we can discretize (Eq. 1) as

(Eq. 6)
$$\begin{bmatrix} w_1 \\ \vdots \\ w_N \end{bmatrix} = L_N \begin{bmatrix} \hat{v}_1 \\ \vdots \\ \hat{v}_N \end{bmatrix}$$
 where $L_N = -D_N^{(2)} + 2q \begin{bmatrix} \cos(2x_1) \\ \cos(2x_j) \\ \cos(2x_N) \end{bmatrix}$

The dispersion relation is shown in Figure 1, we order the eigenvalue as red, blue and black in

order monotone increasing.



Figure 1: the first 11 eigenvalues of Mathieu equation.

Conclusion:

- (1) We can regard potential $V_q(x) = 2q\cos(2x)$ is a perturbation of kinetic operator $-\Delta$, we know eigen-pair of $-u_{xx} = \lambda u$ with periodic B.C. is $\lambda_k = k^2$ for $k = 0, 1, 2, \cdots$ and eigenvector $\{1, \cos kx, \sin kx\}$, this system has degeneracy for $k = 1, 2, \cdots$, say $\cos kx$ and $\sin kx$ have the same energy since combination of both corresponds to forward wave e^{ikx} and backward wave e^{-ikx} . From Figure 1, it is clear that eigen-value locates at $\lambda_k = k^2$ for q = 0 but when q > 0, the degeneracy is broken, or say splitting of eigen-value.
- (2) If we characterize curve $\lambda_k(q)$ as eigen-value of k-th order, then can we estimate the slope
 - of $\frac{d}{dq}\lambda_k(0)$, for example, from Figure 1, $\frac{d}{dq}\lambda_1(0) < 0$ (corresponds to $u_1(0,x) = \cos x$) and $\frac{d}{dq}\lambda_2(0) > 0$ (corresponds to $u_1(0,x) = \sin x$).

From Feynmann theorem (see appendix A), let $H(q) = -\frac{d^2}{dx^2} + 2q\cos(2x)$, then

$$\frac{d}{dq}H(q) = 2\cos(2x), \text{ we have}$$
(1) $\frac{d}{dq}\lambda_0(0) = \langle 1|\frac{dH(0)}{dq}|1\rangle = \int_0^{2\pi} 2\cos(2x)dx = 0$
(2) $\frac{d}{dq}\lambda_1(0) = \langle \sin x|\frac{dH(0)}{dq}|\sin x\rangle = -\frac{\pi}{2}, \text{ corresponding to blue line}$
(3) $\frac{d}{dq}\lambda_2(0) = \langle \cos x|\frac{dH(0)}{dq}|\cos x\rangle = \frac{\pi}{2}, \text{ corresponding to black dashed line.}$

(4)
$$\left\langle \cos kx \left| \frac{dH(0)}{dq} \right| \cos kx \right\rangle = 0$$
 and $\left\langle \sin kx \left| \frac{dH(0)}{dq} \right| \sin kx \right\rangle = 0$ for $k > 1$, hence the slope of other $\frac{d}{dq} \lambda_k(0) = 0$.

Question 1: Can we distinguish the curve corresponds to $\cos kx$ or $\sin kx$?

 if we apply Feymann thorem again, we have

$$\frac{d^{2}}{d\lambda^{2}}E(\lambda) = \langle \psi(\lambda) | \frac{d^{2}}{d\lambda^{2}}H(\lambda) | \psi(\lambda) \rangle + \langle \frac{d}{d\lambda}\psi(\lambda) | \frac{d}{d\lambda}H(\lambda) | \psi(\lambda) \rangle$$

$$+ \langle \psi(\lambda) | \frac{d}{d\lambda}H(\lambda) | \frac{d}{d\lambda}\psi(\lambda) \rangle$$
In our problem $\frac{d^{2}}{dq^{2}}\lambda_{k}(0) = 2\langle \psi_{k}(0) | \frac{dH}{dq} | \frac{d}{dq}\psi_{k}(0) \rangle$, however we don't know $\frac{d}{dq}\psi_{k}(0)$, so

we cannot estimate $\frac{d^2}{dq^2}\lambda_k(0)$.

If we use perturbation theorem (for non-degenerate version, in fact this version is not adequate for this problem since $H_0 = -\frac{d^2}{dx^2}$ is degenerated), then $\Delta_n^{(2)} = \sum_{k \neq n} \frac{|V_{nk}|^2}{E_n^{(0)} - E_k^{(0)}}$, first we consider n = 2 and $|2^{(0)}\rangle = \cos 2x$, then $V_{20} = \int_0^{2\pi} \cos(2x)\cos(2x)dx = \pi$ $V_{2k} = \int_0^{2\pi} \left\{ \frac{\cos kx}{\sin kx} \right\} \cos(2x)\cos(2x)dx = \frac{1}{2} \int_0^{2\pi} \left\{ \frac{\cos kx}{\sin kx} \right\} \cos(4x)dx$, then $V_{24}, \cos 4x = \frac{1}{2} \int_0^{2\pi} \cos^2(4x)dx = \frac{\pi}{2}$ and $V_{2k} = 0$ otherwise. $\Delta_2^{(2)}, \cos 2x = \sum_{k \neq n} \frac{|V_{nk}|^2}{E_2^{(0)} - E_k^{(0)}} = \frac{|V_{20}|^2}{2^2 - 0^2} + \frac{|V_{24}|^2}{2^2 - 4^2} = \frac{11}{48}\pi^2 > 0$. Similarly for $|2^{(0)}\rangle = \sin 2x$, we have $V_{2k} = \int_0^{2\pi} \left\{ \frac{\cos kx}{\sin kx} \right\} \cos(2x)\sin(2x)dx = \frac{1}{2} \int_0^{2\pi} \left\{ \frac{\cos kx}{\sin kx} \right\} \sin(4x)dx$, then $V_{24}, \sin 4x = \frac{\pi}{2}$ and

 $V_{2k} = 0$ otherwise. $\Delta_2^{(2)}, \sin 2x = -\frac{\pi^2}{48} < 0$.

Hence we know curve of even function $|2^{(0)}\rangle = \cos 2x$ is increasing and curve of odd function $|2^{(0)}\rangle = \sin 2x$ s decreasing.

However for
$$n > 2$$
, we have

$$V_{nk}, \cos(nx) = \int_{0}^{2\pi} \left\{ \frac{\cos kx}{\sin kx} \right\} \cos(2x) \cos(nx) dx$$

$$= \frac{1}{2} \int_{0}^{2\pi} \left\{ \frac{\cos kx}{\sin kx} \right\} \left[\cos((n+2)x) + \cos((n-2)x) \right] dx = \begin{cases} \frac{\pi}{2}, & k = n+2, k = n-2\\ 0, & otherwise \end{cases}$$

$$V_{nk}, \sin(nx) = \int_{0}^{2\pi} \left\{ \frac{\cos kx}{\sin kx} \right\} \cos(2x) \sin(nx) dx$$

= $\frac{1}{2} \int_{0}^{2\pi} \left\{ \frac{\cos kx}{\sin kx} \right\} \left[\sin((n+2)x) + \sin((n-2)x) \right] dx = \begin{cases} \frac{\pi}{2}, & k = n+2, k = n-2\\ 0, & otherwise \end{cases}$
$$\Delta_{n}^{(2)} = \frac{\pi^{2}}{4} \left(\frac{1}{n^{2} - (n-2)^{2}} + \frac{1}{n^{2} - (n+2)^{2}} \right) = \frac{2\pi^{2}}{(4n-4)(4n+4)} > 0, \text{ we only know both curves of } |n^{(0)}\rangle = \cos nx \text{ and } |n^{(0)}\rangle = \sin nx \text{ are increasing locally but we cannot distinguish which is}$$

higher one.

