A METHOD TO SOLVE MATRICIAL EQUATIONS OF THE TYPE $\sum_{i=1}^{p} A_i X B_i = C$

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Keywords Matricial equations. Conjugate Gradient Method.

1. INTRODUCTION

The Conjugate Gradient method has been successfully employed to solve linear systems $Ax = b$ where A is symmetric positive definite.

In this paper we present a functional formulation of the method to be applied to matricial equations of the type

$$\sum_{i=1}^{p} A_i X B_i = C \qquad (1)$$

when A_i is a $n \times n$, B_i is a $m \times m$ matrix for every i and C is a $n \times m$ matrix.

The method can be applied when solving equation (1) is equivalent to minimizing a quadratic functional $V : \mathbb{R}^{n \times m} \to \mathbb{R}$.

In Section 2 we present a functional version of the Conjugate Gradient method.

In Section 3 we define the functional V, show the equivalence between solving equation (1) and minimizing V and we set sufficient conditions on A_i and B_i under which the method applies.

In Section 4 we give examples of matricial equations of type (1) which can be solved by our method. We show numerical results obtained from a particular discretization of the heat equation.

2. A FUNCTIONAL FORM OF THE CONJUGATE GRADIENT METHOD

Let Z be a Hilbert Space with inner product $\langle\ ,\ \rangle$ and $V : Z \to R$ a functional on it

$$V(x) = \frac{1}{2}Q(x,x) - P(x) + k$$

where $Q : Z \times Z \to \mathbb{R}$ is a positive-definite, symmetric continuous bi-linear form and

$$P : Z \to \mathbb{R} \quad \text{a continuous linear form.}$$

If we know how to compute grad $V(x)$ and grad $P(x)$ the Conjugate Gradient algorithm to compute

$$\text{Min } V(x) \text{ is the following :}$$

Algorithm 2.1.

Let an arbitratry $x_0 \in Z$ and a given $\varepsilon > 0$
Let $d_0 = -g_0 = -$ grad $V(x_0)$. If $||d_0|| \le \varepsilon$ then x_0 is an approximate solution.
Otherwise for $k = 0, 1, \ldots$

$$x_{k+1} = x_k + \alpha_k d_k$$

where

$$\alpha_k = \frac{\langle g_k, d_k\rangle}{\langle d_k, G_k\rangle} \text{ with } G_k = g_k + \text{ grad } P(x_k)$$

Compute $g_{k+1} =$ grad $V(x_{k+1})$. If $||g_{k+1}|| \le \varepsilon$ then x_{k+1} is an approximate solution. Otherwise $d_{k+1} = -g_{k+1} + \beta_k d_k$ where

$$\beta_k = \frac{\langle g_{k+1}, G_k\rangle}{\langle d_k, G_k\rangle}$$

3. THE FUNCTIONAL V AND THE CONJUGATE GRADIENT METHOD

Let $Z = \mathbb{R}^{n\times m}$ and $A_i \in \mathbb{R}^{n\times n}$, $B_i \in \mathbb{R}^{n\times m}$ $i = 1,2,\ldots,p$

$$X \text{ and } C \in Z$$

We define $V : Z \to \mathbb{R}$ as

$$V(X) = 0.5\sum_{i=1}^{p} tr(A_i X B_i X^t) - tr(C^t X) \tag{2}$$

Inicially we are going to verify that to solve matricial equation (1) is equivalent to find a critical point of V. Next we will see what are the conditions for $V(X) = \frac{1}{2}Q(X,X) - P(X) + k$ where Q is a positive definite symmetric bilinear form, which implies that this critical point is a minimal point of V.

To find a critical point of V we compute the derivative of V in the direction K

$$\text{Der}[V(X)]K = 0.5\sum_{i=1}^{p} tr(A_i K B_i X^t) + 0.5\, tr(A_i X B_i K^t) - tr(C^t K)$$

Since $tr(MN) = tr(NM)$ as long as MN and NM are well defined we have

$$\text{Der}[V(X)]K = 0.5\sum_{i=1}^{p} tr(K B_i X^t A_i) + 0.5\sum_{i=1}^{p} tr(A_i X B_i K^t) - tr(KC^t) =$$

$$= 0.5\sum_{i=1}^{p} tr(A_i^t X B_i^t K^t) + 0.5\sum_{i=1}^{p} tr(A_i X B_i K^t) - tr(CK^t)$$

If we suppose that A_i and B_i are symmetric for every i we have

$$\text{Der}[V(X)]K = \left[\sum_{i=1}^{p} tr(A_i X B_i) - tr(C)\right] K^t = tr\left[\left(\sum_{i=1}^{p}(A_i X B_i - C\right) K^t\right].$$

for every K in Z.

