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Conjugate gradient method for non-positive definite matrix operator

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The conjugate Gradient Method relies on symmetric positive definite property of a matrix operator. In this work, we investigate and establish the case of non-positive symmetric matrix operator using various forms of conversions and transformations on the operator.

Key words: Hilbert Space, Positive Symmetric Matrix, Quadratic Functional, Conjugate, Gradient Method.

INTRODUCTION

Consider the quadratic functional of the form:

$$f(X) = f_0 + \langle a, X \rangle_H + \frac{1}{2} \langle X, AX \rangle_H \quad (1)$$

where A is an $n \times n$ symmetric positive definite constant matrix operator on Hilbert space H , a is a vector in H and f_0 is a constant term. The minimization of the above quadratic form by conjugate gradient Method (CGM) relies on the symmetric positive definite of matrix A . See [6, and 9]. Our attention in this work is on a non-positive symmetric A which can be converted to positive definite through series of approaches. Ibiejugba et al. (2003), Hasdorff (1976) and several others have shown the effect of positive definite matrix on the convergence rate of CGM. It was shown that the CGM converges to optimal value in at most n iteration, where n is the dimension of the matrix operator. This in essence shows that a non-positive definite matrix may not terminate in at most n iteration. For further work see (Abdulrahman, (2007), Andrew and Chelsea, 1977, Enid, 1993, Lipschutz, 1987).

Effect of matrix on the optimal value

The operator arising from the quadratic functional (1) is

always symmetric and became a powerful tool to locate the optimal value. This symmetric matrix may be positive definite, negative definite, Singular point (positive-indefinite) and Saddle point (indefinite) (Jonathan, 1994). While the solution of positive and negative definite are unique, the singular point is as a result of indefinite matrix which does not have a solution. The solution to saddle point can represent the maximum and minimum at the same time. The definiteness of the operator plays a vital role in the optimality conditions.

A symmetric positive or negative definite matrix operator of a quadratic function guarantee a strictly convex function which in the first place show that it is an increasing or decreasing function and in turn give rise to a unique minimum or maximum.

A symmetric semi positive (semi negative) definite matrix operator in turn gives a convex function which may possibly be increasing (decreasing). In this case the open ball center at x^* with radius r is also an optimum. This suggests that there may be infinitely many points within the domain of optimum.

Indefinite matrix is the case where the function may be increasing, decreasing or neither. This is a serious case as we can not initially predict the nature of result that will come out of the computation.

The positive definite matrix guarantees an inverse of the matrix which is also unique, but this does not necessarily hold for indefinite matrix (Lawrence, 1976). We then conclude that indefinite matrix can only affect the uniqueness of the solution and does not necessarily mean it has no solution. The generated CGM by Ibiejugba et al.

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(2003) and Hasdorff (1976) have shown the effect of positive definite operator on the convergence properties of the algorithm.

Effect of matrix conversion on the objective functional

A non-positive definite matrix can be converted to positive definite in a number of ways. These include positive definite completion problem due to Wayne et al. (1993), forcing of indefinite matrix due to Thomas (2001) and matrix transformation.

Positive definite completion problem

In this case we try to find in a symmetric matrix which pair of $a_{ij} = a_{ji}$ can be replaced in order to get a positive definite matrix. Wyne Baret [12] shows that this replacement must be with respect to the dimension of the matrix. In a $n \times n$ matrix the pair of $a_{ij} = a_{ji}$ that will be replaced must be $(n - 2)$, i.e. in a 4×4 matrix $(4 - 2)$ pair can be replace. This replacement has a price on both the objective function and the corresponding system of linear equation. With this $(n - 2)$ it implies that the completion problem can not take care of 2×2 operators. Consider the problem

$$\text{minimize } F_1(X) = 1 - x_1 - x_2 - x_3 + x_1^2 + 2x_2^2 + x_3^2 + 2x_1x_2 + 2x_1x_3$$

This is written in matrix form as

$$\text{Minimize } F_1(X) = 1 - \begin{pmatrix} 1 \\ 1 \\ 1 \end{pmatrix}^T \begin{pmatrix} x_1 \\ x_2 \\ x_3 \end{pmatrix} + \frac{1}{2} \begin{pmatrix} x_1 \\ x_2 \\ x_3 \end{pmatrix}^T \begin{pmatrix} 2 & 2 & 2 \\ 2 & 4 & 0 \\ 2 & 0 & 2 \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \\ x_3 \end{pmatrix}$$

