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A FEW WAYS TO FIND APPROXIMATE SOLUTION TERMS OF THE METHOD OF GENERALIZED SEPARATION OF VARIABLES

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Резюме. Метод узагальненого розділення змінних будує наближення розв'язку задачі у вигляді суми доданків з розділеними змінними. Доданки знаходять послідовно як розв'язки певних мінімізаційних задач. У цій роботі ми розглянемо деякі способи знаходження наступного доданку наближеного розв'язку та наведемо формальний опис алгоритмів методу.

Abstract. The method of generalized separation of variables approximates a problem solution with a series of terms from a set of elements with separated variables. The terms should be found consecutively as solutions of certain minimization problems. In this paper we consider a few possible ways to find the next series term and give a formal description of the method algorithms.

1. Introduction

The method of generalized separation of variables (MGSV) is an iterative approach to approximate a solution of a linear multidimensional equation. According to the method instead of solving a single multidimensional problem we solve a series of one-dimensional problems and build a solution approximation. The method allows to dramatically decrease a computational complexity of problem solution algorithms. Besides a solution approximation is much more compact than the solution itself, i.e. requires less space.

The method has been originally suggested to solve multidimensional integral and matrix equations [1]. In [4,5] the method description is given for integral Fredholm equations.

The main idea of the method is to represent a solution of a linear d-dimensional equation $Au = f$ as a series of terms with separated variables

$$u\left(x_1, \ldots, x_d\right) = \sum_{k=1}^{\infty} \prod_{j=1}^{d} \phi_j^{(k)}\left(x_j\right),$$

which are found consecutively by minimizing the following functional

$$J_k\left(\phi_1, \ldots, \phi_d\right) = \| f - \sum_{l=1}^{k-1} A\left(\phi_1^{(l)} \otimes \cdots \otimes \phi_d^{(l)}\right)^2 \| \to \min.$$

Here A is a linear continuous operator in the corresponding space.

Key words. Method of generalized separation of variables, linear equation, multidimensional problem, approximate solution.

Paper [6] describes the MGSV modification which builds a solution approximation in a slightly different way

$$u = \sum_{k=1}^{\infty} A^* \left(\phi_1^{(k)} \otimes \cdots \otimes \phi_d^{(k)} \right),$$

where A^* is the adjoint of A and the terms of the series are found from

$$J_k \left(\phi_1, \ldots, \phi_d \right) = \| A^{-1} f - \sum_{l=1}^{k-1} A^* \left(\phi_1^{(l)} \otimes \cdots \otimes \phi_d^{(l)} \right)^2 \| \to \min .$$

In [2,3] a convergence of the solution approximation series to the exact equation solution is proven for both MGSV and its modification, respectively.

2. MGSV

Consider d complex separable Hilbert spaces H_j, $j = 1, \ldots, d$. Let's denote with $(\cdot, \cdot)_j$ an inner product in H_j which defines the corresponding norm $\|[\|j]\cdot$. Let H is a tensor product of the given spaces

$$H = \bigotimes_{j=1}^{d} H_j$$

with a norm $\|\cdot\|$ defined by its inner product $(\cdot, \cdot)$.

Note that H is also a complex separable Hilbert space and for any $h_j^{(1)}, h_j^{(2)} \in H_j$, $j = 1, \ldots, d$

$$\left(h_1^{(1)} \otimes \cdots \otimes h_d^{(1)}, h_1^{(2)} \otimes \cdots \otimes h_d^{(2)} \right) = \prod_{j=1}^{d} \left(h_j^{(1)}, h_j^{(2)} \right)_j .$$

Consider a linear operator equation in H

$$Au = f, \tag{1}$$

where $u, f \in H$ and $A \in \mathfrak{L}(H)$ is a linear continuous operator in H such that there exists its continuous inverse operator $\exists A^{-1} \in \mathfrak{L}(H)$. Note that under such conditions the adjoint operator also exists and is continuous in H as well $\exists A^* \in \mathfrak{L}(H)$. Moreover the equation (1) has a unique solution in H.

