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A Model for HOMO–LUMO Gap and Maximum–Weight Matching*

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Abstract

Let G_1, G_2 be simple, connected, invertible graphs. The bridged graph is constructed from G_1 and G_2 by connecting selected pairs of vertices from G_1 and G_2 via new edges. The HOMO-LUMO gap is the difference between the smallest positive and largest negative eigenvalue of its adjacency matrix. The Kekulé pattern coincides with "perfect matching". In view of the importance of these two indices and the generality of results, we consider the HOMO-LUMO gap on the edge-weighted bridged graph. And in order to control structure, we present the integer program of the maximum-weight matching with vertex weight. Then we give a model of HOMO-LUMO gap and maximum-weight matching with the weight coefficient w. The numerical results are presented.

1 Introduction

Let G be a simple, connected graph of order n with adjacency matrix $A(G)$. The eigenvalues of $A(G)$ are called the spectrum of G, where $\lambda_1 \geq \lambda_2 \geq \cdots \geq \lambda_n$. A graph G is invertible if its adjacency matrix $A(G)$ is invertible ([14, 15]).

The spectrum has been used in the H*ü*kel molecular orbital (HMO) theory. A simple linear relation between HMO π-electron energy and graph eigenvalues was discovered by G*ü*nthard and Primas in the 1950s [4] and rediscovered by Cvetković and one of the

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present authors in the 1970s [2]. The π-electron energy levels E_i, $i = 1, 2, \cdots, n$, meets the relation

$$E_i = \alpha + \beta\lambda_i$$

where α and β are constants and $\beta < 0$, λ_i is an eigenvalue of A (A is the adjacency matrix of the molecular structural graph G). We usually express the energy in so-called β-units, in which case $E_i = \lambda_i$. The HOMO-LUMO gap is the difference between the energy of the highest occupied molecular orbital (HOMO) and the energy of the lowest unoccupied molecular orbital (LUMO). The energy $E_{HOMO} = \lambda_k$ where $k = n/2$ for n even and $k = (n+1)/2$ for n odd. The energy $E_{LUMO} = \lambda_{k+1}$ for n even, and $E_{LUMO} = \lambda_k$ for n odd. The HOMO-LUMO gap is $\Delta_{HL} = \lambda_s^+(A) - \lambda_l^-(A)$, where $\lambda_s^+(A)$ is the smallest positive eigenvalue, and $\lambda_l^-(A)$ is the largest negative eigenvalue of the adjacency matrix A. For bipartite graphs it is always correct, and for a number of non-bipartite graphs it also works.

In recent years, the HOMO-LUMO gap based on the spectrum of graph in mathematical chemistry is researched variously. Zhang et al. ([16, 17]) determined the acyclic molecules with greatest HOMO-LUMO separation and further to ordering them. The HOMO-LUMO gaps for some types of molecules were considered [8]. Bojan Mohar [10] provided rather tight lower and upper bounds on the maximum value of the HOMO-LUMO index among all graphs with given average degree. Soňa Pavlíková and Daniel Ševčovič [11] constructed a mixed integer semidefinite program for maximization of the HOMO-LUMO gap and gave the upper and lower bounds for the HOMO-LUMO spectral gap. Li et al. in [9] obtained the bounds of the HOMO-LUMO index, and they indicated that the HOMO-LUMO gap was responsible to the kinetic stability and reactivity of conjugated molecules. Especially, if $\Delta_{HL} = 0$, then the underlying π-electron system is predicted to be extremely reactive and is usually not capable of existence. So we hope the HOMO-LUMO gap is as large as possible.

A Kekulé pattern is a chemical notion which coincides with "perfect matching" in graph theory. The history of Kekulé pattern began in 1865, when August Kekulé invented the structural formula of benzene [13]. Peter John and Horst Sachs [5] described algorithms for calculating the number of Kekulé structures. Wenchen He and Wenjie He [5] gave a review of the Peak-Valley path method which was one of important approaches for investigating Kekulé structures of benzenoid hydrocarbons. The Kekulé pattern is

important for the stability of aromatic system [12].

