Programming to generate geminal configurations

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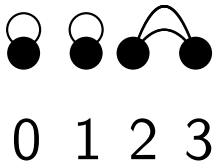
Introduction

- Others make geminal configurations by hand, and they are not totally confident about getting all the cases.
- I made a computer program (using Python) to generate configurations, and check if the results archieved by hand is sufficient.
- In this presentation, I use the following geminal configuration to illustrate the algorithm. Then, I give the results for the other geminal configurations, when the number of nodes are higher.

Representation of curved edges

1. Represent the curves of configuration by a sequence:
   - Example: The graph of



   is represented as the list of:

$$[(0,0),(1,1),(2,3),(2,3)]$$

2. Represent the operation of switching nodes by the permutation (0,1,2,3).
   - Example: Switch 0 to 1 is presented as the list (1,0,2,3), switch 0 to 2 and 1 to 3 is presented as the list (2,3,0,1)
3. Apply an operation to a configuration is illustrated by this example:
   - Operation: g=(2,3,0,1)
   - Configuration: a=[(0,1),(0,2),(1,3),(2,3)]
   - g(a)=[(2,3),(2,0),(3,1),(0,1)]
   - Note that g(a), and a are duplicated configuration

Symbolic Representation of Determinant

1. The determinant of the matrix is represented symbolically:
   - Determinant of a 2×2 matrix:

$$\begin{vmatrix} a & b \\ c & d \end{vmatrix} \rightarrow [(a, d), (b, c)]$$

   - Determinant of a 3×3 matrix:

$$\begin{vmatrix} a & b & c \\ x & y & z \\ m & n & p \end{vmatrix} \rightarrow$$

$$\rightarrow [(a, y, p), (a, z, n), (x, b, p), (x, c, n), (m, b, z), (m, c, y)]$$

2. *Note*:
   - If the matrix is $n \times n$ then the determinant is the list of n! elements
   - The element's signs are all neglected

Algorithm Outline

The algorithm basically has three main steps

- Step 1-Generate the configurations of curved edges.
- Step 2-Generate the symmetry groups.
- Step 3-Remove duplicates configuration of curved edge using the symmetry groups.

Algorithms: Step 1-Generate the configurations of curved edges

1. Construct all the configurations of curved edges by compute symbolically the determinant of the matrix:

$$M = \begin{bmatrix} (0,0) & (0,1) & (0,2) & (0,3) \\ (1,0) & (1,1) & (1,2) & (1,3) \\ (2,0) & (2,1) & (2,2) & (2,3) \\ (3,0) & (3,1) & (3,2) & (3,3) \end{bmatrix}$$

2. Order all the determinant's elements. Rules of ordering are as follows:
   - (a_i, a_j) has $a_i < a_j$
   - $[(a_{00}, a_{01}), (a_{10}, a_{11}), (a_{20}, a_{21}) ...]$ has $a_{00} < a_{10} < a_{20} < ...$
3. Delete the same elements received after ordering.

Algorithms: Step 1-Result

- There are 17 configurations of curved edges in the case 4 dots:

$$
\begin{aligned}
A = [&((0,0),(1,1),(2,2),(3,3)),((0,1),(0,1),(2,3),(2,3)),\\
&((0,1),(0,1),(2,2),(3,3)),((0,1),(0,2),(1,3),(2,3)),\\
&((0,2),(0,3),(1,2),(1,3)),((0,0),(1,2),(1,3),(2,3)),\\
&((0,3),(0,3),(1,1),(2,2)),((0,0),(1,1),(2,3),(2,3)),\\
&((0,0),(1,3),(1,3),(2,2)),((0,0),(1,2),(1,2),(3,3)),\\
&((0,2),(0,2),(1,1),(3,3)),((0,1),(0,2),(1,2),(3,3)),\\
&((0,1),(0,3),(1,2),(2,3)),((0,3),(0,3),(1,2),(1,2)),\\
&((0,1),(0,3),(1,3),(2,2)),((0,2),(0,2),(1,3),(1,3)),\\
&((0,2),(0,3),(1,1),(2,3))]
\end{aligned}
$$

