Implementations of the Levin-Weniger convergence accelerator and applications to problems in physics

Ignacio Porras, Francisco Cordobés-Aguilar

Departamento de Física Atómica, Molecular y Nuclear
Universidad de Granada

Luminy 09 Conference
Outline:

- Introduction.
Outline:

- Introduction.
- A new remainder for the generalized Levin transformation.
Outline:

- Introduction.
- A new remainder for the generalized Levin transformation.
- Attempts to improve stability.
Outline:

- Introduction.
- A new remainder for the generalized Levin transformation.
- Attempts to improve stability.
- Series appearing in few-electron integrals.
Outline:

- Introduction.
- A new remainder for the generalized Levin transformation.
- Attempts to improve stability.
- Series appearing in few-electron integrals.
- Generalizing Čížek et al's generalization of Levin-Weniger transformations.
Outline:

- Introduction.
- A new remainder for the generalized Levin transformation.
- Attempts to improve stability.
- Series appearing in few-electron integrals.
- Generalizing Čížek et al’s generalization of Levin-Weniger transformations.
- Conclusions.
Introduction:

Convergence acceleration is an important problem in many problems in physics.
Convergence acceleration is an important problem in many problems in physics.

Variational calculations in atomic physics: multiple series for the calculation of each matrix element of the Hamiltonian.
Introduction:

- Convergence acceleration is an important problem in many problems in physics.
- Variational calculations in atomic physics: multiple series for the calculation of each matrix element of the Hamiltonian.
- High precision is demanded.
Introduction:

- Convergence acceleration is an important problem in many problems in physics.
- Variational calculations in atomic physics: multiple series for the calculation of each matrix element of the Hamiltonian.
- High precision is demanded.
- Large basis sets: necessity of reducing computing time.
Introduction:

- Convergence acceleration is an important problem in many problems in physics.
- Variational calculations in atomic physics: multiple series for the calculation of each matrix element of the Hamiltonian.
- High precision is demanded.
- Large basis sets: necessity of reducing computing time.
- Crucial problems: negative ions.
For a series $S = \sum_{i=0}^{\infty} a_i$, where $S_n = \sum_{i=0}^{n} a_i$, for which we assume

$$S_n = S + \omega_n \sum_{j=0}^{k-1} \frac{C_j}{(n + \beta)^j}$$
For a series \( S = \sum_{i=0}^{\infty} a_i \), where \( S_n = \sum_{i=0}^{n} a_i \), for which we assume

\[
S_n = S + \omega_n \sum_{j=0}^{k-1} \frac{C_j}{(n + \beta)^j}
\]

Then, multiplying by \( (n + \beta)^{k-1} \) both sides:

\[
(n + \beta)^{k-1} \frac{S_n - S}{\omega_n} = \text{polynomial in } n \text{ of degree } k - 1
\]
Generalized Levin transformed reviewed by Weniger

For a series $S = \sum_{i=0}^{\infty} a_i$, where $S_n = \sum_{i=0}^{n} a_i$, for which we assume

$$S_n = S + \omega_n \sum_{j=0}^{k-1} \frac{C_j}{(n + \beta)^j}$$

Then, multiplying by $(n + \beta)^{k-1}$ both sides:

$$\frac{(n + \beta)^{k-1} S_n - S}{\omega_n} = \text{polynomial in } n \text{ of degree } k - 1$$

And applying the $k$-th power of the difference operator $\Delta^k$:

$$S = \frac{\sum_{j=0}^{k} (-1)^j \binom{k}{j} \frac{(n + j + \beta)^{k-1}}{(n + k + \beta)^{k-1}} \frac{S_{n+j}}{\omega_{n+j}}}{\sum_{j=0}^{k} (-1)^j \binom{k}{j} \frac{(n + j + \beta)^{k-1}}{(n + k + \beta)^{k-1}} \frac{1}{\omega_{n+j}}}$$

A new remainder for g-Levin transformation

Levin’s $u$-transformation: $\omega_n = na_n$ or $\omega_n = (n + \beta)a_n$ (inspired in integrals)
A new remainder for g-Levin transformation

- Levin's \( u \)-transformation: \( \omega_n = n a_n \) or \( \omega_n = (n + \beta) a_n \) (inspired in integrals)

- Formal obtention of a remainder for series for which \( a_n \sim n^{-\alpha} \), using Euler-McLaurin sum rule:

\[
\sum_{i=n}^{\infty} a_i = \int_{n}^{\infty} f(x) \, dx + \frac{1}{2} f(n) - \sum_{k=1}^{m} \frac{B_{2k}}{(2k)!} f(2k-1)(N) + E_m
\]

where
A new remainder for g-Levin transformation

- Levin’s \( u \)-transformation: \( \omega_n = na_n \) or \( \omega_n = (n + \beta)a_n \) (inspired in integrals)

- Formal obtention of a remainder for series for which \( a_n \sim n^{-\alpha} \), using Euler-McLaurin sum rule:

\[
\sum_{i=n}^{\infty} a_i = \int_n^{\infty} f(x) \, dx + \frac{1}{2} f(n) - \sum_{k=1}^{m} \frac{B_{2k}}{(2k)!} f^{(2k-1)}(N) + E_m
\]

where

- \( f(x) \) verifies \( f(i) = a_i \) for \( i = n, n + 1, \ldots \),
A new remainder for g-Levin transformation

