Chapter 5

Monotonic sequences and

a converse of the Cesaro method
5.1 The Cesaro method

The Cesaro method (CM) is one of the older methods\textsuperscript{,}\textsuperscript{4} that is generally used for accelerating
alternating (sawtooth) sequences where the alternate members of the PS, viz. \( S_j \) and \( S_{j+1} \), bracket the limit
point \( S_0 \). The method is based on a very simple idea of \textit{averaging}. Thus, given a PS \{\( S_j \}\}, here one defines
the TS as

\[
T_1 = S_1 , \\
T_2 = \frac{S_1 + S_2}{2} , \\
\vdots \\
T_n = \frac{S_1 + S_2 + \ldots + S_n}{n} = \frac{1}{n} \sum_{j=1}^{n} S_j , \quad n \geq 1
\]  

(5.1)

so that from \( n \) members of the PS, an equal number of members is obtained for the TS. The beauty of the
method lies in the fact that it usually maintains the bracketing nature of the PS in TS also, but with a
tighten bound in the latter case. So, one gradually approaches the limit \( S_0 \) from both above and below. The
method is regular and hence could be applied to both convergent and divergent sequences. Performance of
this method may be illustrated by taking some test examples as follows :

(i) Let us consider an \textit{oscillatory} sequence \((a, b, a, b, \ldots)\). Applying the CM, we obtain the TS as

\[
T_{2a} = \frac{a + b}{2} , \\
T_{2a+1} = \frac{(n + 1)a + nb}{2n + 1} \rightarrow \frac{a + b}{2} \text{ as } n \rightarrow \infty
\]  

(5.2)

The result obviously leads to the value \((a + b)/2\) as the limit of the PS. This is actually an \textit{average} value
and here it is also the exact limit-value of the sequence.

(ii) Now, consider a \textit{sawtooth} divergent sequence, \((1, -1, 2, -2, \ldots)\) which on applying CM gives the TS as

\[
T_{2a} = 0 , \\
T_{2a+1} = \frac{n + 1}{2n} \rightarrow \frac{1}{2} \text{ as } n \rightarrow \infty
\]  

(5.3)
As \( n \to \infty \), the TS leads to an oscillatory sequence here, with lower and upper bounds as 0 and 1/2 respectively. Hence, if we further employ CM on the TS and continue the process, it will ultimately give the limit value as 1/4, by virtue of example (i). Some such uses of the CM have been made in Chapter 4.

However, the method does not apply to monotonic sequences in the sense that it leads to a worse TS. To see it explicitly, let us consider the sequence

\[
S_n = 2 \left(1 - \frac{1}{2^n}\right)
\]

for which \( S_0 = 2 \). The EM also gives the same result by associating the series

\[
\frac{1}{1-x} = 1 + x + x^2 + \ldots , \quad (x = \frac{1}{2})
\]

with the given sequence.

The CM leads in this case to

\[
T_m = 2 - \frac{2}{m} + \frac{1}{m2^m - 1}
\]

which shows immediately that the decay has become slower now compared to the PS, owing to the presence of \( O(1/m) \) term here.

Plainly, however, it is apparent that an averaging improves result only when the values are scattered on both sides of the actual result. This is true in sawtooth cases, not when members of the PS follow a monotonic approach. Thus, it is physically expected as well that CM would perform better only for sawtooth/oscillatory sequences. We shall now explore if it is at all possible to modify CM in order that monotonic sequences may be accelerated.

5.2 The Converse Cesaro method

The converse transformation of CM, as the name indicates, may be obtained by doing the reverse of what we have done in (5.1). Thus, from (5.1) the members of the PS may be regenerated as

\[
S_j = jT_j - (j - 1)T_{j-1}
\]
The converse transformation, after a trivial renaming, looks like

\[ T_j = (j + 1)S_{j+1} - jS_j, \quad j \geq 1. \]  

(5.8)

The expression may also be written in terms of forward difference operator ‘Δ’ (\( \Delta S_j = S_{j+1} - S_j \)) as

\[ T_j = S_{j+1} + j\Delta S_j. \]  

(5.9)

We call it the converse Cesaro method (CCM). A few observations relating to CCM may now be in order:

(i) The scheme is regular, i.e. if \( S_j \to S_0 \) as \( k \to \infty \) holds, we would have \( T_j \to S_0 \) as \( j \to \infty \). This is because convergence requires \( j\Delta S_j \to 0 \) as \( j \to \infty \).

