Vorobyev method of moments
model reduction, convergence, computation

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HPCSE 2015
Soláň, May 2015

Iterative methods ... Why moments ???

Gene Golub, for pushing me to moments
Bernd Fischer, for the beautiful book and much more
Gérard Meurant, for many moment related joint interests
Claude Brezinski, for pointing out the work of Vorobyev
Jörg Liesen, for sharing interests and many years of collaboration
Volker Mehrmann, for inspiration and discussions of moments in control.

Liesen, S, Krylov Subspace Methods, Principles and Analysis, OUP, 2013:

Chapter 2: KSM as projections ... Algorithms.

Chapter 3: KSM as matching moments ... Understanding.

Outline

1. Stieltjes moment problem
2. Vorobyev moment problem
3. Convergence
4. Practical computations?

1 Stieltjes moment problem (1894) of order n

Consider $2n$ real numbers $m_0, m_1, \dots, m_{2n-1}$.
Solve the $2n$ equations

$$\sum_{j=1}^{n} \omega_j^{(n)} \{\theta_j^{(n)}\}^{\ell} = m_\ell \,, \qquad \ell = 0, 1, \dots, 2n-1\,,$$

for the $2n$ real unknowns $\theta_j^{(n)},\ \omega_j^{(n)} > 0\,.$

Is this problem linear?
Does it look easy?
When does it have a solution?

1 Approximation of positive definite linear functionals

Linear functional $\mathcal{L}(x)$ is positive definite on the space of polynomials $\mathcal{P}_n$ of degree at most n if the Hankel matrix M_n of moments

$$\mathcal{L}(x^\ell) = m_\ell, \quad \ell = 0, 1, \dots, 2n$$

is positive definite, i.e., $\Delta_n > 0$, where

$$\Delta_n = |M_n| = \begin{vmatrix} m_0 & m_1 & \cdots & m_n \\ m_1 & m_2 & \cdots & m_{n+1} \\ \vdots & \vdots & \ddots & \vdots \\ m_n & m_{n+1} & \cdots & m_{2n} \end{vmatrix} .$$

Solution of the Stieltjes moment problem of order n exists and it is unique if and only if $\Delta_n > 0$.

1 How to compute?

- Cholesky decomposition of the matrix of moments $M_n = L_n L_n^T$
- The entries of the kth row of the the inverse L_n^{-1} give the coefficients of the kth orthonormal polynomial determined by the positive definite linear functional $\mathcal{L}(x)$ associated with the matrix of moments M_n .
- Roots of the ℓth orthogonal polynomial give the quadrature nodes $\theta_j^{(\ell)}$. The weights $\omega_j^{(\ell)}$ are given by the formula for the interpolatory quadrature.

Gauss-Christoffel quadrature associated with the linear functional $\mathcal{L}(x)$ determined by the positive definite matrix of moments M_n .

1 Generalization to complex Gauss quadrature?

Linear functional $\mathcal{L}(x)$ is quasi-definite on the space of polynomials $\mathcal{P}_n$ of degree at most n if the Hankel matrix M_n of moments

$$\mathcal{L}(x^\ell) = m_\ell, \quad \ell = 0, 1, \ldots, 2n$$

is strongly regular, i.e., $\Delta_j \neq 0\,, \quad j = 0, 1, \ldots, n\,,$ where

$$\Delta_j = \begin{vmatrix} m_0 & m_1 & \cdots & m_j \\ m_1 & m_2 & \cdots & m_{j+1} \\ \vdots & \vdots & \ddots & \vdots \\ m_j & m_{j+1} & \cdots & m_{2j} \end{vmatrix}.$$

S. Pozza, M. Pranic, S (2015), submitted.

Outline

2. Vorobyev moment problem

3. Convergence

4. Practical computations?

Russian Monographs and Texts on Advanced Mathematics and Physics

Volume I
A. I. Khinchin, *A Course of Mathematical Analysis*
Volume II
S. G. Mikhlin, *Linear Integral Equations*
Volume III
P. P. Korovkin, *Linear Operators and Approximation Theory*
Volume IV
L. E. El'sgol'ts, *Differential Equations*
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Volume XVIII
S. B. Pikelner, *Principles of Cosmic Electrodynamics*
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O. V. Kovalev, *Irreducible Representation of Space Groups*

