

EXPLANATION OF APPARENT PARADOXES IN CAVALIERI SAMPLING

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ABSTRACT

To predict the precision of systematic sampling in design stereology is an old problem. In G. Matheron's transitive theory the variance is decomposed into the extension term, which represents the trend and it can be estimated from data, a 'Zitterbewegung' term, which is neglected because it oscillates about zero, and higher order terms which are ignored. Recently, K. Kiêu and coworkers have established a precise connection between the extension term and the smoothness properties of the measurement function (e.g. the 'area function' when estimating a volume from Cavalieri sections), and completing the Zitterbewegung term. The extension term is always a good approximation of the variance when the number of sections is very large, but not necessarily when this number is small. In this paper we propose a more general representation of the variance and we construct a flexible extension term which approximates the variance satisfactorily for an arbitrary number of sections.

Key words: Cavalieri estimator, extension term, object- m , stereology, systematic sampling, Zitterbewegung.

1 INTRODUCTION

Cavalieri sampling is widely used in design stereology to estimate the volume of a bounded object from systematic sections. Error predictions based on Matheron's transitive theory (1965, 1971) have been used over decades — see also Gundersen and Jensen (1987), Cruz-Orive, (1989, 1993). The variance is decomposed into the so called extension term, a Zitterbewegung, and higher order terms. To approximate the variance, only the extension term is used.

In general, the problem is to estimate the integral of a bounded function f , called the measurement function, over a bounded domain, by systematic sampling at abscissas a constant distance T apart. Recently, Kiên Kiêu and coworkers, (Souchet, 1995, Kiêu,

1997 and Kiêu et al, 1998), have found that the extension term is of $O(T^{2m+2})$, where m , called the smoothness constant, is the order of the first non-continuous derivative of f ; they have also completed the Zitterbewegung. Gundersen et al (1998) note that the extension term is a good approximation of the variance when T is small enough. For a practical working range where T is not small, however, the variance may behave quite differently as $O(T^{2m+2})$, and the recent theory does not quite explain this. In this paper we start from a generalized representation of the variance and we allow terms from the Zitterbewegung, and higher order terms, to be recruited into the traditional extension term using precise criteria. As a result, we obtain a flexible extension term for any particular f which approximates the variance satisfactorily for any interesting range of T . For the time being our approach applies to area functions whose form is known analytically (at least at some points, see § 2.2) and is free from measurement errors.

2 SYSTEMATIC SAMPLING ALONG AN AXIS: CURRENT THEORY

2.1 Problem, sampling and unbiased estimation

The target parameter may be the volume Q of a bounded, connected and non-random subset $X \subset \mathbb{R}^3$, namely:

$$Q = \int_{-\infty}^{\infty} f(x) dx, \quad (1)$$

where $f(x)$ denotes the area of the intersection between X and a plane normal to a fixed, conveniently oriented sampling axis, at a point of abscissa x . In a general context, $f : \mathbb{R} \rightarrow \mathbb{R}^+$ is a bounded non-random function, called the measurement function, which is integrable in a bounded domain H and vanishes outside H ; in the Cavalieri context H is the orthogonal linear projection of X on the sampling axis.

An unbiased estimator of Q is:

$$\widehat{Q} = T \cdot \sum_{k \in \mathbb{Z}} f(z + kT) = T \cdot (f_1 + f_2 + \dots + f_n), \quad (2)$$

where z is a uniform random variable in $[0, T)$, T the distance between consecutive planes — for convenience we consider $T \in (0, \text{length}(H))$ — and f_1, f_2, \dots, f_n the section areas at the sampling points which lie in H . The mean value of n is $E(n) = \text{length}(H)/T$.

