Method of Rotated Reference Frames

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Outline
MOTIVATION
(the inverse problems perspective)
Given a data function \( \phi(\rho_s, \rho_d) \) which is measured for multiple pairs \((\rho_s, \rho_d)\), find the absorption coefficient \( \alpha(r) \) inside the slab.
Linearized Integral Equation

\[ \phi(\rho_s, \rho_d) = \int \Gamma(\rho_s, \rho_d; r) \delta \alpha(r) d^3r \]

\[ \phi(\rho_s, \rho_d) = \frac{I(\rho_s, z_s; \rho_d, z_d) - I_0(\rho_s, z_s; \rho_d, z_d)}{I_0(\rho_s, z_s; \rho_d, z_d)} \]

(measurable data-function)

\[ \Gamma(\rho_s, \rho_d) = G_0(\rho_s, z_s; r)G_0(r; \rho_d, z_d) \]

(first Born approximation)

\[ \alpha(r) = \alpha_0 + \delta \alpha(r) \]
How To Invert?

Numerical SVD approach:

\[ \phi_i = \sum_j \Gamma_{ij} \delta \alpha_j \]

\[ \phi = \Gamma \delta \alpha \]
\[ \Gamma^* \phi = \Gamma^* \Gamma \delta \alpha \]
\[ \delta \alpha^+ = \left( \Gamma^* \Gamma \right)^{-1}_{\text{reg}} \Gamma^* \phi \]
Analytical SVD approach: Making use of the translational invariance

\[ \tilde{\phi}(q_s, q_d) = \int \phi(p_s, p_d) e^{i(q_s \cdot p_s + q_d \cdot p_d)} d^2 \rho_s d^2 \rho_d \]

\[ q_s = q / 2 + p, \quad q_d = q / 2 - p; \]

Data function: \( \psi(q, p) = \tilde{\phi}(q / 2 + p, q / 2 - p) \)

\[ \psi(q, p) = \int_0^L g_s(q / 2 + p; z) g_d(q / 2 - p; z) \delta \tilde{\alpha}(q; z) dz \]

\[ \delta \tilde{\alpha}(q; z) dz = \int \delta \alpha(p, z) e^{i p \cdot q} d^2 \rho \]

\[ G_0(p_s, z_s; p, z) = \int \frac{d^2 q}{(2\pi)^2} g_s(q; z) e^{i q \cdot (p - p_s)} \]

\[ G_0(p, z; p_d, z_d) = \int \frac{d^2 q}{(2\pi)^2} g_d(q; z) e^{i q \cdot (p_d - p)} \]
Imaging complex structures with diffuse light
*Optics Express 16*(7), 5048-5060 (2008)
In the case of RTE, we need the plane-wave decomposition of the Greens function, of the form

\[ G_0(r, \hat{s}; r', \hat{s}') = \int \frac{d^2 q}{(2\pi)^2} g(q; z, \hat{s}; z', \hat{s}') e^{iq(r-r')} \]

and the integral kernel

\[ \Gamma(q, p; z) = \int g(q/2 + p; z_s, \hat{z}; z, \hat{s}) g(q/2 - p; z, \hat{s}; z_d, \hat{z}) d^2 s \]

We then get the integral equations of the form

\[ \psi(q, p) = \int_{z_s}^{z_d} \Gamma(q, p; z) \delta \tilde{\alpha}(q; z) dz \]
Motivation Continued
(the spectral methods)
Solve system of equations:

\[(z + W)\langle x \rangle = \langle b \rangle\]

Find \(\sigma(z) = \text{Im} \langle b | x \rangle = \text{Im} \langle b | (z + W)^{-1} | b \rangle\)

for \(M\) different values of \(z\), where

\[z = x + i\delta\] is a complex number

\(W\) is an \(N \times N\) matrix

\(|x\rangle, |b\rangle\) are vectors of length \(N\)
The "naive" method:

1) Choose $z$
2) Make a matrix $A = z + W$
3) Solve $A|x\rangle = |b\rangle$
4) Goto step (1)

Computational complexity: $M \times N^3$
The spectral method:

1) Diagonalize $W$ (find eigenvectors $|n\rangle$ and eigenvalues $w_n$)

2) For every $z$,

$$|x\rangle = \sum_n \frac{|n\rangle\langle n|b\rangle}{z + w_n}; \quad \sigma = \sum_n \frac{c_n^2 \delta}{(x + w_n)^2 + \delta^2}$$

Computational complexity: $N^3 + M \times N^2$

However, if the whole vector $|x\rangle$ is not needed, the complexity may be as low as

$$N^3 + M \times N$$
Spectral Method for the RTE?

\[
\text{RTE: } (\hat{s} \cdot \nabla + \mu_t)I(r, \hat{s}) = \mu_s \int A(\hat{s}, \hat{s}')I(r, \hat{s}')d^2\hat{s}' + \varepsilon(r, \hat{s})
\]

Where is the "spectral variable"?