Additional Volumes in Preparation

Method of Moments in Applied Mathematics

by YU V. VOROBYEV

Translated from the Russian

by BERNARD SECKLER

GORDON AND BREACH SCIENCE PUBLISHERS
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2 The problem of moments in Hilbert space

Let $z_0, z_1, \ldots, z_n$ be $n+1$ linearly independent elements of Hilbert space V. Consider the subspace V_n generated by all possible linear combinations of $z_0, z_1, \ldots, z_{n-1}$ and construct a linear operator $\mathcal{B}_n$ defined on V_n such that

$$
\begin{aligned}
z_1 &= \mathcal{B}_n z_0, \\
z_2 &= \mathcal{B}_n z_1, \\
&\vdots \\
z_{n-1} &= \mathcal{B}_n z_{n-2}, \\
E_n z_n &= \mathcal{B}_n z_{n-1},
\end{aligned}
$$

where $E_n z_n$ is the projection of z_n onto V_n .

2 Approximation of bounded linear operators

Let $\mathcal{B}$ be a bounded linear operator on Hilbert space V. Choosing an element z_0, we first form a sequence of elements $z_1, \ldots, z_n, \ldots$

$$z_0, \; z_1 = \mathcal{B}z_0, \; z_2 = \mathcal{B}z_1 = \mathcal{B}^2 z_0, \; \ldots \; , z_n = \mathcal{B}z_{n-1} = \mathcal{B}^n z_{n-1}, \; \ldots$$

For the present $z_1, \ldots, z_n$ are assumed to be linearly independent. Determine a sequence of operators $\mathcal{B}_n$ defined on the sequence of nested subspaces V_n such that

$$z_1 = \mathcal{B}z_0 = \mathcal{B}_n z_0,$$

$$z_2 = \mathcal{B}^2 z_0 = (\mathcal{B}_n)^2 z_0,$$

$$\vdots$$

$$z_{n-1} = \mathcal{B}^{n-1} z_0 = (\mathcal{B}_n)^{n-1} z_0,$$

$$E_n z_n = E_n \mathcal{B}^n z_0 = (\mathcal{B}_n)^n z_0.$$

2 Model reduction using Krylov subspaces

Using the projection E_n onto V_n we can write for the operators constructed above (here we need the linearity of $\mathcal{B}$)

$$\mathcal{B}_n = E_n \, \mathcal{B} \, E_n \, .$$

The finite dimensional operators $\mathcal{B}_n$ can be used to obtain approximate solutions to various linear problems. The choice of the elements $z_0, \ldots, z_n, \ldots$ as above gives Krylov subspaces that are determined by the operator and the initial element z_0 (e.g. by a partial differential equation, boundary conditions and outer forces).

Challenges:

- Convergence
- Krylov subspace methods in infinite dimensional Hilbert spaces?

3 Convergence

Consider a bounded linear operator $\mathcal{B}$ on Hilbert space V that has a (bounded) inversion, and the problem

$$\mathcal{B}\, u \;=\; f\,.$$

- Since the identity operator on an infinite dimensional Hilbert space is not compact and $\mathcal{B}\mathcal{B}^{-1} = \mathcal{I}\,,$ it follows that $\mathcal{B}$ can not be compact.
- A uniform (norm) limit of finite dimensional approximation operators $\mathcal{B}_n$ is a compact operator.
- Results on strong convergence (pointwise limit)

$$\|\mathcal{B}_n\, w - \mathcal{B}\, w\| \to 0 \quad \forall w \in V\,.$$

3 Analysis of convergence of iterative methods?

Let $\mathcal{Z}_h$ be a numerical approximation of a bounded operator $\mathcal{Z}$ with

