Sparse Moments of Univariate Step Functions and Allele Frequency Spectra

Zvi Rosen¹ · Georgy Scholten² · Cynthia Vinzant³

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Abstract
We study the univariate moment problem of piecewise-constant density functions on the interval [0, 1] and its consequences for an inference problem in population genetics. We show that, up to closure, any collection of \( n \) moments is achieved by a step function with at most \( n - 1 \) breakpoints and that this bound is tight. We use this to show that any point in the \( n \)th coalescence manifold in population genetics can be attained by a piecewise constant population history with at most \( n - 2 \) changes. Both the moment cones and the coalescence manifold are projected spectrahedra and we describe the problem of finding a nearest point on them as a semidefinite program.

Keywords
Moments · Step function · Sample frequency spectrum

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1 Introduction
Given a finite collection \( A \subset \mathbb{N} \), we consider the convex cone \( M(A) \) of all moments \( (m_a)_{a \in A} \) of the form \( m_a = \int x^a d\mu \) where \( \mu \) is a nonnegative Borel measure on the unit interval [0, 1]. For consecutive moments \( A = \{0, 1, 2, \ldots, d\} \), this is a classical object in

Dedicated to Bernd Sturmfels on the occasion of his 60th birthday with gratitude for his academic mentorship.

Zvi Rosen
rosenz@fau.edu

Georgy Scholten
Georgy.Scholten@lip6.fr

¹ Florida Atlantic University, Boca Raton, FL, USA
² Equipe PolSys, Sorbonne Université, LIP6, F-75005, Paris, France
³ University of Washington, Seattle, WA, USA
analysis and real algebraic geometry. The problem of determining membership in the cone \( M(A) \) is known as the truncated Hausdorff moment problem. See, for example, [2, 7, 8, 11].

In this paper we study moments coming from piecewise-constant density functions with the idea of minimizing the number of pieces needed. Formally, we consider the set \( M_k(A) \) as the Euclidean closure of the set of moments \((m_a)_{a \in A}\) where \( m_a = \int_0^1 x^a f(x) \, dx \) and \( f \) is a nonnegative step function with at most \( k \) discontinuities. Our main theorem is the following:

**Main Theorem 1** \( M_k(A) = M(A) \) if and only if \( k \geq |A| - 1 \).

This is the content of Theorem 3 and Corollary 9. The proof involves studying the convex algebraic boundary of these cones and in particular showing that they are simplicial (Corollary 6). When restricting to the moments of monotone density functions, only half as many break points are needed (see Propositions 11 and 12).

**Main Theorem 2** Every \( A \)-moment vector of a monotone density function is the limit of \( A \)-moments of monotone step functions with \( \leq k \) breakpoints if and only if \( k \geq \lfloor |A|/2 \rfloor \).

One of our motivations for studying this problem came from its relation to the coalescence manifold studied by [10]. The coalescence manifold \( C_{n,k} \), formally defined in Section 4, is a set of summary statistics in population genetics, derived from observing \( n \) genomes with a population history consisting of \( k + 1 \) different population sizes. Our last main theorem, appearing as Theorem 13, is that the coalescence manifold \( C_{n,k} \) coincides with an affine section of the moments \( M_k(A) \) for \( A = \{0, 2, \ldots, \binom{n}{2} - 1\} \).

**Main Theorem 3** The coalescence manifold \( C_{n,k} \) is the intersection of \( M_k(A) \) with the hyperplane of points with coordinate sum one for \( A = \{0, 2, \ldots, \binom{n}{2} - 1\} \). That is, \( C_{n,k} = \{(m_a)_{a \in A} \in M_k(A) : \sum_{a \in A} m_a = 1\} \).

The authors in [10] show that the manifold \( C_{n,k} \) stabilizes at \( k = 2n - 2 \), i.e. \( C_{n,2n-2} = C_{n,k} \) for all \( k \geq 2n - 2 \). Together, the main theorems above improve this bound by a factor of two, showing that the coalescence manifolds stabilize at \( k = n - 2 \) and this bound is tight.

The connection with the moment problem also provides a description of \( C_{n,n-2} \) as the projection of a spectrahedron. The problem of finding the nearest point in \( C_{n,n-2} \) to a given point in \( \mathbb{R}^{n-1} \) can then be formulated as a semidefinite program.

This paper is organized as follows. In Section 2, we introduce formal definitions of the moment sets \( M_k(A) \), study their convex and algebraic structure, and prove Main Theorem 1. In Section 3, we analyze analogous questions for moment problems coming from monotone step functions. The definitions and connections with the coalescence manifold \( C_{n,k} \) are given in Section 4. Semidefinite descriptions of these sets are discussed in Section 5. Finally, we end with a discussion of open problems surrounding these interesting sets in Section 6.

## 2 Moments of Step Functions

For \( k \in \mathbb{N} \), let \( S_k \) denote the set of nonnegative step functions on \([0, 1]\) of the form

\[
 f = y_1 1_{[0,s_1]} + \sum_{i=2}^{k+1} y_i 1_{(s_{i-1}, s_i]},
\]

(1)
Let $0 = s_0 < s_1 < \cdots < s_k < s_{k+1} = 1$ and $y_1, \ldots, y_{k+1} \in \mathbb{R}_{\geq 0}$. We note the following properties of $S_k$:

1. $S_k$ is invariant under nonnegative scaling,
2. $S_k \subseteq S_\ell$ when $k \leq \ell$, and
3. $S_k + S_\ell$, defined as $\{f + g \mid f \in S_k, g \in S_\ell\}$, is a subset of $S_{k+\ell}$.

Elements of $S_k$ define nonnegative measures on $[0, 1]$. We will be interested in the possible moments of these measures. Given a finite collection $A \subseteq \mathbb{N}$, we define $M_k(A)$ to be the Euclidean closure of the set of moments arising from density functions in $S_k$:

$$M_k(A) = \left\{ \left( \int_0^1 x^a f(x) dx \right)_{a \in A} : f \in S_k \right\}.$$

One important case is that of consecutive moments $A = \{0, 1, \ldots, d\}$. For any finite collection $A \subseteq \mathbb{N}$, the moment cone $M_k(A)$ can be expressed, up to closure, as the image of $M_k([0, 1, \ldots, \max(A)])$ under the coordinate projection $\pi_A : \mathbb{R}^{\max(A)+1} \to \mathbb{R}^{|A|}$ given by $\pi_A(m_0, \ldots, m_{\max(A)}) = (m_a)_{a \in A}$.

**Remark 1** By linearity of the integral, we see that $M_k(A)$ inherits many properties of $S_k$. That is, $M_k(A)$ is invariant under nonnegative scaling, $M_k(A) \subseteq M_\ell(A)$ when $k \leq \ell$ and $M_k(A) + M_\ell(A) \subseteq M_{k+\ell}(A)$ (here, in the sense of the Minkowski sum), as desired.

We will be interested in comparing this to the full moment cone:

$$M(A) = \left\{ \left( \int_0^1 x^a d\mu \right)_{a \in A} : \mu \text{ is a nonnegative Borel measure on } [0, 1] \right\}.$$

The cone $M(A)$ is dual to the convex cone of univariate polynomials supported on $A$ that are nonnegative on $[0, 1]$, as will be discussed below in Proposition 4.

When $0 \in A$, the closure in the definition of $M(A)$ is not necessary, and the extreme rays of $M(A)$ all come from point evaluations at points in $[0, 1]$. That is, we can write $M(A)$ as the conical hull of the image of $[0, 1]$ under the corresponding moment map:

$$M(A) = \text{conicalHull} \{v_A(t) : t \in [0, 1]\} \quad \text{where } v_A(t) = (t^a)_{a \in A}.$$

In the case $A = \{0, 1, \ldots, d\}$, this equality is a classical result in functional analysis; see, for example, [11, Prop. 10.5]. When $0 \in A$, the convex hull of the moment curve does not contain the origin since the corresponding coordinate is identically equal to one. The conical hull of this set is therefore closed, coinciding with the conical hull of the curve and with $M(A)$. See also [5, Prop. 21].

When $0 \notin A$, this equality only holds up to closure, as the curve parametrized by $v_A(t)$ includes the origin. In this case, $M(A) = \text{conicalHull}[v_A(t) : t \in [0, 1]]$. As we will see below, then we can still write $M(A)$ as the conical hull of a curve segment. Specifically, for $B = \{a - \min(A) : a \in A\}$, $M(A)$ coincides with conicalHull$[v_B(t) : t \in [0, 1]]$.

**Lemma 1** If $A \subseteq \mathbb{N}$ is finite and $B = \{a - \min(A) : a \in A\}$, then $M(A) = M(B)$.

**Proof** Let $b = \min(A)$. For $t \in (0, 1]$, the point $v_A(t)$ can be rewritten as $t^b v_B(t)$, a scalar multiple of $v_B(t)$. It follows that the conical hulls of $\{v_A(t) : t \in (0, 1]\}$ and $\{v_B(t) : t \in (0, 1]\}$ are equal. We observe that the extreme ray $v_B(0)$ of $M(B)$ can be attained in the...
closure of $M(A)$ as the limit of the moment of the step function $f = \varepsilon^{-(b+1)}1_{[0,\varepsilon]}$ as $\varepsilon$ goes to zero:

$$\lim_{\varepsilon \to 0} \int_0^1 x^a f(x) \, dx = \lim_{\varepsilon \to 0} \varepsilon^{-(b+1)} \int_0^\varepsilon x^a \, dx = \lim_{\varepsilon \to 0} \varepsilon^a - \frac{b}{a+1} \begin{cases} \frac{1}{a+1} & \text{if } a = b, \\ 0 & \text{otherwise.} \end{cases}$$

It follows that $v_B(0)$ belongs to $M(A)$. Since $M(B)$ can be written as the union of the cone over $v_A(t)$ for $t \in (0, 1]$ and the ray over $v_B(0)$, the equality between the two cones ensues:

$$M(A) = \text{conicalHull}\{v_A(t) : t \in [0, 1]\} = M(B).$$

Example 1 Consider $A = \{1, 2\}$ and $B = \{0, 1\}$. Then

$$M(B) = \text{conicalHull}\{(1, t) : t \in [0, 1]\} = \text{conicalHull}\{(t, t^2) : t \in [0, 1]\} = M(A).$$

Here, we see the need for taking closures when $0 \notin A$. The point $(1, 0) = v_B(0)$ is not contained in the conical hull of the curve segment $\{(t, t^2) : t \in [0, 1]\}$ but is contained in its closure. See Fig. 1. In this case, the boundary of $M(A) = M(B)$ consists of scalar multiples of $v_B(0)$ and $v_B(1)$, both of which belong to $M_1(A)$, by Proposition 2 below. Arguments below will then show that $M(A) = M_1(A)$.