In view of the importance of the HOMO-LUMO gap and Kekulé pattern, we try to consider them simultaneously. In chemistry, the bond orders are considered as the edge weights of the corresponding graph. So we consider HOMO-LUMO gaps for edge-weighted graphs. And for more general results, we pay attention to the maximum-weight matching, not perfect matching. In order to study how to connect two molecules to get the stability structure, we consider the bridged graph which is constructed from two disjoint invertible graphs by bridging one's vertices to the other's through a bipartite graph.

In this paper, we first give the semidefinite program of the HOMO-LUMO gap and the integer program of maximum-weight matching. Then we give the representation of bridged graphs. Next, we give the semidefinite program of the HOMO-LUMO gap on the edge-weighted bridged graph. And in order to control structure, we consider the integer program of the maximum-weight matching with vertex weight. Then we present a model considering them at the same time. We provide the weight coefficient w, which makes a balance between the HOMO-LUMO gap and maximum-weight matching. At last, we consider three optimizations, and give the numerical results. They show the optimization of HOMO-LUMO gap, the relation between the maximum-weight matching and vertex weight, and show how to make a balance using w, respectively.

2 Semidefinite program of the HOMO-LUMO gap and integer program of maximum-weight matching (MWM)

In this section, suppose the graph G is invertible. The HOMO-LUMO gap is $\Delta_{HL} = \lambda_s^+(A) - \lambda_l^-(A)$, where $\lambda_s^+(A)$ is the smallest positive eigenvalue, and $\lambda_l^-(A)$ is the largest negative eigenvalue of the adjacency matrix A. Then we can obtain([11]):

$$\lambda_s^+(A) = \frac{1}{\lambda_{max}(A^{-1})}, \quad \lambda_l^-(A) = \frac{1}{\lambda_{min}(A^{-1})}$$

where $\lambda_{max}(A^{-1}) > 0$ and $\lambda_{min}(A^{-1}) = -\lambda_{max}(-A^{-1}) < 0$ are the maximum and minimum eigenvalues of the inverse matrix A^{-1}, respectively. We use $\leq$ to denote the *Löwner* partial ordering on symmetric matrices. It means $A \leq B$ iff the matrix $B - A$ is positive semidefinite, that is $B - A \geq 0$. Following [1], [3], the maximal and minimal

eigenvalues of A^{-1} can be expressed as follows:

$$0 < \lambda_{max}(A^{-1}) = \min_{A^{-1} \leq tI} t, \qquad 0 > \lambda_{min}(A^{-1}) = \max_{sI \leq A^{-1}} s$$

Let $\mu = 1/t$, $\eta = -1/s$, then we can get the following equations:

$$\lambda_s^+(A) = \max_{\mu A^{-1} \leq I} \mu, \qquad \lambda_l^-(A) = -\max_{-\eta A^{-1} \leq I} \eta$$

So we get the semidefinite program of the HOMO-LUMO gap for a invertible graph G as follows:

$$\begin{aligned} \Delta_{HL}(A) = \max_{\mu,\eta \geq 0} \ & \mu + \eta \\ s.t. \ & \mu A^{-1} \leq I \\ & -\eta A^{-1} \leq I \end{aligned}$$

The maximum-weight matching is the matching which has maximum weight. The integer program of maximum weight matching (MWM) is:

$$\begin{aligned} \max \ & \sum_{e \in E(G)} c_e x_e \\ s.t. \ & \sum_{v \in e} x_e \leq 1 \quad \forall v \in V(G) \\ & x_e \in \{0,1\} \quad \forall e \in E(G) \end{aligned}$$

where c_e is the weight of the edge e, x_e denotes whether to take the edge e as a matching edge (If $x_e = 1$, it is chosen as a matching edge; If $x_e = 0$, it is not). $V(G)$ ($E(G)$) is the set of vertices (edges) of graph G.

3 Representation of bridged graphs

Let G_1, G_2 be simple, undirected, invertible graphs with n_1, n_2 vertices, respectively. A bridged graph G_B is constructed from disjoint invertible graphs G_1 and G_2 by connecting selected pairs of vertices from G_1 and G_2 via new edges. G_k is the bipartite graph $G(V(G_1), V(G_2))$ with the new edges. The adjacency matrix A_k of G_k is as follows:

$$A_k = \begin{pmatrix} 0 & K \\ K^T & 0 \end{pmatrix}$$

where K is an $n_1 \times n_2$ binary matrix.

