METHODS FOR THE CONSTRUCTION OF EXTRAPOLATION PROCESSES

Herbert H. H. Homeier, Regensburg

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- **General Approach**
- **Iterative Approach**
- **Variational Approach**
- **Perturbative Approach**

MANY THANKS TO

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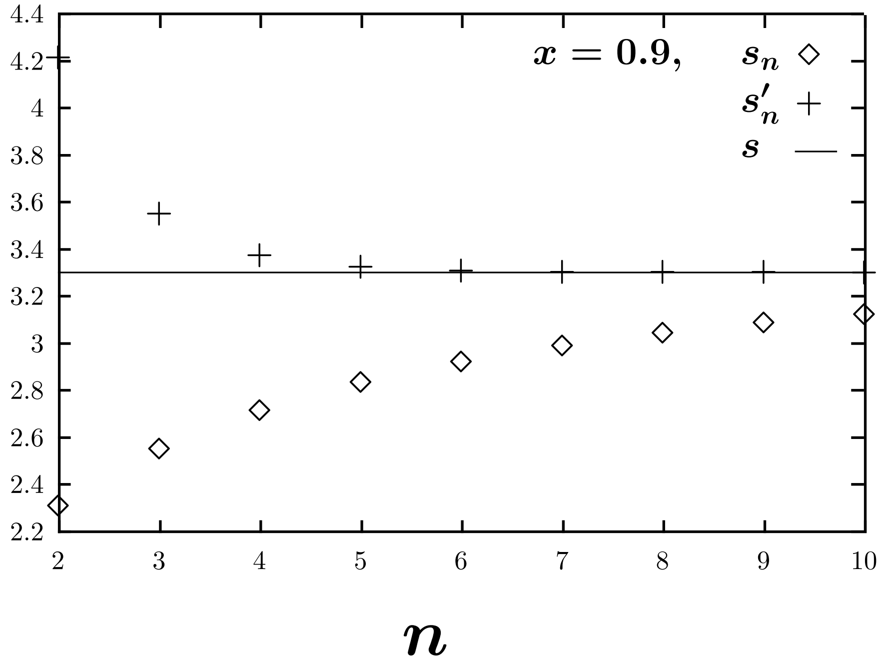
Development of Methods:
Extrapolation Methods

Problem:
Slow Convergence

Example

$$s_n = 1 + \frac{x}{1} + \frac{x^2}{2} + \frac{x^3}{3} + \cdots + \frac{x^n}{n}$$
$$s = \lim_{n \to \infty} s_n = 1 - \ln(1-x)$$



Sequence transformation $\{s'_n\} = T(\{s_n\})$:
Accelerate convergence

Development of Methods: *Extrapolation Methods*

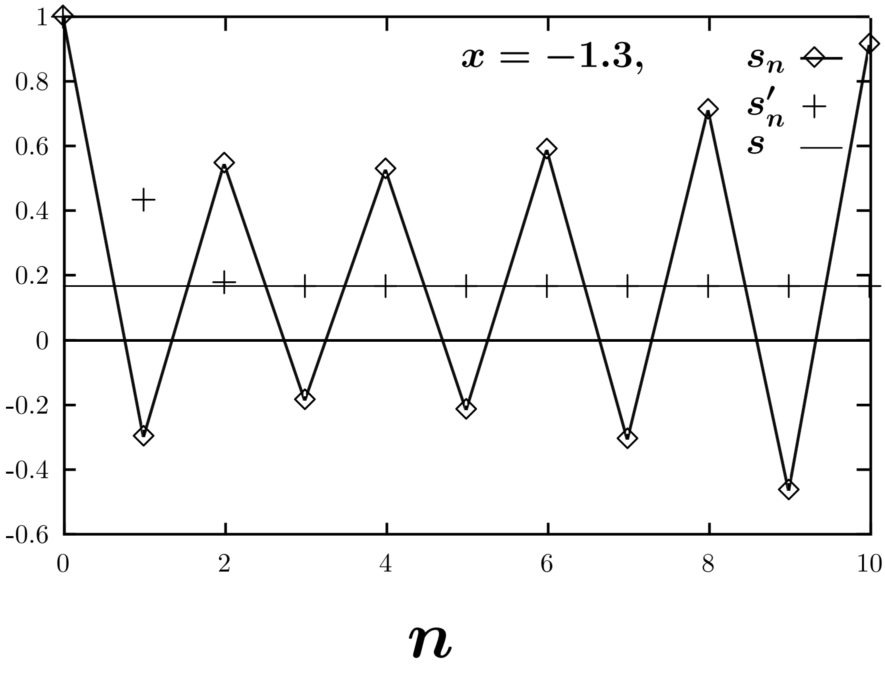
Problem:

