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EXACTNESS AND ORDERING IN DISCRETE CAVALIERI SAMPLING

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ABSTRACT

We study the discrete Cavalieri estimator under systematic sampling from a finite population, which models an object represented by a finite sequence of blocks along a sampling axis. For a fixed population size and a sample size that divides it, we characterize when the estimator has zero variance, namely exactness, through an explicit balance condition that characterizes the zero-variance populations; this turns out to be a simple linear family. We then ask when exactness continues to hold if the sample size is allowed to vary within the even divisors of an even population size. In that case, we prove that exactness across all such even sample sizes necessarily implies the matched-pairs condition that is known to be sufficient at a fixed even sample size. We also derive a variance formula showing that it depends only on how much the sums over certain groups differ from their average. This leads to a concrete partitioning objective for choosing an ordering and helps explain why exact optimization quickly becomes impractical. Guided by this objective and by smooth fractionator practice, we discuss simple heuristics and show that a pairing-based ordering is exact under a simple affine model and remains stable under bounded perturbations.

Keywords: Cavalieri estimator, systematic sampling, finite populations, exactness, matched pairs, smooth fractionator, stereology.

INTRODUCTION

Systematic sampling along a fixed axis is a standard tool in stereology. Under the Cavalieri principle, volume is estimated by summing cross-sectional areas at equally spaced locations, with a random start, see Cruz-Orive and Weibel (1981); Gundersen and Jensen (1987); Baddeley and Jensen (2004). A substantial literature analyzes efficiency and variance prediction in the continuous setting under regularity assumptions, including transitive methods and related approximations, see Mattfeldt (1989); Kiêu *et al.* (1999); García-Fiñana and Cruz-Orive (2000; 2004). Departures from an ideal equidistant grid, for instance uneven spacing or missing sections, have long been discussed in stereology (Cruz-Orive, 1999). More recent work revisits these issues by linking them to variance-correction and quadrature ideas. When the realized section distances are irregular but recorded, one can still derive variance corrections for systematic sampling (Kiderlen and Dorph-Petersen, 2017). Further analyses allow the sampling locations to be genuinely non-equidistant and may include missing observations (dropouts), linking the resulting estimators to randomized Newton–Cotes type quadrature rules (Stehr and Kiderlen, 2020b;a). In addition, Cavalieri estimation can be framed as randomized quadrature for periodic kernels, yielding variance bounds that extend naturally to higher-dimensional settings (Soto Sánchez, 2025).

In many laboratory workflows, the object is first discretized into a finite ordered list of blocks or slabs, and one applies a design-based estimator to that finite population. This paper stays entirely in that discrete finite-population setting. We write N for the population size, n for the sample size, and $T = N/n$ for the systematic period. The discrete Cavalieri estimator is then a systematic estimator of the population total. Exactness, meaning zero variance over the random start, can occur in nontrivial discrete configurations. A clear stereological discussion of constructive exactness patterns, including matched pairs and Murthy–Gundersen type orderings in the smooth fractionator context, is given in Tinajero-Bravo *et al.* (2014) and Gundersen (2002), with Murthy's earlier balanced systematic ideas in Murthy (1967).

Our first goal is to make the discrete exactness mechanism explicit for a fixed sample size. We show that exactness is equivalent to a simple balance condition across the T residue classes modulo T. This yields a transparent linear characterization of the exact populations once N and n are fixed, and it complements the constructions in Tinajero-Bravo *et al.* (2014) by giving a sharp criterion for exactness under systematic sampling.

A second motivation is that, in practice, the number of sampled sections may change because of dropouts or protocol adjustments. This leads naturally to multi-scale questions, namely which populations remain exact for more than one admissible sample size. We formalize this requirement and prove that, when N is even, exactness across all even sample sizes makes the classical matched-pairs structure necessary. This clarifies the gap between exactness at one fixed sample size and exactness that persists across an even family.

Finally, when exactness is not achievable for a fixed collection of values, one wants arrangements with small variance. We derive an exact identity for the variance of the discrete Cavalieri estimator over the random start, showing that it is a scaled empirical variance of the residue-class sums. This gives a concrete objective for arrangement and places the best arrangement task inside a classical family of constrained partitioning problems (Garey and Johnson, 1979). It also explains why "smoothing" orderings help, because any rearrangement that reduces dispersion of these sums reduces the Cavalieri variance exactly. Guided by this identity and by smooth fractionator practice, we discuss simple heuristics that target the same balancing mechanism directly.