(ii) The method now works for monotonic sequences. Let us consider an example of a very familiar monotonic sequence of the form

\[ S_n = S_0 + \frac{A}{n} + \frac{B}{n^2} + \cdots = S_0 + O\left(\frac{1}{n}\right). \]  

(5.10)

Then,

\[ T_n = S_0 - \frac{B}{n(n + 1)} + \cdots = S_0 + O\left(\frac{1}{n^2}\right). \]  

(5.11)

Since the decay has become faster in \( T_n \), members of TS approach \( S_0 \) at a faster rate. Now, if \( A, B, \ldots \) are all positive, \( S_n \) approaches \( S_0 \) from above. But, \( T_n \) would approach the same from below. This shows the importance of bracketing in the present context.

(iii) Even if we consider a more general form\(^6\) for \( S_n \), viz.

\[ S_n = S_0 + \frac{A}{n^\alpha} + \cdots, \]  

(5.12)

one would find that

\[ T_n = S_0 + \frac{A(1-\alpha)}{n^\alpha} + \cdots. \]  

(5.13)

This shows, (a) at \( \alpha = 1 \), CCM would work best and (b) for any \( \alpha > 1 \), \( S_n \) and \( T_n \) would bracket \( S_0 \).

(iv) The scheme may be employed iteratively, if necessary. In CM also, iterative applications are common\(^3\). The expression (5.9) is then expressed in CCM as

\[ T_k^{(m)} = T_{k+1}^{(m-1)} + k \Delta T_k^{(m-1)} \]  

(5.14)
Thus, \( T_k \) in (5.9) is actually equivalent to \( T^{(1)} \).

(v) Finally, we note a close kinship of CCM with the Neville-Aitken extrapolation\(^{26}\). Indeed \( T^{(1)}_k \) in (5.14) is the same as the first Neville-Aitken transform defined by (2.17) in Ref. 26. But, the equivalence is lost for \( m > 2 \). This is because, spirits of the two schemes are basically different.

A demonstrative example may be given here to appreciate the workability of CCM by taking the instance of the \textit{Riemann Zeta function}\(^3\),\(^10\),\(^12\) given by

\[
\zeta(z) = \sum_{n=1}^{\infty} n^{-z} .
\]  

which converges for any \( \Re(z) > 1 \), but the rate is noticeably slow at low \( \Re(z) \). For demonstrative computations, we have chosen the case of \( \zeta(2) \), results of which are shown in Table 5.1. Since \( T^{(1)}_k \) is again monotonic and approaches \( S_0 \) from below, a second transformation \( (T^{(2)}_k) \) has been carried out which tends to \( S_0 \) from above. In such a situation, it is natural to take an average \( (\text{here of } T^{(1)} \text{ and } T^{(2)}) \), as shown in Table 5.1. To assess the worth of adopting the CCM, we have also listed the results obtained by employing DPA in the table. The superiority of CCM, inspite of its extreme simplicity, is evident. A closer look at Table 5.1 also reveals that CCM is much more efficient during the initial stages than later. This may be directly verified. To proceed, consider the PS given in Table 5.1:

\[
S_k = \sum_{n=1}^{k} n^{-z} , 
\]  

By employing CCM, one obtains the TS as

\[
T^{(1)}_k = S_{k+1} + \frac{k}{(k+1)^z} \]  

Equation (5.17) implies (a) for \( z > 1 \), the extra contribution embedded in \( T^{(1)}_k \) decreases as \( k \) increases (which we have just seen) and (b) CCM is more effective for lower \( z \) values, another desirable feature.

5.3 Some results

Calculation of lattice constants in atomic lattices is an important factor in determining the potential energies at a given lattice site and hence the structural stabilities\(^{29-33}\) of different lattices. As we have seen
Table 5.1. Performance of CCM for the sequence (5.16) at $z = 2$ (Exact value $= \frac{1}{8} \pi^2 = 1.644 934$).

