Moment Expansion vs Continued Fraction II [nln96]

Moment expansion of correlation function (see [nln78]):

$$D_0(t) = \sum_{n=0}^{\infty} M_n \frac{(-\imath t)^n}{n!}, \quad M_{2k} \text{ as in [nln85].} \tag{1}$$

Asymptotic expansion and continued-fraction representation:

$$d_0(\zeta) \doteq \int_0^{\infty} dt\, e^{\imath\zeta t} D_0(t) = \imath \sum_{n=0}^{\infty} M_n \zeta^{-(n+1)} = \cfrac{\imath}{\zeta - a_0 - \cfrac{b_1^2}{\zeta - a_1 - \cdots}} \tag{2}$$

Transformation relations between $\{M_n\}$ and $\{a_n, b_n^2\}$ extracted from inspection of the two representation in (2).

- Conversion $\{a_n, b_n^2\} \leftrightarrow \{\Delta_k\}$ in two steps.
- First step: $\{a_n, b_n^2\} \leftrightarrow \{M_n\}$ here.
- Second step: $\{M_{2k}\} \leftrightarrow \{\Delta_k\}$ in [nln85].

Calculating $\{a_n, b_n^2\}$ first is most practical in many applications. Key features of dynamical quantities (bandwidth, gap, singularity structure) are most effectively extracted from $\{\Delta_k\}$.

Forward direction: $\{M_n\} \rightarrow \{a_n, b_n^2\}$

Initialize auxiliary quantities:

$$M_k^{(0)} = (-1)^k M_k, \quad L_k^{(0)} = (-1)^{k+1} M_{k+1}, \quad k = 0, \ldots, 2K. \tag{3}$$

Evaluate sequentially for $k = n, \ldots, 2K-n+1$ (in two successive inner loops) and $n = 1, \ldots, 2K$ (outer loop):

$$M_k^{(n)} = L_k^{(n-1)} - L_{n-1}^{(n-1)} \frac{M_k^{(n-1)}}{M_{n-1}^{(n-1)}}, \qquad L_k^{(n)} = \frac{M_{k+1}^{(n)}}{M_n^{(n)}} - \frac{M_k^{(n-1)}}{M_{n-1}^{(n-1)}}. \tag{4}$$

Identify continued-fraction coefficients among auxiliary quantities:

$$b_n^2 = M_n^{(n)}, \quad a_n = -L_n^{(n)}, \quad n = 0, \ldots, K. \tag{5}$$

Reverse direction: $\{a_n, b_n^2\} \;\to\; \{M_n\}$

Initialize auxiliary quantities, setting $b_0^2 = b_{-1}^2 \doteq 1$:

$$M_n^{(n)} = b_n^2, \quad L_n^{(n)} = -a_n, \quad n = 0, \ldots, K; \tag{6a}$$

$$M_k^{(-1)} = 0, \quad k = 0, \ldots, 2K+1. \tag{6b}$$

Evaluate sequentially for $n = 0, \ldots, \min(K, 2K-j)$ (inner loop) and $j = 0, \ldots, 2K+1$ (outer loop):

$$M_{n+j+1}^{(n)} = b_n^2 L_{n+j}^{(n)} + \frac{b_n^2}{b_{n-1}^2} M_{n+j}^{(n-1)}, \quad L_{n+j+1}^{(n)} = M_{n+j+1}^{(n+1)} - \frac{a_n}{b_n^2} M_{n+j+1}^{(n)}. \tag{7}$$

Identify moments among auxiliary quantities:

$$M_n = (-1)^n M_n^{(0)}, \quad n = 0, \ldots, 2K+1. \tag{8}$$

Results of a few iterations in the forward sequence (left) and in the reverse sequence (right):

$a_0 = M_1$	$M_1 = a_0$
$b_1^2 = M_2 - M_1^2$	$M_2 = a_0^2 + b_1^2$
$a_1 = \dfrac{M_3 - M_1^3}{M_2 - M_1^2} - 2M_1$	$M_3 = (a_0^3 + 2a_0 b_1^2 + b_1^2 a_1)$
$b_2^2 = \dfrac{M_4 - M_1 M_3}{M_2 - M_1^2} - M_2$ $- \left[\dfrac{M_1^3 - M_3}{M_2 - M_1^2} - 2M_1\right]\left[\dfrac{M_1^3 - M_3}{M_2 - M_1^2} + M_1\right]$	$M_4 = b_1^2\left[a_0^2 + a_1^2 + a_0 a_1 + b_1^2 + b_2^2\right]$ $+a_0\left[a_0^3 + 2a_0 b_1^2 + b_1^2 a_1\right]$