2.2 Characterization of the measurement function f

A prerequisite for a proper choice of the variance representations given later is the characterization of f according to Souchet (1995), Kiêu (1997), and Kiêu et al (1998). Given a function $h : \mathbb{R} \rightarrow \mathbb{R}^+$, the amplitude of the jump or 'transition' of the k th derivative $h^{(k)}$ of h at the abscissa x is expressed as follows:

$$Sh^{(k)}(x) = \lim_{y \rightarrow x^+} h^{(k)}(y) - \lim_{y \rightarrow x^-} h^{(k)}(y), \quad (x \in \mathbb{R}, k = 0, 1, \dots). \quad (3)$$

Further, $Dh^{(k)}$ will denote the set of points where $h^{(k)}$ is non-continuous, namely:

$$Dh^{(k)} = \{x_i | Sh^{(k)}(x_i) \neq 0, i \in \mathbb{Z}\}, \quad (k = 0, 1, \dots). \tag{4}$$

The function h , and in particular the measurement function f is (m, p) -piecewise smooth if its support is bounded and if:

- (a). $Df^{(k)} = \emptyset, (k < m)$, that is, all derivatives of f of order less than m are continuous, (i.e., m is the order of the first non-continuous derivative of f).
- (b). For $m \leq k \leq m + p, f^{(k)}$ may have only a finite number of jumps, and they have to be finite.

2.3 Recent variance representations and approximations (K. Kiêu et al)

The classical, well known representation of the variance of \widehat{Q} is:

$$\text{Var}(\widehat{Q}) = T \sum_{k=-\infty}^{\infty} g(kT) - \int_{-\infty}^{\infty} g(h) dh, \tag{5}$$

where g is the covariogram of the measurement function f , namely:

$$g(h) = \int_{-\infty}^{\infty} f(x) f(x + h) dx, \quad (-\infty < h < \infty), \tag{6}$$

(e.g. Moran, 1950). To estimate $\text{Var}(\widehat{Q})$ from data, Matheron (1965) used the classical Euler-MacLaurin summation formula. To allow for transitions of $f(x)$ at points other than the ends of its support, Souchet (1995), Kiêu (1997) and Kiêu et al (1998) have derived a refined version of the Euler-MacLaurin formula which leads to the following variance representation. If f is $(m, p \geq 1)$ -piecewise smooth, then it can be shown that g is $(2m + 1, p)$ -piecewise smooth, (K. Kiêu, personal communication, which corrects his own result in Kiêu, 1997, pp. 53-54), and

$$\text{Var}(\widehat{Q}) = \text{Var}_E(\widehat{Q}) + Z(T) + o(T^{2m+2}). \tag{7}$$

The term $\text{Var}_E(\widehat{Q})$ in the right hand side of the preceding expression is called the extension term, and it constitutes a good approximation of $\text{Var}(\widehat{Q})$ when T is small enough; the extension term has the advantage that it can be estimated from the data if a suitable model is adopted for g . Its expression is:

$$\text{Var}_E(\widehat{Q}) = -T^{2m+2} \cdot \frac{B_{2m+2}}{(2m + 2)!} \cdot Sg^{(2m+1)}(0), \tag{8}$$

where B_{2j} is a Bernoulli number, e.g. $B_1 = -1/2, B_2 = 1/6, B_4 = -1/30, B_6 = 1/42$, etc., and $B_{2j+1} = 0, (j = 1, 2, \dots)$, see Abramowitz and Stegun (1965). Further, the term $Z(T)$ typically exhibits an oscillating behaviour about 0, and it is called the 'Zitterbewegung'. Its expression is:

$$Z(T) = -T^{2m+2} \sum_{\{c \in Dg^{(2m+1)} \setminus 0\}} P_{2m+2,T}(c) \cdot Sg^{(2m+1)}(c), \tag{9}$$

where $P_{j,T}(x) = P_j(x/T - [x/T])$, $[\cdot]$ denotes the integral part of ' \cdot ', $P_j(x) = B_j(x)/j!$, ($j \geq 1$), and $B_j(x)$ is a Bernoulli polynomial (Abramowitz and Stegun, 1965, p. 805); $B_j(0) = B_j$ is the j th Bernoulli number. The oscillating behaviour of $Z(T)$ is inherited from that of the polynomials $P_{j,T}(\cdot)$. The representation of Eqs. (7)-(9) was already given by Kellerer (1989, Eq. (A1.6)).

