Perturbation Monte Carlo estimators and derivatives:

1 Discrete Absorption Weighting (DAW)

Discrete absorption weighting adjusts the photon weight at each collision. In a homogeneous medium, the terminal estimator with discrete absorption weigthing modifies the photon weight at each collision by a factor $\frac{\mu_s}{\mu_t}$. Therefore, if a photon suffers k collisions before being detected, the "modified" terminal estimator with discrete absorption weighting tallies[1]

$$\xi_{DAW} = \begin{cases} \left(\frac{\mu_s}{\mu_t}\right)^k & \text{if the photon exits the tissue at the detector} \\ 0 & \text{otherwise.} \end{cases} \tag{1}$$

This estimator is unbiased, and so $E[\xi_{DAW}] = \int \xi_{DAW} d\nu = I$.

Determination of the perturbed reaction rate I^* using the terminal estimator with discrete absorption weighting is accomplished by modifying the weight at each collision by the appropriate weight factors. If the photon suffers k collisions and is absorbed in the detector volume V, then the resulting weight is

$$\xi^*_{DAW} = \left(\frac{\mu_s}{\mu_t}\right)^k \left(\frac{\mu^*_s/\mu^*_t}{\mu_s/\mu_t}\right)^j \left(\frac{\mu^*_t}{\mu_t}\right)^j \exp\left[-\left(\mu^*_t - \mu_t\right) S\right] \tag{2}$$

$$= \left(\frac{\mu_s}{\mu_t}\right)^k \left(\frac{\mu^*_s}{\mu_s}\right)^j \exp\left[-\left(\mu^*_s + \mu^*_a - \mu_s - \mu_a\right) S\right] \tag{3}$$

where k is the number of collisions prior to detection, j is the number of collisions in the perturbed region and S is the total path length in the perturbed region. If the photon does not get absorbed in V, the estimator scores 0. This estimator is unbiased with respect to the background measure and so $E_\nu[\xi^*_{DAW}] = I^*$.

2 Discrete Absorption Weighting Derivatives

2.1 With respect to μ^*_a

Derivative can be taken directly:

$$\frac{\partial \xi^*_{DAW}}{d\mu^*_a} = \left(\frac{\mu_s}{\mu_t}\right)^k \left(\frac{\mu^*_s}{\mu_s}\right)^j (-S) \exp\left[-\left(\mu^*_s + \mu^*_a - \mu_s - \mu_a\right) S\right] \tag{4}$$

Simplified for numerical stability to (which applies if $j = 1$):

$$\frac{\partial \xi^*_{DAW}}{d\mu^*_a} = \left(\frac{\mu_s}{\mu_t}\right)^k (-S) \left\{\left(\frac{\mu^*_s}{\mu_s}\right) \exp\left[-\left(\mu^*_s + \mu^*_a - \mu_s - \mu_a\right) S/j\right]\right\}^j \tag{5}$$

2.2 With respect to μ^*_s

Taking derivative with respect to μ^*_s gives:

$$\frac{\partial \xi^*_{DAW}}{d\mu^*_s} = \left(\frac{\mu_s}{\mu_t}\right)^k \left\{(j/\mu_s) \left(\frac{\mu^*_s}{\mu_s}\right)^{j-1} \exp\left[-\left(\mu^*_s + \mu^*_a - \mu_s - \mu_a\right) S\right] + \left(\frac{\mu^*_s}{\mu_s}\right)^j (-S) \exp\left[-\left(\mu^*_s + \mu^*_a - \mu_s - \mu_a\right) S\right]\right\} \tag{6}$$

Multiplying by $\left(\frac{\mu_s^*}{\mu_s^*}\right) = 1$ and rearranging terms:

$$\frac{\partial\xi_{DAW}^*}{d\mu_s^*} = \left(\frac{\mu_s}{\mu_t}\right)^k \left\{ \left(\frac{\mu_s^*}{\mu_s^*}\right)\left(\frac{j}{\mu_s}\right)\left(\frac{\mu_s^*}{\mu_s}\right)^{j-1} \exp[-(\mu_s^* + \mu_a^* - \mu_s - \mu_a)S] + \right. \tag{7}$$

$$\left. \left(\frac{\mu_s^*}{\mu_s}\right)^j (-S)\exp[-(\mu_s^* + \mu_a^* - \mu_s - \mu_a)S] \right\} \tag{8}$$

$$= \left(\frac{\mu_s}{\mu_t}\right)^k \left\{ \left(\frac{j}{\mu_s^*}\right)\left(\frac{\mu_s^*}{\mu_s}\right)^j \exp[-(\mu_s^* + \mu_a^* - \mu_s - \mu_a)S] + \right. \tag{9}$$

$$\left. \left(\frac{\mu_s^*}{\mu_s}\right)^j (-S)\exp[-(\mu_s^* + \mu_a^* - \mu_s - \mu_a)S] \right\} \tag{10}$$

$$= \left(\frac{\mu_s}{\mu_t}\right)^k \left(\frac{j}{\mu_s^*} - S\right) \left\{ \left(\frac{\mu_s^*}{\mu_s}\right)^j \exp[-(\mu_s^* + \mu_a^* - \mu_s - \mu_a)S] \right\} \tag{11}$$

Simplified for numerical stability to:

$$\frac{\partial\xi_{DAW}^*}{d\mu_s^*} = \left(\frac{\mu_s}{\mu_t}\right)^k \left(\frac{j}{\mu_s^*} - S\right) \left\{ \left(\frac{\mu_s^*}{\mu_s}\right) \exp[-(\mu_s^* + \mu_a^* - \mu_s - \mu_a)S/j] \right\}^j \tag{12}$$

3 Continuous Absorption Weighting (CAW)

Continuous absorption weighting decays the photon weight continuously along its path length. In a homogenous medium, if the photon's path length from source to exiting the tissue is L, then [1]

$$\xi_{CAW} = \begin{cases} \exp\{-\mu_a L\} & \text{if the photon exits the tissue at the detector} \\ 0 & \text{otherwise.} \end{cases} \tag{13}$$

This estimator is unbiased, and so $E[\xi_{CAW}] = \int \xi_{CAW} d\nu = I$.