No Convergence

Example:

$$s_n = 1 + \frac{x}{1} + \frac{x^2}{2} + \frac{x^3}{3} + \cdots + \frac{x^n}{n}$$

$$s = \lim_{n\to\infty} s_n = 1 - \ln(1-x)$$



Sequence transformation $\{s'_n\} = T(\{s_n\})$:

Achieve convergence

PROBLEMS

- **Extrapolation**
- **Convergence acceleration**
- **Summation of divergent series**
- **No universal method available**
- **Linear methods often not efficient enough**
- **Accuracy of single method unknown in practice**

AIMS

- **problem adapted**
- **nonlinear**
- **efficient**

APPROACH

- **Model sequences**
- **Iteration of simple methods**
- **Comparison of results of various methods**

BASIC PRINCIPLE **EXAMPLE**

Model sequences
$\sigma_n = \sigma + \mathcal{M}_n(\vec{c}, \vec{p}(n))$

$$\sigma_n = \sigma + c\,\omega_n$$

Exact Calculation of σ
$\sigma = T_n(\{\sigma_n\}, \vec{p}(n))$

$$\sigma = \sigma_{n+1} - \omega_{n+1}\frac{\sigma_{n+1} - \sigma_n}{\omega_{n+1} - \omega_n}$$

Sequence transformation for problem $\{s_n\}$
$s'_n = T_n(\{s_n\}, \vec{p}(n))$

$$s'_n = s_{n+1} - \omega_{n+1}\frac{s_{n+1} - s_n}{\omega_{n+1} - \omega_n}$$

Acceleration for
$\{s_n\} \approx \{\sigma_n\}$

$$\frac{s_n - s}{\omega_n} = O(1)$$

ANNIHILATION OPERATORS

$$\sigma_n = \sigma + \omega_n \sum_{j=0}^{k} c_j \phi_j(n)$$

with linear operator

$$\mathcal{O}_n(\phi_j(n)) = 0\,, \qquad j = 0, \ldots, k$$

then

$$\mathcal{O}_n\left(\frac{\sigma_n - \sigma}{\omega_n}\right) = 0$$

or

$$\sigma = \frac{\mathcal{O}_n(\sigma_n/\omega_n)}{\mathcal{O}_n(1/\omega_n)} \Longrightarrow s'_n = \frac{\mathcal{O}_n(s_n/\omega_n)}{\mathcal{O}_n(1/\omega_n)}$$

CONVERGENCE CLASSIFICATION

$$\lim_{n\to\infty} \frac{s_{n+1} - s}{s_n - s} = \rho$$

linearly convergent: $0 < |\rho| < 1$
logarithmically convergent: $\rho = 1$

REMAINDER ESTIMATES

$$\frac{s_n - s}{\omega_n} = O(1)\,, \qquad n \to \infty$$

Series

$$s_n = \sum_{j=0}^{n} a_j \to s\,, \quad n \to \infty$$

Levin

$$\begin{aligned} {}^{t}\omega_n &= a_n\,, \\ {}^{u}\omega_n &= (n+\beta)a_n\,, \qquad \beta > 0\,, \\ {}^{v}\omega_n &= \frac{a_n a_{n+1}}{a_n - a_{n+1}}\,. \end{aligned}$$

Smith and Ford

$${}^{\tilde{t}}\omega_n = a_{n+1}$$

Asymptotically related series

$$\hat{a}_n \sim a_n$$

$$\hat{s}_n = \sum_{j=0}^{n} \hat{a}_j \to \hat{s}\,, \quad n \to \infty$$

Linear remainder estimates

$$\begin{aligned}
{}^{lt}\omega_n &= \hat{a}_n\,, \\
{}^{lu}\omega_n &= (n+\beta)\hat{a}_n\,, \qquad \beta > 0\,, \\
{}^{lv}\omega_n &= \frac{\hat{a}_n \hat{a}_{n+1}}{\hat{a}_n - \hat{a}_{n+1}}\,, \\
{}^{l\tilde{t}}\omega_n &= \hat{a}_{n+1}
\end{aligned}$$

Kummer-type remainder estimate

$${}^{k}\omega_n = \hat{s}_n - \hat{s}$$

Tails

$$T_n = a_{n+1} + a_{n+2} + \cdots = s - s_n$$

$$\begin{aligned}
{}^{\tilde{t}}T_n &= s_{n+1} - s_n = a_{n+1} + 0 + \cdots\,, \\
{}^{l\tilde{t}}T_n &= \hat{s}_{n+1} - \hat{s}_n = \hat{a}_{n+1} + 0 + \cdots\,, \\
{}^{k}T_n &= \hat{s} - \hat{s}_n = \hat{a}_{n+1} + \hat{a}_{n+2} + \cdots\,.
\end{aligned}$$

