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2003 J. Phys. A: Math. Gen. 36 2995

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Random projections and the optimization of an algorithm for phase retrieval

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Received 22 July 2002, in final form 2 October 2002

Published 12 March 2003

Online at stacks.iop.org/JPhysA/36/2995

Abstract

Iterative phase retrieval algorithms typically employ projections onto constraint subspaces to recover the unknown phases in the Fourier transform of an image, or, in the case of x-ray crystallography, the electron density of a molecule. For a general class of algorithms, where the basic iteration is specified by the *difference map*, solutions are associated with fixed points of the map, the attractive character of which determines the effectiveness of the algorithm. The behaviour of the difference map near fixed points is controlled by the relative orientation of the tangent spaces of the two constraint subspaces employed by the map. Since the dimensionalities involved are always large in practical applications, it is appropriate to use random matrix theory ideas to analyse the average-case convergence at fixed points. Optimal values of the γ parameters of the difference map are found which differ somewhat from the values previously obtained on the assumption of orthogonal tangent spaces.

PACS numbers: 02.60.-x, 02.30.Nw, 42.30.Kq

1. Introduction

In two-dimensional interferometric imaging, as well as diffraction from three-dimensional crystals and non-periodic objects, the Fourier modulus of an object is sampled on a discrete and finite grid. To recover the object, additional *a priori* constraints (object support, positivity, atomicity, etc) are imposed in order to ‘retrieve’ the corresponding phases, without which the Fourier synthesis of the object is impossible. A natural setting for computations is the N -dimensional complex Euclidean space E^N , where N is the number of pixels (or voxels) in the finite Fourier transform grid. The most widely used phase retrieval algorithms are formulated as maps $E^N \rightarrow E^N$, which, when used iteratively, impose the Fourier modulus data as well as the *a priori* constraints in the course of recovering the object.

The work reported here concerns the convergence of the phase retrieval algorithm based on the *difference map* [1]:

$$\rho \mapsto D(\rho) = \rho + \beta(\Pi_1 \circ f_2 - \Pi_2 \circ f_1)(\rho). \quad (1)$$

The action of D is to add to the current object, $\rho \in E^N$, a difference of projections Π_1 and Π_2 . In general, the action of a projection on an object ρ is the minimal modification of ρ that restores a particular constraint, where minimality is specified by the standard Euclidean norm in E^N . The two specific constraints considered below are the Fourier modulus constraint, implemented by Π_F , and a ‘fixed’ or ‘atomic’ support constraint, implemented by Π_S . The nonzero real parameter β serves as the step size of the iterations. Convergence of the difference map is crucially dependent on the maps f_1 and f_2 with which the basic projections in (1) are composed:

$$f_i(\rho) = (1 + \gamma_i)\Pi_i(\rho) - \gamma_i\rho \quad (i = 1, 2). \quad (2)$$

The structure of the maps f_i is geometrical, taking ρ to a general point parametrized by γ_i on the line determined by ρ and $\Pi_i(\rho)$. A previous analysis [1] of the convergence of the difference map, greatly simplified by the assumption of orthogonality of the two constraint subspaces near the solution, found

$$\gamma_1^{\text{opt}} = -1/\beta \quad (3a)$$

$$\gamma_2^{\text{opt}} = 1/\beta \quad (3b)$$

as optimal parameter values. The main result reported here is a modification of these values for the more realistic case of constraint subspaces that are not perfectly orthogonal, locally, in the vicinity of the solution.

The presentation is organized as follows. Section 2 reviews the relationship between the fixed points of the difference map and the solution to the associated phase retrieval problem. Explicit expressions for the two chief projections and their linearization are derived in section 3. Convergence of the difference map for a general pair of linearized projections is studied in section 4. Traces encountered in section 4 are averaged in a standard random matrix ensemble in section 5 and compared with averages over object ensembles appropriate for phase retrieval. Results are summarized in section 6.

2. The difference map

A special case of the difference map, the *hybrid input–output map* [2], first appeared in the context of two-dimensional phase retrieval with a fixed support constraint. The generality of the construction for an arbitrary pair of projections [1, 3], and the flexibility in choosing the parameters γ_i [1], was only noticed recently. With $\Pi_1 = \Pi_S$ (support), $\Pi_2 = \Pi_F$ (Fourier modulus), the hybrid input–output map is obtained for the parameter values $\gamma_1 = -1$, $\gamma_2 = 1/\beta$ [1].

A phase retrieval solution ρ^{sol} exists if and only if the difference map has a fixed point ρ^* . This is an immediate consequence of the definition of the difference map. At a fixed point $\rho^* = D(\rho^*)$, the difference of projections in (1) vanishes, and we have

$$\Pi_1 \circ f_2(\rho^*) = \Pi_2 \circ f_1(\rho^*) := \rho^{\text{sol}}. \quad (4)$$

From this follows

$$\Pi_1(\rho^{\text{sol}}) = \Pi_2(\rho^{\text{sol}}) = \rho^{\text{sol}} \quad (5)$$

showing that the object ρ^{sol} satisfies both constraints. Conversely, given ρ^{sol} , the set of fixed points is given by

$$(\Pi_1 \circ f_2)^{-1}(\rho^{\text{sol}}) \cap (\Pi_2 \circ f_1)^{-1}(\rho^{\text{sol}}) \quad (6)$$

a nonempty set since it trivially contains ρ^{sol} .

