Institute for Computational Mathematics
Hong Kong Baptist University

ICM Research Report
09-13

Fast orthogonalization to the kernel of the discrete gradient operator with application to Stokes problem

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Abstract

We obtain a simple tensor representation of the kernel of the discrete d-dimensional gradient operator defined on tensor semi-staggered grids. We show that the dimension of the nullspace grows as $\mathcal{O}(n^{d-2})$, where d is the dimension of the problem, and n is one-dimensional grid size. The tensor structure allows fast orthogonalization to the kernel. The usefulness of such procedure is demonstrated on three-dimensional Stokes problem, discretized by finite-differences on semi-staggered grids, and it is shown by numerical experiments that the new method outperforms usually used stabilization approach.

Key words: Discrete gradient operator, kernel, tensor structure, fast orthogonalization, Stokes problem

1 Introduction

Discrete gradient operator naturally appears in several applications (one of the most important is the numerical solution of the Stokes problem [1,8,7,3]), and it is interesting to study its properties. One of the properties, which is different from the continious case, is the structure of the kernel of the discrete gradient operator. This structure, of course, depends on the discretization of the continuous problem. In the continuous case the dimension of the kernel is

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[1] This work was partially supported by RFBR grants 08-01-00115, 09-01-00565, 09-01-12058, RFBR/DFG grant 09-01-91332 and Priority Research Program of Department of Mathematical Sciences of Russian Academy of Sciences.

one — only the constant function is in it. In the discrete case the situation is more complicated and that has a serious influence on the numerical solution of the corresponding linear systems. In this paper we consider one particular discretization scheme for the gradient which comes from the finite-difference approximation of the Stokes problem. Let us note that the gradient discretization can be enough to have the full discretization of the Stokes problem (i.e. the divergence and the Laplace operator can be obtained from the gradient operator).

We restrict our attention only to tensor-structured grids. Surprisingly, not a lot is known even in this simplest case, for known results see recent book [3]. In two-dimensional case the dimension of the nullspace is 2, and the nullspace vectors are so-called "checkerboard vectors" [4,5], and in three-dimensional case with an $n \times n \times n$ grid the dimension of the kernel is not smaller then $3n-2$ [10], which influences on the convergence rate of the numerical methods and their cost.

In this paper we obtain the tensor structure of the kernel, i.e. the kernel vectors can be represented in a compact tensor form, by using the tensor representation of the discrete gradient operator. Moreover, any vector can be orthogonalized to this kernel in a fast way in $\mathcal{O}(N)$ operations. As an application we consider the numerical solution of the three-dimensional Stokes problem discretized with semi-staggered finite difference scheme, and numerically show that our method attains optimal convergence, and compare its efficiency with the stabilization method [2,9,11].

2 Discretization

2.1 Two-dimensional case

We will use a finite differences approach. First consider two-dimensional case. Our domain is a square $\Omega = [0,1]^2$. As standard in semi-staggered grids approach [6,3], two grids are needed. The first one is a uniform $n_1 \times n_2$ grid in Ω:

$$\Omega^{(1)}_{ij} = [(i - \frac{1}{2})h_1, (j - \frac{1}{2})h_2], \quad i = 1, \ldots, n_1, \quad j = 1, \ldots, n_2,$$

where $h_1 = \frac{1}{n_1}, h_2 = \frac{1}{n_2}$ The function in question (with respect to Stokes problem it is pressure p) will be defined on this grid, while the gradient $\nabla_h p = [B_x p, B_y p]$ of it will be assigned to points

$$\Omega^{(2)}_{ij} = [ih_1, jh_2], \quad i = 1, \ldots, (n_1 - 1), \quad j = 1, \ldots, (n_2 - 1).$$

We have $n_1 n_2$ pressure components and $2(n_1-1)(n_2-1)$ gradient components (since we deal with the planar problem). For simplicity, we suppose further that $n_1 = n_2 = n$ and $h = h_1 = h_2 = \frac{1}{n}$, but all results obtained are valid for $n_1 \neq n_2$. We need discrete analogues of two functions, $B_x p = \frac{\partial p}{\partial x}$ and $B_y p = \frac{\partial p}{\partial y}$. Consider first B_x, B_y is treated analogously. The gradient discretization on semi-staggered grids reads

$$B_x p = \frac{1}{2h}(p_{ij} - p_{(i-1)j} + p_{i(j-1)} - p_{(i-1)(j-1)}), \qquad (1)$$
$$i, j = 1, \dots, n.$$