Example

$$F_m(z) = \sum_{j=0}^{\infty} (-z)^j / j!(2m + 2j + 1) \, ,$$

$$^{k}\omega_n = \left((1 - e^{-z})/z - \sum_{j=0}^{n} (-z)^j/(j+1)! \right) .$$

n	s_n	$^{u}\omega_n$	$^{t}\omega_n$	$^{k}\omega_n$
5	–13.3	0.3120747	0.3143352	0.3132981
6	14.7	0.3132882	0.3131147	0.3133070
7	–13.1	0.3132779	0.3133356	0.3133087
8	11.4	0.3133089	0.3133054	0.3133087
9	–8.0	0.3133083	0.3133090	0.3133087

$z = 8 \, , m = 0$

$_2$J-Transformation

ITERATIVE SEQUENCE TRANSFORMATIONS

Idea:

- **Simple sequence transformation**

$$\{s'_n\} = T(\{s_n\})$$

- **Iteration:**

$$\{s''_n\} = T'(\{s'_n\}), \{s'''_n\} = T''(\{s''_n\}), \ldots$$

- **Example: Aitken Δ^2 method**

$$s_n^{(1)} = s_n - \frac{(s_{n+1} - s_n)^2}{s_{n+2} - 2s_{n+1} + s_n} .$$

Iteration

$$\mathcal{A}_0^{(n)} = s_n ,$$

$$\mathcal{A}_{k+1}^{(n)} = \mathcal{A}_k^{(n)} - \frac{(\mathcal{A}_k^{(n+1)} - \mathcal{A}_k^{(n)})^2}{\mathcal{A}_k^{(n+2)} - 2\mathcal{A}_k^{(n+1)} + \mathcal{A}_k^{(n)}} .$$

Problem:

- **Iteration not unique, for example**

$$s_n^{(k+1)} = T^{(k)}(\{s_n^{(k)}\})$$

with $T^{(0)} = T$.

- **Example**

$$\begin{aligned} \overline{\mathcal{A}}_0^{(n)} &= s_n \,, \\ \overline{\mathcal{A}}_{k+1}^{(n)} &= \overline{\mathcal{A}}_k^{(n)} \\ & \qquad - X_k \, \frac{(\overline{\mathcal{A}}_k^{(n+1)} - \overline{\mathcal{A}}_k^{(n)})^2}{\overline{\mathcal{A}}_k^{(n+2)} - 2\overline{\mathcal{A}}_k^{(n+1)} + \overline{\mathcal{A}}_k^{(n)}} \end{aligned}$$

with $X_0 = 1$ "allowed",
i.e., $X_k = (2k+1)/(k+1)$.

HIERARCHICAL CONSISTENCY

Example:

- Simple transformation:

$$s'_n = s_{n+1} - \omega_{n+1} \frac{s_{n+1} - s_n}{\omega_{n+1} - \omega_n}$$

- Problem: ω'_n ?
- For

$$\sigma_n = \sigma + \omega_n (c_0 + c_1 r_n)$$

  we have

$$\sigma'_n = \sigma - c_1 \frac{\omega_n \omega_{n+1}}{\omega_{n+1} - \omega_n} (r_{n+1} - r_n)$$

- Hence

$$\omega'_n = -\frac{\omega_n \omega_{n+1}}{\omega_{n+1} - \omega_n} (r_{n+1} - r_n)$$

- Iteration $\Longrightarrow \mathcal{J}$ transformation

$$s_n^{(0)} = s_n \,, \qquad \omega_n^{(0)} = \omega_n \,,$$

$$s_n^{(k+1)} = s_n^{(k)} - \omega_n^{(k)} \frac{s_{n+1}^{(k)} - s_n^{(k)}}{\omega_{n+1}^{(k)} - \omega_n^{(k)}} \,,$$

$$\omega_n^{(k+1)} = - \frac{\omega_n^{(k)} \omega_{n+1}^{(k)}}{\omega_{n+1}^{(k)} - \omega_n^{(k)}} \, \delta_n^{(k)} \,,$$

$$\mathcal{J}_n^{(k)}(\{s_n\}, \{\omega_n\}, \{r_n^{(k)}\}) = s_n^{(k)}$$

- for power series,
- very versatile and powerful.
- related to E algorithm with model

$$\sigma_n = \sigma + \sum_{j=0}^{k} c_j \, g_j(n)$$

- **Analysed in**
  H. H. H. Homeier, A hierarchically consistent, iterative sequence transformation, Numer. Algo. 8 (1994) 47-81.
  —, Analytical and numerical studies of the convergence behavior of the $\mathcal{J}$ transformation, J. Comput. Appl. Math. 69 (1996) 81-112.
  —, Determinantal representations for the $\mathcal{J}$ transformation, Numer. Math. 71 (1995) 275-288.