To recover an object using the difference map, one begins with an initial, arbitrary object $\rho(0)$ and generates iterates $\rho(n) = D^n(\rho(0))$ until the norm of the difference

$$\|\rho(n + 1) - \rho(n)\| = \|\beta(\Pi_1 \circ f_2 - \Pi_2 \circ f_1)(\rho(n))\| \tag{7}$$

becomes suitably small. Then, from the approximate fixed point $\rho^* \approx \rho(n)$, the solution ρ^{sol} is obtained using (4). There is no guarantee that, given an arbitrary starting point $\rho(0)$, the iterates will converge on a fixed point. In particular, it may happen that the linearization of the difference map in the neighbourhood of a fixed point has unstable directions. Avoiding this, and instead making fixed points maximally stable in an average sense, is the primary focus of the present work.

The uniqueness of solutions is linked to the tightness of the constraints. In many applications the two constraint subspaces C_1 and C_2 are unions of countably many submanifolds of E^N and their stable intersection properties (i.e. solutions) are functions of their dimensionalities. Thus if $\dim(C_1) + \dim(C_2) > N$, then the set of solutions, $C_1 \cap C_2$, has positive dimension and there is no uniqueness. For phase retrieval to be well posed, the number of *a priori* constraints must be sufficiently large, and the dimensionality of the associated constraint subspace correspondingly small, so that only the empty intersection is stable. In this overconstrained situation a solution will reduce to a single point (or low-dimensional submanifold in the case of symmetries) since a solution is known to exist at the outset.

3. Projections

When the Fourier transform of an object is sampled on a regular grid (fundamentally unavoidable in crystallography, an artefact of CCD array design otherwise), the object can be treated as living on a *periodic* real space grid. The fineness of the grid in real space is determined by the range of the Fourier space sampling. A general point of the periodic real space grid has the form

$$\mathbf{r} = (r_1, r_2, \dots) \quad r_i \in \mathbb{Z}_{m_i} / m_i \tag{8}$$

where the integers m_i give the ranges of the Fourier space sampling for the different components of the Fourier space basis, and \mathbb{Z}_m denotes the set of integers modulo m . Points in Fourier space (relative to a basis which may be non-orthogonal) have the form

$$\mathbf{q} = (q_1, q_2, \dots) \quad q_i \in 2\pi\mathbb{Z}_{m_i}. \tag{9}$$

In crystallography, \mathbf{r} is called a ‘fractional coordinate’, while \mathbf{q} is, up to a factor of 2π , a triplet of Miller indices. The periodicity of the Fourier space grid (9) is an artefact of the regular, grid-like sampling in real space; this artificial periodicity can be tolerated since the modulus of the Fourier transform of real objects becomes negligible at the extremes of the range. With points in real and Fourier spaces defined as above, the components of an arbitrary object in real space, ρ_r , and Fourier space, ρ_q , are related by the unitary transformation (discrete Fourier transform) with matrix elements

$$(\mathcal{F})_{qr} = \frac{1}{\sqrt{N}} \exp(i\mathbf{q} \cdot \mathbf{r}) \tag{10}$$

where $N = m_1 m_2 \dots$ is the total number of real or Fourier space samples.

3.1. Support projection

Object support constraints can take two forms, depending on the application. In phase retrieval with non-periodic objects one normally has *a priori* knowledge of a fixed object support S ,

with the property $\rho_r = 0$ if $r \notin S$. For example, relatively tight bounds on the set S can be derived from the object's autocorrelation [4], as given directly by the Fourier transform of the squared Fourier modulus. In crystallography, on the other hand, it is the *form* of the support that supplies the necessary constraint. Given the number of atoms M , a valid support comprises a union of M very compact sets, say $3 \times 3 \times 3$ arrays of voxels. Although the locations of the individual atomic supports are unknown, the small size of the combined support of all M atoms is a very strong constraint.

In the case of a *fixed object support* the corresponding projection operator is linear and has the following simple form:

$$(\Pi_S)_{rr'} = \sum_{s \in S} \delta_{rs} \delta_{sr'}. \quad (11)$$

It is easily verified that given an arbitrary object ρ , the object $\Pi_S(\rho)$ is the nearest object (in the Euclidean sense) having support S . The corresponding constraint subspace is a linear subspace of E^N with dimensionality $|S|$.

