Learning Direct and Inverse Transmission Matrices

Daniele Ancora
CNR-NANOTEC, Institute of Nanotechnology, Rome Unit, Soft and Living Matter Lab., Piazzale Aldo Moro, 5, 00186, Rome, Italy

Luca Leuzzi
CNR-NANOTEC, Institute of Nanotechnology, Rome Unit, Soft and Living Matter Lab., Piazzale Aldo Moro, 5, 00186, Rome, Italy and Physics Department, Sapienza University, Piazzale Aldo Moro, 5, 00186, Rome, Italy

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Linear problems appear in a variety of disciplines and their application for the transmission matrix recovery is one of the most stimulating challenges in biomedical imaging. Its knowledge turns any random media into an optical tool that can focus or transmit an image through disorder. Here, converting an input-output problem into a statistical mechanical formulation, we investigate how inference protocols can learn the transmission couplings by pseudolikelihood maximization. Bridging linear regression and thermodynamics let us propose an innovative framework to pursue the solution of the scattering-riddle.

A major interest in biomedical imaging is the comprehension of the light scattering through disordered media: many recent studies have achieved light-focusing and image reconstruction even through complex biological tissues [1, 2]. The deterministic nature of the scattering event suggests that turbid devices could be treated as a normal optical tool: the memory effect principle [3] states that tilting the illumination wavefront turns into a translation of the scrambled intensity pattern. This makes the turbid layer acting as an autocorrelation-lens [4], possible to be used for focusing or imaging through -or even behind- opaque walls. More generally, any small variation of the input wavefront results into a small variation of the output in a deterministic and continuous fashion, thus a transmission matrix approach was proposed to describe the process [5]. In analogy with classical optics, the transmission matrix would contain the -yet complicated- rules on how the device acts on a given input, transporting it into a disordered output via a linear combination. Although few important studies were done [6, 7], measuring such matrix is one of the greatest challenges in disordered photonics [8] and could give new insights on the scattering process. Among a number of possible applications, the main interest of the biomedical imaging community is toward its measurement in a disordered multi-mode fiber transmission [9], that would open up their usage against the more fragile and expensive single-mode bundle fibers counterpart in endoscopic devices. Put in simple words, the problem is that whatever we send in the input appears totally randomized at the output, due to the complex photon paths permitted by the complex media. An established option, at the moment, is the method provided by Popoff et al. [6] that relies on the usage of the Hadamard basis for the input to calculate the transmission matrix based on output observations. Since it relies on output sampling on a given input basis, this method is quite specific and, in practice, one needs to accomplish \( T \)-matrix inversion before being able to effectively focus or image through disorder. Our study fits in this scenario: we investigate how statistical inference could offer a novel way to learn the transmission matrix \( T \) of a complex media, unbounded from any basis and even free from matrix inversion. In the following, we will introduce the mathematical model, inspired by a spin-like thermodynamic description of an interacting input/output Hamiltonian. The analogy with spin-glass theory let us borrow a number of statistical tools for the inference of the coupling parameters, tightly linked with the unknown \( T \). In particular, we make use of a pseudolikelihood maximization approach coupled with a progressive parameter decimation scheme [11]. On the other hand, for very sparse matrices one might consider the recent activation technique [12]. The model, in these terms, is scalable to any number of parallel implementations, avoiding exponential complexity for the solution of the inverse problem. At the current stage, we leave our approach general in terms of applicability, promoting it also as a thermodynamic alternative to any linear regression problem [13].

We start considering a linear transmission problem involving a two-edge input-output system (from now on I/O). In these terms, the disordered medium acts as a linear light scrambler, connecting the input \( F^\text{in} \) (described by the index \( \alpha = 1, \ldots, N/2 \)) to the output pattern \( F^\text{out} \) (index \( \gamma = 1, \ldots, N/2 \)) via an intensity transmission matrix \( T \) of the form given by:

\[
F^\text{out}_\gamma = \sum_{\alpha=1}^{N/2} T_{\gamma \alpha} F^\text{in}_\alpha + \sigma_\gamma \epsilon_\gamma. \tag{1}
\]

In Eq. (1), the last factor is a noise term given by the product of \( \epsilon \), a vector containing normally distributed random numbers. The term \( \sigma_\gamma \) rescales the mean square displacement in the channel \( \gamma \). Let us initially set \( \sigma_\gamma = 0, \forall \gamma \). This is a simplified optical model, due to the fact...
that we are connecting the intensities measured from both fiber’s ends rather than treating more appropriately complex electromagnetic fields \[^5 \, ^{13},^{15}\]. With such assumption we are neglecting the phases that cannot be directly measured with current technology, looking only at the modulus squared of the field amplitude at each site. This method would work rigorously with incoherent sources and serves to introduce the statistical framework. In this representation \(T\) is not exactly the electromagnetic transmission matrix of the fiber, but rather a matrix connecting the intensities between the fiber’s ends: however, we will refer to it as an effective-\(T\), leaving the discussion of the more realistic case to further studies. We stress, however, that the present model has the advantage to be easily applicable to any generic experimental I/O pattern.