Numerical example:

$$G_n = \int_0^1 \left\{ \int_{-\infty}^{\infty} \frac{\Gamma/\pi}{(x-\Delta\omega)^2+\Gamma^2} \left(\exp\left[-\frac{Y q^2 \Gamma/\pi}{x^2+\Gamma^2} \right] - 1 \right) \, dx \right\} q^n \, dq$$

Taylor series in $Y \Longrightarrow$ Power series
Acceleration with $\mathcal{J}$ transformation

n	s_n	$s_0^{(n)}$
15	-3047434.	-0.16361565
16	5412146.	-0.16361782
17	-9099655.	-0.16361716
18	14525645.	-0.16361732
19	-22070655.	-0.16361728
20	31994427.	-0.16361729
∞	-0.16361729	-0.16361729

$n=2$, $\Delta\omega=5$, $\Gamma=1$, $Y=100$, $r_k^{(k)}=1/(n+1+k)$, k variant

More general:

- Hierarchy of model sequences: The higher, the more parameters
- Iteration of simple transformation T is consistent, if
  - T is exact for lowest level sequences
  - Variant of T maps higher to lower level

EXAMPLE:
Hierarchy for $\mathcal{J}$ transformation

$$\sigma_n = \sigma + \omega_n \Big(c_0 + c_1 \sum_{n_1=0}^{n-1} \delta_{n_1}^{(0)} + c_2 \sum_{n_1=0}^{n-1} \delta_{n_1}^{(0)} \sum_{n_2=0}^{n_1-1} \delta_{n_2}^{(1)} + \cdots \Big)$$

at level k.

FORMAL DESCRIPTION

- Simple model $\{\boldsymbol{\sigma}_n(\vec{c},\vec{p})\} \rightarrow \boldsymbol{\sigma}(\vec{p})$
- Simple transformation

$$T(\vec{p}\,) : \{\boldsymbol{\sigma}_n(\vec{c},\vec{p}\,)\}_{n=0}^{\infty} \longrightarrow \{\boldsymbol{\sigma}(\vec{p}\,)\}_{n=0}^{\infty}$$

- Hierarchy of model sequences

$$\{\{\boldsymbol{\sigma}_n^{(\ell)}(\vec{c}^{\,(\ell)},\vec{p}^{(\ell)})|\vec{c}^{(\ell)} \in \mathbb{C}^{a^{(\ell)}}\}_{n=0}^{\infty}\}_{\ell=0}^{L}$$

with $a^{(\ell)} > a^{(\ell')}$ for $\ell > \ell'$

- Mapping between levels

$$T(\vec{p}^{\,(\ell)}) : \{\boldsymbol{\sigma}_n^{(\ell)}(\vec{c}^{\,(\ell)},\vec{p}^{\,(\ell)})\}_{n=0}^{\infty} \longrightarrow \{\boldsymbol{\sigma}_n^{(\ell-1)}(\vec{c}^{\,(\ell-1)},\vec{p}^{\,(\ell-1)})\}_{n=0}^{\infty}$$

- Hierarchical consistent transformation

$$T^{(\ell)} = T(\vec{p}^{\,(0)}) \circ T(\vec{p}^{\,(1)}) \circ \ldots \circ T(\vec{p}^{\,(\ell)})$$

METHODS FOR ORTHOGONAL SERIES

- $\mathcal{I}$ **transformation:**
  - **Simple model sequence:**

    $$\sigma_n = \sigma + \omega_n (c \exp(in\nu) + d \exp(-in\nu))$$

  - **Simple sequence transformation**

    $$s'_n = \frac{\dfrac{s_{n+2}}{\omega_{n+2}} - 2\cos(\nu)\,\dfrac{s_{n+1}}{\omega_{n+1}} + \dfrac{s_n}{\omega_n}}{\dfrac{1}{\omega_{n+2}} - 2\cos(\nu)\,\dfrac{1}{\omega_{n+1}} + \dfrac{1}{\omega_n}}$$

  - **Compute ω'_n ?**
  - **More complicated model sequence:**

    $$\sigma_n = \sigma + \omega_n (e^{in\nu}(c_0 + c_1 r_n) + e^{-in\nu}(d_0 + d_1 r_n))$$

    yields

    $$\sigma'_n \approx \sigma + \omega'_n (c' \exp(in\nu) + d' \exp(-in\nu))$$

    $$\omega'_n = \frac{-(r_{n+1} - r_n)}{\dfrac{1}{\omega_{n+2}} - 2\cos(\nu)\,\dfrac{1}{\omega_{n+1}} + \dfrac{1}{\omega_n}}$$

