chapter 4 : computing eigenvalues

4.1 introduction

problem : Given $A$, find $\lambda$ and $x \neq 0$ such that $Ax = \lambda x$.

$\lambda$ : e-value (e.g. frequency, growth rate, energy level)

$x$ : e-vector (e.g. normal mode, principal component, bound state)

thm : Assume $A$ is real and symmetric. Then the e-values $\lambda_i$ are real and the e-vectors $q_i$ form an orthonormal basis, i.e. $q_i^T q_j = 0$ for $i \neq j$, $||q_i||_2 = 1$, and any $x$ can be written as a linear combination of the $q_i$. (pf : omit)

ex : $A = \begin{pmatrix} 2 & -1 \\ -1 & 2 \end{pmatrix}$

$$f_A(\lambda) = \det \begin{pmatrix} 2-\lambda & -1 \\ -1 & 2-\lambda \end{pmatrix} = (2-\lambda)^2 - 1 = \lambda^2 - 4\lambda + 3 = (\lambda-3)(\lambda-1)$$

$\lambda_1 = 3$ : $Ax = 3x \Rightarrow \begin{pmatrix} 2 & -1 \\ -1 & 2 \end{pmatrix}\begin{pmatrix} x_1 \\ x_2 \end{pmatrix} = 3\begin{pmatrix} x_1 \\ x_2 \end{pmatrix}$

choose $x_1 = 1$, then $2x_1 - x_2 = 3x_1 \Rightarrow x_2 = -1, -x_1 + 2x_2 = 3x_2$ ok

$q_1 = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ -1 \end{pmatrix} \Rightarrow ||q_1||_2 = 1$

$\lambda_2 = 1$ : $Ax = x \Rightarrow \begin{pmatrix} 2 & -1 \\ -1 & 2 \end{pmatrix}\begin{pmatrix} x_1 \\ x_2 \end{pmatrix} = \begin{pmatrix} x_1 \\ x_2 \end{pmatrix}$

choose $x_1 = 1$, then $2x_1 - x_2 = x_1 \Rightarrow x_2 = 1, -x_1 + 2x_2 = x_2$ ok

$q_2 = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ 1 \end{pmatrix} \Rightarrow ||q_2||_2 = 1$ , $q_1^T q_2 = 0$ ok

obvious method for computing e-values

step 1. form $f_A(\lambda) = \det(A - \lambda I)$

step 2. solve $f_A(\lambda) = 0$ by the methods of chapter 2

ex : $A = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$ , $\tilde{A} = \begin{pmatrix} 1+\epsilon & 0 \\ 0 & 1-\epsilon \end{pmatrix}$ : perturbed matrix

$$f_A(\lambda) = (1-\lambda)^2 = \lambda^2 - 2\lambda + 1 = 0 \Rightarrow \lambda = 1$$

$$f_{\tilde{A}}(\lambda) = (1+\epsilon-\lambda)(1-\epsilon-\lambda) = \lambda^2 - 2\lambda + 1 - \epsilon^2 = 0 \Rightarrow \lambda = 1 \pm \epsilon$$

1. A change in the elements of $A$ of size $\epsilon$ leads to a change in the e-values of size $\epsilon$.

2. A change in the coefficients of $f_A(\lambda)$ of size $\epsilon^2$ leads to a change in the roots of size $\epsilon$.

3. Hence the roots of $f_A(\lambda)$ depend sensitively on the coefficients, and this implies that the obvious method for computing e-values is unstable.

<u>ex</u> (Wilkinson)

