Lecture 5: Introduction to Inverse Problems

Matrix

Collagen orientation

Fibril diam = 0.5 μm

Cells

Type
- epithelial
- adipose
- fibroblast
- muscle
- hepatocyte

Shape

Nucl/cyto

Mitochondria

Diam = um

#/cell =

Vasculature

Microvasc

Blood volume %

Diam = mm

Fractal dimen = 1.4

Large vessel

Orientation

Shape

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Lecture 5 Outline

• The Ill-Conditioned Nature of Inverse Problems
• Inverse Problem Approaches:
  A. Table Look-up
  B. Based on 1-D Models: Inverse Adding-Doubling
  C. Stochastic RTE-Based: Perturbation and Differential Monte Carlo
• Summary and Take Home Messages
Inverse Problems: Challenges

While forward RTE problems produce unique radiance distributions throughout the tissue...

- In SDA we cannot separate $\mu_s$ from $g$
- Higher order ($P_N$) solvers exhibit similar limitations (similarity theory)

►► inverse RTE problems are inherently ill-conditioned
Inverse Problems: Desiderata

To solve inverse problems we want

1. At least as many measurements as “unknowns” (e.g., $\mu_a$, $\mu_s$)
2. Measurements placed at locations/times where they are very sensitive to changes in optical properties
3. Minimizing redundancy in measurements

Achieving this imposes significant demands on inverse problem-solving
General Inverse Problem Formulation

Given problem input:
\[ I = \{\mu_t, \mu_a, \rho, n, Q, \Gamma, BC, IC, f_1, f_2, \ldots, f_D\} \]
and output:
\[ O = \{I_1, I_2, \ldots, I_D\}, \quad D = \# \text{ of measurements (detectors)} \]

The forward problem map: \( F: I \rightarrow O \)
The inverse problem map: \( F^{-1}: O \rightarrow I \)

In general, \( \|F\| < 1 \) (F is contractive) while \( \|O\| > 1 \) (inverse problem is inherently ill-conditioned).

F depends on choice of model and implementation strategy.
General Approaches to Solving Inverse Problems: Table Look-Up

A. Table Look-up Approach:

- **Determine table** $[I_i, O_{ij}]$ $i=1,...,N; j=1,...,D$: Repeatedly solve forward RTE problems until solution “matches” measured output; interpolate in the table generated, if necessary. Output $O_{ij}$ can be based on exact or approximate methods, analytic or numerical.

- **Extract inverse solution** by “locating it” in the table, or by nonlinear optimization (least squares)
General Approaches to Solving Inverse Problems: Table Look-Up

For fast computation, use formula-based solvers (SDA* for high albedos, pre-computed MC table for low albedos)

SDA-based: a. for homogeneous tissue*; b. for layered tissue**


Inverse problem solvers based on SDA are in widespread use and perform well in the diffusive regime
General Approaches to Solving Inverse Problems: Based on 1-D Models

B. Based on 1D Models

A method called inverse adding-doubling (IAD)* works well in slabs (even layered ones) and can include refractive index mismatches at the boundary. We discuss this method in the context of the 1-D slab problem introduced in Lecture 2.

*S.A. Prahl et. al, Determining the optical properties of turbid media by using the adding-doubling method, A.O., 32, 559-568, 1993.
RTE in 1-D Slab Geometry

Input: \( \mu_a, \mu_s, d, g \), source \( Q_0 = 1 \) at \( x=0 \) \((\mu>0)\)

\[
p(\mu) = p_f \delta(\mu-1) + p_b \delta(\mu+1)
\]
\[
p_f + p_b = 1, \ p_f - p_b = g
\]
\[
d = \text{slab thickness}
\]

\[
L_+(x) = c_1 \exp(\lambda x) + c_2 \exp(-\lambda x)
\]
\[
L_-(x) = d_1 \exp(\lambda x) + d_2 \exp(-\lambda x)
\]

where \( c_1, c_2, d_1, d_2 \) depend on input data and

\[
\lambda = \sqrt{\mu_a(\mu_a + \mu_s')} = \sqrt{\mu_a \mu_{tr}}
\]

In principle we could solve directly for \( \mu_a, \mu_s \) from knowledge of
\( R = L_-(0), \ T = L_+(d) \) but in practice, iterative methods are used
IAD for 1-D Slab

Input: \((\mu_a, \mu_s, g, d)\)

Dimensionless parameters:
\[ a = \frac{\mu_s}{\mu_s + \mu_a}, \quad \tau = d(\mu_s + \mu_a) \]

