A Tutorial on Multivariate $k$-Statistics and their Computation

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Abstract

This document aims to provide an accessible tutorial on the unbiased estimation of multivariate cumulants, using $k$-statistics. We offer an explicit and general formula for multivariate $k$-statistics of arbitrary order. We also prove that the $k$-statistics are unbiased, using Möbius inversion and rudimentary combinatorics. Many detailed examples are considered throughout the paper. We conclude with a discussion of $k$-statistics computation, including the challenge of time complexity, and we examine a couple of possible avenues to improve the efficiency of this computation. The purpose of this document is threefold: to provide a clear introduction to $k$-statistics without relying on specialized tools like the umbral calculus; to construct an explicit formula for $k$-statistics that might facilitate future approximations and faster algorithms; and to serve as a companion paper to our Python library PyMoments [12], which implements this formula.

1 Introduction

Cumulants are a class of statistical moments that succinctly describe univariate and multivariate distributions. Low-order cumulants are quite familiar: first-order cumulants are means, second-order cumulants are covariances, and third-order cumulants are third central moments. But fourth-order cumulants and larger are difficult to express in terms of central or raw moments. Still, higher-order cumulants have found a variety of applications, largely because they preserve the intuition of central moments while also featuring desirable multilinearity and additivity properties. Various applications have exploited these properties to solve problems in statistics, signal processing, control theory, and other fields.

This note concerns the unbiased estimation of cumulants from data. The canonical unbiased estimators of cumulants, known as Fisher’s $k$-statistics, or more simply $k$-statistics, have been around since Fisher’s seminal work on univariate $k$-statistics in 1930 [4] and Wishart and Kendall’s later work extending them to the multivariate case (e.g., [6]). These papers provide formulas for low-order $k$-statistics, and they describe the process of symbol manipulation that can be used to construct higher-order formulas, but they stop short of an explicit, general expression for $k$-statistics. The objective of this note is to provide such an expression, as well as a self-contained derivation.

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The technical content of this paper is not really novel. We highlight the deep connection that cumulants and \( k \)-statistics have with Möbius inversion on the partition lattice, but this connection has been known since at least 1983 [13] and has been noted in subsequent work [11, 7]. The same formulas for multivariate \( k \)-statistics derived here have also been constructed through the umbral calculus [3, 9], though interpreting these formulas requires a nontrivial investment of effort into learning the umbral calculus formalism. Software packages are also available for \( k \)-statistics. \textit{MathStatica}, a proprietary \textit{Mathematica} package, provides methods for symbolic \( k \)-statistic formulas [10]. An R package, \textit{kStatistics} [8], is available to compute multivariate \( k \)-statistics of data samples. Our own library \textit{PyMoments} implements multivariate \( k \)-statistics in Python [12]. Thus, rather than providing new insight into the problem of cumulant estimation, the aim of this paper is to serve as a quick, accessible, and explicit reference for multivariate \( k \)-statistics.

We also hope this paper will invite discussion regarding the efficient computation of \( k \)-statistics. The time complexity of computing these statistics scales poorly with order, so in order to make higher-order \( k \)-statistics useful in real-world applications, it is necessary to optimize their efficiency. We briefly discuss some possible avenues toward efficient computation or approximation of these statistics, but this topic is still under-explored.

The paper is organized as follows. In the remainder of this section, we introduce the preliminary mathematical concepts that are needed to derive \( k \)-statistics, including the definition of cumulants themselves (Section 1.2) and their connection to Möbius inversion on the partition lattice (Section 1.3). Section 2 contains the main results—a definition of and explicit formula for \( k \)-statistics in terms of raw sample moments (Definition 2.1), and a proof of their unbiased estimation that reveals a derivation of these statistics (Section 2.1). The last part of the paper, Section 3, briefly discusses some points on the computational efficiency of evaluating \( k \)-statistics.

\subsection{Preliminaries}

\textbf{Multisets and Multi-indices} A multiset is a set that allows for repeated elements. There are two ways to represent a multiset. The simplest representation is explicit enumeration of the elements, e.g., \([x_1, x_2, \ldots, x_n]\), where it is possible that \( x_i = x_j \). When the universe of possible elements in the multiset is clear from context, another representation is to use a multi-index, which assigns an integer multiplicity to every element in the universe. For example, when we are considering multisets with elements drawn from \( \{1, 2, \ldots, n\} \), we can encode the multiset using a multi-index \( \alpha : \{1, 2, \ldots, n\} \to \mathbb{Z}_{\geq 0} \), where \( \alpha(i) \) is the multiplicity of \( i \) in the multiset. We will often use “multiset generator” notation to describe a multiset; for example, \([i \mod 2 \mid i \in \{1, 2, 3, 4, 5\}] = [0, 0, 1, 1, 1] \).

\textbf{Partitions} A partition of a set \( S \) is a collection of mutually disjoint subsets \( B_1, B_2, \ldots, B_k \subseteq S \), called blocks, such that \( \bigcup_{i=1}^k B_i = S \). We denote partitions as sets of blocks, e.g., \( \pi = \{B_1, B_2, \ldots, B_k\} \). The size of a partition is the number of blocks: \( |\pi| = k \). Given two partitions \( \pi, \rho \) of the same set, we say that \( \pi \) refines \( \rho \), and write \( \pi \leq \rho \), if every block in \( \pi \) is the subset of a block in \( \rho \). The partition lattice \((\Pi_n, \leq)\) is the poset of partitions of the set \( \{1, 2, \ldots, n\} \), with refinement as a partial order. Within the partition lattice, note that the unique partition with one block is the unique maximum element; similarly, the unique partition with \( n \) blocks is the unique minimum element. Figure 1 provides a visual representation of the partition lattice \( \Pi_4 \).