How can we write this equation in the form \((z + W)|I\rangle = |\varepsilon\rangle\) ?

\(\mu_t\) and \(\mu_s\) do not qualify...

We can try to expand \(I(r, \hat{s})\) into a 3D Fourier integral with respect to \(r\) and into the basis of ordinary spherical harmonics \(Y_{lm}(\theta, \varphi)\) with respect to \(\hat{s}\)...

...and see if the equation can be cast into the desired form.
The Conventional Method of Spherical Harmonics

This results in the following system of equations with respect to the vector of the expansion coefficients \( |I(k)\rangle \) (\( k \) - the Fourier variable):

\[
i A^{(x)} k_x |I(k)\rangle + i A^{(y)} k_y |I(k)\rangle + i A^{(z)} k_z |I(k)\rangle + D |I(k)\rangle = |\varepsilon(k)\rangle
\]

\( A^{(x)} \), \( A^{(y)} \), \( A^{(z)} \) are different matrices.

\[
A^{(x)}_{lm, l_m'} = \int \sin \theta \cos \phi Y^*_l m (\theta, \phi) Y_{l_m'} (\theta, \phi) \sin \theta d\theta d\phi , \quad \text{etc.} \quad \text{.....}
\]

“This rather awe-inspiring set of equations … has perhaps only academic interest”.

K.M. Case, P.F. Zweifel, Linear Transport Theory
Rotated Reference Frames

The usual spherical harmonics are defined in the laboratory reference frame. Then $\theta$ and $\varphi$ are the polar angles of the unit vector $\mathbf{s}$ in that frame.

**THE MAIN IDEA:** For each value of the Fourier variable $k$, use spherical harmonics defined in a reference frame whose $z$-axis is aligned with the direction of $k$.

We call such frames "rotated". Spherical harmonics defined in the rotated frame are denoted by $Y(\mathbf{s};\mathbf{k})$. 
Rotation of the Laboratory Frame 
(x,y,z).

\[ Y_{lm}(\hat{s}; \hat{k}) = \sum_{m'=-l}^{l} D_{m'm}^{l}(\varphi_k, \theta_k, 0) Y_{lm'}(\hat{s}) \]

- Wigner D-functions
- Euler angles
- Spherical functions in the laboratory frame
\[(\hat{s} \cdot \nabla + \mu_t)I = \mu_s A I + \varepsilon\]

\[I(\mathbf{r}, \hat{s}) = \int \tilde{I}(\mathbf{k}, \hat{s}) e^{i \mathbf{k} \cdot \mathbf{r}} d^3 k\]

\[\varepsilon(\mathbf{r}, \hat{s}) = \int \tilde{\varepsilon}(\mathbf{k}, \hat{s}) e^{i \mathbf{k} \cdot \mathbf{r}} d^3 k\]

\[(i \mathbf{k} \cdot \hat{s} + \mu_t)\tilde{I} = \mu_s A\tilde{I} + \tilde{\varepsilon}\]

\[\tilde{I}(\mathbf{k}, \hat{s}) = \sum_{l,m} F_{lm}(\mathbf{k}) Y_{lm}(\hat{s}; \hat{k})\]

\[\tilde{\varepsilon}(\mathbf{k}, \hat{s}) = \sum_{l,m} E_{lm}(\mathbf{k}) Y_{lm}(\hat{s}; \hat{k})\]

\[A(\hat{s}, \hat{s}') = \sum_{l,m} A_l Y_{lm}(\hat{s}; \hat{k}) Y^*_{lm}(\hat{s}; \hat{k})\]
\[ ik \sum_{l'm'} R_{lm}^{l'm'} F_{l'm'}(\mathbf{k}) + \sigma_{l} F_{lm}(\mathbf{k}) = E_{lm}(\mathbf{k}) \]

\[ \sigma_{l} = \mu_{a} + \mu_{s}(1-A_{l}) \]

\[ R_{lm}^{l'm'} = \int \hat{s} \cdot \hat{k} \; Y_{lm}^{*}(\hat{s};\hat{k})Y_{l'm'}(\hat{s};\hat{k})d^{2}s = \]

\[ = \delta_{mm'} \left[ b_{l}(m)\delta_{l'=l-1} + b_{l+1}(m)\delta_{l'=l+1} \right] \]

\[ b_{l}(m) = \sqrt{\frac{l^{2} - m^{2}}{4l^{2} - 1}} \]
RTE in the Angular Basis of Rotated Spherical Functions

\[ ikR |I(k)\rangle + D |I(k)\rangle = |E(k)\rangle \]