With Barret's result our $(n - 2)$ here is 1 then it make sense to remove only a pair from the original matrix.

$$\begin{pmatrix} 2 & 2 & 2 \\ 2 & 4 & 0 \\ 2 & 0 & 2 \end{pmatrix} \text{ Can be replaced by } \begin{pmatrix} 2 & 2 & x \\ 2 & 4 & 0 \\ x & 0 & 2 \end{pmatrix} \text{ the principal}$$

minor becomes $H_1 = 2, H_2 = 4$ and $H_3 = 4 - 2x^2$ and all will be greater than zero if $x < \sqrt{2}$. Choosing $x =$

$$1, \begin{pmatrix} 2 & 2 & 1 \\ 2 & 4 & 0 \\ 1 & 0 & 2 \end{pmatrix} \text{ is a positive definite completion of } \begin{pmatrix} 2 & 2 & 2 \\ 2 & 4 & 0 \\ 2 & 0 & 2 \end{pmatrix}.$$

The resulting functional is

$$\text{minimize } F_2(X) = 1 - x_1 - x_2 - x_3 + x_1^2 + 2x_2^2 + x_3^2 + 2x_1x_2 + x_1x_3$$

and Choosing $x = 1.4$,

$$\begin{pmatrix} 2 & 2 & 1.4 \\ 2 & 4 & 0 \\ 1.4 & 0 & 2 \end{pmatrix} \text{ is a positive definite completion of } \begin{pmatrix} 2 & 2 & 2 \\ 2 & 4 & 0 \\ 2 & 0 & 2 \end{pmatrix}.$$

The resulting functional is

$$\text{minimize } F_3(X) = 1 - x_1 - x_2 - x_3 + x_1^2 + 2x_2^2 + x_3^2 + 2x_1x_2 + 1.4x_1x_3$$

This conversion to positive definitely affects the last term of the functional and the effect is be shown in the result.

Forcing of an indefinite matrix to be positive definite

This case quite unique and has a similar problem on the objective function and its corresponding gradient. All the same, an indefinite matrix can be made positive definite by adding a small positive number to the diagonal element. This is done by $A - I\beta$ where I is the identity matrix and β is the smallest positive number. This number will be choosing appropriately so that the resulting matrix will be positive definite (Thomas et al., 2001). In the above example, the smallest possible value is $\beta = 0.5$ and the resulting positive definite matrix is

$$\begin{pmatrix} 2.5 & 2 & 2 \\ 2 & 4.5 & 0 \\ 2 & 0 & 2.5 \end{pmatrix},$$

the resulting functional becomes

$$\text{minimize } F_4(X) = 1 - x_1 - x_2 - x_3 + 1.25x_1^2 + 2.25x_2^2 + 1.25x_3^2 + 2x_1x_2 + 2x_1x_3$$

We can see now that there is effect of 0.25 increases on x_1^2, x_2^2 and x_3^2 which is half of the value added to obtain the positive definite matrix.

Matrix transformation

Transformation of matrix has played a major role in finding solution to some problem where the original problem may not. In this case a non-positive definite matrix A can be made positive definite by

$$(2) \quad B = AA^T$$

B is symmetric and positive definite for non-symmetric and/or non-positive definite matrix A .

The gradient of functional (1) is

$$(3) \quad \nabla f(X) = a^T + AX = 0$$

The replacement A by B does not affect the solution to (1) i.e. equation (3) is equivalent to

$$(4) \quad \nabla f(X) = a^T + BX = 0$$

With equation (4), B is a full matrix which may affect the solution as the dimension of the matrix keeping increasing (John and Karin, 2001). The equivalent of equations (3) and (4) then show that they both minimize the functional (1).

Table 1. Numerical result.