The MGSV approximates the solution of (1) with a series where each term has a special form called *separable* with respect to spaces H_j, $j = 1, \ldots, d$. In other words each term is a tensor product of d elements from $H_1, H_2, \ldots, H_d$ respectively. Let's denote with G a set of separable elements of H with respect to H_j, $j = 1, \ldots, d$

$$G = \left\{ \bigotimes_{j=1}^{d} h_j : \; h_j \in H_j, \; j = 1, \ldots, d \right\},$$

Also we define a set G_A as a mapping A applied to the set G

$$G_A = A(G) = \{ Ag : \; g \in G \} . \tag{2}$$

Thus the MGSV solution approximation series consists of elements from G

$$\sum_{k=1}^{\infty} g_k, \quad g_j \in G, \tag{3}$$

where k-th term is found according to the minimum condition

$$\|f - A\left(\sum_{l=1}^{k-1} g_l + g_k\right)\| = \inf_{g \in G} \|f - A\left(\sum_{l=1}^{k-1} g_l + g\right)\|. \tag{4}$$

The terms of (3) are constructed consecutively and produce a sequence of approximate solutions. The sum of the first k terms of (3) is k-th solution approximation of the equation (1)

$$u_k = \sum_{l=1}^{k} g_l, \quad u_0 = 0_H,$$

where 0_H is a zero vector in H.

k-th term of the series (3) is called k-th approximate solution *improvement*

$$g_k = u_k - u_{k-1}.$$

When we have k-th solution approximation u_k by subtracting Au_k from the right-hand side of the equation (1) we get the very same initial equation (1) but with different right-hard side $f - Au_k$ which is called k-th *residual* equation

$$Au = f - Au_k.$$

Let f_k is a right-hand side of k-th residual equation

$$f_k = f - Au_k = f - A\left(\sum_{j=1}^{k} g_j\right), \quad f_0 = f.$$

In [2] it is proven that at least one such element g_k satisfying (4) exists in H. Therefore there always exists a minimization problem solution of the following functional

$$J_k\left(h_1, \ldots, h_d\right) = \|f_{k-1} - A\left(\bigotimes_{j=1}^{d} h_j\right)\|^2, \quad h_j \in H_j,\ j = 1, \ldots, d. \tag{5}$$

By considering the definition of G_A (2) and the condition (4) it's easy to see that element Ag_{k+1} is the best approximation to the right-hand side of k-th residual equation in the set G_A

$$\|f_k - Ag_{k+1}\| = \inf_{g \in G_A} \|f_k - g\|.$$

Algorithm 1 describes a generic approach of MGSV.

The loop break (iteration stop) condition of algorithm 1

$$\frac{\|f_k\|}{\|f\|} = \frac{\|f - Au_k\|}{\|f\|} < \epsilon,$$

Algorithm 1 MGSV

Require: $f \in H$, $A \in \mathfrak{L}(H)$, $\epsilon > 0$
Ensure: $\|f - A\widetilde{u}\| < \epsilon$
  $k \leftarrow 0$
  $u_0 \leftarrow 0_H$
  repeat
    $k \leftarrow k + 1$
    $g_k \leftarrow$ solution of the (4)
    $u_k \leftarrow u_{k-1} + g_k$
    $f_k \leftarrow f - Au_k$
  until $\frac{\|f_k\|}{\|f\|} < \epsilon$
  $\widetilde{u} \leftarrow u_k$
  return $\widetilde{u}$

can be replaced with alternatives, for example

$$\frac{\|g_k\|}{\|u_{k-1}\|} = \frac{\|u_k - u_{k-1}\|}{\|u_{k-1}\|} < \epsilon.$$

The possible ways to find g_k in algorithm 1 are considered below. In [2] the convergence of approximate solution sequence of the MGSV to the exact solution of the equation (1) is proven.