– Iteration $\Longrightarrow$ $\mathcal{I}$ transformation

$$s_n^{(0)} = s_n \,, \qquad \omega_n^{(0)} = \omega_n$$

$$s_n^{(k+1)} = \frac{\dfrac{s_{n+2}^{(k)}}{\omega_{n+2}^{(k)}} - 2\cos(\nu)\,\dfrac{s_{n+1}^{(k)}}{\omega_{n+1}^{(k)}} + \dfrac{s_n^{(k)}}{\omega_n^{(k)}}}{\dfrac{1}{\omega_{n+2}^{(k)}} - 2\cos(\nu)\,\dfrac{1}{\omega_{n+1}^{(k)}} + \dfrac{1}{\omega_n^{(k)}}}$$

$$\omega_n^{(k+1)} = \frac{-\Delta r_{n+1}^{(k)}}{\dfrac{1}{\omega_{n+2}^{(k)}} - 2\cos(\nu)\,\dfrac{1}{\omega_{n+1}^{(k)}} + \dfrac{1}{\omega_n^{(k)}}}$$

– for Fourier series

– Notice three-term recurrence

$$u_{n+2} - 2\cos(\nu) u_{n+1} + u_n = 0$$

satisfied by $\exp(\pm i n \nu)$
(or $\cos(n\nu)$, $\sin(n\nu)$)

- $\mathcal{K}$ **transformation:**
  - **Simple model sequence :**

$$\sigma_n = \sigma + c\omega_n P_n(\cos(\nu))$$

  - **Three-term recurrence**

$$\zeta_n^{(0)} P_n + \zeta_n^{(1)} P_{n+1} + \zeta_n^{(2)} P_{n+2} = 0 \,.$$

    (ν dependent)
  - **Algorithm (analog to $\mathcal{I}$ transformation)**

$$s_n^{(0)} = s_n \,, \qquad \omega_n^{(0)} = \omega_n \,,$$

$$s_n^{(k+1)} = \frac{\zeta_{n+k}^{(0)} \dfrac{s_n^{(k)}}{\omega_n^{(k)}} + \zeta_{n+k}^{(1)} \dfrac{s_{n+1}^{(k)}}{\omega_{n+1}^{(k)}} + \zeta_{n+k}^{(2)} \dfrac{s_{n+1}^{(k)}}{\omega_{n+1}^{(k)}}}{\zeta_{n+k}^{(0)} \dfrac{1}{\omega_n^{(k)}} + \zeta_{n+k}^{(1)} \dfrac{1}{\omega_{n+1}^{(k)}} + \zeta_{n+k}^{(2)} \dfrac{1}{\omega_{n+1}^{(k)}}}$$

$$\omega_n^{(k+1)} = \frac{\delta_n^{(k)}}{\zeta_{n+k}^{(0)} \dfrac{1}{\omega_n^{(k)}} + \zeta_{n+k}^{(1)} \dfrac{1}{\omega_{n+1}^{(k)}} + \zeta_{n+k}^{(2)} \dfrac{1}{\omega_{n+1}^{(k)}}}$$

$$\mathcal{K}_n^{(k)}(\{\delta_n^{(k)}\}, \{\zeta_n^{(j)}\}, \{s_n\}, \{\omega_n\}) = s_n^{(k)}$$

  - **ν dependent, for orthogonal series.**

MULTIPOLE EXPANSIONS

$$U_Q(\vec{r}) = 4\pi \sum_{\ell m} \frac{1}{r^{\ell+1}} \frac{Y_\ell^m(\vec{r}/r)}{2\ell+1} Q_\ell^{m*}$$

$$Q_\ell^m = \int r'^\ell Y_\ell^m(\vec{r}'/r')\rho(\vec{r}')\,\mathrm{d}^3r'\,,$$

Rotational symmetry

$$U_Q(\vec{r}) = \sum_{\ell=0}^{\infty} P_\ell\left(\frac{\vec{r}\cdot\vec{R}}{r\,R}\right)\frac{q_\ell}{r^{\ell+1}}$$