The jumps of derivatives of g are related to those of f as follows:

$$Sg^{(2m+1)}(c) = (-1)^{m+1} \sum_{\{a \in Df^{(m)}, b \in Df^{(m)} | b-a=c\}} Sf^{(m)}(a) \cdot Sf^{(m)}(b), \quad (10)$$

(Souchet, 1995). Moreover, since g is symmetric, namely $g(h) = g(-h)$, $h \in \mathbb{R}$, it follows that:

$$Sg^{(2j)}(0) = 0, \quad Sg^{(2j+1)}(0) = 2g^{(2j+1)}(0^+), \quad (j = 0, 1, \dots). \quad (11)$$

2.4 Examples and apparent paradoxes

An important consequence of the preceding theory is that the approximation of $\text{Var}(\hat{Q})$ via the extension term, see Eq. (8), depends on the smoothness constant m of the measurement function f . In most applications it was hitherto assumed that $m = 0$, in which case:

$$\text{Var}(\hat{Q}) \approx -\frac{T^2}{6} \cdot g^{(1)}(0^+). \quad (12)$$

K. Kiêu and coworkers have shown that $m = 0$ only if f has at least one finite jump (Fig. 1). In most real cases, however, one would expect f to be continuous and $f^{(1)}$ non-continuous with at least one finite jump, in which case $m = 1$, see Fig. 3, and:

$$\text{Var}(\hat{Q}) \approx \frac{T^4}{360} \cdot g^{(3)}(0^+). \quad (13)$$

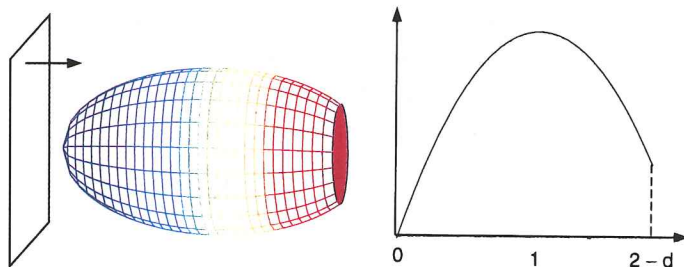


Figure 1. Left: an ellipsoid truncated by a cap of thickness d . Right: the corresponding measurement (section area) function. The horizontal axis is the sampling axis, and the vertical axis is the area of the intersection between the object and a scanning plane (see left) normal to the sampling axis.

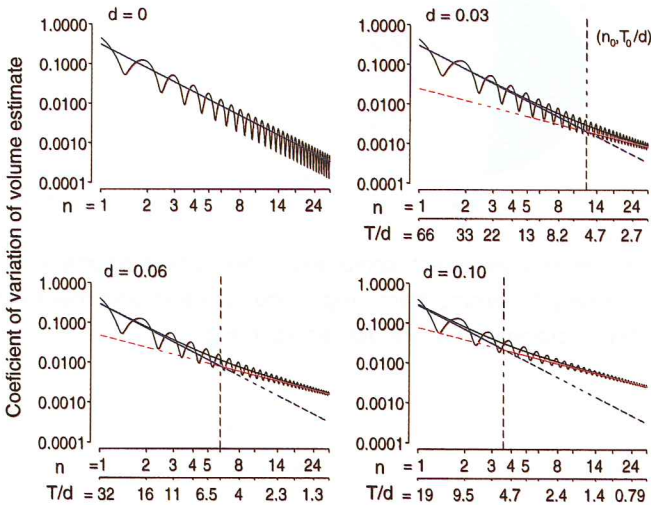


Figure 2. Oscillating curves: true coefficient of variation of the Cavalieri estimator of the volume of the object in Fig. 1 from n sections. Note the change in trend from $O(1/n^4)$ for $T > T_0$, (blue lines) to $O(1/n^2)$ for $T < T_0$, (red lines). See text, § 3.3.

