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New developments of the Extended Quadrature Method of Moments to solve Population Balance Equations

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Abstract

Population Balance Models have a wide range of applications in many industrial fields as they allow accounting for heterogeneity among properties which are crucial for some system modelling. They actually describe the evolution of a Number Density Function (NDF) using a Population Balance Equation (PBE). For instance, they are applied to gas-liquid columns or stirred reactors, aerosol technology, crystallisation processes, fine particles or biological systems. There is a significant interest for fast, stable and accurate numerical methods in order to solve for PBEs, a class of such methods actually does not solve directly the NDF but resolves their moments. These methods of moments, and in particular quadrature-based methods of moments, have been successfully applied to a variety of systems. Point-wise values of the NDF are sometimes required but are not directly accessible from the moments. To address these issues, the Extended Quadrature Method of Moments (EQMOM) has been developed in the past few years and approximates the NDF, from its moments, as a convex mixture of Kernel Density Functions (KDFs) of the same parametric family. In the present work EQMOM is further developed on two aspects. The main one is a significant improvement of the core iterative procedure of that method, the corresponding reduction of its computational cost is estimated to be between 80% and 85%. The second aspect is an extension of EQMOM to two new KDFs used for the approximation, the Weibull and the Laplace kernels. All MATLAB source codes used for this article are provided with this article.

Keywords: Extended Quadrature Method of Moments (EQMOM), Quadrature Based Method of Moments (QBMM), Population Balance, Mathematical modelling, Gauss quadrature

1. Introduction

Population Balance Equations (PBEs) are particular formalisms that allows describing the evolution of properties among heterogeneous populations. They are used to track the size

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distribution of fine particles [1]; the bubble size distribution in gas-liquid stirred-tank reactors or bubble columns [2, 3]; the crystal-size distribution in crystallizers or the distribution of biological cell properties in bioreactors [4, 5], among other examples.

A PBE describes the evolution and transport of a Number Density Function (NDF), under the influence of multiple processes which modify the tracked property distribution (*e.g.* erosion, dissolution, aggregation, breakage, coalescence, nucleation, adaptation, etc.).

One often requires low-cost numerical methods to solve PBEs, for instance when coupling with a flow solver (*e.g.* Computational Fluid Dynamics software). Monte-Carlo methods constitute a stochastic resolution of the population balance and can be applied to such PBE-CFD simulations [6]. Similarly, sectional methods allow direct numerical resolutions of the PBE through the discretisation of the property space [7, 8]. They respectively require a high number of parcels or sections in order to reach high accuracy and are thus often discarded for large-scale simulations.

An interesting alternative approach lies in the field of methods of moments. A PBE, which describes the evolution of a NDF, is transformed in a set of equations which describes the evolution of the moments of that distribution. Moments are integral properties of NDFs, the first low order integer moments are related to the mean, variance, skewness and flatness of the statistical distributions described by NDFs. This approach then reduces the number of resolved variables to a finite set of NDF moments. It also comes with some difficulties when one must compute non-moment integral properties, or point-wise evaluations, of the distribution [9].

To tackle these issues, one can try to recover a NDF from a finite set of its moments. In most cases, this reverse problem has an infinite number of solutions and different approaches exist to identify one or another out of them. Some methods that lead to continuous approximations are the Spline method [10], the Maximum-Entropy approach [9, 11, 12] or the Kernel Density Element Method (KDEM) [13].

More recently, the Extended Quadrature Method of Moments (EQMOM) was proposed as a new approach which is more stable than the previous ones, and yields either continuous or discrete NDFs depending on the moments [1, 14, 15]. EQMOM has been implemented in OpenFOAM [16] for the purpose of PBE-CFD coupling. The core of this method relies on an iterative procedure that is a computational bottleneck.

The current work focuses on EQMOM and develops a new core procedure whose computational cost is significantly lower than previous implementations by reducing both (i) the cost of each iteration and (ii) the total number of required iterations.

The previous core procedure [1] will be recalled before describing how it can be shifted toward the new –cheaper– approach. Both implementations will be compared in terms of computational cost (number of required floating-point operations) and run-time.

Multiple variations of EQMOM exist, the Gauss EQMOM [14, 17], Log-normal EQMOM [18] as well as Gamma and Beta EQMOM [15]. Two new variations, namely Laplace EQMOM and Weibull EQMOM, are proposed along with a unified formalism among all six variations.

The whole source code used to write this article (figures and data generation) is provided as supplementary data, as well as our implementations of EQMOM in the form of a MATLAB functions library [19].

48 **2. Quadrature Based Methods of Moments: QMOM and EQMOM**

49 *2.1. Definitions*

50 Let $d\mu(\xi)$ be a positive measure, induced by a non-decreasing function $\mu(\xi)$ defined on
 51 a support Ω_ξ . This measure is associated to a Number Density Function $n(\xi)$ such that
 52 $d\mu(\xi) = n(\xi)d\xi$. Let \mathbf{m}_N be the vector of the first $N + 1$ integer moments of this measure:

$$\mathbf{m}_N = \begin{bmatrix} m_0 \\ m_1 \\ \vdots \\ m_N \end{bmatrix}, \quad m_k = \int_{\Omega_\xi} \xi^k n(\xi) d\xi \quad (1)$$

53 Three actual supports will be considered: (i) $\Omega_\xi =]-\infty, +\infty[$, (ii) $\Omega_\xi =]0, +\infty[$ and
 54 (iii) $\Omega_\xi =]0, 1[$. For each support, one can define the associated realisable moment space,
 55 $\mathcal{M}_N(\Omega_\xi)$, as the set of all vectors of finite moments \mathbf{m}_N induced by all possible positive
 56 measures defined on Ω_ξ .

57 *2.2. Quadrature Method of Moments*

58 EQMOM is based on the Quadrature Method of Moments (QMOM) that was first in-
 59 troduced by McGraw [20]. It is used to approximate integral properties of a distribution
 60 where only a finite number of its moments is known. By making use of an even number
 61 of moments $2P$, one can compute a Gauss quadrature rule characterised by its weights
 62 $\mathbf{w}_P = [w_1, \dots, w_P]^T$ and nodes $\boldsymbol{\xi}_P = [\xi_1, \dots, \xi_P]^T$ such that:

$$\int_{\Omega_\xi} f(\xi) d\mu(\xi) = \sum_{i=1}^P w_i f(\xi_i) \quad (2)$$

63 holds true if $f(\xi) = \xi^k, \quad \forall k \in \{0, \dots, 2P - 1\}$. Otherwise, this quadrature rule will produce
 64 an approximation of the integral property. The computation of the quadrature rule (*i.e.*
 65 the vectors \mathbf{w}_P and $\boldsymbol{\xi}_P$) is of special interest for us, which is why its two main steps will be
 66 detailed.

67 Any positive measure $d\mu(\xi)$ is associated with a sequence of monic polynomials (*i.e.* poly-
 68 nomial whose leading coefficient equals 1) denoted π_k –with k the order of the polynomial–
 69 such that:

$$\int_{\Omega_\xi} \pi_i(\xi) \pi_j(\xi) d\mu(\xi) = 0, \quad \text{for } i \neq j \quad (3)$$

70 These polynomials are said orthogonal with respect to the measure $d\mu(\xi)$ and are defined
 71 by:

$$\pi_k(\xi) = \frac{1}{c_k} \begin{vmatrix} m_0 & m_1 & \cdots & m_{k-1} & m_k \\ m_1 & m_2 & \cdots & m_k & m_{k+1} \\ \vdots & \vdots & \ddots & \vdots & \vdots \\ m_{k-1} & m_k & \cdots & m_{2k-2} & m_{2k-1} \\ 1 & \xi & \cdots & \xi^{k-1} & \xi^k \end{vmatrix} \quad (4)$$

72 with c_k a constant chosen so that the leading coefficient (of order k) of π_k equals 1, hence
 73 making π_k a monic polynomial.

74 It is known that monic orthogonal polynomials satisfy a three-term recurrence relation
 75 [21]:

$$\pi_{k+1}(\xi) = (\xi - a_k)\pi_k(\xi) - b_k\pi_{k-1}(\xi) \quad (5)$$

76 with a_k and b_k being the recurrence coefficients specific to the measure $d\mu(\xi)$, $\pi_{-1}(\xi) = 0$
 77 and $\pi_0(\xi) = 1$.

78 Let $\mathbf{J}_n(d\mu)$ be the $n \times n$ Jacobi matrix associated to the measure $d\mu$. This is a tridiagonal
 79 symmetric matrix defined as:

$$\mathbf{J}_n(d\mu) = \begin{pmatrix} a_0 & \sqrt{b_1} & & 0 \\ \sqrt{b_1} & a_1 & \ddots & \\ & \ddots & \ddots & \sqrt{b_{n-1}} \\ 0 & & \sqrt{b_{n-1}} & a_{n-1} \end{pmatrix} \quad (6)$$

80 The weights and nodes of the quadrature rule from Eq. (2) are given by spectral properties
 81 of $\mathbf{J}_P(d\mu)$. The nodes ξ_P of the rule are the eigenvalues of $\mathbf{J}_P(d\mu)$. The weights of the rule
 82 are given by:

$$w_i = m_0 v_{1,i}^2 \quad (7)$$

83 where $v_{1,i}$ is the first component of the normalised eigenvector belonging to the eigenvalue
 84 ξ_i . The computation of the quadrature rule (Eq. (2)) then relies on two steps:

- 85 1. The computation of the recurrence coefficients $\mathbf{a}_{P-1} = [a_0, \dots, a_{P-1}]^T$ and $\mathbf{b}_{P-1} =$
 86 $[b_1, \dots, b_{P-1}]^T$.
- 87 2. The computation of the eigenvalues and the normalised eigenvectors of $\mathbf{J}_P(d\mu)$.

88 Multiple algorithms are available in the literature to compute the recurrence coefficients:

- 89 • The Quotient-Difference algorithm [22, 23]
- 90 • The Product-Difference algorithm [24]
- 91 • The Chebyshev algorithm [25]

92 The Chebyshev algorithm was found to be the stablest one of the three [1, 25], its description
 93 is given in Appendix A.

94 2.3. Extended Quadrature Method of Moments

95 The QMOM method is well suited for the approximation of integral properties of the
 96 NDF, which is actually the main purpose of Gauss quadratures. However, in many applica-
 97 tions such as evaporation [9] or dissolution [26] processes, point-wise values of the NDF $n(\xi)$
 98 are required but not directly accessible from the moments. For that purpose, a method is
 99 needed to produce an approximation $\tilde{n}(\xi)$ of the original distribution $n(\xi)$, by knowing only
 100 a finite set of its moments.

101 In a sense, one can consider that the Gaussian quadrature computed with QMOM ap-
 102 proximates $n(\xi)$ as a weighted sum of Dirac distributions:

$$\tilde{n}(\xi) = \sum_{i=1}^P w_i \delta(\xi, \xi_i) \quad (8)$$

103 with the Dirac δ distribution defined by its sifting property

$$\int_{-\infty}^{+\infty} f(\xi) \delta(\xi, \xi_m) d\xi = f(\xi_m) \quad (9)$$

104 For most applications, $n(\xi)$ is expected to be a continuous distribution whilst QMOM
 105 yields monodisperse or discrete polydisperse reconstructions of $n(\xi)$, with $\tilde{n}(\xi) = 0$ for all
 106 values of ξ except some finite number of these values.

107 Many methods were suggested to tackle this problem and to propose a continuous recon-
 108 struction $\tilde{n}(\xi)$ from a finite number of moments \mathbf{m}_N . Some of them are the Spline method
 109 [10], the Maximum-Entropy approach [11, 12, 9] or the Kernel Density Element Method
 110 [13]. Their properties will not be discussed here but one only underlines that they tend to
 111 be unstable, ill-conditioned, or have a high sensitivity to numerical parameters [10, 26, 27].
 112 In particular, none of them can handle the case of a moment set which would be on the
 113 boundary of the realisable moment space $\mathbf{m}_N \in \partial\mathcal{M}_N(\Omega_\xi)$. Such a moment set is associated
 114 to a discrete (or degenerated) distribution and, in this specific case, the solution provided
 115 by QMOM is the only possible reconstruction.

116 Note that a failure –or instabilities– in a numerical method can compromise the integrity
 117 of large-scale simulations. For this reason, Chalons et al. [14], Yuan et al. [15] and Nguyen
 118 et al. [1] proposed a robust and stable method to tackle this reconstruction problem by han-
 119 dling both continuous approximations and discrete solutions. Their approach, the Extended
 120 Quadrature Method of Moments, approximates $n(\xi)$ as a convex mixture of Kernel Density
 121 Functions (KDFs) of the same parametric family:

$$\tilde{n}(\mu) = \sum_{i=1}^P w_i \delta_\sigma(\xi, \xi_i) \quad (10)$$

122 with

- 123 • w_i : the weight of the i -th node, $w_i \geq 0, \forall i \in \{1, \dots, P\}$
- 124 • ξ_i : the location parameter of the i -th node, $\xi_i \in \Omega_\xi, \forall i \in \{1, \dots, P\}$
- 125 • δ_σ : a KDF chosen to perform the approximation, referred later to as the reconstruction
 126 kernel. σ is the shape parameter of the approximation.

127 The computation of the weights $\mathbf{w}_P = [w_1, \dots, w_P]^T$, the nodes $\boldsymbol{\xi}_P = [\xi_1, \dots, \xi_P]^T$ and
 128 the shape parameter σ from the moment set \mathbf{m}_{2P} is performed by the EQMOM moment-
 129 inversion procedure. The improvement of this procedure constitutes the core of this article
 130 and is detailed in section 3.

131 Multiple standard normalized distribution functions can be used as the reconstruction
 132 kernel δ_σ (*e.g.* Gaussian, Log-normal, etc.). A list of them is given in Appendix B. All
 133 of these kernels degenerate into Dirac distribution if their shape parameters are sufficiently
 134 small:

$$\lim_{\sigma \rightarrow 0} \delta_\sigma(\xi, \xi_m) = \delta(\xi, \xi_m) \quad (11)$$

135 This allows EQMOM to perfectly handle the case of a moment set \mathbf{m}_{2P} being on the bound-
 136 ary of the realisable moment space $\partial\mathcal{M}_{2P}(\Omega_\xi)$.

