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Use of genetic algorithms to optimize fiber optic probe design for the extraction of tissue optical properties

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***Abstract*—This paper outlines a framework by which the optimal illumination/collection geometry can be identified for a particular biomedical application. In this study, this framework was used to identify the optimal probe geometry for the accurate determination of tissue optical properties representative of that in the ultraviolet-visible (UV-VIS) spectral range. An optimal probe geometry was identified which consisted of a single illumination and two collection fibers, one of which is insensitive to changes in scattering properties, and the other is insensitive to changes in the attenuation coefficient. Using this probe geometry in conjunction with a neural network algorithm, the optical properties could be extracted with root mean square errors of 0.30 cm^{-1} for the reduced scattering coefficient (tested range of 3-40 cm^{-1}), and 0.41 cm^{-1} for the absorption coefficient (tested range of 0-80 cm^{-1}).**

***Index Terms*—Reflectance, Optical Properties, Fiber Optics, Monte Carlo, Genetic Algorithms**

I. INTRODUCTION

THE diffuse reflectance spectrum, which reflects the absorption and scattering properties of a turbid medium, is sensitive to a number of important physiological indicators and thus, is a useful tool for the early diagnosis of pre-cancers and cancers. The illumination/collection geometry is a critical aspect of tissue diffuse reflectance spectroscopy in that it affects sensitivity to the absorption and scattering properties of the medium, the sensing depth and the signal to noise. Specialized probe geometry designs have been previously shown to be useful in characterizing tissue optical properties from diffuse reflectance spectra [1, 2].

This paper outlines a framework by which the optimal illumination/collection geometry can be identified given a particular design objective. Here, the framework is used to identify the optimal probe geometry for the accurate determination of tissue optical properties representative of that in the ultraviolet-visible (UV-VIS) spectral range. The unique benefits of this approach are (1) no *a priori* information is needed about the tissue absorbers and scatterers, and (2) there is no requirement for complex multiple source-detector separation fiber probe geometries.

II. II. METHODS

A. General Optimization Methodology

The optimization methodology proceeds in the following manner. First, a population of fiber probe geometries was randomly initialized. Next, diffuse reflectance measurements were simulated for each of these probe geometries for a wide range of tissue optical properties using Monte Carlo modeling. The training data set for each of the probe geometries was used to optimize a neural network algorithm to take the diffuse reflectance as an input, and output the optical properties. The optimized neural network algorithm was applied to an independent validation set consisting of simulated diffuse reflectance spectra (for a randomly selected set of optical properties which were not used in training the algorithm) for the same probe geometry. Each probe design was ranked according to how accurately the neural network could retrieve the optical properties from the independent validation data set, and the population of probe designs was iteratively evolved toward the optimal probe geometry using a genetic algorithm. Finally, the unbiased accuracy with which the neural network algorithm can extract optical properties was evaluated on an independent testing data set.

B. Monte Carlo Simulations

The training, validation, and testing data sets described above were generated using Monte Carlo simulations (see [3], for a description of the Monte Carlo model). Optical properties ranging from approximately 3 - 40 for the reduced scattering coefficient (μ_s') and 0 - 80 for the absorption coefficient (μ_a) were used, with the anisotropy factor (g) tested over the range of 0.8 - 0.95. The training data set consisted of 144 sets of optical properties. The validation and testing data sets each consisted of 25 randomly assigned sets of optical properties within the same range.

C. Neural Network Objective Function

A neural network objective function was used to determine the optical properties from the diffuse reflectance measurement. This was chosen because it is useful in

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approximating complex non-linear functions, and has previously been shown effective in extracting optical properties [4]. The neural network consisted of a number of inputs (corresponding to the number of collection fibers), 10 hidden layer neurons having hyperbolic tangent activation functions, and two output neurons having linear activation functions. The inputs to the neural network were the diffuse reflectance from each collection fiber, and the outputs were the optical properties (μ_a and μ_s'). The neural network was trained using the Monte Carlo generated training data set for each probe design using a Levenberg-Marquardt algorithm in Matlab (Mathworks Inc., Natick, MA). A detailed description of this algorithm is available online [5]. The fitness of a particular probe geometry was defined as the root mean square error (RMSE) between the optical properties extracted using the neural network algorithm and the actual optical properties.

