一般化固有値問題の精度保証付き解法

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1. Problems

Let us consider generalized eigenvalue problems as follows:
find the maximum of λ such that

$$Ax = \lambda Bx, \tag{1}$$

where $x \in R^n$, and A, B : matrices in $R^{n\times n}$.

As conserns the numerical verification methods for PDEs which we have developed, we need an upper bound of λ as sharp as possible. Aside from the numerical verification, this situation with the problem (1) often appears in many cases in mathematical science and engineering. Thus we believe that it is significant to investigate calculations for (1) with guaranteed accuracy.

2. Methods for Generalised Eigenvalue Probrems

We restrict the problem (1) such as A : symmetric and B : symmetric and positive definite, and explain three kinds of methods.

First two methods treat problems tranformed to:
find λ such that

$$\lambda = \sup_{y\neq 0} \left|\frac{y^T E y}{y^T y}\right|, \tag{2}$$

$$E := C^{-1} A C^{-T}, \tag{3}$$

where C denotes an $n\times n$ lower triangular matrix obtained by the Cholesky decomposition of B, namely,

$$B = CC^T.$$

Note that this transformation should be executed by a rigorous calculation using interval arithmetic considering the rounding error. Then E is given as an interval matrix. We define $\hat{E}$ by a matrix such that each element is the center of the interval of the corresponding element of E.

1. Method with estimation by Gerschgorin's theorem :
i) Compute an $n\times n$ matrix $\tilde{T}$ which approximately diagonalizes $\hat{E}$ by some suitable method (eg. QR decomposition).
ii) Execute the following calculation rigorously:

$$\tilde{D} := \tilde{T}^T E \tilde{T},$$

$$\tilde{\lambda} := \max_{1\leq i\leq n} \sum_{j=1}^{n} |\tilde{D}_{ij}|.$$

iii) Execute the following calculation rigorously:

$$\tilde{I} := (\tilde{T}\tilde{T}^T)^{-1},$$

$$\lambda_T := \max_{1\leq i\leq n} \sum_{j=1}^{n} |\tilde{I}_{ij}|.$$

Then we have an upper bound of λ as follows:

$$\lambda \leq \tilde{\lambda}\lambda_T. \tag{4}$$

2. Rump's method :

i) Compute an approximate value γ to λ by some favorite method.

ii) Take a positive constant δ, $0 < \delta << 1$ and $\tilde{\gamma} := (1+\delta)\gamma$. Set $X_1 := \tilde{\gamma}I - E$, where I: the identity matrix. Compute an approximation to the Cholesky decomposition of X_1, namely, a lower triangular matrix $\tilde{G}$ such that

$$X_1 \approx \tilde{G}\tilde{G}^T.$$

iii) Execute the following calculation rigorously:

$$\begin{aligned} Y &:= \tilde{G}\tilde{G}^T - X_1 \\ \varepsilon_1 &:= \max_{1\le i\le n} \sum_{j=1}^{n} |Y_{ij}|. \end{aligned}$$

iv) Set $X_2 := \tilde{\gamma}I + E$ and calculate ε_2 in a similar way as ii) and iii).

Then we have an estimation of λ as follows:

$$\lambda \le \tilde{\gamma} + \max(\varepsilon_1, \varepsilon_2).$$

Note that if A is known as positive definite, the process for X_2 can be omitted.

The third method which is a variation of method 2 treats generalized eigenvalue problem directly so that we do not need the tranformation from (1) to (2). We note that method 1 also has a variation which does not need this transformation.

Hereafter λ means

$$\lambda = \sup_{x\ne 0} |\frac{x^T A x}{x^T B x}|.$$

3. Variation of Rump's method:

i) Compute an approximate value γ to λ by some method. Take a positive constant δ_1, $0 < \delta_1 << 1$ and $\tilde{\gamma} := (1+\delta_1)\gamma$. Set $X_1 := \tilde{\gamma}B - A$ and $X_2 := \tilde{\gamma}B + A$.

ii) We will verify that each X_k $(k = 1, 2)$ is positive definite. Compute an approximate value ρ_k to the minimum absolute value of the eigenvalues of X_k and take a positive constant δ_2, $0 < \delta_2 << 1$. Set $\tilde{\rho}_k := (1-\delta_2)\rho_k$ and $Y_k := X_k - \tilde{\rho}_k I$.

iii) For each k, compute an approximation to the Cholesky decomposition of Y_k, namely, a lower triangular matrix $\tilde{G}_k$ such that

$$Y_k \approx \tilde{G}_k\tilde{G}_k^T.$$

iv) Execute the following calculation rigorously:

$$\begin{aligned} Z_k &:= \tilde{G}_k\tilde{G}_k^T - Y_k \\ \varepsilon_k &:= \max_{1\le i\le n} \sum_{j=1}^{n} |(Z_k)_{ij}|. \end{aligned}$$

If $\tilde{\rho_k} - \varepsilon_k > 0$ then X_k is positive definite, and we have an estimation of λ as follows:

$$\lambda \le \tilde{\gamma}$$

In our presentation, we will see the performance of each method in various situations. We use PROFIL, a useful and efficient free software for verified computation based on C^{++} in our calculation.