Let us call 'object- m ' an object whose area function f has smoothness constant m . Note, however, that f , and hence m , may depend on the cutting direction. Fig. 1 represents an ellipsoid with a cap of height d removed. This truncated ellipsoid is an object-0 because its area function has a finite jump corresponding to the planar face of the object parallel to the sampling plane. Therefore, for this object the variance approximation (12) should hold. What happens, then, if d is very small, so that the object cannot be visually distinguished from a complete ellipsoid? Will then Eq. (12) still be better than Eq. (13)? If the answer is 'yes', then the situation will seem illogical (i.e. two nearly indistinguishable objects require very different formulae), whereas, if the answer is 'no', then we would seem to face a theoretical contradiction.

A heuristic explanation is: for the truncated ellipsoid, Eq. (12) holds when the distance T between sections is so small that they can 'feel' that a cap is missing. For larger T , however, the sections will 'see' the object as if it was a complete ellipsoid (object-1), and Eq. (13) will be the better one there. The ranges of T corresponding to each trend vary with d , see Fig. 2. On the other hand, Fig. 4 illustrates the opposite situation, in which the object-1 of Fig. 3 behaves as an object-0 when T is large (so that the sections 'see' the slope of the area function as if it was a jump), and it behaves as an object-1 only when the sections are close enough to appreciate that the area function is really continuous. Again, the corresponding ranges of T vary with the width d of the slope.

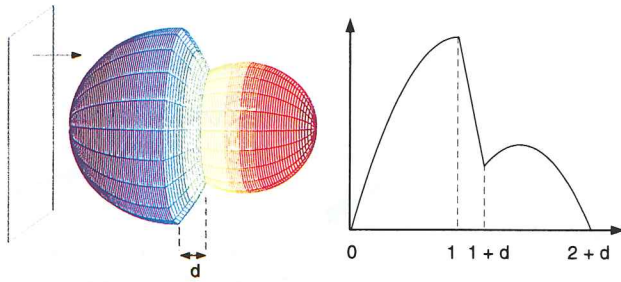


Figure 3. Left: the 'mushroom' object, composed of two sphere fragments of height 1 and a cone fragment of height d joining them. Right: the corresponding measurement (section area) function. The coordinate axes are defined as in Fig. 1.

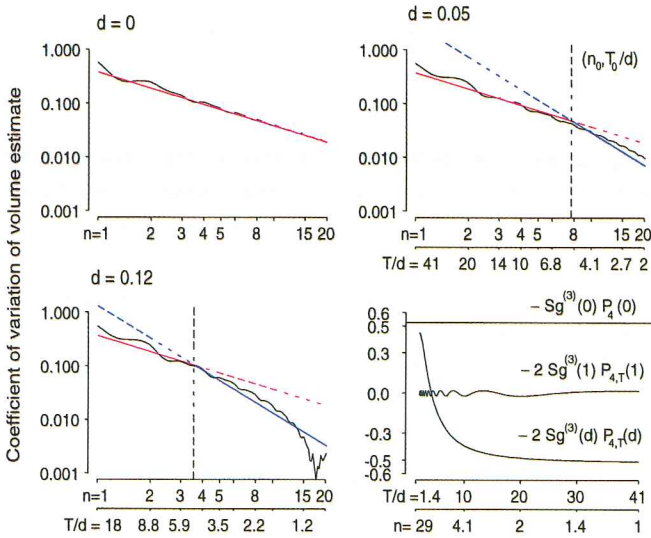


Figure 4. First three panels: the full curves represent the true coefficient of variation of the Cavalieri estimator of the volume of the object in Fig. 3 from n sections. Note the change in trend from $O(1/n^2)$ for $T > T_0$, (red lines), to $O(1/n^4)$ for $T < T_0$, (blue lines). Last panel: the curve in the middle contributes to the Zitterbewegung, whereas the sum of other two, times T^4 , is the approximation (18). See text, § 3.4.

