Some Research Methodologies in Applied and Computational Mathematics

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Some Important Words

Here some suggestions on Research Methodology in Applied and Computational Mathematics shall be discussed. Of course some of you already know such techniques. Note that these techniques are not necessarily correct, also not for writing great papers. It is only for you to learn how to start your own research, to increase your number of publications and to go out of shadow of your advisor. Therefore, please don't be too serious about my words here. My words are not important for your future.

- New Proofs
- Modifications
- Generalizations
- Helps from Other Areas
- Diagram
- Integration and Cooperation among Different Areas

- Refinement

- Groups

- Conclusion

New Proofs

Many theorems have several different proofs. For example,

Necessary and sufficient conditions of Optimality in constrained Optimization have two proofs: KKT condition via dual function (Lagrangian)-Analysis proof; e Fritz John Lemma - Geometrical proof.

Hahn-Banach theorem also has two proofs: Analysis and geometry.

The conjugate gradient method for solving symmetric and positive definite systems can be derived from optimization of quadratic function or from pure linear algebra.

Hence, It is worthwhile to think about new proofs of existing results with at least one of following characteristics:

Simplicity

Different vision (geometry, algebra, analysis or other motivations)

More for teaching

New and smart idea

New Interpretations

Example A: convergence of Filter method:

Paper of Fletcher etc.

Paper of Clovis Gonzaga and Elizabeth Karas

Example B: finite termination of the conjugate gradient method:

All residuals at all steps are mutual orthogonal by optimization

$r_n = 0$ since it is orthogonal to all vectors of base by linear algebra

Modifications

Analyze possibility of modification for conditions of published results; Try to set weaker conditions or more feasible conditions.

Motivation: Technique of proof, or limitation of tools lead the conditions stronger than necessary.

J.Y. Yuan, Study of Comparison theorem of splitting matrices:

$$A = M_1 - N_1 = M_2 - N_2, \qquad M_i^{-1} \text{ existem}$$

$$x_{k+1} = M_1^{-1} N_1 x_k + M_1^{-1} b$$

$$y_{k+1} = M_2^{-1} N_2 y_k + M_2^{-1} b$$

$$x_0 = y_0, \qquad Ax = b$$

If $A^{-1}M_i \geq 0$ e $A^{-1}M_1 \leq A^{-1}M_2$, then

$$\rho(M_1^{-1}N_1) \leq \rho(M_2^{-1}N_2)$$

If $(M_2^{-1}A)^{i+l} \leq (M_1^{-1}A)^i(M_2^{-1}A)^l$

then

$$\rho(M_1^{-1}N_1) \leq \rho(M_2^{-1}N_2)$$

Theorem

If A and $M^*A^{-*}A + N$ satisfy the condition

$$x^*Ax \neq 0 \qquad \frac{x^*(M^*A^{-*}A + N)x}{x^*Ax} > 0$$

for all $x \in E = \{x \in C^n : \quad Hx = \lambda x\}$. Then $\rho(H) < 1$.

Lemma

$$AA^* - H^*A^*AH = (I - H)^*(M^*A + A^*N)(I - H).$$

Theorem

$\rho(H) < 1$ if and only

$$x^*(M^*A + A^*N)x > 0,$$

$$\forall x \in E = \{x \in C^n : \quad Hx = \lambda x\}.$$

Proof

$$x^*A^*Ax - x^*H^*A^*AHx = [(I-H)x]^*(M^*A + A^*N)[(I-H)x]$$

or

$$(1-|\lambda|^2)x^*A^*Ax = |1-\lambda|^2 x^*(M^*A + A^*N)x.$$

$$(1-|\lambda|^2) = |1-\lambda|^2 \frac{x^*(M^*A + A^*N)x}{x^*A^*Ax}.$$

With new (always weaker or/and simpler), the published results should be modified.

Motivations: Most cases, the conditions are necessary for the published results. If we modify those conditions, the results have to be modified.

