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Estimation of arbitrary order central statistical moments by the Multilevel Monte Carlo Method

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Abstract We extend the general framework of the Multilevel Monte Carlo method to multilevel estimation of arbitrary order central statistical moments. In particular, we prove that under certain assumptions, the total cost of a MLMC central moment estimator is asymptotically the same as the cost of the multilevel sample mean estimator and thereby is asymptotically the same as the cost of a single deterministic forward solve. The general convergence theory is applied to a class of obstacle problems with rough random obstacle profiles. Numerical experiments confirm theoretical findings.

Keywords Uncertainty quantification, multilevel Monte Carlo, stochastic partial differential equation, variational inequality, rough surface, random obstacle, statistical moments.

1 Introduction

Estimation of central statistical moments is important for many reasons. The variance (or the standard deviation) is one of the most important characteristics of a random variable, along with the mean. Higher order moments, particularly the third and the fourth moments (or the related skewness and kurtosis) are important in statistical applications, e.g. for tests whether a random variable is normally distributed [7]. Another example is [3], where skewness and kurtosis are utilized in a stopping criteria for a Monte Carlo method. Higher order moments inherit further characterization of a random variable; the problem of determining a probability distribution from its sequence of moments is widely known as the problem of moments [1]. This paper is dedicated to estimation of arbitrary order central statistical moments by means of the Multilevel Monte Carlo method, a non-intrusive sampling-based multiscale approach particularly suitable for uncertainty propagation in complex forward problems.

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To facilitate the presentation, let us consider an abstract well posed forward problem

$$u = S(\ ); \tag{1}$$

where   are model parameters (model input), u is the unique solution of the forward problem (model output) and S is the corresponding solution operator. As an illustrative example, we consider a contact problem between deformable bodies. The quantity of interest (observable) X might be either the solution itself, or some general, possibly nonlinear, continuous functional of the solution $X = F(u)$. Therefore the observable X might be either a spatially varying function (e.g. the displacement of a deformable body or the contact stress) or a scalar quantity (e.g. the size of the actual contact area). Typically, a model description contains probabilistic information about input parameters   and if it is possible to generate samples of , then samples of X may be generated via the forward map $X = F \quad S(\ )$.

However, the solution operator S is usually given implicitly as an inverse of a certain di erential or integral operator and the inverse can only be computedome general, cxi(abe28(e29713()-28(e29

3. Direct evaluation of central moments is no more demanding in terms of the overall computational cost than evaluation the non-centered moments. Particularly useful for stable and efficient numerical evaluation are one-pass update formulae from [15].

In this work we analyze simple and general form MLMC estimators for r-th order central statistical moments introduced in (25) and (29) below. The simple form of the estimators allowing for a unified analysis comes at the expense of a small systematic error which cannot be removed by a simple scaling when r 4, cf. [13, 8]. The rigorous control of this systematic error is presented below.

The paper is structured as follows. After preliminaries in Section 2, we give an overview of the general MLMC framework and the analysis strategy in Section 3. In Section 4 study in detail the MC estimator of arbitrary order central moments and particularly prove convergence of its bias and variance. In Section 5 we apply the developed theory to the MLMC estimator of arbitrary order central moments. Under additional assumptions we prove the same asymptotic work-error relation of the estimator for an arbitrary r-th moment as the same as for the estimation of the expectation value by the multilevel sample mean. In Section 6 we apply the general theory to a class of random obstacle problems (see also [9, 14, 4]). In Section 7 we report on the results of numerical experiments supporting the abstract theory.

2 Function spaces and statistical moments

Let (; ;

and distinguish the special case $H = B^2$, i.e.

$$\text{i) } H = \mathbb{R} \quad \text{or} \quad \text{ii) } H = W^{s,2}(D) \equiv H^s(D). \tag{6}$$

The nonnegative integer s will be fixed throughout the paper therefore is omitted in the notation (5) and (6) for brevity. In both cases, H is a Hilbert space with an inner product $\langle \cdot, \cdot \rangle_H$ and B^p is a Banach space with the a norm $\| \cdot \|_{B^p}$ specified in Table 1 for definiteness.

