Frédérique Laurent

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Characterization of the moment space corresponding to the Levermore basis

Caractérisation de l’espace des moments correspondant à la base de Levermore

Frédérique Laurent\textsuperscript{a, b}

\textsuperscript{a} Laboratoire EM2C, CNRS, CentraleSupélec, Université Paris-Saclay, 3 rue Joliot Curie 91190 Gif-sur-Yvette, France
\textsuperscript{b} Fédération de Mathématiques de CentraleSupélec - FR CNRS 3487, France.
\textit{E-mail:} frederique.laurent@centralesupelec.fr.

\textbf{Abstract.} A complete characterisation of the moment space corresponding to the Levermore basis is given here, through constraints on the moments. The necessary conditions are obtained thanks to classical tools, similar to Hankel determinants. In the mono-variante case, it is well-known that these conditions are sufficient. To generalize this result to multi-variante case, a non-classical constructive proof is given here reducing the problem to several mono-variante ones. However, it is also shown here on an example that the obtained multi-variante closure does not necessarily inherit of the good properties of the mono-variante closure.

\textbf{Résumé.} Une caractérisation complète de l’espace des moments correspondant à la base de Levermore est donnée ici, à travers des contraintes sur les moments. Les conditions nécessaires sont obtenues grâce à des outils classiques, similaires aux déterminants de Hankel. Dans le cas mono-varié, il est bien connu que ces conditions sont suffisantes. Pour généraliser ce résultat à un cas multi-varié, une preuve constructive non classique est donnée ici en se ramenant à des problèmes mono-variés. Cependant, il est également montré ici, sur un exemple, que la fermeture obtenue dans le cas multi-varié n’hérite pas nécessairement des bonnes propriétés de la fermeture mono-variée.

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1. \textbf{Introduction}

Moment closure methods, consisting in transforming a kinetic equation into a system of equations on moments of the number density function (NDF), is used in several applications such as rarefied gas dynamics [8] or dispersed phases of a multiphase flow [1]. Different kinds of closure can then be used, based for example on entropy maximization [4, 7], on quadrature [5] or on
some other reconstructed NDF [1]. In any cases, a finite number of moments is considered, gathered in a sequence called moment sequence. The moment space is the space of the moment sequences corresponding to any finite Borel measure. It is characterized by some constraints on the moments, called realizability conditions. It is usually important to know these realizability conditions, for example to be able to develop realizable numerical schemes, which naturally satisfy these constraints or just to check the realizability of the moments.

In the mono-variate case, where there is only one internal variable, the interior of the moment space is completely characterized by the positivity of the Hankel determinants when considering the sequence of integer moments [3]. But in the multi-variate case, these conditions are not always sufficient. The objective of this paper is to express the realizability conditions in the case of the moment space corresponding to the Levermore basis. The choice of this basis allows to consider moments till order four and to respect Galilean invariance (in particular, it does not single out any direction). Moreover, classical tools, similar to Hankel determinants can still be used to give realizability conditions. In this particular case, a constructive proof allows to show that the determined conditions are sufficient: in the multi-variate case, a measure can be constructed from measures which are solutions of some mono-variate finite moment problems.

It could be a way to generalize to multi-variate cases the closures developed in the mono-variate case. However, it is also shown here on an example that the multi-variate closure does not necessarily inherit of the good properties of the mono-variate closure.

2. Moments, centralized moments, notations

The multi-dimensional space $\mathbb{R}^d$ is considered, with $d > 1$. For any positive measure $d\mu$, let us defined the following moments of order 0 to 4, assuming that they exist and are finite:

$$
M_0(\mu) := \int_{\mathbb{R}^d} d\mu(v), \quad M_1(\mu) := \int_{\mathbb{R}^d} v d\mu(v), \quad M_2(\mu) := \int_{\mathbb{R}^d} vv^T d\mu(v), \quad M_3(\mu) := \int_{\mathbb{R}^d} v(v^T v) d\mu(v), \quad M_4(\mu) := \int_{\mathbb{R}^d} (v^T v)^2 d\mu(v).
$$

They are scalars, vectors and matrix and correspond to the Levermore basis $m(v) = 1, v, v \otimes v, v^2 v, v^4$ [4], even if they are written slightly differently, using only products of matrices and column vectors, $v$ being a column vector, like $M_1$ and $M_3$, whereas $M_2$ is a $d$-by-$d$ matrix and $M_0$ and $M_4$ are some scalars. Moreover, each moment sequence is denoted $M(\mu) = (M_0(\mu), M_1(\mu), M_2(\mu), M_3(\mu), M_4(\mu))$ and the corresponding moment space $\mathcal{M}_d$ is the set of all the $M(\mu)$ corresponding to any finite Borel measure on $\mathbb{R}^d$.