A.M. Ostrowski, On the linear iteration procedures for symmetric matrices (1954)

E. Reich, On the convergence of the classical iterative procedures for symmetric matrices (1949)

K.B. Keller, On the solution of singular and semi-definite linear systems by iteration, SIAM J. Numer. Anal. (1965)

J.M. Ortega and R.J. Plemmons, Extensions of the Ostrowski-Reich Theorem for SOR iterations, LAA (1979)

J.Y. Yuan, The Ostrowski-Reich theorem for SOR iterations: extensions to the rank deficient case, LAA (2000)

Let $A = M - N$. For solving linear system $Ax = b$. There are

$$x_{k+1} = M^{-1}Nx_k + M^{-1}b$$

$$x_k \to x^* \qquad \Leftrightarrow \qquad \rho(M^{-1}N) < 1$$

$$H = M^{-1}N$$

Theorem

If A and $M^*A^{-*}A + N$ satisfy the condition

$$x^*Ax \neq 0 \qquad \frac{x^*(M^*A^{-*}A + N)x}{x^*Ax} > 0$$

for all $x \in E = \{x \in C^n : \quad Hx = \lambda x\}$. Then $\rho(H) < 1$.

Contrary, if $\rho(H) < 1$, then for all $x \in E$, there are

$$x^*Ax \neq 0 \qquad \frac{x^*(M^*A^{-*}A + N)x}{x^*Ax} > 0$$

or

$$x^*Ax = \frac{x^*(M^*A^{-*}A + N)x}{x^*Ax} = 0.$$

Proof

Let λ and x be $Hx = \lambda x$ e $x \in E$. Remind $\lambda \neq 1$ (if not, $Mx = Nx$ implies that A is singular).

Since

$$A - H^*AH = (I - H)^*(M^*A^{-*}A + N)(I - H), \qquad (*)$$

$$x^*Ax - x^*H^*AHx = [(I - H)x]^*(M^*A^{-*}A + N)[(I - H)x]$$

or

$$(1 - |\lambda|^2)x^* A x = |1 - \lambda|^2 x^*(M^* A^{-*} A + N)x.$$

By the condition,

$$(1 - |\lambda|^2) = |1 - \lambda|^2 x^*(M^* A^{-*} A + N)x / x^* A x > 0.$$

Then $|\lambda| < 1$.

Consider singular A. The key problems: x^*Ax can be zero; There does not exist A^{-1}. Now we cannot consider classic convergence concept because $\lambda = 1$ is eigenvalue of H explicitly.

Therefore, We have to think semi-convergence ($\lambda = 1$ is simple eigenvalue of H and other eigenvalues λ of H satisfy $|\lambda| < 1$).

Also we must consider generalized inverse of A.

To get the result, by the proof, the first step is to modify (*).

$$A - H^*AH = (I - H)^*(M^*(A^{+})^*A + N)(I - H), \qquad (**)$$

with condition $R(A) = R(A^*)$.

Theorem

Let $A = M - N$ and $H = M^{-1}N$ with $R(A) = R(A^*)$ and $M : R(A) \to R(A)$. If A and $M^*A^{+*}A + N \neq 0$ satisfy the condition

$$x^*Ax \neq 0 \qquad \frac{x^*(M^*A^{+*}A + N)x}{x^*Ax} > 0$$

for all $x \in E = \{x \in C^n : \quad Hx = \lambda x\} \bigcap R(A)$. Then H is semi-convergent.

Contrary, if H is semi-convergent, then for all $x \in E \bigcap R(A)$, there is

$$x^*Ax \neq 0 \qquad \frac{x^*(M^*A^{+*}A + N)x}{x^*Ax} > 0$$

or

$$x^*Ax = \frac{x^*(M^*A^{+*}A + N)x}{x^*Ax} = 0.$$

Let $A = M - N$ and $H = M^{-1}N$ with $M : R(A^*) \to R(A)$. Then,

- If $M^*A + A^*N$ is positive on $E \bigcap R(A^*)$, then, H is semi-convergent;

- If H is semi-convergent, then, $M^*A + A^*N$ is positive on $E \bigcap R(A^*)$ or $x^*(M^*A + A^*N)x = 0$ for all $x \in N(A)$.

Generalizations

Generalize results from Problem A to Problem B with the same ideas and techniques or similar to solve new problems;

For the generalization, we have to analyze characteristics of Problem B, try to obtain the same results as Problem A. since both problems are different, we must use new techniques, new tools or new ideas which are our contributions. If Problem B can be solved (theoretically or numerically), it also is great contribution.

- J.Y. Yuan, Numerical Methods for generalized least squares problems, JCAM, 1996

- J.Y. Yuan and A.N. Iusem, Preconditioned Conjugate Gradient Methods for Generalized Least Squares Problems, JCAM, 1996.