3 EXACT TREATMENT OF THE APPARENT PARADOXES

3.1 The current approach

Gundersen et al. (1998) construct a few geometrical objects to illustrate 'paradoxes' of a kind similar to those described in the preceding subsection. They show that Eq. (8)

predicts the trend of $\text{Var}(\widehat{Q})$ fairly well provided that a suitable value of m is used in the corresponding range of T , and therefore that Eq. (12) is always satisfactory for an object-0 for small enough T , whereas Eq. (13) is always satisfactory for an object-1 for small enough T , and similarly for other values of m .

3.2 Our approach

The current approach suffers from several shortcomings. First, for a given working range of T corresponding to a small number n of sections, it is *a priori* not clear which value of m should be plugged into Eq. (8) to get a good approximation of $\text{Var}(\widehat{Q})$ in that range. And second, Eq. (8) helps only when m is correctly chosen for a concrete range of T , but it is incapable of explaining the changes in trend of $\text{Var}(\widehat{Q})$ over the whole range of T .

Our approach starts from a generalized version of Eq. (7). Suppose that f is (m, p) -piecewise smooth, with smoothness constant $m = 0, 1, \dots$ and $p = 1, 2, \dots$, both known and fixed. For all N such that $2m + 1 \leq N \leq 2m + p$ we may write:

$$\begin{aligned} \text{Var}(\widehat{Q}) &= \sum_{k=2m+1}^N (-1)^k T^{k+1} \sum_{c \in Dg^{(k)}} P_{k+1,T}(c) \cdot Sg^{(k)}(c) + o(T^{N+1}) \\ &= \sum_{k=2m+1}^N (-1)^k T^{k+1} \left[\frac{B_{k+1}}{(k+1)!} \cdot Sg^{(k)}(0) \right. \\ &\quad \left. + 2 \sum_{\{c \in Dg^{(k)} | c > 0\}} P_{k+1,T}(c) \cdot Sg^{(k)}(c) \right] + o(T^{N+1}). \end{aligned} \tag{14}$$

The preceding formula is a slight adaptation of one given by Souchet (1995, p. 49). An important relation, proved in the Appendix, which generalizes Eq. (10), is:

$$Sg^{(k)}(c) = \sum_{\{i+j=k-1\}} \sum_{\{a \in Df^{(i)}, b \in Df^{(j)} | b-a=c\}} (-1)^{i+1} S f^{(i)}(a) \cdot S f^{(j)}(b), \quad (k \leq 2m + p). \tag{15}$$

The idea is to build up a new extension term from the right hand side of Eq. (14). The criteria to recruit terms from the second summation are as follows. Consider the term $P_{k+1,T}(c) \cdot Sg^{(k)}(c)$.

- *Criterion [1].* If $T \geq c$, then $P_{k+1,T}(c) = P_{k+1}(c/T)$ is a Bernoulli polynomial with one oscillation in $(0 < c/T \leq 1)$. Thus, for each $c \in Dg^{(k)}$ and $c > 0$, the term $P_{k+1,T}(c) \cdot Sg^{(k)}(c)$ will be recruited into the extension term for the range $c \leq T < \text{length}(H)$.
- *Criterion [2].* If $0 < T < c$, then the polynomial $P_{k+1,T}(c) = P_{k+1}(c/T - [c/T])$ exhibits an oscillation about 0 between consecutive integer values of c/T , namely an oscillation in each of the infinity many intervals:

$$T \in \left\{ \left[\frac{c}{j+1}, \frac{c}{j} \right), (j = 1, 2, \dots) \right\}. \tag{16}$$

Thus, for each $c \in Dg^{(k)}$ and $c > 0$, the term $P_{k+1,T}(c) \cdot Sg^{(k)}(c)$ will be recruited into the Zitterbewegung (even if $Sg^{(k)}(c)$ is non-negligible) for the range $0 < T < c$.

