Applied Radiation and Isotopes 70 (2012) 315–323

Contents lists available at SciVerse ScienceDirect

Applied Radiation and Isotopes

journal homepage: www.elsevier.com/locate/apradiso

Estimating statistical uncertainty of Monte Carlo efficiency-gain in the context of a correlated sampling Monte Carlo code for brachytherapy treatment planning with non-normal dose distribution

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ARTICLE INFO

Article history:
Received 8 March 2011
Received in revised form
11 September 2011
Accepted 21 September 2011
Available online 29 September 2011

Keywords:
Monte Carlo
Correlated sampling
Efficiency
Uncertainty
Bootstrap

ABSTRACT

Correlated sampling Monte Carlo methods can shorten computing times in brachytherapy treatment planning. Monte Carlo efficiency is typically estimated via efficiency gain, defined as the reduction in computing time by correlated sampling relative to conventional Monte Carlo methods when equal statistical uncertainties have been achieved. The determination of the efficiency gain uncertainty arising from random effects, however, is not a straightforward task specially when the error distribution is non-normal. The purpose of this study is to evaluate the applicability of the *F* distribution and standardized uncertainty propagation methods (widely used in metrology to estimate uncertainty of physical measurements) for predicting confidence intervals about efficiency gain estimates derived from single Monte Carlo runs using fixed-collision correlated sampling in a simplified brachytherapy geometry. A bootstrap based algorithm was used to simulate the probability distribution of the efficiency gain estimates and the shortest 95% confidence interval was estimated from this distribution. It was found that the corresponding relative uncertainty was as large as 37% for this particular problem. The uncertainty propagation framework predicted confidence intervals reasonably well; however its main disadvantage was that uncertainties of input quantities had to be calculated in a separate run via a Monte Carlo method. The *F* distribution noticeably underestimated the confidence interval. These discrepancies were influenced by several photons with large statistical weights which made extremely large contributions to the scored absorbed dose difference. The mechanism of acquiring high statistical weights in the fixed-collision correlated sampling method was explained and a mitigation strategy was proposed.

1. Introduction

Monte Carlo transport simulations offer a powerful tool to accurately calculate absorbed dose distributions in complex geometries. Such simulations have successfully been used in the past to study the perturbing effects of heterogeneities in typical brachytherapy configurations (Williamson et al., 1993; Kirov et al., 1996). Due to the statistical nature of the Monte Carlo method, the results are associated with an uncertainty that is inversely proportional to the number of photon histories simulated and thus to the computing time. For the purpose of clinical patient dose-planning, where the geometry of the problem varies from patient to patient, the central processing unit (CPU) time of no more than a few minutes is desirable. To achieve this goal, variance reduction techniques therefore need to be exploited. Hedtjärn et al. (2002) tested a fixed-collision correlated sampling method (Rief, 1984; Lux and Koblinger, 1991; Sampson et al., 2009) suitable for use in photon transport codes. In contrast to previous applications of correlated sampling to radiation dosimetry transport (Ma and Nahum, 1993; Holmes et al., 1993) where only the initial trajectory and random number seed of particle histories are fixed, the locations and outcomes of photon collisions, in terms of scattered photon energy and angle, are all fixed and only the particle weights are allowed to vary with the perturbing geometry. Use of the fixed-collision method benefits from the applicability of the kerma approximation in calculating absorbed dose implying that only photon collisions need to be fixed.

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doi:10.1016/j.apradiso.2011.09.015

The efficiency of a Monte Carlo method is inversely proportional to a product of the total CPU time and the variance of the scored quantity. The efficiency gain of a correlated sampling scheme compared to a conventional one is then often defined as the ratio of their efficiencies. Its estimate is a stochastic variable whose realization may differ from the non-stochastic true value; it is affected by uncertainty. Methods for evaluating measurement uncertainty (JCGM, 2009) include: (i) uncertainty frameworks based on the law of propagation of uncertainty, e.g., the GUM report of the Joint Committee for Guides in Metrology (JCGM, 2008b) or Report 1297 from NIST (Taylor and Kuyatt, 1994) hereafter referred to as GUM framework; (ii) standard parametric statistics, in which the probability distribution of the output quantity (efficiency gain estimate in our case) is derived via mathematical analysis, and (iii) Monte Carlo or bootstrapping methods, in which the distribution of the output quantity is established by making random draws from the probability distributions of input quantities (JCGM, 2008b). The parametric statistics approach provides the most accurate predictions if its assumptions about distributions of input quantities are correct. The GUM framework is often used in engineering and applied physics if distributions of output quantities can be approximated by normal or t distributions. In other cases, Monte Carlo sampling may be the only viable alternative. Since the ratio of two random variables (the efficiency gain estimate) may deviate from both the normal and t distributions assumed in the GUM framework, and the asymptotic normality of the means of scored absorbed dose and dose difference often assumed in the parametric statistics approach cannot be guaranteed, it is of interest whether these methods can be used to accurately predict the uncertainty of efficiency gain.

The aim of this work is to evaluate the applicability of the GUM framework and a commonly used parametric statistical model for analysis of variance (the F distribution) for the calculation of uncertainty in fixed-collision correlated Monte Carlo efficiency relative to that of a conventional Monte Carlo code for a typical idealized brachytherapy dose calculation geometry. As the efficiency gain and its uncertainty are closely related to the implementation of the correlated sampling method, the aim is also to analyze the inner working of the method and propose improvements of the current implementation.