The constraint subspace for an *atomic support* is, in contrast, a union of very many linear subspaces, each one corresponding to a different arrangement of atoms. Thus one is really working with a collection of supports S , where the linear projection operator (11) applies to each $S \in \mathcal{S}$. The actual projection operator is nonlinear, returning the element of $\{\Pi_S(\rho) : S \in \mathcal{S}\}$ which minimizes $\|\Pi_S(\rho) - \rho\|$. This complication, however, is not relevant to the local analysis we perform below: only one element of \mathcal{S} contains the solution (given a choice of object origin and enantiomer) and the linear projection (11) can be used for just that one.

3.2. Fourier modulus projection

We consider the situation where a large number of the object's Fourier moduli have been measured to high precision. In this case, the moduli F_q in

$$\rho_q^{\text{sol}} = F_q \exp(i\phi_q) \quad (12)$$

for a large subset Q_{data} of Fourier samples q can be treated as known quantities. The corresponding projection operator is nonlinear but simple when expressed in Fourier space:

$$\tilde{\Pi}_F(\rho_q) = \begin{cases} F_q \frac{\rho_q}{|\rho_q|} & \text{for } q \in Q_{\text{data}} \text{ and } \rho_q \neq 0 \\ F_q & \text{for } q \in Q_{\text{data}} \text{ and } \rho_q = 0 \\ \rho_q & \text{otherwise.} \end{cases} \quad (13)$$

On actual computing machinery, and random initialization, the arbitrary choice of phase made in the second case above never comes up in practice. In crystallography, Q_{data} never includes the origin and frequently also omits 'reflections' q close to the origin. Since in all applications there is a systematic decay of moduli at large spatial frequencies, a significant fraction of the samples near the corners of the Fourier grid (those farthest from the origin) will lack measured values. There is usually no harm in approximating these small moduli by zero, since it is the absolute error that matters in Fourier synthesis. Geometrically, Fourier modulus projection in Fourier space corresponds to projections of the complex numbers ρ_q onto circles with prescribed radii (F_q), for all $q \in Q_{\text{data}}$. A more refined approach, one which takes into account measurement errors and bounds on unmeasured moduli, would involve projections, respectively, onto annuli and disks. When considered together with support projection (11), it is necessary to use the real space form of Fourier modulus projection:

$$\Pi_F = \mathcal{F}^{-1} \circ \tilde{\Pi}_F \circ \mathcal{F}. \quad (14)$$

3.3. Linearized projections

To study convergence, the difference map and the projections from which it is built are linearized about the solution ρ^{sol} . In general, the linearization π of a projection Π is defined by

$$\pi(\eta) := \lim_{\epsilon \rightarrow 0} \frac{\Pi(\rho^{\text{sol}} + \epsilon\eta) - \rho^{\text{sol}}}{\epsilon}. \tag{15}$$

Since object support projection (11) is already linear,

$$\pi_S(\eta) = \Pi_S(\eta). \tag{16}$$

Linearized Fourier modulus projection (13) is diagonal in Fourier space,

$$(\tilde{\pi}_F)_{qq'} = \delta_{qq'} \cdot \begin{cases} \frac{1}{2} - \frac{1}{2} \exp(i2\phi_q)C & \text{for } \mathbf{q} \in Q_{\text{data}} \text{ and } F_q \neq 0 \\ 0 & \text{for } \mathbf{q} \in Q_{\text{data}} \text{ and } F_q = 0 \\ 1 & \text{otherwise} \end{cases} \tag{17}$$

where C is the complex conjugation operator. The second case above, although never strictly encountered with realistic objects, expresses the fact that the rank of the projection effectively decreases by 1 whenever $|\rho_q| \gg F_q$ (projection onto the origin, rather than a circle). This case is included because small (unmeasured) moduli at large spatial frequencies are ubiquitous in practice. Assuming for simplicity, however, that Q_{data} includes all N Fourier samples, and that all the moduli F_q are nonzero, the real space form (14) of linearized Fourier modulus projection is given by

$$(\pi_F)_{rr'} = \frac{1}{2} \delta_{rr'} - \frac{1}{2N} \sum_q \exp(i[2\phi_q - \mathbf{q} \cdot (\mathbf{r} + \mathbf{r}')]C). \tag{18}$$

To facilitate the comparison with random matrix theory, we express π_F in somewhat more compact notation. In the case of real-valued objects, where the operator C can be dropped, we have

$$\pi_F = \frac{1}{2}(1 + U^T U) \tag{19}$$

where the unitary matrix U is defined by

$$(U)_{qr} = \frac{1}{\sqrt{N}} \exp(i(\phi_q - \mathbf{q} \cdot \mathbf{r})). \tag{20}$$

Since for real objects $\phi_{-q} = -\phi_q$, the reality of $U^T U$ follows from

$$(U)_{qr}^* = (U)_{-qr}. \tag{21}$$

When representing complex-valued objects in a $2N$ -dimensional real vector space, a general operator $X + YC$, where X and Y are ordinary matrices, has the block structure,

$$\begin{pmatrix} \text{Re}(X + Y) & \text{Im}(Y - X) \\ \text{Im}(X + Y) & \text{Re}(X - Y) \end{pmatrix} \tag{22}$$

and the projection takes the form

$$\pi_F = \frac{1}{2} \begin{pmatrix} 1 + \text{Re}(U^T U) & \text{Im}(U^T U) \\ \text{Im}(U^T U) & 1 - \text{Re}(U^T U) \end{pmatrix}. \tag{23}$$