Proposition 2 Let $A \subset \mathbb{N}$ be finite and let $B = \{a - \min(A) : a \in A\}$. The points $v_B(0)$ and $v_B(1)$ belong to $M_1(A)$ and for every $t \in (0, 1)$, $v_B(t)$ belongs to $M_2(A)$.

Proof For $0 < t < 1$, and $0 < \varepsilon < 1 - t$, consider the step function in $S_2$ given by

$$f = \varepsilon^{-1}t^{-\min(A)}1_{(t, t+\varepsilon)}.$$ By continuity, the limit of the integral $\int_0^1 x^a f(x) \, dx$ as $\varepsilon \to 0$ equals $\varepsilon^{a-\min(A)}$, thus $M_2(A)$ contains the limit point $v_B(t) = (t^b)_{b \in B}$. Similarly, the limit as $\varepsilon \to 0$ of the A-moment vectors of the step functions $f = (\min(A) + 1)\varepsilon^{-1-\min(A)}1_{[0,\varepsilon]}$ and $f = \varepsilon^{-1}1_{[1-\varepsilon, 1]}$ in $S_1$ are $v_B(0)$ and $v_B(1)$, respectively. Therefore, these vectors belong to $M_1(A)$. □

A corollary of this statement is that $M_k(A) = M(A)$ for $k = 2|A|$. Indeed, by Carathéodory’s Theorem, any point in $M(A)$ is in the conical hull of at most $|A|$ points.
of the form $(t^a)_{a \in A}$ where $t \in [0, 1]$, each of which belongs to $M_2(A)$ by Proposition 2. By Remark 1, the sum of $|A|$ elements from $M_2(A)$ belongs to $M_{2|A|}(A)$, giving $M(A) \subseteq M_{2|A|}(A)$. In fact, $M_k(A)$ fills out the whole moment cone much sooner:

**Theorem 3** If $k \geq |A| - 1$, $M_k(A) = M(A)$.

The proof of this theorem relies on understanding points on the boundary of $M(A)$. The following is a useful characterization that has appeared many times in the literature, e.g. [4, Lemma 3] and [5, Prop. 7]. We include a short proof for the sake of completeness.

**Proposition 4** Let $A \subseteq \mathbb{N}$ be finite with $0 \in A$. If $m = (m_a)_{a \in A}$ belongs to the Euclidean boundary of $M(A)$, then any representing measure $\mu$ on $[0, 1]$ with $m_a = \int x^a d\mu$ has finite support. Specifically, the support of $\mu$ is a subset of the roots contained in $[0, 1]$ of a polynomial nonnegative on $[0, 1]$ and of the form $p(x) = \sum_{a \in A} p_a x^a$. The vector $m$ is a conic combination of the vectors $v_A(r)$ where $r$ ranges over the roots of $p$.

**Proof** Let $\ell : \mathbb{R}^A \to \mathbb{R}$ be a linear function $\ell(v) = \sum_{a \in A} p_a v_a$ defining a supporting hyperplane of $M(A)$ at $m$. That is, $\ell(v) \geq 0$ for all $v \in M(A)$ and $\ell(m) = 0$. Consider the polynomial $p(x) = \ell(v_A(x)) = \sum_{a \in A} p_a x^a$. Since $v_A(t) \in M(A)$ for all $t \in [0, 1]$, $p$ is nonnegative on $[0, 1]$. Furthermore, for any measure $\mu$ with moments $m$,

$$\int p(x) d\mu = \sum_{a \in A} p_a m_a = \ell(m) = 0.$$

The measure $\mu$ is nonnegative and the polynomial $p$ is nonnegative on $[0, 1]$. From this we see that the support of the measure $\mu$ must be contained in the (finite) set of roots $R$ of $p(x)$. Specifically, $\mu = \sum_{r \in R} w_r \delta_r$ for some $w_r \in \mathbb{R}_{\geq 0}$; therefore, $m = \sum_{r \in R} w_r v_A(r)$. \hfill\Box

**Proof of Theorem 3** First, consider a point $m$ in the boundary of $M(A)$. By Lemma 1, $M(A) = M(B)$ where $B = \{a - \min(A) : a \in A\}$, and so $m$ also belongs to the boundary of $M(B)$. By Proposition 4, $m$ is the vector of $B$-moments of a measure $\mu$ supported on the roots of a nonnegative polynomial on $[0, 1]$ of the form $p(x) = \sum_{a \in B} p_a x^a$. Let $b$ be the number of distinct roots of $p$ in the set $[0, 1]$ and $i$ be the number of distinct roots of $p$ in the open interval $(0, 1)$. Then $m$ is in the conical hull of the $b + i$ points given by $v_B(r)$ where $r$ ranges over these roots. By Proposition 2, $m$ belongs to $M_k(A)$ for $k = b + 2i$.

By Descartes’ rule of signs, the number of positive roots of $p$, counting multiplicity, is at most the number of sign changes in the list of coefficients $\{p_a\}_{a \in B}$. If $p_0 \neq 0$, then $p$ has at most $|B| - 1$ roots in $\mathbb{R}_{>0}$. If $p_0 = 0$, then $p$ is the sum of at most $|B| - 1$ nonzero terms and its number of roots in $\mathbb{R}_{\geq 0}$ must be smaller or equal to $|B| - 2$. Note that every root of $p$ in $(0, 1)$ must have even multiplicity greater or equal to 2. All together, this gives $b + 2i \leq |B| - 1 = |A| - 1$.

Now consider $m$ in the interior of $M(A)$. Let $c = (1/(a + 1))_{a \in A} \in M_0(A)$ denote the vector obtained by integrating against the constant step function of height one. Let $\lambda^*$ be the maximum value of $\lambda \in \mathbb{R}$ for which $m - \lambda c$ belongs to $M(A)$. From $m \in M(A)$, we see that $\lambda^* \geq 0$. Moreover, since $M(A)$ is pointed, $-c$ does not belong to $M(A)$, meaning that for sufficiently large $\lambda$, $m - \lambda c$ does not belong to $M(A)$. Since $M(A)$ is closed, it follows that such a maximum $\lambda^*$ must exist.

The point $m - \lambda^* c$ belongs to the boundary of $M(A)$. By the arguments above, $m - \lambda^* c$ belongs to $M_k(A)$ for $k \geq |A| - 1$. Since $c \in M_0(A)$ and

$$m = (m - \lambda^* c) + \lambda^* c,$$
the point \( m \) also belongs to \( M_k(A) \) for \( k \geq |A| - 1 \).

Remark 2 It follows from the proof of Theorem 3 that for all \( k \geq 0 \), \( M_k(A) \) is star convex with respect to the \( A \)-moment of the constant function, \( c = (1/(a + 1))_{a \in A} \). Indeed, since \( c \) belongs to \( M_0(A) \), \( \lambda c + M_k(A) \subseteq M_k(A) \) for all \( \lambda \geq 0 \).

We further characterize the facial structure of the boundary of \( M(A) \). Through a connection to Schur polynomials, we can deduce linear independence among sets of points from the curve of the correct size. See also [5, Section 4].

Proposition 5 For a collection \( A \) of integers \( 0 = a_1 < a_2 < \cdots < a_n \) and any real values \( 0 \leq r_1 < r_2 < \cdots < r_n \leq 1 \), the determinant of the matrix \( S_A(r) \) is strictly positive, where

\[
S_A(r) = \begin{pmatrix}
1 & 1 & \ldots & 1 \\
1 & r_1^{a_2} & & \\
& r_2^{a_2} & \ldots & r_n^{a_2} \\
& & \ldots & \ldots \\
& & & r_n^{a_n}
\end{pmatrix}.
\]

Proof By the bialternant formula for Schur polynomials, the determinant of the matrix \( S_A(r) \) can be expressed as

\[
\det(S_A(r)) = \left( \prod_{1 \leq i < j \leq n} (r_j - r_i) \right) s_\lambda(r_1, \ldots, r_n)
\]

for \( \lambda = (a_n - (n - 1)), a_{n-1} - (n - 2), \ldots, a_1 \), where \( s_\lambda(x_1, \ldots, x_n) \) denotes the Schur polynomial associated to the partition \( \lambda \). By definition, the Schur polynomial \( s_\lambda(x_1, \ldots, x_n) \) is the sum of monomials \( x^T \) over all semistandard Young tableaux \( T \) of shape \( \lambda \). One can observe, either from expanding the determinant of \( S_A(x_1, \ldots, x_n) \) along the first column, or by filling out a semistandard Young Tableau of shape \( \lambda \) without using the number 1, that \( x_1 \) does not appear in all the monomials of the determinant of \( S_A \). It follows that \( \det(S_A(r)) \) is strictly positive for any choice of \( 0 \leq r_1 < r_2 < \cdots < r_n \leq 1 \).

Corollary 6 All proper faces of \( M(A) \) are simplicial.

Proof By Lemma 1, we can assume that \( 0 \in A \). Recall that \( M(A) \) is the conical hull over the curve segment \( \{v_A(t) : t \in [0, 1] \} \) and any proper face \( F \) of this cone can be expressed as the conical hull of some points \( v_A(r_1), \ldots, v_A(r_k) \) where \( 0 \leq r_1 < r_2 < \cdots < r_k \leq 1 \). If \( k > \dim(F) \), then there is a subset of these points of size \( \dim(F) + 1 \leq k \leq n \), which necessarily lie in \( F \) and are therefore linearly dependent, contradicting Proposition 5. Therefore \( k = \dim(F) \) and \( F \) is simplicial.