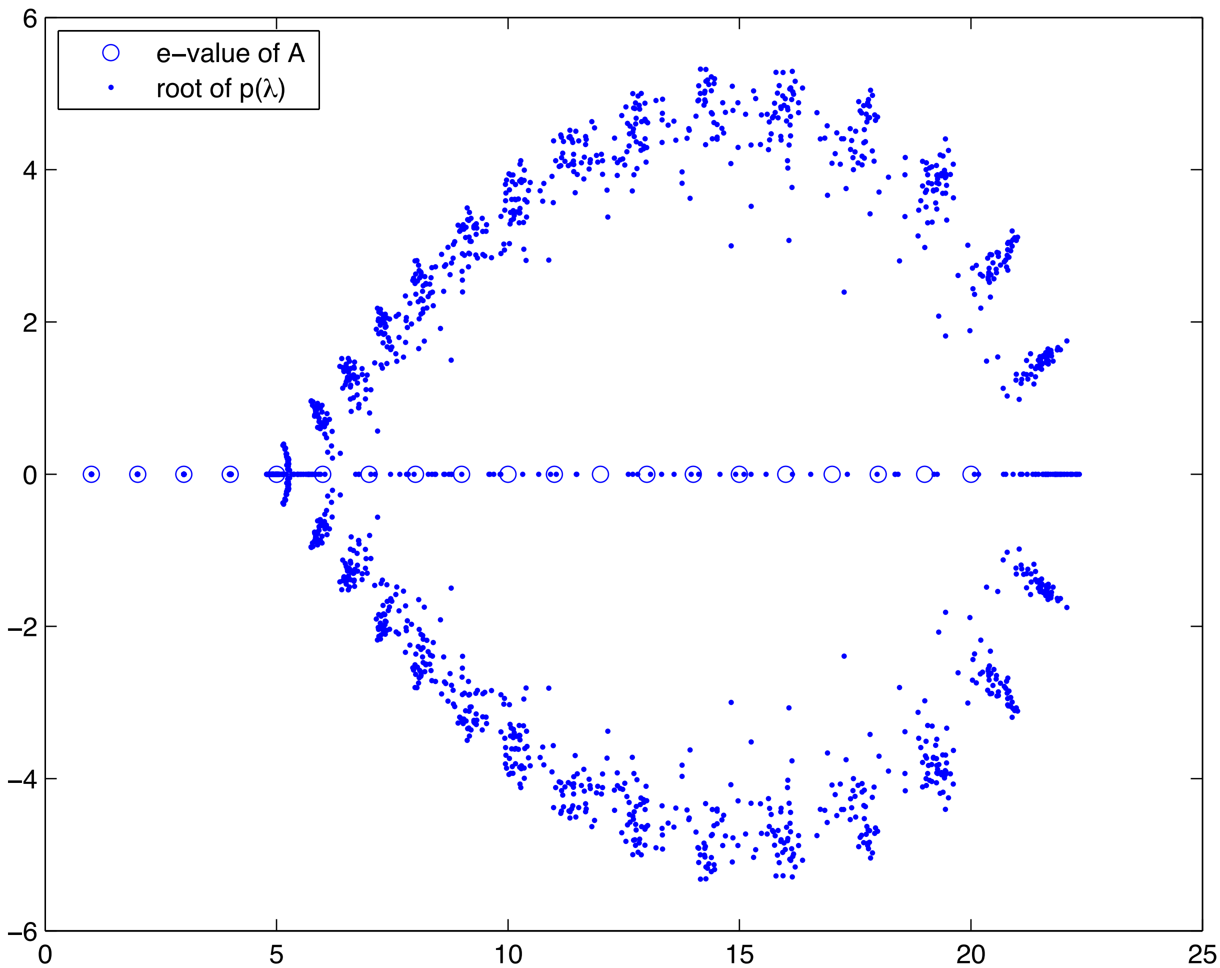
$A = \mathrm{diag}(1, 2, \ldots, 20)$

$f_A(\lambda) = (1-\lambda)(2-\lambda)\cdots(20-\lambda) = \sum_{k=0}^{20} a_k \lambda^k$

set $\tilde{a}_k = a_k(1 + 10^{-10}\epsilon_k)$ , $\epsilon_k \in (0,1)$ : random , $p(\lambda) = \sum_{k=0}^{20} \tilde{a}_k \lambda^k$ , roots $=$ ?

<u>Matlab</u>

```
plot(zeros(1,20),'o'); hold on;
for i=1:100
  r = roots(poly(1:20).*(ones(1,21)+1e-10*randn(1,21)));
  plot(r,'.'); axis([0,25,-6,6]);
end
```




1. This example shows that the roots of the characteristic polynomial are very sensitive to perturbations in the coefficients, and hence solving $f_A(\lambda) = 0$ numerically is not a practical method for computing e-values.

2. question : What method does Matlab use to compute the roots of $p(\lambda)$?

def : Given any $x \neq 0$, define $R_A(x) = \dfrac{x^T A x}{x^T x}$ : Rayleigh quotient. 18 Thurs 3/21

note

1. For $x = q_i$, $R_A(q_i) = \dfrac{q_i^T A q_i}{q_i^T q_i} = \dfrac{q_i^T \lambda_i q_i}{q_i^T q_i} = \lambda_i$.

2. For $x \approx q_i$, $R_A(x)$ is an approximation to $\lambda_i$ and we can derive an error estimate by Taylor expansion. First recall some notation.