Levin’s $u$-transformation: $\omega_n = na_n$ or $\omega_n = (n + \beta)a_n$ (inspired in integrals)

Formal obtention of a remainder for series for which $a_n \sim n^{-\alpha}$, using Euler-McLaurin sum rule:

$$\sum_{i=n}^{\infty} a_i = \int_{n}^{\infty} f(x) \, dx + \frac{1}{2} f(n) - \sum_{k=1}^{m} \frac{B_{2k}}{(2k)!} f^{(2k-1)}(N) + E_m$$

where

- $f(x)$ verifies $f(i) = a_i$ for $i = n, n+1, \ldots$,
- $B_n$ denote the Bernoulli numbers,
A new remainder for g-Levin transformation

- Levin’s \( u \)-transformation: \( \omega_n = na_n \) or \( \omega_n = (n + \beta)a_n \) (inspired in integrals)

- Formal obtention of a remainder for series for which \( a_n \sim n^{-\alpha} \), using Euler-McLaurin sum rule:

\[
\sum_{i=n}^{\infty} a_i = \int_{n}^{\infty} f(x) \, dx + \frac{1}{2} f(n) - \sum_{k=1}^{m} \frac{B_{2k}}{(2k)!} f(2k-1)(N) + E_m
\]

where

- \( f(x) \) verifies \( f(i) = a_i \) for \( i = n, n+1, \ldots \),
- \( B_n \) denote the Bernouilli numbers,
- and \( E_m \) is a remainder term.
If $n$ is large enough and $f(x) \sim \frac{C}{x^\alpha}$:

$$\sum_{i=n}^{\infty} a_i = \frac{C}{\alpha - 1} \frac{1}{n^{\alpha-1}} + \frac{C}{2} \frac{1}{n^\alpha} + \sum_{k=1}^{m} \frac{B_{2k} C'(\alpha)_{2k-1}}{(2k)!} \frac{1}{n^{\alpha+2k-1}} + E_m$$
If $n$ is large enough and $f(x) \sim \frac{C}{x^\alpha}$:

$$\sum_{i=n}^{\infty} a_i = \frac{C}{\alpha - 1} \frac{1}{n^{\alpha-1}} + \frac{C}{2} \frac{1}{n^\alpha} + \sum_{k=1}^{m} \frac{B_{2k}C(\alpha)_{2k-1}}{(2k)!} \frac{1}{n^{\alpha+2k-1}} + E_m$$

We apply this result to the sum:

$$S = \sum_{i=0}^{\infty} a_i = \sum_{i=0}^{n-1} a_i + \sum_{i=n}^{\infty} a_i = S_{n-1} + \sum_{i=n}^{\infty} a_i$$

up to $k$ terms, for the second sum, including for convenience the missing terms $\left(1/n^{\alpha+2k}\right)$.
If \( n \) is large enough and \( f(x) \sim \frac{C}{x^\alpha} \):

\[
\sum_{i=n}^{\infty} a_i = \frac{C}{\alpha - 1} \frac{1}{n^{\alpha-1}} + \frac{C}{2} \frac{1}{n^{\alpha}} + \sum_{k=1}^{m} \frac{B_{2k} C'(\alpha)_{2k-1}}{(2k)!} \frac{1}{n^{\alpha+2k-1}} + E_m
\]

We apply this result to the sum:

\[
S = \sum_{i=0}^{\infty} a_i = \sum_{i=0}^{n-1} a_i + \sum_{i=n}^{\infty} a_i = S_{n-1} + \sum_{i=n}^{\infty} a_i
\]

up to \( k \) terms, for the second sum, including for convenience the missing terms \((1/n^{\alpha+2k})\).

We obtain and estimator for \( S \) that will be denoted by \( Q_0 \).

\[
S_{n-1} = Q_0 + \frac{Q_1}{n^{\alpha-1}} + \frac{Q_2}{n^{\alpha}} + \cdots + \frac{Q_k}{n^{\alpha+k-2}}
\]
Applying this result for \( n, \ldots n + k \), we find a system of equations that can be solved for \( Q_0 \):

\[
Q_0^{(\alpha)}(n, k) = \frac{\sum_{j=0}^{k} \frac{(-1)^j}{j!(k-j)!} (n + j + 1)^{k+\alpha-2} S_{n+j}}{\sum_{j=0}^{k} \frac{(-1)^j}{j!(k-j)!} (n + j + 1)^{k+\alpha-2}}
\]
Applying this result for $n, \ldots n + k$, we find a system of equations than can be solved for $Q_0$:

$$Q_0^{(\alpha)}(n, k) = \frac{\sum_{j=0}^{k} \frac{(-1)^j}{j!(k-j)!} (n + j + 1)^{k+\alpha-2} S_{n+j}}{\sum_{j=0}^{k} \frac{(-1)^j}{j!(k-j)!} (n + j + 1)^{k+\alpha-2}},$$