This lets us assign an index to points on the boundary of \( M(A) \), following [11, Chapter 10.2]. Let \( m \) be a point on the boundary of \( M(A) \). By Corollary 6, there is a unique representation of \( m \) as \( \sum_{j=1}^k w_j v_A(r_j) \) where \( 0 \leq r_1 < \cdots < r_k \leq 1 \) and \( w_1, \ldots, w_k \in \mathbb{R}_{>0} \). We define the index of \( m \), denoted \( \text{ind}(m) \), to be \( b + 2i \) where \( b = \# \{ j : r_j \in [0, 1] \} \) and \( i = \# \{ j : r_j \in (0, 1) \} \). By Proposition 2, any point \( m \) on the boundary of \( M(A) \) belongs to \( M_{\text{ind}(m)}(A) \).
To prove the converse, we must rule out the possibility that \( \mathbf{m} \in M_k(A) \) for \( k < \text{ind}(\mathbf{m}) \). In other words, it is impossible to approach a point \( \mathbf{m} \) on the boundary of \( M(A) \) with moment vectors of step functions with fewer breakpoints than expected.

**Lemma 7** Let \( \mathbf{m} \) be a point on the boundary of \( M(A) \). For \( k < \text{ind}(\mathbf{m}) \), \( \mathbf{m} \) is not an element of \( M_k(A) \). That is, if \( \mathbf{m} \in M_k(A) \), then \( \text{ind}(\mathbf{m}) \leq k \).

**Proof** Note that for any non-zero point \( \mathbf{m} \) in \( M(A) \), \( m_0 > 0 \) and so we can rescale \( \mathbf{m} \) to have \( m_0 = 1 \). We will write \( M_k(A) \cap \{m_0 = 1\} \) as the image of a compact polytope under a polynomial map and check that any point \( \mathbf{m} \) in the image of this map and the boundary of \( M(A) \) has index \( \leq k \).

Any function \( f \in S_k \) can be written as \( f = y_1 1_{[0, s_1]} + \sum_{i=2}^{k+1} y_i 1_{(s_{i-1}, s_i]} \) for some values \( 0 = s_0 < s_1 < \cdots < s_k < s_{k+1} = 1 \) and \( y_i \geq 0 \) for all \( i \). We now introduce transformed \( w \)-coordinates by letting \( w_i = y_i(s_i - s_{i-1}) \) denote the area \( \int_{s_{i-1}}^{s_i} f(x) \, dx \). The corresponding moment in \( M_k(A) \) is given by the image of the point \( (s, w) = (s_1, \ldots, s_k, w_1, \ldots, w_{k+1}) \) under the polynomial map

\[
\mu_A(s, w) = \left( \sum_{i=1}^{k+1} \frac{y_i s_i + 1 - a + 1}{a + 1} \right)_{a \in A} = \left( \sum_{i=1}^{k+1} \frac{w_i a + 1 - a + 1}{a + 1} \right)_{a \in A}.
\]

Note that the constraint that \( m_0 = 1 \) translates into \( \sum_i w_i = 1 \). Consider the polytope

\[
P = \left\{ (s, w) \in \mathbb{R}^{2k+1} \mid 0 \leq s_1 \leq \cdots \leq s_k \leq 1, w_i \geq 0, \sum_{i=1}^{k+1} w_i = 1 \right\},
\]

which is a product of two simplices of dimension \( k \). We claim that \( \mu_A(P) \) equals in the intersection of \( M_k(A) \) with \( \{m_0 = 1\} \). To see this, note that the set of moments of step functions \( f \in S_k \) with \( \int f(x) \, dx = 1 \) coincides with the image, under \( \mu_A \), of points \( (s, w) \in P \) with distinct \( 0 < s_1 < \cdots < s_k < 1 \). The closure of this set is \( M_k(A) \cap \{m_0 = 1\} \), which necessarily coincides with the image of \( P \) under \( \mu_A \), as the image of a compact set under a continuous map is closed.

If \( w_i > 0 \) and \( s_{i-1} < s_i \) for some \( i \), then \( \mu_A(s, w) \) has a representing measure whose support includes the interval \((s_{i-1}, s_i]\) and is therefore not finite. Then by Proposition 4, \( \mathbf{m} \) belongs to the interior of \( M(A) \).

Suppose the point \( \mathbf{m} \) belongs to \( M_k(A) \). Then \( \mathbf{m} = \mu_A(s, w) \) for some \( (s, w) \) in \( P \). Let \( I \) denote the collection of indices \( 1 \leq i \leq k \) for which \( w_i > 0 \). If \( \mathbf{m} \) belongs to the boundary of \( M(A) \), \( s_{i-1} = s_i \) for all \( i \in I \). Then

\[
\mathbf{m} = \mu_A(s, w) = \sum_{i \in I} w_i v_A(s_i).
\]

We can bound \( \text{ind}(\mathbf{m}) \) by bounding the number of distinct values of \( s_i \) that appear. For each \( i \in I \) with \( s_i \in (0, 1) \), \( s_i \) equals \( s_{i-1} \); hence, there are at least two indices \( j \) in \( \{1, \ldots, k\} \) for which \( s_j = s_i \). Trivially, if \( s_i \in (0, 1) \), there is at least one \( j \in \{1, \ldots, k\} \) such that \( s_j = s_i \). Together, these show that

\[
\text{ind}(\mathbf{m}) = \# \{s_i \in (0, 1) : i \in I\} + 2 \cdot (\# \{s_i \in (0, 1) : i \in I\}) \leq k.
\]

\[ \square \]

**Example 2** For \( k = 3 \), consider the point \( (s, w) \in P \subset \mathbb{R}^7 \) given by \( s = (0, 1/2, 1/2) \) and \( w = (1/3, 0, 2/30) \). Note that there is no value of \( y \in \mathbb{R}^4 \) satisfying the equations
\[ w_i = y_i(s_i - s_{i-1}), \text{ as } w_1 > 0 \text{ and } s_1 - s_0 = 0. \] However, we can write \( \mathbf{m} = \mu_A (\mathbf{s}, \mathbf{w}) \) as \( 1/3v_A(0) + 2/3v_A(1/2) \), showing that the index of \( \mathbf{m} \) equals 3. Lemma 7 shows that this is the maximal index of a point in \( M_k(A) \) and the boundary of \( M(A) \).

**Lemma 8** The intersection of \( M_k(A) \) with the Euclidean boundary of \( M(A) \) is a semialgebraic set of dimension \( \leq k \).

**Proof** By Lemma 7, the intersection of \( M_k(A) \) with the Euclidean boundary of \( M(A) \) is the set of boundary points of index \( \leq k \). We can parametrize this as a union of semialgebraic sets, specifically the union over \( \sigma \in \{0, 1\}^2 \) of

\[
\left\{ \sum_{j=1}^{\ell} w_j v_A(r_j) + w_{\ell+\sigma_1} v_A(0) + w_{\ell+\sigma_1+\sigma_2} v_A(1) : r \in (0, 1)^\ell, w \in (\mathbb{R}_{>0})^{\ell+\sigma_1+\sigma_2} \right\},
\]

where, in each set, \( \ell \) is chosen so that \( 2\ell + \sigma_1 + \sigma_2 \leq k \). Here, we use \( r \) to denote the vector \( (r_j)_j \) and \( w \) for the vector \( (w_j)_j \). Note that each set is the image of \( (0, 1)^n \times (\mathbb{R}_{>0})^m \) under a polynomial map where \( n + m \leq k \) and therefore has dimension \( \leq k \).

**Corollary 9** If \( k < |A| - 1 \), \( M_k(A) \neq M(A) \).

**Proof** The cone \( M(A) \) is full-dimensional in \( \mathbb{R}^{|A|} \), in consequence, the cone’s boundary is a hypersurface of dimension \( |A| - 1 \). By Lemma 8, the dimension of the intersection of \( M_k(A) \) with the boundary of \( M(A) \) has dimension \( \leq k \), so for \( k < |A| - 1 \), this cannot be the entire boundary of \( M(A) \).

**Example 3** For \( A = \{0, 2, 5\} \), Theorem 3 and Corollary 9 imply that \( M_k(A) \) equals \( M_2(A) \) for all \( k \geq 2 \) but not for \( k = 1 \). Affine transformations of the intersections of \( M_1(A) \) and \( M_2(A) \) with the affine hyperplane \( \{m_0 = 1\} \) are shown in Fig. 2. See also [10, Fig. 6]. The intersection of \( M_1(A) \) with the boundary of \( M_2(A) \) consists of just two rays, which appear as points in the hyperplane \( \{m_0 = 1\} \). The set \( M_1(A) \) consists of moments of functions with just one breakpoint. Step functions with one breakpoint and total mass one can be parametrized by \( f = \frac{w}{s} \mathbf{1}_{[0,s]} + \frac{1-w}{s-1} \mathbf{1}_{[s,1]} \) for \( s \in (0, 1) \) and \( w \in [0, 1] \). Note that fixing \( w \) and taking the limit as \( s \to 0 \) gives a weighted sum of a point mass at zero and the constant function \( w\delta_0 + (1-w) \mathbf{1}_{[0,1]} \). Similarly, \( s \to 1 \) gives \( w\mathbf{1}_{[0,1]} + (1-w)\delta_1 \).

For \( s = w \in [0, 1] \), the corresponding step function is constant, i.e. \( f = \mathbf{1}_{[0,1]} \) and the moment map sends this line segment to a single point. However, away from this line, the moment map is a homeomorphism to its image in \( M_1(\{0, 2, 5\}) \).