D. *Optimization with Genetic Algorithm*

The goal of the genetic algorithm was to minimize the returned fitness score of probe, thereby selecting the optimal probe geometry for optical property extraction. Genetic algorithms work with a population of solutions. In generating a new solution, operators similar to those of natural evolution such as crossover, mutation, and selection are employed to produce offspring. At each generation, a population of child solutions is generated from the parent population. Parent individuals for the next generation of solutions are chosen based on the process of selection, which is weighted towards the fittest individuals, thereby introducing selective pressure on the population to evolve towards an optimal solution. After termination of the optimization process, the optimal fiber geometry was output by the algorithm. The "GARealGenome" optimization method was employed using the GAlib optimization library; the code and a detailed description are available online [6].

E. *Fiber Probe Geometry Parameters*

Five basic probe designs were tested. The probe consisted of a single illumination fiber, and between two and six collection fibers (a total of five possible configurations). A series of optimizations using the framework described in sections A-D was run to consider each of the five probe configurations separately. In this study, only the fiber diameter and source-detector separations were included as free parameters. Each fiber had a variable diameter, having possible values of 50, 100, 150, 200, 300, 400, and 500 μm (commercially available). The center-to-center distance from the source fiber to each collection fiber was limited to less than 1.5 mm, and greater than the sum of the source and collection fiber radii. All fibers had an NA of 0.22.

III. RESULTS AND DISCUSSION

Table 1 shows the RMSE in μ_a and μ_s' from the testing data sets for the optimal result from each probe configurations. The magnitude of the error was found to be approximately constant over the entire range of optical properties tested. Thus, as the magnitude of the optical properties increase, the percent error decreases. It can be seen that as the number of fibers increases beyond two collection fibers, the RMSE of the testing data set does not decrease. The use of additional fibers leads to over-training of the algorithm. The fiber design having 2 collection fibers provides the best balance between performance and complexity. It consists of a single 500 μm diameter illumination fiber, a 200 μm diameter collection fiber at a center-to-center distance of 380 μm (collection fiber 1), and a 400 μm diameter collection fiber at a center-to-center distance of 1360 μm (collection fiber 2). In developing this algorithm, the case where the source fiber was also used for collection was also considered. It was found that, in general, this geometry did not perform as well.

Figure 1 shows a scatter plot of the extracted vs. expected optical properties obtained from the testing data set for the optimal probe design. The extracted optical properties show minimal deviation from the expected optical properties over the entire range tested for both (a) μ_a and (b) μ_s'. The optical properties could be extracted with an RMSE of 0.41 cm^{-1} for μ_a (tested range of 3-40 cm^{-1}), and 0.30 cm^{-1} for μ_s' (tested range of 3-40 cm^{-1}).

The sensitivity of the RMSE to positioning errors expected in manufacturing this probe was then evaluated. It was found that for a reasonable range of positioning errors (0-500 μm standard deviation), there was a minimal increase in the errors seen. For example, with a 200 μm standard deviation in positioning, the RMSEs were 0.46±0.07 and 0.55±0.35 for μ_a and μ_s', respectively, over the same range as above.

Finally, it is desirable to gain some understanding as to why this particular fiber design performs well. Figure 2 shows a log scale contour plot of the collected diffuse reflectance as a function of μ_t (μ_s+μ_a) and albedo (μ_s/μ_t) for each of the two collection fibers. For collection fiber 1 (Fig. 2(a)) the plot of the diffuse reflectance has roughly vertical contour lines. This indicates the reflectance collected by this fiber is relatively insensitive to changes in μ_t. For collection fiber 2 (Fig. 2(b)), the contour lines roughly follow the lines of constant μ_a. This indicates that the diffuse reflectance is relatively insensitive to changes in μ_s'. As a result of this, the diffuse reflectance collected by fiber 1 gives a direct measure of the albedo and that collected by fiber 2 gives a direct measure of μ_a. μ_s' can be determined directly given these two parameters. This is likely the mechanism by which this probe is effective in extracting optical properties. Note that these relationships appear to break down particularly at low values of μ_t, and in this case the extraction of optical properties would become on a more complex function of the collected reflectance from each fiber, all of which is handled by the neural network function.