$$\|\mathcal{Z} - \mathcal{Z}_h\| = \mathcal{O}(h).$$

Then we have $[(\lambda - \mathcal{Z})^{-1} - (\lambda - \mathcal{Z}_h)^{-1}] = \mathcal{O}(h)$ uniformly for $\lambda \in \Gamma$ if Γ surrounds the spectrum of $\mathcal{Z}$ with a distance of order $\mathcal{O}(h)$ or more, and, for any polynomial p

$$p(\mathcal{Z}) - p(\mathcal{Z}_h) = \frac{1}{2\pi i} \int_\Gamma p(\lambda)[(\lambda - \mathcal{Z})^{-1} - (\lambda - \mathcal{Z}_h)^{-1}]\, d\lambda\,.$$

But the *assumption* $\|\mathcal{Z} - \mathcal{Z}_h\| = \mathcal{O}(h)$ does not hold for any bounded invertible infinite dimensional operator $\mathcal{Z}$.

3 Self adjoint bounded operators

$$\mathcal{B}\,u \;=\; f \qquad \longleftrightarrow \qquad \omega(\lambda),\;\; \int F(\lambda)\,d\omega(\lambda)$$

$$\uparrow \qquad\qquad\qquad\qquad\qquad\qquad \uparrow$$

$$\mathbf{T}_n\,\mathbf{y}_n \;=\; \mathbf{e}_1 \qquad \longleftrightarrow \qquad \omega^{(n)}(\lambda),\;\; \sum_{i=1}^{n} \omega_i^{(n)}\,F\left(\theta_i^{(n)}\right)$$

Using $F(\lambda) = \lambda^{-1}$ gives

$$\int_{\lambda_L}^{\lambda_U} \lambda^{-1}\,d\omega(\lambda) \;=\; \sum_{i=1}^{n} \omega_i^{(n)} \left(\theta_i^{(n)}\right)^{-1} + \frac{\|u - u_n\|_a^2}{\|f\|_V^2}$$

Stieltjes and Vorobyev moment problems are for self-adjoint bounded operators equivalent; infinite dimensional CG (Lanczos).

Outline

4. Practical computations?

4 Operator formulation of PDE BVP

Consider a PDE problem described in the form of the functional equation

$$\mathcal{A}x = b, \quad \mathcal{A} : V \to V^{\#}, \quad x \in V, \quad b \in V^{\#},$$

where the linear, bounded, and coercive operator $\mathcal{A}$ is self-adjoint with respect to the duality pairing $\langle \cdot, \cdot \rangle$.

Standard approach to solving boundary-value problems using the preconditioned conjugate gradient method (PCG) preconditions the algebraic problem,

$\mathcal{A}, \langle b, \cdot \rangle \;\to\; \mathbf{A}, \mathbf{b} \;\to\;$ preconditioning $\;\to\;$ PCG applied to $\mathbf{A}\mathbf{x} = \mathbf{b}$,

i.e., discretization and preconditioning are often considered separately.

4 CG and the Chebyshev method

Convergence bound for the Chebyshev semiiterative method

$$\frac{\|\mathbf{x} - \mathbf{x}_n\|_{\mathbf{A}}}{\|\mathbf{x} - \mathbf{x}_0\|_{\mathbf{A}}} \leq 2 \left(\frac{\sqrt{\kappa(\mathbf{A})} - 1}{\sqrt{\kappa(\mathbf{A})} + 1} \right)^n .$$

Convergence bound for the conjugate gradient method

$$\frac{\|\mathbf{x} - \mathbf{x}_n\|_{\mathbf{A}}}{\|\mathbf{x} - \mathbf{x}_0\|_{\mathbf{A}}} \leq 2 \left(\frac{\sqrt{\kappa(\mathbf{A})} - 1}{\sqrt{\kappa(\mathbf{A})} + 1} \right)^n .$$

It is worth considering the Chebyshev semiiterative method in a HPC environment, where appropriate.

Conclusions

- Vorobyev work was built on the deep knowledge of the previous results.
- It is amazingly thorough and complete as to the coverage and references.
- Published in 1958 (1965), it was much ahead of time. It stimulates new developments for the future.

References

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Thank you for your patience!