Next we explicit calculate eigenmodes

Let
$$u = a_0 + \sum_{n=1}^{\infty} a_n \cos nx + \sum_{n=1}^{\infty} b_n \sin nx$$
, then
 $\cos(2x)u = a_0 \cos(2x) + \sum_{n=1}^{\infty} a_n \cos(nx) \cos(2x) + \sum_{n=1}^{\infty} b_n \sin(nx) \cos(2x)$
 $= a_0 \cos(2x) + \sum_{n=1}^{\infty} \frac{a_n}{2} \left[\cos((n+2)x) + \cos((n-2)x) \right]$
 $+ \sum_{n=1}^{\infty} \frac{b_n}{2} \left[\sin((n+2)x) + \sin((n-2)x) \right]$
 $= \frac{a_2}{2} + \frac{1}{2} (a_1 + a_3) \cos x + \left(a_0 + \frac{a_4}{2} \right) \cos(2x) + \sum_{n=3}^{\infty} \frac{1}{2} (a_{n-2} + a_{n+2}) \cos(nx)$
 $+ \frac{1}{2} (-b_1 + b_3) \sin x + \frac{b_4}{2} \sin(2x) + \sum_{n=3}^{\infty} \frac{1}{2} (b_{n-2} + b_{n+2}) \sin(nx)$

Substitute into $-u_{xx} + 2q\cos(2x)u = \lambda u$, we have $\int aa = \lambda a$

(Eq. 7)
$$\begin{cases} qa_2 = \lambda a_0 \\ 1^2 a_1 + q(a_1 + a_3) = \lambda a_1 \\ 2^2 a_2 + q(2a_0 + a_4) = \lambda a_2 \\ n^2 a_n + q(a_{n-2} + a_{n+2}) = \lambda a_n \end{cases} \text{ and } \begin{cases} 1^2 b_1 + q(-b_1 + b_3) = \lambda b_1 \\ 2^2 b_2 + qb_4 = \lambda b_2 \\ n^2 b_n + q(b_{n-2} + b_{n+2}) = \lambda b_n \end{cases}$$

If we set $\vec{a} = (a_0 | a_1 | a_2 | \cdots | a_n | \cdots)$ and $\vec{b} = (b_0 | b_1 | b_2 | \cdots | b_n | \cdots)$, then we can abbreviate

(Eq. 7) as $\begin{bmatrix} A_{11} \\ A_{22} \end{bmatrix} \begin{pmatrix} a \\ b \end{pmatrix} = \lambda \begin{pmatrix} a \\ b \end{pmatrix}$, say system is decompose into modes of even function (related

to \vec{a} , i.e. $\cos nx$) and modes of odd function (related to \vec{b} , i.e. $\sin nx$). Moreover if we look at (Eq. 7) carefully, it is not difficult to find further decomposition

$$\begin{cases} qa_{2} = \lambda a_{0} \\ 2^{2}a_{2} + q(2a_{0} + a_{4}) = \lambda a_{2} \\ (2k)^{2}a_{2k} + q(a_{2k-2} + a_{2k+2}) = \lambda a_{2k} \end{cases} \text{ and } \begin{cases} 1^{2}a_{1} + q(a_{1} + a_{3}) = \lambda a_{1} \\ (2k+1)^{2}a_{2k+1} + q(a_{2k-1} + a_{2k+3}) = \lambda a_{2k+1} \end{cases}$$

$$\begin{cases} 1^{2}b_{1} + q(-b_{1} + b_{3}) = \lambda b_{1} \\ (2k+1)^{2}b_{2k+1} + q(b_{2k-1} + b_{2k+3}) = \lambda b_{2k+1} \end{cases} \text{ and } \begin{cases} 2^{2}b_{2} + qb_{4} = \lambda b_{2} \\ (2k)^{2}b_{2k} + q(b_{2k-2} + b_{2k+2}) = \lambda b_{2k} \end{cases}$$

Remark 1: such sub-decomposition holds even in truncated matrix. For example, if we denote kinetic operator $Ku = -\frac{d^2u}{dx^2}$ and potential operator $Vu = 2\cos(2x)u$, then for N = 4, $K_a = diag(0,1^2,2^2,3^2,4^2)$, $K_b = diag(1^2,2^2,3^2,4^2)$, $V_a = \begin{pmatrix} 1 \\ 1 & 1 \\ 2 & 1 \\ 1 & 1 \end{pmatrix}$, $V_b = \begin{pmatrix} -1 & 1 \\ 1 & 1 \\ 1 & 1 \end{pmatrix}$ and then $\begin{cases} (K_a + qV_a)a = \lambda a \\ (K_b + qV_b)b = \lambda b \end{cases}$.

Question 2: It is easy to show that $(K_b + qV_b)$ is symmetric but $(K_a + qV_a)$ is not symmetric, we know eigenvalue of $(K_b + qV_b)$ is real, can you show me that eigenvalue of $(K_a + qV_a)$ also real?



Figure 2: eigenmodes of (Eq. 7), red color is even function and blue color is odd function. This figure is the same as Figure 1. For high oscillatory modes, its kinetic energy dominant the system, $\cos kx$ and $\sin kx$ are also near eigenmodes, as seen in right panel, we may called them scattering mode.

Table 1: choose N = 4, $\lambda_k(a)$ denotes eigenvalue computed by $(K_a + qV_a)$ and $\lambda_k(b)$ denotes eigenvalue computed by $(K_b + qV_b)$. This table shows (1) sub-decomposition is correct.