- A.N. Iusem and J.Y. Yuan, Preconditioned SOR Methods for Generalized Least Squares Problems, Acta Mathematica Applicada Sinica, 2000.

To establish iterative methods for solving the generalized least squares problems

$$\min\,(Ax-b)^T W^{-1}(Ax-b)$$

where $A \in R^{m\times n}$ with full rank and $m \geq n$.

Consider problem

$$\min\,(Ax-b)^T W^{-1}(Ax-b)$$

where $A \in R^{m\times n}$ is not full rank and $m \geq n$.

- C.H. dos Santos, B.P.B. Silva and J.Y. Yuan, Direct Iterative Methods for Rank Deficient Generalized Least Squares Problems, JCAM, 2000.

- C.H. dos Santos and J.Y. Yuan, Block SOR methods for rank deficient generalized least squares problems, Inter. J. Computer Math., 1998.

- C.H. dos Santos and J.Y. Yuan, Preconditioned conjugate gradient methods for rank deficient generalized least squares problems, JCAM, 1999.

Apply Method B to solve the same problem which was solved by Method A to establish new algorithms,obtain new results, discover new things and properties and improve existing results.

Consider

$$\min\, (Ax - b)^T W^{-1} (Ax - b)$$

where $A \in R^{m\times n}$ with full rank and $m \geq n$.

Apply the preconditioned conjugate gradient method, study convergence and iterative errors (J.Y. Yuan and A.N. Iusem, Preconditioned Conjugate Gradient Methods for Generalized Least Squares Problems, JCAM, 1996).

Apply the 2-block and 3-block SOR methods for solving the same problem, study the convergence and conditions of convergence. Also make comparison between the block SOR methods and the preconditioned conjugate gradient method (A.N. Iusem and J.Y. Yuan, Preconditioned SOR Methods for Generalized Least Squares Problems, ACTA Mathematica Applicada Sinica, 2000).

The problem can be generalized to a general form: Saddle point problem which was well studied. Many papers discussed different preconditioners for the problem.

Another example Equations of motion of Oldroyd Fluids.

- A.K. Pani, J.Y. Yuan and P. Damázio, On a linearized backward Euler method for the equations of motion of Oldroyd fluids of order one, SIAM, 2006.

- A.K. Pani and J.Y. Yuan, Semidiscrete finite element galerkin approximation to the equations of motion arising in the Oldroyd model, IMA J. Numer. Anal., 2005.

Rolle's Theorem

Let $f \in C[a,\ b]$ and derivative in $(a,\ b)$. If $f(a) = f(b)$, then there exists at least one $c \in (a,\ b)$ such that $f'(c) = 0$.

Naturally we shall ask what happens nif $f(a) \neq f(b)$?

It leads to Mean value Theorem:

Mean value Theorem

Let $f \in C[a,\ b]$ and derivative in $(a,\ b)$. Then there exists at least $c \in (a,\ b)$ such that

$$f'(c) = \frac{f(b) - f(a)}{b - a}.$$

Observation

We can understand

$$f'(c) = \frac{f(b) - f(a)}{b - a}$$

$$\Downarrow$$

$$\frac{f'(c)}{x'} = \frac{f(b) - f(a)}{x(b) - x(a)}$$

Then, what happens if denominator is one uma funtion $g(x)$?

Lagrangian Theorem

Let $f,\ g \in C[a,\ b]$ and derivative in $(a,\ b)$. If $g'(x) \neq 0\ \forall x \in (a,\ b)$, and $g(b) \neq g(a)$, then there exists at least $c \in (a,\ b)$ such that

$$\frac{f'(c)}{g'(c)} = \frac{f(b) - f(a)}{g(b) - g(a)}.$$

Help from Other Areas

Sometimes the point of view, the technique, the idea or the methods from other areas can hep us to solve our problem.

discuss with researchers from different areas,

attend talks of other areas,

Collaborate with researchers from other areas,

Listen critics from other areas.

Bieberbach's conjecture - Branges' Theorem

$$f(z) = z + \sum_{n \geq n} a_n z^n, \qquad |z| \leq 1$$

satisfies

$$|a_n| \leq n \qquad (n = 2, 3, \ldots).$$

was proved in Feb. 1984.

Louis de Branges worked on this conjecture much time without success, and published some papers wtih errors so that his colleagues didn't trust him too much. But he persisted in his work and transformed the problem to the following problem by functional analysis:

$$\int_0^1 {}_2F_1\left({-n,n+a+2, \atop (a+3)/2} st\right) s^{(a-1)/2}(1-s)^{(a-1)/2}\, ds > 0$$

where $a > -1$, $0 < t < 1$, ${}_2F_1$ is geometric function apresented by Jacobian polynomials.