The linearized difference map is defined by

$$d(\eta) := \lim_{\epsilon \rightarrow 0} \frac{D(\rho^{\text{sol}} + \epsilon\eta) - \rho^{\text{sol}}}{\epsilon} \tag{24}$$

and is obtained by replacing the projections Π_1 and Π_2 in D by their linearized counterparts, π_1 and π_2 . The fixed points of d form a linear space that can be directly constructed from the kernels of π_1 and π_2 as follows. From (4) and $\rho^* = \rho^{\text{sol}} + \eta^*$ we have

$$\pi_1 \circ [(1 + \gamma_2)\pi_2 - \gamma_2](\eta^*) = 0 \quad (25a)$$

$$\pi_2 \circ [(1 + \gamma_1)\pi_1 - \gamma_1](\eta^*) = 0. \quad (25b)$$

By forming suitable linear combinations of (25a) and (25b), and making use of the idempotency of π_1 and π_2 , one can show

$$\pi_1(\eta^*) = 0 \quad (26)$$

$$\pi_2(\eta^*) = 0. \quad (27)$$

Thus,

$$\ker(d - 1) = \ker \pi_1 \cap \ker \pi_2 := \ker \pi_\perp \quad (28)$$

where π_\perp is the projection onto the orthogonal complement of the linear space of fixed points. Since it is the projection of the iterates $d^n(\eta)$ by π_\perp that should converge to zero, we consider in the next section the operator

$$d_\perp := \pi_\perp \circ d \circ \pi_\perp. \quad (29)$$

Applying DeMorgan's law (for Euclidean subspaces) to (28), we obtain

$$\ker(1 - \pi_1) \cup \ker(1 - \pi_2) = \ker(1 - \pi_\perp). \quad (30)$$

By using (28) and (30) one easily verifies a set of identities needed in the next section:

$$\pi_i \circ \pi_\perp = \pi_\perp \circ \pi_i = \pi_i \quad (i = 1, 2). \quad (31)$$

Finally, since we confine ourselves to the overconstrained case where

$$\ker(1 - \pi_1) \cap \ker(1 - \pi_2) = \{0\} \quad (32)$$

it follows from (30) that

$$\dim \ker(1 - \pi_1) + \dim \ker(1 - \pi_2) = \dim \ker(1 - \pi_\perp) \quad (33)$$

or equivalently,

$$\text{Tr } \pi_1 + \text{Tr } \pi_2 = \text{Tr } \pi_\perp. \quad (34)$$

4. Convergence of the difference map

With linearization, convergence to the space of fixed points corresponds to the vanishing of the norm of the iterates $(d_\perp)^n(\eta)$, where the map d_\perp was defined in (29). This in turn is guaranteed by a suitable bound on an induced matrix norm of d_\perp . With the standard Euclidean norm on the vector space, the natural choice for the induced matrix norm is the spectral norm:

$$\|d_\perp\|_\infty := \max_{\|\eta\|=1} \|d_\perp(\eta)\|. \quad (35)$$

There are two reasons, however, why the spectral norm may not be the appropriate choice. First, it presents a serious challenge to calculate, even in the limit $N \rightarrow \infty$. Second, although being able to achieve $\|d_\perp\|_\infty < 1$ by a suitable choice of parameters guarantees convergence, it may not be true that minimizing this bound also maximizes the average rate of convergence. An alternative is suggested by the interpretation of $(\|d_\perp\|_\infty)^2$ as the standard ∞ -norm applied

to the eigenvalues of the matrix $d_{\perp}^{\dagger} \circ d_{\perp}$. In particular, the 1-norm of the (non-negative) eigenvalues has the advantage that it is easily calculated:

$$(\|d_{\perp}\|_1)^2 := \frac{1}{N} \text{Tr } d_{\perp}^{\dagger} \circ d_{\perp}. \quad (36)$$

The norm $\|d_{\perp}\|_1$, called the Frobenius norm, gives the root-mean-square change in the Euclidean length of uniformly sampled unit vectors when acted on by d_{\perp} . Although a bound on $\|d_{\perp}\|_1$ does not guarantee convergence, its minimization makes more sense in that it reflects a property of all the eigenvalues rather than just the top of the spectrum. This feature, and its tractable form, leads us to adopt the Frobenius norm as the vehicle for optimizing the difference map; the subscript 1 will subsequently be dropped.