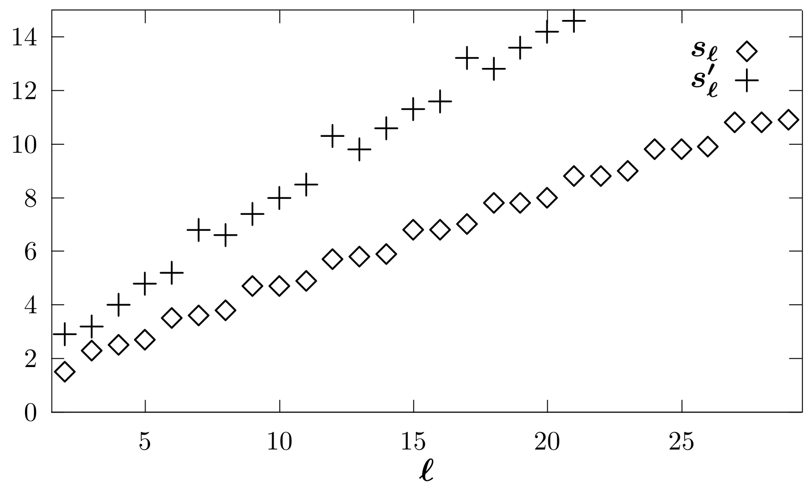
Legendre Expansion

Example

$$\rho(\vec{r}) = \exp(-\alpha r)\exp(-\beta|\vec{r} - \vec{R}|)$$

ℓ	$-\lg\|1 - s_\ell/s\|$	$-\lg\|1 - s'_\ell/s\|$
2	2.6	5.1
4	4.3	9.7
6	5.9	11.5
8	7.6	16.0
10	9.2	16.0

$\mathcal{K}$ **transformation,** $r = 12$, $\theta = 60^o$



Exact digits ($r = 4$, $\theta = 60^o$)

MANYFOLD FREQUENCIES

- Important near singularities
- Increases stability
- Instead of

$$s_0, s_1, s_2, \ldots \;, \omega_0, \omega_1, \omega_2, \ldots$$

take

$$s_{\tau \cdot 0}, s_{\tau \cdot 1}, s_{\tau \cdot 2}, \ldots \;, \omega_{\tau \cdot 0}, \omega_{\tau \cdot 1}, \omega_{\tau \cdot 2}, \ldots$$

- for Fourier and orthogonal series put

$$\nu \longrightarrow \tau \cdot \nu$$

i.e., for $x = \cos \nu$

$$x \longrightarrow x_\tau = \cos(\tau \cdot \arccos x)$$

$$\sum_{\ell=0}^{\infty} \frac{1}{\ell+1} P_{\ell}(x) = \ln \left(1 + \sqrt{\frac{2}{1-x}} \right)$$

$$x = 0.9$$

$\mathcal{K}$ transformation

$\tau = 1$

n	$-\lg \lvert 1 - s_n/s \rvert$	$-\lg \lvert 1 - s'_n/s \rvert$
16	2.07	5.24
18	1.75	6.88
20	1.91	6.58
22	3.59	6.91
24	2.01	6.80

$\tau = 3$

m	n	$-\lg \lvert 1 - s_m/s \rvert$	$-\lg \lvert 1 - s'_n/s \rvert$
48	16	2.51	9.31
54	18	2.45	10.40
60	20	2.48	11.63
66	22	2.59	13.18
72	24	2.80	14.47

ASSOCIATED POWER SERIES

Example:

$$\sum_{n=0}^{\infty} \frac{1+in}{n^2} \cos(n\nu) = \frac{1}{2} \sum_{n=0}^{\infty} \frac{1+in}{n^2} e^{in\nu} + \frac{1}{2} \sum_{n=0}^{\infty} \frac{1+in}{n^2} e^{-in\nu}$$

Accelerate power series separately and add

Adaptable to more complicated examples:

$$\sum \cos((n+1/2)\nu) P_n(\cos\nu')$$

(singular at $\nu = \nu'$) is sum of 4 power series

$$\frac{1}{4} \sum_{n=0}^{\infty} e^{\pm i(n+1/2)\nu} \rho_n^{\pm}(\nu')$$

$$\rho_n^{\pm}(\nu') = P_n(\cos\nu') \pm i \frac{2}{\pi} Q_n(\cos\nu') \sim \frac{\exp(\pm in\nu')}{\sqrt{n}} \times \text{const.}$$

$$\tau = 10, \qquad \nu = 6\pi/10, \qquad \nu' = 2\pi/3$$

near singularity.

n	$-\lg\left|(s_{\tau n} - s)/s\right|$	$-\lg\left|(G_n^{(\tau)} - s)/s\right|$
8	1.3	7.7
12	1.2	14.0
16	1.0	18.1
20	1.5	22.6
24	1.3	27.3
28	1.2	31.2

$G_n^{(\tau)} = \sum_{j=1}^{4} \mathcal{L}_n^{(0)}(1, [p_{j,\tau n}]|_{n=0}, [(\tau n+1)(p_{j,\tau n} -$
$p_{j,(\tau n)-1})]|_{n=0})$

VARIATIONAL METHODS

Problem:
Exact limit invariant under addition of null sequences
Nonlinear sequence transformation usually not !