$$f(x_1, x_2) = f(a_1, a_2) + \frac{\partial f}{\partial x_1}(a_1, a_2)(x_1 - a_1) + \frac{\partial f}{\partial x_2}(a_1, a_2)(x_2 - a_2) + \cdots$$

$$f(x) = f(a) + \nabla f(a) \cdot (x - a) + O(||x - a||^2) \quad , \quad \nabla f = \left(\frac{\partial f}{\partial x_1}, \frac{\partial f}{\partial x_2}\right)$$

$$R_A(x) \;=\; R_A(q_i) \;+\; \nabla R_A(q_i) \cdot (x - q_i) \;+\; O(||x - q_i||^2)$$

$$\nabla R_A(x) \;=\; \nabla\left(\frac{x^T A x}{x^T x}\right) = \frac{x^T x \cdot \nabla(x^T A x) \;-\; x^T A x \cdot \nabla(x^T x)}{(x^T x)^2}$$

$$\nabla(x^T x) \;=\; \nabla(x_1^2 + x_2^2) \;=\; (2x_1, 2x_2) \;=\; 2x^T$$

$$x^T A x \;=\; (x_1, x_2)\begin{pmatrix} a_{11} & a_{12} \\ a_{12} & a_{22} \end{pmatrix}\begin{pmatrix} x_1 \\ x_2 \end{pmatrix} \;=\; a_{11}x_1^2 \;+\; 2a_{12}x_1x_2 \;+\; a_{22}x_2^2$$

$$\nabla(x^T A x) \;=\; (2a_{11}x_1 \;+\; 2a_{12}x_2, 2a_{12}x_1 \;+\; 2a_{22}x_2) \;=\; 2(Ax)^T$$

$$\nabla R_A(x) \;=\; \frac{x^T x \cdot 2(Ax)^T - \; x^T A x \cdot 2x^T}{(x^T x)^2} \;=\; \frac{2}{x^T x}((Ax)^T - R_A(x)x^T)$$

$$\nabla R_A(q_i) \;=\; \frac{2}{q_i^T q_i}((Aq_i)^T - R_A(q_i)q_i^T) \;=\; 2((\lambda_i q_i)^T - \lambda_i q_i^T) \;=\; 0$$

$\Rightarrow\; R_A(x) \;=\; \lambda_i \;+\; O(||x - q_i||^2)$ : quadratic appoximation

4.2 power method

idea : $v$ , $Av$ , $A^2 v$ , ...

algorithm

1. $v^{(0)}$ : given , $||v^{(0)}||_2 = 1$ , $\lambda^{(0)} = (v^{(0)})^T A v^{(0)}$
2. for $k = 1, 2, \ldots$
3. $\quad w \;=\; Av^{(k-1)}$ % this can be done efficiently if $A$ is sparse
4. $\quad v^{(k)} \;=\; w/||w||_2$ % this is done to avoid overflow/underflow
5. $\quad \lambda^{(k)} \;=\; (v^{(k)})^T A v^{(k)}$ % $\lambda^{(k)} \to \lambda_1$ : largest e-value of $A$ in absolute value

$\underline{\text{ex}}$ : $A = \begin{pmatrix} 2 & 1 & 1 \\ 1 & 3 & 1 \\ 1 & 1 & 4 \end{pmatrix} \Rightarrow \begin{cases} \lambda_1 = 5.214320 \\ \lambda_2 = 2.460811 \\ \lambda_3 = 1.324869 \end{cases}$

$$v^{(0)} = \begin{pmatrix} 1 \\ 1 \\ 1 \end{pmatrix} \cdot \tfrac{1}{\sqrt{3}} \Rightarrow \lambda^{(0)} = (v^{(0)})^T A v^{(0)} = 5$$

power method

| $k$ | $\lambda^{(k)}$ | $\lvert\lambda^{(k)} - \lambda_1\rvert$ | $\dfrac{\lvert\lambda^{(k)} - \lambda_1\rvert}{\lvert\lambda^{(k-1)} - \lambda_1\rvert}$ |
|---|---|---|---|
| 0 | 5.000000 | 0.214320 | - |
| 1 | 5.181818 | 0.032502 | 0.151650 |
| 2 | 5.208193 | 0.006127 | 0.188513 |
| $\downarrow$ | $\downarrow$ | $\downarrow$ | $\downarrow$ |
| $\infty$ | $\lambda_1$ | 0 | $(\lambda_2/\lambda_1)^2$ |

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thm : Assume that $|\lambda_1| > |\lambda_2| > \cdots > |\lambda_n|$ and $q_1^T v^{(0)} \neq 0$.