For the examples of Figs. 1, 3 we are concerned only with $m = 0, 1$, and therefore we only have to retain terms up to $N = 3$ in Eq. (14). The corresponding variance approximations are calculated next.

3.3 The truncated ellipsoid: an object-0 that may behave as object-1

The area function f of the object, see Fig. 1, is such that $Df^{(0)} = \{2 - d\}$, whereas $Df^{(1)} = Df^{(2)} = \{0, 2 - d\}$.

Using Criterion [2], for $0 < T < 2 - d$ all terms of the form $P_{k+1,T}(2 - d) \cdot Sg^{(k)}(2 - d)$, ($k = 1, 2, 3$), will contribute to the Zitterbewegung only. On the other hand, by Eq. (11) we have $Sg^{(2)}(0) = 0$. Therefore, Eq. (14) yields the following extension term:

$$\text{Var}(\widehat{Q}) \approx -\frac{T^2}{6} \cdot g^{(1)}(0^+) + \frac{T^4}{360} \cdot g^{(3)}(0^+). \tag{17}$$

Note that the preceding expression is a combination of Eqs. (12) and (13). Whenever $0 < T \leq T_0$, where T_0 depends on d , the first term in the right hand side prevails, agreeing with the fact that the object is an object-0. However, when $T_0 < T < 2 - d$, the second term prevails: the object behaves as an object-1 there (Fig. 2). The threshold T_0 at which the trend changes is obtained by equating the two terms in the right hand side of Eq. (17) and solving for T , namely: $T_0 = [-60 \cdot g^{(1)}(0^+)/g^{(3)}(0^+)]^{1/2}$.

3.4 The 'mushroom': an object-1 that may behave as object-0

From the area function f of the object, see Fig. 3, we see that $Df^{(0)} = \emptyset$ for $d > 0$, (because f is continuous if $d > 0$), whereas $Df^{(1)} = Df^{(2)} = \{0, 1, 1 + d, 2 + d\}$.

By Criterion [2], for each $c \in \{d, 1, 1 + d, 2 + d\}$ the terms $P_{k+1,T}(c) \cdot Sg^{(k)}(c)$, ($k = 1, 2, 3$), contribute to the Zitterbewegung for $0 < T < c$.

By Criterion [1], for $T > d$ the terms $P_{k+1,T}(d) \cdot Sg^{(k)}(d)$, ($k = 1, 2, 3$), contribute to the extension term. However, using Eq. (15) we see that $Sg^{(1)}(c) = Sg^{(2)}(c) = 0$ for all c ; therefore, Eq. (14) yields the following extension term for $T > d$:

$$\text{Var}(\widehat{Q}) \approx -T^4 \cdot P_4(0) \cdot Sg^{(3)}(0) - 2T^4 P_4(d/T) \cdot Sg^{(3)}(d). \tag{18}$$

Using Eq. (15), and assuming that $d \ll 1$, we get $Sg^{(3)}(0) \approx 2[Sf^{(1)}(1)]^2$ and $Sg^{(3)}(d) \approx -[Sf^{(1)}(1)]^2$, so that $Sg^{(3)}(0) \approx -2Sg^{(3)}(d)$ in this particular example (Fig. 4, last panel). Therefore:

$$\begin{aligned} \text{Var}(\widehat{Q}) &\approx -2T^4 \cdot [P_4(d/T) - P_4(0)] \cdot Sg^{(3)}(d) \\ &= -\frac{1}{12} \cdot Sg^{(3)}(d) \cdot d^2 \cdot (T - d)^2, \quad (T > d). \end{aligned} \tag{19}$$

When T is 'fairly larger' than d , then Eq. (19) shows that $\text{Var}(\widehat{Q}) = O(T^2)$, (Fig. 4), which explains why the object behaves as an object-0 when T is fairly larger than the width d of the 'slope' of the area function (Fig. 3). When $T < d$, then the term $P_{1,T}(d) \cdot Sg^{(3)}(d)$ contributes to the Zitterbewegung, and therefore the extension term consists only of the first term in the right hand side of Eq. (18), so that $\text{Var}(\widehat{Q}) = O(T^4)$, and the object behaves as an object-1 for small T . When $d = 0$ we have an object-0 for all $0 < T < 2$, (Fig. 4, first panel).