H	$\langle f, g \rangle_H$	B^p	$\|f\|_{B^p}$
$\mathbb{R}$	fg	$\mathbb{R}$	$|f|$

$W^{s,}$

for the norm on these spaces. Notice that $L^2(\Omega; H)$ is a Hilbert space with inner product

$$\langle X, Y \rangle := \int_\Omega \langle X(\omega), Y(\omega) \rangle_H \, dP$$

occasionally call $V(S)$ the variance of the estimator S. The reason for this slight abuse of terminology is that $V(S) \in \mathbb{R}_+$ is indeed a measure of variation of the quantity S. Furthermore it is consistent with the existing literature on Monte Carlo Methods and, in particular, the well-known splitting of the mean-square error (MSE) of an estimator into the sum of its (squared) bias and the variance

$$\begin{aligned} \|M - S\|^2_{L^2(\Omega;H)} &= \|M - E[S] + E[S] - S\|^2_{L^2(\Omega;H)} \\ &= \|M - E[S]\|^2_{L^2(\Omega;H)} + 2E\langle M - E[S], E[S] - S\rangle_H + \|E[S] - S\|^2_{L^2(\Omega;H)} \\ &= \|M - E[S]\|^2_H + V(S). \end{aligned} \tag{15}$$

Indeed, the inner product is zero since $M - E[S]$ is deterministic and $\langle M - E[S], \cdot\rangle_H$ is a linear functional on H. In order to facilitate the further discussion we introduce the relative root mean-square error

$$\mathrm{Rel}(M; S) := \frac{\|M - S\|_{L^2(\Omega;H)}}{\|M\|_H}.$$

Frequently, in practical applications the approximate evaluation of the quantity M involves some kind of deterministic approximation procedure. In this case the method can be interpreted as a two-stage approximation: there exists a sequence $M_\ell \to M$ converging strongly in H as $\ell \to \infty$, and a family of single level randomized estimators S_ℓ approximating M_ℓ. Then by the triangle inequality we have the upper bound (notice that if $M_L = E[S_L]$, the identity (15) provides a sharper result)

$$\|M - S_L\|_{L^2(\Omega;H)} \le \|M - M_L\|_H + \|M_L - S_L\|_{L^2(\Omega;H)}. \tag{16}$$

This estimate suggests that S_L

$M_L = \sum_{\ell=1}^{L} M_\ell$. Thus, similarly to (16) we obtain

$$\begin{aligned} \|M - S_{ML}\|_{L^2(\Omega;H)} &\le \|M - M_L\|_H + \|M_L - S_{ML}\|_{L^2(\Omega;H)} \\ &\le \|M - M_L\|_H + \sum_{\ell=1}^{L} \|M_\ell - T_\ell\|_{L^2(\Omega;H)}. \end{aligned} \tag{21}$$

where the X_i are independent and identically distributed (iid) samples of X. The estimator (25) is possibly the most natural and intuitive computable sample approximation for $M^r[X]$ with $r \geq 2$. However, as we will prove in Lemma 3 below, the estimator (25) is biased in general. In particular but important cases $r = 2$ and 3, the estimator (25) can be made unbiased with a minor modification. Indeed, the rescaled estimators

$$\tilde{S}^2_M[X] := \frac{M}{M-1} S^2_M[X]; \qquad \tilde{S}^3_M[X] := \frac{M^2}{(M-1)(M-2)} S^3_M[X]; \tag{26}$$

are unbiased, i.e. satisfy $E[\tilde{S}^r_M[X]] = M^r[X]$, for $r = 2; 3$. One might expect that a multiple of $S^r_M[X]$ is an unbiased estimator for higher order central moments as well, but already for $r = 4$ it holds that