The recovery of the matrix \(T\) corresponds to find the solution of all equations (1), such that:

\[
\int \prod_{\gamma=1}^{N/2} dI_{\gamma}^{out} \delta \left( I_{\gamma}^{out} - \Delta \sum_{\alpha=1}^{N/2} T_{\gamma\alpha} I_{\alpha}^{in} \right) = 1. \tag{2}\]

Assuming Gaussian noise-induced uncertainty to the solutions of these equations corresponds to approximate the \(\delta\)-functions in (2) with Gaussian functions having their variance vanishing to zero, so that we can write Eq. (2) as

\[
\lim_{\Delta \to 0} \int \prod_{\gamma=1}^{N/2} dI_{\gamma}^{out} \frac{e^{-\frac{1}{2\Delta^2} \left( I_{\gamma}^{out} - \Delta \sum_{\alpha=1}^{N/2} T_{\gamma\alpha} I_{\alpha}^{in} \right)^2}}{\sqrt{2\pi\Delta^2}} = 1. \tag{3}\]

The mean square displacement \(\Delta\) corresponds to the uncertainty term \(\sigma_\gamma\) in (1). For the sake of simplicity we initially consider the same noise for each channel. Let us call \(\mathcal{H}\) the squared argument on the exponent, that can be readily expressed as:

\[
\mathcal{H} = \sum_{\gamma} \left( I_{\gamma}^{out} - \Delta \sum_{\alpha=1}^{N/2} T_{\gamma\alpha} I_{\alpha}^{in} \right)^2 = \sum_{\gamma} (I_{\gamma}^{out})^2 - 2 \sum_{\gamma,\alpha} I_{\gamma}^{out} T_{\gamma\alpha} I_{\alpha}^{in} + \sum_{\gamma,\alpha,\alpha'} T_{\gamma\alpha} T_{\gamma\alpha'} I_{\alpha}^{in} I_{\alpha'}^{in} = \sum_{i,j} I_i J_{ij} I_j. \tag{4}\]

To reach the matrix formulation (4) we defined a generic vector \(\mathbf{I} = \{ I_{\gamma}^{in}, I_{\alpha}^{out} \} \) of length \(N\) obtained concatenating both the elements of the input and output fields, where both indexes \(i, j = \{ \gamma, \alpha \}\) span the concatenated input and output indexes. Explicitly, the interaction matrix \(J\) has the form of a tensor that contains the transmission matrix and its conjugate as expressed in:

\[
J = \left( \begin{array}{cc} -U & +2T^\dagger \\ +2T & -I \end{array} \right) \tag{5}\]

where \(U = T^\dagger T\) is the input self-coupling Gramian matrix, \(T\) is the transmission matrix defined in Eq. (1) and \(I\) is the identity matrix. \(J\) is the generalized coupling matrix that we will infer with a statistical approach. In this framework the system can be seen as a generalized spin-like I/O model described by the Hamiltonian \(\mathcal{H} = \mathbf{I}^\dagger J \mathbf{I}\).

Giving a statistical interpretation to the Boltzman factor \(e^{-\beta \mathcal{H}}\) in (5), the probability of a coupled input-output realization \(\mathbf{I}\) with a given Hamiltonian disapplying coupling constants \(J_{ij}\) is equal to:

\[
P(\mathbf{I}|J) = \frac{1}{Z(J, \mathbf{I})} \exp \left\{ -\beta \sum_{ij} I_i J_{ij} I_j \right\} \tag{6}\]

where the partition function of the system is:

\[
Z(J, \mathbf{I}) = \int \prod_{k=1}^{N} dI_k e^{-\beta \mathcal{H}(J, \mathbf{I})}. \tag{7}\]

with the definition \(\beta = (2\Delta^2)^{-1}\), to be interpreted as the inverse temperature of the I/O model, relative to the effective noise term in the measurements. Given the probability, we can write the (log-)likelihood that a system with couplings \(\{ J_{ij} \}\) yields the experimental I/O realizations \(\mathbf{I}\):

\[
\mathcal{L} = \text{ln} \left[ P(\mathbf{I}|J) \right]. \tag{8}\]

The set of couplings \(J_{ij}\) that maximizes the likelihood are the ones that most likely represent the observed model \(\mathcal{H}(J, \mathbf{I})\) given all the possible realizations of \(\mathbf{I}\).