DISCRETE MODEL

Let $N \in \mathbb{N}$. A finite population is a vector

$$Y = (y_0, \ldots, y_{N-1})^\top \in \mathbb{R}^N,$$

and the target parameter is the total $Q = \sum_{i=0}^{N-1} y_i$.

Fix $N \in \mathbb{N}$ and a sample size n such that n divides N, and set $T = N/n$. Let Z be uniformly distributed on $\{0, \ldots, T-1\}$. The discrete Cavalieri (systematic) estimator of Q is

$$\widehat{Q}_n \;=\; T \sum_{k=0}^{n-1} y_{Z+kT}.$$

For each $r \in \{0, \ldots, T-1\}$, we write $\widehat{Q}_n(r)$ for the value of $\widehat{Q}_n$ when $Z = r$.

Definition 2.1. *For each $r \in \{0, \ldots, T-1\}$, define the residue class (coset) of indices*

$$I_r \;=\; \{\, r + kT \pmod N : k = 0, \ldots, n-1 \,\}.$$

Define the corresponding residue-class sum

$$S_r \;=\; \sum_{i \in I_r} y_i.$$

Lemma 2.2. *For each $r \in \{0, \ldots, T-1\}$, one has $\widehat{Q}_n(r) = T\,S_r$. Also $\sum_{r=0}^{T-1} S_r = Q$.*

Proof. If the start equals r, the sampled indices are precisely I_r, so $\widehat{Q}_n(r) = T \sum_{i \in I_r} y_i = T\,S_r$. The residue classes form a partition of $\{0, \ldots, N-1\}$, so summing the coset sums gives the population total. □

As an immediate consequence, $\widehat{Q}_n$ is unbiased. Indeed, since Z is uniform on $\{0, \ldots, T-1\}$,

$$\mathbb{E}[\widehat{Q}_n] = \frac{1}{T} \sum_{r=0}^{T-1} \widehat{Q}_n(r) = \frac{1}{T} \sum_{r=0}^{T-1} T\,S_r = Q.$$

See also Madow and Madow (1944) and Cochran (1977) for general systematic-sampling treatments in finite populations.

EXACTNESS FOR A FIXED SAMPLE SIZE

EXACTNESS AS RESIDUE-CLASS BALANCE

Definition 3.1 (Exactness)**.** *The population Y is exact if*

$$\widehat{Q}_n(r) = Q$$

for every start $r \in \{0, \ldots, T-1\}$.

Theorem 3.2 (Exactness and residue-class sums)**.** *A population $Y \in \mathbb{R}^N$ is exact if and only if*

$$S_0 = S_1 = \cdots = S_{T-1} = \frac{Q}{T}. \tag{1}$$

Proof. By Lemma 2.2, exactness is equivalent to $T\,S_r = Q$ for every r. Dividing by T yields Eq. (1). □

Theorem 3.2 provides a concrete way to interpret classical exactness mechanisms in the discrete setting. For example, the matched-pairs condition in Tinajero-Bravo *et al.* (2014) for even N and even sample sizes makes each systematic sample consist of pairs with constant sum, so the coset sums agree automatically. Murthy–Gundersen type orderings can likewise be viewed as practical ways of distributing large and small values across residue classes, often leading to small coset dispersion under monotone trends. In many stereological applications the full population is not known before sampling, but the criterion still serves as a useful benchmark and as guidance for arrangements based on auxiliary size information.

EXACTNESS SUBSPACE AND ITS DIMENSION

Beyond the exactness criterion itself, it is useful to understand how large the class of exact populations is for a given N and sample size n. The balance relations are linear equalities, so the exact populations form a linear subspace of $\mathbb{R}^N$. Making this structure explicit gives an immediate dimension count and clarifies how restrictive exactness becomes as the period T increases.

For each residue class $r \in \{0, \dots, T-1\}$, define the linear functional

$$L_r : \mathbb{R}^N \to \mathbb{R}, \qquad L_r(Y) = S_r = \sum_{i \in I_r} y_i.$$

Collecting these gives a linear map

$$L : \mathbb{R}^N \to \mathbb{R}^T, \qquad L(Y) = \big(S_0, \dots, S_{T-1}\big)^\top,$$

so $L(Y)$ is the vector of residue-class sums. Exactness means that all entries of $L(Y)$ are equal. Equivalently, all differences $S_r - S_0$ vanish. Accordingly, define the linear map $D : \mathbb{R}^T \to \mathbb{R}^{T-1}$ by

$$D(s_0, \dots, s_{T-1})^\top = \big(s_1 - s_0, \dots, s_{T-1} - s_0\big)^\top,$$

and let A be the $(T-1) \times N$ matrix representing the composition $D \circ L$.