$$E[S^4_M[X]] = \frac{M-1}{M^3}\left((M^2 - 3M + 3)M^4[X] + 3(2M-3)M^2[X]^2\right) \tag{27}$$

see e.g. [13,8] (in Lemma 3 below we derive a general representation for $E[S^r_M[X]]$ with an arbitrary r). In this case the unbiased estimate for $M^4[X]$ takes the form

$$\tilde{S}^4_M[X] := \frac{M^2}{(M-2)(M-3)}\left(\frac{M+1}{M-1} S^4_M[X] - 3 S^2_M[X]^2\right). \tag{28}$$

A similar result holds for any r: an unbiased estimator $\tilde{S}^r_M[X]$ can be built as a weighted sum of $S^r_M[X]$ with a nonlinear combination of $S^2_M[X]; \ldots; S^{r-2}_M[X]$. Such representations for $\tilde{S}^r_M[X]$ can be obtained for an arbitrary r and used for a single level Monte Carlo estimation of $M^r[X]$. However, an unbiased estimation for $r \geq 4$ may cause some technical difficulties, as we explain below.

Notice that the above description fits into the abstract framework of Section 3.1. Indeed, suppose that X_ℓ is an approximation to X at level ℓ, then (16) holds with

$$\mathcal{M} := M^r[X]; \qquad \mathcal{M}_L := M^r[X_L]; \qquad \mathcal{S}_L := S^r_M[X_L].$$

We introduce a multilevel estimator

$$S^r_{ML}[X] = \sum_{\ell=1}^{L} S^r_{M_\ell}[X_\ell] - S^r_{M_\ell}[X_{\ell-1}]; \tag{29}$$

where in the summands $S^r_{M_\ell}[X_\ell] - S^r_{M_\ell}[X_{\ell-1}]$ are built from M_ℓ pairs of samples $(X_\ell; X_{\ell-1})_i$, both computed for the same realization of input parameters (the same random event $\omega_i \in \Omega$). This fits into the abstract framework of Section 3.1 with

$$\mathcal{S}_{ML} := S^r_{ML}[X]; \qquad T_\ell := S^r_{M_\ell}[X_\ell] - S^r_{M_\ell}[X_{\ell-1}].$$

Evidently, since the estimator (25) is biased the multilevel estimator (29) is (in general) biased as well, whereas an unbiased estimator can be defined as

$$\tilde{S}^r_{ML}[X] = \sum_{\ell=1}^{L}$$

Applying (40) and the Holder inequality (9) gives us

$$\|X_{\underline{j}} - Y_{\underline{j}}\|_2 = \Big\| \sum_{i=1}^{r} (X_{j_i} - Y_{j_i}) \prod_{k=1}^{i-1} X_{j_k} \prod_{k=i+1}^{r} Y_{j_k} \Big\|_2 \le \sum_{i=1}^{r} c_H^{r-1} \|X - Y\|_{2p} \|X\|_{2q(r-1)}^{i-1} \|Y\|_{2q(r-1)}^{r-i}. \tag{41}$$

Estimating the sum with

$$\sum_{i=1}^{r} \|X\|_{2q(r-1)}^{i-1} \|Y\|_{2q(r-1)}^{r-i} \le \min\Big\{ r \max\big(\|X\|_{2q(r-1)}^{r-1}; \|Y\|_{2q(r-1)}^{r-1}\big);\ (\|X\|_{2q(r-1)} + \|Y\|_{2q(r-1)})^{r-1} \Big\}$$

completes the proof.