Again, determination of the perturbed reaction rate I^* using the terminal estimator with continuous absorption weighting is accomplished by modifying the weight at each collision by the appropriate weight factors.

$$\xi_{CAW}^* = \exp\{-\mu_a L\} \left[\frac{\exp(-\mu_a^* S)}{\exp(-\mu_a S)}\right] \left(\frac{\mu_s^*}{\mu_s}\right)^j \exp\left[-\left(\mu_s^* - \mu_s\right) S\right] \tag{14}$$

$$= \exp\{-\mu_a L\} \left[\exp\left(-\mu_a^* + \mu_a\right) S\right] \left(\frac{\mu_s^*}{\mu_s}\right)^j \exp\left[-\left(\mu_s^* - \mu_s\right) S\right] \tag{15}$$

$$= \exp\{-\mu_a L\} \left(\frac{\mu_s^*}{\mu_s}\right)^j \exp\left[-\left(\mu_s^* + \mu_a^* - \mu_s - \mu_a\right) S\right] \tag{16}$$

where j is the number of collisions in the perturbed region and S is the total path length in the perturbed region.

Note! The weight modifications due to the Nadon-Nikodym derivative for both DAW and CAW are equivalent upon reorganization of terms (for $j \geq 0$). Therefore, derivative factors are equivalent. Just to check...

4 Continuous Absorption Weighting Derivatives (CAW)

4.1 With respect to μ_a^*

Derivative can be taken directly:

$$\frac{\partial \xi^*_{CAW}}{\partial \mu_a^*} = \exp\{-\mu_a L\}(-S)\left(\frac{\mu_s^*}{\mu_s}\right)^j \exp\left[-\left(\mu_s^* + \mu_a^* - \mu_s - \mu_a\right) S\right] \tag{17}$$

Simplified for numerical stability to (which holds for $j = 1$):

$$\frac{\partial \xi^*_{CAW}}{\partial \mu_a^*} = \exp\{-\mu_a L\}(-S)\left\{\left(\frac{\mu_s^*}{\mu_s}\right) \exp\left[-\left(\mu_s^* + \mu_a^* - \mu_s - \mu_a\right) S/j\right]\right\}^j \tag{18}$$

4.2 With respect to μ_s^*

Taking derivative with respect to μ_s^* gives:

$$\begin{aligned}\frac{\partial \xi^*_{CAW}}{\partial \mu_s^*} &= \exp\{-\mu_a L\}(j/\mu_s)\left(\frac{\mu_s^*}{\mu_s}\right)^{j-1} \exp\left[-\left(\mu_s^* + \mu_a^* - \mu_s - \mu_a\right) S\right] + \\ &\left(\frac{\mu_s^*}{\mu_s}\right)^j (-S) \exp\left[-\left(\mu_s^* + \mu_a^* - \mu_s - \mu_a\right) S\right] \end{aligned} \tag{19}$$

Multiplying by $\left(\frac{\mu_s^*}{\mu_s^*}\right) = 1$ and rearranging terms:

$$\frac{\partial \xi^*_{CAW}}{d\mu_s^*} = \exp\{-\mu_a L\}\left\{\left(\frac{\mu_s^*}{\mu_s^*}\right)\left(\frac{j}{\mu_s}\right)\left(\frac{\mu_s^*}{\mu_s}\right)^{j-1} \exp[-(\mu_s^* + \mu_a^* - \mu_s - \mu_a)S] + \right. \tag{20}$$

$$\left. \left(\frac{\mu_s^*}{\mu_s}\right)^j (-S) \exp[-(\mu_s^* + \mu_a^* - \mu_s - \mu_a)S]\right\} \tag{21}$$

$$= \exp\{-\mu_a L\}\left\{\left(\frac{j}{\mu_s^*}\right)\left(\frac{\mu_s^*}{\mu_s}\right)^j \exp[-(\mu_s^* + \mu_a^* - \mu_s - \mu_a)S] + \right. \tag{22}$$

$$\left. \left(\frac{\mu_s^*}{\mu_s}\right)^j (-S) \exp[-(\mu_s^* + \mu_a^* - \mu_s - \mu_a)S]\right\} \tag{23}$$

$$= \exp\{-\mu_a L\}\left(\frac{j}{\mu_s^*} - S\right)\left\{\left(\frac{\mu_s^*}{\mu_s}\right)^j \exp[-(\mu_s^* + \mu_a^* - \mu_s - \mu_a)S]\right\} \tag{24}$$

Simplified for numerical stability to:

$$\frac{\partial \xi^*_{CAW}}{d\mu_s^*} = \exp\{-\mu_a L\}\left(\frac{j}{\mu_s^*} - S\right)\left\{\left(\frac{\mu_s^*}{\mu_s}\right) \exp[-(\mu_s^* + \mu_a^* - \mu_s - \mu_a)S/j]\right\}^j \tag{25}$$

References

[1] C. K. Hayakawa, J. Spanier, and V. Venugopalan. Comparative analysis of discrete and continuous absorption weighting estimators used in Monte Carlo simulations of radiative transport in turbid media. *J. Opt. Soc. Am. A*, 31(2):301–311, 2014.