2. Theory

In this section we introduce the concepts of efficiency gain, correlated sampling, bootstrap method and highest density intervals; they will be needed for an in-depth discussion of the efficiency gain estimate behavior and construction of confidence intervals for that quantity.

2.1. Efficiency and efficiency gain

Let the term "history" denotes a sequence of interactions, initiated by emission of a primary particle by the radioactive source, that the particle experiences as it loses energy. We assume that the Monte Carlo simulation is time independent (does not depend on history number) and interactions in one history are not affected by interactions in previous histories. In mathematical terms, assume that a history i contributes a certain amount Z_i to the scored quantity (e.g., absorbed dose). Z_i is a random variable with a distribution D_Z, mean value $E(Z_i)$ and variance $V(Z_i)$. This distribution and hence the mean value and variance are the same for all histories. Moreover, the Z_i are independent random variables. Under these assumptions, a simulated physical quantity can be estimated by the average $\overline{Z} = (1/n)\sum_{i=1}^{n} Z_i$. Efficiency $\varepsilon_{\overline{Z}}$ of the Monte Carlo method is then conventionally defined as the inverse of the product of the variance $V(\overline{Z})$ of the average $\overline{Z}$ times the computing (CPU) time $t_{\overline{Z}}$:

$$\varepsilon_{\overline{Z}} \equiv [V(\overline{Z})t_{\overline{Z}}]^{-1}. \tag{1}$$

For simplicity we assume that the time $t_{\overline{Z}}$ is a non-stochastic quantity. The efficiency $\varepsilon_{\overline{Z}}$ is a non-stochastic quantity too. Since $V(\overline{Z}) = V(Z)/n$, the efficiency of a run consisting of n histories is independent of the number of histories:

$$\varepsilon_{\overline{Z}} = [V(\overline{Z})t_{\overline{Z}}]^{-1} = [V(Z_1)t_{\overline{Z}}/n]^{-1} = [V(Z_1)t_Z]^{-1}. \tag{2}$$

Here, $t_Z = t_{\overline{Z}}/n$ is the average CPU time per one history.

The efficiency of a sampling scheme is usually quantified in terms of the efficiency gain, γ, defined as a ratio of the efficiency of the tested sampling method, $\varepsilon_{\overline{T}}$, to that of the reference sampling method, $\varepsilon_{\overline{R}}$

$$\gamma \equiv \frac{\varepsilon_{\overline{T}}}{\varepsilon_{\overline{R}}} = \frac{V(\overline{R})t_{\overline{R}}}{V(\overline{T})t_{\overline{T}}} = \frac{V(R)t_R}{V(T)t_T} = \frac{n_R^{-1}V(R\sqrt{t_{\overline{R}}})}{n_T^{-1}V(T\sqrt{t_{\overline{T}}})}, \tag{3}$$

where n_R and n_T are the numbers of histories of the reference and tested methods, respectively. This expresses the reduction in CPU time $t_{\overline{T}}$, that is achieved in obtaining equal uncertainties $V(\overline{T}) = V(\overline{R})$ of the calculated value compared to the corresponding CPU time $t_{\overline{R}}$ using the reference sampling scheme. Alternatively, efficiency gain expresses the increase in statistical precision (reduced variance), that is achieved for equal CPU times $t_{\overline{T}} = t_{\overline{R}}$.

Efficiency gain γ in Eq. (3) is a non-stochastic quantity whose value is typically estimated using the (stochastic) efficiency gain estimate G:

$$G \equiv \frac{n_R^{-1}S_R^2 t_{\overline{R}}}{n_T^{-1}S_T^2 t_{\overline{T}}}, \tag{4}$$

where the estimate of the variance of the reference sampling method, S_R^2, is defined for n_R samples R_i as

$$S_R^2 \equiv \frac{1}{n_R - 1}\sum_{i=1}^{n_R}(R_i - \overline{R})^2 \tag{5}$$

and similarly for the estimate of the variance of the tested sampling method, S_T^2. By introducing variables $X = R\sqrt{t_{\overline{R}}}$ and $Y = T\sqrt{t_{\overline{T}}}$, Eq. (4) can also be written as

$$G = \frac{n_R^{-1}S_X^2}{n_T^{-1}S_Y^2}, \tag{6}$$

where S_X^2 and S_Y^2 are sample variances defined by formula (5). For brevity, we often call calculated samples of the efficiency gain estimate G simply as efficiency gain. This should not lead to a confusion since γ cannot be directly calculated.

2.2. Correlated sampling

The correlated sampling algorithm has been described extensively by Hedtjärn et al. (2002), Sampson et al. (2009): only aspects pertinent to this study will be described here. In correlated sampling, the heterogeneous geometry is treated as a perturbation of the corresponding homogeneous (unperturbed) system, which consists solely of uniform density water. As such, the absorbed dose delivered to the heterogeneous system, $D_{het}(\boldsymbol{x})$, is assumed to be a correction to the absorbed dose delivered, $D_{hom}(\boldsymbol{x})$, in the corresponding homogeneous system:

$$D_{het}(\boldsymbol{x}) = \mathrm{HCF}(\boldsymbol{x}) \cdot D_{hom}(\boldsymbol{x}), \tag{7}$$

where $\mathrm{HCF}(\boldsymbol{x})$ is the heterogeneity correction factor and $\boldsymbol{x}$ denotes the position of a given voxel in a 3D grid constituting the system. An estimate of the HCF calculated by the correlated sampling