Equal to g-Levin formula for $\beta = 1$ and $\omega_n = (n + 1)^{-\alpha+1}$, which is equivalent to $u$-transform in the large $n$-limit.
Applying this result for $n, \ldots, n + k$, we find a system of equations than can be solved for $Q_0$:

$$Q_0^{(\alpha)}(n, k) = \sum_{j=0}^{k} \frac{(-1)^j}{j!(k-j)!} (n + j + 1)^{k+\alpha-2} S_{n+j}$$

$$= \frac{1}{\sum_{j=0}^{k} \frac{(-1)^j}{j!(k-j)!} (n + j + 1)^{k+\alpha-2}}$$

Equal to g-Levin formula for $\beta = 1$ and $\omega_n = (n + 1)^{-\alpha+1}$, which is equivalent to $u$-transform in the large $n$-limit.

For $n$ not large, differences appear.
Applying this result for $n, \ldots n + k$, we find a system of equations than can be solved for $Q_0$:

$$Q_0^{(\alpha)}(n, k) = \frac{\sum_{j=0}^{k} (-1)^j \frac{(n + j + 1)^{k+\alpha-2}}{j!(k-j)!} S_{n+j}}{\sum_{j=0}^{k} \frac{(-1)^j (n + j + 1)^{k+\alpha-2}}{j!(k-j)!}} ,$$

Equal to g-Levin formula for $\beta = 1$ and $\omega_n = (n + 1)^{-\alpha+1}$, which is equivalent to $u$-transform in the large $n$-limit.

For $n$ not large, differences appear.

$\alpha = 2$ leads to Richardson’s convergence accelerator.
Unstability problems:

- Alternating sums of close values in numerator and denominator. Problems when $k$ increases, getting worse as $n$ increases.
Unstability problems:

- Alternating sums of close values in numerator and denominator. Problems when $k$ increases, getting worse as $n$ increases.

- Attempt to improve stability: we assume that differences in the values $P_{n,j} = S_{n+j} - S_n = \sum_{i=n+1}^{n+j} a_i$ are greater than differences between $S_{n+j}$ values, for different $j$, fixed $n$. 
Unstability problems:

- Alternating sums of close values in numerator and denominator. Problems when $k$ increases, getting worse as $n$ increases.

- Attempt to improve stability: we assume that differences in the values $P_{n,j} = S_{n+j} - S_n = \sum_{i=n+1}^{n+j} a_i$ are greater than differences between $S_{n+j}$ values, for different $j$, fixed $n$.

- Summing and subtracting $S_n$ leads to:

$$S = S_n + \sum_{j=1}^{k} (-1)^j \binom{k}{j} \frac{(n + j + \beta)^{k-1}}{(n + k + \beta)^{k-1}} \frac{P_{n,j}}{\omega_{n+j}}$$

$$S = S_n + \frac{1}{\omega_{n+j}} \sum_{j=0}^{k} (-1)^j \binom{k}{j} \frac{(n + j + \beta)^{k-1}}{(n + k + \beta)^{k-1}}$$
Unstability problems:

- Alternating sums of close values in numerator and denominator. Problems when $k$ increases, getting worse as $n$ increases.

- Attempt to improve stability: we assume that differences in the values $P_{n,j} = S_{n+j} - S_n = \sum_{i=n+1}^{n+j} a_i$ are greater than differences between $S_{n+j}$ values, for different $j$, fixed $n$.

- Summing and substracting $S_n$ leads to:

\[
S = S_n + \frac{\sum_{j=1}^{k} (-1)^j \binom{k}{j} (n + j + \beta)^{k-1}}{\sum_{j=0}^{k} (-1)^j \binom{k}{j} (n + k + \beta)^{k-1} } \frac{P_{n,j}}{\omega_{n+j}}
\]

- Čížek, Zamastil and Skála obtained an accelerator in terms of $P_{n,j}$.

Test 1:

\[ S = \sum_{i=1}^{\infty} \frac{1}{i^2} = \frac{\pi^2}{6} \]
Test 1:

\[ S = \sum_{i=1}^{\infty} \frac{1}{i^2} = \frac{\pi^2}{6} \]

For this case, Richardson, \( u \)-Levin and \( Q_0 \) are equivalent.
Test 1:

\[ S = \sum_{i=1}^{\infty} \frac{1}{i^2} = \frac{\pi^2}{6} \]

For this case, Richardson, \( u \)-Levin and \( Q_0 \) are equivalent.

\( \epsilon \): relative error (solid lines: with \( P_{n,j} \), dashed lines: with \( S_{n+j} \))
Test 1:

\[ S = \sum_{i=1}^{\infty} \frac{1}{i^2} = \frac{\pi^2}{6} \]

For this case, Richardson, \( u \)-Levin and \( Q_0 \) are equivalent.