This can be interpreted as a mean value of the first-order difference applied at the level j and at the level $(j-1)$ and averaged to the level $(j - \frac{1}{2})$. This justifies the name "semi-staggered", since the gradient is naturally assigned to the middle point. For our purpose we will need another form of (1). Matrix B_x can be written in a very simple and intuitive way by using tensor notation. Introduce two auxiliary matrices E and Z of size $(n-1) \times n$ which act on a vector as follows:

$$E \begin{pmatrix} p_1 \\ p_2 \\ \dots \\ p_n \end{pmatrix} = \begin{pmatrix} p_2 \\ p_3 \\ \dots \\ p_n \end{pmatrix},$$

and

$$Z \begin{pmatrix} p_1 \\ p_2 \\ \dots \\ p_n \end{pmatrix} = \begin{pmatrix} p_2 \\ p_3 \\ \dots \\ p_{n-1} \end{pmatrix},$$

i.e. E throws out the first component of a vector and Z — the last one. With the help of these matrices it is easy to represent B_x:

$$B_x = \frac{1}{2h}(E \times E - Z \times E + E \times Z - Z \times Z),$$

or

$$B_x = \frac{1}{2h}(E - Z) \times (E + Z).$$

Matrices $(E - Z)$ and $(E + Z)$ play an important role and will be denoted by

G and H respectively, and

$$B_x = \frac{1}{2h} G \times H.$$

Obviously, the second component of the gradient is

$$B_y = \frac{1}{2h}(E+Z) \times (E-Z) = \frac{1}{2h} H \times G.$$

2.2 Three (and more) dimensional case

In three (and more) dimensions everything is treated in the same way. The discrete gradient operators, B_x, B_y, B_z, are expressed in terms of the same matrices G and H:

$$\begin{aligned} B_x &= G \times H \times H, \\ B_y &= H \times G \times H, \\ B_z &= H \times H \times G. \end{aligned} \tag{2}$$

It is obvious how to generalize (2) to many dimensions. In d dimensions the discrete gradient operator $\nabla_h^{(d)}$ is of form

$$\nabla_h^{(d)} = [B_{x_1}^\top, B_{x_2}^\top, \ldots, B_{x_d}^\top]^\top,$$

where the k-th component of the gradient B_{x_k} is

$$B_{x_k} = G \times G \times \ldots \times \underbrace{H}_{k} \times \ldots \times G, \quad k = 1, \ldots, d. \tag{3}$$

Although it may not be as important in applications as planar and spatial cases, nevertheless the tensor representation gives a simple way to discretize the multidimensional gradient operator which appears in certain financial applications [15].

3 Kernel

The tensor structure of the discrete gradient operator suggests us an easy and efficient way to find what we are looking for — the structure of its kernel.

3.1 Two-dimensional case

Let us start from two-dimensional case, where the answer is known [5,10] and show how the kernel can be represented in tensor form. Matrices B_x, B_y have form (up to a constant factor, which we omit here since it does not influence the nullspace)

$$B_x = G \times H, \; B_y = H \times G.$$

We want to find a vector p such that

$$B_x p = 0, \; B_y p = 0,$$

i.e. it belongs both to the kernels of B_x and B_y. Let us seek for a kernel vector of B_x in form $x \times y$, so we have

$$Gx = 0 \text{ or } Hy = 0.$$

Recall that matrices G and H have sizes $(n-1) \times n$, so each of them has at least one vector in the nullspace. It is not difficult to see from the definition of G and H that their kernels have dimension one. Denote the kernel vector of G by a and the kernel vector of H by b, then it can be shown that up to a scaling factor

$$a = (1, 1, \ldots, 1)^\top,$$

while

$$b = (1, -1, 1, \ldots, -1)^\top.$$

Therefore, the kernel of B_x contains vectors of form

$$a \times x + y \times b,$$

where x and y are arbitrary vectors. The dimension of this subspace is $n + n - 1 = 2n - 1$, since the vector $a \times b$ is counted twice. To show that there are no more vectors in it, consider vectors of form

$$a' \times b',$$

where a' is any vector such that $Ga' \neq 0$ and b' is any vector such that $Hb' \neq 0$. The dimension of the space spanned by a' is $n-1$ and spanned by b' is $n-1$, so the dimension of the space spanned by their tensor products is

$$(n-1)(n-1),$$

and there are no kernel vectors in it. Since

$$(n-1)(n-1) + n + n - 1 = n^2$$

is equal to the number of columns of B_x, we have found all kernel vectors of B_x. Analogously, all kernel vectors of B_y have form

$$b \times x' + y' \times a.$$

There are two vectors in the intersection of these two subspaces:

$$a \times b$$

and

$$b \times a,$$

so there are two of them and it is easy to see that these are the "checkerboard" vectors.