137 EQMOM can also be used to compute integral properties of the NDF with high accuracy.
 138 This comes with the introduction of nested quadratures. The main quadrature proposes the
 139 following approximation of integral terms:

$$\int_{\Omega_\xi} f(\xi)n(\xi)d\xi \approx \sum_{i=1}^P w_i \left[\int_{\Omega_\xi} f(\xi)\delta_\sigma(\xi, \xi_i)d\xi \right] \quad (12)$$

140 Moreover, a quadrature rule can be used to approximate the bracketed integral in Eq.
 141 (12). This will be the nested quadrature that actually depends on the kernel $\delta_\sigma(\xi, \xi_m)$. For
 142 instance, Gauss-Hermite quadratures can be used to approximate integrals over a Gaussian
 143 kernel (see Appendix B.1). Nested quadratures then give the following approximation:

$$\int_{\Omega_\xi} f(\xi)n(\xi)d\xi \approx \sum_{i=1}^P w_i \sum_{j=1}^Q \omega_j f\left(\xi_{ij}^{(\sigma)}\right) \quad (13)$$

144 with Q the order of the sub-quadrature, $\boldsymbol{\omega}_Q = [\omega_1, \dots, \omega_Q]^T$ the weights of the sub-quadrature,
 145 and $\xi_{ij}^{(\sigma)}$ the j -th node of the sub-quadrature, taking into account the location and shape
 146 parameters of the i -th main-quadrature node. These nested quadratures are detailed for all
 147 KDFs in Appendix B and Appendix C.

148 3. Moment inversion procedure

149 The EQMOM moment-inversion procedure comes with analytical solutions for some ker-
 150 nels in the case of low-order quadratures. The one-node analytical solutions are detailed for
 151 all kernels in Appendix B. When they exist, the two-nodes analytical solutions are imple-
 152 mented in MATLAB code (see supplementary data) but are not detailed in this article. The
 153 current section is focusing on the numerical procedure used to compute the reconstruction
 154 parameters in absence of an analytical solution.

155 The procedure proposed by Yuan et al. [15] and Nguyen et al. [1] is first recalled in section
 156 3.1. The section 3.2 details how their approach can be shifted toward a new convergence
 157 criteria that will be applied to the specific cases of

- 158 • the *Hamburger* moment problem (section 3.3): NDF defined on the whole phase space
 159 $\Omega_\xi =]-\infty, +\infty[$
- 160 • the *Stieltjes* moment problem (section 3.4): NDF defined on the positive phase space
 161 $\Omega_\xi =]0, +\infty[$

162 • the *Hausdorff* moment problem (section 3.5): NDF defined on the closed support
 163 $\Omega_\xi =]0, 1[$

164 *3.1. Standard procedure*

165 Let \mathbf{m}_N be the vector of the first $N + 1$ integer moments of the measure $d\mu(\xi) = n(\xi)d\xi$,
 166 with $N = 2P$ an even integer:

$$\mathbf{m}_N = \begin{bmatrix} m_0 \\ m_1 \\ \vdots \\ m_N \end{bmatrix}, \quad m_k = \int_{\Omega_\xi} \xi^k n(\xi) d\xi \quad (14)$$

167 The EQMOM moment-inversion procedure aims to identify the parameters σ , $\mathbf{w}_P =$
 168 $[w_1, \dots, w_P]^\top$ and $\boldsymbol{\xi}_P = [\xi_1, \dots, \xi_P]^\top$ such that $\mathbf{m}_N = \widetilde{\mathbf{m}}_N$ with:

$$\widetilde{\mathbf{m}}_N = \begin{bmatrix} \widetilde{m}_0 \\ \widetilde{m}_1 \\ \vdots \\ \widetilde{m}_N \end{bmatrix}, \quad \widetilde{m}_k = \int_{\Omega_\xi} \xi^k \widetilde{n}(\xi) d\xi, \quad \widetilde{n}(\xi) = \sum_{i=1}^P w_i \delta_\sigma(\xi, \xi_i) \quad (15)$$

169 For any value of σ , Yuan et al. [15] identified a procedure which leads to the parameters
 170 \mathbf{w}_P and $\boldsymbol{\xi}_P$ such that $\mathbf{m}_{N-1} = \widetilde{\mathbf{m}}_{N-1}$. The EQMOM moment-inversion problem has then
 171 been reduced to solving a scalar non-linear equation by looking for a root of the function
 172 $D_N(\sigma) = m_N - \widetilde{m}_N(\sigma)$.

173 The approach developed by Yuan et al. [15] and then improved by Nguyen et al. [1] is
 174 based on the fact that, for the KDFs used in EQMOM, it is possible to write the following
 175 linear system:

$$\widetilde{\mathbf{m}}_n = \mathbf{A}_n(\sigma) \cdot \mathbf{m}_n^* \quad (16)$$

176 where $\mathbf{A}_n(\sigma)$ is a lower-triangular $(n + 1) \times (n + 1)$ matrix whose elements depend only on
 177 the chosen KDF and on the value σ , whereas \mathbf{m}_n^* is defined as:

$$\mathbf{m}_n^* = \begin{bmatrix} m_0^* \\ m_1^* \\ \vdots \\ m_n^* \end{bmatrix}, \quad m_k^* = \sum_{i=1}^P w_i \xi_i^k \quad (17)$$

178 By their definition, the moments \mathbf{m}_n^* correspond to the moments of a degenerated dis-
 179 tribution (*i.e.* a finite sum of Dirac distributions), hence these moments will be referred as
 180 the *degenerated moments of the approximation*. Degenerated moments are defined in such a
 181 way that the vectors \mathbf{w}_P and $\boldsymbol{\xi}_P$ can be computed from \mathbf{m}_{2P-1}^* using a Gauss Quadrature
 182 (see 2.2).

183 At this point, one has the basis required to compute the objective function $D_N(\sigma)$ and
 184 to search for its root. The computation of $D_N(\sigma)$ from a vector \mathbf{m}_N is as follow (see also
 185 Fig. 1a):

- 186 1. Compute $\mathbf{m}_{N-1}^*(\sigma) = \mathbf{A}_{N-1}^{-1}(\sigma) \cdot \mathbf{m}_{N-1}$.
- 187 2. Compute the recurrence coefficients $\mathbf{a}_{P-1}^*(\sigma)$ and $\mathbf{b}_{P-1}^*(\sigma)$ by applying the Chebyshev
- 188 algorithm to $\mathbf{m}_{N-1}^*(\sigma)$.
- 189 3. Use the recurrence coefficients to compute the Gaussian quadrature rule $\mathbf{w}_P(\sigma)$ and
- 190 $\boldsymbol{\xi}_P(\sigma)$.
- 191 4. Knowing the parameters σ , $\mathbf{w}_P(\sigma)$ and $\boldsymbol{\xi}_P(\sigma)$ of the reconstruction, compute $\tilde{\mathbf{m}}_N(\sigma)$,
- 192 this can be done easily by:
- 193 • Computing the N-th order degenerated moment of the approximated NDF: $\bar{m}_N^*(\sigma) =$
 - 194 $\sum_{i=1}^P w_i(\sigma) \xi_i(\sigma)^N$.
 - 195 • Multiplying the last line of $\mathbf{A}_N(\sigma)$ and the vector of degenerated moments: $\tilde{\mathbf{m}}_N(\sigma) =$
 - 196 $[0, 0, \dots, 1] \cdot \mathbf{A}_N(\sigma) \cdot [m_0^*(\sigma), \dots, m_{N-1}^*(\sigma), \bar{m}_N^*(\sigma)]^\top$.
- 197 5. Compute $D_N(\sigma) = m_N - \tilde{\mathbf{m}}_N(\sigma)$.

198 For each compatible KDF, it is possible to use the low order moments to compute an

199 upper bound σ_{max} so that the search of a root of D_N is restricted to the interval $\sigma \in [0, \sigma_{max}]$.

200 Then a bounded non-linear equation solver such as Ridder's method can be applied to

201 actually find the root of the function.

202 Two specific cases were discarded in the previous description of the method. First, it

203 happens that the function D_N does not admit any root, in such a case the procedure is

204 switched toward the minimisation of this function in order to reduce the error on the last

205 moment of the approximation.

206 Second, during the computation of $D_N(\sigma)$, one must compute degenerated moments

207 from which the weights and nodes are extracted. If the degenerated moments $\mathbf{m}_{N-1}^*(\sigma)$ turn

208 out not to be realisable on the support Ω_ξ of the NDF, the quadrature performed on this

209 vector will lead to nodes outside Ω_ξ , or even to negative/complex weights. Nguyen et al. [1]

210 then suggest to check for the realisability of the degenerated moments, and if these are not

211 realisable, to set $\tilde{\mathbf{m}}_N(\sigma)$ to a arbitrarily high value such as 10^{100} . This will force the non-

212 linear equation solver to test a lower value of σ in order to bring back the vector $\mathbf{m}_{N-1}^*(\sigma)$

213 within the realisable moment space. However note that this is only a numerical trick to

214 converge toward the actual root, but $D_N(\sigma)$ is actually undefined as soon as $\mathbf{m}_{N-1}^*(\sigma)$ is not

215 realisable.

216 3.2. A new procedure based on moment realisability

217 The reversible linear system linking the raw moments of the approximation $\tilde{\mathbf{m}}_N$ to its

218 degenerated moments \mathbf{m}_N^* is such that a new objective function $D_N^*(\sigma)$ –whose root is the

219 same as that of $D_N(\sigma)$ – can be formulated. Its computation is as follow (see also Fig. 1b):

- 220 1. Compute $\mathbf{m}_N^*(\sigma) = \mathbf{A}_N^{-1}(\sigma) \cdot \mathbf{m}_N$.
- 221 2. Compute a quadrature on the vector $\mathbf{m}_{N-1}^*(\sigma)$ to obtain the vectors $\mathbf{w}_P(\sigma)$ and $\boldsymbol{\xi}_P(\sigma)$.
- 222 3. Compute $\bar{m}_N^*(\sigma) = \sum_{i=1}^P w_i(\sigma) \xi_i(\sigma)^N$.
- 223 4. Compute $D_N^*(\sigma) = m_N^*(\sigma) - \bar{m}_N^*(\sigma)$.

224 The benefit of this new objective function is that it only requires the matrix $\mathbf{A}_N^{-1}(\sigma)$

225 instead of both the matrix $\mathbf{A}_{N-1}^{-1}(\sigma)$ and the last line of $\mathbf{A}_N(\sigma)$. This only increases the

226 clarity of the method, but has hardly no effect on its numerical cost.

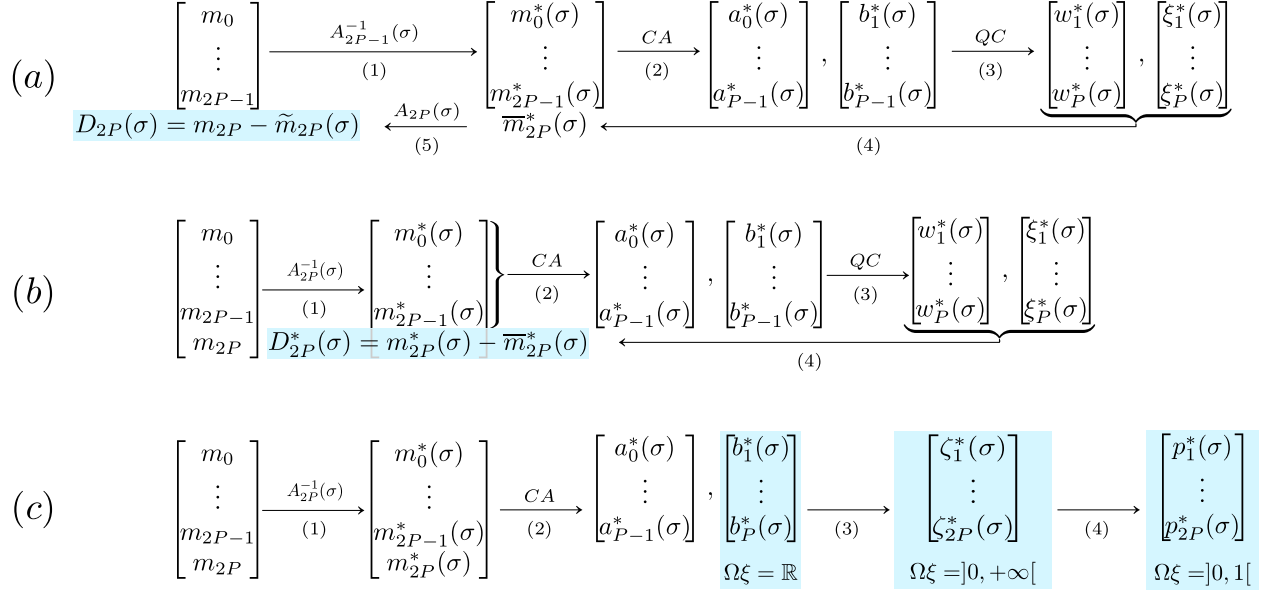


Figure 1: Comparison of the computation of convergence criteria based on (a) $D_N(\sigma)$, (b) $D_N^*(\sigma)$ and (c) the realisability criteria of the support Ω_ξ . CA: Chebyshev Algorithm. QC: Quadrature Computation. The convergence criteria are highlighted in light blue. Inspired by Fig. 1 from Nguyen et al. [1].

227 The point of this alternative approach is however to underline a crucial element for the
 228 new EQMOM implementation: we actually look for a value of σ for which $m_{2P}^*(\sigma) = \overline{m}_{2P}(\sigma)$.
 229 This implies that, for this specific searched σ value, the vector $\mathbf{m}_{2P}^*(\sigma)$ reads

$$\mathbf{m}_{2P}^*(\sigma) = \begin{bmatrix} \sum_{i=1}^P w_i \xi_i^0 \\ \sum_{i=1}^P w_i \xi_i^1 \\ \vdots \\ \sum_{i=1}^P w_i \xi_i^{2P} \end{bmatrix} \quad (18)$$

230 which is, by construction, the vector of the first $2P + 1$ moments of the sum of P Dirac
 231 distributions. Under the condition $\xi_i \neq 0, i \in \{1, \dots, P\}$, the vector $\mathbf{m}_{2P}^*(\sigma)$ will then have
 232 the following specific properties:

- 233 1. The vector $\mathbf{m}_{2P-1}^*(\sigma)$ must be strictly within the realisable moment space $\mathcal{M}_{N-1}(\Omega_\xi)$.
- 234 2. The vector $\mathbf{m}_{2P}^*(\sigma)$ must be on the boundary of the realisable moment space $\mathcal{M}_N(\Omega_\xi)$.