For any moment sequence $M = (M_0, M_1, M_2, M_3, M_4)$ such that $M_0 \neq 0$, let us also define the corresponding central moment sequence $C(M) = (\rho, u, P, q, r)$ by $\rho = M_0$, $u = \frac{1}{M_0} M_1$ and

$$
P = \frac{1}{M_0^2} \left( M_0 M_2 - M_1 M_1^T \right), \quad q = \frac{1}{M_0^3} \left( M_0^2 M_3 - M_0 \text{tr}(M_2) M_1 - 2M_0 M_2 M_1 + 2M_1^T M_1 M_1 \right),
$$

$$
r = \frac{1}{M_0^4} \left( M_0^3 M_4 - 4M_0^2 M_1^T M_3 + 4M_0^2 M_1^T M_2 M_1 + 2M_0 M_1^T M_1 \text{tr}(M_2) - 3 \left( M_1^T M_1 \right)^2 \right).
$$

Then, $P$, $q$ and $r$ are the normalized centered moments of order 2, 3 and 4 corresponding to $M$ and if $M = M(\mu)$ then they are such that:

$$
P = \frac{1}{M_0} \int_{\mathbb{R}^d} (v - u)(v - u)^T d\mu(v), \quad q = \frac{1}{M_0} \int_{\mathbb{R}^d} (v - u)(v - u)^T (v - u)d\mu(v),
$$

$$
r = \frac{1}{M_0} \int_{\mathbb{R}^d} [(v - u)^T (v - u)]^2 d\mu(v).
$$

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For \( M_0 = 0 \), we set \( u = q = 0 \), \( P = 0 \) and \( r = 0 \). Moreover, the moments can be expressed from the central moments: \( M_0 = \rho \), \( M_1 = \rho u \) and
\[
M_2 = \rho (P + uu' ), \quad M_3 = \rho (q + \text{tr}(P)u + 2Pu + u'u'u), \\
M_4 = \rho (r + 4u'q + 2u'u\text{tr}(P) + 4u'Pu + (u'u)^2).
\]
Then, the application \( C \) is one to one from the moment space \( \mathcal{M}_d \) to the central moment space \( \mathcal{C}_d = C(\mathcal{M}_d) \) and, thanks to the change of variable \( w = v - u \), it is equivalent to find a measure corresponding to the non-zero moment sequence \( M \) or to the moment sequence \((1, 0, P, q, r)\) with \( C(M) = (\rho, u, P, q, r) \). We will then focus on the central moment space to characterize the moment space.

3. Characterization of the moment space

Here, the characterisation of the moment space in the mono-variate case is first recalled. Then, necessary realizability conditions are given, expressed through some constraints on \( C \). They are then shown to be sufficient, using a constructive proof.

3.1. Mono-variate case

In the mono-variate case, the central moments are some scalar and are denoted \( C = (\rho, u, p, q, r) \).

**Theorem 1.** \( C = (\rho, u, p, q, r) \in \mathbb{R}^5 - \{(0, 0, 0, 0, 0)\} \) belongs to the central moment space \( \mathcal{C}_1 \) if and only if one of the following conditions is fulfilled:

(i) \( \rho > 0, p = q = r = 0 \).

(ii) \( \rho > 0, p > 0 \) and \( r \geq p^2 + \frac{q^2}{p} \).

The first case (i) corresponds to the moments of a Dirac measure, which is the only possible measure when \( p = 0 \) and the second case (ii) insures the non negativity of the Hankel determinants, an equality in the last equation corresponding to a uniq measure, which is a sum of two weighted Dirac measures.

3.2. Necessary condition

Let us denote \( \mathcal{S}^+_d (\mathbb{R}) \) (\( \mathcal{S}^+_d (\mathbb{R}) \) respectively) the set of all symmetric and positive (and definite respectively) \( d \times d \) matrices with real coefficients. The following lemma gives some conditions on \( C \) to be realizable, i.e. conditions for \( C \in \mathcal{C}_d \).