3.2 Three (and more) dimensional case

Now let us go to the three-dimensional case. Here we have three matrices B_x, B_y, B_z:

$$B_x = G \times H \times H, \; B_y = H \times G \times H, \; B_z = H \times H \times G.$$

The nullspace for B_x is

$$B_x = a \times y_1 \times z_1 + x_2 \times b \times z_2 + x_3 \times y_3 \times b$$

and analogous expressions are for B_y and B_z. Let us "guess" the answer. The vector of form

$$p = x \times b \times b + b \times y \times b + b \times b \times z, \tag{4}$$

with arbitrary vectors x, y and z of length n satisfies

$$B_x p = 0, \; B_y p = 0, \; B_z p = 0,$$

since for each matrix involved we have at least two "letters" b and using $Hb = 0$ we get the zero answer. In this case the dimension of the nullspace is at least $(n + n + n) - 2 = 3n - 2$, since the vector $b \times b \times b$ belongs to all three subspaces that constitute our kernel. To show that there are no more vectors in the nullspace, we have to provide a set of linearly independent vectors that do not belong the kernel.

First, consider vectors of form

$$p = a' \times b' \times c' \tag{5}$$

such that $B_x p \neq 0$. That is fulfilled if $Ga' \neq 0$, $Hb' \neq 0$, $Hc' \neq 0$, and since the dimensions of the nullspaces for G and H are 1, the dimension of the subspace spanned by such p is $(n-1)^3$. Denote this subspace by $\mathcal{L}_1$. Then, again consider vectors of form (5) but such that $B_x p = 0$, and $B_y p \neq 0$. Denote this space by $\mathcal{L}_2$. This holds for three cases:

$$p = p_1 = a \times b_1 \times c_1,$$

$$p = p_2 = a_2 \times b \times c_2,$$
$$p = p_3 = a_3 \times b_3 \times b,$$

where a_1, b_1, c_1, a_2, c_2, a_3, b_3 span subspaces of dimension $n-1$. Such vectors p do not belong to $\mathcal{L}_1$. To count the dimension of the subspace spanned by p in question, notice that these three subspaces have a non-zero intersection, and

$$\dim(\mathrm{span}(p_1) + \mathrm{span}(p_2) + \mathrm{span}(p_3)) = 3(n-1)^2 - 3(n-1),$$

where we subtracted the dimensions of their intersection. For example, space $\mathrm{span}(p_1) \bigcap \mathrm{span}(p_2)$, consists of vectors of form

$$p = a \times b \times c',$$

and its dimension is $(n-1)$. The space $\mathrm{span}(p_1) \bigcap \mathrm{span}(p_2) \bigcap \mathrm{span}(p_3)$ contains only zero vector, since the only possible candidate is $a \times b \times b$, but $Hb = 0$.

Finally, consider the space spanned by vectors of form (5) such that $B_x p = 0$, $B_y p = 0$, $B_z p \neq 0$. It contains vectors of form

$$p_1 = a \times a \times c_1,$$

$$p_2 = a \times b \times c_2,$$
$$p_3 = b \times a \times c_3,$$

spaces spanned by these vectors do not intersect and their union has dimension $3(n-1)$. Denote it by $\mathcal{L}_3$. We have explicitly constructed three non-intersecting subspaces $\mathcal{L}_1, \mathcal{L}_2, \mathcal{L}_3$, which do not contain kernel vectors, and their union has dimension

$$\dim(\mathcal{L}_1 + \mathcal{L}_2 + \mathcal{L}_3) \geq (n-1)^3 + 3(n-1)^2 - 3(n-1) + 3(n-1) = n^3 - 3n + 2,$$

and that finishes the proof.

For the case $d > 3$ we have a similar representation for the kernel vector. If the vector p belongs to the kernel of the d-dimensional gradient operator (3) then

$$p = x_1 \times b \times \ldots \times b + b \times x_2 \times \ldots \times b + \ldots + b \times b \times \ldots \times x_d,$$

where $x_1, x_2, \ldots, x_d$ are arbitrary vectors of corresponding lengths, and it can be shown that the dimension of the kernel is

$$dn^{d-2} - d + 1$$

since the vector $b \times b \times \ldots \times b$ is counted d times.

Thus we have obtained a compact tensor form of the kernel of the discrete gradient operator. Another representation is available [10], but the new form is more convenient for two reasons. The approach of [10] is not easy to generalize to many dimensions, while the tensor representation can be easily constructed in that case. The second reason is that the new representation allows fast orthogonalization procedure, i.e. an arbitrary vector can be orthogonalized to the kernel of the gradient in $\mathcal{O}(N)$ operations. Such operation is important in the applications, we will study it in the next section.

