Andrew Knyazev
Department of Mathematics
University of Colorado at Denver
P.O. Box 173364, Campus Box 170
Denver, CO 80217-3364

Time requested: 45
Andrew.Knyazev@cudenver.edu
http://www-math.cudenver.edu/~aknyazev/
tel: 303 556 8442, fax: 303 556 8550
17 years since degree

Toward the Optimal Preconditioned Eigensolver: Locally Optimal Block Preconditioned Conjugate Gradient Method

Andrew Knyazev

Numerical solution of extremely large and ill conditioned eigenvalue problems is attracting a growing attention recently as such problems are of major importance in applications. They arise typically as discretization of continuous models described by systems of partial differential equations (PDE's). For such problems, preconditioned *matrix-free* eigensolvers are especially effective as the stiffness and the mass matrices do not need to be assembled, but instead can be only accessed through functions of the corresponding vector-matrix products.

It is well recognized that traditional approaches are inefficient for very large eigenproblems. Preconditioning is the key for significant improvement of the performance as it allows one to find a path between Scylla of expensive factorizations and Charybdis of slow convergence. The study of preconditioned linear solvers has become a major focus of numerical analysts and engineers. For eigenvalue computations, preconditioning is much more difficult; and presently there are more questions than answers, even in the symmetric case.

While the mainstream research in the area introduces preconditioning in eigenvalue solvers using preconditioned inner iterations for solving linear systems with shift-and-invert matrices, our approach is to incorporate preconditioning directly into Krylov-based iterations. This results in simple, robust, and efficient algorithms, in many preliminary numerical comparisons superior to inner-outer schemes commonly used at present, e.g., to the celebrated inexact Jacobi-Davidson methods. For symmetric eigenproblems, the suggested Locally Optimal Block Preconditioned Conjugate Gradient (LOBPCG) method not only outperforms the inexact Jacobi-Davidson methods in many cases, but even exhibits properties of the optimal algorithm on the whole class of the preconditioned eigensolvers, which includes most presently known methods; e.g., the generalized Davidson, trace minimization and inexact continuation methods.

To be more specific, let us consider a generalized eigenvalue problem $(A - \lambda B)x = 0$ with real symmetric positive definite matrices A and B, where we are interested in computing p smallest eigenvalues and corresponding eigenvectors. An important class of eigenproblems is that of *mesh eigenproblems*, arising from discretizations of PDE's, e.g., in structural mechanics, where it is usual to call A the *stiffness* matrix, and B the *mass* matrix. To accelerate the convergence, we introduce a *preconditioner* T. In many engineering applications, preconditioned iterative solvers for linear systems $Ax = b$ are already available, and efficient, e.g., multilevel or incomplete factorization based, preconditioners $T \approx A^{-1}$ are constructed. The peculiarity of the preconditioning we recommend is that no eigenproblem specific preconditioners are used.

Instead, we propose the same T be used to solve the eigenvalue problem. We assume that the preconditioner T is *symmetric positive definite.*

We define [2-4] a preconditioned single-vector, for $p = 1$, eigensolver for the pencil $A - \lambda B$ as a generalized polynomial method: $x^{(k)} = P_k(TA, TB)x^{(0)}$, where P_k is a polynomial of the k-th degree of two independent variables, $x^{(0)}$ is an initial guess, and T is a fixed preconditioner. Thus, the approximation $x^{(k)}$ belongs to the generalized Krylov subspace $K_k\left(TA, TB, x^{(0)}\right)$. It is important to realize that this definition is very broad, e.g., it is general enough to embrace most known preconditioned iterative methods for computing the extreme eigenpair, using a fixed preconditioner, no matter what the origin of a particular solver is. Now, one can immediately understand the difficulties, which are emanated from the fact that the Krylov subspace is constructed using polynomials of *two noncommuting matrix variables.* The majority of known tools developed for the Lanczos and PCG methods, most importantly, the theory of orthogonal polynomials, fails us in this case. A novel ground-breaking theory is apparently needed here.

Having our definition of the class of preconditioned eigensolvers, we can introduce the *global optimization* method for computing the first eigenpair by minimizing the Rayleigh quotient $\lambda(x)$ on the generalized Krylov subspace. While this method provides optimal accuracy on the generalized Krylov subspace, it is also exceedingly expensive as the dimension of the subspace grows exponentially and no short-term recurrence to find the optimum is known (and, perhaps, is even possible). For block methods, when $p > 1$, we introduce the generalized block Krylov subspace. The *block global optimization* GLOBAL method computes approximate eigenvectors as corresponding Ritz vectors on this subspace and is used for accuracy benchmarks.

To introduce another benchmark, let us *suppose* that the minimal eigenvalue λ_1 is *already known*, and we just need to compute the corresponding eigenvector x_1, an element of the null–space of the homogeneous system of linear equations $(A - \lambda_1 B)x_1 = 0$. What would be an *ideal* preconditioned method of computing x_1 under the assumption that λ_1 is known? As such, we choose the *standard PCG method.* It is well known that the PCG method can be used to compute a nonzero element of the null–space of a homogeneous system of linear equations with symmetric and nonnegative definite matrix if a nonzero initial guess is used and the preconditioner is symmetric positive definite. This Ideal method is suggested [4] for benchmarking of the accuracy and costs of practical eigenvalue solvers, when $p = 1$.