**Lemma 2.** If \( C = (\rho, u, P, q, r) \in \mathcal{C}_d \), then either \( \rho = 0, u = q = 0, P = 0 \) and \( r = 0 \), or \( \rho > 0 \) and:
\[
P \in \mathcal{S}^+_d (\mathbb{R}), \quad r \det(P) \geq \text{tr}(P)^2 \det(P) + q' \text{adj}(P)q, \tag{2}
\]
where \( \text{adj}(P) \) is the adjugate of \( P \), i.e. the transpose of the cofactor matrix of \( P \).

**Proof.** If \( \rho = 0 \) then \( u = q = 0, P = 0 \) and \( r = 0 \) by convention. Otherwise \( \rho > 0 \) and one can find a positive measure \( \mu \) corresponding to the moment sequence \((1, 0, P, q, r)\). The matrix \( P = \int g(v)Pd\mu(v) \) is necessarily symmetric and positive. Moreover, the measure \( \mu \) defines a scalar product \((g, h) = \int g(v)h(v)d\mu(v) \) on the space \( \mathbb{P}_d \) of polynomial functions \( P(X_1, \ldots, X_d) \) in \( \mathbb{R}^d \) spanned by \( 1, X_1, \ldots, X_d, \sum_{i=1}^d X_i^2 \). Its matrix \( \Delta_d \) in the basis \( 1, X_1, \ldots, X_d, \sum_{i=1}^d X_i^2 \) has then a non-negative determinant:
\[
0 \leq \Delta_d = \begin{vmatrix}
1 & 0 & \text{tr}(P) \\
0 & P & q \\
\text{tr}(P) & q' & r
\end{vmatrix} = \begin{vmatrix}
P & q \\
q' & r
\end{vmatrix} + (-1)^{d+3} \text{tr}(P) \begin{vmatrix}
0 & P \\
\text{tr}(P) & q'
\end{vmatrix}, \tag{3}
\]
the last equality coming from a cofactor expansion along the first row. Then, denoting \( p_{i,j} \) the 
(i, j)-minor of \( P \) and \( q_i \) the coefficients of \( q \), one can write, after some cofactor expansions along 
the last row and last column for the first term of (3) and along the first column for the second 
term of (3):

\[
\Delta_d = - \sum_{i=1}^{d} \sum_{j=1}^{d} (-1)^{i+j} p_{i,j} q_i q_j + r \det(P) - (\tr(P))^2 \det(P) = -q^t \adj(P)q + r \det(P) - \tr(P)^2 \det(P).
\]

This concludes the proof. \( \square \)

One can remark that when \( P \) is definite, then the constraints (2) can be written

\[
P \in \mathcal{S}_d^{++}(\mathbb{R}), \quad r \geq \tr(P)^2 + q^t P^{-1} q.
\]

This necessary condition can also be found in [6] with a similar proof, which type is classical in 
the theory of moments. But it was not shown that it is a sufficient condition and the boundary of 
the moment space was not rigorously characterized. Thus, when \( P \) is singular, equation (4) is no 
more valid and the condition (2) is clearly not sufficient.

**Lemma 3.** Let \( C = \{\rho, u, P, q, r\} \in \mathcal{C}_d \), with \( \rho > 0 \) and \( P \) singular. Then either \( (P, q, r) = (0, 0, 0) \) or 
\( r \geq \tr(P)^2 + q^t R R^t q \), where \( R \) is the matrix whose columns are the orthonormal 
eigenvectors of \( P \) corresponding to non zero eigenvalues.

**Proof.** Let us denote \( p = \rk(P) \) the rank of \( P \). By assumption, \( p < d \). If \( p = 0 \), then \( P = 0 \) 
and necessarily, the measure corresponding to the moment sequence \((1, 0, P, q, r)\) is the Dirac 
measure on \( \mathbb{R}^d \) concentrated at 0. In this case, \( q = 0 \) and \( r = 0 \).

