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Validation of a monte carlo platform for the optical modelling of pulse oximetry

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Abstract. A custom Monte Carlo (MC) platform has been established to generate optophysiological models of mechanisms in pulse oximetry. The current research is an exploration of the process of empirically validating such a platform. With the growing availability and accuracy of tissue optical properties in literatures, MC simulation of light-tissue interaction is providing increasingly valuable information for optical bio-monitoring research. However, the extent of the validity of results from such simulations depends heavily on its agreement with empirical data. The use of images captured from a CMOS camera for the construction of intensity distributions of light transmitted through the human finger has been investigated to compare with corresponding distributions produced in the MC simulations.

1. Introduction

Photoplethysmography (PPG) is an optical biomonitoring technique that non-invasively measures arterial pulsations in-vivo. Its ease of use and convenience make it an attractive area of research in the biomedical and clinical community. Among its applications, pulse oximetry—the determination of arterial oxygen saturation—is the most widespread thanks to its ability to alert the clinician of the presence of hypoxemia in real-time. Pulse oximetry has become a standard of patient monitoring during anaesthesia, in recovery rooms and under intensive care. However, oximeters have a number of factors that lead to inaccurate readings and limit their applicability. As such, these are practable areas of research when attempting to increase the reliability and applicability of the technology. The success of solutions to engineering issues of pulse oximetry depends heavily on the validity of the assumptions used to correlate the PPG signals. The adverse effects of these issues are generally quantified according to the sensitivity and specificity of oximeters under the relevant scenarios, often overlooking the mechanisms leading to such inaccuracies due to the inherent complexity and variability of the physical mechanisms involved. With the increasing availability and accuracy of tissue optical properties in literature, the use of numerical solutions of light propagation in human tissue are providing increasingly valuable insights into such mechanisms.

1.1. Tissue Optical Modeling

The operation principal of current pulse oximeters is commonly described using the Beer-Lambert model, where the measuring site is treated as a blood-filled cuvette with no scattering effects and the light sources are assumed to be monochromatic. The highly scattering nature of human tissue clearly

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contradicts these assumptions, but the model illustrates the common simplification process inherent in the area.

Numerous models that predict photon transport in tissue have been developed,\(^4\) most of which are simplified forms of the radiation transfer theory (RTT). The latter is commonly accepted as a sufficiently strict mathematical description of continuous wave (CW) light propagation in a scattering medium\(^5\) and relies on the absorption and scattering coefficients \(\mu_a\) and \(\mu_s\), and anisotropy factor \(g\) for an optical description of the medium. Monte Carlo (MC) radiation transport techniques are based on the stochastic nature of radiation interactions, and in the context of tissue optics, they provide a numerical solution of the RTT equation. As a finite element method, it is suited for complex geometries and is capable of achieving very high degrees of accuracy at the expense of heavy computational load.

The accuracy of optical propagation models depends heavily on that of the tissue optical properties. In recent years, several substantial investigations have led to the determination of increasingly accurate optical properties of the constituents of PPG monitoring sites in a range of wavelengths.\(^4\)\(^-\)\(^10\)

1.2. Validity of Simulations
In order for a simulation of optical propagation to provide expected results, it contains an accurate geometrical model of the bodies in which the propagation occurs and it must take into account all the physical phenomena involved in the real life process. However, in the case of tissue optical modeling, a complete geometrical description of the tissue body, and consequently, the complex interactions between the mechanisms involved are difficult to achieve using available techniques. Some simplifying assumptions could therefore be made about the process. The degree to which the simulated results under these assumptions correlate with real-life measurements of the system dictates the accuracy of using such assumptions in a theoretical model.

1.3. Aims and Objectives of Study
In the MC simulation work,\(^13\) we proposed the combination of optical properties and standardised models of human anatomy and physiology in MC simulations of light transport to deliver a characterisation of the mechanisms and consequent systematic reduction of the effects of issues with an adverse effect to pulse oximetry. To this end, a MC platform has been created to perform light transport simulations on complex tissue geometries. The current phase of the investigation aims to validate the distributions of transmitted light around the finger acquired through MC simulations by constructing equivalent distributions from images acquired through a CMOS camera. This data will be used to determine the degree of correlation between simulated and empirical data under the assumptions used, and to determine the validity of several methodologies for the validation of such simulations.