\( \epsilon \): relative error (solid lines: with \( P_{n,j} \), dashed lines: with \( S_{n+j} \))

From now on, starting index \( n = 1 \), unless otherwise stated.
\[ _2F_1(1, 1, 5/2, 1) = \sum_{n=0}^{\infty} \frac{n!}{(5/2)^n} = 3 \]
Test 2:

\[ _2 F_1(1, 1, 5/2, 1) = \sum_{n=0}^{\infty} \frac{n!}{(5/2)_n} = 3 \]

\[ a_n \sim n^{-3/2}, \quad \alpha = 3/2. \text{ } u\text{-Levin exact for this series.} \]
Test 2:

\[ _2F_1(1, 1, 5/2, 1) = \sum_{n=0}^{\infty} \frac{n!}{(5/2)_n} = 3 \]

\[ a_n \sim n^{-3/2}, \quad \alpha = 3/2. \quad u\text{-Levin} \text{ exact for this series.} \]
Test 3:

\[ S = \sum_{n=1}^{\infty} \frac{1}{\sqrt{n}} \left( 1 + \frac{1}{n} \right) - \frac{1}{\sqrt{n+1}} \left( 1 + \frac{1}{n+1} \right) = 2 \]
Test 3:

\[ S = \sum_{n=1}^{\infty} \frac{1}{\sqrt{n}} \left( 1 + \frac{1}{n} \right) - \frac{1}{\sqrt{n+1}} \left( 1 + \frac{1}{n+1} \right) = 2 \]

\[ a_n \sim n^{-3/2}, \quad Q_{0}^{3/2} \text{ is exact.} \]
Test 3:

\[ S = \sum_{n=1}^{\infty} \frac{1}{\sqrt{n}} \left( 1 + \frac{1}{n} \right) - \frac{1}{\sqrt{n+1}} \left( 1 + \frac{1}{n+1} \right) = 2 \]

\[ a_n \sim n^{-3/2}, \, Q_0^{3/2} \text{ is exact.} \]
Test 4:

\[ \frac{1}{z} = \sum_{m=0}^{\infty} \hat{k}_{m-1/2}(z) \frac{1}{2^m m!} \]
Test 4:

\[ \frac{1}{z} = \sum_{m=0}^{\infty} \hat{k}_m^{-1/2}(z) \frac{1}{2^m m!} \]

For \( z = 1 \):

\[ 1 = e^{-1} \left[ 1 + \frac{1}{2} \sum_{n=0}^{\infty} M(-n; -2n; 2) \frac{(1/2)^n}{(n + 1)!} \right] ; a_n \sim n^{-3/2} \]
Test 4:

\[ \frac{1}{z} = \sum_{m=0}^{\infty} \hat{k} m - 1/2(z) \frac{1}{2^m m!} \]

For \( z = 1 \):

\[ 1 = e^{-1} \left[ 1 + \frac{1}{2} \sum_{n=0}^{\infty} M(-n; -2n; 2) \frac{(1/2)^n}{(n + 1)!} \right] ; \ a_n \sim n^{-3/2}. \]
Calculations with arbitrary precision:

- MPFR: Multi-Precision Floating-point library with correct Rounding (free distribution, in C language).
Calculations with arbitrary precision:

- MPFR: Multi-Precision Floating-point library with correct Rounding (free distribution, in C language).
Calculations with arbitrary precision:

- MPFR: Multi-Precision Floating-point library with correct Rounding (free distribution, in C language).
- We adjust the number of bits of precision by convenience.
Recall Test 2:

\[ _2F_1(1, 1, 5/2, 1) = \sum_{n=0}^{\infty} \frac{n!}{(5/2)^n} = 3 \]
Recall Test 2:

\[ 2F_1(1, 1, 5/2, 1) = \sum_{n=0}^{\infty} \frac{n!}{(5/2)^n} = 3 \]

Results for 200 bit-precision:
Few electron integrals in atomic calculations

Two electron correlated integrals:

\[ I_2(i, j, l, a, b) = \int \int d\vec{r}_1 d\vec{r}_2 r_1^i r_2^j r_{12}^l e^{-ar_1 - br_2} \]
Few electron integrals in atomic calculations

**Two electron correlated integrals:**

\[
I_2(i, j, l, a, b) = \int \int d\vec{r}_1 d\vec{r}_2 r_1^i r_2^j r_{12}^l e^{-a r_1 - b r_2}
\]

**Usual approach:**

\[
r_{12}^l = \sum_{m=0}^{\infty} R_{l,m}(r_1, r_2) P_m(\cos \theta_{12})
\]

and expansions of \( R_{l,m} \) in terms of \( r_\text{<} = \min\{r_1, r_2\} \) and \( r_\text{>} = \max\{r_1, r_2\} \) (finite sum) or \( r_1 r_2/(r_1 + r_2)^2 \) (infinite sum).
Few electron integrals in atomic calculations

Two electron correlated integrals:

\[ I_2(i, j, l, a, b) = \int \int d\vec{r}_1 d\vec{r}_2 r_1^i r_2^j r_{12}^l e^{-ar_1 - br_2} \]

Usual approach:

\[ r_{12}^l = \sum_{m=0}^{\infty} R_{l,m}(r_1, r_2) P_m(\cos\theta_{12}) \]

and expansions of \( R_{l,m} \) in terms of \( r_\prec = \min\{r_1, r_2\} \) and \( r_\succ = \max\{r_1, r_2\} \) (finite sum) or \( r_1 r_2/(r_1 + r_2)^2 \) (infinite sum).