235 EQMOM procedure will then rely on the realisability of the vector $\mathbf{m}_{2P}^*(\sigma)$ instead of the
 236 computation of the error on the last moment, this will be a cheaper approach. The actual
 237 definition of the realisable moment space of order n , \mathcal{M}_n , depends on the support Ω_ξ of the
 238 NDF. The three classical supports, corresponding to the *Hamburger*, *Stieltjes* and *Hausdorff*
 239 moment problems, come with different constraints on a moment set to ensure its realisability.
 240 The realisability criteria for each of these supports will then be detailed.

241 Fig. 1 sums up the “standard approach” based on $D_N(\sigma)$, the shifted approach, based
 242 on $D_N^*(\sigma)$, as well as the new approach based on the realisability criteria of $\mathbf{m}_{2P}^*(\sigma)$ for all
 243 three supports.

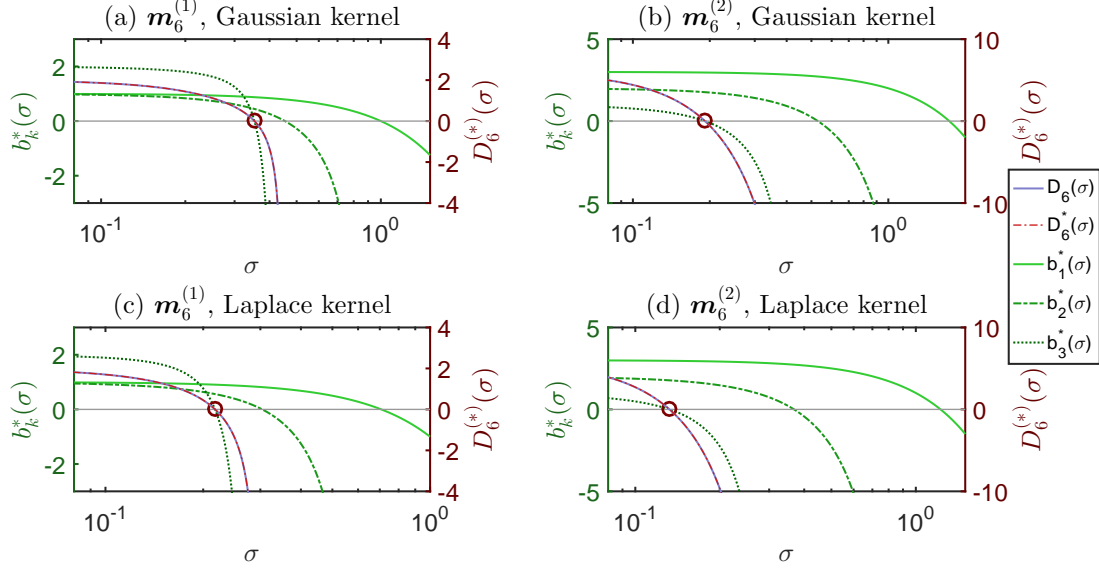


Figure 2: Evolution of the different convergence criteria for both Gaussian (a and b) and Laplace (c and d) kernels depending on σ value. The two initial moment sets are $\mathbf{m}_6^{(1)} = [1 \ 1 \ 2 \ 5 \ 12 \ 42 \ 133]^\top$ and $\mathbf{m}_6^{(2)} = [1 \ 2 \ 7 \ 17 \ 58 \ 149 \ 493]^\top$.

244 3.3. Application to the Hamburger problem

245 As stated in 2.2, it is known that the monic polynomials which are orthogonal to a
 246 measure $d\mu(\xi) = n(\xi)d\xi$ satisfy a three-term recurrence relation (Eq. (5)) with a_k and
 247 $b_k, k \in \mathbb{N}$, the recurrence coefficients specific to the measure $d\mu(\xi)$. The Favard's theorem
 248 [28] and its converse [29] imply that the measure $d\mu(\xi)$ is realisable on $\Omega_\xi =]-\infty, +\infty[$ if
 249 and only if $a_k \in \mathbb{R}$ and $b_k > 0, \forall k \in \mathbb{N}$.

250 One looks for a value of σ such that the associated degenerated moments $\mathbf{m}_{2P-1}^*(\sigma)$
 251 are within the realisable moment space and the moments $\mathbf{m}_{2P}^*(\sigma)$ are on the boundary of
 252 this moment space. Then, if the Chebyshev algorithm is used to compute the recurrence
 253 coefficients $\mathbf{a}_{P-1}^*(\sigma) = [a_0^*(\sigma), \dots, a_{P-1}^*(\sigma)]^\top$ and $\mathbf{b}_P^*(\sigma) = [b_1^*(\sigma), \dots, b_P^*(\sigma)]^\top$ from the vector
 254 $\mathbf{m}_{2P}^*(\sigma)$, the condition of realisability can be written in terms of values of $\mathbf{b}_P^*(\sigma)$: looking for
 255 the EQMOM reconstruction parameters with the Gaussian and Laplace kernels is equivalent
 256 to looking for a value of σ such as:

- 257 • $b_k^*(\sigma) > 0, \quad \forall k \in \{1, \dots, P-1\}$
- 258 • $b_P^*(\sigma) = 0$

259 Fig. 2 makes use of the developments from Appendix B.1 and Appendix B.2, about
 260 the Gaussian and Laplace kernels respectively, to show the evolution of $D_6(\sigma)$, $D_6^*(\sigma)$ and
 261 $b_k^*(\sigma), k \in \{1, 2, 3\}$ for two sets of 7 moments ($P = 3$). This figure illustrates the fact that
 262 indeed the approaches based on $D_N(\sigma)$, $D_N^*(\sigma)$ and $b_P^*(\sigma)$ are equivalent as they share the
 263 same circled root.

264 Let denote σ_k the root of $b_k(\sigma)$. One can notice that the root σ_k lies within the interval
 265 $[0, \sigma_{k-1}]$. We actually observed the existence of all roots σ_k , $k \in \{1, \dots, P\}$ on numerous
 266 (about 10^6) randomly selected moment sets of $N + 1 = 13$ moments, and never observed an
 267 undefined root. The generality of this observation has not been mathematically proved, but
 268 it seems that indeed σ_k is always defined and always lies in $\sigma_k \in [0, \sigma_{k-1}]$, $k \in \{2, \dots, P\}$.
 269 σ_1 is defined analytically.

270 The previous observations were used to design a simple algorithm which allows identifying
 271 the root σ_P . This algorithm is based on the fact that it is possible to check whether a value
 272 σ_t is higher or lower than σ_P at low cost and with no prior knowledge of σ_P value:

- 273 • If $b_k^*(\sigma_t) > 0$, $\forall k \in \{1, \dots, P\}$, then $\sigma_t < \sigma_P$.
- 274 • Otherwise, that is if $\exists k \in \{1, \dots, P\}$, $b_k^*(\sigma_t) < 0$, then $\sigma_t > \sigma_P$.

275 One can then use an iterative approach that will

- 276 1. Check the realisability of the raw moments $\mathbf{m}_{2P} = \mathbf{m}_{2P}^*(0)$ by computing $\mathbf{b}_P^*(0)$ and
 277 checking the positivity of all elements.
- 278 2. Initialise an interval $[\sigma_l^{(0)}, \sigma_r^{(0)}]$ such that $\sigma_l^{(0)} < \sigma_P$ and $\sigma_r^{(0)} > \sigma_P$, and then update
 279 these bounds to shrink the search interval. These initial values will be $\sigma_l^{(0)} = 0$ and
 280 $\sigma_r^{(0)} = \sigma_1$ with σ_1 the analytical solution of $b_1^*(\sigma) = 0$.
- 281 3. Iterate over k
 - 282 (a) Choose $\sigma_t \in [\sigma_l^{(k-1)}, \sigma_r^{(k-1)}]$.
 - 283 (b) Compute $\mathbf{b}_P^*(\sigma_t)$.
 - 284 (c) If all elements of $\mathbf{b}_P^*(\sigma_t)$ are positive, set $\sigma_l^{(k)} = \sigma_t$ and $\sigma_r^{(k)} = \sigma_r^{(k-1)}$.
 - 285 (d) Otherwise, set $\sigma_l^{(k)} = \sigma_l^{(k-1)}$ and $\sigma_r^{(k)} = \sigma_t$.

286 The choice of σ_t at step 3a will be made by trying to locate the root σ_j of $b_j^*(\sigma)$ with j the
 287 index of the first negative element of $\mathbf{b}_P^*(\sigma_r^{(k)})$. Following Nguyen et al. [1] developments,
 288 the use of Ridder's method is advised to select σ_t . This method actually tests two σ values
 289 per iteration. Consequently, the step 3 of the previous algorithm becomes:

- 290 3. Iterate over k
 - 291 (a) Identify j the index of the first negative element of $\mathbf{b}_P^*(\sigma_r^{(k-1)})$.
 - 292 (b) Compute $\sigma_{t_1} = \frac{1}{2} (\sigma_l^{(k-1)} + \sigma_r^{(k-1)})$ and $\mathbf{b}_P^*(\sigma_{t_1})$.
 - 293 (c) Compute $\sigma_{t_2} = \sigma_{t_1} + (\sigma_{t_1} - \sigma_l^{(k-1)}) \frac{b_j^*(\sigma_{t_1})}{\sqrt{b_j^*(\sigma_{t_1})^2 - b_j^*(\sigma_l^{(k-1)}) * b_j^*(\sigma_r^{(k-1)})}}$ and $\mathbf{b}_P^*(\sigma_{t_2})$.
 - 294 (d) Set $\sigma_l^{(k)}$ as the highest value between $\sigma_l^{(k-1)}$, σ_{t_1} and σ_{t_2} such that the correspond-
 295 ing vector \mathbf{b}_P^* contains only positive values.
 - 296 (e) Set $\sigma_r^{(k)}$ as the lowest value between $\sigma_r^{(k-1)}$, σ_{t_1} and σ_{t_2} such that the corresponding
 297 vector \mathbf{b}_P^* contains at least one negative value.

298 Stop the computation if $\sigma_r^{(k)} - \sigma_l^{(k)} < \varepsilon \sigma_1$ or if $b_P^* \left(\sigma_l^{(k)} \right) < \varepsilon b_P^*(0)$, with ε a relative tolerance
 299 (e.g. $\varepsilon = 10^{-10}$). Then compute the weights \mathbf{w}_P and nodes $\boldsymbol{\xi}_P$ of the EQMOM reconstruction
 300 by computing a Gauss quadrature based on the recurrence coefficients $\mathbf{a}_{P-1}^* \left(\sigma_l^{(k)} \right)$ and
 301 $\mathbf{b}_{P-1}^* \left(\sigma_l^{(k)} \right)$.

302 Actual implementations of this algorithm for both kernels are provided as supplementary
 303 data.

304 3.4. Application to the Stieltjes problem

305 It is well known that the realisability of a moment set \mathbf{m}_N on the support $\Omega_\xi =]0, +\infty[$
 306 is strictly equivalent to the positivity of the Hankel determinants $\underline{\mathcal{H}}_{2n+d}$ [30] defined as:

$$\underline{\mathcal{H}}_{2n+d} = \begin{vmatrix} m_d & \cdots & m_{n+d} \\ \vdots & \ddots & \vdots \\ m_{n+d} & \cdots & m_{2n+d} \end{vmatrix} \quad (19)$$

307 with $d \in \{0, 1\}$ and $n \in \mathbb{N}$, $2n + d \leq N$.

308 This condition on the positivity of Hankel determinants can be translated into a condition
 309 on the positivity of the numbers ζ_k [29] defined by :

$$\zeta_k = \frac{\underline{\mathcal{H}}_{k-3} \underline{\mathcal{H}}_k}{\underline{\mathcal{H}}_{k-2} \underline{\mathcal{H}}_{k-1}}, \quad \underline{\mathcal{H}}_j = 1 \text{ if } j < 0 \quad (20)$$

310 These numbers can be directly computed from the recurrence coefficients \mathbf{a}_P and \mathbf{b}_P defined
 311 in 2.2 through the following relations:

$$\zeta_{2k} = \frac{b_k}{\zeta_{2k-1}}, \quad \zeta_{2k+1} = a_k - \zeta_{2k} \quad (21)$$

312 with $\zeta_1 = a_0 = m_1/m_0$.

313 The goal here is to use these realisability criteria to compute the parameters of EQMOM
 314 quadrature with either the Log-normal, the Gamma or the Weibull kernel (see Appendix
 315 B.3, Appendix B.4 and Appendix B.5 respectively). In these cases, one must

- 316 1. Compute $\mathbf{m}_N^*(\sigma) = \mathbf{A}_N^{-1}(\sigma) \cdot \mathbf{m}_N$ with $\mathbf{A}_N(\sigma)$ the matrix associated to the chosen
 317 kernel (see Appendix B.3, Appendix B.4, Appendix B.5).
- 318 2. Apply the Chebyshev algorithm to $\mathbf{m}_N^*(\sigma)$ to access the recurrence coefficients $\mathbf{a}_P^*(\sigma)$
 319 and $\mathbf{b}_P^*(\sigma)$.
- 320 3. Compute $\boldsymbol{\zeta}_N^*(\sigma) = [\zeta_1^*(\sigma), \dots, \zeta_N^*(\sigma)]^T$ using the relations in Eq. (21).