“Measurements” (from exact solution)
\[ R = R(\mu_a, \mu_s, g) = L_-(0) \quad T = T(\mu_a, \mu_s, g) = L_+(d) \]

Henyey-Greenstein scattering
\[ p(\mu_0) = \frac{1 - g^2}{4\pi(1 + g - 2g\mu_0)^{3/2}} \]
\[ \int_{-1}^{1} \mu_0^n p(\mu_0) d\mu_0 = g^n \]

Find \( \mu_a = \mu_a(R,T) \quad \mu_s = \mu_s(R,T) \)

IAD involves iterative strategy
IAD Procedure

- Guess set of optical properties $\mu_a, \mu_s$
- Calculate reflectance $R = L_-(0)$ and (total) transmittance $T = L_+(d)$ from exact formulas
- Compare calculated and measured values
- Test for goodness of fit
- Repeat until a match is found
Table Look-up Approach

A metric is needed to judge how far computed values are from measured values

\[ M_1(\mu_a, \mu_s) = \frac{|R_{\text{calc}} - R_{\text{meas}}|}{R_{\text{meas}}} + \frac{|T_{\text{calc}} - T_{\text{meas}}|}{T_{\text{meas}}} \]

Relative error:

Assumes measurement errors for \( R_{\text{meas}} \) and \( T_{\text{meas}} \) are roughly equal; if not, weighting factors should be introduced

Least squares: \[ M_2(\mu_a, \mu_s) = \frac{(R_{\text{calc}} - R_{\text{meas}})^2}{\sigma^2_{R_{\text{meas}}}} + \frac{(T_{\text{calc}} - T_{\text{meas}})^2}{\sigma^2_{T_{\text{meas}}}} \]

More generally, if \( \alpha = (\mu_a, \mu_s, g, ...) \) denotes the optical properties to be found, we minimize

\[ M_2 = \Xi^2 = \sum_{i=1}^{M} \left[ \frac{R_{\text{calc}, i(\alpha + \Delta \alpha) - R_{\text{meas}, i}}}{\sigma(R_{\text{meas}, i})} \right]^2 \]
1-D Slab Problem

This figure shows total reflection and transmission of index-matched slab as a function of albedo $a$ and anisotropy $g$ for a fixed unscattered transmission value of 10%.

Note the rich information content:
- Uniqueness of inverse solution
- Regions where inversion is likely to be more difficult.

Similarity theory* can be used to facilitate solution representation, based on reduced albedo and optical thickness

\[
a' = \frac{a(1-g)}{1-ag}, \quad \tau' = (1-ag)\tau
\]

1-D Slab Problem

This figure shows total reflection and transmission of a mismatched slab as a function of reduced albedo $a'$ and reduced optical thickness $\tau'$. Scattering is assumed isotropic, $g = 0$.

Note:
- Improved separation of inverse solutions when dependence is expressed in terms of reduced optical parameters.
General Approach to Solving Inverse Problems: Stochastic Perturbation

C. **Stochastic Perturbation Approach:**

   A. **Formulate perturbation model** that treats **variable** input quantities (uses weighted Monte Carlo, Lecture 2)

   B. **Implement** this model (i.e., generate photon biographies) using a **single set** of “baseline” optical properties thought to be in the ballpark

   C. Post-process the stored biographical data and use **least squares optimization** to determine best-fitting values
Stochastic RTE-Based: Perturbation and Differential Monte Carlo

This method relies on use of weighted MC simulation (Lecture 2)


Recall stochastic model \((B, M, \xi)\) where \(\xi = \) weighted Monte Carlo estimator

Recall: the identity
\[
A = \int_B \xi dM = \int_{\Gamma \times S^2} f(r, \Omega)L(r, \Omega)drd\Omega
\]

establishes that sample averages of \(\xi\) converge to \(A\); i.e.,
\[
\frac{1}{N} \sum_{i=1}^{N} \xi(b_i) \rightarrow \int_B \xi dM = E[\xi] = A
\]
Perturbation Monte Carlo

Suppose: measure $M$ is derived from the “background”/baseline simulation (unperturbed tissue); $M^*$ describes the measure that would result from inclusion of any sort of perturbation (darkened spot on skin, tumor) exhibiting different optical properties.