![Fig. 2 The parameter space of \( M_1(A) \) and \( M_1(A) \), \( M_2(A) \) for \( A = \{0, 2, 5\} \)](image-url)
Example 4 Consider $A = \{0, 2, 5, 9\}$. To visualize the moment sets $M_k(A)$ for $k = 1, 2$, we consider their intersections with the affine hyperplane $\{m_0 = 1\}$. Affine transformations of these intersections are shown in Fig. 3. Note that the step functions with at most one breakpoint and total mass one can be written as $\lambda \mathbf{1}_{[0,1]} + (1 - \lambda) \frac{1}{2} \mathbf{1}_{[0,s]} + (1 - \lambda) \frac{1}{1-s} \mathbf{1}_{(s, 1]}$ where $\lambda \in [0, 1]$. The result is a two-dimensional surface in the plane $\{m_0 = 1\}$. The set $M_2(A)$ is full-dimensional, but does not fill up all of $M(A)$. As promised by Lemma 8, the intersection $M_2(A)$ with the boundary of $M(A)$ has dimension $\leq 2$, so its image in $\{m_0 = 1\}$ has dimension $\leq 1$. Indeed, we see this intersection is given by the curve parametrized by $(t^2, t^3, t^6)$ for $t \in [0, 1]$, which appears as the dotted curve segment on the left of Fig. 3, and the line segment between its endpoints $(0, 0, 0)$ and $(1, 1, 1)$. Finally, by Theorem 3, $M_3(A)$ is the full cone $M(A)$. Points on the boundary of $M(A)$ have index $\leq 3$, and so have one of the two forms $w_0 v_A(0) + w_r v_A(r)$ or $w_1 v_A(1) + w_r v_A(r)$ where $r \in [0, 1]$, $w_0, w_1, w_r \in \mathbb{R}_{\geq 0}$.

We will now take a closer look at this example, paying close attention to the boundary of the domain and its image in $M_2(A)$. The domain parametrizes the set of step functions with two breakpoints and total mass one and so consists of the product of two 2-simplices:

$$P = \{(s_1, s_2) : 0 \leq s_1 \leq s_2 \leq 1\} \times \{(w_1, w_2, w_3) \in \mathbb{R}_{\geq 0}^3 : w_1 + w_2 + w_3 = 1\}.$$

Here, $(s_1, s_2)$ parametrize the two breakpoints and $(w_1, w_2, w_3)$ parametrize the proportion of mass in each piece. So the domain is four-dimensional while the image has dimension three. Therefore the generic fiber of the moment map has dimension one.

We can however obtain a generically finite-to-one map by restricting to facets of the polytope $P$. Furthermore, one can check that every point in the image of $P$ is also the image of some point on the boundary of $P$, i.e. $\mu_A(P) = \mu_A(\partial P)$. See [12, Proposition 4.5.3] for details. The boundary of $P$ is composed of six triangular prisms given by $s_1 = 0, s_2 = 1, s_1 = s_2, w_1 = 0, w_2 = 0$, and $w_3 = 0$. We can visualize this by way of a Schlegel diagram via one of its facets, see in Fig. 4.

We make a number of observations about the restriction of the moment map to the boundary of $P$. There are four 2-faces that the moment map collapses to a curve, namely the faces given by $0 = s_1 = s_2, s_1 = s_2 = 1, w_1 = w_2 = 0$, and $w_2 = w_3 = 0$. In addition to these 2-faces, the intersections of the facets of $P$ with the hypersurfaces given by $y_1 = y_2$ and $y_2 = y_3$ sometimes drop dimension under the moment map $\mu_A$. In the $(s, w)$ variables, these correspond to surfaces $(s_2 - s_1) w_1 = s_1 w_2$ and $(1 - s_2) w_2 = s_2 w_3$, respectively. For example, in each of the facets $s_1 = 0$ and $w_1 = 0$, the equation $(1 - s_2) w_2 = s_2 w_3$ cuts out a surface whose image under $\mu_A$ is a curve. For the face $s_1 = 0$, the moments of this surface collapse to the line segment connecting the constant function and the point masses at 0 and for $w_1 = 0$, the image of this surface collapses to the curve segment of moments of

Fig. 3 The sets $M_1(A)$, $M_2(A)$, $M_3(A)$ in $\{m_0 = 1\}$ for $A = \{0, 2, 5, 9\}$
step functions of a single step with $w_1 = 0$. Similarly, the faces $s_2 = 1$ and $w_3 = 0$ each contain a two-dimensional surface cut out by $s_1 w_2 = (1 - s_1) w_1$ whose moments collapse to a line segment—from the constant function to the point mass at 1 for $s_2 = 1$ and a curve segment of moments of a single step with $w_3 = 0$.

Aside from these subsurfaces, the map on the boundary $\partial P$ is locally nondegenerate. Interestingly, the images of these facets can overlap in full-dimensional sets. One consequence is that the fibers of the moment map can be disconnected.

For example, the point $(m_0, m_2, m_5, m_9) = (1, 0.164, 0.054, 0.031)$ belongs to $M_2(A)$ for $A = \{0, 2, 5, 9\}$. Its fiber under $\mu_A$ is a curve in the four-dimensional polytope $P$ from (2). The bold curve segments in Fig. 5 show the $(s_1, s_2)$-coordinates of this curve. In particular, this fiber has at least two connected components. The darker blue region corresponds to the two-dimensional fiber of the point $(m_0, m_2, m_5) = (1, 0.164, 0.054)$ under the corresponding map for $A = \{0, 2, 5\}$. The lighter shade blue region represents the full $(s_1, s_2)$-simplex.

Fig. 5 A disconnected fiber of $\mu_A$, for $A = \{0, 2, 5, 9\}$
3 Increasing and Decreasing Step Functions

In this section, we study the moment cones of non-negative monotone functions on the unit interval [0, 1]. We define the increasing and decreasing moment cones

\[ M^\uparrow(A) = \left\{ \left( \int_0^1 x^a f(x) \, dx \right)_{a \in A} : f \text{ is nonnegative and increasing on } [0, 1] \right\} \quad \text{and} \quad M^\downarrow(A) = \left\{ \left( \int_0^1 x^a f(x) \, dx \right)_{a \in A} : f \text{ is nonnegative and decreasing on } [0, 1] \right\}. \]

Recall that if a function \( f : [0, 1] \to \mathbb{R} \) is monotone, then it is automatically Borel-measurable. As in the non-monotone case, all of these moment vectors can be achieved as a limit of moments of step functions with a bounded number of steps. For \( k \in \mathbb{N} \), let \( S^\uparrow_k \) denote the set of nonnegative, increasing step functions on [0, 1] with at most \( k \) discontinuities. Similarly, let \( S^\downarrow_k \) denote the analogous set of decreasing step functions. This corresponds to requiring \( y_1 \leq y_2 \leq \cdots \leq y_{k+1} \) or \( y_1 \geq y_2 \geq \cdots \geq y_{k+1} \) in (1).

Similarly, for finite \( A \subset \mathbb{N} \), we consider the \( A \)-moments of these step functions,

\[ M^\Box_k(A) = \left\{ \left( \int_0^1 x^a f(x) \, dx \right)_{a \in A} : f \in S^\Box_k \right\} \quad \text{for } \Box \in \{\uparrow, \downarrow\}. \]

Just as with \( M_k(A) \), we see that the set \( M^\Box_k(A) \) is invariant under nonnegative scaling, \( M^\Box_k(A) \subseteq M^\Box_{k+\ell}(A) \) when \( k \leq \ell \) and \( M^\Box_k(A) + M^\Box_{\ell}(A) \subseteq M^\Box_{k+\ell}(A) \).

As in the non-monotone case, we can understand the cones \( M^\Box(A) \) as the conical hull of curve segments.

**Definition 1** We define maps \( \gamma^\uparrow_A \) and \( \gamma^\downarrow_A \) from \([0, 1]\) to \( \mathbb{R}^{|A|} \) where, for \( t \in [0, 1] \), \( \gamma^\uparrow_A(t) \) and \( \gamma^\downarrow_A(t) \) are the \( A \)-moment vectors of the step functions \((1/(1-t))1_{(t,1]} \) and \((1/t_{\min(A)+1})1_{[0,t]} \), respectively. For every \( a \in A \), the \( a \)th coordinate of these maps are given by

\[
\left( \gamma^\uparrow_A(t) \right)_a = \frac{1}{1-t} \int_t^1 x^a \, dx = \frac{1}{a+1} \sum_{i=0}^a t^i
\]

and

\[
\left( \gamma^\downarrow_A(t) \right)_a = \frac{1}{t_{\min(A)+1}} \int_0^t x^a \, dx = \frac{1}{a+1} t^{a-\min(A)}. \]

We observe that \( \gamma^\uparrow_A(0) = \gamma^\uparrow_A(1) = (1/(a+1))_{a \in A} \) corresponds to the moment vector of the constant function \( 1_{[0,1]} \). The other endpoints correspond to point masses. Specifically, \( \gamma^\uparrow_A(1) = \nu_A(1) \) is the moment vector of a point mass at \( t = 1 \) and \( \gamma^\downarrow_A(0) = \frac{1}{\min(A)+1} \nu_B(0) \) for \( B = \{a - \min(A) : a \in A \} \) corresponds to a point mass at \( t = 0 \).

**Remark 3** The conical hull over \( \{\gamma^\Box_A(t) : t \in [0, 1]\} \) is closed because this curve is compact and does not contain the origin. Indeed, for \( \Box = \uparrow \), the \( a \)th coordinate of \( \gamma^\uparrow_A(t) \) is \( \geq (1/a+1) \) for all \( t \). For \( \Box = \downarrow \), the \( \min(A) \)-th coordinate of \( \gamma^\downarrow_A(t) \) is identically \( 1/(\min(A)+1) \).

**Lemma 10** For \( \Box \in \{\uparrow, \downarrow\} \), the cone \( M^\Box(A) \) equals \( \text{conicalHull}\{\gamma^\Box_A(t) : t \in [0, 1]\} \).
Proof Since \( M(A) \) is a convex cone containing the point \( \gamma_A(t) \) for all \( t \), it automatically contains the conical hull of this curve.