<table>
<thead>
<tr>
<th>$k$</th>
<th>$S_k$</th>
<th>$T_{k-1}^{(1)}$</th>
<th>$T_{k-2}^{(2)}$</th>
<th>Avg.</th>
<th>DPA$^9$</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>1.0</td>
<td>-</td>
<td>-</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td>3</td>
<td>1.36</td>
<td>1.583</td>
<td>1.667</td>
<td>1.625</td>
<td>1.45</td>
</tr>
<tr>
<td>5</td>
<td>1.46</td>
<td>1.623</td>
<td>1.681</td>
<td>1.642</td>
<td>1.552</td>
</tr>
<tr>
<td>7</td>
<td>1.51</td>
<td>1.634</td>
<td>1.654</td>
<td>1.644</td>
<td>1.590</td>
</tr>
<tr>
<td>9</td>
<td>1.54</td>
<td>1.638</td>
<td>1.650</td>
<td>1.644</td>
<td>1.609</td>
</tr>
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<td>21</td>
<td>1.60</td>
<td>1.644</td>
<td>1.648</td>
<td>1.644</td>
<td>1.644</td>
</tr>
<tr>
<td>31</td>
<td>1.61</td>
<td>1.644</td>
<td>1.645</td>
<td>1.644</td>
<td>1.644</td>
</tr>
</tbody>
</table>
in Chapter 2, the evaluation of these lattice constants involves infinite sums\(^{30-32}\). Thus, for example, for regular SC lattice the expression has the form

\[
S(m) = \lim_{j \to \infty} S_j(m) = \sum_{M,N,P=-j}^{j} \frac{1}{(\sqrt{M^2 + N^2 + P^2})^m}
\]  

(5.18)

where \(M, N, P\) are integers, not all zero, and \(m\) usually takes values from 4 to 15. Similar expressions for other lattices like BCC, FCC etc. may be found in Chapter 2. We also pointed out there that a cubical development of the infinite lattice is far more convenient than a radial development, in so far as the applicability of STT is concerned. Since the PS in such cases follow a monotonic character, it seems worthwhile to explore how CCM may handle the acceleration process. So, Table 5.2 shows the results for regular cubic lattices at \(m = 4\) where convergence is slowest. Here, the first transform \(T_j^{(1)}\) obtained by employing CCM gives a lower bound to \(S(m)\). Hence, CCM is applied for the second time to obtain \(T_j^{(2)}\) whereby an upper bound to the \(S(m)\) is obtained. As evident from the table, both the upper and lower bounds gradually improve, along with their averages. Besides its bounding property, the method also provides more balanced estimates for all the cases in comparison with the estimates of the continuum approximation\(^{32,35}\), another simple alternative in this context (see, e.g. Chapter 2 for elaboration on this point). Thus, the latter method, in which the infinite sum in (5.18) is truncated at some \(j\) value and the effect of the remainder is taken through an integral, yields results\(^{35}\) given in Table 5.3. We note at this point some inconsistencies in these results: (i) Although \(S_4^{(3)}\) should provide better estimates than \(S_4^{(1)}\), in case of SC lattice we observe the reverse. (ii) \(S_4^{(3)} > S_4^{(1)}\) for SC and BCC, but the opposite inequality holds for FCC. (iii) Such estimates do not provide any bounding property. On the other hand, CCM provides balanced estimates; \(T^{(1)}\) gradually increases while \(T^{(2)}\) shows a gradual decrease. Simply, by taking \(k = 10\), one obtains very reasonable estimates which are free from the inconsistencies mentioned above. Table 5.2 gives the average values (Avg.) wherefrom this may be checked. However, the extreme simplicity of CCM forbids it from furnishing high quality estimates for which one should opt for far more sophisticated methods, as considered in Chapter 2 and will be considered again in Chapter 6. One may employ CCM in quite a few other contexts. While we have concentrated here on atomic LS problem, some more examples will be chosen in Chapter 7.
Table 5.2. Evaluation of lattice constants $S(m)$ for various cubic lattices by CCM at $m = 4$.