Idea:
Restore invariance variationally for certain null sequences x_n

$$s'_n = f(\{s_n + \alpha x_n\})$$

$$\frac{\partial s'_n}{\partial \alpha} = 0$$

Example:

Aitken Δ^2 method

$$s_n^{(1)} = s_n - \frac{(\Delta s_n)^2}{\Delta^2 s_n}\,.$$

Use $s_n \to s_n + \alpha x_n$ **with** $\lim_{n\to\infty} x_n = 0$

$$s_n^{(1)} \to s_n^{(1)}(\alpha) = s_n + \alpha x_n - \frac{(\Delta s_n + \alpha \Delta x_n)^2}{\Delta^2 s_n + \alpha \Delta x_n}.$$

Choose α **such that** $s_n^{(1)}(\alpha)$ **is stationary:**

$$\left.\frac{\partial s_n^{(1)}}{\partial \alpha}\right|_{\alpha=\alpha_0} = 0$$

Result: For $s_n = 10 + 1/n^2$ **new method accelerates** ($O(n^{-3})$ **error), but Aitken does not(!) accelerate convergence.**

Example

$$s'_n = \sum_{j=0}^{k} c_j s_{n+j} \,, \qquad \sum_{j=0}^{k} c_j = 1$$

Put

$$s_n \to s_n + \sum_{\nu=1}^{k} \alpha_\nu x_n^{(\nu)}$$

Saddle point $\Longrightarrow$ Linear system

$$\frac{\partial s'_n}{\partial \alpha_\mu} = \sum_{j=0}^{k} c_j x_{n+j}^{(\mu)} = 0$$

Result identical to E algorithm !

$$s'_n = \frac{\begin{vmatrix} s_n & \dots & s_{n+k} \\ x_n^{(1)} & \dots & x_{n+k}^{(1)} \\ \vdots & \ddots & \vdots \\ x_n^{(k)} & \dots & x_{n+k}^{(k)} \end{vmatrix}}{\begin{vmatrix} 1 & \dots & 1 \\ x_n^{(1)} & \dots & x_{n+k}^{(1)} \\ \vdots & \ddots & \vdots \\ x_n^{(k)} & \dots & x_{n+k}^{(k)} \end{vmatrix}}$$

PERTURBATIONAL METHODS

Rayleigh-Schrdinger Perturbation Theory

$$H = H + \beta V$$

yields

$$E^{(n)} = E_0 + \beta E_1 + \ldots + \beta^n E_n$$

Goldhammer-Feenberg

$$H = (1 - \alpha)H_0 + [V + \alpha H_0]$$

yields

$$E^{(n)}(\alpha) = E_0(\alpha) + \beta E_1(\alpha) + \ldots + \beta^n E_n(\alpha)$$

Choose α variationally
(True E is α-independent)

$$\frac{\partial E^{(n)}(\alpha)}{\partial \alpha} = 0$$

For $n = 3$ solution is $\alpha = E_3/E_2 \longrightarrow$ Feenberg series

$$F_n = E^{(n)}(E_3/E_2)$$

EFFECTIVE CHARACTERISTIC POLYNOMIALS

Čížek

$$P_n(E) = \det \left|\langle \phi_j | H | \phi_k \rangle - E\,\delta_{j,k}\right| = \sum_{j=0}^{n} E^j \sum_{k=0}^{n-j} f_{n,j,k} \beta^k$$

Obtain f's from perturbation series

$$P_n(E_0 + \beta E_1 + \beta^2 E_2 + \ldots) = O(\beta^{n(n+3)/2})$$

Zero of P_2:

$$\Pi_2 = E_0 + E_1 + \frac{E_2^2}{2} \frac{E_2 - E_3}{E_2\,E_4 - E_3^2} + \frac{E_2^2}{2} \frac{\sqrt{(E_2 - E_3)^2 - 4\,(E_2\,E_4 - E_3^2)}}{E_2\,E_4 - E_3^2}$$

Invariant under Feenberg scaling

$$\Pi_2(E_0, \ldots, E_4) = \Pi_2(E_0(\alpha), \ldots, E_4(\alpha))\,.$$

Scaling property

$$\Pi_2(c\,E_0, \ldots, c\,E_4) = c\,\Pi_2(E_0, \ldots, E_4)\,.$$

MANY-BODY PERTURBATION THEORY

Dissociation barrier (kJ/mol) for

$$H_2CO \longrightarrow H_2 + CO$$

Method	Minimum	Transition state	Barr.
$E_0 + E_1$	-113.912879	-113.748693	431.1
E_2	-114.329202	-114.182435	385.3
E_3	-114.334186	-114.185375	390.7
E_4	-114.359894	-114.219892	367.6
F_4	-114.360838	-114.220603	368.2
[2/2]	-114.362267	-114.223409	364.6
Π_2	-114.364840	-114.227767	359.9
Best Estimate			360

(TZ2P Basis at MP2 Geometries)

ITERATION SEQUENCES

Fixed-point equation

$$x = \Psi(x)$$

Direct Iteration

$$x_0,\ x_1 = \Psi(x_0), \ldots,\ x_{n+1} = \Psi(x_n), \ldots$$

Cycling

$$s_0 = x_{\text{Start}}, s_1 = \Psi(s_0), \ldots, s_k = \Psi(s_{k-1})$$
$$x_{\text{Start}} = \mathcal{T}(s_0, \ldots, s_k)$$

