A NEW APPROACH TO NUMERICAL ALGORITHMS

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Introduction

• In this paper we developed a new Lanczos algorithm on the Grassmann manifold.

• This work comes in the wake of the article by A. Edelman, T. A. Arias and S. T. Smith, “The geometry of algorithms with orthogonality constraints”

Introduction

• The Grassmann and Stiefel manifolds are based on orthogonality constraints

• The Lanczos method and the conjugate gradients method are closely related

• One of the main problems of the Lanczos method is the loss of orthogonality
Numerical linear algebra problems

- The problem of computing eigenvalues, eigenvectors and invariant subspaces is always present in areas as diverse as Engineering, Physics, Computer Sciences and Mathematics.

- Lately, it has been verified that the iterations of eigenvalues and eigenvectors problems are best analyzed in some special spaces.

- A bridge between the geometry of the abstract spaces and the well known algorithms of numerical linear algebra.

Optimization Problem

- The optimization problem of the estimative of the invariant subspaces is made explicit with a geometric approach.

- However a geometrical treatment on the Grassmann manifold appropriate for numerical linear algebra is not present in standard references.
Grassmann Manifold

- \( \text{Gr}(p,n) - \text{Grassmann Manifold} : \)
  \[ p \text{-dimensional subspaces in } \mathbb{R}^n \]

- Identify matrix algorithms that induce iterations on the Grassmann manifold

- Translate abstractly defined Grassmannian algorithms into tractable numerical algorithms

- Use suitable matrix representations that facilitate convergence analysis

Iterations on the Grassmann Manifold

- One possible way to represent numerically an element \( \mathcal{Y} \) of \( \text{Gr}(p,n) \) consists of specifying an \( n \times p \) full column rank matrix \( Y \) whose columns span the space \( \mathcal{Y} \), and we can write
  \[ \mathcal{Y} = \text{span}(Y) \]

- \( \mathcal{Y} \) is called the column space of \( Y \)

- The set of all the matrices that have the same column space is a fiber over \( Y \)
Iterations on the Grassmann Manifold

- We have an iteration on the Grassmann Manifold if a fiber is mapped into a fiber.

- The concept of the fiber bundle structure allows us to describe the relationship between subspaces and matrices representations.

Lanczos on the Grassmann manifold

- The Lanczos algorithm is a method for computing some eigenvalues of a large symmetric matrix $A$ and their eigenvectors.

- The idea consists in building a sequence of nested subspaces $\text{span} \ x, Ax, A^2x, ...$ and solving the eigenproblem reduced to these subspaces.
Algorithm Grassmann-Lanczos (GL)

Let $A$ be an symmetric matrix $n \times n$
Consider $\mathcal{Y}$ an $p$-dimensional subspace of $\mathbb{R}^n$ i.e.,

$$\mathcal{Y} \in \text{Gr}(p, n)$$

The algorithm produce a sequence of subspaces

$$\text{Gr}(p, n) \rightarrow \text{Gr}(p, n)$$

$$\mathcal{Y} \rightarrow \mathcal{Y}_+$$

1. Pick an orthonormal matrix $Y, n \times p$, being $\mathcal{Y} = \text{span}(Y)$
2. Create an orthonormal basis $Q$ for the Krylov subspace
   $$\mathcal{K}_m(Y) = \text{span} \ Y, AY, ..., A^{m-1}Y$$
3. Calculate the matrix Rayleigh quotient $M = Q^T A Q$ that represents the projection of $A$ into $\mathcal{K}_m(Y)$
4. Calculate $X$, an orthonormal basis for the $p$-dimensional dominated eigenspace of $M$
5. Let $\mathcal{Y}_+$ be the span of $QX$
Algorithm Grassmann-Lanczos (GL)

- Doesn’t have a function that maps fibers to fibers
- The algorithm is defined as a mapping
- This algorithm is well-defined
  \[ \text{Gr}(p, n) \rightarrow \text{Gr}(p, n) \]

Conclusion and Future Work

- This paper offers a new approach to the Lanczos algorithm
- Lanczos algorithm is a very competitive method whose main problem is the loss of orthogonality, but the introduction of Grassmann manifolds seems to solve this problem
- This method might be easily implemented by blocks
Conclusion and Future Work

- We believe that this method is competitive in sequential computation, and also in parallel computing.
- Until now, as far as we know, people haven’t though of Lanczos as a subspace iteration.
- We intend to obtain new convergence results and make extensive comparisons with other Grassmannian methods.

References


References


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Thank you
Teşekkür ederim
Obrigado