Data-Compatible T-Matrix Completion (DCTMC)

A new numerical method for solving nonlinear inverse problems

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Motivation 1: Local Minima

\[ F[V] = \Phi \]

\[ \chi = D[F[V] - \Phi] + \lambda^2 D[\Phi - \Phi_{\text{guess}}] \]

Theoretical model

Object

Data

Wave in

Wave out

\[ V(r) \]
Motivation 2: Large Data Sets

\[ \chi = D[F[V] - \Phi] + \lambda^2 D[\Phi - \Phi_{\text{guess}}] \]

\[ N_s = L^2 \]
\[ N_d = L^2 \]
\[ N = N_s N_d = L^4 \]
Algebraic Structure of the Inverse Problem

\[ A(I - V\Gamma)^{-1}VB = \Phi \]

Every variable is a matrix!

\( A, B, \Gamma \) -- different restrictions of the same unperturbed Green's function \( G_0 \)

\( \sum_d \) Surface of detectors

\( \Omega \)

\( \sum_s \) Surface of sources

\[ r_1, r_1', r_2, r_2' \in \Omega; r_s \in \sum_s; r_d \in \sum_d \]
Let us view T-matrix as the fundamental unknown and use the one-to-one Correspondence between $T$ and $V$.

\[ A(I - V\Gamma)^{-1}VB = \Phi \]

\[ T[V] = (I - V\Gamma)^{-1}V \]

\[ V[T] = (I + TV)^{-1}T \]

\[ ATB = \Phi \]
Main Idea

(1) First, we define a class of kernels $V(r, r')$ that are compatible with the data. This is the only instance when the data are used, and it turns out that the size of the data set is not a limiting factor for this step.

(2) Then we iteratively reduce the off-diagonal norm of $V(r, r')$ while making sure that $V(r, r')$ remains within the class of “data-compatible” kernels.

(3) Once the ratio of the off-diagonal and diagonal norms of $V(r, r')$ is deemed sufficiently small, we compute $\sigma(r) = \int V(r, r') \, d^3r'$. This gives an approximate numerical solution to the nonlinear ISP.
The Experimental T-Matrix

\[
A = \sum_{\mu=1}^{N_d} \sigma^A_{\mu} \langle \phi^A_{\mu} \rvert g^A_{\mu} \rangle
\]

\[
B = \sum_{\mu=1}^{N_s} \sigma^B_{\mu} \langle \phi^B_{\mu} \rvert g^B_{\mu} \rangle
\]

\[
ATB = \Phi
\]

\[
\sigma^A_{\mu} \sigma^B_{\nu} \tilde{T}_{\mu\nu} = \tilde{\Phi}_{\mu\nu}, \\
1 \leq \mu \leq N_d, \\
1 \leq \nu \leq N_s
\]

\[
\tilde{\Phi}_{\mu\nu} = \langle \phi^A_{\mu} \rvert \Phi \rvert g^B_{\nu} \rangle, \quad 1 \leq \mu \leq N_d, \\
1 \leq \nu \leq N_s
\]

\[
\tilde{T}_{\mu\nu} = \langle g^A_{\mu} \rvert \Phi \rvert \phi^B_{\nu} \rangle, \quad 1 \leq \mu, \nu \leq N_{\nu}
\]

\[
\tilde{T} = R_A^* T R_B = R[T] \quad \text{,} \quad T = R^{-1}[\tilde{T}]
\]

\[
\tilde{T} = \begin{bmatrix}
\tilde{T}_{\mu\nu} & \frac{\Phi_{\mu\nu}}{\sigma^A_{\mu} \sigma^B_{\nu}} & M_A \\
M_B & UNKNOWN
\end{bmatrix}
\]

\[
\tilde{T}_{\text{exp}} = \begin{bmatrix}
\tilde{T}_{\mu\nu} & \frac{\Phi_{\mu\nu}}{\sigma^A_{\mu} \sigma^B_{\nu}} & M_A \\
M_B & UNKNOWN
\end{bmatrix}
\]

\[
T_{\text{exp}} = A^+ \Phi B^+
\]
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Data-compatible T-matrix Representation: SV $kT$