Otherwise \( p > 0 \) and we introduce an orthogonal matrix \( Q \) such that \( D = Q^t P Q \) is diagonal:

\[
D = \text{diag}(d_1, \ldots, d_p, 0, \ldots, 0).
\]

The columns of \( Q \) are the eigenvectors of \( P \). The change of variable \( w = Q^t v \) allows to find a positive measure \( \mu \) corresponding to the moment sequence \((1, 0, D, q, r)\), 
with \( \bar{q} = Q^t q \). If \( \bar{R} \) is the matrix of the orthogonal projection from \( \mathbb{R}^d \) to \( \mathbb{R}^p \), then \( \mu(w) = \mu_1(\bar{R}w) \otimes \delta \), 
where \( \delta \) is the Dirac measure on \( \mathbb{R}^{d-p} \) concentrated at 0. Moreover, the moment sequence of \( \mu_1 \) is 
then \((1, 0, \bar{R}D \bar{R}^t, \bar{R}q, r)\), since \( \bar{R}D \bar{R}^t = \text{diag}(d_1, \ldots, d_p) \). And since \( \bar{R}^t D \bar{R} \) is definite, then, from 
Lemma 2:

\[
r \geq \left( \sum_{i=1}^{p} d_i \right)^2 + \bar{q}^t (\bar{R} \bar{R}^t)^{-1} \bar{R}q = \tr(P)^2 + q^t Q \bar{R} \bar{R}^t Q^{-1} \bar{R}q.
\]

Denoting \( R = \bar{Q} \bar{R} \), this concludes the proof. \( \square \)

### 3.3. Sufficient condition

The objective of this section is to show that the conditions given above are sufficient to charac-
terize the moment space. First, let us consider the case where \( P \) is definite.

**Lemma 4.** If \( C = \{\rho, u, P, q, r\} \) is such that \( \rho > 0 \), \( P \in \mathcal{S}_d^{++}(\mathbb{R}) \) and \( r \geq \tr(P)^2 + q^t P^{-1} q \), then \( C \in \mathcal{C}_d \).

**Proof.** We introduce an orthogonal matrix \( Q \) such that \( D = Q^t P Q \) is diagonal and denote \( d_j \) the 
eigenvectors of this diagonal, which are positive and \( \bar{q}_i \) the coefficients of \( \bar{q} = Q^t q \). Then, the 
inequality on \( r \) can be rewritten:

\[
r \geq \left( \sum_{j=1}^{d} d_j \right)^2 + \sum_{j=1}^{d} \bar{q}_j^2 d_j = \sum_{j=1}^{d} \left( d_j^2 + \bar{q}_j^2 \frac{d_j}{d_i} \right) + \sum_{j=1}^{d} \sum_{k \neq j} d_j d_k.
\]

Let us then denote

\[
\Delta = r - \sum_{j=1}^{d} \left( d_j^2 + \bar{q}_j^2 \frac{d_j}{d_i} \right) - \sum_{j=1}^{d} \sum_{k \neq j} d_j d_k.
\]
in such a way that \( \Delta \geq 0 \). Let us also denote, for \( i = 1, \ldots, d \)
\[
    r_j = d_j^2 + \frac{\bar{q}_j^2}{d_j} + \delta_j, \quad \delta_j = \frac{\Delta}{d_j},
\]
in such a way that
\[
    r_j \geq d_j^2 + \frac{\bar{q}_j^2}{d_j}, \quad \sum_{j=1}^d r_j + \sum_{j=1}^d \sum_{k \neq j} d_j d_k = r.
\]
The moment sequence \((1, 0, d_j, \bar{q}_j, r_j)\) is then realizable and one can find a corresponding positive measure \( \mu_j(w_j) \) on \( \mathbb{R} \). Let us then introduce \( \mu(w) = \mu_1(w_1) \otimes \mu_2(w_2) \otimes \cdots \otimes \mu_d(w_d) \), which defines a positive measure on \( \mathbb{R}^d \). Its zeroth order moment is 1 and its first order moments are 0. Moreover,
\[
\left( \int_{\mathbb{R}^d} w w' d\mu(w) \right)_{i,j} = \int_{\mathbb{R}^d} w_i w_j d\mu(w) = d_i \delta_{i,j},
\]
where \( \delta_{i,j} \) is one if \( i = j \) and zero otherwise,
\[
\left( \int_{\mathbb{R}^d} w \|w\|^2 d\mu(w) \right)_{j} = \int_{\mathbb{R}^d} w_j \sum_{k=1}^d w_k^2 d\mu(w) = \int_{\mathbb{R}} w_j^2 d\mu_j(w_j) = \bar{q}_j,
\]
and
\[
\int_{\mathbb{R}^d} \|w\|^4 d\mu(w) = \int_{\mathbb{R}^d} \sum_{j=1}^d \sum_{k=1}^d w_j^2 w_k^2 d\mu(w) = \sum_{j=1}^d r_j + \sum_{j=1}^d \sum_{k \neq j} d_j d_k = r.
\]
So, the change of variable \( v = Qw \) allows to define a measure corresponding to the moment sequence \((1, 0, P, q, r)\). This concludes the proof. \( \square \)

In the case where \( P \) is not definite, but non zero, one have the following result.