For the other direction, consider a monotone function \( f : [0, 1] \to \mathbb{R} \). We can construct a sequence of step functions \( f_n \) converging uniformly to \( f \) on \([0, 1]\). For example, we may take \( f_n = \sum_{i=1}^n \frac{M}{n} \mathbf{1}_{T_i} \), where \( M \in \{ f(0), f(1) \} \) is the maximal value of \( f \) on \([0, 1]\) and \( \mathbf{1}_{T_i} \) is the indicator function of the set \( T_i \) of \( x \in [0, 1] \) with \( f(x) \geq iM/n \). That is \( f_n(x) = \frac{M}{n} \cdot \lceil \frac{n}{M} f(x) \rceil \). Note that \( |f_n - f| \leq M/n \) and so \( f_n \) converges uniformly to \( f \) on \([0, 1]\). It follows that for any \( a, x^a f_n \) converges uniformly to \( x^a f \) and so the integral \( \int_0^1 x^a f_n(x) dx \) converges to \( \int_0^1 x^a f(x) dx \).

Note that the set \( T_i \) defined above has the form \( [s_i, 1] \) or \([s_i, 1] \) if \( f \) is increasing and \([0, s_i] \) or \([0, s_i] \) if \( f \) is decreasing for some \( s_i \in [0, 1] \). The moment vector of \( f_n \) therefore is a conic combination of the points \( \gamma_{A(t)}(s_i) \) for the appropriate \( \in \{ \uparrow, \downarrow \} \). Taking \( n \to \infty \) shows that the moment vector of \( f \) belongs to the closure of the conical hull of \( \gamma_A(t) : t \in [0, 1] \).

Therefore, the moment cone corresponding to nonnegative, increasing step functions on \([0, 1] \) belongs to the closure of the conical hull of \( \gamma_A(t) : t \in [0, 1] \). By definition, \( M(A) \) is the closure of this set and so also belongs to the closure of this conical hull. Similarly, \( M(A) \) belongs to the closure of the conical hull of \( \gamma_A(t) : t \in [0, 1] \). By Remark 3, both of these conical hulls are already closed.

\[ \square \]

Proposition 11 If \( k \geq \left\lfloor \frac{|A|}{2} \right\rfloor \), then \( M_k(A) = M(A) \) and \( M^1_k(A) = M^1(A) \).

Proof Our proof proceeds similarly to that of Theorem 3. Let \( \mathbf{m} \) be a point of the boundary of \( M(A) \). We want to express \( \mathbf{m} \) as the A-moment of an increasing step function of the fewest steps possible. Let \( \ell : \mathbb{R}^A \to \mathbb{R} \) define a supporting hyperplane of \( M(A) \) at \( \mathbf{m} \), so that \( \ell \geq 0 \) on \( M(A) \) and \( \ell(\mathbf{m}) = 0 \). By Lemma 10, \( M(A) \) is the conical hull of points on this curve, with \( \ell = 0 \). We use this to show that \( \mathbf{m} \) belongs to \( M_k(A) \) for \( k \geq \left\lfloor \frac{|A|}{2} \right\rfloor \).

(\( \downarrow \)) Let \( p(x) = \ell \left( \gamma_A^1(x) \right) = \sum_{a \in A} \frac{p_a}{a+1} x^{a-min(A)} \). The polynomial \( p \) is nonnegative on \([0, 1] \). By Descartes’ rule of signs, \( p \) has at most \( |A| - 1 \) positive roots, counting multiplicity, and if \( p_{min(A)} = 0 \), then it has at most \( |A| - 2 \). Let \( i \) denote the number of distinct roots of \( p \) in \((0, 1) \) and \( b = 1 \) if \( p(0) = 0 \) and \( 0 \) otherwise. Since each interior root of \( p \) must have multiplicity \( \geq 2 \), this gives \( 2i + b \leq |A| - 1 \). Note that \( \gamma_A^1(t) \in M_k(A) \) for all \( t \in [0, 1] \) and belongs to \( M_k(A) \) for \( t = 1 \). Therefore \( \mathbf{m} \) belongs to \( M_k(A) \) for \( k = i + b \leq \frac{1}{2} (|A| - 1 + b) \). The bound follows from the integrality of \( i + b \) and \( b \in \{0, 1\} \).

(\( \uparrow \)) Let \( p(x) = \ell \left( \gamma_A^1(x) \right) = \sum_{a \in A} \frac{p_a}{a+1} \sum_{i=0}^a x^i \), which is a polynomial nonnegative on \([0, 1] \). Again, by Descartes’ rule of signs, \( p \) has at most \( |A| - 1 \) positive roots, counting multiplicity. If \( i \) is the number of distinct roots of \( p \) in \((0, 1) \) and \( b = 0 \) if \( p(1) = 0 \) and \( 0 \) otherwise, this gives that \( 2i + b \leq |A| - 1 \). As before, \( \gamma_A^1(t) \in M_k(A) \) for all \( t \in (0, 1) \) and belongs to \( M_k(A) \) for \( t = 0 \). Therefore \( \mathbf{m} \) belongs to \( M_k(A) \) for \( k = i + b \leq \frac{1}{2} (|A| - 1 + b) \leq \frac{1}{2} |A| \).

Now consider \( \mathbf{m} \) in the interior of \( M(A) \) and let \( \mathbf{c} \) be the moment vector of the constant function \( \mathbf{1}_{[0, 1]} \). Let \( \lambda^* \) be the maximum value of \( \lambda \in \mathbb{R} \) for which \( \mathbf{m} - \lambda \mathbf{c} \) belongs to \( M(A) \). Since \( \mathbf{m} \in M(A) \), we know that \( \lambda^* \geq 0 \), and for sufficiently large \( \lambda \), \( \mathbf{m} - \lambda \mathbf{c} \notin M(A) \).
Thus \( m - \lambda^*c \) belongs to the boundary of \( M_k^{\Box}(A) \), which is equal to the boundary of \( M_k^{\Box}(A) \) by the argument above. Hence, \( m \) also belongs to \( M_k^{\Box}(A) \).

Proposition 12 For all \( k < \left\lfloor \frac{|A|}{2} \right\rfloor \), the cone \( M_k^{\Box}(A) \) is a proper subset of \( M^{\Box}(A) \).

Proof Any point in the cone \( M_k^{\Box}(A) \subset \mathbb{R}^{|A|} \) is a conic combination of \( k \) points on the boundary curve \( \gamma^\Box_A \), each contributing two degrees of freedom, and the point corresponding to the image of the constant step function \( \gamma^\Box_A(0) = \gamma^\Box_A(1) \), contributing a single degree of freedom. Therefore, the semialgebraic set \( M_k^{\Box}(A) \) has dimension at most \( \min\{2k + 1, |A|\} \).

The cone \( M^{\Box}(A) \) is full-dimensional in \( \mathbb{R}^{|A|} \). Let \( n = \lfloor |A|/2 \rfloor \) so that \( |A| \) is 2\( n \) or 2\( n + 1 \). In either case, we observe that for \( k \leq n - 1 \), the dimension of \( M_k^{\Box}(A) \) is less than or equal to \( 2n - 1 \), hence it cannot fill up all of \( M^{\Box}(A) \).

Example 5 For \( A = \{0, 2, 5\} \), \( M_1^{\downarrow}(A) \) and \( M_1^{\uparrow}(A) \) are depicted respectively as the red and blue regions of \( M_1^{\Box}(A) \) and \( M_2^{\Box}(A) \) in Fig. 2. As expected, they are attained with step functions of a single step. For \( A = \{0, 2, 5, 9\} \), \( M_1^{\downarrow}(A) \) is a union of \( M_1^{\uparrow}(A) \) and \( M_1^{\downarrow}(A) \), shown on the left in Fig. 3. Since \( 1 < 2 = \lfloor |A|/2 \rfloor \), these sets are not full dimensional and so cannot fill up \( M^{\downarrow}(A) \) or \( M^{\uparrow}(A) \). For \( k = 2 = \lfloor |A|/2 \rfloor \), \( M_2^{\uparrow}(A) = M^{\uparrow}(A) \) and \( M_2^{\downarrow}(A) = M^{\downarrow}(A) \). These form (yellow and orange) parts of the full dimensional set \( M_2^{\Box}(A) \) shown in the middle of Fig. 3.

4 Connection with Coalescence Manifold

The motivation for studying moments of step functions comes from the field of population genetics. A central problem in this area is:

Question 1 Given a sample of \( n \) genotypes from a present-day population, what inferences can be drawn regarding the history of that population?

Our approach to the problem is to fix a function \( p(t) \) describing effective population size \( t \) years (or other time units) before the present. We then compute, as a function of \( p \), a vector of invariants \( c \) associated to the genome sample. Understanding the relationship between \( p \) and \( c \) will allow us to infer likely values of \( p \) based on measured data.

Following [1] and [10], we model the natural process of the production of a sample of \( n \) genotypes as follows. For more details and discussion of the biological motivation, we refer the reader to [1] and [10].

– We first create a genealogical tree connecting \( n \) individuals, going backwards in time. We say that the lineages of two samples coalesce when they reach a common ancestor. In this model, the coalescence of each pair of lineages is viewed as a Poisson point process with rate parameter \( 1/p(t) \), where \( p(t) \) is the effective population size at time \( t \) before present. (Heuristically, looking at the previous generation and picking parents at random, there is a \( 1/p(t) \) chance that two lineages will pick the same parent.) The result is a rooted tree on \( n \)-leaves in which the lengths of edges represent time between individuals.
– After the genealogical tree is specified, mutations are distributed on the tree as a Poisson point process with constant rate relative to branch length. The “infinite-sites model” is used, so that repeated mutation at a given site is disallowed, which is a good model for large genomes.

**Definition 2** Fixing a population history, and defining the random process as above, we define random variables:

- The *sample frequency spectrum* (also known as the *site* or *allele frequency spectrum*), abbreviated SFS, is the vector of random variables \((X_{n,b})_{b=1,\ldots,n-1}\) where \(X_{n,b}\) denotes the number of mutations that are shared by exactly \(b\) out of the \(n\) individuals.
- The *coalescence vector* is the vector \((T_{i,i})_{i=2,\ldots,n-1}\) of the time at which a sample of size \(i\) has exactly \(i\) distinct lineages, i.e. the time until the first coalescence.

For a fixed population function \(p\), taking expectations gives the population invariants \(\xi_{n,b} = \mathbb{E}[X_{n,b}]\) and \(c_i = \mathbb{E}[T_{i,i}]\).