Now we consider the edge-weighted invertible graphs G_1, G_2 whose edge-weighted adjacency matrices are A_1, A_2, respectively. The corresponding binary adjacency matrices are $\overline{A_1}$ and $\overline{A_2}$. For the edge-weighted bridged graph G_B, the edge-weighted adjacency matrix A_B of G_B is:

$$A_B = \begin{pmatrix} A_1 & K \\ K^T & A_2 \end{pmatrix}$$

where A_1, A_2 are both symmetric invertible matrices.

Then the corresponding binary adjacency matrix $\overline{A_B}$ of G_B is:

$$\overline{A_B} = \begin{pmatrix} \overline{A_1} & K \\ K^T & \overline{A_2} \end{pmatrix}$$

According to [11], if G_1, G_2 are invertible graphs, then the graph G_B is invertible iff $S = A_1 - KA_2^{-1}K^T$ (the Schur complement) is invertible. In this case, we get

$$A_B^{-1} = \begin{pmatrix} A_1 & K \\ K^T & A_2 \end{pmatrix}^{-1} = \begin{pmatrix} S^{-1} & -S^{-1}KA_2^{-1} \\ -A_2^{-1}K^TS^{-1} & A_2^{-1} + A_2^{-1}K^TS^{-1}KA_2^{-1} \end{pmatrix} = Q^T \begin{pmatrix} S^{-1} & 0 \\ 0 & A_2^{-1} \end{pmatrix} Q$$

where Q is an invertible matrix with the inverse $Z = Q^{-1}$ given by:

$$Q = \begin{pmatrix} I & -KA_2^{-1} \\ 0 & I \end{pmatrix}, \quad Z = \begin{pmatrix} I & KA_2^{-1} \\ 0 & I \end{pmatrix}$$

4 A model for HOMO-LUMO gap and MWM

In this section, we propose a model of HOMO-LUMO gap and MWM. We consider the semidefinite program of HOMO-LUMO gap on the edge-weighted bridged graph G_B first. For $\mu \geq 0$, we have $\mu A_B^{-1} \leq I$ iff $\mu Z^T A_B^{-1} Z \leq Z^T Z$, which means

$$\mu \begin{pmatrix} S^{-1} & 0 \\ 0 & A_2^{-1} \end{pmatrix} \leq Z^T Z = \begin{pmatrix} I & KA_2^{-1} \\ A_2^{-1}K^T & I + A_2^{-1}K^TKA_2^{-1} \end{pmatrix}$$

We can do a similar operation for $-\eta A^{-1} \leq I$. Considering that the bipartite graph G_k is not empty, we obtain the constraint $\sum_{i,j} K_{ij} \geq 1$. So we get the semidefinite program of the HOMO-LUMO gap as follows:

$$\max_{\mu,\eta \geq 0, K} \ \mu+\eta$$

$$s.t. \quad \begin{pmatrix} I - \mu S^{-1} & KA_2^{-1} \\ A_2^{-1}K^T & I - \mu A_2^{-1} + A_2^{-1}K^TKA_2^{-1} \end{pmatrix} \geq 0 \tag{4.1}$$

$$\begin{pmatrix} I + \eta S^{-1} & KA_2^{-1} \\ A_2^{-1}K^T & I + \eta A_2^{-1} + A_2^{-1}K^TKA_2^{-1} \end{pmatrix} \geq 0 \tag{4.2}$$

$$S = A_1 - KA_2^{-1}K^T \tag{4.3}$$

$$K_{ij} \in \{0,1\}, \quad \forall i \in [n_1], j \in [n_2] \tag{4.4}$$

$$\sum_{i,j} K_{ij} \geq 1, \quad \forall i \in [n_1], j \in [n_2] \tag{4.5}$$

In chemistry, since sometimes we need some structure to appear, we consider the vertex weight. Since the vertex weight has some influence on the real meaning of HOMO-LUMO gap, we only consider it for maximum-weight matching to control the structure. Assume that the vertex-weighted matrices of G_1, G_2 are W_1, W_2, respectively. They are diagonal matrices where every element is the weight of vertex.