4.2 Estimation of the building blocks (31) and (32)

In this section we obtain upper bounds for (31) and (32) required later on in convergence theorem for the multilevel estimator in the forthcoming Section 5. The following notation will be essential in the forthcoming analysis. Let $r \ge 2$ be an integer and $1 \le k \le r$. Denote $m := \min(k+1; r)$. For an m-multiindex $\underline{j} = (j_1; \dots; j_m) \in \wedge_M^m$ we define its extension to an r-multiindex by

$$E(\underline{j}) = \begin{cases} (j_1; \dots; j_k; \underbrace{j_{k+1}; \dots; j_{k+1}}_{r-k \text{ times}}); & k < r; \\ (j_1; \dots; j_r); & k = r. \end{cases} \tag{42}$$

Notice the alternative expression: $m = k + 1 - \delta_{k;r}$ where δ_{kr} is the Dirac delta. These definitions and notation (34) allow for a compact representation of the sample estimator (25) as a sum products. Indeed, opening the brackets in (25) we observe

$$S_M^r[X] = \sum_{k=0}^{r} \frac{(-1)^k}{M^{k+1-\delta_{k;r}}} \binom{r}{k} \sum_{\underline{j} \in \wedge_M^{k+1-\delta_{k;r}}} X_{E(\underline{j})}. \tag{43}$$

The following lemma provides the quantitative structure for the bias of the estimator $S_M^r[X]$.

Lemma 3 Suppose X is a sufficiently smooth random field so that its statistical moments of any order up to $r \ge 2$ exist. Then it holds that

$$E[S_M^r[X]] = M^r[X] + M^{-1}\Big(\frac{r(r-1)}{2} M^{r-2}[X] M^2[X] - r M^r[X]$$

where the constants $c(\underline{j};M;r)$ are independent of X. This set of constants is non-unique, however, there exist $c(\underline{j};M;r)$ such that for $r \geq 4$

$$\sum_{\underline{j}\in\Xi^r_M} |c(\underline{j};M;r)| \leq 2\sum_{k=3}^{r-2} M^{-\lceil \frac{k}{2}\rceil}\binom{r}{k}(k-1)^{k-1} + (r-1)^r M^{-\lceil \frac{r}{2}\rceil}. \tag{45}$$

Proof We assume w.l.o.g. that $E[X] \equiv M^1[X] = 0$, since estimator $S^r_M[X]$ and central moments are independent of the value $E[X]$. Notice that (44) is satisfied when $r = 2$. Indeed, (45) implies that the sum over $\underline{j}\in\Xi^2_M$ vanish and therefore, since $M^0[X] \equiv 1$, the identity (44) is equivalent to

$$E\left[S^2_M[X]\right] = M^2[X] + M^{-1}\left(M^0[X]M^2[X] - 2M^2[X]\right) = \frac{M-1}{M}M^2[X] \tag{46}$$

Analogously, for $r = 3$ the estimate (44) is equivalent to

$$E\left[S^3_M[X]\right] = M^3[X] - \frac{3}{M}M^3[X] + \frac{2}{M^2}M^3[X]. \tag{47}$$

and for $r = 4$ we have

$$\begin{aligned} E\left[S^4_M[X]\right] &= M^4[X] + \frac{1}{M}(6M^2[X]^2 - 4M^4[X]) + \frac{1}{M^2}(6M^4[X] - 15M^2[X]^2) \\ &\quad + \frac{1}{M^3}(9M^2[X]^2 - 3M^4[X]). \end{aligned} \tag{48}$$

Representations (46), (47) and (48) hold true in view of (26),(27) and the assertion of the lemma follows for $2 \leq r$

the identity (54) follows by the counting argument similar to the proof of Lemma 1. Utilizing the estimate (37) we get the upper bound

$$\begin{aligned}
&\sum_{k=4}^{r-2} \frac{1}{M^k}\binom{r}{k}\left(|\mathcal{J}_M^k| + k|\mathcal{J}_M^{k-1}|\right)\\
&\quad\le \sum_{k=4}^{r-2} \frac{1}{M^k}\binom{r}{k}\left((k-1)^{k-1}M^{\lfloor\frac{k}{2}\rfloor} + k(k-2)^{k-2}(M-1)^{\lfloor\frac{k-1}{2}\rfloor}\right)\\
&\quad\le \sum_{k=4}^{r-2} 2M^{-\lceil\frac{k}{2}\rceil}\binom{r}{k}(k-1)^{k-1}.
\end{aligned}$$

