Efficient eigensolvers and their applications

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There are many applications that give rise to matrix eigenvalue problems. These span from traditional areas of analysis of vibrations, stability of an electrical network, and physical applications related to e.g. quantum mechanical systems, to the more nascent areas of data analysis and machine learning. In addition to the basic definitions and results, concepts and techniques that make eigensolvers efficient include the Eigenstructure-preserving transformations (shift, invert, shift & invert, polynomial), subspace projection, deflation and restarting techniques. Numerical algorithms often integrate all these ingredients. These algorithms include:

- **Power Method**. Perhaps the highest profile application of this method is the calculation of Google PageRank.

ALGORITHM: POWER METHOD

1. Choose a nonzero initial vector $\mathbf{v}^{(0)}$
2. For $k = 1, 2, \ldots,$ until convergence, Do:
   $\mathbf{v}^{(k)} = \frac{1}{\alpha_k}\mathbf{A}\mathbf{v}^{(k-1)}$
   $\alpha_k =$ the component of $\mathbf{A}\mathbf{v}^{(k-1)}$ with largest modulus.
3. EndDo

- **QR Algorithm** and its practical variants (e.g. with shifts), resulting from the *Schur form* theorem which states that any matrix is unitarily similar to a triangular matrix from which we can read off the eigenvalues.

ALGORITHM: QR WITHOUT SHIFTS[a]

1. Until $\mathbf{A}$ *becoming sufficiently close to being upper triangular*, Do:
   Compute the QR factorization $\mathbf{A} = \mathbf{QR}$
   Set $\mathbf{A} := \mathbf{RQ}$
2. EndDo

[a] Never used in practice

- **Rayleigh-Quotient Iteration** or, in general, the Min-Max theorem (Courant-Fischer).

MIN-MAX THEOREM

The k^{th} largest eigenvalues of a Hermitian matrix $\mathbf{A}$ is characterized by

$$\lambda_k = \max_{S,\, \dim(S)=k} \quad \min_{\mathbf{v}\in S,\, \mathbf{v}\neq 0} \frac{(\mathbf{A}\mathbf{v}, \mathbf{v})}{(\mathbf{v}, \mathbf{v})}.$$

As a consequence, the largest and smallest eigenvalues are

$$\lambda_1 = \max_{\mathbf{v}\neq 0} \frac{(\mathbf{A}\mathbf{v}, \mathbf{v})}{(\mathbf{v}, \mathbf{v})}, \;\; \lambda_n = \min_{\mathbf{v}\neq 0} \frac{(\mathbf{A}\mathbf{v}, \mathbf{v})}{(\mathbf{v}, \mathbf{v})}.$$

For certain applications, e.g. error analysis for Galerkin-type methods, we need to evaluate the smallest eigenvalue or bound it from below. Moreover, this task often exists for a parameter-dependent family of matrices having an affine structure

$$\mathbf{A}(\boldsymbol{\mu}) = \sum_{q=1}^{Q} \theta_q(\boldsymbol{\mu}) \mathbf{A}_q.$$

In this setting, even the most efficient eigensolver might become infeasible due to the sheer number of eigenproblems there are to solve. The Successive Constraint Method [3, 2] was invented to address this difficulty by interpreting this problem as a Q-dimensional linear program

$$\lambda_n(\boldsymbol{\mu}) = \min_{\mathbf{v}\neq 0} \left(\sum_{q=1}^{Q} \theta(\boldsymbol{\mu}) \frac{(\mathbf{A}_q \mathbf{v}, \mathbf{v})}{(\mathbf{v}, \mathbf{v})} \right) := \min_{\mathbf{v}\neq 0} \left(\sum_{q=1}^{Q} \theta(\boldsymbol{\mu}) y_q \right).$$

A small number of constraints, partially resulting from the resolution of the exact eigenvalues $\lambda_n(\boldsymbol{\mu})$ at judiciously selected parameter values $\{\boldsymbol{\mu}^1, \cdots, \boldsymbol{\mu}^n\}$, are then enforced. The result is a set of rigorous and tight lower and upper bounds for $\lambda_n(\boldsymbol{\mu})$ for any $\boldsymbol{\mu}$, that are obtained with an expense *independent of* the size of $\mathbf{A}(\boldsymbol{\mu})$.

Directions of project

The overarching goal is the thorough investigation of the above algorithms or others that interest you, and their application. These are the **possible** steps/deliverables:

- Study various applications of Eigen value problems, in particular quantum mechanics. Chapter 10 of the book [5] and the review paper [6] are good references.
- Study the standard PageRank algorithm and its variants, and implement your own version before applying it to the ICERM webpages. The paper [4] serves as a good starting point.
- Study the linear program based Successive Constraint Method (SCM) [3, 2] for a fast evaluation of rigorous bounds of the extremal eigenvalues for parametric, symmetric, and positive definite matrices.
- **Challenging.** Algorithms in [3, 2] are for extremal eigenvalues. Can you extend them to the intermediate ones that are close to the extremes?
- Investigate the approach in [1] to obtain the spectra of matrices without solving eigenvalue problems.

References

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[2] Yanlai Chen, Jan S. Hesthaven, Yvon Maday, and Jerónimo Rodríguez, *A monotonic evaluation of lower bounds for inf-sup stability constants in the frame of reduced basis approximations*, Comptes Rendus Mathématique. Académie des Sciences. Paris **346** (2008), no. 23-24, 1295–1300. MR 2473311

[3] D. B. P. Huynh, G. Rozza, S. Sen, and A. T. Patera, *A successive constraint linear optimization method for lower bounds of parametric coercivity and inf-sup stability constants*, Comptes Rendus Mathématique. Académie des Sciences. Paris **345** (2007), no. 8, 473–478. MR 2367928

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[5] Yousef Saad, *Numerical methods for large eigenvalue problems: revised edition*, vol. 66, Siam, 2011.

[6] Yousef Saad, James R Chelikowsky, and Suzanne M Shontz, *Numerical methods for electronic structure calculations of materials*, SIAM review **52** (2010), no. 1, 3–54.