Now we only need to prove the integration is positive for all $n \geq 2$.

Brange asked help of Gautschi who verified numerically the result till $n \leq 40$. Brange was very happy with the result because in general people confirmed the result only for $n = 2, \ldots, 8$.

On Feb. 29, 1984, Gautschi called Askey, specialist at special functions. At the beginning Askey that it would be impossible because complex inequality cannot be proved by only real analysis, finally he agreed to think about the problem.

At the same night, Gautschi received call from Askey who said that the result is the special case of his result with Gasper published in 1976. (Amer. J. Math., 98(1976) 709-737).

Then, in 1985, North Europe Acta Mathematica published Branges' paper: **A proof of the Bieberbach Conjetura**

Computational fluid mechanics + numerical linear algebra + optimization

Diagram

Sometimes we design one diagram (or table) which can give us many helps to create new ideas.

Ostrowski-Reich Theorem

Necessary and sufficient convergence conditions of iterative methods for solving $Ax = b$ where $A = M - N$:

$$x_{k+1} = M^{-1}Nx_k + M^{-1}b$$

$$\begin{array}{ccc} A \quad \text{(SPD)} & \Longrightarrow & A \quad \text{SPSD} \\ \text{O} - \text{R}, 1949, 1954 & & \text{Keller}, 1965 \\ \Downarrow & & \\ A \quad \text{NSPD} & ? \rightarrow & A \quad \text{singular} \\ \text{O} - \text{P}, 1979 & & \text{Yuan}, 2000 \end{array}$$

In nonlinear optimization, nonlinear conjugate gradient methods exist several forms. The difference of the forms is the choice of β_k which influences the convergence of the method.

β_k is function of $\|g_k\|^2$, $g_k^T y_{k-1}$, $\|g_{k-1}\|^2$, $d_{k-1}^T y_{k-1}$ e $-g_{k-1}^T d_{k-1}$ whose combinations result in the following methods:

	$\|g_k\|^2$	$g_k^T y_{k-1}$
$\|g_{k-1}\|^2$	FR	PRP
$d_{k-1}^T y_{k-1}$	DY	HS
$-g_{k-1}^T d_{k-1}$	CD	LS

FR – Fletcher-Reevves, PRP – Polak-Ribiére-Polyak, DY – Dai-Yuan, HS – Hestenes-Stiefel, CD – Conjugate Descent.

Consider inexact gradient method using interpolation. We can obtain the similar results. Think one-dimensional problem. We have 4 interpolation conditions $f(0)$, $f(-1)$, $f'(0)$, and $f'(-1)$. For quadratic interpolation, we only need 3 conditions. Then, we can have various combinations corresponding to different inexact methods.

Integration and Cooperation

- Between Pure Mathematics and Applied Mathematics
- Among Mathematics and Physics, Chemistry etc.
- Between Mathematics and Engineering
- Among Mathematics and medicine, pharmacology, psychology, economics, etc.

Example: Generalization of results from generalized inverse matrices to groups, semi-groups and algebra.

Example: Computational Fluid Mechanics. Cuminato and his Ph.D. student use Crank-Nicolson method with explicit cooperation of boundary conditions. The numerical simulation gives some conjecture that the method is stable with some parameter $\alpha \in (0,\ 2)$, and unstable when $\alpha \geq 2$. Unfortunately they proved that the conjecture is true only for $\alpha \in (0,\ 1/8)$ and $\alpha \to \infty$. At that time, Yuan was visiting the group. They discussed the problem with Yuan. Yuan tried some numerical linear algebra technique to extend their result to $\alpha \in (0,\ 3/5)$. It still was not good enough. After two night thinking, Yuan used combination of optimization techniques and numerical linear algebra techniques to proved the conjecture successfully.

Refinement

For the same problem, we improve our result step by step with different techniques and ideas.

Example, round-off error analysis of eigenvalue problem, and matrix decomposition etc. Each paper gives sharp upper bounds.

Group

The idea research group consists of

$$\textbf{Idea} + \textbf{Technique} + \textbf{Implementation} + \textbf{English}.$$

Conclusion

Using examples to illustrate several techniques of research methodology in Applied and Computational Mathematics.