Resolution of Large Scale Hermitian Eigenproblem using YML Workflow Framework

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Extended Abstract

We make use of the YML workflow global computing environment [3] to compute a few eigenvalues of a hermitian matrix A. The limits and advantages of the large-scale environments for the concerned algorithms will be highlighted. We consider two projection methods based on the numerical integration and the Padé approximants. The first one proposed by T. Sakurai and H. Sugiura [2] allows to approach m eigenvalues of the generalized eigenproblem $(A - \lambda B)x = 0$ when the second, called Padé-Rayleigh-Ritz (PRR) [1], permits the computation of m approximated eigenvalues of $(A - \lambda I)x = 0$. When B and A are the identity and a hermitian matrices respectively, both of theses methods allow to approach a few eigenvalues of A.

In the Sakurai-Sugiura method, one can find the eigenvalues being inside of a domaine which can be a circle defined by a radius ρ and a center γ by solving $(H_m^{<} - \lambda \widetilde{H}_m)x = 0$. The matrices $H_m^{<} = (\mu_{i+j-1})_{i,j=1}^{m}$ and $\widetilde{H}_m = (\mu_{i+j-2})_{i,j=1}^{m}$ are the $m \times m$ Hankel ones whose elements μ_k are obtained by the N-trapezoidal approximation of an integral of $u^H(zI-A)^{-1}v$ function. Let N be a positive integer and $\omega_j = \gamma + \rho.\exp(\frac{2\pi ij}{N})$, for $j = 0, \ldots N-1$. We have $\mu_k = \frac{1}{N}\sum_{j=0}^{N-1}(\omega_j - \gamma)^{k+1} f(\omega_j)$ for $k = 0, 1, \ldots$ where $f(\omega_j) = u^H(\omega_j I - A)^{-1})v$. Let V_m be the Vandermonde matrix with respect to the eigenvalues $\xi_1, \ldots, \xi_m$ of $(H_m^{<} - \lambda \widetilde{H}_m)$. Then the eigenvector q_j associated to the eigenvalue λ_i can be computed by $s_k V_m^{-T}$ where $s_k = \frac{1}{N}\sum_{j=0}^{N-1}(\omega_j - \gamma)^{k+1} u f(\omega_j)$, for $k = 0, \ldots, m-1$.

Algorithm Sakurai-Sugiura (**input:** u, v, N, m, γ, ρ **output:** $\lambda_1, \ldots, \lambda_m, q_1, \ldots, q_m$)

1. set $\omega_j = \gamma + \rho.\exp(\frac{2\pi ij}{N})$, for $j = 0, \ldots N-1$

2. $y_j = ((\omega_j I - A)^{-1})v$, for $j = 0, \ldots N-1$

3. $f_j = u^H y_j$, for $j = 0, \ldots N-1$

4. Compute μ_k, for $k = 0, \ldots 2m-1$

5. Compute the eigenvalues $\xi_1, \ldots, \xi_m$ of $H_m^{<} - \lambda \widetilde{H}_m$

6. Compute $q_1, \ldots, q_m$ by the above equation.

7. Set $\lambda_j \gamma + \xi_j$ for $j = 0, \ldots m-1$

In the PRR method, one makes use of the Padé approximants and Krylov subspace $span(x, Ax, \ldots, A^{m-1}x)$ in the projection methods for computing a few eigenvalues of a hermitian matrix A. This process consists of approximating the poles of $R_x(\lambda) = ((I - \lambda A)^{-1}x, x)$, the mean value of the resolvant of A, by those of $[m-1/m]_{R_x}(\lambda)$, where $[m-1/m]_{R_x}(\lambda)$ is the Padé approximant of order m of the function $R_x(\lambda)$. This is equivalent to approximating the eigenvalues of A by the roots of $Q_m(\lambda)$ the polynomial of degree m of the denominator of $[m-1/m]_{R_x}(\lambda)$. This projection method provides a simple way to determine the minimum polynomial of x in the Krylov subspace method.

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Let

$$\Delta(i,j) \quad = \quad \begin{pmatrix} C_{i+0} & \dots & C_{i+j} \\ C_{i+1} & \dots & C_{i+j+1} \\ & \dots & \\ C_{i+j} & \dots & C_{i+2j} \end{pmatrix}.$$

for $i, j = 0, 1, \dots$. Let $c = -(C_m, C_{m+1}, \dots, C_{2m-1})^t$ and $Q_m(\lambda) = \lambda^m + b_{m-1}\lambda^{m-1} + \dots + b_0$ whose the companion matrix is:

$$H_m = \begin{pmatrix} -b_{m-1} & -b_{m-2} & \dots & -b_1 & -b_0 \\ 1 & 0 & \dots & 0 & 0 \\ 0 & 1 & \dots & 0 & 0 \\ \vdots & \vdots & \dots & \vdots & \vdots \\ 0 & 0 & \dots & 1 & 0 \end{pmatrix}$$

Then we can approach m distinct eigenvalues of A and their corresponding eigenvectors by the following computation steps:

Algorithm PRR (**input:** $y_0 = x/ \parallel x \parallel$, m **output:** $\lambda_1, \dots, \lambda_m$, $q_1, \dots, q_m$)

1. Compute $C_{2k-1} = (y_k, y_{k-1})$, $C_{2k} = (y_k, y_k)$ where $y_k = Ay_{k-1}$, for $k = 1, m-1$

2. Solve the linear system: $\Delta(0, m-1)b = c$

3. Compute the eigenvalues λ_i of the matrix H_m

4. Compute the vectors z_i of $(\Delta(1, m-1) - \lambda_i \Delta(0, m-1))z_i = 0$

5. Compute the approximated eigenvectors $[q_1, \dots, q_m] = [y_1, \dots, y_m][z_1, \dots, z_m]$.

The expensive part of these algorithms relays to an n-order matrix inversion in the first one and $m/2$ n-order matrix-vector products in the second one. We will analyse the distribution of these algorithms for the large-scale architectures. The results of our experiments in the YML workflow global computing environment using omniRPC middleware will be presented. The iterative version of these methods in viewpoint of efficiency and the number of iterations to obtain convergence will be compared.

Keywords : *projection method, large-scale computation, global computing environment*

References

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