2. Materials and Methods

2.1. Simulation Settings
An accurate 3D anatomical model (Zygote Media Group, USA) of a male adult finger was used to numerically resolve the RTT equation for the case of a single LED lightsource at 633nm and 850nm, placed near the standard position found in commercial probes. The simulation results were used to distinguish localised light intensities that vary due to the cardiovascular cycle from those that are static, thus providing a means to construct static and dynamic intensity distributions mapped to the surface of the finger. Sensor responses were generated by scanning a square bucket of arbitrary size in 0.1mm steps from -1 to 1 mm longitudinally and from 0 to 360º circumferentially.

Simulations were configured in accordance to a series of simplifying assumptions. Internal reflection and refraction between boundaries was disregarded, with the exception of that between epidermis and air. The contribution of bone structures was simplified by disregarding their volumetric optical properties and only taking into account surface reflectance. The diffusion approximation of
RTT, also known as the $P_1$ approximation,\textsuperscript{6} was used for all volumetric optical parameters in the simulation in order to reduce the raytracing time by a factor of five, and rays were traced using spatial and angular Sobol sampling\textsuperscript{12} to increase the convergence rate of the data.

Table I: Optical properties used for MC raytraces, sources of data, and ratios used to determine the coefficients at 850 nm.

<table>
<thead>
<tr>
<th>Tissue Type</th>
<th>$\mu_a (\text{mm}^{-1})$</th>
<th>$\mu_s' (\text{mm}^{-1})$</th>
<th>$\mu_a (\text{mm}^{-1})$</th>
<th>$\mu_s' (\text{mm}^{-1})$</th>
<th>References</th>
</tr>
</thead>
<tbody>
<tr>
<td>Epidermis</td>
<td>0.43</td>
<td>2.25</td>
<td>0.22</td>
<td>1.69</td>
<td></td>
</tr>
<tr>
<td>Dermis</td>
<td>0.27</td>
<td>3.37</td>
<td>0.14</td>
<td>2.52</td>
<td></td>
</tr>
<tr>
<td>Dermis plexus superficialis</td>
<td>0.33</td>
<td>3.46</td>
<td>0.12</td>
<td>2.59</td>
<td>Tuchin\textsuperscript{5}</td>
</tr>
<tr>
<td>Dermis</td>
<td>0.27</td>
<td>3.37</td>
<td>0.14</td>
<td>2.53</td>
<td></td>
</tr>
<tr>
<td>Dermis plexus profundus</td>
<td>0.34</td>
<td>3.49</td>
<td>0.12</td>
<td>2.62</td>
<td></td>
</tr>
<tr>
<td>Subcutaneous fat</td>
<td>0.06</td>
<td>1.2</td>
<td>0</td>
<td>0.98</td>
<td>Tuchin\textsuperscript{5}</td>
</tr>
<tr>
<td>Nerve fibre</td>
<td>0.1</td>
<td>0.53</td>
<td>0.08</td>
<td>1.7</td>
<td>Tuchin\textsuperscript{5}</td>
</tr>
<tr>
<td>Muscle</td>
<td>0.1</td>
<td>0.53</td>
<td>0.05</td>
<td>0.35</td>
<td>Tuchin\textsuperscript{5}</td>
</tr>
<tr>
<td>Whole blood (S$_{O_2}$=97%, hct=0.41)</td>
<td>0.66</td>
<td>1.7</td>
<td>1.3</td>
<td>1.58</td>
<td>Tuchin\textsuperscript{5}</td>
</tr>
<tr>
<td>Bone</td>
<td>0.54</td>
<td>0.22</td>
<td>0.54</td>
<td>0.18</td>
<td>Ugnell\textsuperscript{19}</td>
</tr>
</tbody>
</table>

Lastly, the modulation due to main arterial vessels was assumed to make a significant contribution to the time-varying portion of the PPG signals, where the modulation due to perfusion was assumed homogeneous and could thus be accounted for as a factor of the former time varying portion. The modulation used in simulation is simplified to a change in absorption as opposed to a change in main vessel diameter. From a raytracing perspective, the changes in intensity of rays transilluminating main arteries are treated as the source of AC distributions, where the true AC signal is represented as an arbitrary portion of these changes in intensity.