The number of partitions on \( \Pi_n \) with size \( |\pi| = k \) is given by \textit{Stirling’s number of the second kind},
and is given by
\[
\binom{n}{k} = \frac{1}{k!} \sum_{i=0}^{k-1} (-1)^i \binom{k}{i} (k - i)^n
\]
for positive \( n \). The total number of partitions in \( \Pi_n \) is known as Bell’s number:
\[
B_n = |\Pi_n| = \sum_{k=1}^{n} \binom{n}{k}
\]

**General Notation**  Given two non-negative integers \( k \leq n \), the falling factorial is the quantity
\[
(n)_k = n(n - 1) \cdots (n - k + 1).
\]

### 1.2 Cumulants

We begin with a formal definition of cumulants and (implicitly) a review of our notational conventions. Given a random vector \( X = (X_1, X_2, \cdots, X_n) \), where \( X_i \) are scalar random variables, define the moment generating function \( M_X : \mathbb{R}^n \to \mathbb{R} \) and the cumulant generating function \( K_X : \mathbb{R}^n \to \mathbb{R} \) by
\[
M_X(t) = \mathbb{E} \left[ e^{t^\top X} \right], \quad K_X(t) = \log M_X(t)
\]
Assuming that $M_X(t)$ and $K_X(t)$ admit Taylor expansions about $t = 0_n$, we can write

$$
M_X(t) = 1 + \sum_{i=1}^{n} m_{[i]} t_i + \frac{1}{2} \sum_{i,j=1}^{n} m_{[i,j]} t_i t_j + \sum_{i,j,k=1}^{n} m_{[i,j,k]} t_i t_j t_k + \cdots
$$

$$
K_X(t) = \sum_{i=1}^{n} \kappa_{[i]} t_i + \frac{1}{2} \sum_{i,j=1}^{n} \kappa_{[i,j]} t_i t_j + \sum_{i,j,k=1}^{n} \kappa_{[i,j,k]} t_i t_j t_k + \cdots
$$

where the coefficients $m_{\alpha}$ and $\kappa_{\alpha}$ are defined for any multiset from the indices $\{1, 2, \ldots, n\}$. The coefficients in the expansion of the moment generating function are familiar—for example, where the coefficients

$$
m_{[i,j,k]} = \frac{\partial^3 M_X(t)}{\partial t_i \partial t_j \partial t_k} \bigg|_{t=0_n} = E \left[ \frac{\partial^3}{\partial t_i \partial t_j \partial t_k} e^{t^\top X} \right] \bigg|_{t=0_n} = E [X_i X_j X_k]
$$

is a third-order raw moment. Of course, this relationship holds true in general: the coefficients $m_{\alpha}$ in the expansion of the moment generating function are precisely the raw moments of $X$.

Cumulants are defined similarly, as coefficients in the Taylor expansion of $K_X(t)$. Formally, given any multiset from $\{1, 2, \ldots, n\}$, or equivalently, given any multi-index $\alpha$ on $\{1, 2, \ldots, n\}$, we define the cumulant

$$
\kappa_{\alpha}(X) = \frac{\partial^{|\alpha|} K_X(t)}{\partial t_1^{\alpha_1} \partial t_2^{\alpha_2} \cdots \partial t_n^{\alpha_n}} \bigg|_{t=0_n}
$$

as the coefficient of the term $\frac{1}{|\alpha|} t_1^{\alpha_1} t_2^{\alpha_2} \cdots t_n^{\alpha_n}$ in the series expansion of $K_X(t)$. The order of a cumulant is the size $|\alpha|$. Low-order cumulants have familiar interpretations, as the next few examples demonstrate:

**Example 1.1** (First-Order Cumulants). Consider a single random variable $X_i$. The first-order cumulant of this variable is

$$
\kappa_{[i]}(X) = \frac{\partial K_X(t)}{\partial t_i} \bigg|_{t=0_n} = \frac{1}{M_X(t)} \frac{\partial M_X(t)}{\partial t_i} \bigg|_{t=0_n} = m_{[i]} = E[X_i]
$$

Thus, first-order cumulants are identical to first-order raw moments, i.e., means. △

**Example 1.2** (Second-Order Cumulants). Consider a pair of random variables $X_i, X_j$, possibly repeating. The second-order cumulant of this pair of variables is

$$
\kappa_{[i,j]}(X) = \frac{\partial^2 K_X(t)}{\partial t_i \partial t_j} \bigg|_{t=0_n} = \frac{1}{M_X(t)} \frac{\partial^2 M_X(t)}{\partial t_i \partial t_j} - \frac{1}{M_X(t)^2} \frac{\partial M_X(t)}{\partial t_i} \frac{\partial M_X(t)}{\partial t_j} \bigg|_{t=0_n} = m_{[i,j]} - m_{[i]} m_{[j]}
$$

Thus, second-order cumulants are identical to covariances. △
Example 1.3 (Third-Order Cumulants). Consider a triple of random variables $X_i, X_j, X_k$, possibly repeating. After evaluating and simplifying the appropriate third derivative, we find that

$$\kappa_{[i,j,k]}(X) = \left. \frac{\partial^3 K_X(t)}{\partial t_i \partial t_j \partial t_k} \right|_{t=0} = 2m_{[i]}m_{[j]}m_{[k]} - m_{[i]}m_{[j]} - m_{[j]}m_{[i,k]} - m_{[i]k} + m_{[i,j,k]}$$

In particular, if $X_i = X_j = X_k$, we obtain the third univariate cumulant of the random variable $X_i$:

$$\kappa_{[i,i,i]}(X) = 2\mathbb{E}[X_i^3] - 3\mathbb{E}[X_i]\mathbb{E}[X_i^2] + \mathbb{E}[X_i^3]$$

$$= \mathbb{E}[(X_i - \mathbb{E}[X_i])^3]$$

$$= \text{var}(X_i)^{3/2}\text{skew}(X_i)$$

where skew(·) is the moment coefficient of skewness. In other words, third univariate cumulants are identical to third central moments, thereby quantifying the skewness of a distribution.

1.3 Cumulants, Raw Moments, and Möbius Inversion

As the previous three examples suggest, cumulants and raw moments are closely related—after all, cumulants and raw moments are the series coefficients of functions related by a log transform. High-order derivatives of the logarithm result in an abundance of terms, which rapidly get out of hand when trying to derive high-order cumulants manually. Fortunately, by invoking the multivariate version of Faà di Bruno’s formula, we can use some powerful ideas from combinatorics to compactly represent these computations. This subsection will reveal a general formula for expression cumulants in terms of raw moments, which will prove useful in our later derivation of $k$-statistics.