Moreover, it holds that

$$\frac{2}{M^2}\binom{r}{2} + \frac{4}{M^2}\binom{r}{3} \le 2M^{-2}\binom{r}{3}2^2; \quad (r-1)M^{-r}|\mathcal{J}_M^r| \le M^{-\lceil\frac{r}{2}\rceil}(r-1)^r$$

and thereby the proof is complete.

Lemma 4 Let $X, Y : \Omega \to H$ be two sufficiently smooth random variables with H the Hilbert space $\mathbb{R}$ or $W^{s,2}(D)$. For $r \ge 2$ the estimate

$$\|M^r[X] - M^r[Y] - E[S_M^r[X] - S_M^r[Y]]\|_H \le \frac{r(r+1)}{2M}(1 + \varepsilon_b(M;r))K(X,Y;r) \tag{55}$$

holds, where $K(X,Y;r)$ is the upper bound in Lemma 2. We have $\varepsilon_b(M;r) \in O(M^{-1})$ and for $r > 3$ the estimate holds for

$$\varepsilon_b(M;r) = \frac{2}{r(r+1)}\left(2\sum_{k=3}^{r-2} M^{-\lceil\frac{k}{2}\rceil+1}\binom{r}{k}(k-1)^{k-1} + (r-1)^r M^{-\lceil\frac{r}{2}\rceil}\right) \tag{56}$$

and $\varepsilon_b(M;r) = 0$ for $r = 2, 3$.

Proof Assume w.l.o.g. that $E[X] = E[Y] = 0$. Then by Lemma 3 and the triangle inequality, we obtain

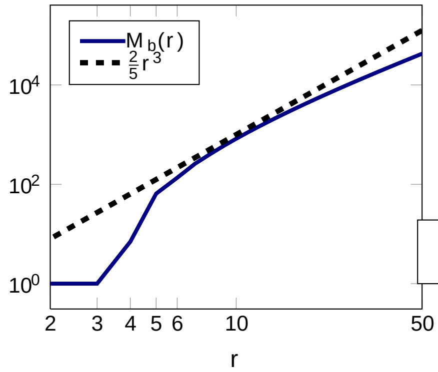
$$\begin{aligned}
&\|M^r[X] - M^r[Y] - E[S_M^r[X] - S_M^r[Y]]\|_H\\
&\quad\le M^{-1}\frac{r(r-1)}{2}\|M^{r-2}[X]M^2[X] - M^{r-2}[Y]M^2[Y]\|_H\\
&\quad\quad + M^{-1}r\|M^r[X] - M^r[Y]\|_H + \sum_{\mathbf{j}\in\mathcal{J}_M^r}|c(\mathbf{j};M;r)|\|E[X_{\mathbf{j}} - Y_{\mathbf{j}}]\|_H.
\end{aligned}$$

We first apply Lemma 2 to estimate the norms in H and then Lemma 3 to bound the sum over $\mathcal{J}_M^r$ and gain ε_b for $r > 3$. For $r = 2, 3$ we have $\varepsilon_b(r) = 0$ due to (46) and (47). Thus the Lemma is proved.

Lemma 5 Let $X, Y : \Omega \to H$ be two sufficiently smooth random variables with H the Hilbert space $\mathbb{R}$ or $W^{s,2}(D)$. For $r \ge 2$ the estimate

$$V(S_M^r[X] - S_M^r[Y]) \le M^{-1}(r+1)^2(1 + \varepsilon_v(M;r))K(X,Y;r)^2 \tag{57}$$