Definition 3.3 (Exactness subspace). *Define*

$$\mathscr{E}_{N,n,T} \; = \; \{Y \in \mathbb{R}^N : AY = 0\}.$$

Proposition 3.4. *The following holds*

$$\mathscr{E}_{N,n,T} = \{Y \in \mathbb{R}^N : Y \text{ is exact}\}.$$

Proof. By construction, $AY = 0$ holds exactly when $S_r - S_0 = 0$ for every $r = 1, \dots, T-1$, that is, when all coset sums are equal. By Theorem 3.2, this is equivalent to exactness. ☐

Corollary 3.5. *The subspace $\mathscr{E}_{N,n,T}$ has codimension $T-1$ in $\mathbb{R}^N$. Equivalently,*

$$\dim \mathscr{E}_{N,n,T} = N - (T-1).$$

Proof. The linear map L is onto $\mathbb{R}^T$. Indeed, given any $s \in \mathbb{R}^T$, define Y by setting $y_{r+kT} = s_r/n$ for all r and k. Then $S_r = s_r$, so $L(Y) = s$. The difference map D is onto $\mathbb{R}^{T-1}$, since for any $d \in \mathbb{R}^{T-1}$ one may take $s_0 = 0$ and $s_r = d_r$ for $r = 1, \dots, T-1$. Therefore $\operatorname{rank}(A) = \operatorname{rank}(D \circ L) = T-1$, and $\ker(A) = \mathscr{E}_{N,n,T}$ has codimension $T-1$. ☐

This section settles the fixed-sample-size exactness question. In many protocols the intended sample size may change, so it is natural to ask which populations remain exact when n varies. We take this up next.

MULTI-SCALE EXACTNESS AND MATCHED PAIRS

In practice, the sample size is not always decided once and for all. One may plan to take n sections but end up with fewer because some sections are lost, or because the workload or the available tissue limits the number of observations. From a design-based viewpoint, it is then natural to ask for which populations the systematic Cavalieri estimator remains exact for more than one admissible sample size.

Definition 4.1 (Multi-scale exactness). *We say that a population Y is multi-scale exact over a collection of admissible sample sizes if it is exact for every n in that collection.*

Matched pairs are a classical sufficient condition for exactness when both N and n are even, and they play a central role in the discrete discussion of Tinajero-Bravo *et al.* (2014). That paper also notes that, for one fixed even sample size n, exactness may still occur without matched pairs. The next theorem shows that the situation changes when exactness is required uniformly across all even sample sizes dividing N.

Theorem 4.2. *Let $N = 2M$. Then Y is exact for every even sample size n such that $n \mid N$ if and only if there exists $\mu \in \mathbb{R}$ such that*

$$y_{k+M} + y_k \; = \; 2\mu \quad \text{for all } k \in \{0, \dots, M-1\}. \qquad (2)$$

Proof. Assume first that Y is exact for every even $n \mid N$. In particular, it is exact for $n = 2$. In that design the period is $T = M$, so each residue class contains exactly two indices, namely $I_r = \{r, r+M\}$. Therefore $S_r(Y) = y_r + y_{r+M}$. By Theorem 3.2, these two-term sums are constant in r. Denote their common value by 2μ, which yields Eq. (2).

Conversely, assume Eq. (2) holds and let n be any even divisor of N, with period $T = N/n$. Since $N = 2M$, one has $M = (n/2)T$. Fix a coset

$$I_r = \{r + kT : k = 0, \dots, n-1\}.$$

Adding M to an index in I_r amounts to adding $(n/2)T$, hence it stays within the same coset. Therefore the elements of I_r can be grouped into $n/2$ disjoint pairs of the form $(r+kT,\ r+(k+n/2)T)$, each with sum 2μ by Eq. (2). It follows that $S_r(Y) = (n/2) \cdot 2\mu = n\mu$, which does not depend on r. By Theorem 3.2, Y is exact for this n. ☐

Requiring exactness simultaneously for many sample sizes is therefore a strong constraint. For even N, Theorem 4.2 shows that exactness across all even sample sizes makes a global pairing symmetry around the mean necessary, whereas exactness at a single chosen n may still occur without it. When such symmetry is absent, exactness is no longer the right baseline, and the practical question becomes how the variance depends on the ordering of the values. The next section gives an identity that makes this dependence explicit in terms of dispersion of the residue-class sums.