It is a bit simpler to start in the reverse direction, writing raw moments in terms of cumulants, and then using Möbius inversion to obtain our desired expressions. Writing raw moments in terms of cumulants is really a straightforward application of Faà di Bruno’s generalization of the chain rule:

Lemma 1.4 (Faà di Bruno’s Formula). Let $n$ and $k$ be positive integers, and let $f : \mathbb{R} \to \mathbb{R}$ and $g : \mathbb{R}^k \to \mathbb{R}$ be a pair of functions that are differentiable to order $n$. Then

$$\frac{\partial^n f(g(x))}{\partial x_1 \partial x_2 \cdots \partial x_n} = \sum_{\pi \in \Pi_n} f(|\pi|)(g(x)) \prod_{B \in \pi} \prod_{i \in B} \frac{\partial |B| g(x)}{\partial x_i}$$

where $f^{(j)}(\cdot)$ denotes the $j$th derivative, $\pi$ loops through every partition of the set $\{1, 2, \ldots, n\}$, $B$ loops through each block in a given partition, and $i$ loops through each element of $\{1, 2, \ldots, n\}$ contained within a given block.

See [5] for an overview and proof of this formula (as well as a different discussion of the application we are about to see). Equation (1.2) is an entrypoint that will allow us to apply the combinatorics of the partition lattice to the study of cumulants.

In order to write raw moments in terms of cumulants, we can express $M_X(t) = f(g(t))$, where
\[f(\cdot) = \exp(\cdot) \text{ and } g(t) = K_X(t).\] Therefore, applying (1.2), we obtain

\[
m_{[i_1, i_2, \ldots, i_k]} = \frac{\partial^n e^{K_X(t)}}{\partial t_{i_1} \partial t_{i_2} \cdots \partial t_{i_k}} \bigg|_{t=0} = \sum_{\pi \in \Pi_k} \frac{d\exp(y)}{dy} \bigg|_{y=K_X(0)} \left( \prod_{B \in \pi} \frac{\partial^{|B|} K_X(t)}{\prod_{j \in B} \partial t_j} \bigg|_{t=0} \right)\]

\[
= \sum_{\pi \in \Pi_k} \prod_{B \in \pi} \frac{\partial^{|B|} K_X(t)}{\prod_{j \in B} \partial t_j} \bigg|_{t=0}
\]

We recognize the inner derivative as a cumulant of the random vector \(X = (X_1, X_2, \ldots, X_n)\), in particular, the cumulant corresponding to the multiset of indices \([i_j | j \in B]\). Therefore, simplifying this equation, we can express the raw moment in terms of cumulants, as follows:

\[
m_{[i_1, i_2, \ldots, i_k]} = \sum_{\pi \in \Pi_k} \prod_{B \in \pi} \kappa_{[i_j | j \in B]} 
\] (1.3)

Let us consider some small examples of this formula:

**Example 1.5** (Low-Order Raw Moments). Let us consider how to construct first-order and second-order raw moments from cumulants. Given any particular random variable \(X_i\) from the vector \(X = (X_1, X_2, \ldots, X_n)\), we know that \(m_{[i]} = \kappa_{[i]}\), either by applying (1.3) or recalling Example 1.1. Next, given a pair of (possibly identical) random variables \(X_{i_1}, X_{i_2}\) from the vector, we use (1.3) to compute

\[
m_{[i_1, i_2]} = \sum_{\pi \in \Pi_2} \prod_{B \in \pi} \kappa_{[i_j | j \in B]} = \prod_{B \in \{\{1\}, \{2\}\}} \kappa_{[i_j | j \in B]} + \prod_{B \in \{\{1,2\}\}} \kappa_{[i_j | j \in B]} = \kappa_{[i_1]} \kappa_{[i_2]} + \kappa_{[i_1, i_2]}
\]

Combining these two results, we see that

\[
\kappa_{[i_1, i_2]} = m_{[i_1, i_2]} - \kappa_{[i_1]} \kappa_{[i_2]} = m_{[i_1, i_2]} - m_{[i_1]} m_{[i_2]} = \text{cov}(X_{i_1}, X_{i_2})
\]

replicating our conclusion from Example 1.2. △

This example hints at the possibility of inverting (1.3) to express cumulants as functions of central moments. It turns out that stating a general formula for this inversion is straightforward, thanks to Möbius inversion. The general topic of Möbius inversion on posets is beyond the scope of this note, but many good lecture notes are available online for an easy introduction (for example, [2]), or the reader may refer to a text like Aigner [1] for a more detailed and rigorous discussion. Fortunately, Möbius inversion on the partition lattice is a standard example in this area of combinatorics, so we can cut to the chase and state the needed result:

**Lemma 1.6** (Möbius Inversion on the Partition Lattice: Part I). Consider two functions \(f, g : \Pi_n \to \mathbb{R}\). The following are equivalent:

\[(i) \quad f(\pi) = \sum_{\rho \leq \pi} g(\rho), \quad \forall \pi \in \Pi_n \] (1.4)
\[
g(\pi) = \sum_{\rho \leq \pi} (-1)^{|\rho|-1}(|\rho| - 1)! f(\rho), \quad \forall \pi \in \Pi_k \tag{1.5}
\]

Lemma 1.6 provides a handy formula to invert sums over refinements of a given element of the partition lattice. While not immediately obvious, Lemma 1.6 can be used to invert (1.3), leading to the following result:

**Theorem 1.7 (Cumulants from Raw Moments).** Consider the raw moments \(m\) and cumulants \(\kappa\) of a random vector \(X = (X_1 \; X_2 \; \cdots \; X_n)\). For any multiset \([i_1, i_2, \ldots, i_k]\) from the indices \(\{1, 2, \ldots, n\}\), the corresponding cumulant can be expressed in terms of the raw moments by

\[
\kappa_{[i_1, i_2, \ldots, i_k]} = \sum_{\pi \in \Pi_k} (-1)^{|\pi|-1}(|\pi| - 1)! \prod_{B \in \pi} m_{[i_j \mid j \in B]} \tag{1.6}
\]

**Proof.** Define two maps \(f_k, g_k : \Pi_k \to \mathbb{R}\) by

\[
g_k(\pi) = \prod_{B \in \pi} \kappa_{[i_j \mid j \in B]}
\]

and

\[
f_k(\pi) = \prod_{B \in \pi} m_{[i_j \mid j \in B]}
\]