In practice implementations of MGSV consider a discrete case of the equation (1). Assume H_j is a n_j-dimensional space, $j = 1, \ldots, d$. Since H is a tensor product of $H_1, H_2, \ldots, H_d$ it is a n-dimensional space where

$$n = \dim H = \prod_{j=1}^{d} \dim H_j = \prod_{j=1}^{d} n_j.$$

Now the equation (1) is equivalent to a system of n linear equations. In general a space required to store a solution of the equation linearly depends on the number of dimensions n, i.e. the required storage is

$$\mathcal{O}\left(\prod_{j=1}^{d} n_j\right). \tag{6}$$

On the other hand since space H has a special structure a single term of the MGSV approximate solution consumes only

$$\mathcal{O}\left(\sum_{j=1}^{d} n_j\right) \tag{7}$$

of the storage. If we increase number of dimensions in all spaces $H_1, H_2, \ldots, H_d$ simultaneously expression (6) will grow exponentially while expression (7) will grow linearly. Thus as long as the number of terms in the solution approximation is relatively small MGSV produces a compact (in terms of the storage) solution approximation of the equation (1).

In a discrete case MGSV is closely related to approximations of a multidimensional tensor with a product of one-dimensional tensors (vectors) [7]. Indeed, elements u and f can be viewed as d-dimensional tensors of $n_1 \times \cdots \times n_d$ size and operator A as $(2d)$-dimensional tensor of $n_1 \times \cdots \times n_d \times n_1 \times \cdots \times n_d$ size. Then in order to find k-th solution improvement we have to minimize a function with d one-dimensional vector parameters

$$J_k\left(x_1, \ldots, x_d\right) = \left\| f_{k-1} - A\left(x_1 \otimes \cdots \otimes x_d\right)\right\|^2. \tag{8}$$

Here $x_j = \left(x_j^{(1)}, \ldots, x_j^{(n_j)}\right)$ is a one-dimensional vector of coordinates in H_j, $j = 1, \ldots, d$. The norm of d-dimensional tensor t of $n_1 \times \cdots \times n_d$ size can be, for example,

$$\|t\| = \sqrt{\sum_{\substack{1 \le k_j \le n_j \\ 1 \le j \le d}} |t_{k_1, \ldots, k_d}|^2}, \quad t \in H.$$

The function (8) is a polynomial of total degree $2d$ with m variables

$$x_1^{(1)}, \ldots, x_1^{(n_1)}, \ldots, x_d^{(1)}, \ldots, x_d^{(n_d)}.$$

Here

$$m = \sum_{j=1}^{d} n_j.$$

3. Alternating Least Squares

Let's consider the minimization problem of functional (5). In general the problem is nonlinear and can be solved using any nonlinear functional minimization methods. However note that if in (5) we fix all parameter values except of one h_j, $1 \le j \le d$ then we get a functional of a single parameter $h_j \in H_j$ which minimization problem is linear.

Similarly if we fix values of all polynomial (8) variables except of $x_j^{(1)}$, ..., $x_j^{(n_j)}$, $1 \le j \le d$ then we get a quadratic polynomial of n_j variables. The minimization of such polynomial can be done by solving a system of n_j linear equations with n_j variables. This leads us to the method of alternating least squares which can be used to approximate the next term of MGSV series.

The idea of *Alternating Least Squares* method (ALS) is to choose an initial values of (5) variables, fix all of them and then cyclically iterate over the variables, release one of them, solve a linear minimization problem and adjust the current variable value. Algorithm 2 describes a generic approach of ALS method.