VARIANCE VIA RESIDUE-CLASS SUMS

Exactness is the zero-variance ideal. When exactness is not achievable for a given collection of values, the practical question is how the ordering of those values along the axis affects $\mathrm{var}(\widehat{Q}_n)$. The next identity answers this exactly by expressing the variance in terms of the residue-class sums.

Proposition 5.1. *The following holds*

$$\mathrm{var}(\widehat{Q}_n) \;=\; T\sum_{r=0}^{T-1}\Big(S_r-\frac{Q}{T}\Big)^2. \tag{3}$$

Proof. By Lemma 2.2, one has $\widehat{Q}_n(r) = T\,S_r$. Also $\mathbb{E}[\widehat{Q}_n] = Q$. Since Z is uniform on $\{0,\dots,T-1\}$,

$$\begin{aligned}\mathrm{var}(\widehat{Q}_n) &= \frac{1}{T}\sum_{r=0}^{T-1}\big(\widehat{Q}_n(r)-Q\big)^2\\ &= \frac{1}{T}\sum_{r=0}^{T-1}T^2\Big(S_r-\frac{Q}{T}\Big)^2\\ &= T\sum_{r=0}^{T-1}\Big(S_r-\frac{Q}{T}\Big)^2,\end{aligned}$$

which is Eq. (3). □

The right-hand side of Proposition 5.1 is a sum of squares. Therefore $\mathrm{var}(\widehat{Q}_n) = 0$ holds exactly when all residue-class sums equal Q/T, which is the balance condition from Theorem 3.2.

More importantly for what follows, the variance formula shows that the arrangement matters only through the dispersion of the residue-class sums around their mean. This observation leads directly to a partitioning formulation of the arrangement problem.

BEST ARRANGEMENT AS A PARTITIONING PROBLEM

Definition 6.1 (Arrangement)**.** *Fix a finite population Y with values $y_0,\dots,y_{N-1}$ (values may repeat). An arrangement of these values along the sampling axis is a permutation π of $\{0,\dots,N-1\}$, which produces the arranged vector*

$$Y_\pi = \big(y_{\pi(0)},\dots,y_{\pi(N-1)}\big)^\top.$$

In stereological language one often thinks of this as choosing an ordering of the population units before systematic sampling. The practical question of finding a best possible arrangement is discussed in the stereological literature, see, e.g., Gundersen (2002); Tinajero-Bravo *et al.* (2014), and it goes back at least to early work in systematic sampling (Sethi, 1965). Proposition 5.1 shows that, in the discrete model, the variance depends on the arrangement only through the T residue-class sums.

Any arrangement π determines which values fall into each residue class modulo T. Equivalently, it determines which original indices contribute to each residue class. For $r \in \{0,\dots,T-1\}$, we define

$$I_{r,\pi} = \{\pi(r+kT) : k = 0,\dots,n-1\},$$

so $I_{r,\pi}$ is the set of original indices whose values appear in the residue-class positions $r, r+T,\dots,r+(n-1)T$ of the arranged vector Y_π. Also, we define the corresponding residue-class sum by

$$S_{r,\pi} \;=\; \sum_{k=0}^{n-1} y_{\pi(r+kT)} \;=\; \sum_{i\in I_{r,\pi}} y_i.$$

With this in mind, we consider the objective as a function of the arrangement,

$$F(\pi) \;=\; \sum_{r=0}^{T-1}\Big(S_{r,\pi}-\frac{Q}{T}\Big)^2, \tag{4}$$

where $Q = \sum_{i=0}^{N-1} y_i$.

To make the dependence on π explicit in the estimator, write

$$\widehat{Q}_{n,\pi} \;=\; T\sum_{k=0}^{n-1} y_{\pi(Z+kT)},$$

so that the only randomness is the start Z. Then Proposition 5.1 gives

$$\mathrm{var}(\widehat{Q}_{n,\pi}) \;=\; T\,F(\pi).$$

Thus minimizing the Cavalieri variance over π is equivalent to minimizing $F(\pi)$, meaning to making the T residue-class sums as equal as possible.