Defining $\langle P,Q\rangle_V = tr(PQ^t)$

$$\text{Der}[V(X)]K = \left\langle \sum_{i=1}^{p} A_i X B_i - C, K \right\rangle_V$$

Then X is a critical point of V if and only if

$$\mathrm{Der}[V(X)]K = 0 \quad \forall K \in Z \text{ , that is iff } \sum_{i=1}^{p} A_i X B_i = C \, .$$

Furthermore by Riez's theorem

$$\text{(3)} \qquad \mathrm{grad}\, V(X) = \sum_{i=1}^{p} A_i X B_i - C \, .$$

Defining $Q : ZXZ \to I\!R$ by

$$\text{(4)} \qquad Q(X,Y) = tr(\sum_{i=1}^{p} A_i X B_i Y^t)$$

and

$$P : Z \to I\!R$$

by

$$P(X) = tr(C^t X), \quad C \in Z$$

we have

$$V(X) = \frac{1}{2} Q(X,X) - P(X).$$

If Q is positive definite, symmetric, bilinear then the critical point of V will be a minimal point and the conjugate gradient method (Algorithm 2.1) can be applied.

It is not difficult to prove that $Q(X,Y)$ is bilinear and symmetric.

The theorem below set the conditions on A_i and B_i for the symmetric and bilinear form Q to be positive-definite.

Theorem: Let X_k , $1 \le k \le nm$ be an element of the canonical basis of $I\!R^{n.m}$, that is X_k is a $n \times m$ matrix with all elements zero except for $x_{r,s} = 1$, where

$$r = \begin{cases} \text{quotient of the division of } k \text{ by } m \text{ if the rest is zero} \\ \text{or} \\ (\text{quotient of the division of } k \text{ by } m) + 1 \text{ if the rest is not zero} \end{cases}$$

$$s = k - (r-1)m \, .$$

Then the symmetric, bilinear form Q defined by (4) is positive definite if and only if

$$D = d_{\ell j} = Q(X_\ell, X_j) \;\; n.m \times n.m$$

is positive definite

Proof: $d_{\ell j} = Q(X_\ell, Y_j) = \sum_{i=1}^{p} tr(A_i X_\ell B_i Y_j^t)$

Then for every $X \in Z$, $X = \sum_{s=1}^{n\times m} v_s X_s$ and $v = (v_s)_{n.m\times 1}$ is a vector of $I\!R^{n\times m}$.

$$Q(X,X) = Q\left(\sum_{s=1}^{n\times m} v_s X_s \, , \, \sum_{s=1}^{n\times m} v_s X_s\right) = \sum_{i,j=1}^{n\times m} v_i, v_j Q(X_i, X_j) = v^t D v \, .$$

To prove that D is positive definite we can use Sylvester's theorem stated below.

Theorem: A matrix $A = a_{ij}$, $n \times n$ is positive definite if and only if $\Delta_\ell > 0$, $\ell = 1, 2, \ldots, n$ where Δ_ℓ is the principal minor of order ℓ of matrix A.

If the dimensions n and m are big this verification is cumbersome even if p is small.

In next Section we will present classes of matrices where it is easy to see that $Q(X,Y)$ is positive definite and a practical example where we apply our method.

4. EXAMPLES

4.1. THE EQUATION $C^tCX + CXD^t + C^tXD + XDD^t = E$

If $p = 4\lambda$ and $\sum_{i=1}^{p} A_i X B_i$ can be grouped as $\sum_{j=1}^{\lambda} P_j$ where

$$P_j = A_{1j}XB_{1j} + A_{2j}XB_{2j} + A_{3j}XB_{3j} + A_{4j}XB_{4j}$$

with

$$\begin{array}{ll} A_{1j} = C_j^tC_j & B_{1j} = I \\ A_{2j} = C_j & B_{2j} = D_j^t \\ A_{3j} = C_j^t & B_{3j} = D_j \\ A_{4j} = I & B_{4j} = D_jD_j^t \end{array}$$

then

$$Q(X,X) = \sum_{j=1}^{\lambda} tr(S_j)$$

where

$$\begin{aligned} S_j &= A_{1j}XB_{1j}X^t + A_{2j}XB_{2j}X^t + A_{3j}XB_{3j}X^t + A_{4j}XB_{4j}X^t \\ &= (C_jX + XD_j)(C_jX + XD_j)^t = F_jF_j^t \end{aligned}$$

and $Q(X,X) \geq 0 \ \forall X$.