4 Orthogonalization

In two dimensions no special effort is needed, since only two vectors are in the nullspace and their analytical representation is known. For the case $d \geq 3$ dimensions the number of vectors is $dn^{d-2} - d + 1$ and some special approach is required. We will focus on three-dimensional case, since the generalization to $d > 3$ dimensions is technical.

Suppose we have some vector p of appropriate size and we want to orthogonalize it to the kernel of $\nabla_h^{(3)}$, i.e. find a vector p' in the orthogonal complement to the Ker $\nabla_h^{(3)}$ that minimizes $||p - p'||$. In order to do this, we subtract from p some vector from the kernel:

$$p' = p - \alpha \times b \times b - b \times \beta \times b - b \times b \times \gamma,$$

where α, β, γ have to be found from the orthogonality conditions, i.e.

$$(p', e_i \times b \times b) = 0, \quad (p', b \times e_j \times b) = 0, \quad (p', b \times b \times e_k) = 0, \qquad (6)$$

for $i, j, k = 1, \ldots n$. In what follows we will assume that b is normalized, i.e.

$$||b|| = 1.$$

It is natural to treat p as a three-dimensional $n \times n \times n$ array p_{ijk}. Then equations (6) can be rewritten as a system of equations for α, β, γ:

$$\begin{aligned}
&\sum_{j,k=1}^{n} p_{ijk} b_j b_k = \alpha_i + b_i \widehat{b} + b_i \widehat{\gamma}, \quad i = 1, \dots, n.\\
&\sum_{k,i=1}^{n} p_{ijk} b_k b_i = \beta_j + b_j \widehat{\alpha} + b_j \widehat{\gamma}, \quad j = 1, \dots, n.\\
&\sum_{i,j=1}^{n} p_{ijk} b_i b_j = \gamma_k + b_k \widehat{\alpha} + b_k \widehat{\beta}, \quad k = 1, \dots, n,
\end{aligned} \tag{7}$$

where

$$\widehat{\alpha} = \sum_{i=1}^{n} \alpha_i b_i, \quad \widehat{\beta} = \sum_{j=1}^{n} \beta_j b_j \quad \widehat{\gamma} = \sum_{k=1}^{n} \gamma_k b_k.$$

If we multiply the first equation of (7) by b_i and sum over i we obtain a simple equation:

$$\widehat{\alpha} + \widehat{\beta} + \widehat{\gamma} = c = \sum_{i,j,k=1}^{n} p_{ijk} b_i b_j b_k.$$

The same equations are obtained from the second and the third equation of (7), so we have one equation for three unknowns. It is quite natural since we have the dimension of the nullspace equal to $n + n + n - 2 = 3n - 2$ but $n + n + n = 3n$ orthogonality conditions. To simplify the final expression, let $\widehat{\alpha} = \widehat{\beta} = \widehat{\gamma} = \frac{c}{3}$. Then

$$\begin{aligned}
c &= \sum_{i,j,k=1}^{n} p_{ijk} b_i b_j b_k \qquad (8)\\
\alpha_i &= \sum_{j,k=1}^{n} p_{ijk} b_j b_k - \frac{2c}{3} b_i, \quad i = 1, \dots, n,\\
\beta_j &= \sum_{k,i=1}^{n} p_{ijk} b_k b_i - \frac{2c}{3} b_j, \quad j = 1, \dots, n,\\
\gamma_k &= \sum_{i,j=1}^{n} p_{ijk} b_i b_j - \frac{2c}{3} b_k, \quad k = 1, \dots, n,\\
p'_{ijk} &= p_{ijk} - \alpha_i b_j b_k - b_i \beta_j b_k - b_i b_j \gamma_k, \quad i, j, k = 1, \dots, n,
\end{aligned}$$

are the final orthogonalization formulae. If we recall that up to a scaling factor $b_i = (-1)^i$, then the computations require no multiplications but $5n^3$ additions and subtractions. The obtained orthogonalization procedure is simple and fast. Now we will show its effectiveness by applying to the numerical solution of the Stokes problem.