(2) Large q deviate $\cos kx$ or $\sin kx$ to its neighbor

	0	1	2	3	4
$q=0.1, \lambda_k(a)$	-0.0050	4.0042	16.0008	9.0013	1.0987
q = 0.1	0.9988	0	-0.0250	0	0.0001
$u_{1} = (a_{1}, a_{2}, \cdots, a_{n})$	0	-0.9999	0	0.0127	0
u_k (u_0, u_1, \dots, u_4)	-0.0499	0	-0.9997	0	0.0083
	0	0.0127	0	0.9999	0
	0.0003	0	0.0083	0	1.0000
$q=15, \lambda_k(a)$	-22.1808	10.1268	32.0540	-2.9029	27.9029
<i>q</i> = 15	0.5327	0	-0.4752	0	0.3235
$u_{1} = (a_{2}, a_{2}, \cdots, a_{n})$	0	0.6216	0	0.7833	0
u_k (u_0, u_1, \dots, u_4)	-0.7877	0	-0.3208	0	0.6914
	0	-0.7833	0	0.6216	0
	0.3095	0	0.8193	0	0.6460
$q=0.1, \lambda_k(b)$		0.8988	3.9992	9.0012	16.0008
q = 0.1		-0.9999	0	-0.0123	0
$u_{1} = (h_{1}, h_{2}, \cdots, h_{n})$		0	1.0000	0	0.0083
u_k ($v_1, v_2,, v_4$)		0.0123	0	-0.9999	0
		0	-0.0083	0	1.0000
$q=15, \lambda_k(b)$		-21.4011	-6.1555	16.4011	26.1555
q = 15		-0.8968	0	0.4425	0
$u_{1} = (h_{1}, h_{2}, \cdots, h_{n})$		0	0.8281	0	0.5606
$[u_k (v_1, v_2,, v_4)]$		0.4425	0	0.8968	0
		0	-0.5606	0	0.8281

(3) Splitting of degenerate eigenmodes at q = 0

Choose N = 42, and q = 15, we plot first 4 eigenmode in even configuration $(K_a + qV_a)a = \lambda a$ and odd configuration $(K_b + qV_b)b = \lambda b$ in frequency space and also in physical space. In Figure 4, support of dominant frequency components only locates near neighbor and the root of eigenmode is 0, 2, 4, 6 in order. In Figure 5, support of dominant frequency components only locates near neighbor also and the root of eigenmode is 1, 3, 5, 7 in order.

	0	1	2	3	4
$q=15, \lambda_k(a)$	-22.5130	-8.1011	5.0780	16.5874	25.3751
$q=15, \lambda_k(b)$		-22.5130	-8.0993	5.1166	17.0373

Observation 1: even eigenmode $u_{k,evev}(\pi) \sim 0$ (odd eigenmode is odd symmetric with respect to $x = \pi$, so $u_{k,odd}(\pi) = 0$), when eigenvalue $\lambda_k < \max V = 2q = 30$, why? From Figure 3, the first 4 eigenvalue is smaller than $\max V$, but we know $\langle E \rangle = \langle T \rangle + \langle V \rangle$ for average $\langle \cdot \rangle$ over any domain where $\langle T \rangle = \langle u_k | \left(-\frac{d^2}{dx^2} \right) | u_k \rangle$ is kinetic energy and $\langle V \rangle = \langle u_k | 2q \cos 2x | u_k \rangle$ is potential energy, since $\langle T \rangle > 0$, we must have $\lambda_k = \langle E \rangle > \langle V \rangle$, but V attains maximum at $x = \pi$ and then we must have $u_k(\pi) \sim 0$ to guarantee $\lambda_k > \int_{-\infty}^{\pi+\delta} V u_k^2 dx \, .$ 6



Figure 3: for first 4 eigenmode, eigenvalue (energy) is smaller than maximum of potential energy, so eigen-function must be near zero at midpoint where potential energy attains maximum.



Figure 4: even eigenmode, left panel is eigenmode of combination of frequency space, right panel is eigenmode in physical space.



Figure 5: odd eigenmode, left panel is eigenmode of combination of frequency space, right panel is eigenmode in physical space.

Observation 2: if we reflect graph ($x < \pi$) of first even eigenmode, then the graph is the same as first odd eigenmode. I think this is due to

- (1) sub-decomposition, say $\{1, \cos(2kx)\}$ corresponding to $\{\sin((2k+1)x)\}$ and $\left\{\cos\left((2k+1)x\right)\right\}$ corresponding to $\left\{\sin\left(2kx\right)\right\}$.
- (2) When $q \gg k^2$ for k : eigenmode, then potential dominants λ_k and
- (3) Nodal set matching, say "if we reflect $\cos(2kx)$ about $x = \pi$, then we must have one more nodal point $x = \pi$, this would match sin((2k+1)x)". Of course we need Sturn-Liouville theorem to make sure nodal set is increasing without jump.



Example 2 (Airy function): From http://en.wikipedia.org/wiki/Airy_function

In mathematics, the Airy function Ai(x) is a special function named after the British astronomer <u>George Biddell Airy</u>. The function Ai(x) and the related function Bi(x), which is also called an Airy function, are solutions to the <u>differential equation</u> $u_{xx} = xu$ for $x \in R$ known as the Airy equation or the Stokes equation. This is the simplest second-order linear differential equation with a turning point (a point where the character of the solutions changes from oscillatory to exponential).

Question 3: Why Airy function is exponential decay for x > 0 and oscillates at x < 0, like Figure 6?

<ans> Informally, we can relate $u_{xx} = xu$ (Airy's governing equation) to two kinds second order

equation
$$(u_{xx} = xu) \sim \begin{cases} u_{xx} + k^2 u = 0 & \text{for } x < 0 \\ u_{xx} = k^2 u & \text{for } x > 0 \end{cases} \sim \begin{cases} u \in \{\sin x, \cos x\} & \text{for } x < 0 \\ u \in sp\{e^x, e^{-x}\} & \text{for } x > 0 \end{cases}$$
. However formally

we require Sturn-Livoulle comparison theorem.

$$(\text{Eq. 8}) \quad Ai(x) = \frac{1}{\pi} \int_0^\infty \cos\left(\frac{t^3}{3} + xt\right) dt$$

$$(\text{Eq. 9}) \quad Bi(x) = \frac{1}{\pi} \int_0^\infty \exp\left(-\frac{t^3}{3} + xt\right) + \sin\left(\frac{t^3}{3} + xt\right) dt$$
Asymptotic behavior for $x \gg 1$

$$(\text{Eq. 10}) \quad Ai(x) \sim \frac{1}{2\sqrt{\pi}x^{1/4}} \exp\left(-\frac{2}{3}x^{3/2}\right) \text{ and } Ai(-x) \sim \frac{1}{\sqrt{\pi}x^{1/4}} \sin\left(\frac{2}{3}x^{3/2} + \frac{\pi}{4}\right)$$

$$(\text{Eq. 11}) \quad Bi(x) \sim \frac{1}{\sqrt{\pi}x^{1/4}} \exp\left(\frac{2}{3}x^{3/2}\right) \text{ and } Bi(-x) \sim \frac{1}{\sqrt{\pi}x^{1/4}} \cos\left(\frac{2}{3}x^{3/2} + \frac{\pi}{4}\right)$$

Further function value at tuning point x = 0

(Eq. 12)
$$Ai(0) = \frac{1}{3^{2/3}\Gamma(2/3)}, \quad \frac{d}{dx}Ai(0) = \frac{1}{3^{1/3}\Gamma(1/3)}$$

(Eq. 13) $Bi(0) = \frac{1}{3^{1/6}\Gamma(2/3)}, \quad \frac{d}{dx}Bi(0) = \frac{3^{1/6}}{\Gamma(1/3)}$



Figure 6: airy function Ai(x) is exponential

decay for x > 0 but has infinite number of oscillations that decay with algebraically in amplitude $x^{-1/4}$ for x < 0.