Let \(\hat{1}_k = \{1, 2, \ldots, k\}\) be the maximum partition in \(\Pi_k\). Then (1.3) can be re-written \(f_k(\hat{1}_k) = \sum_{\rho \leq \hat{1}_k} g_k(\rho)\), since the set \(\Pi_k\) is precisely the set of refinements of \(\hat{1}_k\). In fact, this is enough to conclude that \(f_k(\pi) = \sum_{\rho \leq \pi} g_k(\rho)\) for all \(\pi \in \Pi_k\). This is because we can write

\[
f_k(\pi) = \prod_{B \in \pi} f_B(\hat{1}_B)
\]

where \(\hat{1}_B\) is the maximum element of the lattice of partitions of \(B\), and \(f_B\) is defined similar to \(f_k\), but on the elements of \(B\) instead of \(\{1, 2, \ldots, k\}\). Invoking (1.3), we have that \(f_B(\hat{1}_B) = \sum_{\rho_B \leq \hat{1}_B} g_B(\rho_B)\) (where \(g_B\) is defined similar to \(g_k\)), so that

\[
f_k(\pi) = \prod_{B \in \pi} \sum_{\rho_B \leq \hat{1}_B} g_B(\rho_B) = \sum_{\rho_1 \leq \hat{1}_B} \sum_{\rho_2 \leq \hat{1}_B} \cdots \sum_{\rho_{|\pi|} \leq \hat{1}_B} \prod_{B \in \pi} g_B(\rho_B) = \sum_{\rho \leq \pi} g_k(\rho)
\]

since the set of all tuples of refinements \((\rho_1, \rho_2, \ldots, \rho_{|\pi|})\) is isomorphic to the product of lattices \(\Pi_{|\pi|} \cdots \Pi_{|\pi|}\), which is itself isomorphic to the set of all refinements of \(\pi\). Thus \(f_k\) and \(g_k\) satisfy (1.4), so we invoke the M\"{o}bius inversion in Lemma 1.6 to obtain (1.5). In particular, evaluating (1.5) on \(\hat{1}_k\), we obtain

\[
g_k(\hat{1}_k) = \sum_{\rho \leq \hat{1}_k} (-1)^{|\rho|-1}(|\rho| - 1)! f_k(\rho)
\]

\[
= \sum_{\rho \in \Pi_k} (-1)^{|\rho|-1}(|\rho| - 1)! \prod_{B \in \pi} m_{[i_j \mid j \in B]}
\]

But \(g_k(\hat{1}_k) = \kappa_{[i_1, i_2, \ldots, i_k]}\), so we obtain (1.6). \(\square\)
2 Multivariate $k$-Statistics

Now that we have examined multivariate cumulants, our next challenge is to estimate them from a sample. Once again, suppose that we have a random vector $X = (X_1, X_2, \cdots, X_n)^\top$, distributed according to some joint distribution $F$. Further suppose that, instead of knowing $F$, all we have is an i.i.d. sample $x_1, x_2, \ldots, x_N$ from this distribution, where $x_t \in \mathbb{R}^n$. We would like to estimate the cumulants of $X$ using some statistic, i.e., some function of the data $x_1, x_2, \ldots, x_N$.

It turns out that we can obtain an unbiased estimate of each cumulant using raw sample moments. For each multiset $[i_1, i_2, \ldots, i_k]$ of the indices $\{1, 2, \ldots, n\}$, the corresponding raw sample moment is the statistic given by

$$
\hat{m}_{[i_1, i_2, \ldots, i_k]} = \frac{1}{N} \sum_{t=1}^{N} x_{t,i_1} x_{t,i_2} \cdots x_{t,i_k} \tag{2.1}
$$

Because the observations in the sample are independent, $\hat{m}_{[i_1, i_2, \ldots, i_k]}$ is an unbiased estimator for the raw moment $m_{[i_1, i_2, \ldots, i_k]}$. Furthermore, we can use raw sample moments to obtain an unbiased estimates of cumulants:

**Definition 2.1 ($k$-Statistic).** Consider the random vector $X = (X_1, X_2, \cdots, X_n)^\top$ and some multiset $[i_1, i_2, \ldots, i_k]$ from the indices $\{1, 2, \ldots, n\}$. Given a sample of $X$ with at least $N \geq k$ observations, the corresponding $k$-statistic is given by

$$
k_{[i_1, i_2, \ldots, i_k]} = \sum_{\pi \in \Pi_k} (-1)^{|\pi|-1} c_\pi \prod_{B \in \pi} \hat{m}_{[j \in B]} \tag{2.2}
$$

where we define a positive coefficient for each partition in $\Pi_k$ by

$$
c_\pi = N^{|\pi|} \sum_{B_1} \sum_{B_2} \cdots \sum_{B_{|\pi|}} \frac{(\sum_{j=1}^{|\pi|} b_j - 1)!}{(N)^{\sum_{j=1}^{|\pi|} b_j}} \left( \prod_{j=1}^{|\pi|} \binom{|B_j|}{b_j} (b_j - 1)! \right), \quad \forall \pi \in \Pi_k \tag{2.3}
$$

and $B_1, B_2, \ldots, B_{|\pi|}$ are the blocks of the partition $\pi$. \(\triangle\)

Equation (2.2) is a linear combination of products of raw sample moments (which are computed from the data). The linear combination itself involves a sum over the partition lattice with coefficients of alternating sign, which hints at Möbius inversion. Indeed, we can derive the $k$-statistic by using Möbius inversion to correct the bias of products of raw sample moments. We provide a much more detailed derivation in the next section, when we prove that $k$-statistics are unbiased:

**Theorem 2.2 ($k$-Statistics are Unbiased Estimators of Cumulants).** Consider the random vector $X = (X_1, X_2, \cdots, X_n)^\top$, and let $[i_1, i_2, \ldots, i_k]$ be any multiset of the indices $\{1, 2, \ldots, n\}$. The $k$-statistic computed from any i.i.d. sample of $X$ with at least $k$ observations is an unbiased estimator of the cumulant, i.e.,

$$
\mathbb{E} [k_{[i_1, i_2, \ldots, i_k]}] = \kappa_{[i_1, i_2, \ldots, i_k]}
$$