5 Numerical experiments

As a test problem we consider the Stokes problem with Dirichlet boundary conditions in the unit cube $\Omega = [0,1]^3$:

$$\begin{aligned} -\triangle v + \nabla p &= f, \\ \operatorname{div} v &= 0, \\ v_{|\partial\Omega} &= 0. \end{aligned} \tag{9}$$

For the discretization of the continuous problem we use semi-staggered grids which was firstly introduced in [6]. In this case the discretization can be obtained solely from the discretization of the gradient. The gradient $B = \nabla_h = [B_x, B_y, B_z]$ is defined by the formula (2), the divergence operator is the transpose to it and the "consistent" discretization of the Laplace operator is

$$\triangle_h = \nabla_h \nabla_h^\top,$$

which is the discrete analogue to the $\triangle = \operatorname{div}\nabla$ equation. The obtained saddle-point system

$$\begin{pmatrix} A & B \\ B^\top & 0 \end{pmatrix} \begin{pmatrix} v \\ p \end{pmatrix} = \begin{pmatrix} f \\ 0 \end{pmatrix}, \; p \in \Omega_{ijk}^{(1)}, \; v \in \Omega_{ijk}^{(2)}, \tag{10}$$

is solved by the reduction to the Schur complement [1] with matrix S of form

$$S = B^\top A^{-1} B. \tag{11}$$

Since the gradient operator B has a large nullspace, so has S, and we seek for the *normal solution* which is orthogonal to the kernel of S (which coincides with the kernel of B), and apply conjugate gradients for the matrix S. At each step of CG we orthogonalize to the kernel of B by using formulae (8) (this is equivalent to solving the system with S restricted to the orthogonal complement to the kernel of B). The matrix-by-vector product with S is required at each iteration step, and it is performed implicitly by solving the system with the matrix A which is done by using Fast Fourier Transform (i.e. S is not formed explicitly). As a model example, we consider the analytical solution of form

$$\begin{aligned} v_1 &= x + x^2 + xy + x^3 y, \\ v_2 &= y + xy + y^2 + x^2 y^2, \\ v_3 &= -2z - 3xz - 3yz - 5x^2 yz, \\ p &= xyz + x^3 y^3 z - \frac{5}{32}, \end{aligned}$$

and the right hand side is obtained from the equations directly. Using known analytical solution, we can estimate the accuracy.

We compare the orthogonalization method with the stabilization approach [2,11]. The stabilization approach results in replacing the (2,2) block in the saddle-point system by certain 27-point discretization of Laplace operator with Neumann boundary conditions, so the additional cost $27N$ is higher than for the orthogonalization step $5N$ [2].

We compare methods in terms of CG iterations and solution accuracy. The stopping criteria for CG is set to 10^{-8}. The results are presented in Table 1.

h	E_{ort}	E_{stab}	Iter (ort)	Iter (stab)
1/16	7.30e-05	2.39e-04	23	28
1/32	2.01e-05	7.18e-05	23	31
1/64	5.26e-06	1.93e-05	23	33
1/128	1.34e-06	5.01e-06	23	33

Table 1
Comparison of orthogonalization and stabilization methods for model problem

This model example shows that the fast orthogonalization method proposed in this paper outperforms the stabilization approach both in the number of iterations and in the solution accuracy. For test problems with other right-hand sides the situation is similar.

Remark. The number of iterations with the orthogonalization method for the model problem is independent of the mesh size. For small values of $N = n^3$ we can compute the spectrum of S numerically. From the theory we know that the spectrum of S contains $(3n - 2)$ zero eigenvalues. It is an experimental fact, that there are also $(n - 2)^3$ eigenvalues equal to 1, and the smallest non-zero eigenvalue is bounded from below by a constant, independent of n. We currently do not have the proof of this fact, so it is a hypothesis. If the hypothesis is true, the CG method with orthogonalization for a matrix S is equivalent to the CG method for a matrix with a clustered spectrum. This matrix has $(n-2)^3$ eigenvalues equal to one and the smallest eigenvalue is bounded from below by a constant, independent of n. This results in fast convergence. However, the proof of the hypothesis is required and it is a subject of the ongoing work.

[2] However, the complexity is negligible in both cases, since the solution of Poisson equation takes most of the time on each iteration step.

6 Conclusions and future work

In this paper we presented a compact tensor form for the kernel of the discrete gradient operator defined on semi-staggered grids in arbitrary dimension. The tensor structure allows fast orthogonalization to the kernel, which can be used in the numerical solution of the Stokes problem. We demonstrated the efficiency of such approach on a three-dimensional example, and showed that it outperforms traditionally used stabilization approach.

The tensor structure of the kernel makes it natural to use tensor representation also for vectors during the iterative process. The application of recently introduced tensor-train (TT) format [13,12,14] in conjunction with the mesh-independent iterational method will lead to the significant reduction in numerical cost for solving problems, which include the solution of the Stokes problem as a subproblem. The preliminary results show the benefit of such approach and will be presented in forthcoming papers.

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