A straightforward calculation, making repeated use of (31), gives

$$\|d_{\perp}\|^2 = t_{\perp} + 2\beta[\gamma_1 t_2 - \gamma_2 t_1 + (\gamma_2 - \gamma_1)t_{12}] + \beta^2 [\gamma_1^2 t_2 + \gamma_2^2 t_1 + (2 + 2(\gamma_1 + \gamma_2) - (\gamma_1 - \gamma_2)^2)t_{12} - 2(1 + \gamma_1)(1 + \gamma_2)t_{1212}] \quad (37)$$

where

$$t_1 := (\text{Tr } \pi_1)/N \quad (38a)$$

$$t_2 := (\text{Tr } \pi_2)/N \quad (38b)$$

$$t_{\perp} := (\text{Tr } \pi_{\perp})/N = t_1 + t_2 \quad (38c)$$

$$t_{12} := (\text{Tr } \pi_1 \circ \pi_2)/N \quad (38d)$$

$$t_{1212} := (\text{Tr } \pi_1 \circ \pi_2 \circ \pi_1 \circ \pi_2)/N. \quad (38e)$$

Since (37) is quadratic in the γ_i and non-negative, it has a unique minimum where the partial derivatives $\partial(\|d_{\perp}\|^2)/\partial\gamma_i$ vanish. The optimal γ_i are given by the following expressions:

$$\gamma_1^{\text{opt}} = -\frac{(t_1 - t_{12})(t_2 - t_{1212}) - (t_{12} - t_{1212})(t_1 - 2t_{12} + t_{1212})\beta}{[t_1(t_2 - t_{12}) + t_{12}(2t_{1212} - t_2) - t_{1212}^2]\beta} \quad (39a)$$

$$\gamma_2^{\text{opt}} = \frac{(t_2 - t_{12})(t_1 - t_{1212}) - (t_{12} - t_{1212})(t_2 - 2t_{12} + t_{1212})\beta}{[t_2(t_1 - t_{12}) + t_{12}(2t_{1212} - t_1) - t_{1212}^2]\beta}. \quad (39b)$$

The Frobenius norm (37) evaluated for these parameter values is

$$\|d_{\perp}\|^2 = t_{\perp} + \left\{ (t_1 - t_{12})(t_2 - t_{12})(2t_{1212} - t_1 - t_2) + 2(t_2 - t_1)(t_{12} - t_{1212})^2\beta + [(t_{12} - t_{1212})(2t_1 t_2 - 3t_{12}(t_1 + t_2) + 4t_{12}^2 + t_{1212}(t_1 + t_2 - 2t_{12}))\beta^2] \right\} / \{t_1 t_2 - t_{12}(t_1 + t_2 - 2t_{1212}) - t_{1212}^2\}. \quad (40)$$

When the linearized constraint subspaces are orthogonal, as was assumed in [1], the product traces t_{12} and t_{1212} vanish and one recovers the result $\gamma_1^{\text{opt}} = -1/\beta$, $\gamma_2^{\text{opt}} = 1/\beta$. Using (38c) in (40), one obtains $\|d_{\perp}\|^2 = 0$ for this case. This simple result could have been anticipated since for the given values of the γ_i and orthogonal subspaces ($\pi_1 \circ \pi_2 = 0$) one has the simplification $d = 1 - \pi_1 - \pi_2 = 1 - \pi_{\perp}$, and hence $d_{\perp} = 0$.

5. Average traces of projection products

Because our convergence measure $\|d_{\perp}\|^2$ is linear in the traces t_{12} and t_{1212} , using instead an average of these traces with respect to a particular class of objects will provide parameters for the optimum average-case convergence. The projections that appear in these traces can be

expressed as $\pi = O^T P O$, where P is a fixed canonical projection and O is an orthogonal matrix. The actual matrices O that apply to the projections considered earlier comprise subensembles in the space of orthogonal matrices. For π_S (object support) O is a permutation matrix, while for π_F (Fourier modulus) O belongs to a continuous family of orthogonal matrices defined implicitly by (19) or (23). Traces of products of $\pi_1 = O_1^T P_1 O_1$ and $\pi_2 = O_2^T P_2 O_2$ only depend on the relative orthogonal matrix $O = O_1 O_2^T$. In the absence of detailed knowledge of the appropriate subensemble for O , we might consider the average over the complete, group invariant ensemble:

$$\langle t_{12} \rangle := \frac{1}{N} \langle \text{Tr } P_1 O^T P_2 O \rangle \quad (41a)$$

$$\langle t_{1212} \rangle := \frac{1}{N} \langle \text{Tr } P_1 O^T P_2 O P_1 O^T P_2 O \rangle. \quad (41b)$$

There are highly sophisticated methods [5, 6] for evaluating these standard random matrix averages which rely solely on symmetry. Here we quote the limiting forms for large N ; details of the calculation are given in the appendix:

$$\lim_{N \rightarrow \infty} \langle t_{12} \rangle = t_1 t_2 \quad (42a)$$

$$\lim_{N \rightarrow \infty} \langle t_{1212} \rangle = t_1^2 t_2 + t_1 t_2^2 - t_1^2 t_2^2. \quad (42b)$$

In the remainder of this section these formulae are compared with explicit averages over actual *object ensembles* (and $\pi_1 = \pi_S, \pi_2 = \pi_F$). If the random matrix theory results (42a), (42b) are reproduced, then the problem of choosing optimal parameters is greatly simplified since (37) will then only depend on the dimensionalities of the constraint subspaces (t_1 and t_2).