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APPENDIX: PROOF OF EQ. (15)

We use the notation introduced in § 2 and § 3.2 throughout. We start from a variant of Euler-MacLaurin’s formula given by Souchet (1995):

$$\begin{aligned} \widehat{Q} - Q &= T \sum_{k \in \mathbb{Z}} f(z + kT) - \int_{\mathbb{R}} f(x) dx \\ &= \sum_{i=m}^{m+p-1} (-1)^i T^{i+1} \cdot \sum_{a \in Df^{(i)}} P_{i+1,T}(a - z) \cdot Sf^{(i)}(a) + o(T^{m+p}). \end{aligned} \tag{I.1}$$

The desired variance is $\text{Var}(\widehat{Q}) = \mathbb{E}(\widehat{Q} - Q)^2$, the expectation being with respect to the uniform random variable z . Thus:

$$\begin{aligned} \text{Var}(\widehat{Q}) &= \mathbb{E} \left[\sum_{i=m}^{m+p-1} (-1)^i T^{i+1} \sum_{a \in Df^{(i)}} P_{i+1,T}(a - z) \cdot Sf^{(i)}(a) + o(T^{m+p}) \right]^2 \\ &= \sum_{k=2m}^{2m+p-1} (-1)^k T^{k+2} \sum_{\{i+j=k\}} \sum_{\{a \in Df^{(i)}, b \in Df^{(j)}\}} \mathbb{E} \left[P_{i+1,T}(a - z) \cdot P_{j+1,T}(b - z) \right] \\ &\quad \cdot Sf^{(i)}(a) \cdot Sf^{(j)}(b) + o(T^{2m+p+1}). \end{aligned} \tag{I.2}$$

Further, similarly as in Kiêu (1997, pp. 45–46) we have:

$$\begin{aligned} \mathbb{E} \left[P_{i+1,T}(a - z) \cdot P_{j+1,T}(b - z) \right] &= \int_0^T P_{i+1,T}(a - z) \cdot P_{j+1,T}(b - z) \frac{dz}{T} \\ &= (-1)^i \cdot P_{i+j+2,T}(b - a), \end{aligned} \tag{I.3}$$

which, substituted into the right hand side of Eq. (I.2) yields:

$$\begin{aligned} \text{Var}(\widehat{Q}) &= \sum_{k=2m+1}^{2m+p} (-1)^{k-1} T^{k+1} \sum_{\{i+j=k-1\}} \sum_{\{a \in Df^{(i)}, b \in Df^{(j)}\}} (-1)^i \cdot P_{k+1,T}(b - a) \\ &\quad \cdot Sf^{(i)}(a) \cdot Sf^{(j)}(b) + o(T^{2m+p+1}) \end{aligned} \tag{I.4}$$

On the other hand, setting $N = 2m + p$ in Eq. (14) we obtain:

$$\begin{aligned} \text{Var}(\widehat{Q}) &= T \sum_{k \in \mathbb{Z}} g(kT) - \int_{\mathbb{R}} g(x) dx \\ &= \sum_{k=2m+1}^{2m+p} (-1)^k T^{k+1} \cdot \sum_{c \in Dg^{(k)}} P_{k+1,T}(c) \cdot Sg^{(k)}(c) + o(T^{2m+p+1}), \end{aligned} \tag{I.5}$$

(Souchet, 1995), which, compared with Eq. (I.4) yields Eq. (15).