- **Scalar spectral parameter**
- **Block-tridiagonal real symmetric matrix**
- **Diagonal matrix**
  \[ S_{lm,l'm'} = \delta_{ll'}\delta_{mm'}[\mu_a + \mu_s(1 - A_l)] \]
- **Source term**
- **Parameters of the phase function. (For the HG model, \( A_l = g^l \))**
Let $D = SS$

$$W = S^{-1}RS^{-1}$$

$$
\begin{align*}
&ikR\left|I(\mathbf{k})\right\rangle + D\left|I(\mathbf{k})\right\rangle = \left|E(\mathbf{k})\right\rangle \\
&(ikW + 1)S\left|I(\mathbf{k})\right\rangle = S^{-1}\left|E(\mathbf{k})\right\rangle \\
&\left|I(\mathbf{k})\right\rangle = S^{-1}(1 + ikW)^{-1}S^{-1}\left|E(\mathbf{k})\right\rangle \\
&W\left|\psi_\mu\right\rangle = \lambda_\mu\left|\psi_\mu\right\rangle \\
&\left|I(\mathbf{k})\right\rangle = \sum_\mu \frac{S^{-1}\left|\psi_\mu\right\rangle\left\langle\psi_\mu\right|S^{-1}\left|E(\mathbf{k})\right\rangle}{1 + ik\lambda_\mu}
\end{align*}
$$
The Spectral Solution

\[ I(r, \hat{s}) = \sum_{lm} \frac{1}{\sqrt{\sigma_l}} \int \sum_{\mu} \frac{\langle lm | \psi_\mu \rangle \langle \psi_\mu | S^{-1} | E(k) \rangle Y_{lm}(\hat{s}; \hat{k})}{1 + ik \lambda_\mu} e^{ik \cdot r} d^3 k \]

\[ \varepsilon(r, \hat{s}) = \delta(r - r_0) \delta(\hat{s} - \hat{s}_0) \]

\[ E_{lm}(k) = \frac{1}{(2\pi)^3} e^{-ik \cdot r_0} Y_{lm}^*(\hat{s}_0; \hat{k}) \]

The integral is not easy… but doable.

\[ G_0(\mathbf{r}, \hat{\mathbf{s}}; \mathbf{r}_0, \hat{\mathbf{s}}_0) = \sum_{m=-\infty}^{\infty} \sum_{l,l'=-|m|}^{\infty} Y_{lm}(\hat{\mathbf{s}}; \hat{\mathbf{R}}) \chi_{ll'}^m(R) Y_{l'm}^*(\hat{\mathbf{s}}_0; \hat{\mathbf{R}}) \]

\[ \chi_{ll'}^m(R) = \frac{(-1)^{\frac{m}{2}}}{2\pi \sqrt{\sigma_l \sigma_{l'}}} \sum_{M=-\overline{l}}^{\overline{l}} (-1)^M \sum_{n, \lambda_n > 0} \frac{\langle l | \phi_n(M) \rangle \langle \phi_n(M) | l' \rangle}{\lambda_n^3(M)} \]

\[ \times \sum_{j=0}^{\overline{t}} C_{l,M,l',-M}^{l'-l'+2,j,0} C_{l,m,l',-m}^{l'-l'+2,j,0} k_{l'-l'+2,j} \left( \frac{R}{\lambda_n(M)} \right) \]

\[ \overline{t} = \min(l, l') \]

\[ \mu = (M, n) \]

\[ \langle lm | \psi_{Mn} \rangle = \delta_{mm} \langle l | \phi_n(M) \rangle \]
FIG. 1: Eigenvalues of the matrices $W(M)$ for the following parameters: $\mu_a = 0.03\text{cm}^{-1}$, $\mu_s = 500\text{cm}^{-1}$, $g = 0.98$. These parameters are typical for biological tissues in the near-infrared spectral range. (a) All eigenvalues of $W(0)$ vs the eigenvalue number $n$. (b) The maximum eigenvalues of the matrices $W(M)$ vs $M$. In simulations, infinite matrices $W(M)$ have been truncated so that the size of each matrix was $N = 10^3$. 
* If $|\lambda| < 1 / \mu_t$ - continuous spectrum