Table 2: zero of Airy function from http://mathworld.wolfram.com/AiryFunctionZeros.html

root	1st	2nd	3th	4th	5th	6th
Ai(x)	-2.33811	-4.0875	-5.52056	-6.7867144	-7.94413	-9.02265
Bi(x)	-1.17371	-3.27109	-4.83074	-6.16985	-7.37676	-8.49195

If we want to use Chebyshev node to interpolate Airy function, then it has difficulty since domain of Airy function is $x \in R$, even we can truncate x > 0 for x = L since Airy function decays exponentially for x > 0, however we cannot truncate x < 0 for x = -L since Airy function is oscillates for x < 0 and decay slowly about $x^{-1/4}$. Now if we sample x = -L is root of airy function and image $Ai(L) \sim 0$, then we can approximate Airy function by solving

(Eq. 14) $u_{xx} = xu$, u(L) = u(-L) = 0

The existence of solution of (Eq. 14) is equivalent to following:

Let x = Ly, $y \in [-1,1]$, u(x) = U(y), then (Eq. 14) is equivalent to

(Eq. 15)
$$U_{yy} = L^3 y U$$
, $u(1) = u(-1) = 0$

At first glance, (Eq. 15) is generalized eigenvalue problem $Au = \lambda Bu$, why? Let us discretize (Eq. 15) under Chebyshev node, then $A = \tilde{D}_N^2$, $B = diag(y_1, y_2, \dots, y_{N-1})$, $\lambda = L^3$. Let eigen-pair be $\{\lambda_k, U_k\}$, and $u_k(x) = U_k(y)$, define $L_k = \lambda_k^{1/3}$.

Remark 2: In fact, Ai(L) > 0 and Bi(L) > 0, hence our eigen-function u_k is combination of Ai(x), Bi(x), say $u_k(x) = Ai(x) - \beta_k Bi(x)$ satisfying $u_k(L_k) = 0$. So $\beta_k = \frac{Ai(L_k)}{Bi(L_k)}$, in order

to estimate coefficient β_k , we use asymptotic estimate of Ai(x), Bi(x) (i.e (Eq. 10) and (Eq.

11)),
$$\frac{Ai(x)}{Bi(x)} \sim \frac{\frac{1}{2\sqrt{\pi}x^{1/4}}\exp\left(-\frac{2}{3}x^{3/2}\right)}{\frac{1}{\sqrt{\pi}x^{1/4}}\exp\left(\frac{2}{3}x^{3/2}\right)} \sim \frac{1}{2}\exp\left(-\frac{4}{3}x^{3/2}\right), \ \beta_k \sim \frac{1}{2}\exp\left(-\frac{4}{3}\sqrt{\lambda_k}\right).$$
 Moreover since

 $u_k(-L_k) = 0$, we have $Ai(-L_k) = \beta_k Bi(-L_k)$, from Figure 6, we know $|Bi(x)| \le |Bi(0)| \le 0.5$, hence $|Ai(-L_k)| \le \frac{1}{2}\beta_k$. This means the value of β_k determine the accuracy of approximation to Airy function.



Figure 7: the more grids, the more accurate airy function is. When N = 12, the shape of eigen-function is far away from Airy function.

Question 4: If we don't scale eigen-function u_5 , then u_5 is multiple of Ai, see Figure 8, why?



Figure 8: $u_5(0) = 0.6629$ but

Ai(0) = 0.355. Eigen-function is multiple of

Airy function.

<ans> As far as equation is concerned, u_5 is also eigen-function when we do scaling, in MATLAB, it do norm normalization such that $||u_5|| = 1$, this is a degree of freedom since $Ai(0) = \frac{1}{\pi} \int_0^\infty \cos\left(\frac{t^3}{3}\right) dt$. after we do scaling $u_5 \leftarrow u_5 \frac{Ai(0)}{u_5(0)}$, then $||Ai - u_5||_\infty = 5.5117e-008$ and $||Ai - u_5||_\infty = 5.2487e-008$.

$Dl(L_k)$							
	1st	2nd	3th	4th	5th	6th	
λ_k	12.8239	68.3153	168.2478	312.5917	501.3484	734.5180	
$L_k = \lambda_k^{1/3}$	2.3407	4.0880	5.5206	6.7867	7.9441	9.0227	
β_k	0.0042	8.1822e-006	1.5416e-008	2.8910e-011	5.4121e-014	1.0123e-016	
$Ai(L_k)$	0.0204	7.9326e-004	3.2070e-005	1.3215e-006	5.5033e-008	2.3073e-009	
$Bi(L_k)$	5.1675	99.4736	2.1142e+003	4.6254e+004	1.0264e+006	2.2969e+007	
True β_k	0.004	7.9746e-006	1.5169e-008	2.8570e-011	5.3618e-014	1.0045e-016	

Table 3: N = 48, we use MATLAB built-in function AIRY to compute $Ai(L_k) = airy(L_k)$ and $Bi(L_k) = airy(2, L_k)$, then compute true $\beta_k = \frac{Ai(L_k)}{Bi(L_k)}$.

Example 3 (Laplace eigenvalue with Dirichlet B.C.)

(Eq. 16) $-\Delta u + f(x, y)u = \lambda u$, -1 < x, y < 1 and u = 0 on the boundary

Case 1:
$$f = 0$$
, then $\lambda_{k,m} = \frac{\pi^2}{4} (k^2 + m^2)$, $u_{k,m} = \sin\left(\frac{\pi}{2}k(x+1)\right) \sin\left(\frac{\pi}{2}m(y+1)\right)$

We plot first 4 eigen-pair in Figure 9, 2nd and 3rd eigenmode are degenerated due to 2-fold symmetry in domain and Laplacian operation is rotational symmetry. Here 2-fold symmetry means that if we rotate domain by 90 degree, then the problem is the same.



 $-\Delta_{u,v}u = \lambda u$, for -1 < u, v < 1 and u = 0 on the boundary.

Remark 3: in case of degenerate eigenmodes, the choice of eigenvector is arbitrary. Here MATLAB choose eigenvector with nodal line approximately along diagonal, due to orthogonality property of degenerate eigenmode, both eigenvector has nodal line along diagonal.

Case 2: $f = \exp(y - x - 1)$, since f is not 2-fold symmetry, so degeneracy is broken, in fact, $\sup (f) \approx \{(x, y) \in [-1, 1]^2 : y \ge x + 1\}$ is left upper corner, see Figure 10.



Figure 10: support of f is concentrated at upper left corner, with 1/8 of the domain. fis not 2-fold symmetry, so we expect that degeneracy does not happen.

From Courant-Fisher theorem (minimum property of spectrum of Hermitain operator), we expect that eigenvector would avoid fall into $\operatorname{supp}(f)$, see Figure 11.



Figure 11: first 4 eigenmodes for

 $f = \exp(y - x - 1)$, eigenvalues are

distinct.

Remark 4: such barrier function f is equivalent to solve eigenvalue problem in non-supp(f),

say
$$-\Delta u = \lambda u$$
, $(x, y) \in [-1, 1]^2 - \operatorname{supp}(f)$ and $u = 0$ on the boundary.

