数理逍遥 II[16C1115] Topics in Mathematics。
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Chapter 4: Eigenvalue problem 固有値問題

Submit by Friday February 10^{th} (16:00) to 数学事務・図書館 602 with the アンケート

Preliminary, 子文

Let A be an invertible matrix with n distinct eigenvalues in absolute values: $|\lambda_1| > |\lambda_2| > \cdots > |\lambda_n|$. A の絶対値固有値が相異なると想定し、それを $|\lambda_1| > |\lambda_2| > \cdots > |\lambda_n|$ と書く。

The QR-method to approximate all the eigenvalues of the matrix A requires to compute a lot of QR-decompositions. The Gram-Schmidt orthonormalization method is slow and numerically unstable: the output matrix Q may not have orthogonal columns even for quite good approximations. A の固有値を全て近似する QR 法において、多くの QR 分解を計算する必要である。普段の Gram-Schmidt(正規）直交化過程は遅くて数値的に不安定だと知られている：直交だと期待する行列 Q は、実際によい近似を使ってもその行が互いに直交だとは限らない。

A faster common better method is due to Francis & Kublanovskaya (around 1960): Francis 氏と Kublanovskaya 氏により、効率と数値的により安定な方法を導入した：

- Tridiagonalize the matrix A into a tridiagonal symmetric matrix T (often possible see Exercises 1, 2).
  A を三重対角化して、対称な三重対角行列 T を得る。T と A は同じ固有値を持つ。
- Then apply the QR -method to the matrix T instead of A. It produces only tridiagonal symmetric matrices (Exercise 3,b)) and we can apply the fast QR-decomposition for tridiagonal matrices using Givens rotations matrices (Exercise 3,a)).
  それから、A の代わりに三重対角行列 T に QR 法を適用する。それで対称な三重対角行列の専用 QR 分解 (Givens 回転行列) を使うことができ、速くて数値的に安定あ QR 法を与える。

1 Tridiagonalization by Householder method (... 法を用いた三重対角化)

Let $u \in \mathbb{R}^n$ of norm 1 ($\|u\|_2 = 1$) be the *Householder vector* of the *Householder matrix* $H_u = I - 2uu^T \in \mathrm{Mat}_{n\times n}(\mathbb{R})$.

a) Show that $H_u^T = H_u$ and $H_u^2 = I$. (Thus, H_u is orthoganal and symmetric and $H_u^{-1} = H_u$).

b) Show that $H_u.u = -u$ and that $H_u.v = v$ if $v \in \langle u\rangle^\perp$ (that is H_u is the matrix of a *reflection* ＝鏡像 of axis u).

c) (Tridiagonalization=三重対角化 of a symmetric matrix. Step 1.) Write

$$A = \begin{pmatrix} a_{1,1} & a_{1,2} & a_{1,3} & \cdots \\ a_{1,2} & a_{2,2} & a_{2,3} \cdots & \\ a_{1,3} & a_{3,2} & a_{3,3} & \cdots \\ \vdots & \ddots & \ddots & \ddots \end{pmatrix}. \tag{1}$$

Let $s^2 = a_{1,2}^2 + \cdots + a_{1,n}^2$ with $\mathsf{sgn}(s) = -\mathsf{sgn}(a_{1,2})$.
Define $\vec{r} = (0, a_{1,2} - s, a_{1,3}, \ldots, a_{1,n})^T \in \mathbb{R}^n$ and let $u = \vec{r}/\|\vec{r}\|_2$.

Then $A.H_u = \begin{pmatrix} a_{1,1} & *_{1,2} & 0 & \cdots \\ a_{1,2} & & & \\ \vdots & & B & \\ a_{1,n} & & & \end{pmatrix}$ with $B \in \mathrm{Mat}_{n-1,n-1}(\mathbb{R})$.

Consider the symmetric matrix $A = \begin{pmatrix} 1 & 1 & 1 & 1 \\ 1 & 2 & 2 & 2 \\ 1 & 2 & 3 & 3 \\ 1 & 2 & 3 & 4 \end{pmatrix}$.

(i) Use the formula above to construct the vector $\vec{r}$ and compute $\|\vec{r}\|_2^2$.

(ii) Write the matrix: $\vec{r}.\vec{r}^T$.

(iii) Compute the first line and first column *only* of the matrix product $A.(\vec{r}.\vec{r}^T)$. (don't need the whole matrix).