The slowest convergent resulting series happens when \( l = -2 \) (relativistic and lower bound calculations)
Particular case:

\[ I_2(-2, -1, -2, a, b) = \frac{8\pi^2}{b} \left\{ \frac{\pi^2}{3} - \left[ \ln \left(1 + \frac{a}{b}\right) \right]^2 \right. \]

\[ + \quad \text{Li}_2 \left(1 - \frac{a}{b}\right) - \text{Li}_2 \left(\frac{b}{b+a}\right) \right\} \quad [1] \]
Particular case:

\[ I_2(-2, -1, -2, a, b) = \frac{8\pi^2}{b} \left\{ \frac{\pi^2}{3} - \left[ \ln \left(1 + \frac{a}{b}\right) \right]^2 \right. \]

\[ + \quad \text{Li}_2 \left(1 - \frac{a}{b}\right) - \text{Li}_2 \left(\frac{b}{b+a}\right) \} \quad [1] \]

Last two terms cancel some digits if \( x = a/b \) is small.
Particular case:

\[
I_2(-2, -1, -2, a, b) = \frac{8\pi^2}{b} \left\{ \frac{\pi^2}{3} - \left[ \ln \left(1 + \frac{a}{b}\right) \right]^2 \right. \\
+ \left. \text{Li}_2 \left(1 - \frac{a}{b}\right) - \text{Li}_2 \left(\frac{b}{b + a}\right) \right\} \quad [1]
\]

Last two terms cancel some digits if \(x = a/b\) is small.

\[
S(x) = \text{Li}_2 \left(1 - x\right) - \text{Li}_2 \left(\frac{1}{1 + x}\right) = \sum_{n=1}^{\infty} \frac{1}{n^2} \left[ (1 - x)^n - \left(\frac{1}{1 + x}\right)^n \right]
\]
Particular case:

\[ I_2(-2, -1, -2, a, b) = \frac{8\pi^2}{b} \left\{ \frac{\pi^2}{3} - \left[ \ln \left(1 + \frac{a}{b}\right) \right]^2 + \text{Li}_2 \left(1 - \frac{a}{b}\right) - \text{Li}_2 \left(\frac{b}{b+a}\right) \right\} \quad [1] \]

Last two terms cancel some digits if \( x = a/b \) is small.

\[ S(x) = \text{Li}_2 \left(1 - x\right) - \text{Li}_2 \left(\frac{1}{1+x}\right) = \sum_{n=1}^{\infty} \frac{1}{n^2} \left[ (1 - x)^n - \left(\frac{1}{1+x}\right)^n \right] \]

Very slowly convergent series if \( x \) is small
(Rydberg states, Hydride ion).
Particular case:

\[ I_2(-2, -1, -2, a, b) = \frac{8\pi^2}{b} \left\{ \frac{\pi^2}{3} - \left[ \ln \left(1 + \frac{a}{b}\right) \right]^2 \right. \]

\[ + \quad \text{Li}_2 \left(1 - \frac{a}{b}\right) - \text{Li}_2 \left(\frac{b}{b+a}\right) \} \quad [1] \]

Last two terms cancel some digits if \( x = a/b \) is small.

\[ S(x) = \text{Li}_2 \left(1 - x\right) - \text{Li}_2 \left(\frac{1}{1+x}\right) = \sum_{n=1}^{\infty} \frac{1}{n^2} \left[ (1 - x)^n - \left(\frac{1}{1+x}\right)^n \right] \]

Very slowly convergent series if \( x \) is small
(Rydberg states, Hydride ion).

Test 5: $S(x = 0.001)$

- Use of $\alpha = 3/2$, although $a_n$ does not behave as a negative power.
Test 5: $S(x = 0.001)$

- Use of $\alpha = 3/2$, although $a_n$ does not behave as a negative power.

- $(n = 20)$
Three electron integrals

\[ I_3(i, j, k, l, m, n, a, b, c) = \int \int \int d\vec{r}_1 d\vec{r}_2 d\vec{r}_3 r_1^i r_2^j r_3^k r_{12}^l r_{23}^m r_{31}^n e^{-ar_1 - br_2 - cr_3} \]
Three electron integrals

\[ I_3(i, j, k, l, m, n, a, b, c) = \int \int \int d\vec{r}_1 d\vec{r}_2 d\vec{r}_3 r_i^1 r_j^2 r_k^3 r_{12}^l r_{23}^m r_{31}^n e^{-ar_1 - br_2 - cr_3} \]

- Multiple series when expanding \( r_{ij} \), even more when avoiding \( r_<, r_> \)
  
  (project with F.W. King and C. H. Leong).
Three electron integrals

\[ I_3(i, j, k, l, m, n, a, b, c) = \int \int \int d\mathbf{r}_1 d\mathbf{r}_2 d\mathbf{r}_3 r_1^i r_2^j r_3^k r_{12}^l r_{23}^m r_{31}^n e^{-ar_1 - br_2 - cr_3} \]

Multiple series when expanding \( r_{ij} \), even more when avoiding \( r_1, r_2 \) (project with F.W. King and C. H. Leong).