321 One actually looks for σ such that

- 322 • $\zeta_k^*(\sigma) > 0, \quad \forall k \in \{1, \dots, N-1\}$
- 323 • $\zeta_N^*(\sigma) = 0$

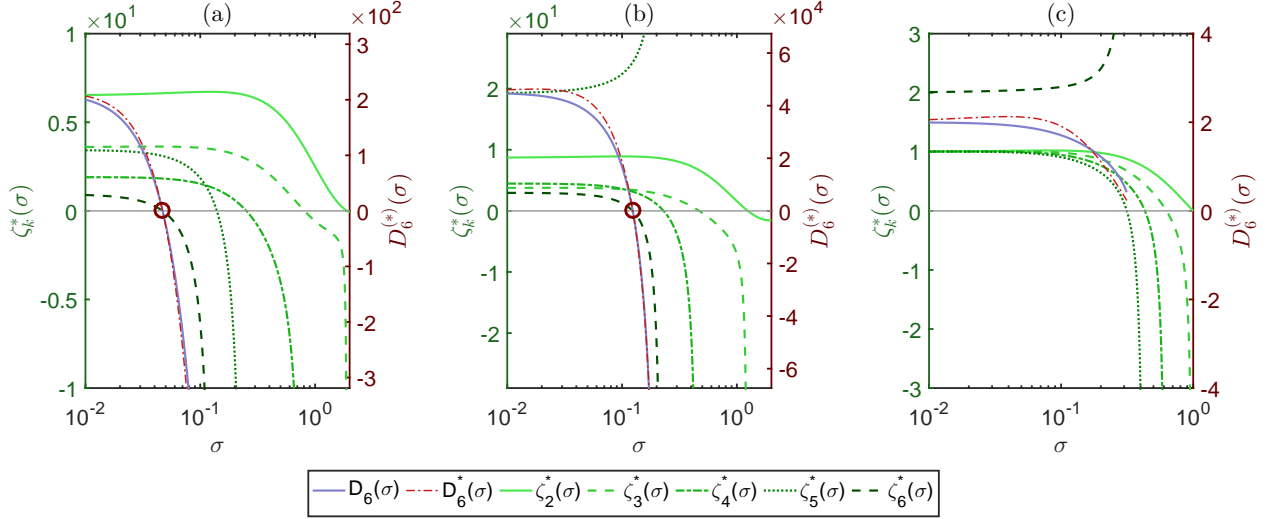


Figure 3: Evolution of the different convergence criteria for the Weibull kernel depending on σ value. The initial moment sets are $\mathbf{m}_6^{(a)} = [1 \ 1.5 \ 12 \ 131 \ 15200 \ 18033 \ 2.16e5]^\top$, $\mathbf{m}_6^{(b)} = [1 \ 5.5 \ 78 \ 1285 \ 22225 \ 4.05e5 \ 7.88e6]^\top$ and $\mathbf{m}_6^{(c)} = [1 \ 1 \ 2 \ 5 \ 14 \ 42 \ 133]^\top$.

324 Let σ_k be the root of $\zeta_k^*(\sigma)$. In all cases, the root σ_2 is defined, analytically for the
 325 Log-normal and Gamma kernels, and numerically for the Weibull kernel. Fig. 3 shows the
 326 evolution of $D_6(\sigma)$, $D_6^*(\sigma)$ and $\zeta_6^*(\sigma)$ for three moment sets when the developments relative
 327 to the Weibull (see Appendix B.5) kernel are used. Three situations can be observed on that
 328 figure:

- 329 1. All roots σ_k , $k \in \{2, \dots, N\}$ are defined (Fig. 3a).
- 330 2. Some intermediary roots σ_k , $k \in \{3, \dots, N-1\}$, are not defined but the root σ_N still
 331 exists (Fig. 3b).
- 332 3. The root σ_N is not defined (Fig. 3c).

333 These three cases can be observed for the Gamma and Log-normal kernels too.

334 In the first two cases, when σ_N exists, the EQMOM approximation is well defined. The
 335 last case –where $\zeta_N^*(\sigma)$ admits no root in $[0, \sigma_{N-1}]$ – actually corresponds to the case described
 336 by Nguyen et al. [1] where $D_N(\sigma)$ did not admit any root either. In this case, it was suggested
 337 to minimise $D_N(\sigma)$ in order to reduce the difference between m_N and $\tilde{m}_N(\sigma)$ as much as
 338 possible.

339 $D_N(\sigma)$ tends to be a decreasing function, but is undefined as soon as any element of
 340 $\zeta_{N-1}^*(\sigma)$ is negative. The minimum of $D_N(\sigma)$ is then usually located at the highest order
 341 defined root. For instance, in the case shown in Fig. 3c, the minimum of $D_6(\sigma)$ is located
 342 at the root σ_5 of $\zeta_5^*(\sigma)$.

343 The moment-inversion procedure for reconstruction kernels defined on $\Omega_\xi =]0, +\infty[$ is
 344 then reduced to the identification of the defined root σ_k , $k \in \{2, \dots, N\}$, of highest index.
 345 The algorithm proposed in section 3.3 already converges toward this root and only requires
 346 little adjustments:

- 347 1. Check the realisability of the raw moments $\mathbf{m}_{2P} = \mathbf{m}_{2P}^*(0)$ by computing $\zeta_N^*(0)$ and
348 checking the positivity of all elements.
- 349 2. Initialise an interval $[\sigma_l^{(0)}, \sigma_r^{(0)}]$ with $\sigma_l^{(0)} = 0$ and $\sigma_r^{(0)} = \sigma_2$ with σ_2 the solution of
350 $\zeta_2^*(\sigma) = 0$.
- 351 3. Iterate over k
- 352 (a) Identify j the index of the first negative element of $\zeta_N^*(\sigma_r^{(k-1)})$.
- 353 (b) Compute $\sigma_{t_1} = \frac{1}{2}(\sigma_l^{(k-1)} + \sigma_r^{(k-1)})$ and $\zeta_N^*(\sigma_{t_1})$.
- 354 (c) Compute $\sigma_{t_2} = \sigma_{t_1} + (\sigma_{t_1} - \sigma_l^{(k-1)}) \frac{\zeta_j^*(\sigma_{t_1})}{\sqrt{\zeta_j^*(\sigma_{t_1})^2 - \zeta_j^*(\sigma_l^{(k-1)})^* \zeta_j^*(\sigma_r^{(k-1)})}}$ and $\zeta_N^*(\sigma_{t_2})$.
- 355 (d) Set $\sigma_l^{(k)}$ as the highest value between $\sigma_l^{(k-1)}$, σ_{t_1} and σ_{t_2} such that the correspond-
356 ing vector ζ_N^* contains only positive values.
- 357 (e) Set $\sigma_r^{(k)}$ as the lowest value between $\sigma_r^{(k-1)}$, σ_{t_1} and σ_{t_2} such that the corresponding
358 vector ζ_N^* contains at least one negative value.

359 Stop the computation if $\sigma_r^{(k)} - \sigma_l^{(k)} < \varepsilon \sigma_1$ or if $\zeta_N^*(\sigma_l^{(k)}) < \varepsilon \zeta_N^*(0)$, with ε a relative tolerance
360 (*e.g.* $\varepsilon = 10^{-10}$). Then compute the weights \mathbf{w}_P and nodes ξ_P of the EQMOM reconstruction
361 by computing a Gaussian-quadrature based on the recurrence coefficients $\mathbf{a}_{P-1}^*(\sigma_l^{(k)})$ and
362 $\mathbf{b}_{P-1}^*(\sigma_l^{(k)})$.

363 3.5. Application to the Hausdorff problem

364 The moments of a distribution defined on the closed support $\Omega_\xi =]0, 1[$ must obey two
365 sets of conditions in order to be within the realisable moment space [12, 23]. The moment
366 set \mathbf{m}_N is interior to the realisable moment space associated to the support $\Omega_\xi =]0, 1[$ if
367 and only if:

- 368 • $\underline{\mathcal{H}}_k > 0$, $\forall k \in \{0, \dots, N\}$
- 369 • $\overline{\mathcal{H}}_k > 0$, $\forall k \in \{1, \dots, N\}$

370 with $\underline{\mathcal{H}}_k$ defined in Eq. (19) and $\overline{\mathcal{H}}_k$ defined by

$$371 \overline{\mathcal{H}}_{2n+d} = \begin{vmatrix} m_{d-1} - m_d & \cdots & m_{n+d-1} - m_{n+d} \\ \vdots & \ddots & \vdots \\ m_{n+d-1} - m_{n+d} & \cdots & m_{2n+d-1} - m_{2n+d} \end{vmatrix} \quad (22)$$

372 Leaving aside the obvious condition $\underline{\mathcal{H}}_0 = m_0 > 0$, the conditions $\overline{\mathcal{H}}_k > 0$ and $\underline{\mathcal{H}}_k > 0$
373 induce a lower bound m_k^- and an upper bound m_k^+ for the values of m_k , $k \in \{1, \dots, N\}$.
374 Consequently, one can define the canonical moments of the distribution $\mathbf{p}_N = [p_1, \dots, p_N]^T$
as

$$p_k = \frac{m_k - m_k^-}{m_k^+ - m_k^-} \quad (23)$$

375 A moment set \mathbf{m}_N is realisable if and only if the associated canonical moment set \mathbf{p}_N lies
 376 in the hypercube $]0, 1[^N$. The canonical moments can be computed through the recurrence
 377 relation [31]:

$$p_k = \frac{\zeta_k}{1 - p_{k-1}} \quad (24)$$

378 with ζ_k defined in Eq. (20) and $p_1 = m_1$.

379 In the case of the Beta kernel (see Appendix B.6), one is looking for a value of σ such
 380 that the vector $\mathbf{p}_N^*(\sigma)$ has the following properties:

- 381 • $p_k^*(\sigma) \in]0, 1[$, $\forall k \in \{1, \dots, N-1\}$
- 382 • $p_N^*(\sigma) = 0$

383 $\mathbf{p}_N^*(\sigma)$ is computed from the vector $\boldsymbol{\zeta}_N^*(\sigma)$ which is deduced from the recurrence coef-
 384 ficients $\mathbf{a}_{P-1}^*(\sigma)$ and $\mathbf{b}_P^*(\sigma)$. These are computed –like previously– through the Chebyshev
 385 algorithm applied to the vector $\mathbf{m}_N^*(\sigma) = \mathbf{A}_N^{-1}(\sigma) \cdot \mathbf{m}_N$.

386 Fig. 4 shows the evolution of the canonical moments and the convergence criteria $D_6(\sigma)$
 387 and $D_6^*(\sigma)$ for four different sets of 7 moments with the developments relative to the Beta
 388 kernel (see Appendix B.6). Each of these sets corresponds to one of the four situations
 389 encountered when dealing with Beta EQMOM:

- 390 • Fig. 4a: the root σ_N of $D_N(\sigma)$, $D_N^*(\sigma)$ and $p_N^*(\sigma)$ exists and can be identified through
 391 a similar procedure than that described in sections 3.3 and 3.4.
- 392 • Fig. 4b: the root σ_N is not defined but the minimum of $D_N(\sigma)$ is located at the σ
 393 value for which $\mathbf{p}_{N-1}^*(\sigma)$ is on the boundary of the hypercube $]0, 1[^{N-1}$.
- 394 • Fig. 4c: $D_N(\sigma)$, $D_N^*(\sigma)$ and $p_N^*(\sigma)$ admit multiple roots.
- 395 • Fig. 4d: the root σ_N is defined, but there is a range $]\sigma_{v_1}, \sigma_{v_2}[$ with $\sigma_{v_2} < \sigma_N$, highlighted
 396 in light grey, such that in this interval the convergence criteria are undefined because
 397 $\forall \sigma \in]\sigma_{v_1}, \sigma_{v_2}[$, $\mathbf{p}_{N-1}^*(\sigma) \notin]0, 1[^{N-1}$.

398 The algorithm proposed in sections 3.3 and 3.4 can still be applied here by replacing the
 399 convergence criteria by the canonical moments, and by checking that the values of $\mathbf{p}_N^*(\sigma)$ all
 400 lie in the interval $]0, 1[$ instead of checking only for positivity:

- 401 1. Check the realisability of the raw moments $\mathbf{m}_{2P} = \mathbf{m}_{2P}^*(0)$ by computing $\mathbf{p}_N^*(0)$ and
 402 checking that all elements lie in $]0, 1[$.
- 403 2. Initialise an interval $[\sigma_l^{(0)}, \sigma_r^{(0)}]$ with $\sigma_l^{(0)} = 0$ and $\sigma_r^{(0)} = \sigma_2$ with σ_2 the analytical
 404 solution of $p_2^*(\sigma) = 0$.
- 405 3. Iterate over k
 - 406 (a) Identify j the index of the first element of $\mathbf{p}_N^*(\sigma_r^{(k-1)})$ that is either negative or
 407 higher than 1.
 - 408 (b) Compute $\sigma_{t_1} = \frac{1}{2}(\sigma_l^{(k-1)} + \sigma_r^{(k-1)})$ and $\mathbf{p}_N^*(\sigma_{t_1})$.

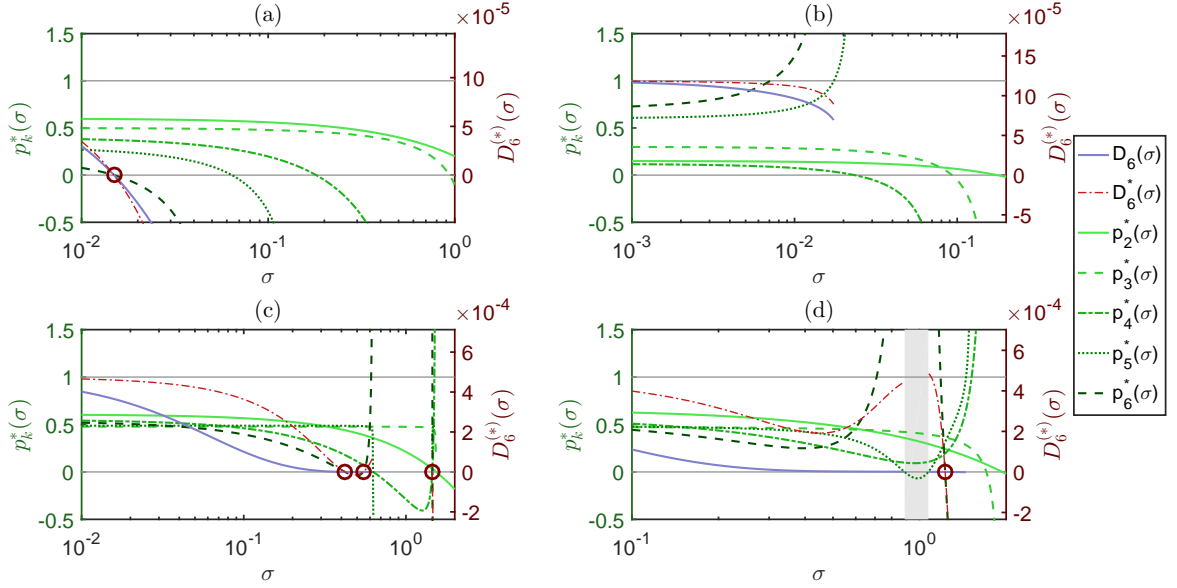


Figure 4: Evolution of the different convergence criteria for the Beta reconstruction kernel and four initial moment sets. These sets can be found in the figure source code provided as supplementary data.