Unfortunately \(\mathcal{L}\) is very difficult to maximize due to an exponential complexity growth as a function of the number of parameters to be inferred. It is convenient in this case, to consider a less computational expensive approach by introducing the log-pseudolikelihood function.
We proceed fixing all intensities except the \( i \)-th, and we write the conditioned probability of a value of \( I_i \) given the values of all the other pixels \( I_{\setminus i} \):

\[
P(I_i|I_{\setminus i}) = \frac{P(I_i, I_{\setminus i})}{P(I_{\setminus i})}.
\]  

The function \( H \) is separable in \( N \) independent partial functions \( H_i \) as

\[
H = \sum_{i=1}^{N} \left[ I_i \sum_{j \neq i} J_{ij} I_j + I_i^2 J_{ii} \right] = \sum_{i=1}^{N} H_i
\]  

We further define \( A_i \equiv -\beta_i \) and \( B_i \equiv \beta_i \sum_{j \neq i} J_{ij} I_j \) such that

\[
\beta_i H_i = I_i B_i |I_{\setminus i}| - I_i^2 A_i.
\]  

We notice that we leave the parameters \( \beta_i \) free to variate for each pseudo-likelihood, to quantify the noise at each channel independently. In fact, thermodynamically, this factor could be seen as an inverse channel temperature for \( i = N/2 + 1, \ldots, N \) (when it is expected \( J_{ii} = 1 \)). By definition, the \( A_i \geq 0 \), \( \forall i \), guaranteeing the convergence of the partition function. Using Eq. (10) we write the pseudolikelihood of the variable \( i \) as

\[
P(I_i|I_{\setminus i}) = \frac{e^{H_i(I_{\setminus i})}}{Z_i(I_{\setminus i})}
\]  

\[
Z_i(I_{\setminus i}) = \int dI_i e^{H_i(I_{\setminus i})} = \int dx e^{-A_i x^2 + B_i |I_{\setminus i}| x}
\]

and the log-pseudolikelihood per element \( i \) is:

\[
\mathcal{L}_i = \ln P(I_i|I_{\setminus i}) = \beta_i H_i - \ln Z_i.
\]

Two approaches are available at this stage: we minimize all the \( \mathcal{L}_i \) in function of the coupling matrix \( J \) using some regularization [14], or we minimize their sum

\[
\mathcal{P} \mathcal{L} \equiv \sum_{i=1}^{N} \mathcal{L}_i
\]

that we refer to as total log-pseudolikelihood function. The latter is commonly followed by a decimation procedure [11], in which we recursively set to zero small couplings until the total pseudolikelihood is not substantially affected by such change.

It is obvious that \( \mathcal{L}_i \) strictly depends upon the integration extremes of the partition function. The choice of the integral extremes in Eq. (12) has to take into account all the possible intensities allowed by the system. Although the intensity treated are always in a limited range, we found that the general choice of integrating along the whole real axis works for the intensity ranges tested. Thus, the undefined integral (12) can be calculated between \((-\infty, \infty)\):

\[
Z_i = \sqrt{\frac{\pi}{4A}} e^{\frac{B}{2A}} \text{erf} \left( \frac{B + 2AI_i}{\sqrt{4A}} \right) \bigg|_{-\infty}^{+\infty} = 2 \sqrt{\frac{\pi}{4A}} e^{\frac{B^2}{4A}}.
\]

This simple operational choice for the extremes turns out to be the most effective against more strict integration ranges (see Ref. [19] for details), leading to:

\[
\mathcal{L}_i = I_i B_i |I_{\setminus i}| - I_i^2 A_i - \frac{1}{2} \ln \left( \frac{\pi}{4A_i} \right) - \ln 2.
\]