Alternatively as a loop break condition in algorithm 2 a relatively small current value of functional (5) can be used instead

$$\frac{J_k\left(h_1^{(l)}, \ldots, h_d^{(l)}\right)}{J_k\left(h_1^{(0)}, \ldots, h_d^{(0)}\right)} < \epsilon.$$

Algorithm 2 ALS

Require: $f_{k-1} \in H$, $A \in \mathfrak{L}(H)$, $h_j^{(0)} \in H_j$, $j = 1, \ldots, d$, $\epsilon > 0$
  $l \leftarrow 0$
  repeat
    $l \leftarrow l + 1$
    for $j = 1$ to d **do**
      fix all variable values of (5) except of h_j and solve

$$J_k\left(h_1^{(l)}, \ldots, h_{j-1}^{(l)}, h_j, h_{j+1}^{(l-1)}, \ldots, h_d^{(l-1)}\right) \longrightarrow \min$$

      $h_j^{(l)} \leftarrow$ the linear minimization problem solution
    end for
  until

$$\frac{\|h_1^{(l)} \otimes \cdots \otimes h_d^{(l)} - h_1^{(l-1)} \otimes \cdots \otimes h_d^{(l-1)}\|}{\|h_1^{(l-1)} \otimes \cdots \otimes h_d^{(l-1)}\|} < \epsilon$$

  for $j = 1$ to d **do**
    $\widetilde{h_j} \leftarrow h_j^{(l)}$
  end for
  return $\widetilde{h_1} \otimes \widetilde{h_2} \otimes \ldots \otimes \widetilde{h_d}$

Consider a numerical sequence

$$\left\{J_k\left(h_1^{(l)}, \ldots, h_d^{(l)}\right)\right\}_{l=0}^{\infty}. \tag{9}$$

According to algorithm 2 the given sequence is monotonically non-increasing

$$\forall l \geq 1 \quad J_k\left(h_1^{(l)}, \ldots, h_d^{(l)}\right) \leq J_k\left(h_1^{(l-1)}, \ldots, h_d^{(l-1)}\right).$$

Since (9) is bounded by zero it converges to some non-negative number L

$$\exists L \geq 0 : \lim_{l \to \infty} J_k\left(h_1^{(l)}, \ldots, h_d^{(l)}\right) = L.$$

However in general sequence (9) does not converge to the infimum of functional (5).

The method of alternating least squares is simple for understanding and implementation, but does not guarantee a convergence to the solution of minimization problem of (5). Besides the method outcome might strongly depend on the initial values $h_1^{(0)}, h_2^{(0)}, \ldots, h_d^{(0)}$.

Note that in some cases a convergence to the minimization problem solution can be proven. For example if the following condition holds

$$\begin{aligned}
&\forall f_{k-1} \in H \quad \forall j, l \quad 1 \leq j < l \leq d \\
&\qquad \forall h_1 \in H_1 \quad \forall h_2 \in H_2 \quad \ldots \quad \forall h_d \in H_d \quad \forall \hat{h_j} \in H_j \quad \forall \hat{h_l} \in H_k \\
&\qquad J_k(h_1, \ldots, h_j, \ldots, h_l, \ldots, h_d) > J_k(h_1, \ldots, \hat{h_j}, \ldots, \hat{h_l}, \ldots, h_d) \quad \Rightarrow \\
&\qquad J_k(h_1, \ldots, h_j, \ldots, h_l, \ldots, h_d) > J_k(h_1, \ldots, h_j, \ldots, \hat{h_l}, \ldots, h_d) \quad \wedge
\end{aligned}$$

$$J_k(h_1,\ldots,h_j,\ldots,h_l,\ldots,h_d) > J_k(h_1,\ldots,\hat{h_j},\ldots,h_l,\ldots,h_d) \quad \wedge$$
$$J_k(h_1,\ldots,\hat{h_j},\ldots,h_l,\ldots,h_d) > J_k(h_1,\ldots,\hat{h_j},\ldots,\hat{h_l},\ldots,h_d) \quad \wedge$$
$$J_k(h_1,\ldots,h_j,\ldots,\hat{h_l},\ldots,h_d) > J_k(h_1,\ldots,\hat{h_j},\ldots,\hat{h_l},\ldots,h_d)$$

then the sequence produced by ALS converges to the (5) minimization problem solution.