- 409 (c) If $j < N$ and $p_j^* \left(\sigma_r^{(k-1)} \right) > 1$
- 410 • Compute $\sigma_{t_2} = \sigma_{t_1} + \left(\sigma_{t_1} - \sigma_l^{(k-1)} \right) \frac{q_j^* \left(\sigma_{t_1} \right)}{\sqrt{q_j^* \left(\sigma_{t_1} \right)^2 - q_j^* \left(\sigma_l^{(k-1)} \right) * q_j^* \left(\sigma_r^{(k-1)} \right)}}$ and $\mathbf{p}_N^* \left(\sigma_{t_2} \right)$,
- 411 with $q_j^* \left(\sigma \right) = 1 - p_j^* \left(\sigma \right)$.
- 412 (d) Else, that is if $j = N$ or $p_j^* \left(\sigma_r^{(k-1)} \right) < 0$
- 413 • Compute $\sigma_{t_2} = \sigma_{t_1} + \left(\sigma_{t_1} - \sigma_l^{(k-1)} \right) \frac{p_j^* \left(\sigma_{t_1} \right)}{\sqrt{p_j^* \left(\sigma_{t_1} \right)^2 - p_j^* \left(\sigma_l^{(k-1)} \right) * p_j^* \left(\sigma_r^{(k-1)} \right)}}$ and $\mathbf{p}_N^* \left(\sigma_{t_2} \right)$.
- 414 (e) Set $\sigma_l^{(k)}$ as the highest value between $\sigma_l^{(k-1)}$, σ_{t_1} and σ_{t_2} such that the correspond-
- 415 ing vector \mathbf{p}_N^* lies in $]0, 1[^N$.
- 416 (f) Set $\sigma_r^{(k)}$ as the lowest value between $\sigma_r^{(k-1)}$, σ_{t_1} and σ_{t_2} such that the corresponding
- 417 vector \mathbf{p}_N^* does not lie in $]0, 1[^N$.

418 Stop the computation if $\sigma_r^{(k)} - \sigma_l^{(k)} < \varepsilon \sigma_2$ or if $p_N^* \left(\sigma_l^{(k)} \right) < \varepsilon p_N^* \left(0 \right)$, with ε a relative

419 tolerance (e.g. $\varepsilon = 10^{-10}$). As previously, once convergence is achieved, the weights \mathbf{w}_P and

420 nodes $\boldsymbol{\xi}_P$ of the reconstruction can be obtained by computing a Gaussian quadrature rule

421 based on the recurrence coefficients $\mathbf{a}_{P-1}^* \left(\sigma_l^{(k)} \right)$ and $\mathbf{b}_{P-1}^* \left(\sigma_l^{(k)} \right)$.

422 This algorithm will converge to the root σ_N for cases similar to Fig. 4a; to the minimum

423 of $D_N(\sigma)$ for cases similar to Fig. 4b; to one of the multiple roots for cases similar to Fig.

424 4c. In the case illustrated in Fig. 4d, the algorithm may or may not identify the existing

425 root, depending on whether one of the intermediate tested σ values lies in the greyed area.

426 One could try to develop a more robust algorithm, that will always find the root if it
 427 is defined, even in the case shown in Fig. 4d. An other improvement would be to ensure
 428 a consistent result when multiple roots exist, for instance by converging toward the lowest
 429 root, so that a small perturbation in the raw moments will only cause a small change on the
 430 resulting σ value. Nothing prevents the current algorithm from converging toward one root
 431 for a moment set and toward another one after a small perturbation of this set which could
 432 induce instabilities in large-scale simulations. Note that these limitations already existed in
 433 previous EQMOM implementations and do not result from the new approach developed in
 434 this article.

435 4. Comparison of EQMOM approaches

436 4.1. Method

437 The new EQMOM moment-inversion procedure only requires computation of the realis-
 438 ability criteria of the vector of degenerated moments $\mathbf{m}_{2P}^*(\sigma)$ in order to identify σ . These
 439 computations were already performed in the original approach [1] to ensure the realisability
 440 of the vector $\mathbf{m}_{2P-1}^*(\sigma)$ prior to the quadrature computation and ulterior steps.

441 It is therefore obvious that the new approach will always require a lower number of
 442 floating point operations (FLOP). In order to quantify this reduction on FLOP number, and
 443 the actual performance gain, two implementations of the Gauss EQMOM moment-inversion
 444 procedure are compared.

445 The first tested implementation is the one described in Fig. 1b, whose computational cost
 446 is similar to that of Nguyen et al. [1]. As it only requires the matrix $\mathbf{A}_{2P}^{-1}(\sigma)$, it will benefit
 447 the same optimizations as the second approach as far as the linear system is concerned. The
 448 second tested implementation is the one described in section 3.3, based on the realisability
 449 of $\mathbf{m}_{2P}^*(\sigma)$ through the computation of the recurrence coefficients $\mathbf{a}_{P-1}^*(\sigma)$ and $\mathbf{b}_P^*(\sigma)$.

450 Both approaches are implemented in MATLAB [19] functions which take as input a vector
 451 of moments (size $2P + 1 \times 1$) and returns the vectors \mathbf{w}_P , $\boldsymbol{\xi}_P$ (size $P \times 1$) and the scalar
 452 σ . These implementations integrate a simple FLOP counter distinguishing each operation
 453 (+, -, *, /, exp, $\sqrt{\quad}$) and counting the number of call to these operations for each step of
 454 computation (linear system, Chebyshev algorithm, quadrature computation and others).

455 In order to evaluate the number of operations used in the computation of the eigenvalues
 456 and eigenvectors of the Jacobi matrix (Eq. (6)), the Jacobi and the Francis algorithms
 457 which are suited for symmetric matrices [32] are used in place of the MATLAB built-in “eig”
 458 function [19]. Finally, the number of tested σ values (*i.e.* the number of calls to the linear
 459 system $\mathbf{m}_{2P}^*(\sigma) = \mathbf{A}_{2P}^{-1}(\sigma) \cdot \mathbf{m}_{2P}$) is measured too.

460 10^4 realisable sets of 11 moments were randomly generated through a two step process:

461 1. Generate two random vectors \mathbf{a}_4 and \mathbf{b}_5 .

- 462 • Elements of \mathbf{a}_4 are distributed along a normal distribution: $a_k \sim \mathcal{N}(0, 25)$, $k \in$
 463 $\{0, \dots, 4\}$.
- 464 • Elements of \mathbf{b}_5 are distributed along an exponential distribution $b_k \sim \text{Exp}(5)$, $k \in$
 465 $\{1, \dots, 5\}$.

466 2. Use a reversed Chebyshev algorithm to compute the vector of moments \mathbf{m}_{10} corre-
467 sponding to \mathbf{a}_4 and \mathbf{b}_5 .

468 A routine applied both moment-inversion procedures on all generated moment sets and
469 varied the actual number of moments $2P + 1 \in \{5, 7, 9, 11\}$. This routine also measured the
470 wall-time of each of these calls.

471 4.2. Results

472 Results of the comparison are given in Table 1. The Jacobi algorithm was the fastest one
473 to compute the eigenvalues and eigenvectors in the cases $P = 2$ and $P = 3$ whilst the Francis
474 algorithm was faster for $P = 4$ and $P = 5$. Table 1 only shows the results corresponding
475 to that fastest algorithm for each case, in order to have the lowest estimate in FLOP and
476 run-time gain between both implementations.

477 The first main observation is a decrease in the number of tested σ values. This decrease
478 is due to the fact that in the former approach, if $\mathbf{m}_{N-1}^*(\sigma)$ turns out not to be realisable, the
479 objective function is set to a arbitrarily high negative value. The use of such an arbitrary
480 value slows down the convergence of the non-linear equation solver. Meanwhile, the new
481 approach never makes use of arbitrary values, all the elements of the vector $\mathbf{b}_P^*(\sigma)$ are used
482 one after the other which yields a better choice of the next tested σ value.

483 The second observation was expected and is a significant drop in the total number of
484 FLOP. This is mainly justified by the fact that the quadrature computation is only called
485 once in the new approach whilst it is called for most tested σ values in the former moment-
486 inversion procedure. This quadrature, which consists in the computation of the eigenvalues
487 and eigenvectors of a tridiagonal symmetric matrix, is the most expensive operation used in
488 the EQMOM moment-inversion procedure.

489 Overall, one observes a net decrease in the number of floating-point operations and in
490 the computation run-time of 80% to 85% for these implementations of Gauss EQMOM and
491 the tested 10^4 moment sets.

492 5. Conclusion

493 The first developments relative to the Extended Quadrature Method of Moments are
494 quite recent [14]. Most of these developments were dedicated to widening the use of this
495 method to new application cases, in particular by adding new reconstruction kernels to
496 the EQMOM formalism, and to demonstrate its stability and accuracy compared to other
497 methods. This article summarised all of these developments, relative to the Gaussian kernel
498 [14], to the Log-normal kernel [18] and to the Gamma and Beta kernels [15]. It was also
499 shown that at least two other kernels are perfectly compatible with the EQMOM formalism:
500 the Laplace and Weibull kernels. In a previous work, the solution of a PBE in some specific
501 setups was a Laplace-like distribution [27]. Moreover, the Weibull distribution is often met
502 in the modelling of biological systems. We then hope that the scientific community will find
503 a good use for these developments.

504 The youth of EQMOM explains that there is still room left for improvements. The
505 core of this method –the moment-inversion procedure– is an iterative process which is its
506 computational bottleneck. Nguyen et al. [1] proposed some modifications, compared to

Table 1: Table of comparison of the Gauss EQMOM implementations corresponding to Fig. 1b and 1c. The count of FLOP details the operations related to (i) the matrix-vector product $\mathbf{A}_{2P}^{-1}(\sigma) \cdot \mathbf{m}_{2P}$, (ii) the Chebyshev Algorithm (CA), (iii) the Quadrature Computation (QC) and (iv) a miscellaneous category. Results are given as mean \pm standard-deviation.

		$P = 2$	$P = 3$	$P = 4$	$P = 5$
New approach	$\mathbf{A}_{2P}^{-1}(\sigma)$	282 \pm 123	843 \pm 210	1842 \pm 328	3418 \pm 527
	CA	227 \pm 92	564 \pm 134	1146 \pm 195	2026 \pm 301
	FLOP QC	52 \pm 1	546 \pm 56	1225 \pm 144	2151 \pm 213
	Misc.	93 \pm 37	100 \pm 23	116 \pm 19	131 \pm 18
	Total	654 \pm 252	2053 \pm 357	4328 \pm 536	7727 \pm 834
	Evaluations	15 \pm 6	17 \pm 4	19 \pm 3	21 \pm 3
Run-time (ms)		6 \pm 3	13 \pm 5	23 \pm 6	33 \pm 7
Former approach	$\mathbf{A}_{2P}^{-1}(\sigma)$	298 \pm 164	1095 \pm 391	2683 \pm 741	5352 \pm 1450
	CA	223 \pm 115	724 \pm 246	1662 \pm 442	3184 \pm 836
	FLOP QC	823 \pm 421	9485 \pm 3245	23734 \pm 5387	46870 \pm 10002
	Misc.	228 \pm 119	395 \pm 137	634 \pm 155	959 \pm 224
	Total	1572 \pm 818	11700 \pm 3939	28713 \pm 6467	56365 \pm 12138
	Evaluations	16 \pm 8	21 \pm 7	27 \pm 7	32 \pm 9
Run-time (ms)		15 \pm 9	73 \pm 30	105 \pm 28	162 \pm 40
Gain in	FLOP	58.4% \pm 26.9%	82.5% \pm 6.6%	84.9% \pm 3.9%	86.3% \pm 3.3%
	Evaluations	6.3% \pm 60.0%	19.0% \pm 33.0%	29.6% \pm 21.4%	34.4% \pm 20.7%
	Run-time	60.0% \pm 31.2%	82.2% \pm 10.0%	78.1% \pm 8.2%	79.6% \pm 6.6%

507 previous implementations, in order to stabilise the method and to speed-up its resolution,
508 namely the use of Ridder’s method instead of bounded-secant or dichotomic methods to
509 solve the non-linear problem, and the realisability checks performed prior to the quadrature
510 computation.

511 Further improvements were proposed by shifting the resolution toward a new paradigm.
512 This results in a significant decrease in computational cost of about 80% – 85% in terms
513 of required floating-point operations. This resulted in our MATLAB implementations in a
514 similar gain in terms of computation wall-time.

515 In multiple works [1, 15, 27], EQMOM has been compared to other methods (Maximum
516 Entropy approach or sectional methods) and exhibited (i) similar accuracy even with a lower
517 number of resolved variables, and (ii) faster or comparable computation times. The new
518 improvements of EQMOM will make it even more competitive as its stability and accuracy
519 are kept while reducing the gap in terms of numerical cost between EQMOM and other
520 cheaper methods such as Gauss or Gauss-Radau quadratures.

521 We strongly believe that transparency about these developments will help further refine-
522 ments of EQMOM. For that reason, all sources used to generate figures and data in this article
523 are provided as supplementary data. We also release all our EQMOM source codes both with
524 this article and in an open-access GIT repository (url: <https://gitlab.com/open-eqmom>).
525 It will be updated as well as supplemented with implementations of EQMOM in languages
526 other than MATLAB. In the case of the Beta reconstruction kernel, some suggestions for
527 further improvements in terms of accuracy and stability were listed in section 3.5. These

528 will be tackled in ulterior work.