(iv) Deduce that $H_u.A = A - 2A\frac{\vec{r}.\vec{r}^2}{\|\vec{r}\|_2^2} = \begin{bmatrix} 1 & -\sqrt{3} & 0 & 0 \\ 1 & & & \\ 1 & & B & \\ 1 & & & \end{bmatrix}$ (the first column is unchanged, and $B \in \mathrm{Mat}_{3,3}(\mathbb{R})$).

(v) Deduce that $H_u.A.H_u = \begin{bmatrix} 1 & -\sqrt{3} & 0 & 0 \\ -\sqrt{3} & & & \\ 0 & & C & \\ 0 & & & \end{bmatrix}$, where $C \in \mathrm{Mat}_{3,3}(\mathbb{R})$ is symmetric. (don't need to compute C).

d) By repeating this process on the symmetric matrix $C \in \mathrm{Mat}_{3,3}(\mathbb{R})$ above, we can *tridiagonalize* = 三重対角化する the matrix A into a tridiagonal matrix T. For a general matrix A as in (1), we need $n-2$ Houselholder transformations denoted H_{u_i}, $i = 1, \ldots, n-2$.

$$T = H_{u_{n-2}}.H_{u_{n-3}}.\cdots.H_{u_1}.A.H_{u_1}.\cdots.H_{u_{n-3}}.H_{u_{n-2}}$$

$\to$ Show that $H_{u_1}.\cdots.H_{u_{n-3}}.H_{u_{n-2}}$ is symmetric orthogonal. Deduce that T and A have the same eigenvalues.

2 Tridiagonal matrices

Let $A = \begin{bmatrix} a_1 & b_1 & 0 & \cdots & 0 \\ c_1 & a_2 & b_2 & 0 & \vdots \\ & \ddots & \ddots & \ddots & \\ \vdots & 0 & c_{n-2} & a_{n-1} & b_{n-1} \\ 0 & \cdots & 0 & c_{n-1} & a_n \end{bmatrix}$ be a tridiagonal invertible matrix.

a) (reduction to the symmetric case: 対称の場合に帰着する)

Assume that $\mathsf{sgn}(b_i) = \mathsf{sgn}(c_i)$ for all $i = 1, \ldots, n-1$ (sgn= sign = 符号 : $\mathsf{sgn}(a) = -1$ or 1 or 0 when $a < 0$ or $a > 0$ or $a = 0$).

Let $D = \begin{bmatrix} d_1 & & 0 \\ & \ddots & \\ 0 & & d_n \end{bmatrix}$ be a diagonal invertible matrix. How to choose d_i so that $B = D.A.D^{-1}$ is tridiagonal and *symmetric* ?

→ Why B and A have the same eigenvalues?

b) According to Question a) we can assume A symmetric:

$$A = \begin{pmatrix} a_1 & b_1 & 0 & \cdots & 0 \\ b_1 & a_2 & b_2 & 0 & \vdots \\ 0 & \ddots & \ddots & \ddots & 0 \\ \vdots & 0 & b_{n-2} & a_{n-1} & b_{n-1} \\ 0 & \cdots & 0 & b_{n-1} & a_n \end{pmatrix}. \tag{2}$$

→ Suppose that there is a $b_i \approx 0$. How can we split the eigenvalue problem of A into two smaller ones? もしも $b_i \approx 0$ ならば、どうやって A の固有値問題をより小さな行列の二つに分解できるか。

c) According to Questions a),b) we can assume that all b_i are non zero.

Let $p_k(\lambda)$ be the characteristic polynomial (固有多項式) of the k-th principal minor of A (第 k 目の主小行列). For example $p_1(\lambda) = \lambda - a_1$, and $p_n(\lambda) = p_A(\lambda)$ is the characteristic polynomial of A).

(i) Let $p_0(\lambda) = 1$. Show the recurrence relation (帰納な公式): $p_{k+1}(\lambda) = (\lambda - a_{k+1})p_k(\lambda) - b_k^2 p_{k-1}(\lambda)$ holds.

(ii) Deduce the following three properties (we say that the sequence of polynomials $(p_0(\lambda), p_1(\lambda), \ldots, p_{n-1}(\lambda), p_n(\lambda))$ is a *Sturm sequence*, or has the *Sturm property*).

-1- None of the polynomials $p_k(\lambda)$ is zero.

-2- For any $\lambda_0 \in \mathbb{C}$, for any $1 \leq k \leq n-1$, $p_k(\lambda_0) = p_{k+1}(\lambda_0)$ is impossible.

-3- Given $\lambda_0 \in \mathbb{R}$, if $p_k(\lambda_0) = 0$, then $\mathsf{sgn}(p_{k-1}(\lambda_0)) = -\mathsf{sgn}(p_{k+1}(\lambda_0))$.