Definition 6.2 (Best arrangement problem)**.** *Given values $y_0,\dots,y_{N-1}$ and a sample size n such that n divides N, the best arrangement problem is to find an arrangement π that minimizes $F(\pi)$ in Eq.* (4).

Proposition 6.3. *The best arrangement problem is NP-hard.*

Proof. We reduce from 3-Partition, which is NP-complete; see (Garey and Johnson, 1979). Given an instance with integers $a_1,\dots,a_{3m}$ and target B, set $N = 3m$, $n = 3$, $T = m$, and $y_i = a_{i+1}$ for $i = 0,\dots,3m-1$. Then $Q = \sum_{i=1}^{3m} a_i = mB$, hence $Q/T = B$. An arrangement π has objective value $F(\pi) = 0$ if and only if each residue-class sum equals B, which is equivalent to a partition of $\{a_i\}$ into m triples each summing to B. Since $F(\pi) \geq 0$ for all π, the optimum of F is zero if and only if there exists an arrangement π with $F(\pi) = 0$. Therefore deciding whether the optimum of F is zero solves 3-Partition, and the best arrangement problem is NP-hard. $\square$

From a computational viewpoint, NP-hardness means that one should not expect a general method that finds a globally optimal arrangement efficiently for all inputs. In particular, exact optimization typically becomes impractical beyond small sizes, which matches the qualitative message already emphasized in early discussions of best possible arrangements (Sethi, 1965; Gundersen, 2002). This motivates simple heuristics that aim to reduce residue-class dispersion directly, which we discuss next.

RESIDUE-CLASS HEURISTICS

Proposition 5.1 shows that, in the discrete model, the variance is controlled entirely by the residue-class sums $S_{r,\pi}$. Equivalently, for fixed N and n, minimizing $\mathrm{var}(\widehat{Q}_{n,\pi})$ over arrangements π is the same as minimizing the coset dispersion objective $F(\pi)$ from Section 6. In particular, any ordering that brings the sums $S_{r,\pi}$ closer to each other reduces $\mathrm{var}(\widehat{Q}_{n,\pi})$ exactly. This provides a concrete way to interpret the intuition behind balanced systematic sampling and the smooth fractionator (Murthy, 1967; Gundersen, 2002). In practice one typically does not know the y_i in advance, but one may have auxiliary size information (e.g. block volume or weight) that can be used to build an ordering with better residue-class balance.

We describe two simple rules that construct an arrangement π by assigning values to the residue-class positions $r, r+T,\dots,r+(n-1)T$ for each $r \in \{0,\dots,T-1\}$. To describe the rules compactly, let $y_{(1)} \leq \cdots \leq y_{(N)}$ denote the ordered population values (order statistics). The output of each rule is a permutation π, hence an arranged vector

$$Y_\pi = (y_{\pi(0)},\dots,y_{\pi(N-1)})^\top .$$

GREEDY BALANCING OF RESIDUE-CLASS SUMS

A natural baseline is to place large values first and repeatedly assign the next value to the currently lightest residue class. Initialize T residue classes, each with current partial sum 0 and with 0 assigned values. Process the values in decreasing order $y_{(N)}, y_{(N-1)},\dots,y_{(1)}$. At each step, assign the next value to a residue class whose current partial sum is minimal among those that still have fewer than n assigned values. If there is a tie, choose the smallest residue-class index r.

This produces T ordered lists of assigned values, one list per residue class. To turn this assignment into a permutation, we keep the values within each residue class in the order in which they were assigned. We then fill the arranged vector by residue classes, placing the first assigned value for class r at position r, the second at position $r+T$, and so on, until position $r+(n-1)T$. The resulting arrangement is denoted π_{greedy}.

This rule is greedy in the standard algorithmic sense, since it makes the locally best choice given the current partial sums. The same idea is classical in load balancing and multiprocessor scheduling, where one assigns the next job to the least loaded machine (Graham, 1966); see also Pinedo (2016). Here the load is the current residue-class sum, and the goal is to keep the T loads as even as possible.

From a practical viewpoint, this baseline has two simple advantages. First, it is completely generic and does not rely on a specific shape such as a monotone trend. Second, it can be driven by auxiliary measurements, so it is still meaningful when the y_i are unknown but correlated proxies are available. In such settings it provides a fast and transparent way to reduce $F(\pi)$ at least locally, and it can also serve as an initializer for local-improvement schemes that target further reductions of F.