Remark 5: If we regard f is a perturbation of $-\Delta u = \lambda u$ and regard it as a parameter, then we expect to connect (2) in in Figure 9 and (2) in Figure 11, also connect (3) in in Figure 9 and (3) in Figure 11. Since 3^{rd} eigenvector in $-\Delta u = \lambda u$ has large portion in supp(f), so it has large deviation in eigenvalue (from 5 to 5.54891) since it need to suppress eigenvector in supp(f), see Figure 12.



Figure 12: due to barrier f, eigenvector of left panel is suppressed in supp(f) to become eigenvector in right panel.

Question 5 (Exercise 1): for f = 0, we can first report 4 eigenvalues, the first 4 eigenvalues has 12 digits accuracy even simulation grid is 16×16 , but 5-th eigenvalue has only 9 digits, why?

	1	2	3	4
$\lambda_{k,m}rac{4}{\pi^2}$	2.00000000000006	5.0000000000337	5.000000000355	8.0000000000668
$\operatorname{exact} \lambda_{k,m} \frac{4}{\pi^2}$	2 = (1,1)	5 = (1, 2)	5 = (2,1)	8=(2,2)

Table 4: eigenvalues of $-\Delta u = \lambda u$ on grid 16×16.

	5	6	7	8
$\lambda_{k,m}rac{4}{\pi^2}$	10.0000000131679	10.0000000131718	13.0000000132017	13.0000000132038
$\operatorname{exact} \lambda_{k,m} \frac{4}{\pi^2}$	10 = (1,3)	10 = (3,1)	13 = (2,3)	13 = (3, 2)

Recall interpolation theorem

Theorem 1(Newton Approximation, see p224, p213[1]): Assume that $P_n(x)$ is Lagrange

polynomial (or Newton polynomial) to interpolate f(x) such that $f(x) = P_n(x) + E_n(x)$. If $f \in C^{n+1}[a,b]$, then for each $x \in [a,b]$, there corresponds a number $c = c(x) \in (a,b)$ such that error term

(Eq. 17)
$$E_n(x) = \frac{f^{(n+1)}(c)}{(n+1)!} \prod_{j=0}^n (x-x_j).$$

If we choose Chebyshev nodes, that $\max \left| \prod_{j=0}^{n} (x - x_j) \right| \le \frac{1}{2^n}$, then error formula (Eq. 17) becomes

(Eq. 18)
$$|E_n(x)| \le \frac{\|f^{(n+1)}\|_{\infty}}{2^n(n+1)!}$$

In our problem, eigenmodes are $\sin(\tau x)$, if we set $f(x) = \sin(\tau x)$, then $||f^{(n+1)}|| = \tau^{n+1}$, so

$$\left|E_{n}\left(x\right)\right| \leq \frac{\tau^{n+1}}{2^{n}\left(n+1\right)!}$$

Table 5: Let n = 16, we compute $|E_{16}(x)|$ with several parameter $\tau = \frac{\pi}{2}k$. This shows that

good approximation to	sin	$\left(\frac{\pi}{2}kx\right)$	for	k = 1, 2	up to 12 digits.
-----------------------	-----	--------------------------------	-----	----------	------------------

k	1	2	3	4	5
$ E_{16}(x) $	9.2574e-017	1.2134e-011	1.1955e-008	1.5904e-006	7.0628e-005

k	6	7	8	9	10
$ E_{16}(x) $	0.0016	0.0215	0.2085	1.5439	9.2574

Question 6 (exercise 2): $A \otimes (B \otimes C) = (A \otimes B) \otimes C$, true or false?

<ans> from http://en.wikipedia.org/wiki/Kronecker_product

$$A \otimes B = \begin{bmatrix} a_{11}B & \cdots & a_{1n}B \\ \vdots & \ddots & \vdots \\ a_{m1}B & \cdots & a_{mn}B \end{bmatrix} \text{ for } A \in R^{m \times n}, \ B \in R^{p \times q}, \ A \otimes B \in R^{mp \times nq}$$

The Kronecker product is a special case of the tensor product, so it is bilinear and associative

(1)
$$A \otimes (B+C) = (A \otimes B) + (A \otimes C)$$

(2)
$$(A+B)\otimes C = (A\otimes B) + (B\otimes C)$$

(3)
$$(kA) \otimes B = A \otimes (kB) = k (A \otimes B)$$

$$(4) \quad A \otimes (B \otimes C) = (A \otimes B) \otimes C$$

But The Kronecker product is not <u>commutative</u>, $A \otimes B \neq B \otimes A$ in general.

Question 7 (exercise 3) : Find lowest eigenvalue of $-\Delta u = \lambda u$ in $[-1,1]^3$ with u = 0 on the

boundary, estimate size of matrix, accuracy of eigenvalue and time to do "eig". We know

eigenmode is $\lambda_{k,m,l} = \frac{\pi^2}{4} (k^2 + m^2 + l^2)$ and $u_{k,m,l} = \sin(kx)\sin(my)\sin(lz)$ for $k, m, l = 1, 2, \cdots$

Source code is F:\course\2008spring\spectral_method\matlab\p23_2.m and we construct L by L = -kron(kron(D2,I), I) - kron(kron(I,D2), I) - kron(I, kron(I,D2)).



Figure 13: sparse pattern of matrix L, with N = 6, dimension of L is $5^3 = 125$

Table 6: experiment platform is quartet 1.

	<i>N</i> = 6	<i>N</i> = 8	N = 12
dimension	125	343	1331
Time to eig	0.024341 s	0.206931 s	7.321695 s
$\lambda_{\min}rac{4}{\pi^2}$	3.000024016211470	2.999999862669497	2.999999999998820
$\left(\lambda_{\min}-\lambda_{1,1,1}\right)\frac{4}{\pi^2}$	2.4016e-005	1.373305034135797e-07	1.179500941361766e-12

Table 7: we estimate $|E_n(x)|$ for $\tau = \frac{\pi}{2}$ (lowest eigenvalue $\lambda_{1,1,1}$). This is consistent with

$$\left(\lambda_{\min} - \lambda_{1,1,1}\right) \frac{4}{\pi^2}$$
 filed in **Table 6**.

	<i>N</i> = 6	N = 8	N = 12
$E_{16}(x)$	7.3152e-005	6.2672e-007	1.3897e-011

Question 8 (exercise 4): continue exercise 3, but use "eigs" in MATLAB to solve eigenvalue of large sparse matrix, we can replace "eye" by "speye" to generate sparse identity matrix, then matrix L becomes sparse also.

Source code: F:\course\2008spring\spectral_method\matlab\p23_3.m

Table 8: experiment platform is quartet 1.