Now, we consider the integer program of MWM on the vertex-weighted graph G_B. Let $\overline{X} = \{\overline{X}_{ij}\}_{(n_1+n_2)\times(n_1+n_2)}$ be the matching matrix, where $\overline{X}_{ij} \in \{0,1\}$ (if $\overline{X}_{ij} = 1$, it means we choose edge e_{ij} as a matching edge; if $\overline{X}_{ij} = 0$, it is not chosen). Obviously, it is a symmetric matrix, $\overline{X}_{ij} = \overline{X}_{ji}$. So the vertex-weighted matching matrix X is:

$$X = W\overline{X}W, \quad W = \begin{pmatrix} W_1 & 0 \\ 0 & W_2 \end{pmatrix}$$

where W is the vertex-weighted matrix of G_B. Then we obtain the integer program of MWM on the vertex-weighted graph G_B:

$$\max_X \ \frac{1}{2}\sum_{i,j} X_{ij}$$

$$s.t. \quad X = W\overline{X}W \tag{4.6}$$

$$\sum_j \overline{X}_{ij} \leq 1, \quad \forall i \in [n_1 + n_2] \tag{4.7}$$

$$\overline{X}_{ij} = \{0,1\}, \quad \forall i,j \in [n_1 + n_2] \tag{4.8}$$

$$\overline{X}_{ij} = \overline{X}_{ji}, \quad \forall i,j \in [n_1 + n_2] \tag{4.9}$$

In view of the matching edges being included in the existing edges, so we need to add a constraint. Let $\overline{A_B} = \{\overline{A^B}_{ij}\}_{(n_1+n_2)\times(n_1+n_2)}$ be the binary adjacency matrix of G_B. We have

$$\overline{A_B} = \begin{pmatrix} \overline{A_1} & K \\ K^T & \overline{A_2} \end{pmatrix}$$

Then we can get the constraint:

$$\overline{X}_{ij} \leq \overline{A^B}_{ij}, \quad \forall i,j \in [n_1 + n_2] \tag{4.10}$$

Based on the importance of HOMO-LUMO gap and Kekulé pattern, and in order to get more general results, so we consider the HOMO-LUMO gap and MWM simultaneously. The optimization model is:

$$\max_{\mu,\eta\geq 0,K,X} \ \mu+\eta+w\cdot\frac{1}{2}\sum_{i,j}X_{ij}$$

with constraints (4.1)−(4.10), where w is the weight coefficient to make a balance between the HOMO-LUMO gap and MWM.

In order to compute fast, we need to make some changes and relaxations. Because the matrices K^TK and $S=A_1-KA_2^{-1}K^T$ exist, the constraints (4.1), (4.2) are nonconvex.

We use a new variable C, where $C=K^TK$. We notice $K_{ij}=\{0,1\}$ is equivalent to $K_{ij}(1-K_{ij})=0$, i.e. $K_{ij}=K_{ij}^2$. We can get

$$C_{jj}=\sum_i K_{ij}^2=\sum_i K_{ij} \tag{4.11}$$

The nonconvex constraint $C=K^TK$ can be relaxed by a convex matrix inequality constraint $C\geq K^TK$. Notice that the inequality constraint with (4.11) is tight: Assume $L=C-K^TK$, then $L\geq 0$. We know $L_{jj}=C_{jj}-\sum_i K_{ij}=0$. It means $diag(L)=0$. So we can get $L=0$ and $C=K^TK$. According to the Schur complement theorem [7], the inequality constraint can be rewritten as follows:

$$\begin{pmatrix} C & K^T \\ K & I \end{pmatrix}\geq 0$$

where I is an $n_1\times n_1$ identity matrix.