**Lemma 5.** If \( C = \{\rho, u, P, q, r\} \) is such that \( \rho > 0 \), \( P \in \mathcal{S}^+_d(\mathbb{R}) - \{0\} \) and \( r \geq \text{tr}(P)^2 + q' R (R' P R)^{-1} R' q \), where \( R \) is the matrix whose columns are the orthonormal eigenvectors of \( P \) corresponding to non zero eigenvalues, then \( C \in \mathcal{C}_d \).

**Proof.** Let us denote \( p = \text{rk}(P) \). The proof is similar than the previous one excepts that the measure \( \mu \) is given by: \( \mu(w) = \mu_1(w_1) \otimes \cdots \otimes \mu_p(w_p) \otimes \delta \otimes \cdots \otimes \delta. \) \( \square \)

In fact, this last result is also valid for \( P \in \mathcal{S}^{++}_d(\mathbb{R}) - \{0\} \) and all the lemma together allow to completely characterize the central moment space. Thus, for any scalars \( \rho \) and \( r \), vectors of \( \mathbb{R}^d \) \( u \) and \( q \) and matrix \( P \), one have the following result.

**Theorem 6.** \( C = (\rho, u, P, q, r) \neq (0, 0, 0, 0, 0) \) belongs to the central moment space \( \mathcal{C}_d \) if and only if one of the following conditions is fulfilled:
\begin{enumerate}
    \item[(i)] \( \rho > 0 \), \( (P, q, r) = (0, 0, 0) \).
    \item[(ii)] \( \rho > 0 \), \( P \in \mathcal{S}^+_d(\mathbb{R}) - \{0\} \) and \( r \geq \text{tr}(P)^2 + q' R (R' P R)^{-1} R' q \), where \( R \) is the matrix whose columns are the orthonormal eigenvectors of \( P \) corresponding to the non zero eigenvalues.
\end{enumerate}

Let us remark that the interior of the moment space is then given by:
\[
\mathcal{M}_d = \{M, C(M) = (\rho, u, P, q, r), \rho > 0, P \in \mathcal{S}^{++}_d(\mathbb{R}), r > \text{tr}(P)^2 + q' P^{-1} q\}.
\]
4. Remark on the use of the reconstruction of the proof for a moment method

The constructive proof of the Theorem uses essentially a solution of the mono-variate Hamburger moment problem with five integer moments. This last problem has some solutions in the literature, which have good properties when used to close moment equations corresponding to the transport part of the kinetic equation in 1D:

\[ \partial_t f + v \partial_x f = 0. \]  \hspace{1cm} (10)

The moment sequence \( \mathbf{M} = (M_0, \ldots, M_4)^t \) approximating \( \int_{\mathbb{R}} (1, v, v^2, v^3, v^4) f(t, x, v) dv \) is then solution of

\[ \partial_t \mathbf{M} + \partial_x F(\mathbf{M}) = 0, \quad F(\mathbf{M}) = (M_1, M_2, M_3, M_4, \overline{M}_5)^t, \]  \hspace{1cm} (11)

with \( \overline{M}_5(t, x) = \int_{\mathbb{R}} v^5 f(t, x, v) dv \), where \( f \) is defined from the moment sequence \( \mathbf{M}(t, x) \). For example, the Gaussian-EQMOM [1] reconstruction or the HyQMOM reconstruction [2] lead to hyperbolic problems. But their extension to the multi-dimensional case is far from trivial.

In the multi-variate reconstruction of the proof, a keypoint is a sort of repartition of \( r \) in the \( r_j \), through \( \delta_j \) in (7). In the proof, \( \delta_j = \Delta / d \) is used, but other values can be used as soon as \( \sum_{j=1}^d \delta_j = \Delta \): for example \( \delta_j = d_j \Delta / \text{tr}(\mathbf{P}) \) or \( \delta_j = d_j^2 \Delta / \text{tr}(\mathbf{P}^2) \). However, none of the performed reconstructions allowed to obtain an unconditional hyperbolic system when using the Gaussian-EQMOM reconstruction or the HyQMOM reconstruction for each mono-variate case.

References