	<i>N</i> = 6	<i>N</i> = 8	N = 12
Time to eigs	0.244953 s	0.031894 s	0.248721 s

$\lambda_{\min} \frac{4}{2}$	3.000024016211436	2.999999862669430	2.999999999998738
$\frac{\pi^2}{\left(\lambda_{\min}-\lambda_{1,1,1}\right)\frac{4}{\pi^2}}$	2.401621143599542e-05	1.373305700269611e-07	1.261657445184028e-12

EIGS Find a few eigenvalues and eigenvectors of a matrix using ARPACK EIGS(A,K,SIGMA) return K eigenvalues based on SIGMA 'LM' or 'SM' - Largest or Smallest Magnitude For real symmetric problems, SIGMA may also be: 'LA' or 'SA' - Largest or Smallest Algebraic 'BE' - Both Ends, one more from high end if K is odd For nonsymmetric and complex problems, SIGMA may also be: 'LR' or 'SR' - Largest or Smallest Real part 'LI' or 'SI' - Largest or Smallest Imaginary part

Example 4 (harmonic oscillator with complex coefficient):

(Eq. 19) $Lu = -u_{xx} + cx^2u$, $c \in C$ Although we have analytical solution $\lambda_k = \sqrt{c}(2k+1)$ and $u_k = \exp(-\sqrt{c}x^2/2)H_k(c^{1/4}x)$ for $k = 0, 1, 2, \cdots$ where H_k is the kth Hermite polynomial, operator L is not normal and then we don't expect that eigenfunctions form an orthonormal basis, this means that eigenfunctions form ill-conditioned basis. Under such operator, system may be ill-conditioned (like ill-conditioned matrix), we need to consider deviation of perturbation. In operator sense, we call **pseudo-spectra**.

Definition 1: for each $\varepsilon > 0$, the $\varepsilon - pseudospectrum$ of matrix A is the subset of the complex plane $\Lambda_{\varepsilon}(A) = \left\{ z \in C : \left\| (zI - A)^{-1} \right\| \ge 1/\varepsilon \right\}$ for some physical norm. When z_0 is eigenvalue of A, we adopt $\left\| (z_0I - A)^{-1} \right\| = \infty$, say $z_0 \in \Lambda_{\varepsilon}(A)$. Alternatively $\Lambda_{\varepsilon}(A)$ can be characterized by eigenvalues of perturbed matrix $\Lambda_{\varepsilon}(A) = \left\{ z \in C : z = eig(A + E) \text{ for some } \| E \| \le \varepsilon \right\}$

Remark 6: if we use 2-norm, then $\Lambda_{\varepsilon}(A) = \{z \in C : \sigma_{\min}(zI - A) \le \varepsilon\}$ since $||A||_2 = \sqrt{\rho(A^H A)}$.

Now we choose c = 1+3i and compute contour plot of $\sigma_{\min}(zI-L) = \varepsilon$ for $\varepsilon = 10^{-0.5}, 10^{-1}, 10^{-1.5}, \dots, 10^{-4}$. In Figure 14, eigenvalues distributed along a ray with angle $\arg(c)$ but distribution of pseudo-spectra is broad for large eigenvalues. We may say such large eigenvalues are doubtful since smaller perturbation of system would cause large deviation of eigenvalue.



Question 9 (exercise 7): in exercise 6.8 we consider $D_N^{N+1} = 0$ theoretically, but in numerically we don't have such property, our experimental data is

Table 9: use MATLAB, first number is double precision, second number is double-double and third number is quad-double.

	<i>N</i> = 5	<i>N</i> = 10	<i>N</i> =15	<i>N</i> = 20
$(\mathbf{D}^N)^{N+1}$	9.8017E-011	4.8672E-002	1.0941E+009	4.8124E+019
	3.7644E-27	3.3708E-18	2.7839E-8	1.7886E+2
	5.1923E-60	6.6438E-51	3.2691E-40	4.6363E-31
$cond(D^N,2)$	1.6810E+017	2.1488E+017	6.8901E+016	3.0900E+017
$\det(D^N)$	1.0232E-012	1.3201E-006	-2.5372E+001	4.0785E+009
$\max\left(\max\left(D^{N}\right)\right)$	10.4721	40.8635	91.5231	162.4476

When N = 20, we require quad-double precision to avoid accumulation of rounding error. Now we plot eigenvalue of D_{20} and its pseudospectra for $\varepsilon = 10^{-2}, 10^{-3}, \dots, 10^{-16}$, then $\max |\Lambda(D_{20})| = 3.5025$ and $\min |\Lambda(D_{20})| = 31.8496$. If we write $D_{20} = E\Lambda E^{-1}$, then $\min (svd(E)) = 4.1688e-015$, $\max (svd(E)) \sim 3$. *E* is ill-conditioned basis. $cond(E^{-1}E) = 1.03$ is still good but $cond(EE^{-1}) = 393$. If we set $M = E\Lambda^{21}E^{-1}$, then cond(M) = 1.9E + 13 and $||M||_2 = 1.1E + 20$. Even we set $\Delta = D_{20} - E\Lambda E^{-1}$, then $cond(\Delta) = 1.7E + 5$ and $||\Delta||_2 = 68$. This means that result of "eig" may not be convinced.



Figure 15: eigenvalue of D_{20} is blue points, which is distributed around a circle with radius about 3.5025 but pseudo-spectra is broad.

In http://www.scholarpedia.org/article/Pseudospectrum

Question 10: Why do we need pseudospectra?

Pseudospectra are of importance in connection with many problems. One of the most prominent of these problems is equations of the form $\dot{x} = Ax$ or $x_{n+1} = Ax_n$, which lead to the study of the semi-groups e^{tA} and A^n . Eigenvalues and spectra can be employed to understand e^{tA} and A^n as $t \to \infty$ and $n \to \infty$, respectively. However, the behavior of the norms $\|e^{tA}\|_2$ and $\|A^n\|_2$ over the entire range of t, n is controlled through theorems of the type of the Kreiss matrix theorem by the resolvent norm $\|(A - \lambda I)^{-1}\|_2$.

Case 1: *A* is normal, satisfying $A^*A = AA^*$, then $\left\| (A - \lambda I)^{-1} \right\|_2 = 1/\operatorname{dist}(\lambda, \sigma(A))$ and so $\left\| (A - \lambda I)^{-1} \right\|_2$ is completely determined by $\sigma(A)$ alone. **Case 2:** *A* is not normal, then from [1], let the spectral abscissa of *A* be defined by $\alpha(A) = \sup \{ \operatorname{Re} z : z \in \Lambda(A) \}$, then $e^{t\alpha(A)} \le \left\| e^{tA} \right\| \le \kappa(V) e^{t\alpha(A)}$ for all $t \ge 0$. Here $\kappa(V) = \|V\| \|V^{-1}\|$ denotes condition number of a "matrix of eigenvector" *V* of *A*. From [2], if *A* is diagonalizable, then $\|A^k\|_p \le \kappa_p(V) \rho(A)^k$ and also if one use Cauchy integral representation of A^k (which involves a contour integral of the resolvent), then one can show that

(Eq. 20) $\left\|A^{k}\right\|_{2} \leq \frac{1}{\varepsilon} \rho_{\varepsilon} \left(A\right)^{k+1}$

where ε – *pseudospectral* radius

(Eq. 21) $\rho_{\varepsilon}(A) = \max\{|z|: z \in \Lambda_{\varepsilon}(A)\}$

Remark 7: physical interpretation of pseudospectra from [1]

Consider a time-dependent driven system $\frac{du}{dt} = Au + e^{zt} f$, the solution is $u(t) = e^{zt} (zI - A)^{-1} f$, if $z \in \Lambda_{\varepsilon}(A)$, this means or certain choices of f, $\frac{\|u(t)\|}{\|e^{zt}f\|} \sim \|(zI - A)^{-1}\| = \frac{1}{\varepsilon}$. In other words, a system governed by a normal operator exhibits **resonance** only if the forcing frequency is close to

the spectrum, however a system governed by a nonnormal operator may exhibit resonance or **pseudo-resonance** at frequencies far from the spectrum, like Figure 14.