According to [11], let G be an undirected vertex-labeled graph on m vertices with an invertible adjacency matrix A. G is arbitrarily bridgeable over the first $\{1,\cdots,k_A\}$ vertices of G if the $k_A\times k_A$ upper principal sub-matrix is a null matrix, i.e. $(A^{-1})_{ij}=0$ for all $i,j=[k_A]$. So we assume G_2 is arbitrarily bridgeable, then if the $n_1\times n_2$ matrix K satisfies: $K_{ij}=0$ for $j=k_{A_2}+1,\cdots,n_2$, we have $KA_2^{-1}K^T=0$, i.e. $S=A_1$. Based on it, constraints (4.1), (4.2) are as follows:

$$\begin{pmatrix} I-\mu A_1^{-1} & KA_2^{-1} \\ A_2^{-1}K^T & I-\mu A_2^{-1}+A_2^{-1}CA_2^{-1} \end{pmatrix}\geq 0$$

$$\begin{pmatrix} I+\eta A_1^{-1} & KA_2^{-1} \\ A_2^{-1}K^T & I+\eta A_2^{-1}+A_2^{-1}CA_2^{-1} \end{pmatrix}\geq 0$$

So we can obtain the optimization model of the HOMO-LUMO gap and MWM with linear matrix constraints and integer constraints:

$$\max_{\mu,\eta\geq 0,K,C,X} \ \mu+\eta+w\cdot\frac{1}{2}\sum_{i,j}X_{ij}$$

$$s.t. \quad \begin{pmatrix} I-\mu A_1^{-1} & KA_2^{-1} \\ A_2^{-1}K^T & I-\mu A_2^{-1}+A_2^{-1}CA_2^{-1} \end{pmatrix} \geq 0 \tag{4.12}$$

$$\begin{pmatrix} I+\eta A_1^{-1} & KA_2^{-1} \\ A_2^{-1}K^T & I+\eta A_2^{-1}+A_2^{-1}CA_2^{-1} \end{pmatrix} \geq 0 \tag{4.13}$$

$$\begin{pmatrix} C & K^T \\ K & I \end{pmatrix} \geq 0 \tag{4.14}$$

$$C_{jj}=\sum_i K_{ij} \tag{4.15}$$

$$K_{ij}=0, \quad \forall i\in[n_1], j\in\{k_{A_2}+1,\cdots,n_2\} \tag{4.16}$$

$$K_{ij}\in\{0,1\}, \quad \forall i\in[n_1], j\in[n_2] \tag{4.17}$$

$$\sum_{i,j}K_{ij}\geq 1, \quad \forall i\in[n_1], j\in[n_2] \tag{4.18}$$

$$\sum_j \overline{X}_{ij}\leq 1, \quad \forall i\in[n_1+n_2] \tag{4.19}$$

$$\overline{X}_{ij}=\{0,1\}, \quad \forall i,j\in[n_1+n_2] \tag{4.20}$$

$$\overline{X}_{ij}=\overline{X}_{ji}, \quad \forall i,j\in[n_1+n_2] \tag{4.21}$$

$$X=W\overline{X}W \tag{4.22}$$

$$\overline{A_B}=\begin{pmatrix} \overline{A_1} & K \\ K^T & \overline{A_2} \end{pmatrix} \tag{4.23}$$

$$\overline{X}_{ij}\leq \overline{A^B}_{ij}, \quad \forall i,j\in[n_1+n_2] \tag{4.24}$$

5 Numerical results

In this section, to illustrate the applicability of the proposed model, we consider three cases: optimization of HOMO-LUMO gap, optimization of MWM, comprehensive optimization of HOMO-LUMO gap and MWM. Some examples have been solved using SeDumi solver within the Yalmip MATLAB. In view of organic molecules, carbon is very important. So in this section, we consider the max degree. We denote max degree by d. We add the constraint: $\sum_j \overline{A^B}_{ij} \leq d, \ \forall i\in[n_1+n_2]$, where $d=3$. When we

consider the optimization of MWM, comprehensive optimization of HOMO-LUMO gap and MWM, in order to get matching edges as much as possible, we add the constraint: $\frac{1}{2}\sum_{i,j}\overline{X}_{ij} \geq \frac{n+m-1}{2}$.