We now introduce [1-4] single-vector, $p = 1$, LOPCG method for the pencil $A - \lambda B$:

$$x^{(i+1)} = w^{(i)} + \tau^{(i)}x^{(i)} + \gamma^{(i)}x^{(i-1)},\ w^{(i)} = T(Ax^{(i)} - \lambda^{(i)}Bx^{(i)}),\ \lambda^{(i)} = \lambda(x^{(i)}),\ \gamma^{(0)} = 0, \quad (1)$$

with scalar iteration parameters $\tau^{(i)}$ and $\gamma^{(i)}$ chosen using an idea of *local optimality*, namely, select $\tau^{(i)}$ and $\gamma^{(i)}$ that minimize the Rayleigh quotient $\lambda(x^{(i+1)})$ by using the Rayleigh–Ritz (RR) method. Dropping the vector $x^{(i-1)}$ from (1) turns it into the steepest descent and dramatically slows it down, according to our numerical tests [2,3,6]. However, adding more vectors $x^{(i-2)}$, etc. to the scheme (1) does not increase the speed as shown in numerical simulations [6] for a FEM approximation of the Laplacian preconditioned with a $V(2,2)$ multigrid. Moreover, in a different set of numerical tests [4] the LOPCG converges with the same speed and is practically as efficient as the Ideal method. There is no explanation for these observations yet.

The LOBPCG is simply a block, for $p > 1$, version of (1), where all $3p$ vectors span the RR trial subspace. The LOBPCG, numerically compared with the GLOBAL method for a model problem with $p = 3$, mysteriously is able to reproduce essentially the same optimal approximation quality of the GLOBAL, even though dimensions of the block generalized Krylov subspace in GLOBAL are: $9, 21, 45, 93, 189, 381, 765$, while the LOBPCG method uses local optimization only on 9-dimensional subspace on every step. A rigorous theoretical explanation of excellent convergence of the LOBPCG remains challenging and needs innovative mathematical ideas. The best presently known theoretical convergence rate estimate is proved in 2001 in an extensive four-parts paper, see [5] and references there, but it still does not capture some important convergence properties of the LOBPCG.

We also provide results of numerical comparison of the LOBPCG with inexact Jacobi-Davidson, Generalized Davidson, Preconditioned Lanczos and inexact Rayleigh Quotient Iterations, suggesting that LOBPCG is practically one of the top preconditioned eigensolvers.

A MATLAB code of the LOBPCG method and the Preconditioned Eigensolvers Benchmarking are available at http://www-math.cudenver.edu/~aknyazev/software/CG/ . Parallel versions using PETSc and Hypre are in progress; preliminary numerical results are provided.

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A brief biography, a list of recent publications, etc.

Education:

- Ph.D. in Numerical Mathematics, Ph.D. advisor - V.I. Lebedev. Institute of Numerical Mathematics Russian Academy of Sciences, 1985
- B.A. and M.S. in Computer Science and Cybernetics, M.S. advisor - E.G. D'yakonov. Moscow State University, Dept. Cybernetics and Computer Science, 1981

Employment:

- Center for Computational Math., University of Colorado at Denver Director, 1999-2001
- Department of Mathematics, University of Colorado at Denver Associate Professor, 1994-present
- Courant Institute of Mathematical Sciences, New York University: Visitor, 1992-1994
- Institute of Numerical Mathematics Russian Academy of Sciences: Senior Scientist, 1983-1992
- Moscow Physico-Technical Institute (Moscow Institute of Physics and Technology), FPFE, Assistant Professor,
- 1985-1991 Moscow State University, Dept. Mathematics and Mechanics, Instructor, 1986-1988
- Moscow Institute of Engineering and Physics, Instructor, 1982-1985
- Kurchatov's Institute of Atomic Energy, Nuclear Reactors: Software Engineer, 1981-1983

Over 30 papers and reports were published. Selected papers:

- A. V. Knyazev, Merico E. Argentati, Principal Angles between Subspaces in an A-Based Scalar Product: Algorithms and Perturbation Estimate. Accepted to SISC, 2001.
- Andrew Knyazev and Klaus Neymeyr, Efficient solution of symmetric eigenvalue problems using multigrid preconditioners in the locally optimal block conjugate gradient method. Accepted to the Copper Mountain issue of ETNA, 2001.
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Selected conferences:

- Miniworkshop: Preconditioning in Eigenvalue Computations (organizer), 03.03. - 09.03.2002, Oberwolfach.

- PRISM'2001, May 21-23, 2001, University of Nijmegen, The Netherlands.

- III International Workshop on Accurate Solution of Eigenvalue Problems, July 3-6, 2000, Hagen, Germany.

- FIFTH US NATIONAL CONGRESS ON COMPUTATIONAL MECHANICS, August 4-6, 1999, University of Colorado at Boulder: MiniSymposium Very Large Eigenvalue Problems (organizer).

- SIAM 45th Anniversary Meeting, July 14-18, 1997, Stanford University: Minisymposium Preconditioned Methods for Large Eigenproblems (organizer).

- XII HOUSEHOLDER SYMPOSIUM, Lake Arrowhead, USA, 1993

- Eigenwertaufgaben in Natur- und Ingenieurwissenschaften und ihre numerische Behandlung, Oberwolfach, 1990.

- XI HOUSEHOLDER SYMPOSIUM, Tylosand, SWEDEN, 1990.

Awards:

- Teaching Excellence Award for the College of Liberal Arts and Sciences at the University of Colorado at Denver, 2000

- Faculty Research Fellowship, University of Colorado at Denver, 2000

- Researcher/Creative Artist Award for the College of Liberal Arts and Sciences at the University of Colorado at Denver, 1999

- CU-Denver nominee for the University of Colorado President's Faculty Excellence Award for Advancing Teaching and Learning through Technology, 1999