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The Best Constant of Discrete Sobolev Inequality on a Weighted Truncated Tetrahedron

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Abstract

The best constant of discrete Sobolev inequality on the truncated tetrahedron with a weight which describes 2 kinds of spring constants or bond distances. Main results coincides with the ones of known results by Kametaka *et al*. under the assumption of uniformity of the spring constants. Since the buckyball fullerene C60 has 2 kinds of edges, destruction of uniformity makes us proceed the application to the chemistry of fullerenes.

Keywords

The Best Constant, Sobolev Inequality, Discrete Laplacian, Weighted Graph, Truncated Polyhedron

1. Introduction

Sobolev inequality known as Sobolev embedding theorem plays an important role in the theory of PDEs. Brezis [1, Chap.IX] gave some constant of Sobolev inequality, and mentioned that the best constant was known and complex. Talenti [2] and Marti [3] studied the best constant by use of variational methods.

Kametaka and his coworkers studied the best constant of Sobolev inequality in view of the boundary value problem [4]-[8], and then they studied discrete Sobolev inequality [9]-[13] aiming to application to the C60 buckyball fullerene [14]. Table 1 is a summary of Kametaka school; in this table, R*n* stands for the regular *n*-hedron, and T*n* stands for the truncated *n*-hedron. In classical geometry, each truncated *n*-hedra is known as a member of Archimedean polyhedra. Note that the works of Kametaka school on each polyhedron is under the assumption of uniformity of the spring constants.

On the other hand, in chemistry of fullerenes [15], the structure of the fullerenes is studied in detail. [16]-[18] tell us that the bond lengths of the C60 buckyball fullerene are of 2 kinds. So, in prospects for application to the chemistry of fullerenes, the assumption of uniformity of the spring constants should be thrown away.

This article concerns with the best constant of discrete Sobolev inequality on T4 with 2 kinds of spring constants, in other words, a weighted T4 graph. The results of Kametaka school for R4 [10] and T4 [12] are generalized in the next section. The outline of this article follows the paper of Kametaka school on R*n* [10].

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2. Discrete Laplacian and Discrete Sobolev Inequality

2.1. Main Results

Consider the truncated tetrahedron T4. It has 12 vertices, and let us number the vertices 0, 1, …, 11 as in **Figure 1**, similar to [12]. Put

$$\mathbf{u} = {}^t(u_0, u_1, \ldots, u_{11}) \in \mathbb{C}^{12} \text{ and } \mathbf{1} = {}^t(1,1,\ldots,1) \in \mathbb{C}^{12}.$$

Define the bond matrix B_{ij}, as in **Figure 2**, by

$$(B_{ij})_{ii} = (B_{ij})_{jj} = 1, \quad (B_{ij})_{ij} = (B_{ij})_{ji} = -1, \quad (B_{ij})_{kl} = 0 \text{ for } k,l \notin \{i,j\}.$$

Note that $|u_i - u_j|^2 = \mathbf{u}^* B_{ij} \mathbf{u}$. Let us represent each edge of T4 by the couple of the numbers of both vertices, identifying (j,i) with (i,j). Put

$$e_1 = \{(0,1),(2,11),(3,6),(4,5),(7,10),(8,9)\},$$

$$e_2 = \{(0,4),(4,8),(8,0),(1,2),(2,3),(3,1),(5,6),(6,7),(7,5),(9,10),(10,11),(11,9)\}.$$

e_1 is the set of original edges of R4, and e_2 is the set of edges of T4 created by the truncation. Let us denote r the ratio of the spring constant of each egde of e_2 to one of each edge of e_1, and introduce 2 kinds of the Sobolev energies as follows:

$$E(\mathbf{u}) = \sum_{(i,j)\in e_1} |u_i - u_j|^2 + r \sum_{(i,j)\in e_2} |u_i - u_j|^2, \quad E(a,\mathbf{u}) = E(\mathbf{u}) + a \sum_{0\le j\le 11} |u_j|^2.$$

Here, $a > 0$ is a dumping parameter. Define the weighted discrete Laplacian

$$A = \sum_{(i,j)\in e_1} B_{ij} + r \sum_{(i,j)\in e_2} B_{ij}.$$

A is also represented as follows:

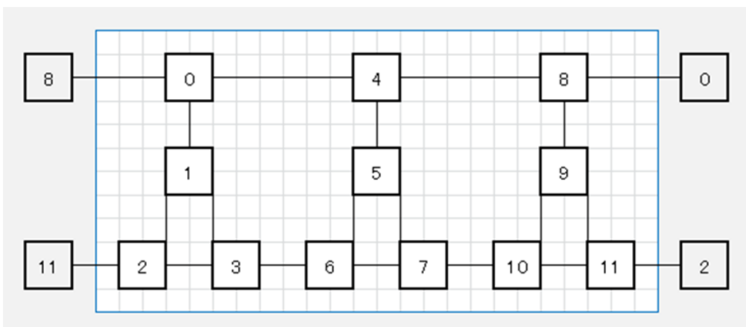

Figure 1. Numbering of the vertices of T4.