Papers [7–9] consider problems of multidimensional tensor decomposition with tensor products of one-dimensional vectors where the numerical ALS method [10, 11] is widely used. Some efficiency improvement techniques are described in [12] while the initial ALS value selection problem is considered in [13].

There are numerous of alternative methods which share the same basic idea with ALS. In [14] some of such methods are compared with ALS:

- DTLD (direct trilinear decomposition);
- ATLD (alternating trilinear decomposition);
- SWATLD (self-weighted alternating trilinear decomposition);
- PALS (pseudo alternating least squares);
- ACOVER (alternating coupled vectors resolution);
- ASD (alternating slice-wise diagonalization);
- ACOMAR (alternating coupled matrices resolution).

According to the paper conclusions none of the methods is superior to ALS in terms of a convergence to the exact solution.

Table 1 contains numerical results of MGSV with ALS for the following equation

$$Au \equiv \int_0^1 \int_0^1 \cos\left(\widehat{x}\widehat{y} + x^2 - y^2\right) u\left(\widehat{x},\widehat{y}\right) \mathrm{d}\widehat{x}\mathrm{d}\widehat{y} - 4u\left(x,y\right) = \sin\left(x^2+y^2\right). \quad (10)$$

For both algorithms $\epsilon = 10^{-5}$. The first column corresponds to MGSV iteration index k, the second column shows the value $\frac{\|f_{k-1}\|}{\|f\|}$ and each of the following columns contains the value

$$\frac{\|f_{k-1} - A\left(h_1^{(l)} \otimes \ldots \otimes h_d^{(l)}\right)\|}{\|f\|}$$

after the l-th iteration of ALS.

Tabl. 1. Numerical results for equation (10)

k	before ALS	$l=1$	$l=2$	$l=3$	$l=4$	$l=5$	$l=6$
1	1.000000	0.344960	0.158934	0.153180	0.153133	0.153133	0.153133
2	0.153133	0.147828	0.025094	0.007752	0.007494	0.007493	0.007493
3	0.007493	0.001684	0.000297	0.000293	0.000293		
4	0.000293	0.000288	0.000035	0.000011	0.000010		

4. Nonlinear Least Squares

Better approximation accuracy can be obtained by using *Nonlinear Least Squares* methods (NLS). These gradient methods minimize nonlinear function (8). In particular NLS representatives are Gauss-Newton method [15, 16], damped Gauss-Newton method [17, 18] and PMF methods [19].

Algorithm 3 describes a generic approach of NLS methods for minimization of nonlinear multivariable function (8).

Algorithm 3 NLS

Require: $f_{k-1} \in H$, $A \in \mathfrak{L}(H)$, $\epsilon > 0$
  $l \leftarrow 0$
  $x^{(0)} \leftarrow$ initial value $\{x^{(0)}$ is a variable vector of function (8)$\}$
  repeat
    $l \leftarrow l + 1$
    $x^{(l)} = x^{(l-1)} - \phi\left(x^{(l-1)}\right)$ $\{\phi$ is a mapping which depends on J_k and a particular method$\}$
  until $\frac{\|x^{(l)} - x^{(l-1)}\|}{\|x^{(l-1)}\|} < \epsilon$
  $\widetilde{x} \leftarrow x^{(l)}$
  return $\widetilde{x}$

NLS methods are mostly generalizations and modifications of Newton method. At each iteration based on a gradient we look for an optimal vector and length of the next step.

NLS methods in general produce more accurate approximations than ALS methods, they do not guarantee a convergence to the global minimum of function (8) though. However NLS methods are inferior to ALS in terms of computational complexity. Numerical results provided in [12, 18] show that NLS methods are slower and require more storage than ALS.

5. Stetter-Möller Matrix Method Modification

Papers [20, 21] consider modifications of *Stetter-Möller matrix method* [22, 23] which allows to find a global minimum of a multivariable higher degree polynomial. Suggested approaches lead a polynomial minimization problem to a generalized eigenvalue problem. A set of points where the polynomial global minimum is achieved has several connected components. For each such connected component the method finds at least one point. There are no special application requirements, i.e. the method finds a minimum for an arbitrary polynomial. Thus the method can be used to find a global minimum of function (8).