We begin by calculating the traces of the two projections. From (11) and (16) we have

$$t_S = (\text{Tr } \pi_S) / N = |S| / N := \sigma \quad (43)$$

where σ is the fraction of pixels or voxels in the support S .

For traces involving the linearized Fourier modulus projection (18) we need to understand the action of the conjugation operator C . In the case of real-valued objects all traces may be evaluated in a real vector space of dimension N , and C can be replaced by the identity. For complex-valued objects traces are evaluated in a $2N$ -dimensional real vector space where the representation of a general operator $X + YC$ has the block form (22). Normalizing the matrix trace of (22) by an extra factor of $\frac{1}{2}$ gives us the identity

$$\text{Tr}(X + YC) := \text{Tr}(\text{Re } X) \quad (44)$$

where the trace on the right is an ordinary matrix trace. Another useful identity involving C is

$$(X + YC)(W + ZC) = (XW + YZ^*) + (XZ + YW^*)C \quad (45)$$

where X, Y, W and Z are ordinary matrices.

Use of identity (44) on (18) gives us immediately

$$t_F = (\text{Tr } \pi_F) / N = \frac{1}{2} \quad (46)$$

in the case of complex-valued objects. For real-valued objects we have

$$(\text{Tr } \pi_F) / N = \frac{1}{2} - \frac{1}{2N^2} \sum_q \exp(i2\phi_q) \left[\sum_r \exp(-i2\mathbf{q} \cdot \mathbf{r}) \right]. \quad (47)$$

The inner sum in (47) vanishes unless the components of \mathbf{q} satisfy $q_i \equiv 0 \pmod{\pi m_i}$, and there are at most 4 (two dimensions) or 8 (three dimensions) such points. In more concrete

terms, the second term in (47) subtracts the number of samples \mathbf{q} which do not possess a continuous phase when the object is real. This correction is negligible in the $N \rightarrow \infty$ limit and we recover the complex-object result (46).

We consider next the first product trace computed earlier using random matrix theory. In the complex-object case, identities (44) and (45) give us immediately

$$t_{\text{SF}} = (\text{Tr } \pi_S \circ \pi_F) / N = \frac{\sigma}{2} \tag{48}$$

in agreement with the random matrix result (42a), even without averaging. For real-valued objects we have

$$(\text{Tr } \pi_S \circ \pi_F) / N = \frac{\sigma}{2} - \frac{1}{2N} \sum_{\mathbf{q}} \exp(i2\phi_{\mathbf{q}}) \Sigma_{-2\mathbf{q}} \tag{49}$$

where

$$\Sigma_{\mathbf{q}} := \frac{1}{N} \sum_{\mathbf{s} \in S} \exp(i\mathbf{q} \cdot \mathbf{s}) \tag{50}$$

defines the Fourier transform of the support’s characteristic function.

The second term in (49) is a correction to the naive random matrix theory result and in general does not vanish. To check whether it vanishes in an average-case sense, we consider two object ensembles distinguished by the nature of their support. If the support is a known fixed set S , say a rectangle or disk in two dimensions, then $\Sigma_{-2\mathbf{q}}$ is a constant in the ensemble average of (49) and we can focus on the average of $\exp(i2\phi_{\mathbf{q}})$. The minimal *a priori* knowledge of the object in real space is that the individual pixel (or voxel) values ρ_r in the support are independently distributed according to a known distribution. For this object ensemble it is straightforward to calculate the distribution of the Fourier transform components $\rho_{\mathbf{q}}$. Excepting a fraction of samples \mathbf{q} which vanishes as $N \rightarrow \infty$ (near $\mathbf{q} = 0$ or associated with facets in the support), the complex numbers $\rho_{\mathbf{q}}$ are isotropic Gaussian random variables with mean zero and corrections that decay in the limit $N \rightarrow \infty$. Consequently, the average of the phases $\exp(i2\phi_{\mathbf{q}})$ in (49) vanishes in the same limit, as does the correction (since $|\Sigma_{\mathbf{q}}| \leq \sigma$, independent of N).