PAIRING EXTREMES AND BALANCING PAIR SUMS

When both N and n are even, a second rule is often more effective for monotone or nearly monotone profiles. First form the extreme pairs

$$(y_{(1)}, y_{(N)}),\ (y_{(2)}, y_{(N-1)}),\ \dots,\ (y_{(N/2)}, y_{(N/2+1)}),$$

and treat each pair as an indivisible item with pair sum $s_k = y_{(k)} + y_{(N+1-k)}$. Process the pairs in increasing order of k, that is, start from $\big(y_{(1)}, y_{(N)}\big)$ and end with $\big(y_{(N/2)}, y_{(N/2+1)}\big)$.

Distribute these $N/2$ pair items into the T residue classes by greedy balancing of the running sums of pair sums. At each step, assign the next pair to a residue class whose current pair-sum total is minimal among those that still have fewer than $n/2$ pairs. If there is a tie, choose the smallest residue-class index r.

This produces T ordered lists of assigned pairs. To turn this into an arrangement, keep the pairs within each residue class in the order in which they were assigned. Within each pair, place the smaller value first. Then, for each residue class r, place the first pair into positions r and $r+T$, the second pair into positions $r+2T$ and $r+3T$, and continue until filling the n positions $r, r+T, \ldots, r+(n-1)T$. This convention defines a deterministic permutation, which we denote by π_{pair}.

The motivation is simple. Pairing a small value with a large one partly cancels the leading trend, so the pair sums typically vary much less than the original values. Balancing these pair sums then aims directly at residue-class balance and therefore at reducing $F(\pi)$. This is closely in line with the smoothing rationale behind the Murthy–Gundersen ordering, also known as the smooth fractionator in Gundersen (2002). In terms of the ordered values $y_{(1)} \leq \cdots \leq y_{(N)}$, it is obtained by listing the odd order statistics in increasing order and then the even order statistics in decreasing order. That is, one can take π_{sf} so that

$$Y_{\pi_{\text{sf}}} = \big(y_{(1)}, y_{(3)}, \ldots, y_{(N-1)}, y_{(N)}, y_{(N-2)}, \ldots, y_{(2)}\big).$$

Like the pairing heuristic, this ordering spreads small and large values across the residue classes. For monotone or near-monotone profiles, that spreading tends to make the residue-class sums more similar and therefore reduces $F(\pi)$.

Proposition 7.1. *Assume that N and n are even and that $n \mid N$. Set $T = N/n$. Suppose the ordered values satisfy $y_{(k)} = a + b(k-1)$ for some $a, b \in \mathbb{R}$. Then the pairing heuristic is exact. In particular, we have $\operatorname{var}(\widehat{Q}_{n,\pi_{\text{pair}}}) = 0$.*

Proof. For each k,

$$\begin{aligned} s_k = y_{(k)} + y_{(N+1-k)} &= a + b(k-1) + a + b(N-k) \\ &= 2a + b(N-1), \end{aligned}$$

so all pair sums are equal. Each residue class receives exactly $n/2$ pairs, hence every residue class has the same total sum. Therefore the residue-class sums $S_{r,\pi_{\text{pair}}}$ coincide, and Theorem 3.2 yields exactness. □

Proposition 7.2. *Assume that N and n are even and that $n \mid N$. Set $T = N/n$. Let $a, b \in \mathbb{R}$ and suppose the ordered values satisfy $y_{(k)} = a + b(k-1) + \varepsilon_k$, with $|\varepsilon_k| \leq \delta$ for all k. Let $S_{r,\pi_{\text{pair}}}$ be the residue-class sums produced by the pairing heuristic. Then, it holds $|S_{r,\pi_{\text{pair}}} - Q/T| \leq 2n\delta$ for all r, hence $F(\pi_{\text{pair}}) \leq 4Tn^2\delta^2$ and*

$$\operatorname{var}(\widehat{Q}_{n,\pi_{\text{pair}}}) \leq 4T^2n^2\delta^2.$$

Proof. Define $s = 2a + b(N-1)$. For each k,

$$s_k = y_{(k)} + y_{(N+1-k)} = s + (\varepsilon_k + \varepsilon_{N+1-k}),$$

so $|s_k - s| \leq 2\delta$. Each residue-class sum is the sum of $n/2$ pair sums, so for every r,

$$\left| S_{r,\pi_{\text{pair}}} - \frac{n}{2}s \right| \leq \frac{n}{2} \cdot 2\delta = n\delta.$$