The summands are only nonzero when


$M_b(r)$
$\frac{2}{5}r^3$
10^4
10^2
10^0
2
3
4
5
6
10
50
r

where we have the estimate

$$M_e(r) \leq \max(M_b(r), M_v(r), 2r^2). \tag{68}$$

Proof Due to (15) we have

$$\begin{aligned}\|M^r[X] - S_M^r[X_L]\|_2^2 &= \|M^r[X] - E[S_M^r[X_L]]\|_H^2 + V(S_M^r[X_L])\\ &\leq 2\|M^r[X] - M^r[X_L]\|_H^2 + 2\|M^r[X_L] - E[S_M^r[X_L]]\|_H^2 + V(S_M^r[X_L]).\end{aligned}$$

by applying the triangle inequality in the second step. Using Lemma 4 and Lemma 5 we gain

$$\begin{aligned}\|M^r[X] - S_M^r[X_L]\|_2^2 &\leq 2\|M^r[X] - M^r[X_L]\|_H^2\\ &\quad + M^{-2}\frac{r^2(r+1)^2}{2}c_H^{2(r-1)}\|X_L\|_{2r}^{2r}(1+\varepsilon_b(M, rM\end{aligned}$$

6 A random obstacle problem

We apply the abstract framework developed above to a class of obstacle problems with rough random obstacles. In this section we briefly introduce the mathematical framework (see [4, Sect. 6, 8] for further details) and present results of numerical experiments in Section 7.

Let D R^d be a bounded convex domain, $\in C(D)$, 0 on ∂D a continuous function and $f \in L^2(D$

The solution $u_\ell(\omega)$ is unique, cf. [11]. Moreover, according to [4] it holds that

$$\|u - u_\ell\|_{L^{2p}(\Omega;W^{1,2p}(D))} \lesssim h_\ell^{\frac{1}{p}} \left(\|f\|_{L^{2p}(\Omega;L^2(D))} + \|\psi\|_{L^{2p}(\Omega;H^2(D))}\right) \tag{84}$$

for $1 \le p \le \infty$ provided $f \in L^{2p}(\Omega;L^2(D))$ and $\psi \in L^{2p}(\Omega;H^2(D))$, see [4] for details.

Instead of only having a random obstacle and a random volume force, one might also have to model random material parameters. For such formulations and related convergence results see [9,14].

In this paper we are particularly interested in the case of rough random obstacles representing e.g. the uneven structure of asphalt read surfaces. We utilize a rough obstacle model from [16], representing of the obstacle $\psi(x)$ as a Fourier series

$$\psi(x) = \sum_q B_q(H)\cos(q \cdot x + \phi_q); \tag{85}$$

where $x \in [0;L]^2$ for simplicity. The sum is over all $q \in \frac{2\pi}{L}\mathbb{Z}^2$, the amplitudes $B_q(H)$ depend on the frequency q and the so called Hurst coefficient $H \in [0;1]$. The ϕ_q are independent random variables, uniformly distributed in $[0;2\pi)$. Isotropic self-affine obstacles obey the law

$$B_q(H) \propto \begin{cases} |q|^{-(H+1)}; & q_\ell \le |q| \le q_s \\ 0; & \text{otherwise}. \end{cases} \tag{86}$$

As obstacle for the numerical experiments in the following section we use the surface (85) with particular parameters

$$\begin{aligned} B_q(H) &= \frac{\pi}{25}(2\pi\max(|q|;q_l))^{-(H+1)}; \qquad q_0 \le |q| \le q_s; \\ q_0 &= 1; \quad q_l = 10; \quad q_s = 26; \end{aligned} \tag{87}$$

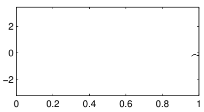


Fig. 2 Self affine surfaces $\psi(x)$ in 1d with $H = 1; 0.5$ and 0 (left column, from top to bottom). The right column shows the magnification of the box on the left.