In the case of an atomic support, although the actual support S is not known, one does know that S is the union of a given number M of very compact sets associated with atoms. In the equal-atom ensemble there is an approximate relationship

$$\Sigma_{\mathbf{q}} \approx \frac{A(\mathbf{q})}{\sqrt{N}} \rho_{\mathbf{q}} \tag{51}$$

where $A(\mathbf{q})$ is a smooth real-valued function (form factor) independent of N . The approximation in (51) arises from shifts (by fractions of voxels) of the atomic centres relative to their individual supports. To bound the sum in (49) we replace each term by its modulus and use (51)

$$\frac{1}{2N} \left| \sum_{\mathbf{q}} \exp(i2\phi_{\mathbf{q}}) \Sigma_{-2\mathbf{q}} \right| < \frac{1}{2N} \sum_{\mathbf{q}} \frac{|A(2\mathbf{q})|}{\sqrt{N}} |\rho_{2\mathbf{q}}|. \tag{52}$$

The root-mean-square of the modulus $|\rho_{2\mathbf{q}}|$ can be calculated in the standard atomic ensemble where M atom centres are uniformly and independently distributed; the result, $|\rho_{2\mathbf{q}}|_{\text{rms}} = O(\sqrt{M/N})$, ($2\mathbf{q} \neq 0$) shows that the correction is negligible for $N \rightarrow \infty$ and fixed resolution ($M/N = \text{const}$). We conclude that explicit averaging in the standard equal-atom ensemble, as in the fixed support ensemble, reproduces the random matrix theory result (42a):

$$\langle t_{\text{SF}} \rangle = \frac{\sigma}{2}. \tag{53}$$

Finally, we turn to the trace of the product of four projection operators. For complex-valued objects we obtain

$$t_{\text{SFSF}} = (\text{Tr } \pi_S \circ \pi_F \circ \pi_S \circ \pi_F) / N = \frac{\sigma}{4} + \frac{1}{4N} \sum_{q, q'} \exp(i2(\phi_q - \phi_{q'})) \Sigma_{q'-q}^2 \quad (54)$$

and for real objects,

$$t_{\text{SFSF}} = (\text{Tr } \pi_S \circ \pi_F \circ \pi_S \circ \pi_F) / N = \frac{\sigma}{4} - \frac{1}{2N} \sum_q \exp(i2\phi_q) \Sigma_{-2q} + \frac{1}{4N} \sum_{q, q'} \exp(i2(\phi_q + \phi_{q'})) \Sigma_{-q'-q}^2. \quad (55)$$

We recognize the single sum in (55) as the sum in (49), which was already argued to be negligible when averaged over the standard object ensembles with fixed or atomic support. However, the averages of the double sums for the fixed support ensemble, both in (54) and (55), can deviate from the random matrix theory result (42b). In fact, the latter is recovered in both cases by retaining only the diagonal terms in the double sums ($\mathbf{q} = \mathbf{q}'$ in (54), $\mathbf{q} = -\mathbf{q}'$ in (55)). Since the contributions of the near-diagonal terms is not diminished in the $N \rightarrow \infty$ limit, there will be non-negligible corrections that depend on details of the ensemble (support shape, distribution of object values, etc). The most we can conclude for the *fixed support ensemble* without these details is

$$\langle t_{\text{SFSF}} \rangle = \frac{\sigma}{4} + O(\sigma^2) \quad (56)$$

a result that may be useful for small object support.

The neglect of non-diagonal terms in the double sum may be easier to justify rigorously for the atomic support ensemble. Considering only the case of real atoms (55), we first use (51) to write

$$\Sigma_{-q'-q}^2 \approx \frac{|A(-\mathbf{q}' - \mathbf{q})|^2}{N} |\rho_{-q'-q}|^2 \exp(-2i\phi_{q'+q}). \quad (57)$$

Now, since $|\rho_{-q'-q}|_{\text{rms}}^2 = O(M/N)$ for $\mathbf{q} + \mathbf{q}' \neq 0$, the non-diagonal terms have moduli which scale as N^{-2} (at constant resolution). To argue that the $O(N^2)$ non-diagonal terms in the double sum have a negligible ensemble average, we consider the phase of a general term:

$$\exp(i2(\phi_q + \phi_{q'} - \phi_{q'+q})). \quad (58)$$

Atomic ensemble averages of *triplet phase invariants* such as (58) are studied at length in the statistical theory of structure factors in crystallography [7]; they are found to vanish in the limit of many atoms, or equivalently, $N \rightarrow \infty$ when the resolution is fixed. There are three exceptions to this general result, when $\mathbf{q} = 0$, $\mathbf{q}' = 0$, or $\mathbf{q}' + \mathbf{q} = 0$. The latter corresponds to the diagonal contribution in the double sum of (55) which we will retain. The two other cases lead to single sums whose moduli can be shown to be negligible by arguments identical to those used for the sum in (52). In summary, this non-rigorous argument leads us to believe that for the *atomic support ensemble*

$$\langle t_{\text{SFSF}} \rangle = \frac{\sigma}{4} + \frac{\sigma^2}{4} \quad (59)$$

in agreement with the random matrix theory result (42b).