  If $|\lambda| > 1 / \mu_t$ - discrete spectrum

* Bounds on the diffuse eigenvalue $\lambda_d = \max[\lambda_n(0)]$

  $$D = c\mu_a \lambda_d^2$$

  $$\sqrt{\beta_1^2 + \beta_2^2} \leq \lambda_d \leq \beta_1 + \beta_2$$

  $$\beta_i = \frac{b_i(0)}{\sqrt{\sigma_i \sigma_{i-1}}}; \quad \beta_1 = \frac{1}{\sqrt{3\mu_a [\mu_a + (1 - A_1)\mu_s]}};$$

  $$\beta_2 = \frac{2}{\sqrt{15[\mu_a + (1 - A_1)\mu_s][\mu_a + (1 - A_2)\mu_s]}}$$

* Bound on the gap: $\Delta \lambda = \lambda_d - \lambda_{\text{next largest}}$

  $$\Delta \lambda \geq \max[\sqrt{\beta_1^2 + \beta_2^2} - \beta_2 - \beta_3, 0]$$
Density, Current, and the Fick’s Law

\[ u(r) = \frac{1}{c} \int I(r, \hat{s}) d^2s ; \quad J(r) = \frac{1}{c} \int I(r, \hat{s}) \hat{s} d^2s \]

\[ u(r) = \frac{1}{c} \sum_{l=0}^{\infty} \sqrt{2l + 1} \lambda^0_{0l}(r) P_l(\hat{s}_0 \cdot \hat{r}) \]

\[ J(r) = \frac{\hat{r}}{\sqrt{3}} \sum_{l=0}^{\infty} \sqrt{2l + 1} \lambda^0_{1l}(r) P_l(\hat{s}_0 \cdot \hat{r}) \]

If \( \kappa = \frac{r}{\Delta \lambda} \frac{\lambda_d}{\lambda_{\text{next largest}}} \ll 1 \), then

\[ J = -D \nabla u , \quad \text{where} \quad D = c \mu_a \lambda_d^2 \]
Angular dependence of the specific intensity for forward (a) and backward (b) propagation obtained at $l_{\text{max}} = 21$, $g = 0.98$ and $\mu_a/\mu_s = 6 \cdot 10^{-5}$. The distance to the source $z$ is assumed to be positive for forward propagation and negative for backward propagation.
Infinite Space, Point Uni-Directional (Sharply-Peaked) Source

(b) off-axis propagation

Two cases:

a) \( \hat{s} \) in the \( xy \) plane

b) \( \hat{s} \) in the \( yz \) plane
Angular distribution of specific intensity for off-axis propagation (relatively small absorption)
Parameters: $g = 0.98$ and $\mu_a/\mu_s = 6 \cdot 10^{-5}$ (a), (b), $= 0.03$ (c), (d).
Angular distribution of specific intensity for off-axis propagation (relatively large absorption)
Parameters: $g = 0.98$ and $\mu_a/\mu_s = 0.2$. 
Plane-Wave Decomposition

\[ I(\mathbf{r}, \mathbf{s}) = \sum_{lm} \frac{1}{\sqrt{\sigma_l}} \int \sum_{\mu} \left| \langle \psi \rangle_{\mu} \right| \left| \psi_{\mu} \right\rangle \frac{E(\mathbf{k})}{1 + i \mathbf{k} \lambda_{\mu}} Y_{lm}(\mathbf{s} ; \mathbf{k}) \right] e^{i \mathbf{k} \cdot \mathbf{r}} d^3 k \]

\[ G_0(\mathbf{r}, \mathbf{s}; \mathbf{r}_0, \mathbf{s}_0) = \sum_{lm, l'm'} \int \frac{d^2 q}{(2\pi)^2} e^{i \mathbf{q} \cdot (\mathbf{r}-\mathbf{r}_0)} Y_{lm}(\mathbf{s} ; \mathbf{z}) g_{l'm'}(\mathbf{q}; \mathbf{z}, \mathbf{z}_0) Y_{l'm}^*(\mathbf{s}_0 ; \mathbf{z}) \]

\[ g(\mathbf{q}; \mathbf{z}, \mathbf{z}_0) = \int_{-\infty}^{\infty} \frac{dk_z}{2\pi} e^{i k_z (z-z_0)} D(\mathbf{q} + \mathbf{z} k_z) K\left( \sqrt{q^2 + k_z^2} \right) D^\dagger(\mathbf{q} + \mathbf{z} k_z) \]