An example of equations of this type for which $Q(X,X) = 0$ if and only if $X = 0$ are equations ($\lambda = 1, C_1 = C, D_1 = D$) with C and D $n \times n$ such that $\det A \neq 0$ where A is the $n^2 \times n^2$ matrix

$$A = \begin{bmatrix} M_1 & P_{12} & P_{13} \cdots & P_{1n} \\ P_{21} & M_2 & & \\ \vdots & & \ddots & \\ P_{n1} & & & M_n \end{bmatrix}$$

with $M_i = c_{ii}I + D^t$ and $P_{ij} = c_{ij}I$.

4.2. THE EQUATION $\sum_{i=1}^{p} A_i X A_i = C$

$$p \geq n^2 \ , \ \ n = \dim A_i \ \text{ for every } i$$

For equations of this type we see that

$$Q(X,X) = \sum_{i=1}^{p} tr(A_i X A_i X^t) = \sum_{i=1}^{p} [tr(A_i X)]^2$$

Then $Q(X,X)$ is positive-definite if rank$(M) = n^2$ where M is the matrix $p \times n^2$ with the n^2 elements of line j being the elements of A_j, that is, line j of M is $(a_{11}^j a_{12}^j \cdots a_{1n}^j a_{12}^j a_{22}^j \cdots a_{2n}^j a_{13}^j a_{23}^j a_{33}^j \cdots a_{3n}^j \cdots a_{nn}^j)$.

4.3. THE EQUATION $BXC + DXE = G$

Equations of this type arise from the discretization by Finite Elements of the variational formulation of

$$(5) \qquad \begin{cases} \Delta u = f \ \text{ in } \ \Omega = [a,b] \times [c,d] \subset \mathbb{R}^2 \\ u = 0 \ \text{ in } \ \partial\Omega \end{cases}$$

In the variational formulation solving (5) is equivalent to solving

$$(6) \qquad \text{Min } g(u) = \text{Min} \int_\Omega 0.5 \left[\left(\frac{\partial u}{\partial x} \right)^2 \right] + \left(\frac{\partial u}{\partial y} \right)^2 - fu \right] dxdy$$

Taking

$$\Delta x = \frac{b-a}{n+1} \ , \ \Delta y = \frac{d-c}{m+1} \ , \ \varphi_i(x) \ , \ \psi_j(y)$$

as finite elements basis such that

$$\varphi_i(a) = \varphi_i(b) = 0 \ , \ \ 1 \leq i \leq n$$
$$\psi_j(c) = \psi_j(d) = 0 \ , \ \ 1 \leq j \leq m$$

then an approximate solution is

$$u(x,y) \approx \sum_{i=1}^{n}\sum_{j=1}^{m} a_{ij}\varphi_i(x)\psi_j(y)\,. \tag{7}$$

Taking (7) into (6) we have

$g(u) \approx V(X) = 0.5\,tr(BXCX^t) + 0.5\,tr(DXEX^t) - tr(G^tX)$ with

X being a $n \times m$ matrix with elements a_{ij}

B a $n \times n$ matrix $b_{ij} = \int_a^b \varphi_i'(x)\varphi_j'(x)dx = b_{ji}$

C a $m \times m$ matrix $c_{ij} = \int_a^d \varphi_i(y)\psi_j(y)dy = c_{ji}$

D a $n \times m$ matrix $d_{ij} = \int_a^b \varphi_i(x)\varphi_j(x)dx = d_{ji}$

E a $m \times m$ matrix $\ell_{ij} = \int_c^d \psi_i'(y)\psi_j'(y)dy = \ell_{ji}$

G a $n \times m$ matrix $g_{ij} = \int_a^b \int_c^d \varphi_i(x)\psi_j(y)f(x,y)dxdy$

It is not difficult to see that

$Q(X,X) = 0.5\,tr(BXCX^t) + 0.5\,tr(DXEX^t) = 0$ if and only if $X = 0$.

We can extend the method to equations

$$\text{(8)}\quad \begin{cases} \sum_{r=1}^{2}\sum_{s=1}^{2} \dfrac{\partial}{\partial x_r}\left(\alpha_{rs}\dfrac{\partial u}{\partial x_s}\right) = f \text{ in } \Omega \text{ with } \overline{\alpha} = (\alpha_{rs}) \text{positive definite} \\ u = 0 \text{ in } \partial\Omega \end{cases}$$

whose variational formulation is

$$\begin{cases} \text{Min } \int_\Omega \{0.5 \sum_{r=1}^{2}\sum_{s=1}^{2} \alpha_{rs}(x_1,x_2)\dfrac{\partial u}{\partial x_r}\dfrac{\partial u}{\partial x_s} - uf\}dx_1dx_2 = \text{ Min } g(u) \\ u = 0 \text{ in } \partial\Omega\,. \end{cases}$$

We have

$$g(u) = 0.5\sum_{i=1}^{2}\sum_{j=1}^{2} tr(B_{ij}XCX^t) - tr(G^tX)$$

with

$$B_{ij} = \int_a^b \int_c^d \alpha_{ij}(x_1x_2)\varphi_1'(x_1)\varphi_j(x_1)dx_1dx_2$$

a $n \times n$ matrix and C, X, G as in the previous case.