5.1 Optimization of HOMO–LUMO gap

Let the weight coefficient $w = 0$. We get the objective function $\max\limits_{\mu,\eta\geq 0,K,C}\ \mu+\eta$ with constraints $(4.12)-(4.18)$. G_1 and G_2 are depicted in Figure 1: (a). Then G_2 is arbitrarily bridgeable on $\{V_1\},\{V_2\},\{V_3\},\{V_4\},\{V_5\},\{V_1,V_3\},\{V_2,V_3\}\cdots$ We obtain the results with the bridging vertices $\{V_1,V_3\}$ (simply, {1,3}) of G_2 in Figure 2: (a). From the figure, the bridging way is $G_2:3\to G_1:5$. The maximum HOMO-LUMO gap is 0.631749.

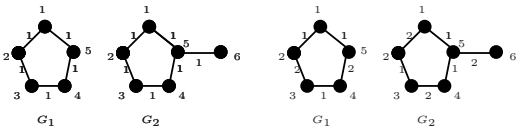


Figure 1. the edge-weighted invertible graphs G_1, G_2

As shown in Figure 1: (b), let the edge weights of G_1, G_2 be $\{1,2,1,2,1\}$ and $\{2,1,2,1,1,2\}$, respectively. Then the results with the bridging vertices $\{1,3\}$ are shown in Figure 2: (b). The bridging way is $G_2:1\to G_1:1$, $G_2:3\to G_1:3$. The maximum HOMO-LUMO gap is 1.455941.

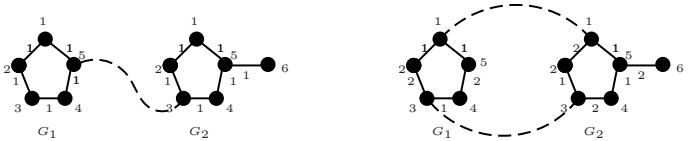
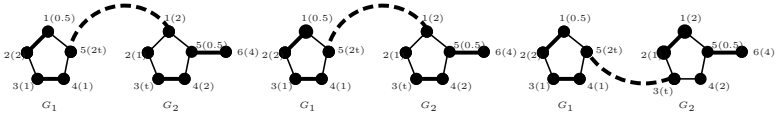


Figure 2. the results of optimal bridging way and HOMO-LUMO gap (HL)

5.2 Optimization of MWM

We use vertex weight to control the matching structure and ensure some structure appear. So we consider the relation between the maximum-weight matching and vertex weight. We consider the objective function $\max\limits_{X}\ \frac{1}{2}\sum\limits_{i,j}X_{ij}$ with constraints $(4.16)-(4.24)$. Assume that the vertex-weighted matrices W_1, W_2 of G_1 and G_2 are $diag(0.5,2,1,1,2)$ and

$diag(2, 1, 1, 2, 0.5, 4)$, respectively. We choose the bridging vertices $\{1, 3\}$. From Figure 3: (a), we can see that the bridging way is $G_2 : 1 \to G_1 : 5$. The matching edges are denoted by thick lines. There may be no edge between $G_2 : 3$ and $G_1 : 5$, although the bridging way is not unique. In order to ensure that the structure appears, we consider to add the vertex weights of $G_2 : 3$ and $G_1 : 5$. We denote the multiple by t. It means the weights of $G_2 : 3$ and $G_1 : 5$ are t, $2t$, respectively. Then we get the results in Figure 3: (b), (c). When $t = \{3, 4, 5 \cdots\}$, the optimal bridging way is $G_2 : 3 \to G_1 : 5$. In fact, when t is around 2.7, it arrives the threshold to ensure that the edge between $G_2 : 3$ and $G_1 : 5$ appears.



(a) $t = \{1\}$ (b) $t = \{2\}$ (c) $t = \{3, 4, 5 \cdots\}$

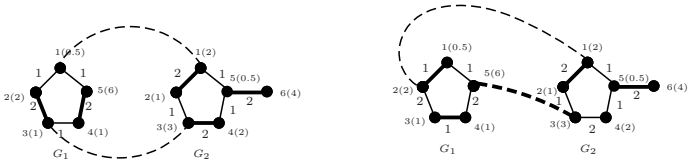
Figure 3. the relation between MWM and vertex weight

5.3 Comprehensive optimization of HOMO-LUMO gap and MWM

Now we consider the comprehensive optimization of HOMO-LUMO gap and MWM. Let G_1, G_2 be the edge-weighted graphs as shown in Figure 1: (b) with $W_1 = diag(0.5, 2, 1, 1, 6)$ and $W_2 = diag(2, 1, 3, 2, 0.5, 4)$. Then we compute the optimal value with bridging vertices $\{1, 3\}$ and different weight coefficient w.