In conclusion, the fiber-optic probe design strategy described in this manuscript resulted in a fairly simple illumination and collection geometry that is capable of extracting the optical properties of a medium from the diffuse reflectance spectra with RMSEs of 0.41 cm^{-1} (tested range of 0-80 cm^{-1}) and 0.30 cm^{-1} (tested range of 3-40 cm^{-1}), for μ_a and μ_s', respectively. This approach could also be easily extended to other applications, such as fluorescence sensing, or extraction of optical properties from layered media.

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Fiber Design	RMSE – testing (cm^{-1})		Optimal Geometry	
	μ_a	μ_s'	Illumination Diameter (μm)	Diameter – Source Detector Separation Pairs for Each Collection Fiber (μm)
2 collection fibers	0.41	0.30	500	(200-380) (400-1360)
3 collection fibers	0.47	0.32	200	(200-610) (500-1330) (500-440)
4 collection fibers	0.46	0.34	400	(50-550) (400-530) (50-1180) (300-1230)
5 collection fibers	0.40	0.29	400	(200-640) (300-1120) (400-490) (500-1190) (50-700)

Table 1: Root mean square errors (RMSE) in μ_a and μ_s' and optimal probe geometries are shown for each of the optimized probe configurations.

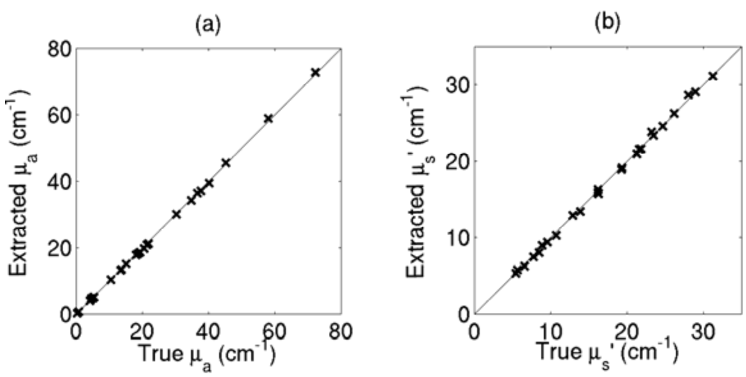

Figure 1: Scatter plots of the extracted vs. expected optical properties for the (a) absorption coefficient and (b) reduced scattering coefficient. The solid line is the line of perfect agreement. These results are for the fiber design with 2 collection fibers.

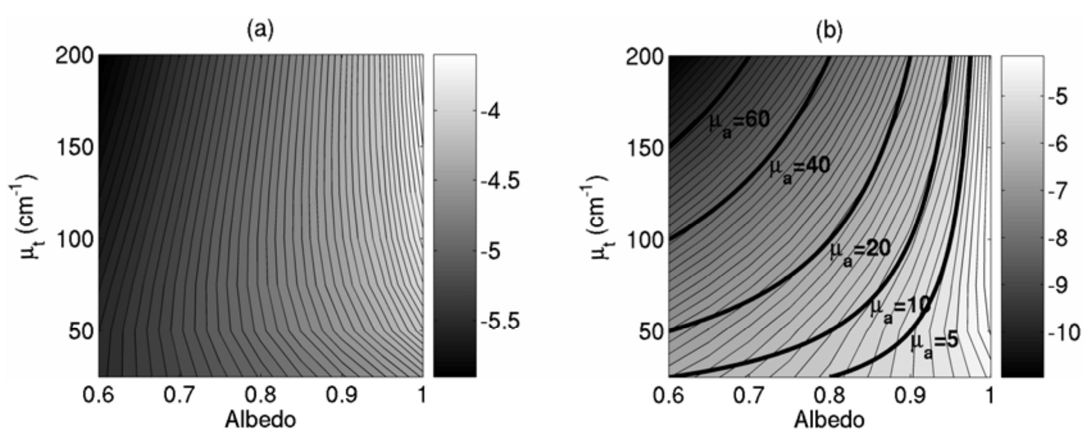

Figure 2: Log contour plots of the collected diffuse reflectance from (a) fiber 1 and (b) fiber 2. It can be seen that the contour lines in (a) roughly follow the vertical lines of equal albedo, while the contour lines in (b) roughly follow the lines of equal μ_a (bold lines).