First, we will consider some lower-order examples of multivariate $k$-statistics.
Example 2.3 (First-Order $k$-Statistics). The partition lattice $\Pi_1$ consists of only one element $\{\{1\}\}$, so first-order $k$-statistics are easily computed as

$$k_{[i]} = c_{\{1\}} \hat{m}_{[i]} = \hat{m}_{[i]}$$

Thus, as expected from Example 1.1, first-order $k$-statistics are merely sample means. △

Example 2.4 (Second-Order $k$-Statistics). The partition lattice $\Pi_2$ consists of two elements: $\{\{1, 2\}\}$, and $\{\{1\}, \{2\}\}$. The corresponding coefficients are

$$c_{12} = N^1 \left( \frac{(0)!}{(N)_1} \left\{ \begin{array}{c} 3 \\ 1 \end{array} \right\} (0)! + \frac{(1)!}{(N)_2} \left\{ \begin{array}{c} 2 \\ 1 \end{array} \right\} (1)! \right) = 1 + \frac{1}{N - 1} = \frac{N}{N - 1}$$

and

$$c_{1|2} = N^2 \left( \frac{(1)!}{(N)_2} \left\{ \begin{array}{c} 1 \\ 1 \end{array} \right\} \left\{ \begin{array}{c} 1 \\ 1 \end{array} \right\} (0)!(0)! \right) = \frac{N^2}{N(N - 1)} = \frac{N}{N - 1}$$

Therefore

$$k_{[1, i]} = \frac{N}{N - 1} (\hat{m}_{[1, i]} + \hat{m}_{[1]} \hat{m}_{[i]})$$

which we recognize as the classical unbiased estimator for covariance. Of course, this is exactly what we should expect after Example 1.2. △

Example 2.5 (Third-Order $k$-Statistics). The partition lattice $\Pi_3$ has five elements: $\{\{1, 2, 3\}\}$, $\{\{1\}, \{2, 3\}\}$, $\{\{2\}, \{1, 3\}\}$, $\{\{3\}, \{1, 2\}\}$, and $\{\{1\}, \{2\}, \{3\}\}$. We first compute the respective coefficients $c_{123}, c_{1[23]}$, $c_{2[13]}$, $c_{3[12]}$, and $c_{1|2|3}$:

$$c_{123} = N^1 \left( \frac{(0)!}{(N)_1} \left\{ \begin{array}{c} 3 \\ 1 \end{array} \right\} (0)! + \frac{(1)!}{(N)_2} \left\{ \begin{array}{c} 3 \\ 2 \end{array} \right\} (1)! + \frac{(2)!}{(N)_3} \left\{ \begin{array}{c} 3 \\ 3 \end{array} \right\} (2)! \right) = 1 + \frac{3}{N - 1} + \frac{4}{(N - 1)(N - 2)}$$

$$c_{1[23]} = N^2 \left( \frac{(1)!}{(N)_2} \left\{ \begin{array}{c} 1 \\ 1 \end{array} \right\} \left\{ \begin{array}{c} 2 \\ 1 \end{array} \right\} (0)!(0)! \right) = \frac{N}{N - 1} + \frac{2N}{(N - 1)(N - 2)}$$

$$c_{1|2|3} = N^3 \left( \frac{(2)!}{(N)_3} \left\{ \begin{array}{c} 1 \\ 1 \end{array} \right\} \left\{ \begin{array}{c} 1 \\ 1 \end{array} \right\} \left\{ \begin{array}{c} 1 \\ 1 \end{array} \right\} (0)!(0)!(0)! \right) = \frac{2N^2}{(N - 1)(N - 2)}$$

Note that $c_{ij}$ depends only on the number and size of each block, and not the blocks themselves, so $c_{1|23} = c_{2[13]} = c_{3[12]}$. Substituting these coefficients into (2.2) and simplifying, we obtain

$$k_{[i_1, i_2, i_3]} = c_{123} \hat{m}_{[i_1, i_2, i_3]} + c_{1[23]} (\hat{m}_{[i_1]} \hat{m}_{[i_2, i_3]} + \hat{m}_{[i_2]} \hat{m}_{[i_1, i_3]} + \hat{m}_{[i_1]} \hat{m}_{[i_2, i_3]}) + c_{1|2|3} \hat{m}_{[i_1]} \hat{m}_{[i_2]} \hat{m}_{[i_3]}$$

$$= \frac{N^2}{(N - 1)(N - 2)} (\hat{m}_{[i_1, i_2, i_3]} - \hat{m}_{[i_1]} \hat{m}_{[i_2, i_3]} - \hat{m}_{[i_2]} \hat{m}_{[i_1, i_3]} - \hat{m}_{[i_1]} \hat{m}_{[i_2, i_3]} + 2\hat{m}_{[i_1]} \hat{m}_{[i_2]} \hat{m}_{[i_3]})$$

In particular, if $X_{i_1} = X_{i_2} = X_{i_3}$, we obtain the third univariate $k$-statistic

$$k_{[i, i, i]} = \frac{N^2}{(N - 1)(N - 2)} \left( \hat{m}_{[i, i, i]} - 3\hat{m}_{[i]} \hat{m}_{[i, i]} + \hat{m}_{[i]}^3 \right)$$

△
2.1 Proof of Theorem 2.2

The general outline of the proof is as follows. We will first note that, while raw sample moments are unbiased estimators of raw moments, it is still the case that products of raw sample moments provide biased estimates for products of raw moments. The first step will be to quantify this bias. Second, we will once again use Möbius inversion over the partition lattice to obtain an unbiased estimator of products of raw moments, in terms of products of raw sample moments. Finally, we will substitute this estimator into (1.6) and simplify.

