Computing 1152 cases?
You better use a computer!

Son Nguyen

under the guide of Dr. Martin Mohlenkamp
Ohio University, Mathematics Department

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We need to compute integrals that include terms like:
\[
\sum_{a \neq b} w_1(|\gamma_a - \gamma_b|) \sum_{m \neq n} w_1(|\gamma_m - \gamma_n|) \sum_{u \neq v} w_1(|\gamma_u - \gamma_v|)
\]
Depending whether \(a, b, m, n, u, v\) are distinct or overlap, we have overall 1154 cases to compute.
When all indices are distinct we have the following case, which also serve as the general expression:
\[
\sum \sum \sum \int \int \int \int \int \\
\sum_{a,b} w_1(|\gamma_a - \gamma_b|) w_2(|\gamma_m - \gamma_n|) w_3(|\gamma_u - \gamma_v|) \\
\phi_a(\gamma_a) \phi_b(\gamma_b) \phi_m(\gamma_m) \phi_n(\gamma_n) \phi_u(\gamma_u) \phi_v(\gamma_v) \Delta \\
d\gamma_a d\gamma_b d\gamma_m d\gamma_n d\gamma_u d\gamma_v
\]
Where $\Delta$ is:

$$
\begin{array}{cccccccc}
\theta_a(\gamma_a) & \theta_a(\gamma_b) & \theta_a(\gamma_m) & \theta_a(\gamma_n) & \theta_a(\gamma_u) & \theta_a(\gamma_v) \\
\theta_b(\gamma_a) & \theta_b(\gamma_b) & \theta_b(\gamma_m) & \theta_b(\gamma_n) & \theta_b(\gamma_u) & \theta_b(\gamma_v) \\
\theta_m(\gamma_a) & \theta_m(\gamma_b) & \theta_m(\gamma_m) & \theta_m(\gamma_n) & \theta_m(\gamma_u) & \theta_m(\gamma_v) \\
\theta_n(\gamma_a) & \theta_n(\gamma_b) & \theta_n(\gamma_m) & \theta_n(\gamma_n) & \theta_n(\gamma_u) & \theta_n(\gamma_v) \\
\theta_u(\gamma_a) & \theta_u(\gamma_b) & \theta_u(\gamma_m) & \theta_u(\gamma_n) & \theta_u(\gamma_u) & \theta_u(\gamma_v) \\
\theta_v(\gamma_a) & \theta_v(\gamma_b) & \theta_v(\gamma_m) & \theta_v(\gamma_n) & \theta_v(\gamma_u) & \theta_v(\gamma_v) \\
\end{array}
$$

Although the analysis can be done by hand, to actually implement these formulas requires automatic generation of all the cases.  
→ **It is hard to do by hand!**
So how to compute those things?

1. Generate all the cases, which is called by geminal, that (*) can take by comparing the values of indices, then group them by their similarity. This is done using Algorithm 1.

2. For each geminal: Expand the determinant Δ, and group them by their similarity. This task is done using Algorithm 2.

3. The next step is to apply reductions to the resulting cases. This is a work in progress. See the other poster.

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Notations

1. Geminals are presented by list of pair. E.g: \((0, 1), (1, 2), (2, 3)\) means:

\[
\sum a \sum b \sum n \int \int \int w_1(\gamma_a - \gamma_b) w_2(\gamma_a - \gamma_n) 3(\gamma_b - \gamma_n) \phi_a(\gamma_a) \phi_b(\gamma_b) \phi_n(\gamma_n)
\]

\[
\begin{vmatrix}
\theta_a(\gamma_a) & \theta_a(\gamma_b) & \theta_a(\gamma_n) \\
\theta_b(\gamma_a) & \theta_b(\gamma_b) & \theta_b(\gamma_n) \\
\theta_n(\gamma_a) & \theta_n(\gamma_b) & \theta_n(\gamma_n)
\end{vmatrix} d\gamma_a d\gamma_b d\gamma_n
\]

2. crea(x): Return a list containing \(x\) and the length of \(x\) plus 1.

\( [0, 1] \rightarrow [0, 1, 2] \)

3. detg(x): Return a list contains all elements of the determinant of \(x\).

\[
\begin{bmatrix}
a & b \\
c & d
\end{bmatrix} \rightarrow [(a, d, 1), (b, c, -1)],
\]

4. order1(x): Order \(x\) by the first number in its elements.