3 QR method

Theorem 1 *Given a symmetric tridiagonal invertible matrix A as in (2), with $b_i \neq 0$ for all $i = 1, \ldots, n-1$. Its QR-decomposition $A = QR$ verifies:*

$$Q = \begin{pmatrix} q_{1,1} & q_{1,2} & \cdots & \cdots & q_{1,n} \\ q_{2,1} & q_{2,2} & q_{2,3} & \cdots & q_{2,n} \\ 0 & \ddots & \ddots & \ddots & \vdots \\ 0 & \cdots & q_{n-2,n-2} & q_{n-1,n-1} & q_{n-1,n} \\ 0 & \cdots & 0 & q_{n,n-1} & q_{n,n} \end{pmatrix} \quad R = \begin{pmatrix} z_1 & s_1 & r_1 & 0 & \cdots & 0 \\ 0 & z_2 & s_2 & r_2 & 0 & \vdots \\ 0 & \ddots & \ddots & \ddots & \ddots & 0 \\ 0 & \cdots & 0 & z_{n-2} & s_{n-2} & r_{n-2} \\ 0 & \cdots & \cdots & 0 & z_{n-1} & s_{n-1} \\ 0 & \cdots & \cdots & \cdots & 0 & z_n \end{pmatrix} \tag{3}$$

can be computed fast using $n-1$ Givens rotattion *matrices.*

a) (the first Givens rotation P_1 on a tridiagonal matrix). Let $A = \begin{pmatrix} 3 & 1 & 0 \\ 1 & 3 & 1 \\ 0 & 1 & 3 \end{pmatrix}$

Let $\cos\theta_1 = \frac{a_1}{\sqrt{a_1^2+b_1^2}} = \frac{3}{\sqrt{3^2+1^2}} = \frac{3}{\sqrt{10}}$ and $\sin\theta_1 = \frac{b_1}{\sqrt{a_1^2+b_1^2}} = \frac{1}{\sqrt{3^2+1^2}} = \frac{1}{\sqrt{10}}$,

and $P_1 := \begin{pmatrix} \cos\theta_1 & \sin\theta_1 & 0 \\ -\sin\theta_1 & \cos\theta_1 & \\ 0 & 0 & 1 \end{pmatrix}$.

$\rightarrow$ Compute $A^{(1)} = P_1 A$. We obtain a matrix $\begin{pmatrix} z_1 & s_1 & r_1 \\ 0 & x_2 & y_2 \\ 0 & 1 & 3 \end{pmatrix}$ for some values z_1, s_1, r_1, x_2, y_2.

(参考までに 2nd Givens rotation P_2) By taking $\cos\theta_2 = \frac{x_2}{\sqrt{x_2^2+1^2}} \approx 0.92998$

$\sin\theta_2 = \frac{1}{\sqrt{x_2^2+1^2}} \approx 0.36761$, and the Givens rotation matrix $P_2 = \begin{pmatrix} 1 & 0 & 0 \\ 1 & \cos\theta_2 & \sin\theta_2 \\ 0 & -\sin\theta_2 & \cos\theta_2 \end{pmatrix}$,

we define: $R = P_2 P_1 A = P_2 A^{(1)}$ since it is upper triangular: $R = \begin{pmatrix} \sqrt{10} & \frac{3}{2}\sqrt{10} & \frac{\sqrt{10}}{10} \\ 0 & 2.72 & 1.98 \\ 0 & 0 & 2.44 \end{pmatrix}$.

We then have $Q = P_2^T . P_1^T = \begin{pmatrix} 0.95 & -0.29 & 0.12 \\ 0.32 & 0.88 & -0.35 \\ 0 & 0.37 & 0.93 \end{pmatrix}$.

b) In the QR-method, we define $A_0 = A$ and:

for $k = 0, 1, 2, \ldots$ repeat:

1. compute the QR-decomposition of A_k : $A_k = Q_k R_k$
2. define $A_{k+1} = R_k Q_k$

$\rightarrow$ Prove that $A_1 = R_0 Q_0$ and $A_0 = A$ have the same eigenvalues.

c) To compute *fast* the QR-decomposition of $A_1, A_2, A_3, \ldots$ by using Givens rotations, all computed matrices $A_1, A_2, \ldots$ should be tridiagonal symmetric (as A_0)...

$\rightarrow$ Prove that if Q_0 and R_0 both have the shape given in (3) of Theorem 1, then $R_0 Q_0$ is tridiagonal symmetric.