In practice, the SFS is more frequently discussed as a summary statistic, but the coalescence vector is simpler to use in computations. Fortunately, Griffiths and Tavaré [6, (1.3)] proved that they are related by a linear transformation \(A_n\), a matrix entirely determined by the sample size \(n\). Therefore, we focus on the coalescence vector \(c = (c_i)_i\).

**Definition 3** We make the reasonable assumption that \(p(t)\) is bounded below by 0 and bounded above by a fixed \(P\). By applying integration by parts and change of variables to the expected value of an exponential distribution, Polanski and Kimmel [9] give the following expression for \(c_i\) in terms of \(p(t)\):

\[
c_i(p) = \int_0^\infty \tilde{p}(\tau) \exp\left[-\left(c_i^2(\tau)\right)\tau\right] d\tau, \tag{3}
\]

where \(\tilde{p}(\tau) = p(R^{-1}_p(\tau))\) and \(R_p(t) = \int_0^t \frac{1}{p(x)} dx\). See also [10, (1)]. Because \(0 < p(t) < P\), the function \(R_p\) is strictly increasing and unbounded; thus, it is a bijection from \(\mathbb{R}_{\geq 0}\) to \(\mathbb{R}_{\geq 0}\), with a well-defined inverse. We call \(\tilde{p}(\tau)\) the *transformed population history*.

The coalescence vector can thus be considered a function from the space of (bounded) population history functions to \(\mathbb{R}^{n-1}\). Since the former space is infinite-dimensional and the latter is finite-dimensional, it is natural to restrict our attention to a finite-dimensional space of population history functions. A common choice for this, motivated by injectivity considerations in [1], is

\[
\tilde{S}_k = \{\text{nonnegative step functions on } \mathbb{R}_{\geq 0} \text{ with at most } k \text{ breakpoints}\}.
\]

**Definition 4** Let \(n, k\) be integers with \(n \geq 2\) and \(k \geq 0\). The *coalescence manifold* \(C_{n,k}\) is the Euclidean closure of the set of vectors \(\tilde{c}(p) = c(p)/\|c(p)\|_1\) for all \(p \in \tilde{S}_k\). Here, \(c(p) = (c_2(p), \ldots, c_n(p))\) where \(c_i(p)\) is defined as in (3).

Because the vectors are normalized to have sum one, the coalescence manifold lives in the simplex \(\Delta^{n-1}\). Note that this definition deviates slightly from the definition in [10] by allowing \(k\) breakpoints instead of \(k\) epochs (i.e. constant intervals). This shifts the index down by one. We now connect back to the moment cones studied above.
Theorem 13  Let \( A = \{ \binom{i}{2} - 1 : i = 2, \ldots, n \} \). The coalescence manifold \( C_{n,k} \) equals the intersection of the cone \( M_k(\mathbb{A}) \) with the affine hyperplane of points with coordinate sum equal to one:

\[
C_{n,k} = \left\{ \mathbf{m} \in M_k(\mathbb{A}) : \sum_{a \in A} m_a = 1 \right\}.
\]

Before we prove the theorem, we demonstrate two lemmas that will simplify the proof.

Lemma 14  Define \( \tilde{\mathbf{p}}(\tau) \) as in (3). Then \( \mathbf{p}(\tau) \in \tilde{S}_k \) if and only if \( \tilde{\mathbf{p}}(\tau) \in \tilde{S}_k \).

Proof  Let \( 0 = s_0 < \cdots < s_{k-1} < s_k \) be the sequence of breakpoints of \( \mathbf{p}(\tau) \). The function \( R_{\mathbf{p}}(t) \) is a monotone increasing function, so the conditions below are equivalent:

\[
s_j < t \leq s_{j+1} \iff R_{\mathbf{p}}(s_j) < R_{\mathbf{p}}(t) \leq R_{\mathbf{p}}(s_{j+1}).
\]

Since \( \mathbf{p} \) is constant on \((s_j, s_{j+1}]\), the transformed history \( \tilde{\mathbf{p}}(\tau) = \mathbf{p}(R_{\mathbf{p}}^{-1}(\tau)) \) is constant on \((R_{\mathbf{p}}(s_j), R_{\mathbf{p}}(s_{j+1})]\). This implies that there are still at most \( k \) breakpoints.

For the reverse direction, repeat the argument with \( R_{\mathbf{p}}^{-1} \) in place of \( R_{\mathbf{p}} \).

Lemma 15  Let \( q \) be a strictly positive step function in \( \tilde{S}_k \). Then, there exists \( \mathbf{p} \) in \( \tilde{S}_k \) such that \( q(\tau) = \mathbf{p}(R_{\mathbf{p}}^{-1}(\tau)) \) where \( R_{\mathbf{p}}(t) = \int_0^t \frac{1}{\tilde{\mathbf{p}}(\tau)} d\tau \) as above.

Proof  Let \( Q(t) = \int_0^t q(x) dx \). We claim the desired function is \( \mathbf{p}(t) = q(\tau^{-1}(t)) \). First, note that because \( q \) is strictly positive and takes only finitely many values, it is bounded away from zero. Therefore, \( Q \) is strictly increasing and takes all values in \([0, \infty)\). Its inverse \( \tau^{-1} \) therefore exists and is also increasing with range \([0, \infty)\). It follows that \( \mathbf{p} \) takes the same values in the same order as \( q \). In particular, \( \mathbf{p} \in \tilde{S}_k \).

To check that \( q(t) = \mathbf{p}(R_{\mathbf{p}}^{-1}(t)) \), we first show that \( R_{\mathbf{p}}(Q(t)) = t \) for all \( t \geq 0 \). By definition,

\[
R_{\mathbf{p}}(Q(t)) = \int_0^t \frac{Q(t)}{\mathbf{p}(x)} dx = \int_0^t \frac{Q(t)}{q(\tau^{-1}(x))} dx = \int_0^t \frac{1}{q(w)} q(w) dw = t.
\]

The penultimate equation comes from substituting \( x = Q(w) \) and \( dx = q(w) dw \). Since both \( Q \) and \( R_{\mathbf{p}} \) are invertible, we see that \( t = Q^{-1}(R_{\mathbf{p}}^{-1}(t)) \) for all \( t \). Applying \( q \) to both sides then gives the claim.

Proof of Theorem 13  We show that the set of coalescence vectors coming from population histories in \( \tilde{S}_k \) is equal to the set of moments in \( M_k(\mathbb{A}) \) summing to 1. The equality of the two closures is then automatic.

Assume \( \mathbf{p} \in \tilde{S}_k \). From Lemma 14, \( \tilde{\mathbf{p}} \) is also in \( \tilde{S}_k \). Starting with (3), we substitute \( u = e^{-\tau} \) to obtain:

\[
\mathbf{c}_i(\mathbf{p}) = \int_0^1 \tilde{\mathbf{p}}^*(u) u^{(\binom{i}{2} - 1)} du, \quad \text{where } \tilde{\mathbf{p}}^*(u) = \mathbf{p}(R_{\mathbf{p}}^{-1}(- \ln(u))).
\]

The function \( \tilde{\mathbf{p}}^* \) is piecewise-constant on \([0, 1]\) with at most \( k \) breakpoints, so is in \( \tilde{S}_k \); therefore, the quantity \( \mathbf{c}_i \) is the \((\binom{i}{2} - 1)\)-th moment of \( \tilde{\mathbf{p}}^* \). This implies that \( \mathbf{c} \) is in \( M_k(\mathbb{A}) \) where \( A = \{ \binom{i}{2} - 1 : i = 2, \ldots, n \} \). Normalizing \( \mathbf{c} \) is equivalent to scaling \( \tilde{\mathbf{p}}^* \) so we may assume its sum is already equal to 1.
Conversely, up to closure, any moment vector in $M_k(A)$ summing to 1 comes from some $f \in S_k$. Changing our domain to $\mathbb{R}_{>0}$ gives $q(\tau) = f(e^{-\tau})$ in $\tilde{S}_k$. By Lemma 15, there exists $\mathbf{p} \in \tilde{S}_k$ that gives the transformed population history $q$.

**Example 6** Consider the population function $\mathbf{p}(t) = p_1 \cdot \mathbf{1}_{[0,b_1]} + p_2 \cdot \mathbf{1}_{(b_1,b_2]} + p_3 \cdot \mathbf{1}_{(b_2,\infty)}$ where $p_1, p_2, p_3, b_1, b_2 \in \mathbb{R}_{>0}$ with $b_1 < b_2$ and we fix $p_2 > p_1 > p_3$. The function $R_p(t)$ is piecewise linear, given by $R_p(t) = \int_0^t \frac{1}{p(x)} \, dx = \frac{t}{p_1} \mathbf{1}_{[0,b_1]} + \left( \frac{t - b_1}{p_2} + \frac{b_1}{p_1} \right) \mathbf{1}_{(b_1,b_2]} + \left( \frac{t - b_2}{p_3} + \frac{b_2 - b_1}{p_2} + \frac{b_1}{p_1} \right) \mathbf{1}_{(b_2,\infty)}$. This function is unbounded and strictly increasing with $R_p(0) = 0$, so it has an inverse $R_p^{-1}$ that is also increasing and unbounded on $\mathbb{R}_{\geq 0}$. The function $\tilde{p}(\tau) = \mathbf{p}(R_p^{-1}(\tau))$ is still piecewise constant with two break points $R_p(b_1) = b_1/p_1$ and $R_p(b_2) = (b_2 - b_1)/p_2 + b_1/p_1$, obtained by solving $R_p^{-1}(\tau) = b_i$. The $i$th entry of the coalescence vector is then

$$c_i = \int_0^\infty \tilde{p}(\tau) e^{(\tau)} \, d\tau = \int_0^1 \tilde{p}^*(u) u^{(i)}(1) - 1 \, du \quad \text{where} \quad \tilde{p}^*(u) = \tilde{p}(-\ln(u)).$$

The second equality comes from the change of coordinates $u = e^{-\tau}$. Note that $\tilde{p}^*$ is the step function given by

$$\tilde{p}^* = p_3 \cdot \mathbf{1}_{(0,s_1]} + p_2 \cdot \mathbf{1}_{(s_1,s_2]} + p_1 \cdot \mathbf{1}_{(s_2,1]} \quad \text{where} \quad s_1 = e^{-R_p(b_2)} \text{ and } s_2 = e^{-R_p(b_1)}.$$ 

The graphs of $\mathbf{p}$ and $\tilde{p}^*$ for the values $(p_1, p_2, p_3) = (2, 3, 1)$ and $(b_1, b_2) = (2, 5)$ are shown in Fig. 6. In this case, the break points of $\tilde{p}^*$ are $e^{-R_p(b_2)} = e^{-2}$ and $e^{-R_p(b_1)} = e^{-1}$.