Question 11 (exercise 5): consider a circular membrane of radius 1 that vibrates according to the second-order wave equation $y_{tt} = \Delta y = \frac{1}{r} (ry_r)_r + \frac{1}{r^2} y_{\theta\theta}$, y(r=1,t) = 0, written in polar coordinate. Separating variable leads to consideration of solution $y(r,\theta,t) = u(r)e^{im\theta}e^{iwt}$ with u(r) satisfying

(Eq. 22)
$$-\frac{1}{r}(ru_r)_r + \frac{m^2}{r^2}u = w^2u, \ u_r(0) = u(1) = 0$$

This is a form of Bessel's equation, and solution are Bessel function $J_m(wr)$ where w has property $J_m(w) = 0$.

Remark 8: If we define x = wr, then (Eq. 22) becomes

(Eq. 23)
$$x^2 \frac{d^2 u}{dx^2} + x \frac{du}{dx} + (x^2 - m^2)u = 0$$
, $u_x(0) = u(w) = 0$.
Solution is Bessel function $J_m(x) = \frac{1}{\pi} \int_0^{\pi} \cos(mt - x\sin t) dt$ normalized by $\int_0^{\infty} J_m(x) dx = 1$.



Figure 16: $J_1(x)$ don't has vanished flux component at origin.

From http://en.wikipedia.org/wiki/Bessel_function

$$J_m(x) \to \frac{1}{\Gamma(m+1)} \left(\frac{x}{2}\right)^m \text{ for } x \to 0 \text{, hence } \frac{d}{dx} J_m(x) \to \frac{1}{2(m-1)!} \left(\frac{x}{2}\right)^{m-1}.$$
 This means that $\frac{d}{dx} J_m(0) = 0 \text{ for } m \neq 1, \text{ see Figure 16.}$

Now we want to use spectral method to find eigenvalue w under given m.

First we scale domain into [-1,1], let us define x = -1 + 2r or say $r = \frac{1}{2}(x+1)$, then

(Eq. 24)
$$-\frac{d^2u}{dx^2} - \frac{1}{x+1}\frac{du}{dx} + \frac{m^2}{(x+1)^2}u = \left(\frac{w}{2}\right)^2 u, \ u_x(-1) = u(1) = 0.$$

Next we need to impose Neumann condition $u_x(-1) = 0$. As usual, we sample Chebyshev grid on $x_j = \cos(j\pi / N)$ for $j = 0, 1, 2, \dots, N$. At x=1 (j=0), we delete a row and a column of the differentiation matrix

At x = -1 (j = N), we impose B.C $u_x(-1) = 0$ according to D_N .

Then we will solve $N \times N$ linear system which N-1 equations enforce

 $-\frac{d^2u}{dx^2} - \frac{1}{x+1}\frac{du}{dx} + \frac{m^2}{(x+1)^2}u = \left(\frac{w}{2}\right)^2 u \text{ on interior point } j = 1, 2, \dots, N-1 \text{ and } 1 \text{ equation is}$ $u_x(-1)=0.$



Figure 17: we fix $v_0 = 0$ and for each interior point, we have equation, at final point at x = -1, we must impose constraint $u_x(-1) = 0$. The same setting holds for D_N .



$$\frac{1}{(x+1)^2} u |_{x_1 \cdots x_{N-1}} = \underbrace{\begin{pmatrix} 1 \\ x_1 + 1 \end{pmatrix}^2}_{(x_1+1)^2} | \begin{pmatrix} 0 \\ 0 \\ \vdots \\ 1 \\ (x_{N-1}+1)^2 \end{pmatrix} | \begin{pmatrix} v_1 \\ v_2 \\ \vdots \\ v_{N-1} \\ v_N \end{pmatrix}$$

Figure 19: $\frac{m^2}{(x+1)^2}u$ on interior point, note that we fill zero for last variable v_N

$$0 = u_x \left(-1\right) = \left[D_N \left(N+1, 2:(N+1)\right) \right] \left[\begin{array}{c} v_1 \\ v_2 \\ \vdots \\ v_{N-1} \\ v_N \end{array} \right]$$
 Figure 20: constraint $u_x \left(-1\right) = 0$, we can express u_N in terms of $u_1 \cdots u_{N-1}$

Finally we have

(Eq. 25)
$$\begin{bmatrix} L \\ D_N (N+1,2:N+1) \end{bmatrix} \begin{pmatrix} u_{1:N-1} \\ u_N \end{pmatrix} = \begin{pmatrix} \lambda & u_{1:N-1} \\ 0 \end{pmatrix} \text{ where } \lambda = \left(\frac{w}{2}\right)^2 > 0.$$

Last equation comes from constraint $u_x(-1) = 0$, and we can express u_N in terms of $u_{1:N-1}$, say

$$u_{N} = \frac{-1}{D_{N}(N+1,N+1)} D_{N}(2:N) \begin{bmatrix} u_{1} \\ \vdots \\ u_{N-1} \end{bmatrix} = G \begin{bmatrix} u_{1} \\ \vdots \\ u_{N-1} \end{bmatrix}, \text{ then we can remove constraint in (Eq. 25)}$$

$$(\text{Eq. 26}) \quad L_{(N-1)\times N} \begin{bmatrix} I_{N-1} \\ G_{1\times(N-1)} \end{bmatrix} \begin{bmatrix} u_{1} \\ \vdots \\ u_{N-1} \end{bmatrix} = \lambda \begin{bmatrix} u_{1} \\ \vdots \\ u_{N-1} \end{bmatrix}$$

Table 10: zeros of $J_n(x)$ from <u>http://mysite.du.edu/~jcalvert/math/bessels.htm</u>

S	N=0	N=1	N=2	N=3	N=4	N=5
1	2.405	3.832	5.135	6.379	7.586	8.780
2	5.520	7.016	8.147	9.760	11.064	12.339
3	8.654	10.173	11.620	13.017	14.373	15.700
4	11.792	13.323	14.796	16.224	17.616	18.982
5	14.931	16.470	17.960	19.410	20.827	22.220
6	18.071	19.616	21.117	22.583	24.018	25.431
7	21.212	22.760	24.270	25.749	27.200	28.628
8	24.353	25.903	27.421	28.909	30.371	31.813
9	27.494	29.047	30.571	32.050	33.512	34.983