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629 **Appendix A. Chebyshev algorithm**

630 The Chebyshev algorithm allows to compute the three-term recurrence coefficients of the
 631 monic polynomials orthogonal to a measure $d\mu(\xi)$ whose moments are given by the vector
 632 $\mathbf{m}_N = [m_0, \dots, m_N]$. This version of the algorithm fills column-wise a $N + 1 \times \lceil \frac{N+1}{2} \rceil$ matrix
 633 denoted \mathbf{S} .

634 First, fill the first column with the moments $S_{i,0} = m_i$, compute $a_0 = m_1/m_0$ and fill the
 635 second column with $S_{i,1} = S_{i+1,0} - a_0 S_{i,0}$, $\forall i \in \{1, \dots, N - 1\}$.

636 Then iterate for $j \in \{2, \dots, \lceil \frac{N-1}{2} \rceil\}$:

$$\begin{aligned}
 a_{j-1} &= \frac{S_{j,j-1}}{S_{j-1,j-1}} - \frac{S_{j-1,j-2}}{S_{j-2,j-2}} \\
 b_{j-1} &= \frac{S_{j-1,j-1}}{S_{j-2,j-2}} \\
 S_{i,j} &= S_{i+1,j-1} - a_{j-1} S_{i,j-1} - b_{j-1} S_{i,j-2}, \quad i \in \{j, \dots, N - j\}
 \end{aligned}$$

637 **Appendix B. Kernels for EQMOM**

638 There exists multiple variations of the EQMOM method depending on the Kernel Density
 639 Function that is used for the reconstruction in Eq. (15). This section details the specificities
 640 of multiple KDF that were found to be compatible with the EQMOM procedure. It details
 641 for each kernel

- 642 1. the actual expression of that kernel $\delta_\sigma(\xi, \xi_m)$;
- 643 2. the expression of its moments;
- 644 3. the matrix $\mathbf{A}_n(\sigma)$ that allows the transfer between the raw moments of the reconstruction
 645 $\widetilde{\mathbf{m}}_n$ and its degenerated moments \mathbf{m}_n^* ;
- 646 4. the nested quadrature rules suiting this kernel;
- 647 5. the analytical solutions available for one-node EQMOM ($P = 1$).

648 Two-nodes analytical solutions exist for the Gaussian, Gamma, Laplace and Log-normal
 649 kernels and are accessible using the same methodology than that used by Chalons et al. [14]
 650 for the Gaussian kernel. These solutions are not detailed here but are implemented in the
 651 MATLAB code given in supplementary data.

652 All definitions of matrices $A_n(\sigma)$ are given using zero-offset. The element of the first line
 653 and column of this matrix then reads $A_{0,0}(\sigma)$.

654 *Appendix B.1. Gaussian kernel*

655 *Appendix B.1.1. Definition*

656 The Gaussian kernel $\delta_\sigma^{(G)}(\xi, \xi_m)$ was first used in EQMOM by Chalons et al. [14]. It is
 657 defined on $\Omega_\xi =]-\infty, +\infty[$ by

$$\delta_\sigma^{(G)}(\xi, \xi_m) = \frac{1}{\sigma\sqrt{2\pi}} \exp\left(-\frac{(\xi - \xi_m)^2}{2\sigma^2}\right) \tag{B.1}$$

658 *Appendix B.1.2. Moments and linear system*

659 Moments of the Gaussian kernel are given by:

$$\int_{-\infty}^{+\infty} \xi^k \delta_\sigma^{(G)}(\xi, \xi_m) d\xi = \sum_{j=0}^{\lfloor k/2 \rfloor} \frac{k!}{j!(k-2j)!} \left(\frac{\sigma^2}{2}\right)^j \xi_m^{k-2j} \quad (\text{B.2})$$

660 Moments of the distribution $\tilde{n}(\xi) = \sum_{i=1}^P w_i \delta_\sigma^{(G)}(\xi, \xi_i)$ are given by the linear system

$$\tilde{\mathbf{m}}_n = \mathbf{A}_n^{(G)}(\sigma) \cdot \mathbf{m}_n^* \quad (\text{B.3})$$

661 with

$$A_{i,j}^{(G)}(\sigma) = \begin{cases} 0 & \text{if } j > i \text{ or } (i-j \bmod 2) = 1 \\ \frac{i!}{\left(\frac{i-j}{2}\right)!j!} \left(\frac{\sigma^2}{2}\right)^{\frac{i-j}{2}} & \text{otherwise} \end{cases} \quad (\text{B.4})$$

662 The inverse of this matrix is given by:

$$A_{i,j}^{(G)-1}(\sigma) = \begin{cases} 0 & \text{if } j > i \text{ or } (i-j \bmod 2) = 1 \\ \frac{i!}{\left(\frac{i-j}{2}\right)!j!} \left(-\frac{\sigma^2}{2}\right)^{\frac{i-j}{2}} & \text{otherwise} \end{cases} \quad (\text{B.5})$$

663 which translates, for the case $n = 4$ into:

$$\begin{bmatrix} \tilde{m}_0 \\ \tilde{m}_1 \\ \tilde{m}_2 \\ \tilde{m}_3 \\ \tilde{m}_4 \end{bmatrix} = \begin{pmatrix} 1 & & & & 0 \\ & 1 & & & \\ \sigma^2 & 0 & 1 & & \\ & 0 & 3\sigma^2 & 0 & 1 \\ 3\sigma^4 & 0 & 6\sigma^2 & 0 & 1 \end{pmatrix} \cdot \begin{bmatrix} m_0^* \\ m_1^* \\ m_2^* \\ m_3^* \\ m_4^* \end{bmatrix} \quad (\text{B.6})$$

$$\begin{bmatrix} m_0^* \\ m_1^* \\ m_2^* \\ m_3^* \\ m_4^* \end{bmatrix} = \begin{pmatrix} 1 & & & & 0 \\ & 1 & & & \\ -\sigma^2 & 0 & 1 & & \\ & 0 & -3\sigma^2 & 0 & 1 \\ 3\sigma^4 & 0 & -6\sigma^2 & 0 & 1 \end{pmatrix} \cdot \begin{bmatrix} \tilde{m}_0 \\ \tilde{m}_1 \\ \tilde{m}_2 \\ \tilde{m}_3 \\ \tilde{m}_4 \end{bmatrix} \quad (\text{B.7})$$

664 *Appendix B.1.3. Moment preserving nested quadrature*

665 The approximation of integral properties using Gauss EQMOM is performed through the
666 following nested quadrature:

$$\int_{-\infty}^{+\infty} f(\xi) n(\xi) d\xi \approx \frac{1}{\sqrt{\pi}} \sum_{i=1}^P w_i \sum_{j=1}^Q \omega_j f(\xi_i + \sigma \lambda_j \sqrt{2}) \quad (\text{B.8})$$

667 with \mathbf{w}_P , $\boldsymbol{\xi}_P$ and σ the EQMOM reconstruction parameters computed from \mathbf{m}_{2P} ; $\boldsymbol{\omega}_Q$ and
668 $\boldsymbol{\lambda}_Q$ are the weights and nodes of a Q -nodes Gauss-Hermite quadrature rule (see Appendix
669 C).

670 *Appendix B.1.4. Single node analytical solution*

671 The case $P = 1$ has the following analytical solution:

$$\begin{aligned} w_1 &= m_0 \\ \xi_1 &= \frac{m_1}{m_0} \\ \sigma &= \frac{\sqrt{m_2 m_0 - m_1^2}}{m_0} \end{aligned}$$

672 *Appendix B.2. Laplace kernel*

673 *Appendix B.2.1. Definition*

674 The Laplace kernel $\delta_\sigma^{(\lambda)}(\xi, \xi_m)$ is defined on $\Omega_\xi =]-\infty, +\infty[$ by

$$\delta_\sigma^{(\lambda)}(\xi, \xi_m) = \frac{1}{2\sigma} \exp\left(-\frac{|\xi - \xi_m|}{\sigma}\right) \quad (\text{B.9})$$

675 *Appendix B.2.2. Moments and linear system*

676 Moments of the Laplace kernel are given by

$$\int_{-\infty}^{+\infty} \xi^k \delta_\sigma^{(\lambda)}(\xi, \xi_m) d\xi = \sum_{j=0}^k \frac{k!}{(k-j)!} \frac{1 + (-1)^j}{2} \xi_m^{k-j} \sigma^j \quad (\text{B.10})$$

677 Moments of the distribution $\tilde{n}(\xi) = \sum_{i=1}^P w_i \delta_\sigma^{(\lambda)}(\xi, \xi_i)$ are given by the linear system

$$\tilde{\mathbf{m}}_n = \mathbf{A}_n^{(\lambda)}(\sigma) \cdot \mathbf{m}_n^* \quad (\text{B.11})$$

678 with

$$A_{i,j}^{(\lambda)}(\sigma) = \begin{cases} 0 & \text{if } j > i \text{ or } (i - j \pmod{2}) = 1 \\ \frac{i!}{j!} \sigma^{i-j} & \text{otherwise} \end{cases} \quad (\text{B.12})$$

679 The inverse matrix is defined by

$$A_{i,j}^{(\lambda)-1}(\sigma) = \begin{cases} 1 & \text{if } i = j \\ -(j+1)(j+2)\sigma^2 & \text{if } i = j+2 \\ 0 & \text{otherwise} \end{cases} \quad (\text{B.13})$$

680 which translates for $n = 6$ into

$$\begin{pmatrix} \tilde{m}_0 \\ \tilde{m}_1 \\ \tilde{m}_2 \\ \tilde{m}_3 \\ \tilde{m}_4 \\ \tilde{m}_5 \\ \tilde{m}_6 \end{pmatrix} = \begin{pmatrix} 1 & & & & & & 0 \\ 0 & 1 & & & & & \\ \frac{2!\sigma^2}{0!} & 0 & 1 & & & & \\ 0 & \frac{3!\sigma^2}{1!} & 0 & 1 & & & \\ \frac{4!\sigma^4}{0!} & 0 & \frac{4!\sigma^2}{2!} & 0 & 1 & & \\ 0 & \frac{5!\sigma^4}{1!} & 0 & \frac{5!\sigma^2}{3!} & 0 & 1 & \\ \frac{6!\sigma^6}{0!} & 0 & \frac{6!\sigma^4}{2!} & 0 & \frac{6!\sigma^2}{4!} & 0 & 1 \end{pmatrix} \cdot \begin{pmatrix} m_0^* \\ m_1^* \\ m_2^* \\ m_3^* \\ m_4^* \\ m_5^* \\ m_6^* \end{pmatrix} \quad (\text{B.14})$$

$$\begin{pmatrix} m_0^* \\ m_1^* \\ m_2^* \\ m_3^* \\ m_4^* \\ m_5^* \\ m_6^* \end{pmatrix} = \begin{pmatrix} 1 & & & & & & 0 \\ 0 & 1 & & & & & \\ -2\sigma^2 & 0 & 1 & & & & \\ & -6\sigma^2 & 0 & 1 & & & \\ & & -12\sigma^2 & 0 & 1 & & \\ & & & -20\sigma^2 & 0 & 1 & \\ 0 & & & & -30\sigma^2 & 0 & 1 \end{pmatrix} \cdot \begin{pmatrix} \tilde{m}_0 \\ \tilde{m}_1 \\ \tilde{m}_2 \\ \tilde{m}_3 \\ \tilde{m}_4 \\ \tilde{m}_5 \\ \tilde{m}_6 \end{pmatrix} \quad (\text{B.15})$$

681 *Appendix B.2.3. Moment preserving nested quadrature*

682 The approximation of integral properties using Laplace EQMOM is performed through
683 the following nested quadrature:

$$\int_{-\infty}^{+\infty} f(\xi)n(\xi)d\xi \approx \sum_{i=1}^P w_i \sum_{j=1}^Q \omega_j f(\xi_i + \sigma\lambda_j) \quad (\text{B.16})$$

684 with \mathbf{w}_P , $\boldsymbol{\xi}_P$ and σ the EQMOM reconstruction parameters computed from \mathbf{m}_{2P} ; $\boldsymbol{\omega}_Q$ and
685 $\boldsymbol{\lambda}_Q$ are the weights and nodes of a Q -nodes ‘‘Gauss-Laplace’’ quadrature rule (see Appendix
686 C).

687 *Appendix B.2.4. Single node analytical solution*

688 The case $P = 1$ has the following analytical solution:

$$\begin{aligned} w_1 &= m_0 \\ \xi_1 &= \frac{m_1}{m_0} \\ \sigma &= \sqrt{\frac{m_2 m_0 - m_1^2}{2m_0^2}} \end{aligned}$$

689 *Appendix B.3. Log-normal kernel*

690 *Appendix B.3.1. Definition*

691 The Log-normal kernel $\delta_\sigma^{(L)}(\xi, \xi_m)$ was first used in EQMOM by Madadi-Kandjani and
692 Passalacqua [18]. It is defined on $\Omega_\xi =]0, +\infty[$ by

$$\delta_\sigma^{(L)}(\xi, \xi_m) = \frac{1}{\sigma \xi \sqrt{2\pi}} \exp\left(-\frac{(\log(\xi) - \log(\xi_m))^2}{2\sigma^2}\right) \quad (\text{B.17})$$

693 *Appendix B.3.2. Moments and linear system*

694 Moments of the Log-normal kernel are given by

$$\int_0^{+\infty} \xi^k \delta_\sigma^{(L)}(\xi, \xi_m) d\xi = \xi_m^k z^{k^2} \quad \text{with } z = e^{\sigma^2/2} \quad (\text{B.18})$$

695 Moments of the distribution $\tilde{n}(\xi) = \sum_{i=1}^P w_i \delta_\sigma^{(L)}(\xi, \xi_i)$ are given by

$$\tilde{m}_k = m_k^* z^{k^2} \quad (\text{B.19})$$

696 This can be translated into a linear system

$$\tilde{\mathbf{m}}_n = \mathbf{A}_n^{(L)}(\sigma) \cdot \mathbf{m}_n^* \quad (\text{B.20})$$

697 with $\mathbf{A}_n^{(L)}(\sigma)$ a diagonal matrix:

$$A_{i,j}^{(L)}(\sigma) = \begin{cases} z^{i^2} & \text{if } i = j \\ 0 & \text{otherwise} \end{cases} \quad (\text{B.21})$$

698 whose inverse matrix is directly given by

$$A_{i,j}^{(L)-1}(\sigma) = \begin{cases} z^{-i^2} & \text{if } i = j \\ 0 & \text{otherwise} \end{cases} \quad (\text{B.22})$$

699 *Appendix B.3.3. Low cost nested quadrature*

700 A variable change allows approximating integral properties over a LogN EQMOM recon-
701 struction using Gauss-Hermite quadratures [18]:

$$\int_0^{+\infty} f(\xi) n(\xi) d\xi \approx \frac{1}{\sqrt{\pi}} \sum_{i=1}^P w_i \sum_{j=1}^Q \omega_j f\left(\xi_i \exp\left(\sigma \lambda_j \sqrt{2}\right)\right) \quad (\text{B.23})$$

702 with \mathbf{w}_P , $\boldsymbol{\xi}_P$ and σ the EQMOM reconstruction parameters computed from \mathbf{m}_{2P} ; $\boldsymbol{\omega}_Q$ and
703 $\boldsymbol{\lambda}_Q$ are the weights and nodes of a Q -nodes Gauss-Hermite quadrature rule (see Appendix
704 C).

