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

Yoshikatsu Sasaki

Department of Mathematics, Hiroshima University, Higashi-Hiroshima, Japan
Email: sasakiyo@hiroshima-u.ac.jp

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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, Rn stands for the regular n-hedron, and Tn 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 Rn [10].

2. Discrete Laplacian and Discrete Sobolev Inequality

2.1. Main Results

Consider the truncated tetrahedron $T_4$. It has 12 vertices, and let us number the vertices 0, 1, ..., 11 as in Figure 1, similar to [12]. Put

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

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 $|u_i - u_j|^2 = u_i^* B_{ij} u_j$. Let us represent each edge of $T_4$ 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 $R_4$, and $e_2$ is the set of edges of $T_4$ created by the truncation. Let us denote $r$ the ratio of the spring constant of each edge of $e_2$ to one of each edge of $e_1$, and introduce 2 kinds of the Sobolev energies as follows:

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

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:

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

Figure 1. Numbering of the vertices of $T_4$. 

Figure 2. Bond matrix.
By use of the weighted Laplacian defined as above, the Sobolev energies are written as follows:

\[ E(u) = u^* A u, \quad E(a, u) = u^* (A + aI) u. \]

The eigenvalues of \( A \) are as follows:

\[
\begin{align*}
0, & \quad 3, & \quad 3, & \quad 2, & \quad 3, & \quad 2, & \quad 3, & \quad \frac{2 + 3r - \sqrt{D}}{2} , & \quad \frac{2 + 3r - \sqrt{D}}{2} , & \quad \frac{2 + 3r + \sqrt{D}}{2} , & \quad \frac{2 + 3r + \sqrt{D}}{2}, \\
\end{align*}
\]

where \( D = 4 - 4r + 9r^2 \). Let us stand \( \lambda_0, \lambda_1, \ldots, \lambda_{11} \) for the eigenvalues of \( A \). Note that \( 0 \) is a simple eigenvalue of \( A \) with the corresponding eigenvector \( 1 = (1, 1, \ldots, 1) \in \mathbb{C}^{12} \), and \( E_0 = \frac{1}{12} 1'1 \) 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

\[ AG_* = G_* A = I - E_0, \quad G_* E_0 = E_0 G_* = 0. \]

\( G_* \) is the Penrose-Moore generalized 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 \( u \in \mathbb{C}^{12} \) such that, for every \( u \in \mathbb{C}^{12} \) satisfying \( 1'u = 0 \), the discrete Sobolev inequality

\[ \left( \max_{l \in \mathcal{J}^{11}} |u_j| \right)^2 \leq CE(u) \]

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

\[ C_0(r) = \frac{1}{12} \sum_{l \in \mathcal{J}^{11}} \frac{1}{\lambda_j} = \frac{52 + 168r + 81r^2}{144r(2 + 3r)}. \]

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

\[ \left( \max_{l \in \mathcal{J}^{11}} |u_j| \right)^2 \leq CE(a, u) \]

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

\[ C_a(r) = \frac{1}{12} \sum_{l \in \mathcal{J}^{11}} \frac{1}{\lambda_j + a} = \frac{1}{12} \left\{ \frac{1}{a} + \frac{2}{a + 3r} + \frac{3}{a + 2 + 3r} + \frac{3(2a + 2 + 3r)}{(3a + 4r) + a(a + 2)} \right\}. \]

**Remark.** \( C_0(r) \) in Theorem 1 coincides 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.
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].

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<thead>
<tr>
<th></th>
<th>R4</th>
<th>R6</th>
<th>R8</th>
<th>R12</th>
<th>R20</th>
</tr>
</thead>
<tbody>
<tr>
<td>The best constant</td>
<td>$3/16 \approx 0.1875$</td>
<td>$29/96 \approx 0.30208$</td>
<td>$13/72 \approx 0.18056$</td>
<td>$137/300 \approx 0.45667$</td>
<td>$7/36 \approx 0.19444$</td>
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<tr>
<th></th>
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<th>T8</th>
<th>T12</th>
<th>T20</th>
</tr>
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<tbody>
<tr>
<td>The best constant</td>
<td>$301/720 \approx 0.41806$</td>
<td>$173/288 \approx 0.60069$</td>
<td>$1019/2016 \approx 0.50546$</td>
<td>$- 239741/376200 \approx 0.63727$</td>
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2.2. Proof

Let $q_j$ be the normalized eigenvectors of $A$, i.e. $Aq_j = \lambda_j q_j$, $q_j^* q_k = \delta_{jk}$, where $\delta_{jk}$ is the Kronecker’s delta. $Q = (q_0, q_1, \ldots, q_{11})$ is unitary. Let $E_t = q_t q_t^*$. Put $\delta_j = '(\delta_{1k}, \ldots, \delta_{11k})$ $(0 \leq k \leq 11)$. We have

$I = QQ^* = \sum_{i \leq k \leq 11} E_i$, $A = QDQ^* = \sum_{i \leq k \leq 11} \lambda_i E_i = \sum_{i \leq k \leq 11} \lambda_i E_i$.

Note that $\sum_{0 \leq j \leq 11} \delta_j E_j \delta_j = \sum_{0 \leq j \leq 11} \delta_j q_j q_j^* \delta_j = q_j q_j^*$ =1. Then, $0 \leq \forall j_0 \leq 11$,

$$C_0 = \sum_{0 \leq j \leq 11} \delta_j E_j \delta_j = \sum_{0 \leq j \leq 11} \delta_j q_j q_j^* \delta_j = q_j q_j^* = 1.$$

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

$$(u, v)_A = (Au, v) = v^* Au, \quad \|u\|_A^2 = (u, u)_A = u^* Au = E(u).$$

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

$$u_j = (u, G \delta_j)_A \quad (0 \leq j \leq 11).$$

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

Proof of Lemma. Since $G_* = G_0$ and $E_0 u = 0$ $(u \in \mathbb{C}^{12})$, we have

$$(u, G \delta_j)_A = (Au, G \delta_j) = \delta_j G A u = \delta_j (I - E_0) u = \delta_j u = u_j.$$
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 $\mathbb{R}^n$ 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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References