We begin by examining the expected value of raw sample moments:

**Lemma 2.6** (Bias of Products of Raw Sample Moments). Consider the random vector \( X = (X_1, X_2, \cdots, X_n)^\top \), and consider some multiset \([i_1, i_2, \ldots, i_k]\) from the indices \(\{1, 2, \ldots, n\}\). For every \(\pi \in \Pi_k\), we have

\[
\mathbb{E} \left[ \prod_{B \in \pi} \hat{m}_{[i_j | j \in B]} \right] = \frac{1}{N^{|\pi|}} \sum_{\rho \geq \pi} (N)^{|\rho|} \prod_{C \in \rho} m_{[i_j | j \in C]} \tag{2.4}
\]

**Proof.** Our first step is to switch the order of sums and products, as follows:

\[
\mathbb{E} \left[ \prod_{B \in \pi} \hat{m}_{[i_j | j \in B]} \right] = \frac{1}{N^{|\pi|}} \mathbb{E} \left[ \prod_{B \in \pi} \sum_{t=1}^N \prod_{j \in B} x_{t,j} \right] = \frac{1}{N^{|\pi|}} \sum_{t_1=1}^N \sum_{t_2=1}^N \cdots \sum_{t_{|\pi|}=1}^N \mathbb{E} \left[ \prod_{j=1}^{|\pi|} \prod_{\ell \in B_j} x_{j,\ell} \right]
\]

Note that the inner expectation depends on which of the observations \(t_1, t_2, \ldots, t_{|\pi|}\) are identical, since observations at distinct times are independent, allowing us to factor the expected value. With this in mind, we will partition the hypercube of \(t\)-indices that we are summing over into equivalence classes, based on partitions of the set \(\{1, 2, \ldots, |\pi|\}\). Given such a partition \(\sigma = \{C_1, C_2, \ldots, C_{|\sigma|}\}\), we define the equivalence class \([\sigma]\) as the set of index tuples \((t_1, t_2, \ldots, t_{|\pi|})\) with the following property: for all \(i, j \in \{1, 2, \ldots, |\pi|\}\), we have that \(t_i = t_j\) if and only if \(i, j \in C\) for some block \(C \in \sigma\). In other words, the blocks of \(\sigma\) represent elements of the \(t\)-index that are identical. Clearly each of the \(N^{|\pi|}\) index tuples in the sum belong to some equivalence class \([\sigma]\). Furthermore, each equivalence class contains \((N)^{|\sigma|}\) elements: \(N\) possible values for indices in the first block, \(N - 1\) possible values in the second block, and so on.

For all \((t_1, t_2, \ldots, t_{|\pi|}) \in [\sigma]\), we have the following property:

\[
\mathbb{E} \left[ \prod_{j=1}^{|\pi|} \prod_{\ell \in B_j} x_{j,\ell} \right] = \prod_{C \in \sigma} \mathbb{E} \left[ \prod_{j \in C} \prod_{\ell \in B_j} X_{j,\ell} \right] = \prod_{C \in \sigma} \mathbb{E} \left[ \prod_{\ell \in \bigcup_{j \in C} B_j} X_{\ell} \right] = \prod_{C \in \sigma} m_{[i_j | \ell \in \bigcup_{j \in C} B_j]}
\]

This follows because the expected value factors along the blocks of \(\sigma\), since the blocks have pairwise-distinct times, and thus the observations in each block are pairwise independent. Then we can write

\[
\mathbb{E} \left[ \prod_{B \in \pi} \hat{m}_{[i_j | j \in B]} \right] = \frac{1}{N^{|\pi|}} \sum_{\sigma \in \Pi_{|\pi|}} (N)^{|\sigma|} \prod_{C \in \sigma} m_{[i_j | \ell \in \bigcup_{j \in C} B_j]} \prod_{B \in \pi}
\]
The final step is to note that there is a bijection between partitions of \( \{1,2,\ldots,|\pi|\} \) and partitions of \( \{1,2,\ldots,k\} \) that are coarser than \( \pi \). This bijection is easy to see: for each block \( C \in \sigma \), replace all of the blocks in \( \pi \) with coarser blocks \( \bigcup_{j \in C} B_j \), resulting in a coarser partition \( \rho \geq \pi \). Due to this bijection, we can re-write the sum over \( \sigma \) as a sum over coarser partitions \( \rho \geq \pi \), obtaining (2.4). \( \square \)

Equation (2.4) has a somewhat familiar form—a sum over partitions that are coarser than \( \pi \). Recall from the proof of Theorem 1.7 that we used Möbius inversion to invert a sum over partitions that refine \( \pi \). While the direction of the sum makes a difference—we cannot use Lemma 1.6 in this case—the partition lattice still admits a Möbius inversion formula to invert (2.4). Once again, we will state the needed formula here, and direct the interested reader to a combinatorics text like [1]:

**Lemma 2.7** (Möbius Inversion on the Partition Lattice: Part II). Consider two functions \( f, g : \Pi_n \to \mathbb{R} \). For two partitions \( \pi \leq \rho \in \Pi_n \), let \( \Sigma(\pi, \rho) \) denote the set of \( \rho \) partitions that, when applied to the blocks of \( \rho \), yield the refinement \( \pi \). Then the following are equivalent:

\[(i) \quad f(\pi) = \sum_{\rho \geq \pi} g(\rho), \quad \forall \pi \in \Pi_n \quad (2.5)\]

\[(ii) \quad g(\pi) = \sum_{\rho \geq \pi} \left( (-1)^{|\pi|-|\rho|} \prod_{\sigma \in \Sigma(\pi, \rho)} (|\sigma| - 1)! \right) f(\rho), \quad \forall \pi \in \Pi_n \quad (2.6)\]

The set \( \Sigma(\pi, \rho) \) may cause some confusion, so it is worth considering an example before we proceed. Consider two partitions of \( \Pi_5 \): \( \pi = \{\{1\}, \{2\}, \{4\}, \{3,5\}\} \), and \( \rho = \{\{1,2,3,5\}, \{4\}\} \). Clearly \( \pi \) is a refinement of \( \rho \). Furthermore, we can obtain \( \pi \) from \( \rho \) by partitioning each block of \( \rho \). Let \( \sigma_1 \) represent the partition of \( \{1,2,3,5\} \) into \( \{\{1\}, \{2\}, \{3,5\}\} \), and let \( \sigma_2 \) be the partition of \( \{4\} \) into \( \{\{4\}\} \). The set \( \Sigma(\pi, \rho) = \{\sigma_1, \sigma_2\} \) is the collection of these two partitions.