$$B_{ij} = \begin{pmatrix} & & & & \\ & 1 & -1 & & \\ & -1 & 1 & & \\ & & & & \end{pmatrix}.$$

Figure 2. Bond matrix.

$$A = \begin{cases} 1+2r & (i=j) \\ -1 & ((i,j)\in e_1) \\ -r & ((i,j)\in e_2) \\ 0 & (\text{otherwise}) \end{cases}.$$

By use of the weighted Laplacian defined as above, the Sobolev energies are written as follows:

$$E(\mathbf{u}) = \mathbf{u}^* A\mathbf{u}, \quad E(a,\mathbf{u}) = \mathbf{u}^*(A+aI)\mathbf{u}.$$

The eigenvalues of A are as follows:

$$0, 3r, 3r, 2+3r, 2+3r, 2+3r, \frac{2+3r-\sqrt{D}}{2}, \frac{2+3r-\sqrt{D}}{2}, \frac{2+3r-\sqrt{D}}{2}, \frac{2+3r+\sqrt{D}}{2}, \frac{2+3r+\sqrt{D}}{2}, \frac{2+3r+\sqrt{D}}{2},$$

where $D = 4-4r+9r^2$. Let us stand $\lambda_0 = 0, \lambda_1, \dots, \lambda_{11}$ for the eigenvalues of A. Note that 0 is a simple eigenvalue of A with the corresponding eigenvector $\mathbf{1} = {}^t(1,1,\dots,1) \in \mathbb{C}^{12}$, and $E_0 = \frac{1}{12}\mathbf{1}\,{}^t\mathbf{1}$ is the projection matrix to the eigenspace corresponding to the eigenvalue 0. Let us introduce the Green matrix of A by

$$G(a) = (A+aI)^{-1}.$$

For the Green matrix, there exists a unique matrix G_* satisfying

$$AG_* = G_* A = I - E_0, \quad G_* E_0 = E_0 G_* = O.$$

G_* is the Penrose-Moore genelarized inverse matrix of A, and is called the pseudo green matrix of A. We see that

$$G_* = \lim_{a\to+0}\left(G(a) - a^{-1}E_0\right).$$

Theorem 1. There exists a positive constant C independent of $\mathbf{u}\in\mathbb{C}^{12}$ such that, for every $\mathbf{u}\in\mathbb{C}^{12}$ satisfying ${}^t\mathbf{1}\mathbf{u} = 0$, the discrete Sobolev inequality

$$\left(\max_{0\le j\le 11} |u_j|\right)^2 \le CE(\mathbf{u})$$

holds. Among such C, the best constant $C_0 = C_0(r)$ is

$$C_0(r) = \frac{1}{12}\sum_{1\le j\le 11}\frac{1}{\lambda_j} = \frac{52+168r+81r^2}{144r(2+3r)}.$$

Theorem 2. There exists a positive constant C independent of $\mathbf{u}\in\mathbb{C}^{12}$ such that, for every $\mathbf{u}\in\mathbb{C}^{12}$, the discrete Sobolev inequality

$$\left(\max_{0\le j\le 11} |u_j|\right)^2 \le CE(a,\mathbf{u})$$

holds. Among such C, the best constant $C_a = C_a(r)$ is

$$C_a(r) = \frac{1}{12}\sum_{0\le j\le 11}\frac{1}{\lambda_j + a} = \frac{1}{12}\left\{\frac{1}{a} + \frac{2}{a+3r} + \frac{3}{a+2+3r} + \frac{3(2a+2+3r)}{(3a+4)r + a(a+2)}\right\}.$$

Remark. $C_0(r)$ in Theorem 1 coinsides with $C_0 = \frac{301}{720}$ for $r=1$ which appears in [12] for T4, and with $C_0 = \frac{3}{16}$ for $r\to\infty$, which appears in [10] for R4. So, the main result covers the results by Kametaka school (cf. **Table 1**).

Table 1. The best constants on polyhedra known by Kametaka school. (a) Regular *n*-hedron (=R*n*) [10]; (b) Truncated *n*-hedron (=T*n*) [9] [12].

(a)

	R4	R6	R8	R12	R20
The best constant	3/16 ≒ 0.1875	29/96 ≒ 0.30208	13/72 ≒ 0.18056	137/300 ≒ 0.45667	7/36 ≒ 0.19444

(b)

	T4	T6	T8	T12	T20
The best constant	301/720 ≒ 0.41806	173/288 ≒ 0.60069	1019/2016 ≒ 0.50546	-	239741/376200 ≒0.63727

2.2. Proof

Let $\mathbf{q}_j$ be the normalized eigenvectors of A, *i.e.* $A\mathbf{q}_k = \lambda_k \mathbf{q}_k$, $\mathbf{q}_j^* \mathbf{q}_k = \delta_{jk}$, where δ_{jk} is the Kronecker's delta. $Q = (\mathbf{q}_0, \mathbf{q}_1, \ldots, \mathbf{q}_{11})$ is unitary. Let $E_k = \mathbf{q}_k \mathbf{q}_k^*$. Put $\boldsymbol{\delta}_k = {}^t(\delta_{1k}, \cdots, \delta_{11,k})$ $(0 \le k \le 11)$. We have

$$I = QQ^* = \sum_{0 \le k \le 11} E_k, \quad A = QDQ^* = \sum_{0 \le k \le 11} \lambda_k E_k = \sum_{1 \le k \le 11} \lambda_k E_k.$$