\[ K(w) = \sum_{\mu} \frac{S^{-1} \left| \psi_{\mu} \right\rangle \left| \psi_{\mu} \right\rangle S^{-1}}{1 + i w \lambda_{\mu}} ; \quad D(\mathbf{k}) = e^{-i \varphi_k J_z} e^{-i \theta_k J_y} \]

\[ \cos \theta_k = \frac{k_z}{\sqrt{q^2 + k_z^2}} \]
\[
g_{l'm'}(q; z, z_0) = \frac{e^{-i(m-m')\varphi_q}}{\sqrt{\sigma_l\sigma_{l'}}} \left[ \text{sgn}(z - z_0) \right]^{l+l'+m+m'} \sum_{m_1 = -l}^l \sum_{m_2 = -l'}^{l'} \sum_{\mu, \lambda_\mu > 0} d_{m_1 m_2}^l \left[ i \tau(q\lambda_\mu) \right] \\
\times \left\langle lm_1 | \psi_\mu \right\rangle \frac{e^{-Q_\mu(q)|z-z_0|}}{\lambda_\mu^2 Q_\mu(q)} \left\langle \psi_\mu | l'm_2 \right\rangle d_{m_1 m_2}^{l''} \left[ i \tau(q\lambda_\mu) \right]
\]

\[Q_\mu(q) = \sqrt{q^2 + 1 / \lambda_\mu^2}\]

\[\cos[i\tau(x)] = \sqrt{1 + x^2}, \quad \sin[i\tau(x)] = -ix\]

\[D_{mm'}^{l}(\alpha, \beta, \gamma) = e^{-i\alpha} d_{mm'}^{l}(\beta) e^{-i\gamma}\]
Evanescent Waves

Plane waves:

\[ I_k = e^{-k \cdot r} \ F_k(\hat{s}), \quad k \cdot k = 1 / \lambda^2, \quad k = k \hat{n} \]
\[ \hat{n} \ - \ real \ unit \ vector \]

\[ F_k(\hat{s}) = \sum_{lm} \langle lm | \psi_\mu \rangle Y_{lm}(\hat{s}; \hat{k}) \]

Evanescent waves:

\[ k = -i q \pm \hat{z} \sqrt{q^2 + 1 / \lambda^2}, \quad q \cdot \hat{z} = 0, \quad k \cdot k = 1 / \lambda^2 \]

\[ k_z = \pm \sqrt{q^2 + 1 / \lambda^2_n} \]
\[
I_{kMn} = \exp\left(-\frac{\hat{k} \cdot \hat{r}}{\lambda_{Mn}}\right) \sum_{lm} Y_{lm}(\hat{s}; \hat{z}) \frac{\exp(-im\varphi_k)}{\sqrt{\sigma_l}} d^l_{mM}(\theta_k) \langle l | \phi_n(M) \rangle
\]
(plane wave modes)

\[
I^{(\pm)}_{qMn} = \exp[iq \cdot \rho - Q_{Mn}(q)z] \sum_{lm} Y_{lm}(\hat{s}; \hat{z}) \frac{\exp(-im\varphi_q)}{\sqrt{\sigma_l}} (-1)^{l+m} d^l_{m,-M}(\theta_k) \langle l | \phi_n(M) \rangle
\]
(evanescent modes)

\[
G_0(r, \hat{s}; r_0, \hat{s}_0) = \sum_{Mn} \int \frac{d^2q}{(2\pi)^2} I^{(\pm)}_{qMn}(r, \hat{s}) V_{qMn} I^{(\pm)}_{-qMn}(r_0, -\hat{s}_0)
\]

\[
V_{qMn} = \frac{1}{Q_{Mn}(q)\lambda_{Mn}^2}
\]
Half-space problem

$Z > 0$
Scattering medium
Propagation described by the RTE

$\varphi < 0$
Non-scattering medium

\[ I = \int \frac{d^2 q}{(2\pi)^2} \sum_{Mn} A_{Mn}(q) I_{qMn}^{(+)} \]
\[
\frac{\mu_a}{\mu_s} = 6.0 \times 10^{-5}, \quad g = 0.98.
\]
CONCLUSIONS

- The method of rotated reference frames takes advantage of all symmetries of the RTE (symmetry with respect to rotations and inversions of the reference frame).
- The angular and spatial dependence of the obtained solutions is expressed in terms of analytical functions.
- The analytical part of the solution is of considerable mathematical complexity. This is traded for relative simplicity of the numerical part. We believe that we have reduced the numerical part of the computations to the absolute minimum allowed by the mathematical structure of the RTE.
Publications:


Available on the web at

http://whale.seas.upenn.edu/vmarkel/papers.html