705 Parameters of this nested quadrature do not depend on σ of the main quadrature nodes
706 $\boldsymbol{\xi}_P$. Consequently, $\boldsymbol{\omega}_Q$ and $\boldsymbol{\lambda}_Q$ only need to be computed once. It is worth noting that this
707 quadrature does not preserve the moments of the distribution and only yields exact results
708 for $f(\xi) = \log(\xi)^k$, $k \in \{0, \dots, 2 \min(P, Q) - 1\}$.

709 *Appendix B.3.4. Moment preserving nested quadrature*

[16] suggested the use of Gauss-Wigert quadratures [33] to preserve the moments of a

LogN EQMOM reconstruction:

$$\int_0^{+\infty} f(\xi)n(\xi)d\xi \approx \sum_{i=1}^P w_i \sum_{j=1}^Q \omega_j^{(\sigma)} f\left(\xi_i \lambda_j^{(\sigma)}\right) \quad (\text{B.24})$$

710 with \mathbf{w}_P , $\boldsymbol{\xi}_P$ and σ the EQMOM reconstruction parameters computed from \mathbf{m}_{2P} ; $\omega_Q^{(\sigma)}$ and
 711 $\lambda_Q^{(\sigma)}$ are the weights and nodes of a Q -nodes Gauss-Wigert quadrature rule of parameter σ
 712 (see Appendix C). This quadrature rule must be computed for each value of σ , *i.e.* for each
 713 LogN EQMOM reconstruction.

714 *Appendix B.3.5. Single node analytical solution*

715 The case $P = 1$ has the following analytical solution:

$$\begin{aligned} w_1 &= m_0 \\ \xi_1 &= \sqrt{\frac{m_1^4}{m_2 m_0^3}} \\ \sigma &= \sqrt{\log\left(\frac{m_2 m_0}{m_1^2}\right)} \end{aligned}$$

716 *Appendix B.4. Gamma kernel*

717 *Appendix B.4.1. Definition*

718 The Gamma kernel $\delta_\sigma^{(\Gamma)}(\xi, \xi_m)$ was first used in EQMOM by Yuan et al. [15]. It is defined
 719 on $\Omega_\xi =]0, +\infty[$ by

$$\delta_\sigma^{(\Gamma)}(\xi, \xi_m) = \frac{\xi^{(l-1)} \exp(-\xi/\sigma)}{\Gamma(l)\sigma^l} \quad \text{with } l = \frac{\xi_m}{\sigma} \text{ and } \Gamma(x) = \int_0^{+\infty} t^{x-1} e^{-t} dt \quad (\text{B.25})$$

720 *Appendix B.4.2. Moments and linear system*

721 Moments of the Gamma kernel are given by

$$\int_0^{+\infty} \xi^k \delta_\sigma^{(\Gamma)}(\xi, \xi_m) d\xi = G_k(\xi_m, \sigma) = \begin{cases} 1 & \text{if } k = 0 \\ \prod_{j=0}^{k-1} (\xi_m + j\sigma) & \text{otherwise} \end{cases} \quad (\text{B.26})$$

722 Moments of the distribution $\tilde{n}(\xi) = \sum_{i=1}^P w_i \delta_\sigma^{(\Gamma)}(\xi, \xi_i)$ are given by the linear system

$$\widetilde{\mathbf{m}}_n = \mathbf{A}_n^{(\Gamma)}(\sigma) \cdot \mathbf{m}_n^* \quad (\text{B.27})$$

723 with

$$A_{i,j}^{(\Gamma)}(\sigma) = \begin{cases} 0 & \text{if } j > i \text{ or } i = 0 \text{ or } j = 0 \\ 1 & \text{if } i = 0 \text{ and } j = 0 \\ A_{i-1,j-1}^{(\Gamma)}(\sigma) + (i-1)\sigma A_{i-1,j}^{(\Gamma)}(\sigma) & \text{otherwise} \end{cases} \quad (\text{B.28})$$

724 The inverse of this matrix is given by

$$A_{i,j}^{(\Gamma)-1}(\sigma) = \begin{cases} 0 & \text{if } j > i \text{ or } i = 0 \text{ or } j = 0 \\ 1 & \text{if } i = 0 \text{ and } j = 0 \\ A_{i-1,j-1}^{(\Gamma)-1}(\sigma) - j\sigma A_{i-1,j}^{(\Gamma)-1}(\sigma) & \text{otherwise} \end{cases} \quad (\text{B.29})$$

725 which translates, for the case $N = 6$ into

$$\begin{bmatrix} \tilde{m}_0 \\ \tilde{m}_1 \\ \tilde{m}_2 \\ \tilde{m}_3 \\ \tilde{m}_4 \\ \tilde{m}_5 \\ \tilde{m}_6 \end{bmatrix} = \begin{pmatrix} 1 & & & & & & 0 \\ & 1 & & & & & \\ & & 1\sigma & & & & \\ & & & 3\sigma & & & \\ & & & & 1 & & \\ & & & & & 6\sigma & 1 \\ & & & & & & 10\sigma & 1 \\ & & & & & & & 15\sigma & 1 \end{pmatrix} \cdot \begin{bmatrix} m_0^* \\ m_1^* \\ m_2^* \\ m_3^* \\ m_4^* \\ m_5^* \\ m_6^* \end{bmatrix} \quad (\text{B.30})$$

$$\begin{bmatrix} m_0^* \\ m_1^* \\ m_2^* \\ m_3^* \\ m_4^* \\ m_5^* \\ m_6^* \end{bmatrix} = \begin{pmatrix} 1 & & & & & & 0 \\ & 1 & & & & & \\ & & -\sigma & & & & \\ & & & \sigma^2 & & & \\ & & & & -3\sigma & & \\ & & & & & 7\sigma^2 & -6\sigma & 1 \\ & & & & & & -10\sigma & 1 \\ & & & & & & & -15\sigma & 1 \end{pmatrix} \cdot \begin{bmatrix} \tilde{m}_0 \\ \tilde{m}_1 \\ \tilde{m}_2 \\ \tilde{m}_3 \\ \tilde{m}_4 \\ \tilde{m}_5 \\ \tilde{m}_6 \end{bmatrix} \quad (\text{B.31})$$

726 *Appendix B.4.3. Low cost nested quadrature*

727 A Gauss-Laguerre quadrature can be used to approximate integral properties over a
728 Gamma EQMOM reconstruction:

$$\int_0^{+\infty} f(\xi)n(\xi)d\xi \approx \sum_{j=1}^Q \omega_j f(\sigma\lambda_j) \sum_{i=1}^P \frac{w_i}{\Gamma\left(\frac{\xi_i}{\sigma}\right)} \lambda_j^{\frac{\xi_i}{\sigma}-1} \quad (\text{B.32})$$

729 with \mathbf{w}_P , $\boldsymbol{\xi}_P$ and σ the EQMOM reconstruction parameters computed from \mathbf{m}_{2P} ; $\boldsymbol{\omega}_Q$ and
730 $\boldsymbol{\lambda}_Q$ are the weights and nodes of a Q -nodes Gauss-Laguerre quadrature rule of parameter
731 $\alpha = 0$ (see Appendix C). The advantage of this quadrature is that it only requires $\boldsymbol{\omega}_Q$ and
732 $\boldsymbol{\lambda}_Q$ to be computed once. However, this quadrature will not preserve the moments of the
733 distribution.

734 *Appendix B.4.4. Moment preserving nested quadrature*

735 A generalized Gauss-Laguerre quadrature preserves the moments of a Gamma EQMOM
736 reconstruction:

$$\int_0^{+\infty} f(\xi)n(\xi)d\xi \approx \sum_{i=1}^P \frac{w_i}{\Gamma\left(\frac{\xi_i}{\sigma}\right)} \sum_{j=1}^Q \omega_j^{(\alpha_i)} f\left(\sigma\lambda_j^{(\alpha_i)}\right) \quad (\text{B.33})$$

737 with \mathbf{w}_P , $\boldsymbol{\xi}_P$ and σ the EQMOM reconstruction parameters computed from \mathbf{m}_{2P} ; $\boldsymbol{\omega}_Q^{(\alpha_i)}$ and
 738 $\boldsymbol{\lambda}_Q^{(\alpha_i)}$ are the weights and nodes of a Q -nodes Gauss-Laguerre quadrature rule of parameter
 739 $\alpha_i = \frac{\xi_i}{\sigma} - 1$ (see Appendix C).

740 The accuracy of this quadrature comes with a cost related to the computation of $\boldsymbol{\omega}_Q^{(\alpha_i)}$
 741 and $\boldsymbol{\lambda}_Q^{(\alpha_i)}$ for each value of α_i .

742 *Appendix B.4.5. Single node analytical solution*

743 The case $P = 1$ has the following analytical solution:

$$\begin{aligned} w_1 &= m_0 \\ \xi_1 &= \frac{m_1}{m_0} \\ \sigma &= \frac{m_2}{m_1} - \frac{m_1}{m_0} \end{aligned}$$

744 *Appendix B.5. Weibull kernel*

745 *Appendix B.5.1. Definition*

746 The Weibull kernel $\delta_\sigma^{(W)}(\xi, \xi_m)$ is defined on $\Omega_\xi =]0, +\infty[$ by

$$\delta_\sigma^{(W)}(\xi, \xi_m) = \frac{1}{\sigma\xi_m} \left(\frac{\xi}{\xi_m}\right)^{\frac{1-\sigma}{\sigma}} \exp\left(-\left(\frac{\xi}{\xi_m}\right)^{1/\sigma}\right) \quad (\text{B.34})$$

747 *Appendix B.5.2. Moments and linear system*

748 Moments of the Weibull kernel are given by

$$\int_0^{+\infty} \xi^k \delta_\sigma^{(W)}(\xi, \xi_m) d\xi = \xi_m^k \Gamma(1 + k\sigma) \quad (\text{B.35})$$

749 Moments of the distribution $\tilde{n}(\xi) = \sum_{i=1}^P w_i \delta_\sigma^{(W)}(\xi, \xi_i)$ are given by

$$\tilde{m}_k = m_k^* \Gamma(1 + k\sigma) \quad (\text{B.36})$$

750 This can be translated into a linear system

$$\tilde{\mathbf{m}}_n = \mathbf{A}_n^{(W)}(\sigma) \cdot \mathbf{m}_n^* \quad (\text{B.37})$$

751 with $\mathbf{A}_n^{(W)}(\sigma)$ a diagonal matrix:

$$A_{i,j}^{(W)}(\sigma) = \begin{cases} \Gamma(1 + i\sigma) & \text{if } i = j \\ 0 & \text{otherwise} \end{cases} \quad (\text{B.38})$$

752 whose inverse matrix is directly given by

$$A_{i,j}^{(W)^{-1}}(\sigma) = \begin{cases} \frac{1}{\Gamma(1+i\sigma)} & \text{if } i = j \\ 0 & \text{otherwise} \end{cases} \quad (\text{B.39})$$

753 *Appendix B.5.3. Low cost nested quadrature*

754 A Gauss-Laguerre quadrature can be used to approximate integral properties over a
755 Weibull EQMOM reconstruction:

$$\int_0^{+\infty} f(\xi)n(\xi)d\xi \approx \sum_{i=1}^P w_i \sum_{j=1}^Q \omega_j f(\xi_i \lambda_j^\sigma) \quad (\text{B.40})$$

756 with \mathbf{w}_P , $\boldsymbol{\xi}_P$ and σ the EQMOM reconstruction parameters computed from \mathbf{m}_{2P} ; $\boldsymbol{\omega}_Q$ and
757 $\boldsymbol{\lambda}_Q$ are the weights and nodes of a Q -nodes Gauss-Laguerre quadrature rule of parameter
758 $\alpha = 0$ (see Appendix C). The advantage of this quadrature is that it only requires $\boldsymbol{\omega}_Q$ and
759 $\boldsymbol{\lambda}_Q$ to be computed once. However, this quadrature will not preserve the moments of the
760 distribution and only yields exact results for $f(\xi) = \xi^{k/\sigma}$, $k \in \{0, \dots, 2 \min(P, Q) - 1\}$

761 *Appendix B.5.4. Moment preserving nested quadrature*

762 One can produce a Gauss quadrature that preserves the moments of Weibull EQMOM
763 approximations:

$$\int_0^{+\infty} f(\xi)n(\xi)d\xi \approx \sum_{i=1}^P w_i \sum_{j=1}^Q \omega_j^{(\sigma)} f(\xi_i \lambda_j^{(\sigma)}) \quad (\text{B.41})$$

764 with \mathbf{w}_P , $\boldsymbol{\xi}_P$ and σ the EQMOM reconstruction parameters computed from \mathbf{m}_{2P} ; $\boldsymbol{\omega}_Q^{(\sigma)}$ and
765 $\boldsymbol{\lambda}_Q^{(\sigma)}$ are the weights and nodes of a Q -nodes ‘‘Gauss-Weibull’’ quadrature rule of parameter
766 σ (see Appendix C). The weights and nodes of the nested quadrature need to be computed
767 for each value of σ , *i.e.* for each Weibull EQMOM approximation of the NDF.