Corresponds to new iteration function:

$$y_{n+1} = \mathcal{T}(y_n, \Psi(y_n), \ldots, \Psi(\Psi(\ldots \Psi(y_n))))$$

ORNSTEIN-ZERNIKE-EQUATION

- **Classical many-particle systems (fluids)**
- **Pair distribution function** $g(r) = 1 + h(r)$

- **Integral equation**

$$h = c + \rho\, h * c$$

$$g(r) = \exp(-\beta u(r) + h(r) - c(r) + E(r))$$

- **Bridge diagrams** $E(r) \Longrightarrow$ **Closure relations**

- **Solution on lattice with FFT:** $\boldsymbol{\Gamma_i = (h(r_i) - c(r_i))r_i,\ r_i = i\Delta r}$

$$\vec{\Gamma} = \Psi(\vec{\Gamma})$$

via

- **direct iteration**
- **direct iteration + vector extrapolation**

- **Extrapolation reduces CPU time by up to 50 %**
- **Extrapolation useful to achieve convergence**

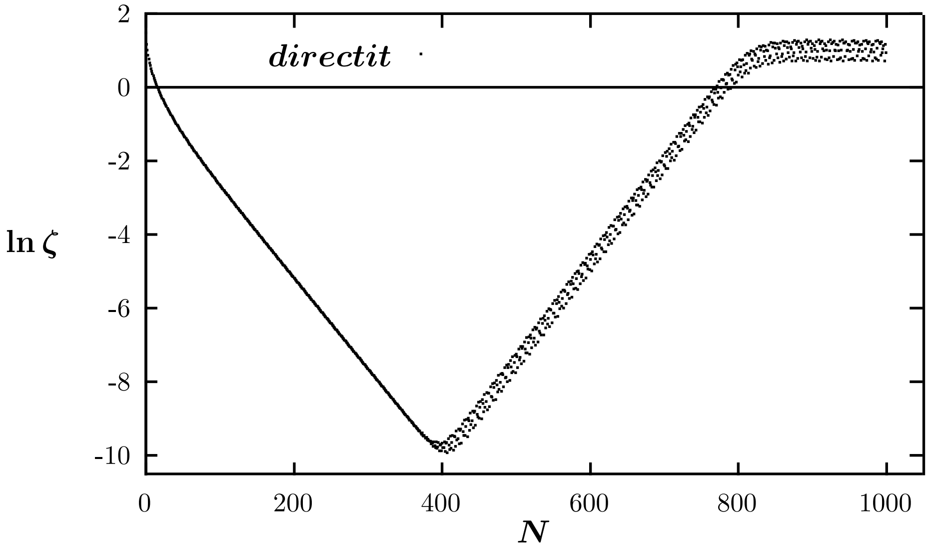


Figure 1: Unstable Fixed-point of Direct Iteration (Hard spheres, high density)

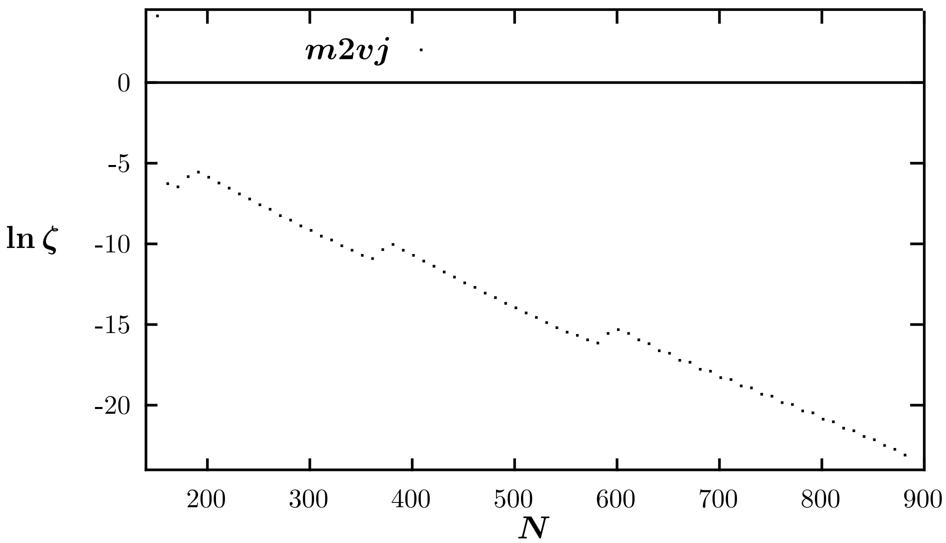


Figure 2: Convergence of the Cycling Method