2.2. Validation Platform

For validation of such results, the conditions used for simulation were reproduced as accurately as possible. A CMOS camera (Mightex, USA) was mounted on a rotating platform that allowed the camera to maintain a constant distance and alignment with respect to the subject’s finger (Fig.1). Sets of 200 frames were captured at 40 fps for both red and infrared illumination, between 90° and 270° in 9° steps, where 180° is the standard transmittance mode sensor position with respect to the light source. For each of the sets, the mean peak-to-peak intensity and mean intensity was determined from windows of size 10*10 pixels, resulting in two additional frames representing the AC and DC intensity distributions of that set. Finally, the AC and DC frames were trimmed and concatenated to form continuous intensity distributions from 90° to 270°.
3. Results

Both simulation and validation results are representative of the \textit{in-vivo} measurement of a transmission-mode pulse oximeter on a measuring site with an arterial oxygen saturation of 97%.

The SNR in a photoplethysmographic signal is proportional to the peak-to-peak AC intensity. Figure 2 shows that the strongest pulsatile signals can be found at ±90° to 120° of the light source position and a dip in intensity can be found at 180° for both simulation and validation data. Simulation data shows an asymmetry due to a 1mm offset of the light source from the centre of the finger, while CMOS data shows a negligible asymmetry.

Comparison of figures 2 and 3 shows that while empirical data maintains the dip found in AC signals when normalised by the DC signals, simulation data levels out. This is indicative of a higher inaccuracy in simulated DC signals than AC signals. Nevertheless, AC/DC ratios show significant correlation.

Figure 4 shows the ratio of ratios along the circumference of the finger for simulated and empirical data. The nearly identical stability between simulated and empirical ratio of ratios indicates further correlation between simulated and real-life data.

The mean AC/DC values before normalisation are 0.37 and 0.34 for red and infrared simulation data, and 0.036 and 0.063 for red and infrared empirical data, which yields a ratio of ratios of 1.1 and 0.57 for simulation and empirical data respectively.

![Figure 2. Normalised peak-to-peak AC signals for simulation and empirical data.](image-url)
Figure 3. Normalised AC/DC ratios for simulation and empirical data.

Figure 4. Ratio of ratios for data scaled to 97% $\text{SpO}_2$ ($R=0.5$)

4. Discussion and Future Work

Empirical validation of the simulation platform detailed in previous work\textsuperscript{[23]} proves to be a challenging step. Arbitrary selection of a factor of 0.1 for AC signals accounts for the offset between the simulated and empirical ratios. However, offset between ratios of ratios cannot be comprehensively explained. The relativity of simulated intensities due to the unitless output and the use of arbitrary factors, makes it difficult to determine which of the signal components deviate from the expected values. Nevertheless, the high correspondence between intensity distributions indicate a predictable output. Both AC signals and AC/DC signals show a high correspondence despite the asymmetry found in simulation data, without which the signals would be likely to correlate further.

Empirical data shows a significant amount of noise. Although the use of a CMOS camera allows for a more complete visualisation of intensity distributions, the platform does not allow the simultaneous recording of signals from all positions, thus allowing quasistatic physiological changes to be recorded. In addition to this, a low SNR due to the limitations of the CMOS camera made it necessary for a light source of multiple LEDs to be used, thus increasing the difference between simulation and empirical conditions, and still not fully resolving the SNR issue. The next stage of platform development involves the use of custom photodiode arrays as a solution to all of these issues.

The geometric model used for simulation is treated as a generic representation of an adult male finger, and as such is prone to being a source of error when comparing the results to corresponding empirical results from a specific subject. An advisable step would be to construct and use anatomical
models from functional magnetic resonance imaging (fMRI) scans of a subject’s finger to ensure the maximum correspondence during validation.

Before performing any further validation, it is necessary to ensure the maximum possible accuracy of both simulated and recorded data. Further validation can include the use of lasers as approximations of point sources. Upon the completion of validation, the derivation of equations to characterise changes in light-source and sensor positions as well as changes in optical properties will be attempted.

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References