Next, we apply this new Möbius inversion formula to invert (2.4), obtaining an unbiased estimator for products of sample moments:

**Lemma 2.8** (Unbiased Estimation of Products of Sample Moments). Consider the random vector \( X = (X_1 \ X_2 \ \cdots \ X_n) \top \), and consider some multiset \( [i_1, i_2, \ldots, i_k] \) from the indices \( \{1,2,\ldots,n\} \). For every \( \pi \in \Pi_k \), define a statistic

\[
\hat{m}_\pi = \frac{1}{(N)^{|\pi|}} \sum_{\rho \geq \pi} \left( -1 \right)^{|\pi|-|\rho|} N^{|\rho|} \prod_{\sigma \in \Sigma(\rho, \pi)} (|\sigma| - 1)! \prod_{C \in \rho} \hat{m}_{[i_j | j \in C]} \quad (2.7)
\]

where \( B_1, B_2, \ldots, B_{|\pi|} \) are the blocks of \( \pi \). Then \( \hat{m}_\pi \) is an unbiased estimator of the product of raw moments \( \prod_{B \in \pi} m_{[i_j | \in B]} \), i.e.,

\[
\mathbb{E}[\hat{m}_\pi] = \prod_{B \in \pi} m_{[i_j | \in B]} \quad (2.8)
\]
Proof. Let us define two functions \( f, g : \Pi_k \to \mathbb{R} \) by

\[
    f(\pi) = N^{\vert\pi\vert} \mathbb{E} \left[ \prod_{B \in \pi} \hat{m}_{i[j \in B]} \right]
\]

\[
    g(\pi) = (N)^{\vert\pi\vert} \prod_{B \in \pi} m_{i[j \in B]}
\]

In terms of these functions, Lemma 2.6 states that

\[
    f(\pi) = \sum_{\rho \geq \pi} g(\rho), \quad \forall \pi \in \Pi_k
\]

Therefore, applying the Möbius inversion in Lemma 2.7, we obtain (2.6). Substituting in the definitions of \( f \) and \( g \) yields

\[
    (N)^{\vert\pi\vert} \prod_{B \in \pi} m_{i[j \in B]} = \sum_{\rho \geq \pi} (-1)^{\vert\pi\vert - \vert\rho\vert} \mathbb{E} \left[ \prod_{\sigma \in \Sigma(\rho, \pi)} \left( \left( \frac{\left( -1 \right)^{\vert\sigma\vert - 1} N^{\vert\sigma\vert} \prod_{\sigma \in \Sigma(\rho, \pi)} \left( \left|\sigma\right| - 1\right)! \hat{m}_{i[j \in C]} \right) \right) \right]
\]

for all \( \pi \in \Pi_k \), from which we immediately conclude (2.8).

We can now, at long last, use Lemma 2.8 to prove that \( k \)-statistics are unbiased estimators for cumulants.

Proof (Theorem 2.2). Substituting (2.8) into (1.6), we see that Theorem 2.8 and Lemma 1.7 together imply that

\[
    \mathbb{E} \left[ \sum_{\pi \in \Pi_k} (-1)^{\vert\pi\vert - 1} \hat{m}_\pi \right] = \kappa_{[i_1, i_2, \ldots, i_k]}
\]

Expanding \( \hat{m}_\pi \) using its definition (2.7), we obtain

\[
    Q \triangleq \mathbb{E} \left[ \sum_{\pi \in \Pi_k} \frac{(-1)^{\vert\pi\vert - 1} (\vert\pi\vert - 1)!}{(N)^{\vert\pi\vert}} \sum_{\rho \geq \pi} (-1)^{\vert\pi\vert - \vert\rho\vert} N^{\vert\rho\vert} \prod_{\sigma \in \Sigma(\rho, \pi)} \left( \left|\sigma\right| - 1\right)! \hat{m}_{i[j \in C]} \right] = \kappa_{[i_1, i_2, \ldots, i_k]}
\]

where we have defined \( Q \) as a placeholder for the expected value, for notational compactness. The remainder of the proof is to simplify \( Q \) down to \( k_{[i_1, i_2, \ldots, i_k]} \) in (2.2).
The first thing to do is manipulate the sum, as follows:

\[
Q \triangleq \sum_{\pi \in \Pi_k} \sum_{\rho \geq \pi} \frac{(-1)^{\rho-1}(|\pi|-1)!N^{\rho}}{(N)^{|\pi|}} \left( \prod_{\sigma \in \Sigma(\rho, \pi)} \frac{(|\sigma|-1)!}{(N)^{|\sigma|}} \right) \prod_{C \in \rho} \hat{m}_{[i,j] \in C}
\]

\[
= \sum_{\rho \in \Pi_k} \sum_{\pi \leq \rho} \frac{(-1)^{\rho-1}(|\pi|-1)!N^{\rho}}{(N)^{|\pi|}} \left( \prod_{\sigma \in \Sigma(\rho, \pi)} \frac{(|\sigma|-1)!}{(N)^{|\sigma|}} \right) \prod_{C \in \rho} \hat{m}_{[i,j] \in C}
\]

\[
= \sum_{\rho \in \Pi_k} (-1)^{\rho-1}N^\rho \left( \sum_{\pi \leq \rho} \frac{(|\pi|-1)!}{(N)^{|\pi|}} \prod_{\sigma \in \Sigma(\rho, \pi)} \frac{(|\sigma|-1)!}{(N)^{|\sigma|}} \right) \prod_{C \in \rho} \hat{m}_{[i,j] \in C}
\]

Because the refinements of \( \rho \) are isomorphic to the product of lattices \( \Pi_{|C_1|} \times \Pi_{|C_2|} \times \cdots \times \Pi_{|C_\rho|} \) (where each of the lattices corresponds to the partitions of a block of \( \rho \)), we can replace the sum over \( \rho \leq \rho \) with a sum over tuples of partitions in this product:

\[
R \triangleq \sum_{\pi \leq \rho} \frac{(|\pi|-1)!}{(N)^{|\pi|}} \prod_{\sigma \in \Sigma(\rho, \pi)} (|\sigma|-1)! = \sum_{\sigma_1 \in \Pi_{|C_1|}} \sum_{\sigma_2 \in \Pi_{|C_2|}} \cdots \sum_{\sigma_\rho \in \Pi_{|C_\rho|}} \frac{\prod_{j=1}^{\rho} (\sum_{j=1}^{\rho} |\sigma_j|-1)!}{(N)^{\sum_{j=1}^{\rho} |\sigma_j|}} \prod_{j=1}^{\rho} (|\sigma_j|-1)!
\]