Averaging over r gives

$$\begin{aligned} \left| \frac{Q}{T} - \frac{n}{2}s \right| &= \left| \frac{1}{T} \sum_{r=0}^{T-1} \left(S_{r,\pi_{\text{pair}}} - \frac{n}{2}s \right) \right| \\ &\leq \frac{1}{T} \sum_{r=0}^{T-1} \left| S_{r,\pi_{\text{pair}}} - \frac{n}{2}s \right| \leq n\delta. \end{aligned}$$

In addition, combining the two inequalities yields $|S_{r,\pi_{\text{pair}}} - Q/T| \leq 2n\delta$. The upper bounds on $F(\pi_{\text{pair}})$ and $\operatorname{var}(\widehat{Q}_{n,\pi_{\text{pair}}})$ follow from Eq. (4) and Proposition 5.1. □

ILLUSTRATIVE EXAMPLES

The following examples are fully explicit. They illustrate how exactness can arise in the discrete setting, how multi-scale exactness restricts the population structure, and how different orderings affect the variance through the residue-class sums. Throughout, residue classes are taken modulo T, as in the discrete model described above. When we compare different orderings of the same values, we use the notation $\widehat{Q}_{n,\pi}$ introduced in the discussion of best arrangements.

Example 8.1 (Exactness without matched pairs)**.** *Let $N = 12$, $n = 4$, and $T = 3$. Consider*

$$Y = (1, 0, 2, 2, 1, 2, 3, 4, 2, 4, 5, 4).$$

The residue classes are $\{0, 3, 6, 9\}$, $\{1, 4, 7, 10\}$, and $\{2, 5, 8, 11\}$. Their sums are $1+2+3+4 = 10$, $0+1+4+5 = 10$, and $2+2+2+4 = 10$. Hence Y is exact by Theorem 3.2. However, matched pairs with $M = 6$ do not hold because $y_0 + y_6 = 4$ while $y_3 + y_9 = 6$. This shows that matched pairs are not needed for exactness for a fixed systematic design.

Example 8.2 (Matched pairs and multi-scale exactness)**.** *Let* $N = 12$ *and* $M = 6$*. Let* $\mu = 5$ *and define*

$$Y = (1,2,3,4,5,6,\,9,8,7,6,5,4),$$

so $y_{k+6} + y_k = 10$ *for* $k = 0,\dots,5$*. By Theorem 4.2, the population is exact for every even sample size dividing* 12*, that is* $n \in \{2,4,6,12\}$*.*

Example 8.3 (Exact ordering for an odd sample size)**.** *Let* $N = 9$*,* $n = 3$*, and* $T = 3$*, and consider the values* $1,2,\dots,9$ *arranged as*

$$Y = (1,2,3,\,5,6,4,\,9,7,8).$$

Since $Q = 45$*, one has* $Q/T = 15$*. The residue-class sums are* $1+5+9 = 15$*,* $2+6+7 = 15$*, and* $3+4+8 = 15$*. Hence the estimator is exact even though* N *and* n *are odd and matched pairs are not available.*

Example 8.4 (Comparing orderings on a monotone profile)**.** *Let* $N = 12$*,* $n = 4$*, and* $T = 3$*, and consider the values* $1,2,\dots,12$*.*

Take the identity ordering π_{id}*, so* $Y_{\pi_{\mathrm{id}}} = (1,2,\dots,12)$*. The residue-class sums are* $(22,26,30)$*. Since* $Q = 78$ *and* $Q/T = 26$*, Proposition 5.1 yields*

$$\operatorname{var}(\widehat{Q}_{n,\pi_{\mathrm{id}}}) = 3\left[(-4)^2 + 0^2 + 4^2\right] = 96.$$

Now consider an ordering produced by the pairing heuristic

$$Y_{\pi_{\mathrm{pair}}} = (1,3,5,\,12,10,8,\,2,4,6,\,11,9,7).$$

Its residue-class sums are $(26,26,26)$*, hence* $\operatorname{var}(\widehat{Q}_{n,\pi_{\mathrm{pair}}}) = 0$*. This matches Proposition 7.1, since the ordered values follow an affine trend.*