Let us examine a particular case:

\[ I_3(i, j, k, l, 0, 0, a, a, c) = \frac{(4\pi)^3}{\Gamma(-l/2)} \frac{(k + 2)! (i + j + l + 5)!}{c^{k+3} a^{i+j+l+6}} S_l(i, j) \]

where

\[ S_l(i, j) = \sum_{n=0}^{\infty} \frac{\Gamma(n - l/2) \Gamma(i + n + 3) \Gamma(j + n + 3)}{\Gamma(n + 2) \Gamma(n + 3 + (i + j)/2) \Gamma(n + 3 + (i + j + 1)/2)} \]
Three electron integrals

\[ I_3(i, j, k, l, m, n, a, b, c) = \int \int \int d\vec{r}_1 d\vec{r}_2 d\vec{r}_3 r_1^i r_2^j r_3^k r_{12}^l r_{23}^m r_{31}^n e^{-ar_1 - br_2 - cr_3} \]

Multiple series when expanding \( r_{ij} \), even more when avoiding \( r_\prec, r_\succ \) (project with F.W. King and C. H. Leong).

Let us examine a particular case:

\[ I_3(i, j, k, l, 0, 0, a, a, c) = \frac{(4\pi)^3}{\Gamma(-l/2)} \frac{(k + 2)! (i + j + l + 5)!}{c^{k+3} a^{i+j+l+6}} S_l(i, j) \]

where

\[ S_l(i, j) = \sum_{n=0}^{\infty} \frac{\Gamma(n - l/2) \Gamma(i + n + 3) \Gamma(j + n + 3)}{\Gamma(n + 2) \Gamma(n + 3 + (i + j)/2) \Gamma(n + 3 + (i + j + 1)/2)} \]

The general term behaves as \( n^{-(l+5)/2} \). In practical variational calculations, the worst case is \( l = -1 \), for which \( a_n \sim n^{-2} \).
\( S_{-1}(i, j) \) can be summed up exactly, and the remainder is known, for particular values of \( i \) and \( j \).
\( S_{-1}(i, j) \) can be summed up exactly, and the remainder is known, for particular values of \( i \) and \( j \).

We will study the remainder for small values of \( i \) and \( j \) and trying to extrapolate the best accelerator.
\( S_{-1}(i, j) \) can be summed up exactly, and the remainder is known, for particular values of \( i \) and \( j \).

We will study the remainder for small values of \( i \) and \( j \) and trying to extrapolate the best accelerator.

\( S_{-1}(0, 0) \):

\[
S - S_n = (n + 2) a_n \left[ 1 - \frac{5}{4(n + 2)} - \frac{3}{8(n + 2)^2} \right]
= n^{-1} \left[ 1 - \frac{9}{8(n + 3/2)} - \frac{5}{8(n + 5/2)} \right]
\]
\( S_{-1}(i, j) \) can be summed up exactly, and the remainder is known, for particular values of \( i \) and \( j \).

We will study the remainder for small values of \( i \) and \( j \) and trying to extrapolate the best accelerator.

\( S_{-1}(0, 0) \):

\[
S - S_n = (n + 2) a_n \left[ 1 - \frac{5}{4(n + 2)} - \frac{3}{8(n + 2)^2} \right] = n^{-1} \left[ 1 - \frac{9}{8(n + 3/2)} - \frac{5}{8(n + 5/2)} \right]
\]

\( u \)-Levin exact for \( \beta = 2 \).
Other cases

$S_{-1}(1, 1)$:

$$
S - S_n = (n + 2) a_n \left[ 1 - \frac{13/8}{n + 2} - \frac{13/8}{(n + 2)^2} - \frac{5/8}{n + 3} \right]
$$

$$
= n^{-1} \left[ 1 - \frac{15/16}{n + 3/2} - \frac{3/8}{n + 5/2} - \frac{7/16}{n + 7/2} \right]
$$
Other cases

- $S_{-1}(1, 1)$:

\[
S - S_n = (n + 2) a_n \left[ 1 - \frac{13/8}{n + 2} - \frac{13/8}{(n + 2)^2} - \frac{5/8}{n + 3} \right]
\]

\[
= n^{-1} \left[ 1 - \frac{15/16}{n + 3/2} - \frac{3/8}{n + 5/2} - \frac{7/16}{n + 7/2} \right]
\]

- $S_{-1}(2, 0)$:

\[
S - S_n = (n + 2) a_n \left[ 1 - \frac{17/16}{n + 2} - \frac{3/8}{(n + 2)^2} - \frac{7/16}{n + 4} \right]
\]

\[
= n^{-1} \left[ 1 - \frac{21/16}{n + 3/2} - \frac{5/8}{n + 5/2} + \frac{7/16}{n + 7/2} \right]
\]
Other cases

- \( S_{-1}(1, 1) \):
  \[
  S - S_n = (n + 2)\, a_n \left[ 1 - \frac{13/8}{n + 2} - \frac{13/8}{(n + 2)^2} - \frac{5/8}{n + 3} \right]
  = n^{-1} \left[ 1 - \frac{15/16}{n + 3/2} - \frac{3/8}{n + 5/2} - \frac{7/16}{n + 7/2} \right]
  \]