**Remark 4** Note that because $\mathbf{p}(t)$ denotes the population size at time $t$ before the present, a population increasing over time corresponds to a function $\mathbf{p}(t)$ decreasing as a function of $t$, i.e. $\mathbf{p}(t)$ has coefficients $p_1 > p_2 > p_3$ in the notation of the example above. Note that $\mathbf{p}(t)$ is decreasing in $t$ if and only if $\tilde{p}(\tau)$ is decreasing in $\tau$. The parametrization $u = e^{-\tau}$ reverses direction and so the function $\tilde{p}^*(u)$ is then increasing as a function of $u$. In these coordinates, $u = 0$ corresponds to “infinitely long ago” ($t = \infty$) and $u = 1$ corresponds to the present ($t = 0$). Therefore, coalescence vectors of populations growing over time are moments of increasing step functions on $[0, 1]$.

Theorem 13 allows us to apply our results from $M_k(A)$ to $C_{n,k}$.

**Corollary 16** $C_{n,n - 2} = C_{n,k}$ for all $k \geq n - 2$ and $C_{n,n - 3} \subsetneq C_{n,n - 2}$.

**Proof** For $A = \left\{ \begin{pmatrix} 1 \\ i \\ \vdots \\ n \end{pmatrix} : i = 2, \ldots, n \right\}, |A| = n - 1$. By Theorem 3, $M_k(A)$ equals $M(A)$ for all $k \geq n - 2$. In particular, $M_{n-2}(A) = M_k(A)$ for all $k \geq n - 2$. Intersecting with

![Fig. 6](https://example.com/fig6.png)
the hyperplane \( \{ m : \sum_{a \in A} m_a = 1 \} \) gives that \( C_{n,n-2} = C_{n,k} \) for all \( k \geq n - 2 \). By Corollary 9, \( M_k(A) \neq M(A) \) for \( k < |A| - 1 = n - 2 \). Hence \( M_{n-3}(A) \neq M(A) \).

Since \( M(A) = M_{n-2}(A) \), intersecting with the hyperplane \( \{ m : \sum_{a \in A} m_a = 1 \} \) gives that \( C_{n,n-2} \neq C_{n,n-3} \). \( \square \)

Affine transformations of the sets \( C_{5,1}, C_{5,2} \) and \( C_{5,3} \) are shown in Fig. 3. As promised, \( C_{5,3} \) is convex and \( C_{5,k} \) is a strict subset for \( k < 3 \).

## 5 Connections with Semidefinite Programming

In this section, we describe how to write the moment cone \( M(A) \) and coalescence manifold \( C_{n,n-2} \) as projections of spectrahedra. This gives rise to natural algorithms for testing membership and finding nearest points in these sets based on semidefinite programming. Formally, a spectrahedron is a set of the form \( \{ x \in \mathbb{R}^n : A_0 + \sum_{i=1}^n x_i A_i \succeq 0 \} \) where \( A_0, \ldots, A_n \) are real symmetric matrices and \( X \succeq 0 \) denotes that the matrix \( X \) is positive semidefinite. These are the feasible sets of semidefinite programs. See e.g. [2, Chapters 5 and 6]. Python code for computing the nearest point in \( C_{n,n-2} \) to an arbitrary point in \( \mathbb{R}^{n-1} \) is available at: 

https://github.com/gescholt/DistanceToCoalescenceManifold

As the full moment cone, \( M([0, 1, \ldots, d]) \) plays a prominent role in this section, we abbreviate it by \( M[d] \).

**Theorem 17** (Theorems 10.1 and 10.2 [11]) For any \( d \in \mathbb{Z}_+ \), the cone \( M([d]) \) is a spectrahedron. If \( d = 2e \) is even, then

\[
M[d] = \left\{ m \in \mathbb{R}^{d+1} : (m_{i+j})_{0 \leq i,j \leq e} \geq 0 \text{ and } (m_{i+j+1} - m_{i+j+2})_{0 \leq i,j \leq e-1} \geq 0 \right\},
\]

and if \( d = 2e + 1 \) is odd, then

\[
M[d] = \left\{ m \in \mathbb{R}^{d+1} : (m_{i+j+1})_{0 \leq i,j \leq e} \geq 0 \text{ and } (m_{i+j} - m_{i+j+1})_{0 \leq i,j \leq e} \geq 0 \right\}.
\]

**Corollary 18** For any finite set of integers \( A \subset \mathbb{N} \), the convex cones \( M(A), M^\uparrow(A) \) and \( M^\downarrow(A) \) are projections of the spectrahedron \( M[\max(A)] \).

**Proof** Let \( d = \max(A) \). Note that by definition, \( M(A) \) equals the closure of the projection of \( M[d] \) under the map \((m_0, m_1, \ldots, m_d) \mapsto (m_a)_{a \in A} \). As discussed in Section 2, for \( 0 \in A \), this projection is closed and otherwise, we replace \( A \) with \( B = \{ a - \min(A) : a \in A \} \) as in Lemma 1. By Theorem 17, \( M[d] \) is a spectrahedron.

More generally, consider any finite collection of polynomials \( p_1, \ldots, p_n \in \mathbb{R}[x]_{\leq d} \). We claim that the conical hull of the curve parameterized \( p : [0, 1] \to \mathbb{R}^n \) where \( p(t) = (p_1(t), \ldots, p_n(t)) \) is the image of \( M[d] \) under a linear map. Specifically, consider the linear map \( \pi : \mathbb{R}^{d+1} \to \mathbb{R}^n \) taking \((m_0, m_1, \ldots, m_d)\) to \((\sum_{j=0}^d p_{ij} m_j)_{i \in [n]}\) where \( p_i(x) = \sum_{j=0}^d p_{ij} x^j \). For any \( t \in [0, 1] \), \( p(t) \) equals \( \pi(v_d(t)) \) where \( v_d(t) \) equals \((1, t, t^2, \ldots, t^d)\). Since \( M[d] \) is the conical hull of \( \{ v_d(t) : t \in [0, 1] \} \), the conical hull of \( \{ p(t) : t \in [0, 1] \} \) is the image of \( M[d] \) under \( \pi \).

Note that the coordinates of both \( \gamma^\uparrow_A(t) \) and \( \gamma^\downarrow_A(t) \) are given by polynomials in \( t \) of degree \( \leq d \). Then by Lemma 10 and the arguments above, both \( M^\uparrow(A) \) and \( M^\downarrow(A) \) can be written as the image of \( M[d] \) under a linear map. \( \square \)
Example 7 For \( A = \{0, 2, 5, 9\} \), we write \( M(A), M^\uparrow(A) \) and \( M^\downarrow(A) \) as projections of the spectrahedron \( M[9] \). By Theorem 17, this is given by the set of \( m = (m_0, \ldots, m_9) \) in \( \mathbb{R}^{10} \) for which the matrices

\[
\begin{pmatrix}
m_1 & m_2 & m_3 & m_4 & m_5 \\
m_2 & m_3 & m_4 & m_5 & m_6 \\
m_3 & m_4 & m_5 & m_6 & m_7 \\
m_4 & m_5 & m_6 & m_7 & m_8 \\
m_5 & m_6 & m_7 & m_8 & m_9 \\
\end{pmatrix}
\quad \text{and} \quad
\begin{pmatrix}
m_0 - m_1 & m_1 - m_2 & m_2 - m_3 & m_3 - m_4 & m_4 - m_5 \\
m_1 - m_2 & m_2 - m_3 & m_3 - m_4 & m_4 - m_5 & m_5 - m_6 \\
m_2 - m_3 & m_3 - m_4 & m_4 - m_5 & m_5 - m_6 & m_6 - m_7 \\
m_3 - m_4 & m_4 - m_5 & m_5 - m_6 & m_6 - m_7 & m_7 - m_8 \\
m_4 - m_5 & m_5 - m_6 & m_6 - m_7 & m_7 - m_8 & m_8 - m_9 \\
\end{pmatrix}
\]

are positive semidefinite. We obtain \( M(A) \) as the image of this cone under the linear map \( m \mapsto (m_0, m_2, m_5, m_9) \). Similarly, the cones \( M^\uparrow(A) \) and \( M^\downarrow(A) \) are the images of \( M[9] \) under the (respective) maps

\[
m \mapsto \left( m_0, \frac{1}{3} \sum_{i=0}^{2} m_i, \frac{1}{6} \sum_{i=0}^{5} m_i, \frac{1}{10} \sum_{i=0}^{9} m_i \right) \quad \text{and} \quad m \mapsto \left( m_0, \frac{m_2}{3}, \frac{m_5}{6}, \frac{m_9}{10} \right).
\]

Corollary 19 Given a point in \( \mathbb{R}^{|A|} \), testing its membership in any of the cones \( M(A), M^\uparrow(A) \) or \( M^\downarrow(A) \) is equivalent to testing the feasibility of a semidefinite program in \( \leq d + 1 \) variables with two matrix constraints, each of size \( \leq 2 \), where \( d = \max(A) \).

Corollary 20 For \( k \geq n - 2 \), the coalescence manifold \( C_{n,k} \) is the projection of a spectrahedron. Testing membership in \( C_{n,k} \) is equivalent to testing the feasibility of a semidefinite program in \( \leq n^2/2 \) variables with two matrix constraints, each of size \( \leq n^2/4 \).