Since $\overline{\alpha}$ is positive definite, $Q(X, X) = 0$ if and only if $X = 0$.

4.4. AN APPROXIMATE SOLUTION OF THE HEAT EQUATION.

Lopes and Zago [5], present a numerical method for the approximate solution of heat equation

$$(9) \qquad \begin{cases} \dfrac{\partial u}{\partial t} = \dfrac{\partial^2 u}{\partial x^2} \\ u(0,t) = u(1,t) = 0 \\ u(x,0) = u_0(x) \quad 0 \le t \le T \quad j \le x \le 1 \end{cases}$$

Using the dual extremum principles of Noble and Sewell [6], we can transform (9) into a pair of restricted minimization and maximization problems.

Approximating these extremum principles by linear finite element basis both in time and space we got irrestricted maximum and minimum problems. The discretized problem consists of finding max $V(X)$ where

$$V : R^{(n-1)\times(m+1)} \quad \to R \text{ is}$$

$$V(X) = 0.5tr(CXRX^tS) + 0.5\, tr(EXFX^t)$$

$$+0.5tr(CXY_TX^t) + 0.5\, tr(CXY_0X^t) - tr(\overline{D}X\overline{1})$$

with

$$x_0 = 0\,,\ x_1 = \Delta x, \ldots, x_n = n\Delta x$$
$$t_0 = 0\,,\ t_1 = \Delta t, \ldots, t_m = m\Delta t = T$$

X is the matrix of unknowns (coefficients of the linear combination of the basis functions).

C, R, S, E, F are symmetric matrices whose elements are the integrals of products of basis functions and derivatives of basis functions.

$\overline{D}$ is a $(n-1)\times(n-1)$ matrix with the initial condition of the problem

$$\overline{1} = \begin{bmatrix} 1 & 1 & 1 & 1 & \cdots & 1 \\ 0 & 0 & \cdots & \cdots & \cdots & 0 \\ \vdots & & & & & \vdots \\ 0 & 0 & \cdots & \cdots & \cdots & 0 \end{bmatrix}_{(m+1)\times(n-1)}$$

$$Y_0 = \begin{bmatrix} 1 & 0 & 0 & & 0 \\ 0 & 0 & & & 0 \\ \vdots & & \ddots & & \\ 0 & & & & 0 \end{bmatrix}_{(m+1)\times(m+1)}$$

$$Y_T = \begin{bmatrix} 0 & 0 & \cdots & 0 \\ & & & \\ \vdots & & \cdots & 1 \end{bmatrix}_{(m+1)\times(m+1)}$$

They proved that the bilinear form associated to V is continuous, symmetric and positive definite and that

$$\operatorname{grad} V(X) = SCXR + EXF + CX(Y_T + Y_0) - (\overline{1}\,\overline{D})^t$$

The functional formulation of the Conjugate Gradient Method here presented was used to solve the problem with good numerical results.
We solved problem (9) with

$$u_0(x) = \sin \pi x\,.$$

The exact solution is $u(x,t) = \sin \pi x e^{-\pi^2 t}$. In Table 4.1 we present our results.

i) $||\text{error}||_\infty$ – is the maximun norm computed in the matriz ERT with

$$ERT_{ij} = u(x_i, t_j) - \tilde{u}(x_i, t_j)$$

and $\tilde{u}(x, j)$ is our approximate solution.

ii) $\Delta x = \frac{1}{n}$

iii) $\Delta t = \frac{1}{m} \quad (T = 1)$

iv) Dim – X matrix dimension: $(n-1)\times(m+1)$.

v) Iter –number of iterations made by Conjugate Gradient untill $||\text{grad } V(X)||_\infty \leq 5 * 10^{-6}$.

Δx	Δt	$\|\|error\|\|_\infty$	Dim	Iter
0.5	0.25	0.1965079	5	5
0.25	0.125	0.0625	27	11
0.125	0.0625	0.01812518	119	31
0.0625	0.03125	0.004675627	495	63
0.03125	0.015625	0.001188576	2015	111

Table 4.1 – Results obtained applying the proposed method to equation (9) with $u_0(x) = \sin \pi x$

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