- \( S_{-1}(2, 0) \):
  \[
  S - S_n = (n + 2)\, a_n \left[ 1 - \frac{17/16}{n + 2} - \frac{3/8}{(n + 2)^2} - \frac{7/16}{n + 4} \right]
  = n^{-1} \left[ 1 - \frac{21/16}{n + 3/2} - \frac{5/8}{n + 5/2} + \frac{7/16}{n + 7/2} \right]
  \]

- \( S_{-1}(2, 2) \):
  \[
  S - S_n = (n + 2)\, a_n \left[ 1 - \frac{477/256}{n + 2} - \frac{45/128}{(n + 2)^2} + \frac{45/64}{n + 3} + \frac{105/256}{n + 4} \right]
  = n^{-1} \left[ 1 - \frac{105/128}{n + 3/2} - \frac{75/128}{n + 5/2} - \frac{76/128}{n + 7/2} - \frac{45/128}{n + 9/2} \right]
  \]
For a series for which:

\[ S_n = S + \omega_n \sum_{j=0}^{k-1} \frac{C_j}{(n + \beta)_j} \]
Weniger transformation

For a series for which:

\[ S_n = S + \omega_n \sum_{j=0}^{k-1} \frac{C_j}{(n + \beta)_j} \]

Then, multiplying by \((n + \beta)_{k-1}\) both sides:

\[ (n + \beta)_{k-1} \frac{S_n - S}{\omega_n} = \text{polynomial in } n \text{ of degree } k - 1 \]
Weniger transformation

For a series for which:

\[ S_n = S + \omega_n \sum_{j=0}^{k-1} \frac{C_j}{(n + \beta)_j} \]

Then, multiplying by \((n + \beta)_{k-1}\) both sides:

\[(n + \beta)_{k-1} \frac{S_n - S}{\omega_n} = \text{polynomial in } n \text{ of degree } k - 1\]

And applying \(\Delta^k\) to this equation:

\[
S = \frac{\sum_{j=0}^{k} (-1)^j \binom{k}{j} \frac{(n + j + \beta)_{k-1}}{(n + k + \beta)_{k-1}} \frac{S_{n+j}}{\omega_{n+j}}}{\sum_{j=0}^{k} (-1)^j \binom{k}{j} \frac{(n + j + \beta)_{k-1}}{(n + k + \beta)_{k-1}} \frac{1}{\omega_{n+j}}}\]
Generalization

For a series for which:

\[ S_n = S + \omega_n \left[ C_0 + \frac{C_{11}}{n + \beta_1} + \frac{C_{12}}{(n + \beta_1)^2} + \cdots + \frac{C_{1p_1}}{(n + \beta_1)^{p_1}} + \cdots \right. \]

\[ + \left. \frac{C_{l1}}{n + \beta_l} + \frac{C_{l2}}{(n + \beta_l)^2} + \cdots + \frac{C_{lp_l}}{(n + \beta_l)^{p_l}} + \cdots \right] \]
Generalization

For a series for which:

\[ S_n = S + \omega_n \left[ C_0 + \frac{C_{11}}{n + \beta_1} + \frac{C_{12}}{(n + \beta_1)^2} + \cdots + \frac{C_{1p_1}}{(n + \beta_1)^{p_1}} + \cdots \right. 
+ \left. \frac{C_{l_1}}{n + \beta_l} + \frac{C_{l_2}}{(n + \beta_l)^2} + \cdots + \frac{C_{l_{p_l}}}{(n + \beta_l)^{p_l}} + \cdots \right] \]

Multiplying by \((n + \beta_1)^{p_1} \cdots (n + \beta_l)^{p_l}\) and applying \(\Delta^k\) with \(k = p_1 + p_2 + \cdots p_l + 1\)

\[ S = \frac{\sum_{j=0}^{k} (-1)^j \binom{k}{j} \frac{(n + j + \alpha_1) \cdots (n + j + \alpha_k)}{(n + k + \alpha_1) \cdots (n + k + \alpha_k)} S_{n+j}}{\sum_{j=0}^{k} (-1)^j \binom{k}{j} \frac{(n + j + \alpha_1) \cdots (n + j + \alpha_k)}{(n + k + \alpha_1) \cdots (n + k + \alpha_k)} \frac{1}{\omega_{n+j}}} \]

where \(\alpha_1 = \cdots \alpha_{p_1} = \beta_1, \alpha_{p_1+1} = \cdots \alpha_{p_1+p_2} = \beta_2, \text{ and so on.}\)
Generalization

For a series for which:

\[ S_n = S + \omega_n \left[ C_0 + \frac{C_{11}}{n + \beta_1} + \frac{C_{12}}{(n + \beta_1)^2} + \cdots + \frac{C_{1p_1}}{(n + \beta_1)^{p_1}} + \cdots \right. \]

\[ + \frac{C_{l_1}}{n + \beta_l} + \frac{C_{l_2}}{(n + \beta_l)^2} + \cdots + \frac{C_{l_{p_l}}}{(n + \beta_l)^{p_l}} + \cdots \]

Multiplying by \((n + \beta_1)^{p_1} \cdots (n + \beta_l)^{p_l}\) and applying \(\Delta^k\) with \(k = p_1 + p_2 + \cdots p_l + 1\)

\[ S = \sum_{j=0}^{k} \left( -1 \right)^j \binom{k}{j} \frac{(n + j + \alpha_1) \cdots (n + j + \alpha_k)}{(n + k + \alpha_1) \cdots (n + k + \alpha_k)} \left[ S_{n+j} \right. \]

\[ \left. \frac{1}{\omega_{n+j}} \right] \]

where \(\alpha_1 = \cdots \alpha_{p_1} = \beta_1, \alpha_{p_1+1} = \cdots \alpha_{p_1+p_2} = \beta_2\), and so on.