	Optima value	Exact	CGM1	CGM2
Problem 1	x_1^*	0.5	0.1875	0.5
	x_2^*	0	0.1875	0
	x_3^*	0	0.1875	0
	$f(X^*)$	-0.25	-0.2813	-0.25
	NITR	-	1	3
Problem 2	x_1^*	0	0.2143	0
	x_2^*	0.25	0.2143	0.25
	x_3^*	0.5	0.2143	0.5
	$f(X^*)$	-0.375	-0.3214	-0.375
	NITR	-	1	3
Problem 3	x_1^*	-10	0.2027	-10
	x_2^*	5.25	0.2027	5.25
	x_3^*	7.5	0.2027	7.5
	$f(X^*)$	-1.375	-0.3041	-1.375
	NITR	-	1	3
Problem 4	x_1^*	-22	0.1714	-22
	x_2^*	10	0.1714	10
	x_3^*	18	0.1714	18
	$f(X^*)$	-3	-0.2571	-3
	NITR	-	1	3
Problem 5	x_1^*	0.5	0.2681	0.5
	x_2^*	4.44E-16	0.1814	6.66E-15
	x_3^*	8.88E-16	0.2143	2.36E-15
	$f(X^*)$	-0.25	-0.2680	-0.25
	NITR	-	19	3

Main result

In this section, we provide various forms of conversions and transformation of a functional with non positive definite matrix operator. Consider.

Problem 1:

$$\minimize F_1(X) = f_{0(1)} - x_1 - x_2 - x_3 + x_1^2 + 2x_2^2 + x_3^2 + 2x_1x_2 + 2x_1x_3$$

Problem 2:

$$\minimize F_1(X) = f_{0(2)} - x_1 - x_2 - x_3 + x_1^2 + 2x_2^2 + x_3^2 + 2x_1x_2 + 2x_1x_3$$

Problem 3:

$$\minimize F_3(X) = f_{0(3)} - x_1 - x_2 - x_3 + x_1^2 + 2x_2^2 + x_3^2 + 2x_1x_2 + 1.4x_1x_3$$

Problem 4:

$$\text{minimize } F_4(X) = f_{0(4)} - x_1 - x_2 - x_3 + 1.25x_1^2 + 2.25x_2^2 + 1.25x_3^2 + 2x_1x_2 + 2x_1x_3$$

Problem 5: problem1 with gradient (4)

Description of CGM algorithm

The conventional conjugate gradient method is used to minimize the quadratic functional (1), the CGM algorithm is describe as follows:

CGM1

- i choose X_0
- ii compute $\nabla F(X_0) = g_0$
 $p_0 = -g_0$
- iii compute $X_{i+1} = X_i + \alpha_i p_i$; $\alpha_i = \frac{g_i^T g_i}{p_i^T A p_i}$
 $g_{i+1} = g_i + \alpha_i A p_i$
if $g_{i+1} = 0$ or $g_{i+1} - g_i \leq \epsilon$ then
- iv compute $\beta_{i+1} = \frac{g_{i+1}^T g_{i+1}}{g_i^T g_i}$
 $p_{i+1} = -g_i + \beta_{i+1} p_i$

CGM2

This is as a result of the modification of the descent $p_{i+1} = -g_{i+1} + \beta_{i+1} p_i$ due to Omolehin et al. (2006), due to these results, the convergence of some functional is expected in at most two iterations.

Using the two CGM algorithms to solve problems 1 - 5 above and comparing the result with the exact value obtained by matrix inverse method. We have the following table of results: (Table 1)

The results in this table represent the optimal value without f_0 . This is done in order to reconcile the optimal value, since f_0 does not take part in the minimization process but in the optimal value. This is the reason why different value of f_0 are used for different problem presented. Now, for the exact, we have,

$$F_1(X^*) = -0.25 + f_{0(1)}$$

$$F_2(X^*) = -0.375 + f_{0(2)}$$

$$F_3(X^*) = -1.375 + f_{0(3)}$$

$$F_4(X^*) = -3 + f_{0(4)}$$

$$F_5(X^*) = -0.25 + f_{0(1)}$$

For all the functional to be equal i.e. $F_1(X^*) = F_2(X^*) = F_3(X^*) = F_4(X^*) = F_5(X^*)$, Problem 1 being the original functional will assume $f_{0(1)} = 0$ then, $f_{0(2)} = 0.125$, $f_{0(3)} = 1.125$ and $f_{0(4)} = 2.75$.

DISCUSSION AND RESULT

The operator of problem1 is non-positive definite, while the operators for the other problems are positive definite. The results of CGM2 obtained at third iteration are exact while that of CGM1 diverges as the first iteration gives the closest value to optimum. The result of CGM1 that is different came from Problem 1, Problem 2, Problem 3, Problem 4, Problem 5 which occurred at 19th iteration without satisfying the termination criteria. In our next work we extend this to higher dimensional operator while at the same time reducing the difference noticed between the functional.

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