\([(0, 1), (2, 3), (1, 2)] \rightarrow [(0, 1), (1, 2), (2, 3)]\)
Notations

1. **order2(x):** Order each elements in x.
   \[ [(0, 1), (3, 2), (2, 1)] \rightarrow [(0,1), (2,3), (1,2)] \]

2. **Grouping duplicate:** If \( \alpha = [(0, 1), (1, 2), (2, 1), 3] \), and \( \beta = [(0, 1), (1, 2), (1, 2), 4] \), and \( \alpha, \beta \) are duplicates, then grouping \( \alpha \) and \( \beta \) means replacing \( \alpha \) and \( \beta \) by \( \gamma = [(0, 1), (1, 2), (2, 1), 7] \)

3. **Corresponding Matrix:** Let \( \alpha \) be \( [(0, 1), (1, 2), (2, 1), 3] \). The corresponding matrix of \( \alpha \) is:

\[
\begin{bmatrix}
(0,0) & (0,1) & (0,2) \\
(1,0) & (1,1) & (1,2) \\
(2,0) & (2,1) & (2,2)
\end{bmatrix}
\]
Algorithm 1

Step 1: Generate all elements in form of \([(0, 1), (m, n), (u, v)]\) that satisfies:
- \(m = crea(0, 1)\);
- \(n = crea(0, 1, m)\);
- \(u = crea(0, 1, m, n)\);
- \(v = crea(0, 1, m, n, u)\);
- \(m \neq n; u \neq v\)

Step 2: Order the output in step 1 by function \(order2\), and group duplicates.

Step 3: Interchange \(0 \leftrightarrow 1\), and apply function \(order2\) to the output in step 2 to group duplicates.

Step 4: Interchange \(2 \leftrightarrow 3\) and then apply function \(order2\) for elements that contains 2, 3 in the output of step 3 to group duplicates.
There are 16 geminals:

1. $(0, 1), (2, 3), (0, 3), 8$
2. $(0, 1), (2, 3), (2, 4), 4$
3. $(0, 1), (0, 2), (1, 3), 8$
4. $(0, 1), (0, 1), (2, 3), 2$
5. $(0, 1), (2, 3), (2, 3), 2$
6. $(0, 1), (0, 2), (0, 1), 8$
7. $(0, 1), (0, 1), (1, 2), 8$
8. $(0, 1), (2, 3), (0, 4), 4$
9. $(0, 1), (1, 2), (0, 2), 8$
10. $(0, 1), (1, 2), (1, 3), 8$
11. $(0, 1), (1, 2), (3, 4), 4$
12. $(0, 1), (0, 2), (2, 3), 8$
13. $(0, 1), (2, 3), (4, 5), 1$
14. $(0, 1), (2, 3), (0, 1), 2$
15. $(0, 1), (0, 2), (0, 2), 8$
16. $(0, 1), (0, 1), (0, 1), 4$
Algorithm 2

1 **Step 1.** Create symmetry group for each geminals in the output of Part 1.1.
   - For a geminal $\alpha$, generate a set $G$ containing all possible permutations that can be an element of group symmetry of $\alpha$.
   - Apply an element, $g$, in $G$, to $\alpha$, and order the outcome by \textit{order2} to get $\beta$.
   - If $\alpha \equiv \beta$, put $g$ in to the group symmetry of $\alpha$.

2 **Step 2:** Apply the group symmetry on each elements of the determinant.
   - For a geminal $\alpha$, compute $\text{det}_g(D_\alpha)$, where $D_\alpha$ is a corresponding matrix of $\alpha$, to obtain the list $D$.
   - Order $D$ by \textit{order1}, and group duplicates to get the list $F$.
   - Apply the group symmetry of $\alpha$ to the first element, $F_0$, in $F$ to obtain $F_{01}$. Order $F_{01}$ by \textit{order1}.
   - Compare $F_{01}$ to the rest of $F$ to group duplicates. Save the elements obtained in a list $A$.
   - Delete $F_{01}$ and its duplicates.
   - Repeat this procedure until the $F$ empty. The final output is $A$.

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Symmetry Group

Eight geminals have identity symmetry group. Follows are symmetry group of the other 8 geminals, the identity was excluded for simplicity:

<table>
<thead>
<tr>
<th>Geminals</th>
<th>Group Symmetry</th>
</tr>
</thead>
<tbody>
<tr>
<td>(0, 1), (2, 3), (2, 4)</td>
<td>(1, 0, 2, 3, 4)</td>
</tr>
<tr>
<td>(0, 1), (0, 1), (2, 3)</td>
<td>(0, 1, 3, 2), (1, 0, 2, 3), (1, 0, 3, 2)</td>
</tr>
<tr>
<td>(0, 1), (2, 3), (2, 3)</td>
<td>(0, 1, 3, 2), (1, 0, 2, 3), (1, 0, 3, 2)</td>
</tr>
<tr>
<td>(0, 1), (2, 3), (0, 4)</td>
<td>(0, 1, 3, 2, 4)</td>
</tr>
<tr>
<td>(0, 1), (1, 2), (3, 4)</td>
<td>(0, 1, 2, 4, 3)</td>
</tr>
<tr>
<td>(0, 1), (2, 3), (4, 5)</td>
<td>(0, 1, 2, 3, 5, 4), (0, 1, 3, 2, 4, 5), (1, 0, 3, 2, 5, 4)</td>
</tr>
<tr>
<td></td>
<td>(0, 1, 3, 2, 5, 4), (1, 0, 2, 3, 4, 5), (1, 0, 2, 3, 5, 4)</td>
</tr>
<tr>
<td></td>
<td>(1, 0, 3, 2, 4, 5)</td>
</tr>
<tr>
<td>(0, 1), (2, 3), (0, 1)</td>
<td>(0, 1, 3, 2), (1, 0, 2, 3), (1, 0, 3, 2)</td>
</tr>
<tr>
<td>(0, 1), (0, 1), (0, 1)</td>
<td>(1, 0)</td>
</tr>
</tbody>
</table>
Follows are the results for those geminals does not have identity symmetry.