For comparison, the smooth fractionator ordering is

$$Y_{\pi_{\mathrm{sf}}} = (1,3,5,7,9,11,\,12,10,8,6,4,2).$$

It yields the same residue-class sums $(26,26,26)$*, hence* $\operatorname{var}(\widehat{Q}_{n,\pi_{\mathrm{sf}}}) = 0$*. A greedy balancing run can also produce an exact ordering, for instance*

$$Y_{\pi_{\mathrm{greedy}}} = (12,11,10,\,7,8,9,\,6,5,4,\,1,2,3),$$

again with residue-class sums $(26,26,26)$*.*

Example 8.5 (One-point perturbation and variance drop)**.** *Let* $N = 12$*,* $n = 4$*, and* $T = 3$*, and consider the values* $1,2,\dots,11,13$*.*

Now, with the identity ordering π_{id}*,* $Y_{\pi_{\mathrm{id}}} = (1,2,\dots,11,13)$ *has residue-class sums* $(22,26,31)$*. Here* $Q = 79$ *and* $Q/T = 79/3$*, so Proposition 5.1 gives*

$$\operatorname{var}(\widehat{Q}_{n,\pi_{\mathrm{id}}}) = 3\left[\left(22 - \frac{79}{3}\right)^2 + \left(26 - \frac{79}{3}\right)^2 + \left(31 - \frac{79}{3}\right)^2\right] = 122.$$

A pairing-based ordering is

$$Y_{\pi_{\mathrm{pair}}} = (1,3,5,\,13,10,8,\,2,4,6,\,11,9,7).$$

It has residue-class sums $(27,26,26)$*, hence*

$$\operatorname{var}(\widehat{Q}_{n,\pi_{\mathrm{pair}}}) = 3\left[\left(27 - \frac{79}{3}\right)^2 + 2\left(26 - \frac{79}{3}\right)^2\right] = 2.$$

For this dataset, the smooth fractionator ordering

$$Y_{\pi_{\mathrm{sf}}} = (1,3,5,7,9,11,\,13,10,8,6,4,2)$$

produces the same residue-class sums $(27,26,26)$*, hence the same variance* 2*. A greedy run can also return an ordering with these sums, for instance*

$$Y_{\pi_{\mathrm{greedy}}} = (13,11,10,\,7,8,9,\,4,6,5,\,3,1,2).$$

Taken together, the examples support two simple takeaways. Exactness in the discrete model is a fixed-design balance effect. It can happen without a global symmetry such as matched pairs, as in Example 8.1, and it can also happen for odd N and odd sample sizes, as in Example 8.3. When exactness is required across the whole even family of sample sizes, the situation is more rigid and matched pairs become necessary, as in Example 8.2 and Theorem 4.2.

When exactness does not hold, the variance identity shows that the key quantity is how well an ordering balances the residue-class sums. Examples 8.4 and 8.5 show this directly. A monotone ordering can have a noticeable variance, while orderings produced by pairing, by greedy balancing, or by the Murthy–Gundersen smooth fractionator can make the residue-class sums nearly equal and lead to a much smaller variance.

CONCLUSION AND FUTURE WORK

This paper gives a discrete, design-based view of Cavalieri sampling in which both exactness and variance are governed by the residue-class sums. For a fixed systematic design, exactness is equivalent to a simple balance condition, and the corresponding class of exact populations has an explicit linear structure and dimension. When exactness is required uniformly across the even family of sample sizes, the matched-pairs property becomes necessary.

Beyond the exactness criterion, the same residue-class sums also provide an exact variance identity. Proposition 5.1 shows that for any ordering the variance depends only on how dispersed these sums are. This offers a concrete way to interpret classical orderings such as matched pairs or the Murthy–Gundersen scheme, and it provides a clear target when one builds orderings from auxiliary size information while the y_i themselves are not observable before sampling.

The variance via residue-class sums also turns the best possible arrangement problem into a concrete optimization problem and helps explain why globally optimal orderings are hard to obtain at realistic sizes. We therefore focus on simple balancing heuristics. The pairing heuristic comes with guarantees in a transparent model, since it is exact for affine trends and remains stable under bounded perturbations, while the greedy rule provides a natural baseline when one simply aims to reduce dispersion directly.

As future work, it would be useful to test and refine these heuristics under realistic conditions, for instance when values are only partly observable before sampling, auxiliary measurements are noisy, or some sections are missing. Large, carefully designed computational experiments could then compare ordering rules on equal footing and clarify when each one works best. On the computational side, a more direct study of the objective function behind the best arrangement problem would be valuable, especially how much it improves under simple local swaps and how often such moves get close to the optimum.

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