Note that $\sum_{0 \le j \le 11} {}^t\boldsymbol{\delta}_j E_k \boldsymbol{\delta}_j = \sum_{0 \le j \le 11} {}^t\boldsymbol{\delta}_j \mathbf{q}_k \mathbf{q}_k^* \boldsymbol{\delta}_j = \mathbf{q}_k \mathbf{q}_k^* = 1$. Then, $0 \le \forall j_0 \le 11$,

$$C_0 = {}^t\boldsymbol{\delta}_{j_0} G_* \boldsymbol{\delta}_{j_0} = \frac{1}{12} \sum_{0 \le j \le 11} {}^t\boldsymbol{\delta}_j G_* \boldsymbol{\delta}_j = \frac{1}{12} \sum_{0 \le j \le 11} {}^t\boldsymbol{\delta}_j \sum_{1 \le k \le 11} \lambda_k^{-1} E_k \boldsymbol{\delta}_j$$
$$= \frac{1}{12} \sum_{1 \le k \le 11} \lambda_k^{-1} \sum_{0 \le j \le 11} {}^t\boldsymbol{\delta}_j E_k \boldsymbol{\delta}_j = \frac{1}{12} \sum_{1 \le k \le 11} \lambda_k^{-1}.$$

Definition. For any $\mathbf{u}, \mathbf{v} \in \mathbb{C}^{12}$, we define

$$(\mathbf{u}, \mathbf{v})_A := (A\mathbf{u}, \mathbf{v}) = \mathbf{v}^* A\mathbf{u}, \quad \| \mathbf{u} \|_A^2 := (\mathbf{u}, \mathbf{u})_A = \mathbf{u}^* A\mathbf{u} = E(\mathbf{u}).$$

Lemma. For every $\mathbf{u} \in \mathbb{C}^{12}$, we have the reproducing equality as follows:

$$u_j = (\mathbf{u}, G_* \boldsymbol{\delta}_j)_A \quad (0 \le j \le 11).$$

Remark. So, G_* is the reproducing kernel on $\mathbb{C}^{12}$.

Proof of Lemma. Since $G_*^* = G_*$ and $E_0 \mathbf{u} = 0$ $(\mathbf{u} \in \mathbb{C}^{12})$, we have

$$(\mathbf{u}, G_* \boldsymbol{\delta}_j)_A = (A\mathbf{u}, G_* \boldsymbol{\delta}_j) = {}^t\boldsymbol{\delta}_j G_* A\mathbf{u} = {}^t\boldsymbol{\delta}_j (I - E_0)\mathbf{u} = {}^t\boldsymbol{\delta}_j \mathbf{u} = u_j.$$

Proof of Theorems. Applying the Schwarz inequality to the reproducing equality, we have

$$| u_j |^2 \le \| \mathbf{u} \|_A^2 \| G_* \boldsymbol{\delta}_j \|_A^2 = \| G_* \boldsymbol{\delta}_j \|_A^2 \, E(\mathbf{u}).$$

Using $E_0 G_* = O$, we have

$$\| G_* \boldsymbol{\delta}_j \|_A^2 = {}^t\boldsymbol{\delta}_j G_* A G_* \boldsymbol{\delta}_j = {}^t\boldsymbol{\delta}_j (I - E_0) G_* \boldsymbol{\delta}_j = {}^t\boldsymbol{\delta}_j G_* \boldsymbol{\delta}_j = C_0.$$

Then we obtain discrete Sobolev inequality:

$$\left(\max_{0 \le j \le 11} | u_j | \right)^2 \le C_0 E(\mathbf{u}).$$

Then, for $\mathbf{u} = G_* \boldsymbol{\delta}_{j_0}$,

$$\left(\max_{0\le j\le 11} |u_j|\right)^2 \le C_0{}^2.$$

$$C_0{}^2 \le ({}^t\boldsymbol{\delta}_j G_* \boldsymbol{\delta}_j)^2 \le \left(\max_{0\le j\le 11} |u_j|\right)^2,$$

Combining it with the trivial inequality

We obtain the conclusion of Theorem 1. Theorem 2 is similarly proved.

3. Discussion and Prospects

Kametaka school says that the high symmetry of R*n* or T*n* allows us to compute the exact expression of the best constant. However, the introduction of our weight does not destroy the computability of this problem because our weighted Laplacian is still symmetric matrix. Whether our model with weight is appropriate or not is another problem. It depends on what kind of problem we want to apply our model to.

And, after this article, the author wish to study the T*n* for n = 6, 8, 12, 20, and application to the interaction of fullerene and another molecules. The high symmetry move us to its beauty however, the destruction of the symmetry also fascinates us.

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