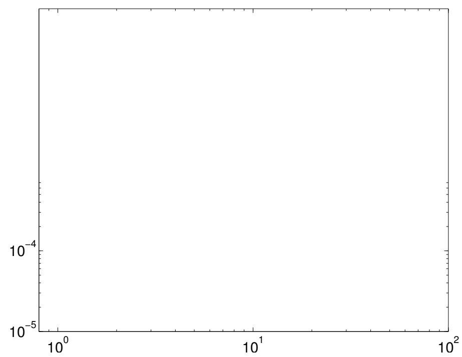


Fig. 3 The values of $B_q(H)$ for ψ defined in (87) in double logarithmic scale. H indicates the height of the plateau and the slope for $q_\ell \le q \le q_s$.

where the sum in (85) now runs over Z^2 (see Figure 3). To gain a randomly rough obstacle we model H as a random variable as well as all phase shifts $'_q$:

$$H \quad U(0;1); \quad '_q \quad U(0;2\ ); \quad q_0 \quad j\,qj \quad q_s: \tag{88}$$

Those random variables are assumed to be mutually independent. Two realizations of this obstacle are plotted in the next section (Figures 4 and 5). We refer to [16] and our previous work [4] for further details on this model.

7 Numerical Experiments

In this section we report on results of numerical experiments for the model obstacle problem described above with $D = [\ 1;1]^2$, $f = \ 5$, $uj_{@D} = \frac{1}{2}$ and random obstacle parametrized by (x) as described in Section 6. In Fig. 4 and 5 we show two realizations of the obstacle pro le and the corresponding solutions for the case of high and low roughness respectively. The computations involve the hierarchy of the nite element spaces $V_`$ de ned in (83) with meshes $T_`$. The coarsest triangulation T_1 consists of four congruent triangles sharing $(0;0)$ as a vertex. Finer meshes $T_{`+1}$ are de ned recursively as the uniform red re nement of coarser meshes $T_`$ by halving the edge of each element so that $h_` \quad N_`^{\frac{1}{2}}$.

As a solver we implemented di erent variants of the Monotone Multigrid Method described in [12]; the Multilevel Subset Decomposition Algorithm appeared to be the best for our model problem. For this algorithm a log-linear cost has been proved, cf. [17], [14, Section 4.5]. In our experiments we observe almost linear complexity, see Fig. 8 indicating that $\quad 1$ in (73).

We mention that e cient updating of a single level estimator of higheratorts Meth343(m6428(w(m642nglvi394(E642nask.4

is a space of polynomials of degree r. Notice, however, that $V_{\cdot}^{r}$ is not required for solving the discrete formulation, but only for evaluating the estimator S_{ML}^{r} [u] (cf. [4] for estimation of the variance). Therefore the computational cost associated with the use of the high order space $V_{\cdot}^{r}$ is negligible.

Obviously, this issue does not appear when estimating higher order statistical moments of scalar quantities. In this paper we report on convergence results for the r-th central statistical moments of the size of the coincidence set

$$(!\ ) = f\,x : u$$

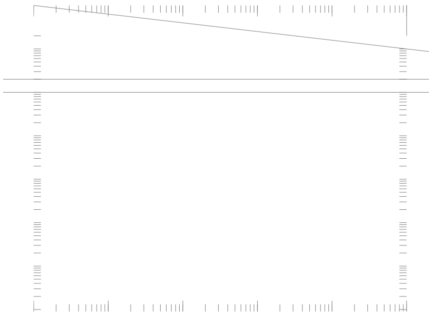


Fig. 6 Convergence of the bias part of the estimator for the rst six moments.

Fig. 7 Convergence of the variance of the level corrections (the variance part of the estimator)

Fig. 8]TJ/F17 7.9701 Tf 32870420 Td [(CAv30(verag)-3273tima)-3273tio-3272cormput

which is a consequence of the above mentioned condition. Starting from the third level we observe an almost uniform distribution of the runtime over the refinement levels whereas the number of samples M_ℓ decays exponentially with increasing level index.

Finally we show the convergence of two consecutive approximation of the first,