<table>
<thead>
<tr>
<th>Lattice</th>
<th>$k$</th>
<th>$S_k$</th>
<th>$T_{k-1}^{(1)}$</th>
<th>$T_{k-2}^{(2)}$</th>
<th>Avg.</th>
</tr>
</thead>
<tbody>
<tr>
<td>SC</td>
<td>1</td>
<td>9.89</td>
<td>-</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td></td>
<td>2</td>
<td>12.43</td>
<td>14.97</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td></td>
<td>3</td>
<td>13.58</td>
<td>15.87</td>
<td>16.77</td>
<td>16.32</td>
</tr>
<tr>
<td></td>
<td>4</td>
<td>14.22</td>
<td>16.17</td>
<td>16.77</td>
<td>16.47</td>
</tr>
<tr>
<td></td>
<td>5</td>
<td>14.64</td>
<td>16.30</td>
<td>16.71</td>
<td>16.51</td>
</tr>
<tr>
<td></td>
<td>10</td>
<td>15.54</td>
<td>16.48</td>
<td>16.57</td>
<td>16.531</td>
</tr>
<tr>
<td></td>
<td>21</td>
<td>16.05</td>
<td>16.52</td>
<td>16.544</td>
<td>16.532</td>
</tr>
<tr>
<td></td>
<td>31</td>
<td>16.20</td>
<td>16.527</td>
<td>16.538</td>
<td>16.532</td>
</tr>
<tr>
<td>BCC</td>
<td>1</td>
<td>14.62</td>
<td>-</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td></td>
<td>2</td>
<td>17.89</td>
<td>21.17</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td></td>
<td>3</td>
<td>19.27</td>
<td>22.01</td>
<td>22.84</td>
<td>22.42</td>
</tr>
<tr>
<td></td>
<td>4</td>
<td>22.02</td>
<td>22.28</td>
<td>22.84</td>
<td>22.56</td>
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<td></td>
<td>5</td>
<td>20.50</td>
<td>22.41</td>
<td>22.79</td>
<td>22.60</td>
</tr>
<tr>
<td></td>
<td>10</td>
<td>21.52</td>
<td>22.58</td>
<td>22.69</td>
<td>22.635</td>
</tr>
<tr>
<td></td>
<td>21</td>
<td>22.09</td>
<td>22.63</td>
<td>22.651</td>
<td>22.638</td>
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<tr>
<td></td>
<td>31</td>
<td>22.27</td>
<td>22.633</td>
<td>22.644</td>
<td>22.638</td>
</tr>
<tr>
<td>FCC</td>
<td>1</td>
<td>15.72</td>
<td>-</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td></td>
<td>2</td>
<td>19.41</td>
<td>23.10</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td></td>
<td>3</td>
<td>21.07</td>
<td>24.38</td>
<td>25.67</td>
<td>25.03</td>
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<tr>
<td></td>
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<td>24.82</td>
<td>25.68</td>
<td>25.25</td>
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<td>23.90</td>
<td>25.26</td>
<td>25.41</td>
<td>25.335</td>
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<td>24.64</td>
<td>25.32</td>
<td>25.346</td>
<td>25.338</td>
</tr>
<tr>
<td></td>
<td>31</td>
<td>24.86</td>
<td>25.33</td>
<td>25.346</td>
<td>25.338</td>
</tr>
</tbody>
</table>
Table 5.3. Behaviour of approximate estimates of $S_m$ with decreasing continuum contributions at $m = 4$.

<table>
<thead>
<tr>
<th></th>
<th>SC</th>
<th>BCC</th>
<th>FCC</th>
</tr>
</thead>
<tbody>
<tr>
<td>$S_4^{(1)}$</td>
<td>16.5894</td>
<td>21.8035</td>
<td>25.6756</td>
</tr>
<tr>
<td>$S_4^{(2)}$</td>
<td>16.6412</td>
<td>22.6333</td>
<td>25.3451</td>
</tr>
<tr>
<td>Exact</td>
<td>16.5323</td>
<td>22.6387</td>
<td>25.3383</td>
</tr>
</tbody>
</table>
5.4 Concluding remarks

Our objective here has been to extend the scope of a simple method like CM to include monotonic sequences so that one simply and quickly obtains an approximate estimate of the limit point from a low-order input data of the PS. We propose what we call CCM to achieve this end.

Like the CM, CCM also provides a bounding property in the TS, though it starts with a monotonic PS. This feature gives the method a distinct advantage. The method may well be applied iteratively to this end.

The method is perhaps the simplest among the STT available to accelerate monotonic sequences. This also explains its limitation in providing high-quality results. However, due to the bounding nature of the method, one can easily guess the limit of the PS, i.e. a rough estimate of $S_0$.

Finally, the strategy itself is of considerable theoretical and philosophical interest. It signifies, while averaging improves convergence of an alternating sequence, a monotonic one is accelerated by 'undoing' such an averaging process.