This is a generalization (including \(\omega_n\)) of the generalization of Levin and Weniger transform by Čížek-Zamastil-Skála, also studied by Weniger.
**Generalization**

For a series for which:

\[ S_n = S + \omega_n \left[ C_0 + \frac{C_{11}}{n + \beta_1} + \frac{C_{12}}{(n + \beta_1)^2} + \cdots + \frac{C_{1p_1}}{(n + \beta_1)^{p_1}} + \cdots \right. \]

\[ + \left. \frac{C_{l1}}{n + \beta_l} + \frac{C_{l2}}{(n + \beta_l)^2} + \cdots + \frac{C_{lp_l}}{(n + \beta_l)^{p_l}} + \cdots \right] \]

Multiplying by \((n + \beta_1)^{p_1} \cdots (n + \beta_l)^{p_l}\) and applying \(\Delta^k\) with \(k = p_1 + p_2 + \cdots p_l + 1\)

\[
S = \sum_{j=0}^{k} (-1)^j \binom{k}{j} \frac{(n + j + \alpha_1) \cdots (n + j + \alpha_k)}{(n + k + \alpha_1) \cdots (n + k + \alpha_k)} \frac{S_{n+j}}{\omega_{n+j}}
\]

where \(\alpha_1 = \cdots \alpha_{p_1} = \beta_1, \alpha_{p_1+1} = \cdots \alpha_{p_1+p_2} = \beta_2,\) and so on.

This is a generalization (including \(\omega_n\)) of the generalization of Levin and Weniger transform by Čížek-Zamastil-Skála, also studied by Weniger.
Application:

For $S_{-1}(i, j)$ sums, previous formula can be applied:
Application:

- For $S_{-1}(i, j)$ sums, previous formula can be applied:

- **Case 1:** Use $\omega_n = (n + 2)a_n$ and $\alpha_1 = \alpha_2 = 2$, $\alpha_3 = \alpha_4 = 3$, ...
Application:

- For $S_{-1}(i, j)$ sums, previous formula can be applied:
  - Case 1: Use $\omega_n = (n + 2)a_n$ and $\alpha_1 = \alpha_2 = 2$, $\alpha_3 = \alpha_4 = 3, \ldots$
  - Case 2: Use $\omega_n = n^{-1}$ and $\alpha_i = i + 1/2$
Application:

- For $S_{-1}(i, j)$ sums, previous formula can be applied:
  - **Case 1:** Use $\omega_n = (n + 2)a_n$ and $\alpha_1 = \alpha_2 = 2, \alpha_3 = \alpha_4 = 3, \ldots$
  - **Case 2:** Use $\omega_n = n^{-1}$ and $\alpha_i = i + 1/2$
  - $S_1(1, 1)$:

![Graph](image)
Conclusions:

\[ \omega_n = (n + \beta)^{-\alpha + 1} \] is a interesting alternative to \( u \)-Levin when \( a_n \sim n^{-\alpha} \).
Conclusions:

- \( \omega_n = (n + \beta)^{-\alpha + 1} \) is an interesting alternative to \( u \)-Levin when \( a_n \sim n^{-\alpha} \)

- Use of differences of partial sums instead of \( S_{n+j} \) improves slightly the optimal result.
Conclusions:

- \( \omega_n = (n + \beta)^{-\alpha + 1} \) is a interesting alternative to \( u \)-Levin when \( a_n \sim n^{-\alpha} \)

- Use of differences of partial sums instead of \( S_{n+j} \) improves slightly the optimal result.

- Multiple precision calculations are required for some very slowly converging series.
Conclusions:

- $\omega_n = (n + \beta)^{-\alpha+1}$ is an interesting alternative to $u$-Levin when $a_n \sim n^{-\alpha}$

- Use of differences of partial sums instead of $S_{n+j}$ improves slightly the optimal result.

- Multiple precision calculations are required for some very slowly converging series.

- Generalization of the transformation of Čížek et al. is adequate for the three-electron integral problem.
Conclusions:

- \( \omega_n = (n + \beta)^{-\alpha + 1} \) is an interesting alternative to \( u \)-Levin when \( a_n \sim n^{-\alpha} \)

- Use of differences of partial sums instead of \( S_{n+j} \) improves slightly the optimal result.

- Multiple precision calculations are required for some very slowly converging series.

- Generalization of the transformation of Čížek et al. is adequate for the three-electron integral problem.

- Weniger’s treatment using \( \Delta^k \) is a powerful formalism for the design of convergence accelerators.