Then $||v^{(k)} - (\pm q_1)|| = O\left(\left|\dfrac{\lambda_2}{\lambda_1}\right|^k\right)$ , $|\lambda^{(k)} - \lambda_1| = O\left(\left|\dfrac{\lambda_2}{\lambda_1}\right|^{2k}\right)$.

pf : $v^{(0)} = \alpha_1 q_1 + \alpha_2 q_2 + \cdots + \alpha_n q_n$ , where $\alpha_i = q_i^T v^{(0)}$

$$\begin{aligned} v^{(k)} = \beta_k A^k v^{(0)} &= \beta_k \left(\alpha_1 A^k q_1 + \alpha_2 A^k q_2 + \cdots + \alpha_n A^k q_n\right) \\ &= \beta_k \left(\alpha_1 \lambda_1^k q_1 + \alpha_2 \lambda_2^k q_2 + \cdots + \alpha_n \lambda_n^k q_n\right) \\ &= \beta_k \lambda_1^k \left(\alpha_1 q_1 + \alpha_2 \left(\frac{\lambda_2}{\lambda_1}\right)^k q_2 + \cdots + \alpha_n \left(\frac{\lambda_n}{\lambda_1}\right)^k q_n\right) \end{aligned}$$

$\Rightarrow$ $v^{(k)} \to \pm q_1$ as $k \to \infty$ , $\pm$ depends on sign$(\lambda_1)$ ok

note

1. The error is reduced by a constant factor in each step.

2. If $\alpha_1 = q_1^T v^{(0)} = 0$, then $v^{(k)} \to \pm q_2$ , $\lambda^{(k)} \to \lambda_2$.

3. If $A = \frac{1}{h^2}\text{trid}(-1, 2, -1)$, the matrix form of $-D_+D_-$, then $w = Av$, can be coded as a loop.

for $i = 1 : n$; $w_i = (-v_{i-1} + 2v_i - v_{i+1})/h^2$; end % assuming $v_0 = v_{n+1} = 0$

This is more efficient than forming $A$ and computing $w = Av$ by direct matrix-vector multiplication.

<u>question</u> : How can the other eigenvalues be obtained?

<u>4.3 inverse power method</u>

idea : apply power method to $A^{-1}$

1. $Aq_i = \lambda_i q_i \;\Rightarrow\; A^{-1}q_i = \lambda_i^{-1} q_i$ : same e-vectors , reciprocal e-values

The largest e-value of $A^{-1}$ is $\lambda_n^{-1}$.

2. $w = A^{-1}v \;\Leftrightarrow\; Aw = v$

<u>algorithm</u>

1. $v^{(0)}$ : given , $||v^{(0)}||_2 = 1$
2. for $k = 1, 2, \ldots$
3. solve $Aw = v^{(k-1)}$ % e.g. $LU$ factorization, etc.
4. $v^{(k)} = w/||w||_2$
5. $\lambda^{(k)} = (v^{(k)})^T A v^{(k)}$

<u>ex</u> : $A = \begin{pmatrix} 2 & 1 & 1 \\ 1 & 3 & 1 \\ 1 & 1 & 4 \end{pmatrix} \Rightarrow \begin{cases} \lambda_1 = 5.214320 \\ \lambda_2 = 2.460811 \\ \lambda_3 = 1.324869 \end{cases}$ , $v^{(0)} = \begin{pmatrix} 1 \\ 1 \\ 1 \end{pmatrix} \cdot \frac{1}{\sqrt{3}}$

<u>inverse power method</u>

| $k$ | $\lambda^{(k)}$ | $\lvert\lambda^{(k)} - \lambda_3\rvert$ | $\dfrac{\lvert\lambda^{(k)} - \lambda_3\rvert}{\lvert\lambda^{(k-1)} - \lambda_3\rvert}$ |
|---|---|---|---|
| 0 | 5.000000 | 3.675131 | - |
| 1 | 3.816327 | 2.491457 | 0.677923 |
| 2 | 1.864903 | 0.540034 | 0.216754 |
| $\downarrow$ | $\downarrow$ | $\downarrow$ | $\downarrow$ |
| $\infty$ | $\lambda_3$ | 0 | hw |

<u>summary</u>

1. power method : $\lambda^{(k)} \to \lambda_1$ , convergence factor $= (\lambda_2/\lambda_1)^2$

   inverse power method : $\lambda^{(k)} \to \lambda_n$ , convergence factor = hw

2. How to compute the other $\lambda_i$? Several methods are discussed in Math 571.

a) shifted inverse power method : $(A - \mu I)^{-1}$

b) $QR$ method

$A^{(0)} = Q^{(0)}R^{(0)}$ , $Q$ : orthogonal ($Q^TQ = I$), $R$ : upper triangular

$A^{(1)} = R^{(0)}Q^{(0)} = Q^{(1)}R^{(1)}$ : same e-values as $A$

$\ldots$

$A^{(k)} \to$ diagonal

3. recall : What method does Matlab use to compute the roots of a polynomial?

   answer : `type roots` , ...