<table>
<thead>
<tr>
<th>Geminals</th>
<th>Before</th>
<th>After</th>
</tr>
</thead>
<tbody>
<tr>
<td>(0, 1), (2, 3), (2, 4)</td>
<td>120</td>
<td>66</td>
</tr>
<tr>
<td>(0, 1), (0, 1), (2, 3)</td>
<td>24</td>
<td>10</td>
</tr>
<tr>
<td>(0, 1), (2, 3), (2, 3)</td>
<td>24</td>
<td>10</td>
</tr>
<tr>
<td>(0, 1), (2, 3), (0, 4)</td>
<td>120</td>
<td>66</td>
</tr>
<tr>
<td>(0, 1), (1, 2), (3, 4)</td>
<td>120</td>
<td>66</td>
</tr>
<tr>
<td>(0, 1), (2, 3), (4, 5)</td>
<td>720</td>
<td>120</td>
</tr>
<tr>
<td>(0, 1), (2, 3), (0, 1)</td>
<td>24</td>
<td>10</td>
</tr>
<tr>
<td>(0, 1), (0, 1), (0, 1)</td>
<td>2</td>
<td>2</td>
</tr>
</tbody>
</table>
What about this?

\[ \sum_{a,b} \sum_{m,n} \int \int \int \int \int \]

\[ w_1(|\gamma_a - \gamma_b|) w_2(|\gamma_m - \gamma_n|) V(r_u) \]

\[ \phi_a(\gamma_a) \phi_b(\gamma_b) \phi_m(\gamma_m) \phi_n(\gamma_n) \phi_u(\gamma_u) \Delta d\gamma_a d\gamma_b d\gamma_m d\gamma_n d\gamma_u \]

Where \( \Delta \) is:

\[
\begin{bmatrix}
\theta_a(\gamma_a) & \theta_a(\gamma_b) & \theta_a(\gamma_m) & \theta_a(\gamma_n) & \theta_a(\gamma_u) \\
\theta_b(\gamma_a) & \theta_b(\gamma_b) & \theta_b(\gamma_m) & \theta_b(\gamma_n) & \theta_b(\gamma_u) \\
\theta_m(\gamma_a) & \theta_m(\gamma_b) & \theta_m(\gamma_m) & \theta_m(\gamma_n) & \theta_m(\gamma_u) \\
\theta_n(\gamma_a) & \theta_n(\gamma_b) & \theta_n(\gamma_m) & \theta_n(\gamma_n) & \theta_n(\gamma_u) \\
\theta_u(\gamma_a) & \theta_u(\gamma_b) & \theta_u(\gamma_m) & \theta_u(\gamma_n) & \theta_u(\gamma_u)
\end{bmatrix}
\]
The two algorithms also work!

Nine distinct geminals has been found, and here are the detailed results:

<table>
<thead>
<tr>
<th>Geminals</th>
<th>Before</th>
<th>After</th>
</tr>
</thead>
<tbody>
<tr>
<td>(0, 1), (1, 2), (0)</td>
<td>6</td>
<td>6</td>
</tr>
<tr>
<td>(0, 1), (1, 2), (1)</td>
<td>6</td>
<td>6</td>
</tr>
<tr>
<td>(0, 1), (0, 2), (3)</td>
<td>24</td>
<td>24</td>
</tr>
<tr>
<td>(0, 1), (2, 3), (1)</td>
<td>24</td>
<td>14</td>
</tr>
<tr>
<td>(0, 1), (2, 3), (4)</td>
<td>120</td>
<td>38</td>
</tr>
<tr>
<td>(0, 1), (2, 3), (3)</td>
<td>24</td>
<td>14</td>
</tr>
<tr>
<td>(0, 1), (0, 1), (1)</td>
<td>2</td>
<td>2</td>
</tr>
<tr>
<td>(0, 1), (0, 2), (1)</td>
<td>6</td>
<td>2</td>
</tr>
<tr>
<td>(0, 1), (0, 2), (2)</td>
<td>6</td>
<td>6</td>
</tr>
</tbody>
</table>
Conclusions

- We have eliminated overall 840 cases from 1154 cases, and established sufficient data to move to the next step of computing those geminals.
- In the next step, all those cases will be reduced one more time down to where we can use the reduction properties to compute them.

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