768 *Appendix B.5.5. Single node numerical solution*

769 The parameters w_1 , ξ_1 and σ of the one-node Weibull EQMOM must be solution of the
770 following system:

$$\begin{aligned} m_0 &= w_1 \\ \frac{m_1}{\Gamma(1 + \sigma)} &= w_1 \xi_1 \\ \frac{m_2}{\Gamma(1 + 2\sigma)} &= w_1 \xi_1^2 \end{aligned}$$

771 The first equation gives $w_1 = m_0$ but no explicit solution exists for the two other equations.
772 One can however notice that $s = \frac{\sigma}{1+\sigma}$ must be a root of

$$G(s) = \frac{m_2 m_0}{m_1^2} - \frac{\Gamma(\frac{1+s}{1-s})}{\Gamma(\frac{1}{1-s})^2} \quad (\text{B.42})$$

773 which is monotonous, defined on $s \in [0, 1[$ and has the following limits

$$G(0) = \frac{m_2 m_0}{m_1^2} > 0$$

$$\lim_{s \rightarrow 1^-} G(s) < 0$$

774 $G(s)$ then admits a single root that can be computed numerically with the Ridder's method.
775 One can also narrow down, at a very low cost, the search interval $[0, 1[$ by using the property

$$g_n = G\left(\frac{n}{n+1}\right) = \frac{m_2 m_0}{m_1^2} - \frac{(2n)!}{(n!)^2} \quad (\text{B.43})$$

776 with n an integer, which induces the following recurrence relation:

$$g_n = c - h_n \quad (\text{B.44})$$

$$h_{n+1} = \left(4 - \frac{2}{n+1}\right) h_n \quad (\text{B.45})$$

777 with $c = \frac{m_2 m_0}{m_1^2}$ and $h_1 = 2$.

778 The proposed algorithm to identify the root of $G(s)$ is

- 779 1. Compute $c = \frac{m_2 m_0}{m_1^2}$
- 780 • if $c < 1$, cancel the operation as the moments are not realisable;
 - 781 • if $c = 1$, $s = 0$ is the root of $G(s)$;
 - 782 • if $c < 2$, set $s_l = 0$, $v_l = c - 1$, $s_r = \frac{1}{2}$ and $v_r = c - 2$ and go to step 3.
 - 783 • otherwise, set $s_l = 0$, $v_l = c - 1$ and go to step 2.
- 784 2. Initialise $i = 1$, $h = 2$ and iterate
- 785 (a) increment i by 1;
 - 786 (b) compute $h = h * \left(4 - \frac{2}{i}\right)$
 - 787 • if $h = c$, then $s = \frac{i}{i+1}$ is a root of $G(s)$;
 - 788 • if $h < c$, set $s_l = \frac{i}{i+1}$ and $v_l = c - h$;
 - 789 • if $h > c$, set $s_r = \frac{i}{i+1}$, $v_r = c - h$ and go to step 3.
- 790 3. Apply the Ridder's method to $G(s)$ on the interval $[s_l, s_r]$
- 791 (a) compute $s_{t_1} = \frac{1}{2}(s_l + s_r)$ and $v_{t_1} = G(s_{t_1})$;
 - 792 (b) compute $s_{t_2} = s_{t_1} + (s_{t_1} - s_l) \frac{v_{t_1}}{\sqrt{v_{t_1}^2 - v_l v_r}}$ and $v_{t_2} = G(s_{t_2})$;
 - 793 (c) set s_l the highest value between s_l , s_{t_1} and s_{t_2} whose image by G is positive;
 - 794 (d) set s_r the lowest value between s_r , s_{t_1} and s_{t_2} whose image by G is negative;
 - 795 (e) stop the computation if $v_l < \varepsilon(c - 1)$ with ε a relative tolerance (*e.g.* $\varepsilon = 10^{-10}$)
 - 796 and consider s_l as a root of $G(s)$.

797

Once the root of $G(s)$ is identified, compute

$$\sigma = \frac{s}{1-s}$$

$$\xi_1 = \frac{m_1}{m_0 \Gamma(1+\sigma)}$$

798

Note that each iteration of the Ridder's method requires two computations of $G(s)$, that implies four computations of the Gamma function –which is quite expensive– by iteration.

799

800

This explains the interest of the second step which allows to narrow down the research interval at hardly no cost.

801

802 *Appendix B.6. Beta kernel*

803 *Appendix B.6.1. Definition*

804

The Beta kernel $\delta_\sigma^{(\beta)}(\xi, \xi_m)$ was first used in EQMOM by Yuan et al. [15]. It is defined on $\Omega_\xi =]0, 1[$ by

805

$$\delta_\sigma^{(\beta)}(\xi, \xi_m) = \frac{\xi^{(l-1)}(1-\xi)^{(m-1)}}{B(l, m)} \quad \text{with } l = \frac{\xi_m}{\sigma} \text{ and } m = \frac{1-\xi_m}{\sigma} \quad (\text{B.46})$$

806

with $B(l, m) = \int_0^1 x^{(l-1)}(1-x)^{(m-1)} dx$ the beta function.

807 *Appendix B.6.2. Moments and linear system*

808

Moments of the Beta kernel are given by

$$\int_0^1 \xi^k \delta_\sigma^{(\beta)}(\xi, \xi_m) d\xi = H_k(\xi_m, \sigma) = \begin{cases} 1 & \text{if } k = 0 \\ \prod_{j=0}^{k-1} \left(\frac{\xi_m + j\sigma}{1+j\sigma} \right) & \text{otherwise} \end{cases} \quad (\text{B.47})$$

809

Moments of the distribution $\tilde{n}(\xi) = \sum_{i=1}^P w_i \delta_\sigma^{(\beta)}(\xi, \xi_i)$ are given by the linear system

$$\tilde{\mathbf{m}}_n = \mathbf{A}_n^{(\beta)}(\sigma) \cdot \mathbf{m}_n^* \quad (\text{B.48})$$

810

with the elements of $\mathbf{A}_n^{(\beta)}(\sigma)$ being computed from the elements of the matrix relative to

811

Gamma EQMOM, $\mathbf{A}_n^{(\Gamma)}(\sigma)$:

$$A_{i,j}^{(\beta)}(\sigma) = \frac{A_{i,j}^{(\Gamma)}(\sigma)}{F_i(\sigma)} \quad (\text{B.49})$$

$$F_i(\sigma) = \begin{cases} 1 & \text{if } i \leq 1 \\ (1 + (i-1)\sigma)F_{i-1}(\sigma) & \text{otherwise} \end{cases} \quad (\text{B.50})$$

812

The inverse of this matrix is also easily defined from $\mathbf{A}_n^{(\Gamma)-1}(\sigma)$:

$$A_{i,j}^{(\beta)-1}(\sigma) = A_{i,j}^{(\Gamma)-1}(\sigma)F_j(\sigma) \quad (\text{B.51})$$

813 *Appendix B.6.3. Low cost nested quadrature*

814 A Gauss-Legendre quadrature can be used to approximate integral properties over a Beta
815 EQMOM reconstruction:

$$\int_0^1 f(\xi)n(\xi)d\xi \approx \frac{1}{2} \sum_{i=1}^P \frac{w_i}{B(\alpha_i+1, \beta_i+1)} \sum_{j=1}^Q \omega_j f\left(\frac{1-\lambda_j}{2}\right) \left(\frac{1-\lambda_j}{2}\right)^{\alpha_i} \left(\frac{1+\lambda_j}{2}\right)^{\beta_i} \quad (\text{B.52})$$

816 with \mathbf{w}_P , $\boldsymbol{\xi}_P$ and σ the EQMOM reconstruction parameters computed from \mathbf{m}_{2P} ; $\boldsymbol{\omega}_Q$ and
817 $\boldsymbol{\lambda}_Q$ are the weights and nodes of a Q -nodes Gauss-Legendre quadrature rule (see Appendix
818 C); $\alpha_i = \frac{\xi_i - \sigma}{\sigma}$ and $\beta_i = \frac{1 - \xi_i - \sigma}{\sigma}$. This nested quadrature only requires $\boldsymbol{\omega}_Q$ and $\boldsymbol{\lambda}_Q$ to be
819 computed once, but will not preserve the moments of the distribution.

820 *Appendix B.6.4. Moment preserving nested quadrature*

821 A Gauss-Jacobi quadrature will preserve the moments of the distribution:

$$\int_0^1 f(\xi)n(\xi)d\xi \approx 2^{\frac{\sigma-1}{\sigma}} \sum_{i=1}^P \frac{w_i}{B(\alpha_i+1, \beta_i+1)} \sum_{j=1}^Q \omega_j^{(\alpha_i, \beta_i)} f\left(\frac{1-\lambda_j^{(\alpha_i, \beta_i)}}{2}\right) \quad (\text{B.53})$$

822 with \mathbf{w}_P , $\boldsymbol{\xi}_P$ and σ the EQMOM reconstruction parameters computed from \mathbf{m}_{2P} ; $\boldsymbol{\omega}_Q^{(\alpha_i, \beta_i)}$ and
823 $\boldsymbol{\lambda}_Q^{(\alpha_i, \beta_i)}$ are the weights and nodes of a Q -nodes Gauss-Jacobi quadrature rule of parameters
824 $\alpha_i = \frac{\xi_i - \sigma}{\sigma}$ and $\beta_i = \frac{1 - \xi_i - \sigma}{\sigma}$ (see Appendix C). The moment-preserving property of this
825 quadrature comes with the need to compute $\boldsymbol{\omega}_Q^{(\alpha_i, \beta_i)}$ and $\boldsymbol{\lambda}_Q^{(\alpha_i, \beta_i)}$ for each node of the main
826 Beta EQMOM quadrature.

827 *Appendix B.6.5. Single node analytical solution*

828 The case $P = 1$ has the following analytical solution:

$$\begin{aligned} w_1 &= m_0 \\ \xi_1 &= \frac{m_1}{m_0} \\ \sigma &= \frac{m_1^2 - m_0 m_2}{m_0(m_2 - m_1)} \end{aligned}$$

829 **Appendix C. Gaussian quadratures**

830 A Q -node Gaussian quadrature allows to approximate a function integral as a weighted
831 sum of pointwise values of this function over an interval I :

$$\int_I f(x)p(x)dx \approx \sum_{j=1}^Q \omega_j f(\lambda_j) \quad (\text{C.1})$$

832 $p(x)$ is a weight function, and the quadrature rule yields accurate integral evaluations if
833 $f(x) = x^k$, $k \in \{0, \dots, 2Q - 1\}$. The computation of the weights $\boldsymbol{\omega}_Q$ and nodes $\boldsymbol{\lambda}_Q$ is
834 performed as detailed in 2.2 by considering polynomials that are orthogonal with respect to
835 the weight function $p(x)$.

836 Table C.1 details for each Gauss quadrature:

- 837 • the weight function $p(x)$;
- 838 • the integration support I ;
- 839 • the computation of recurrence coefficients \mathbf{a}_{Q-1} and \mathbf{b}_{Q-1} ;
- 840 • the zero-th order moment P_0 of $p(x)$.

841 The recurrence coefficients are used to construct the Jacobi matrix \mathbf{J}_Q associated with
842 $p(x)$ on I (see Eq. 6). The nodes $\boldsymbol{\lambda}_Q$ are the eigenvalues of \mathbf{J}_Q , and the weights $\boldsymbol{\omega}_Q$ are given
843 by $\omega_j = P_0 v_{1,j}^2$ with $v_{1,j}$ the first component of the normalised eigenvector belonging to the
844 eigenvalue λ_j .

Table C.1: Specifics of Gauss quadratures used for EQMOM nested quadratures.

Gauss-	I	$p(x)$	\mathbf{a}_Q and \mathbf{b}_Q	P_0
Hermite	\mathbb{R}	$\exp(-x^2)$	$a_k = 0$ $b_k = k/2$	$\sqrt{\pi}$
Laplace ^c	\mathbb{R}	$\exp(- x)/2$	Apply Chebyshev algorithm to \mathbf{P}_{2Q-1} with $P_k = \begin{cases} 0 & \text{if } k \text{ odd} \\ k! & \text{if } k \text{ even} \end{cases}$	1
Laguerre ^f	\mathbb{R}^+	$x^\alpha \exp(-x)$	$a_0 = 1 + \alpha$ $a_k = 2 + a_{k-1}$ $b_k = k(k + \alpha)$	$\Gamma(1 + \alpha)^d$
Wigert ^{a,f}	\mathbb{R}^+	$\frac{1}{\gamma x \sqrt{2\pi}} \exp\left(\frac{\log^2(x)}{2\gamma^2}\right)$	$a_k = ((z^2 + 1)z^{2k} - 1)z^{2k-1}$ $b_k = (z^{2k} - 1)z^{6k-4}$ $z = \exp(\gamma^2/2)$	1
Weibull ^{a,f}	\mathbb{R}^+	$\gamma x^{\gamma-1} \exp(-x^\gamma)$	Apply Chebyshev algorithm to \mathbf{P}_{2Q-1} with $P_k = \Gamma(1 + k/\gamma)$	1
Legendre ^b	$] -1, 1[$	1	$a_k = 0$ $b_k = \frac{k^2}{4k^2 - 1}$	2
Jacobi ^{b,f}	$] -1, 1[$	$(1-x)^\alpha (1+x)^\beta$	$a_k = \frac{\beta^2 - \alpha^2}{\delta_k(\delta_k + 2)}$ $b_k = \frac{4k(k+\alpha)(k+\beta)(k+\alpha+\beta)}{\delta_k^2(\delta_k^2 - 1)}$ $\delta_k = 2k + \alpha + \beta$	$2^{\alpha+\beta+1} \times B(\alpha+1, \beta+1)^e$

^aWilck [33]. ^bShen et al. [34]. ^c Not standard Gauss-quadrature. ^d $\Gamma(x) = \int_0^{+\infty} t^{x-1} e^{-t} dt$. ^e $B(x, y) = \frac{\Gamma(x)\Gamma(y)}{\Gamma(x+y)}$. ^f $\alpha > -1, \beta > -1, \gamma > 0$.