Table 1 shows the computational results with weight coefficient, optimal value, HOMO–LUMO gap, w·MWM (MWM), bridging way and matching way. From it, we can see that the bridging way and matching way change as w increases. As shown in Figure 4, the dashed lines are the bridging ways and the thick lines are matching edges. Obviously, when w is small, the optimal value depends on the HOMO-LUMO gap. So the matching is not maximum. When w is large, the matching is more important, so the bridging way changes and the HOMO-LUMO gap is not optimal. Specially, $w = 0.008$ is the threshold value of w. In addition, if w is large enough, there is always the bridging way: $G_2 : 3 \to G_1 : 5$.

But for G_1, G_2 with $W_1 = diag(0.5, 2, 1, 1, 2)$ and $W_2 = diag(2, 1, 1, 2, 0.5, 4)$, the optimal bridging way does not change any more. As shown in Figure 5, the HOMO-



(a) $0 \leq w < 0.008$ (b) $w \geq 0.008$

Figure 4. the results of different weight coefficient w with $W_1 = diag(0.5, 2, 1, 1, 6)$ and $W_2 = diag(2, 1, 3, 2, 0.5, 4)$

LUMO gap and MWM can be maximum simultaneously. The optimal bridging way is independent of w. And $G_1 : 5$ is not connected by $G_2 : 3$.

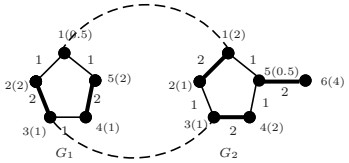


Figure 5. the results of different weight coefficient w with $W_1 = diag(0.5, 2, 1, 1, 2)$ and $W_2 = diag(2, 1, 1, 2, 0.5, 4)$

In a word, w makes a balance between the HOMO-LUMO gap and MWM. When w is small enough, the HOMO-LUMO gap is more important, so the bridging way will make it as large as possible. When w is large enough, the bridging way will get the maximum-weight matching. If there is a bridging way to make the HOMO-LUMO gap and MWM maximum at the same time, then w can not influence it. We also provide a way by changing vertex weight to control the structure.

Table 1. the computational results with various weight coefficient w

weight coefficient	optimal value	HOMO-LUMO gap	$w \cdot MWM$(MWM)	bridging way:$G_2 \to G_1$	matching way
0.004	1.527941	1.4559	0.072(18)	$1 \to 1; 3 \to 3$	$G_1 : 2-3, 4-5; G_2 : 1-2, 3-4, 5-6$
0.006	1.563941	1.4559	0.108(18)	$1 \to 1; 3 \to 3$	$G_1 : 2-3, 4-5; G_2 : 1-2, 3-4, 5-6$
0.008	1.609365	1.4174	0.192(24)	$1 \to 2; 3 \to 5$	$G_1 : 1-2, 3-4; G_2 : 1-2, 5-6; G_1 : 5-G_2 : 3$
0.02	1.897365	1.4174	0.48(24)	$1 \to 2; 3 \to 5$	$G_1 : 1-2, 3-4; G_2 : 1-2, 5-6; G_1 : 5-G_2 : 3$
0.05	2.617365	1.4174	1.2(24)	$1 \to 2; 3 \to 5$	$G_1 : 1-2, 3-4; G_2 : 1-2, 5-6; G_1 : 5-G_2 : 3$
0.1	3.817365	1.4174	2.4(24)	$1 \to 2; 3 \to 5$	$G_1 : 1-2, 3-4; G_2 : 1-2, 5-6; G_1 : 5-G_2 : 3$
0.2	6.217365	1.4174	4.8(24)	$1 \to 2; 3 \to 5$	$G_1 : 1-2, 3-4; G_2 : 1-2, 5-6; G_1 : 5-G_2 : 3$

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