Diagonal interaction-compatible T-matrix Representation: RS $T'_k$

Diagonal interaction-compatible T-matrix Representation: SV $\tilde{T}'_k$

Data-compatible T-matrix Representation: SV $\tilde{T}_k$

First iteration

Subsequent iterations

SVD of $A$ and $B$

Shortcut 1: Fast Rotations

Shortcut 2: Fast $T \rightarrow D$

The Bottleneck

1. $\mathcal{R}^{-1}$

2. $T^{-1}$

3. $\mathcal{D}$

4. $\mathcal{T}$

5. $\mathcal{R}$

6. $\mathcal{O}$

Exit if condition is met

Data
$\Phi$

Diagonal interaction matrix (not data-compatible) $D_k$

Data-compatible interaction matrix (off-diagonal) $V_k$

$T_k$

$\tilde{T}_k$

$k \rightarrow k + 1$

$kT'$

$\tilde{T}'_k$
Computational Shortcut: Fast Rotations

5: \( \tilde{T}_k' = R[T_k'] \)
6: \( \tilde{T}_{k+1} = \mathcal{O}[\tilde{T}_k'] \) \( \mathcal{O}[\tilde{T}] = \mathcal{M}[\tilde{T}] + \tilde{T}_{\text{exp}} = \tilde{T} - \mathcal{N}[\tilde{T}] + \tilde{T}_{\text{exp}} \)
1: \( T_{k+1} = R^{-1}[\tilde{T}_{k+1}] \) \( \mathcal{M}[\tilde{T}] + \mathcal{N}[\tilde{T}] = \tilde{T} \)

\[ T_{k+1} = R^{-1}[\mathcal{O}[R[T_k']]] = T_k' + T_{\text{exp}} - R^{-1}[\mathcal{N}[R[T_k']]] \]

\[ R^{-1}[\mathcal{N}[R[T]]] = P_A (P_A^* T P_B) P_B^* \]
Operation of “Diagonalization” and Linear Reconstructions

\[ D = \mathcal{D}[V] \]
\[ D_{ij} = \delta_{ij} \sum_{j} w(r_{ij}) V_{ij} \]

If \( w(r_{ij}) = \delta_{ij} \), we can analyse the algorithm in the linear regime:

\[ |v_{k+1}\rangle = |v_{\text{exp}}\rangle + (I - W)|v_k\rangle \]

\[ W_{ij} = (P^*_A P_A)_{ij} (P^*_B P_B)_{ji} \]

Vector containing the diagonal part of \( V \)

Fixed point: \( |v_\infty\rangle = W^{-1} |v_{\text{exp}}\rangle \)

Tikhonov regularization: \( W \rightarrow W + \lambda^2 I \)

Practical tip: Richardson iteration is a very slow way to arrive at the linearized solution. Use direct solver of CG to compute linearized solution and then use this result as an initial guess for the nonlinear iterations.
Diffraction tomography:

\[ G_0(r, r') = \frac{\exp(ik|r - r'|)}{|r - r'|} \]

Contrast:

\[ \chi(r) = \frac{\varepsilon(r) - 1}{4\pi} \]
No improvements: 900 iterations

\[
\chi_0 = 0.00175 \quad \chi_0 = 0.0175 \quad \chi_0 = 0.175 \quad \chi_0 = 0.875 \quad \chi_0 = 1.75
\]
With improvements: 70 iterations

- Start from linearized reconstruction (can be computed fast using our method)
- Use weighted summation to the diagonal for “force-diagonalization”
- Use reciprocity of source-detector pairs to improve symmetry of the experimental T-matrix
- Method starts to break down due to incorrect assignment of non-interacting voxels (this can be avoid altogether – not a problem of convergence)
Diffusion tomography:

\[
G_0(r, r') = \frac{\exp\left(-k |r - r'|\right)}{|r - r'|}
\]

Contrast:

\[
\delta \alpha(r) = \frac{\alpha(r) - \alpha_0}{\alpha_0}
\]

Optical depth: \(kL \approx 2\)

Noise: \(2\%\)
Target far

\[ \chi_0 = 0.001 \quad \chi_0 = 0.01 \quad \chi_0 = 0.1 \quad \chi_0 = 1.0 \quad \chi_0 = 2.0 \]
Target near

\[ \chi_0 = 0.001 \quad \chi_0 = 0.01 \quad \chi_0 = 0.1 \quad \chi_0 = 1.0 \quad \chi_0 = 2.0 \]
DCTMC works when Newton-Gauss fails (Convergence of Levenberg-Marquardt Iterations for the inverse diffraction problem, moderate contrast 0.0175)
CONCLUSIONS

• DCTMC works for nonlinear ISP with fairly strong nonlinearity
• DCTMC is, unfortunately, a complicated method: it requires many tweaks, attention to detail, and good programming to work
• As any other method, DCTMC breaks at some point. Not every nonlinear ISP can be solved!
• Please listen to Howard Levinson at 15:15 today (this room)

Under consideration in Phys. Rev. E