Algorithms: Step 2-Generate the symmetry groups

We will consider the case:

1. Establish the list G_0 of the generators:

   $$G_0 = [g_0, g_1, g_2, g_3] = [(0,1,2,3),(1,0,2,3),(0,1,3,2),(2,3,0,1)]$$

2. Create matrix G_1 from the list G_0:

g_0g_0	g_0g_1	g_0g_2	g_0g_3
g_1g_0	g_1g_1	g_1g_2	g_1g_3
g_2g_0	g_2g_1	g_2g_2	g_2g_3
g_3g_0	g_3g_1	g_3g_2	g_3g_3

3. Remove the duplicates from elements of matrix G_1 to establish the list G_1: $G_1 = [g_{10}, g_{11}, .., g_{1k}]$
4. In the similar procedure, create the list G_2 from the list G_1
5. Keep generating G_3, G_4.. until the length of G_n is equal to the length of G_{n+1}, at this point we have generated the whole groups.

Algorithms: Step 2-Result

- There are 8 group elements in this case:

$$
\begin{aligned}
G = [&(1,0,3,2),(2,3,0,1),\\
&(3,2,0,1),(3,2,1,0),\\
&(0,1,2,3),(1,0,2,3),\\
&(0,1,3,2),(2,3,1,0)]
\end{aligned}
$$

Algorithms: Step 3-Remove duplicates configurations of curved edge using the symmetry groups

1. Apply G[0] to A[0] to get G[0](A[0])
2. Reorder (using the rules already mentioned) G[0](A[0]) to get K
3. Check K with all A[i]:
   - If K=A[i], delete A[i]
   - If K $\neq$ A[i], keep A[i]
4. Redo the above steps with G[1], G[2],...
5. Put A[0] into F (empty list)
6. Put the remaining A[i] into A_1
7. Redo the previous procedure with A_1
8. Keep doing this procedure until the list A_k is empty
9. F is the list that contains all the distinct configurations.

Algorithms: Step 3-Result

- There are 8 distinct configurations in the case of 4 dots

- This result is the same as the result calculated by hand

$$
\begin{aligned}
F = [&((0,0),(1,1),(2,2),(3,3)),\\
&((0,1),(0,1),(2,3),(2,3)),\\
&((0,1),(0,1),(2,2),(3,3)),\\
&((0,1),(0,2),(1,3),(2,3)),\\
&((0,2),(0,3),(1,2),(1,3)),\\
&((0,0),(1,2),(1,3),(2,3)),\\
&((0,3),(0,3),(1,1),(2,2)),\\
&((0,3),(0,3),(1,2),(1,2))]
\end{aligned}
$$

Result for case of 5 nodes 

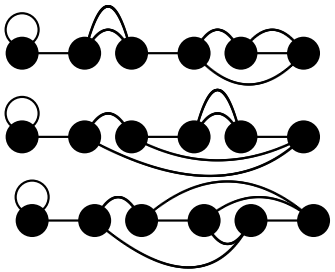
- In case of:

- By hand, they found 20 configurations.
- By computer, I have 21 configurations.
- After coordinating with Dhinali, I found that they missed this one:

Result for case of 6 nodes 

- In the case:

- By hand, they found 32 configurations; however 2 of them are duplicates. By computer, I found 33 ones.
- The 3 new ones I found are:



Computers beat humans!

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Conclusion

- Generating by hand missed some configurations, especially when the number of nodes increase.
- Symmetry groups are useful in finding the duplicates.
- So far, I have done 3 cases. There are still other cases to do.
- Finally, I wish to express my gratitude to Dr Martin J. Mohlenkamp for providing the idea for the algorithm, and helping me while I write the program.