By definition, \(-\mathcal{L}_i\) are convex functions that can be minimized using a quasi-Newton method. We implement the algorithm in a MATLAB environment, with the minFunc routine for the L-BFGS function optimization [20]. To test the model and the inference procedure we choose a squared matrix having a side length of \( w = 12 \) px, both for the input and output signal, turning into \( N = 2w^2 = 288 \) total intensity values. For this system, \( T \) is a \( w^2 \times w^2 \) matrix with \( w^4 = 20736 \) coupling parameters to be estimated. On the other side, we are optimizing the cost function of the system, Eq. (4) via the coupling matrix \( J \), that now has \( k = (2w^2)^2 = 82944 \) parameters (not all independent). We generate data to analyze through transmission matrices \( T \) built with a random activation of 20% of its elements (set equal to 1). The value of each element is then, rescaled by the number of total active parameters per row, so that \( \sum_{\gamma=1}^{N/2} T_{\gamma \gamma} = 1 \). In this way, selecting a random input intensity distribution in the range of \( I_i^{in} \in [0,1] \), also gives \( I_i^{out} \in [0,1] \). We stress that, however, the results presented in the following are general, with no restriction for intensity range nor matrix dimension. To the output we add a Gaussian noise of null mean and mean square displacement in the range of \( \sigma = [0,0.5] \), running independent optimization per each \( \sigma \). With this procedure we create a sample of \( M = 5000 \) couples of input and outputs for the inference.

The green curve in Fig. 2 represents the first minimization of Eq. (14), with all the parameters free to variate,
the quality of the focusing rapidly drops already around in a focusing experiment to transmit a Gaussian function comes systematically larger. However, when using red line. The two curves follow the same trend up to a values of the non-zero inferred elements can vary) with a points and the error on the true network (though var-

The best number of couplings minimize the BIC and serves to rule out the noise is non-zero. In Fig 4, part b we show how the object reconstructed is recognizable by the eye practically with respect to the inverse of the inferred $T$, as soon as the noise is non-zero. In Fig 4, part b we show how the object reconstructed is recognizable by the eye practically for any noise. Compared against the results of the direct $T$ calculation, we observe that denser matrices seem more robust to noise in all cases considered, though dedicated studies are required before making a general statement out of this evidence.

Finally, it is important to notice that $\beta_{\gamma>N/2}$ plays the role of an inverse temperature in the inference process. It is the effective noise variance per each channel, that in the output part turns into $\beta_{\gamma} \rightarrow 1/2/\sigma_{\gamma}$, where we now consider an explicit dependence of the noise on the channel, cf. Eq. (3) (see also Ref. [19] for details). This information is automatically inferred in the diagonal part of $J$ and serves to rule out $T$ and $U$, giving information about the transmission efficiency through the disordered channel.

The model developed let us estimate I/O intensity coupling matrices via a machine learning approach and several benefits emerge from the usage of pseudolikelihood formulation. First of all, the pseudolikelihood can be calculated -and minimized- per each $i$-th element, making the computation scalable and trivially parallel, linearly depending on hardware resources (such as numbers of CUDA cores or independent GPUs). Moreover, the model is directly applicable for the estimation of the inverse coupling matrix $T^{-1}$, rather than using matrix inversion or time reversal approaches [8, 21], experimentally extremely sensitive to noise. Due to its self consistent nature, the model gives us two further important information, such as the noise-estimation per channel (given by the diagonal part of the output-output coupling $J$) and the balance criteria in the input-input Gramian matrix $U$, which can be used to monitor algorithm convergence and as halt criteria. Lastly, our procedure can be generalized to any I/O system in any linear-regression scenarios. Here we considered intensi-
ties to provide a protocol ready to process experimental data, but the model can be extended straightforwardly to complex fields [5, 14], and it is possible to add polarization, i.e., vectorial waves, and wavelength dependence of $T$ elements as further (linearly scalable) degrees of freedom. In the case of complex fields, the problem of the phase measurements is still present, but we could overcome it by integrating out the partition function over all the possible phases. In this case the pseudolikelihood formulation is more complicated, but the approach would be identical. In fact, rather than focusing on the exact model, this letter wants to introduce a first statistical framework for the $T$-estimation. The usage of statistical models let us interpret the $T$-recovery problem in terms of the minimization of the entropy of a system described by the coupling $J$, thus into a thermodinamical problem, borrowing a number of tools coming from statistical mechanics. Thus, it opens up numerous opportunities, such as the study on the influence of the noise in the inference process up to study possible presence of phase transitions in terms of $T$-matrix sparsity. This could lead to important characterization of structured focusing patterns [22, 23] via its intrinsic transmission properties, or to study Anderson localization in 2D optical disordered systems [24, 25], besides offering a statistical framework to study light propagation through opaque media.

FIG. 4. Image reconstruction quality using the inferred $T^{-1}$ in log-scale. It is possible to notice how the inversion of the direct $T$ immediately degrades the reconstruction quality at low noise level, while the inference of the inverse transmission is highly stable up to the whole noise range studied.
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