Table 11: compute first 6 eigenvalues $w_1 \sim w_6$ by $w_k = 2\sqrt{\lambda_k}$ where λ_k is eigenvalue of (Eq. 26), we list eigenvalue for different grid points N = 5, 10, 15, 20

m = 0	N = 5	N = 10	N = 15	N= 20
w ₁	2.4048	2.4048	2.4048	2.4048
<i>w</i> ₂	5.4961	5.5201	5.5201	5.5201
w ₃	9.1697	8.6537	8.6537	8.6537
w ₄	12.2953	11.7931	11.7915	11.7915
<i>W</i> ₅		14.8901	14.9309	14.9309
W ₆		18.4337	18.0711	18.0711
m = 1	N = 5	N = 10	N = 15	N= 20
w ₁	3.8283	3.8312	3.8317	3.8317
<i>w</i> ₂	6.8948	7.0148	7.0153	7.0155
<i>W</i> ₃	11.9241	10.1703	10.1731	10.1733
w ₄	13.7284	13.3299	13.3227	13.3235
<i>W</i> ₅		16.3106	16.4696	16.4702
W ₆		20.4061	19.6132	19.6154

Question 12: We know $\frac{d}{dx}J_1(0) \neq 0$, but our eigenvalue of m=1 is so close to root of J_1 ?

Question 13 (exercise 6): continue exercise 5, we want to design a membrane with radius dependent physical properties such that these $w_2 = 2w_1$ (or say $\lambda_2 = 4\lambda_1$). Consider the modified boundary value problem

$$(\text{Eq. 27}) \quad -\frac{1}{r} \left(p(r) r u_r \right)_r + \frac{m^2}{r^2} u = w^2 u, \quad u_r(0) = u(1) = 0$$

where $p(r) = 1 + \alpha \sin^2(\pi r) > 1$ on $r \in (0,1)$.
We rewrite (Eq. 27) as $-p(r) u_{rr} - \frac{q(r)}{r} u_r + \frac{m^2}{r^2} u = w^2 u$ where $q(r) = \frac{d}{dr} (rp) = p + rp'$,
 $p' = \pi \alpha \sin(2\pi r)$. Again set $x = -1 + 2r$ $(r = \frac{1}{2}(x+1))$, then
(Eq. 28) $-p(r) u_{xx} - \frac{q(r)}{x+1} u_x + \frac{m^2}{(x+1)^2} u = \left(\frac{w}{2}\right)^2 u$

First, we plot first eigenvalue $w_1(\alpha)$ and second 1/2 times eigenvalue $\frac{1}{2}w_2(\alpha)$ as function of α , (here we choose $\alpha = 0:0.01:1$) and find intersection point $\alpha \approx 0.77$, see Figure 21. (source code: F:\course\2008spring\spectral_method\matlab\chap9_ex6.m)

Second we use Bisection method to determine critical value of α up to 6 digits, then $\alpha = 0.7695318$.

 $Source\ code:\ F:\ course\ 2008 spring\ spectral_method\ matlab\ chap9_ex6_v2.m$



Figure 21: two curves intersect at $\alpha \approx 0.77$

Reference

[1] Pseudospectra of Linear Operator, Lloyd N. Trefethen, F:\course\2008spring\spectral_method

[2] Matrix powers in finite precision arithmetic, Nicolas, F:\course\2008spring\matrix_comp

Theorem 2 (Hellmann-Feynman): let $H(\lambda)$ be a Hermitian operator which depends on a real parameter λ , let $|\psi(\lambda)\rangle$ be the normalized eigenket of $H(\lambda)$ with $E(\lambda)$: (Eq. 29) $H(\lambda)|\psi(\lambda)\rangle = E(\lambda)|\psi(\lambda)\rangle$ under $\langle \psi(\lambda)||\psi(\lambda)\rangle = 1$ Then $\frac{d}{d\lambda}E(\lambda) = \langle \psi(\lambda)|\frac{d}{d\lambda}H(\lambda)|\psi(\lambda)\rangle$ **<proof>** $\frac{d}{d\lambda}E(\lambda) = \frac{d}{d\lambda}\langle \psi(\lambda)|H(\lambda)|\psi(\lambda)\rangle + \langle \psi(\lambda)|\frac{d}{d\lambda}H(\lambda)|\psi(\lambda)\rangle + \langle \psi(\lambda)|H(\lambda)|\frac{d}{d\lambda}\psi(\lambda)\rangle$ $= E(\lambda)\langle \frac{d}{d\lambda}\psi(\lambda)||\psi(\lambda)\rangle + \langle \psi(\lambda)|\frac{d}{d\lambda}H(\lambda)|\psi(\lambda)\rangle + E(\lambda)\langle \psi(\lambda)||\frac{d}{d\lambda}\psi(\lambda)\rangle$ $\langle \psi(\lambda)||\psi(\lambda)\rangle = 1$ implies $0 = \frac{d}{d\lambda}\langle \psi(\lambda)||\psi(\lambda)\rangle = \langle \frac{d}{d\lambda}\psi(\lambda)||\psi(\lambda)\rangle + \langle \psi(\lambda)||\frac{d}{d\lambda}\psi(\lambda)\rangle$

Theorem 3 (time-independent perturbation theorem, non-degenerate case): consider $|n^{(0)}\rangle$ is eigenket of $H_0 |n^{(0)}\rangle = E_n^{(0)} |n^{(0)}\rangle$ with eigenvalue $E_n^{(0)}$ and assume $|n^{(0)}\rangle$ is complete, say $I = |n^{(0)}\rangle \langle n^{(0)}|$. Assume spectrum of H_0 is non-degenerate, then consider perturbed problem (Eq. 30) $(H_0 + \lambda V) |n\rangle_{\lambda} = E_n^{(\lambda)} |n\rangle_{\lambda}$

We assume $|n\rangle_{\lambda}$ and $E_n^{(\lambda)}$ are analytic over λ under following sense (Eq. 31) $|n\rangle_{\lambda} = |n^{(0)}\rangle + \lambda |n^{(1)}\rangle + \lambda^2 |n^{(2)}\rangle + \cdots$ (Eq. 32) $\Delta_n = E_n - E_n^{(0)} = \lambda \Delta_n^{(1)} + \lambda^2 \Delta_n^{(2)} + \cdots$ Then we have correction

(Eq. 33)
$$\Delta_n^{(1)} = V_{nn}$$
 and $\Delta_n^{(2)} = \sum_{k \neq n} \frac{|V_{nk}|^2}{E_n^{(0)} - E_k^{(0)}}$
(Eq. 34) $|n^{(1)}\rangle = \sum_{k \neq n} |k^{(0)}\rangle \frac{V_{kn}}{E_n^{(0)} - E_k^{(0)}}$ and
(Eq. 35) $|n^{(2)}\rangle = \sum_{k \neq n} \sum_{l \neq n} |k^{(0)}\rangle \frac{V_{kl}V_{ln}}{\left(E_n^{(0)} - E_k^{(0)}\right)\left(E_n^{(0)} - E_l^{(0)}\right)} - \sum_{k \neq n} |k^{(0)}\rangle \frac{V_{nn}V_{kn}}{\left(E_n^{(0)} - E_k^{(0)}\right)^2}$