Here \( R \) is another placeholder for the middle term of this equation. Now, observe that the dependence of this sum on \( \sigma_j \) is entirely through the size of \( \sigma_j \). Furthermore, for a given size \( b_j = |\sigma_j| \), there are \( \binom{|C_j|}{b_j} \) partitions of size \( b_j \) in \( \Pi_{|C_j|} \). Therefore, we simplify

\[
R = \sum_{b_1=1}^{|C_1|} \sum_{b_2=1}^{|C_2|} \cdots \sum_{b_\rho=1}^{|C_\rho|} \frac{\prod_{j=1}^{\rho} (\binom{|C_j|}{b_j}) (b_j-1)!}{(N)^{\sum_{j=1}^{\rho} b_j}} = \frac{c_\rho}{N^\rho}
\]

invoking the definition of \( c_\rho \) from (2.3). Replacing \( R \) with the right side of this equation in our last expression for \( Q \), we obtain

\[
Q = \sum_{\rho \in \Pi_k} (-1)^{\rho-1}c_\rho \prod_{C \in \rho} \hat{m}_{[i,j] \in C} = k_{[i_1, i_2, \ldots, i_k]}
\]

which completes the proof. \( \square \)

### 3 Computational Notes

We will end our discussion of \( k \)-statistics with some comments on their computation. The core of (2.2) is a for loop over the elements of \( \Pi_k \), the cardinality of which is given by Bell’s number, \( B_k \). The left plot in Figure 2 shows how Bell’s number scales with \( k \). At \( k = 5 \), the for loop only needs to process 52 iterations, fast enough to perform repeated estimation within a bootstrapping scheme, for example. By \( k = 10 \), the for loop must process almost 116,000 iterations—under a minute on a modern laptop, but certainly long enough to make many repeated calculations cumbersome. By \( k = 20 \), we are up to roughly the number of cells in the human body. Roughly speaking, fifth-order \( k \)-statistics are about as
In order to make higher-order \( k \)-statistics more useful, a reasonable truncation of the sum in (2.2) would be highly desirable. One possible approach is to examine the formula in the large \( N \) limit. Looking at (2.3) as \( N \to \infty \), we see that \( c_\pi \to (|\pi| - 1)! \) since the \( b_1 = b_2 = \cdots = b_{|\pi|} = 1 \) term of this sum dominates. Furthermore, the raw sample moment factors converge on the sample moments (i.e., \( \hat{m}_{[i,j] \in C} \to m_{[i,j] \in C} \)), which have no asymptotic dependence on \( N \). With some prior knowledge of the distribution, it may be possible to establish a hierarchy of summands \( (|\rho| - 1)! \prod_{C \in \rho} m_{[i,j] \in C} \) in the large \( N \) limit, allowing for a corresponding truncation of the sum in (2.2). Of course, this depends highly on the raw moments of the distribution, and sufficient prior knowledge of these moments may defeat the purpose of using \( k \)-statistics in the first place.

Instead of truncating the sum, another avenue to speed up the computation may be to approximate the coefficients themselves, e.g., by assuming \( c_\pi \approx (|\pi| - 1)! \) for large \( N \). However, we suggest that approximating \( c_\pi \) has little effect on the efficiency, and that a better approach is to simply cache computed values of the coefficients. The key is to observe that \( c_\pi \) depends on the number and size of each block, but not the blocks in and of themselves, so many terms of the (2.2) sum will have identical value of the coefficients. As noted by [8], the collections of block sizes in \( \Pi_k \) actually correspond to integer partitions of \( k \), so it is sufficient to compute and store one value of \( c_\pi \) per integer partition. The power of this trick lies in the fact that the number of integer partitions (called the partition number), \( p(k) \), is much smaller than Bell’s number \( B_k \), at least when \( k \) is of moderate size or larger. The right plot in Figure 2 shows how \( p(k) \) scales with \( k \) much slower than \( B_k \). For example, computing fifth-order \( k \)-statistics only requires evaluating and storing \( p(5) = 7 \) unique values of \( c_\pi \). Tenth-order \( k \)-statistics involve \( p(10) = 42 \) unique values. And \( k \)-statistics of order 20, which are intractable due to the size of \( |\Pi_{20}| \), would require only 627 unique values of the coefficients. In other words, the number of unique \( c_\pi \)

\[1\] Another problem with high-order \( k \)-statistics is statistical—the variance of the \( k \)-statistic scales poorly with order. As \( k \) increases, the necessary sample size \( N \) increases very quickly, leading to slower computation and infeasible data requirements. Variances of \( k \)-statistics are beyond the scope of this document.
values is very small compared to the size of $|\Pi_k|$, so precise evaluation and storage of these coefficients is cheap.

We also note that (2.2) is easy to vectorize, i.e., it is straightforward to evaluate $k$-statistics on several different samples simultaneously. This vectorization is useful when evaluating $k$-statistics within a resampling scheme, like jackknifing or bootstrapping. The computation is amenable to vectorization due to the simple nature of the operations involved: linear combination (after computing the $c_\pi$ coefficients), multiplication, and power sums are basic operations that are supported in most libraries for array math.

Finally, we take this moment to advertise PyMoments [12], our own Python library for computing multivariate $k$-statistics. PyMoments automatically caches the $c_\pi$ coefficients, saving them in a tree-based data structure that can be re-used between different $k$-statistic evaluations (provided that the sample size $N$ is the same). PyMoments also supports vectorized computation of $k$-statistics. Of course, we are open to feedback on how to improve this library.

4 Conclusion

This document has provided an explicit expression for multivariate $k$-statistics, allowing for unbiased estimation of multivariate cumulants. We were also able to prove the lack of bias using fairly rudimentary combinatorics, and we provided a light discussion on the computational aspect of $k$-statistics. It is our hope that readers may be able to push some of the ideas of this paper forward into new, more efficient algorithms and applications involving $k$-statistics.

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