Values of $\xi$ can be regarded as photon “weights” arising in the simulation prescribed by the probability measure $M$. If the measure $M$ is changed to $M^*$, the identity

$$\int_B \xi^* \, dM = \int_B \xi \, dM^*$$

will be valid if $\xi^* = \xi \frac{dM^*}{dM}$ and shows how to adjust the weights correctly in the simulation prescribed by $M^*$.
Perturbation Monte Carlo

This idea can be used to play “what if” games, such as: What if we double the absorption in the suspicious region? How would the photon weights change in the simulation? To understand this, suppose $M$ is defined by a baseline simulation and $M^*$ represents any perturbation of optical properties in the tissue model. The identity

$$\int_{\Omega} \xi^* \, dM = \int_{\Omega} \xi \, dM^*$$

where

$$\xi^* = \xi \frac{dM^*}{dM}$$

shows how to convert an estimator $\xi$ that would be “correct” (i.e., unbiased) in the perturbed simulation $M^*$ to one $\xi^*$ that is “correct” within the baseline simulation $M$. 
Perturbation Monte Carlo

To appreciate what the formula $\xi^* = \xi \frac{dM^*}{dM}$ means, think of $\frac{dM^*}{dM}$ as a generalization of the Jacobian used for changing variables under an ordinary integral sign. In fact, the integrals with respect to $M$ or $M^*$ are actually computed as a sum of ordinary multiple integrals according to the model equivalence theory (outlined in Lecture 2).

This idea can be made very concrete in practice.
Perturbation Monte Carlo

For example,

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

expresses one way to correct the estimator \( \xi \) from a "baseline" MC simulation (using CAW) with optical properties \((\mu_s, \mu_t)\) to one \( \xi^* \) that is corrected for perturbed optical properties \((\mu_s^*, \mu_t^*)\) in any portion \( V \) of the tissue. (\( j = \# \) collisions in \( V \), \( S = \) distance traversed in \( V \))
Differential Monte Carlo

This formula
\[ \xi^* = \xi_{CAW} \left( \frac{\mu_s^*}{\mu_s} \right)^j \exp[-(\mu_s^* - \mu_s)S] \exp[(-\mu_a^* - \mu_a)S)] \]

can also be (exactly) differentiated to obtain sensitivity coefficients.

►► provides derivatives used by gradient-based least squares optimization routines, which are more robust (e.g., Levenberg-Marquardt)

►► pMC/dMC produces accurate predictions of optical properties more generally. It could also be used to predict other changes \((g, \text{layer thickness})\)
pMC/dMC Flow Chart

Schematic of pMC/dMC computations

Experimental Measurements

conventional Monte Carlo \( u_a, u_s \)

determine \( \chi^2 \)

pMC calculation of \( \xi \) using \( \hat{u}_a, \hat{u}_s \)

determine new \( \hat{u}_a, \hat{u}_s \) using pMC derivative calc.

Converged?

yes

Predicted \( \hat{u}_a, \hat{u}_s \)

no
Optical Property Recovery: Cervical Lesions

Problem: identify relative changes in optical properties in two layers from a given set of measurements. Six detectors are positioned at surface to more accurately capture information from both epithelial and stromal layers.

Schematic of two-layer cervical problem geometry

**Optical Property Recovery: Cervical Lesions**

The background or baseline optical properties:

\[ \mu_a = 0.0341 \text{ mm}^{-1}, \quad \mu_s = 6.11 \]

We chose \( \mu_a \) perturbations ranging from 33\% - 300\% of background values in both layers, \( \mu_s \) perturbations ranging from 70\% - 130\%.

Schematic of two-layer cervical problem geometry
Uses of pMC/dMC: Optical Property Recovery

(a) Predicted optical properties for \( \mu_a \) perturbations in the top layer (a) and in the bottom layer (b)

Note excellent decoupling of changes in \( \mu_a \) from changes in \( \mu_s \)
Uses of pMC/dMC: Optical Property Recovery

Predicted optical properties for $\mu_s$ perturbations in the top layer (a) and in the bottom layer (b)

Again note excellent decoupling
Summary and Take Home Messages

1. Fast inverse problem solutions can be based on formulas and table look-up
2. When exact solutions are not available, perturbation Monte Carlo can be used
3. As a Monte Carlo technique, pMC is valid for any geometry and fully heterogeneous tissue
4. pMC requires only a single set of photon biographies plus a post-processor that is fast

Addressing inverse problems uses all VTS tools
GUI Interaction E – Inverse Problem Solving

In this last GUI interaction

• you are asked to use both SDA and Monte Carlo inverse problem solvers to predict optical properties using spatially-resolved measurements

• you can experiment with the number and placement of such detectors in order to see the impact on the quality of recovered optical properties – have fun!

and thanks for your participation in the 2011 VP Workshop!!