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Note

On "A New Splitting to Solve a Large Hermitian Eigenproblem"

In a recent paper [1], one of us (CMMN) presented an efficient iterative scheme for determining the lowest eigenvalues and corresponding eigenvectors of a Hermitian matrix, H, whose leading principal minor, A, provides a good approximation to the desired eigensolution. The procedure involves the inversion of the matrix:

$$(A-\lambda_s I - r_s^1 I)$$

where λ_s is an estimate of an eigenvalue of H, and r_s^1 is a small parameter chosen to avoid the singularities of

$$(A-\lambda_s I).$$

The first point of this note is to emphasise that the r_s parameters need not be real. Indeed this is crucial because, for many of our matrices, choosing r_s real caused serious problems in converging on the desired eigensolution. Under investigation, we observed that this was due to λ_s lying amongst a series of closely spaced eigenvalues of A, in which case there was no suitably small real value for r_s.

When H is real-symmetric, for computational efficiency one would like to constrain the eigenvector iterates to be real. This would appear to prohibit the use of complex r_s. However, we propose that the imaginary parts of the iterates are simply dropped. This is equivalent to averaging the result of using r_s and r_s^*. We refer to Eqs. (2.4a) and (2.4b) of [1] and assume that the iterate from the previous step, x_s, is real. Then, we see that whereas using r_s yields x_{s+1}, complex conjugating throughout, r_s^* yields x_{s+1}^*. If we can assume that x_{s+1} and x_{s+1}^* are good iterates, we may reasonably assume that their average (i.e., just the real part, $\bar{x}_{s+1}$), is also a good iterate. In particular, the Rayleigh quotient estimate for the eigenvalue, λ_{s+1}, is the same for $\bar{x}_{s+1}$ as it is for x_{s+1} and x_{s+1}^*. Adopting this scheme, we are able to keep to a minimum the amount of complex arithmetic required.

The Rayleigh quotient and subspace matrices are efficiently calculated using $\bar{x}_{s+1}$. The Rayleigh quotient becomes

$$\lambda_{s+1}=\frac{\bar{x}_{s+1}^{1T}\operatorname{Re}((\lambda_s+r_s^1)x_{s+1}^1)+\bar{x}_{s+1}^{1T}C\bar{x}_{s+1}^2+2\bar{x}_{s+1}^{2T}U\bar{x}_{s+1}^2+\bar{x}_{s+1}^{2T}D\bar{x}_{s+1}^2}{\bar{x}_{s+1}^T\bar{x}_{s+1}}$$

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and the subspace matrix becomes

$$H^*_{s+1} = \bar{X}^{1T}_{s+1}\,\mathrm{Re}((\Lambda_s + R^1_s)X^1_{s+1}) + (\bar{X}^{1T}_{s+1}C\bar{X}^2_{s+1})^T + \bar{X}^{2T}_{s+1}D\bar{X}^2_{s+1} + \bar{X}^{2T}_{s+1}U\bar{X}^2_{s+1} + (\bar{X}^{2T}_{s+1}U\bar{X}^2_{s+1})^T$$

with

$$S^*_{s+1} = \bar{X}^T_{s+1}\bar{X}_{s+1}.$$

Note that these expressions are slightly different from the corresponding ones for the straight application of r_s, and that the fully complex vector, x_{s+1}, is still required, though only for evaluating the first term in λ_{s+1} or H^*_{s+1}.

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Reference

1. C. M. M. Nex, *J. Comput. Phys.* **70**, 138 (1987).

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