Let p is a m-variable polynomial of total degree $2d$

$$p(x_1, \ldots, x_m) \in \mathbb{R}[x_1, \ldots, x_m]. \tag{11}$$

Consider a polynomial

$$p_\lambda(x_1, \ldots, x_m) = p(x_1, \ldots, x_m) + \lambda\left(x_1^{2(d+1)} + \ldots + x_m^{2(d+1)}\right), \quad \lambda > 0.$$

According to [20] the global minimum data of (11) can be retreived from p_λ when $\lambda \to 0$.

A polynomial global minimum can be found from the first order conditions by considering its values in critical points. For p_λ if $\lambda > 0$ is fixed this leads to a system of polynomial equations in Gröbner basis [24] which has a finite number of solutions. Thus the Stetter-Möller matrix method can be used.

First, we build matrices $(A_{x_1}, \ldots, A_{x_m})$. Eigenvalues of these matrices which correspond to a common eigenvector form a critical point of polynomial p_λ. Here matrix A_{x_k} $(1 \leq k \leq m)$ represents an operator of multiplication by x_k in quotient space $\mathbb{R}[x_1, \ldots, x_m]/I$ where I is an ideal formed by first order partial derivatives of p_λ.

For an arbitrary polynomial $r(x_1, \ldots, x_m)$ matrix $A_r = r(A_{x_1}, \ldots, A_{x_m})$ contains values of polynomial r in critical points of polynomial p_λ.

Algorithm 4 describes one of the possible approach implementations.

Algorithm 4 Stetter-Möller Matrix Method Modification

Require: $p(x_1, \ldots, x_m) \in \mathbb{R}[x_1, \ldots, x_m]$, $\lambda > 0$, $\epsilon > 0$
  $l \leftarrow 0$
  $\lambda_0 \leftarrow \lambda$
  $\left(x_1^{(0)}, \ldots, x_m^{(0)}\right) \leftarrow (0, \ldots, 0)$
  $v_0 \leftarrow p\left(x_1^{(0)}, \ldots, x_m^{(0)}\right)$
  repeat
    $l \leftarrow l + 1$
    $\lambda_l \leftarrow \frac{\lambda_{l-1}}{2}$
    compute matrices $\left(A_{x_1}^{(l)}, \ldots, A_{x_m}^{(l)}\right)$ for polynomial p_{λ_l}
    compute matrix $A_p^{(l)} = p\left(A_{x_1}^{(l)}, \ldots, A_{x_m}^{(l)}\right)$
    $v_l \leftarrow$ minimum value of $A_p^{(l)}$
    $\left(x_1^{(l)}, \ldots, x_m^{(l)}\right) \leftarrow$ the corresponding vector, i.e. $p\left(x_1^{(l)}, \ldots, x_m^{(l)}\right) = v_l$
  until $\frac{|v_l - v_{l-1}|}{|v_0|} < \epsilon$
  $(\widetilde{x_1}, \ldots, \widetilde{x_m}) \leftarrow \left(x_1^{(l)}, \ldots, x_m^{(l)}\right)$
  return $(\widetilde{x_1}, \ldots, \widetilde{x_m})$

A drawback of the described method is the size of matrix A_r which is equal to $(2d+1)^m$ and grows exponentially with m. However modern ways to solve generalized eigenvalue problems which are based on Jacobi-Davidson or Arnoldi methods [25, 26] do not require a construction of matrix A_r. Thus one of the suggested method modifications [20, 21] can be used instead.

Stetter-Möller matrix method modification unlike ALS and NLS methods always finds a global minimum of a function. However it requires a lot of computational resources. Thus in practice quite often ALS or NLS methods are preferred despite they are not perfectly accurate.

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