Proof By Theorem 13 and Corollary 16, for all \( k \geq n - 2 \), the coalescence manifold \( C_{n,k} \) equals the intersection of \( M(A) \) with the affine hyperplane \( \sum_{a \in A} m_a = 1 \) where \( A = \{0, 1, \ldots, n\} \). By Corollary 18, \( M(A) \) is the projection of \( M[d] \) where \( d = \binom{n}{2} - 1 \). It follows that \( C_{n,k} \) is the projection of the points in \( M[d] \) satisfying the affine linear equation \( \sum_{a \in A} m_a = 1 \). The intersection of a spectrahedron with an affine linear space is again a spectrahedron and so \( C_{n,k} \) is the projection of a spectrahedron.

The spectrahedron \( M[d] \) is defined by two linear matrix inequalities of size \( \leq d + 1 \). There are at most \( d + 1 = \binom{n}{2} \leq n^2/2 \) variables. \( \square \)

Similarly, given a point \( p \in \mathbb{R}^{n-1} \), we can use a semidefinite program to find the nearest point in \( C_{n,k} \) for sufficiently large \( k \). This comes from the description of \( C_{n,k} \) above and the fact that distance minimization can be phrased as a semidefinite program (see, e.g. [3]).

Specifically, given \( x \in \mathbb{R}^{n-1} \), the \( n \times n \) matrix

\[
\frac{\lambda}{(x - p)^T \Id_{n-1} + \Id_{n-1}}
\]

is positive semidefinite if and only if \( \|x - p\|^2 \leq \lambda \), where \( \Id_{n-1} \) denotes the \( (n - 1) \times (n - 1) \) identity matrix. Given a set \( S \subset \mathbb{R}^{n-1} \), suppose that \( \lambda^* \) and \( x^* \) obtain the minimum

\[
\min_{\lambda \in \mathbb{R}, x \in S} \lambda \quad \text{such that} \quad \left( \frac{\lambda}{(x - p)^T \Id_{n-1}} \right) \geq 0.
\]

Then \( x^* \) is (one of) the nearest points in \( S \) to \( p \) and the distance \( \|x^* - p\|^2 \) is \( \sqrt{\lambda^*} \). In particular, if the set \( S \) is the projection of a spectrahedron, then this minimization problem is a semidefinite program.
Corollary 21 Given \( p \in \mathbb{R}^{n-1} \), the problem of finding the closest point to \( p \) in \( C_{n,k} \) for sufficiently large \( k \) is equivalent to solving a semidefinite program in \( \leq n^2/2 \) variables with three matrices of size \( \leq n^2/4 \).

Example 8 For \( n = 5 \) and \( k \geq 3 \), \( C_{5,k} \) equals the set of points in \( M(\{0, 2, 5, 9\}) \) with \( m_0 + m_2 + m_5 + m_9 = 1 \). Projecting from \( M[9] \), we see that \( C_{5,k} = \{ (m_0, m_2, m_5, m_9) \in \mathbb{R}^4 : m_0 + m_2 + m_5 + m_9 = 1 \} \) and \( \exists (m_1, m_3, m_4, m_6, m_7, m_8) \in \mathbb{R}^6 \) such that \( (m_j)_{j=0,...,9} \in M[9] \).

Let \( A(m) \) and \( B(m) \) denote the two \( 5 \times 5 \) matrices appearing in Example 7. Then \( M[9] \) is the set of points \( m \in \mathbb{R}^{10} \) for which \( A(m) \succeq 0 \) and \( B(m) \succeq 0 \). Given a point \( p = (a, b, c, d) \in \mathbb{R}^4 \), we can find the closest point in \( C_{5,k} \) by solving the following semidefinite program with 10 parameters and three \( 5 \times 5 \) linear matrix constraints:

\[
\begin{aligned}
\min_{\lambda, m_0, \ldots, m_9} & \quad \lambda \\
\text{such that} & \quad m_0 + m_2 + m_5 + m_9 = 1, \quad A(m) \succeq 0, \quad B(m) \succeq 0, \\
& \quad \begin{pmatrix}
\lambda & m_0 - a & m_2 - b & m_5 - c & m_9 - d \\
m_0 - a & 1 & 0 & 0 & 0 \\
m_2 - b & 0 & 1 & 0 & 0 \\
m_5 - c & 0 & 0 & 1 & 0 \\
m_9 - d & 0 & 0 & 0 & 1
\end{pmatrix} \succeq 0.
\end{aligned}
\]

If \( (\lambda^*, m^*) \) denotes the points achieving this minimum, then \( (m_0^*, m_2^*, m_5^*, m_9^*) \) is the closest point in \( C_{5,k} \) to \( p \) with distance \( \sqrt{\lambda^*} \).

6 Discussion and Open Questions

One takeaway from Section 2 is that, for \( k \geq n - 2 \), the points on the boundary of \( C_{n,k} \) correspond to moment vectors of point evaluations on \([0, 1]\). However these do not correspond to biologically meaningful population functions! Indeed, these can only come from limits of functions with increasingly high spikes over increasingly short lengths of time. A point in the interior of \( C_{n,k} \) can come from several different population functions, some of which are more biologically plausible than others. One natural question from this standpoint is how to pick the right population history from the fiber of a coalescence vector.

Question 2 Given a point \( m \) in the interior of \( M_k(A) \), how can we find the “best” step function \( f \in S_k \) with moment vector \( m \)?

Here, there is some natural flexibility in the notion of “best”. Ideally it should be biologically plausible and also easy to compute. For plausibility, it might be reasonable to try to bound or minimize the ratios \( y_{i+1}/y_i \) of consecutive population sizes. One step towards this would be to understand the structure of the fibers of the moment map \( \mu_A \).

For \( k = 2 \) and \( A = \{0, 2, 5\} \), the \( (s_1, s_2) \)-coordinates of the fibers of some points in \( M_2(A) \) are shown in Fig. 7.

To understand the fibers, it may also help to relate the combinatorial structure of the polytope \( P \) (which is a product of two \( k \)-dimensional simplices) to the semi-algebraic and
combinatorial structure of $M_k(A)$. For example, the boundary of $M_2([0, 2, 5, 9])$, seen in Fig. 3, comes from some of the two-dimensional faces of the four-dimensional polytope $P$.

**Question 3** How does the facial structure of $P$ relate to the boundary of $M_k(A)$, for $k < |A| - 1$?

Finally, Section 5 gives an algorithm for testing membership in $M(A)$, which coincides with $M_k(A)$ for $k \geq |A| - 1$. It would be desirable to be able to test membership for smaller $k$ as well.

**Question 4** Given a point $p \in \mathbb{R}^{|A|}$, can one effectively test its membership in $M_k(A)$ for $k < |A| - 1$?

These sets are not convex and may have complicated semialgebraic structure (Fig. 3). One possibility would be to exploit the following connection to low rank matrix completion.

Consider a step function $f = y_1 \mathbf{1}_{[0,s_1]} + \sum_{i=2}^{k+1} y_i \mathbf{1}_{(s_{i-1},s_i]}$ in $\mathcal{S}_k$. In a slight abuse of notation, we define its derivative to be $f' = \sum_{i=1}^k (y_{i+1} - y_i)\delta_{s_i}$, which is a signed weighted sum of delta functions. For $j \in A$, let $m'_j$ denote the $j$th moment of the signed measure given by $f'$:

$$m'_j = \int_0^1 x^j f'(x) dx = \sum_{i=1}^k (y_{i+1} - y_i)(s_i)^j.$$
One can check that for any \( j, m'_j = f(1) - jm_{j-1} \). In particular, we can write differences of consecutive moments of the derivative \( f' \) in terms of moments of \( f \), namely \( m'_j - m'_{j+1} = (j + 1)m_j - jm_{j-1} \).

In the case of full moments \( A = \{0, 1, \ldots, d\} \), this lets us bound the value of \( k \) by the rank of the moment matrix corresponding to the moments of \( (x - x^2)f'(x) \). Specifically, for \( m \in \mathbb{R}^A \), define the matrix

\[
\mathcal{M}(m) = \left( (j + \ell + 2)m_{j+\ell+1} - (j + \ell + 1)m_{j+\ell} \right)_{0 \leq j, \ell \leq \lfloor (d-1)/2 \rfloor}.
\]

**Proposition 22** If \( m = \left( \int_0^1 x^j f(x) \, dx \right)_j \) for \( f \in S_k \), then \( \text{rank}(\mathcal{M}(m)) \leq k \).

**Proof** As noted above, we can rewrite the \((j, \ell)\)th entry of \( \mathcal{M}(m) \) as

\[
\mathcal{M}(m)_{j,\ell} = (j + \ell + 2)m_{j+\ell+1} - (j + \ell + 1)m_{j+\ell} = m'_j + \ell + 1 - m'_{j+\ell+2} = \sum_{i=1}^{k} (y_{i+1} - y_i)(s_i - s_i^2)s_i^{j+\ell}.
\]

Therefore \( \mathcal{M}(m) \) equals \( \sum_{i=1}^{k} (y_{i+1} - y_i)(s_i - s_i^2)v(t_i)v(t_i)^T \) for \( e = \lfloor (d - 1)/2 \rfloor \) and \( v(t) = (1, t, t^2, \ldots, t^e)^T \). In particular, \( \mathcal{M}(m) \) is a sum of \( k \) matrices of rank one and so has rank \( \leq k \). \( \Box \)

Note that if the values of \( y_i \) are increasing then this is a sum of positive semidefinite rank one matrices, in which case the rank of \( \mathcal{M}(m) \) will equal \( k \), but if the values \( y_{i+1} - y_i \) have different signs, this might not be the case. Regardless, this suggests the following approach.

**Question 5** Given \((m_a)_{a \in A} \in M(A)\), when does the following low-rank matrix completion find the minimum \( k \) for which \((m_a)_{a \in A} \) belongs to \( M_k(A) \)?

\[
\text{Minimize } \text{rank}(\mathcal{M}(m)) \text{ such that } A(m) \succeq 0, B(m) \succeq 0.
\]

Here, \( A \) and \( B \) are the matrices introduced in Theorem 17 and the minimization is taken over all \( m \in \mathbb{R}^{\lfloor 0, 1, \ldots, \max(A) \rfloor} \) for which \( m_a = m_a \) for all \( a \in A \).

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