6. Optimal parameter values

The results of the previous section show that random matrix averaging, of the traces of products of projections, reproduces for the most part the averages over the actual object ensembles encountered in standard phase retrieval applications (fixed and atomic support). This greatly simplifies the expressions for the optimal γ parameters of the difference map (39a), (39b), since all the traces are explicit functions of just the traces $t_S = \sigma$ and $t_F = \frac{1}{2}$:

$$\gamma_S^{\text{opt}} = -\frac{4 + (2 + \beta)\sigma + \beta\sigma^2}{\beta(4 - \sigma + \sigma^2)} \quad (60a)$$

$$\gamma_F^{\text{opt}} = \frac{6 - 2\sigma - \beta(2 - 3\sigma + \sigma^2)}{\beta(4 - \sigma + \sigma^2)}. \quad (60b)$$

Following the discussion of uniqueness in section 2, phase retrieval with a support constraint is well posed when $t_S + t_F < 1$, which requires that the support fraction satisfies $0 < \sigma < \frac{1}{2}$. As noted in section 5, with the fixed support ensemble the average of t_{SFSF} (54), (55) may differ from the random matrix average by terms proportional to σ^2 , and the coefficients of σ^2 in the above formulae will change accordingly. For the atomic support ensemble the formulae as written are more reliable. Moreover, in the principal atomic support application, crystallography, there is a large dimensionality asymmetry of the two-constraint subspaces as expressed by the statement $\sigma \ll \frac{1}{2}$. For this important application one may therefore take the $\sigma \rightarrow 0$ limit:

$$\gamma_S^{\text{opt}} \stackrel{\sigma \rightarrow 0}{=} -\frac{1}{\beta} \quad (61a)$$

$$\gamma_F^{\text{opt}} \stackrel{\sigma \rightarrow 0}{=} \frac{3 - \beta}{2\beta}. \quad (61b)$$

The Frobenius norm (40) in this limit is given by

$$\|d_{\perp}\|^2 \stackrel{\sigma \rightarrow 0}{=} \frac{\sigma}{8}(3 + 2\beta + 3\beta^2). \quad (62)$$

The numerical constants in (61b) and (62) can be traced to the numerical value of $t_F = \frac{1}{2}$, the only trace with a finite value in the $\sigma \rightarrow 0$ limit. Recalling the discussion in section 3.3 and the interpretation of $t_F N$ as the dimensionality of the Fourier modulus constraint subspace, the exact value $\frac{1}{2}$ is certainly an oversimplification. As a first improvement in the evaluation of $\text{Tr } \pi_F$ one should exclude contributions from samples \mathbf{q} for which the corresponding modulus $F_{\mathbf{q}}$ is negligible. In crystallography, for example, only the samples within an ellipsoid about the origin have non-negligible $F_{\mathbf{q}}$, effectively reducing the rank of the Fourier modulus projection by a fraction given approximately (in three dimensions) by $\pi/6 \approx 0.52$; thus $t_F \approx 0.26$. Given the uncertainty in t_F we give formulae for the optimal γ parameters for general t_F :

$$\gamma_S^{\text{opt}} \stackrel{\sigma \rightarrow 0}{=} -\frac{1}{\beta} \quad (63a)$$

$$\gamma_F^{\text{opt}} \stackrel{\sigma \rightarrow 0}{=} \frac{1 + t_F(1 - \beta)}{\beta}. \quad (63b)$$

Acknowledgments

The author thanks Orlando Alvarez and Piet Brouwer for help with the random matrix averages, and the referee for exceptionally constructive criticism. Additional thanks go to the Center

for Experimental and Constructive Mathematics, where the calculations were performed, and the Aspen Center for Physics, where this article was prepared. This work was supported by the National Science Foundation under grant ITR-0081775.

Appendix

Averages over products of matrix elements of $N \times N$ orthogonal matrices O ($N > 1$), such as

$$X_{pq}^{ij} = \langle O^i_p O^j_q \rangle \quad (\text{A.1})$$

can always be expressed as tensor products of Kronecker- δ 's having the correct invariance properties. The latter follow from the invariance of the group integration measure with respect to the change of variables $O \rightarrow LOR$, where L and R are independent orthogonal matrices. For the example above, the statement of invariance becomes

$$L^i_{i'} L^j_{j'} X^{i'j'}_{p'q'} R^{p'}_p R^{q'}_q = X^{ij}_{pq} \quad (\text{A.2})$$

with general solution

$$X_{pq}^{ij} = a \delta^{ij} \delta_{pq} \quad (\text{A.3})$$

where a is an undetermined constant. By contracting the indices i and j , whereupon the left-hand side of (A.3) corresponds to $\langle (O^T O)_{pq} \rangle = \delta_{pq}$, consistency requires

$$a = 1/N. \quad (\text{A.4})$$

Using this method for the product of four matrix elements,

$$X_{pqrs}^{ijkl} = \langle O^i_p O^j_q O^k_r O^l_s \rangle \quad (\text{A.5})$$

we find

$$\begin{aligned} X_{pqrs}^{ijkl} = & a_1 (\delta^{ij} \delta^{kl} \delta_{pq} \delta_{rs} + \delta^{ik} \delta^{jl} \delta_{pr} \delta_{qs} + \delta^{il} \delta^{jk} \delta_{ps} \delta_{qr}) + a_2 (\delta^{ij} \delta^{kl} \delta_{pr} \delta_{qs} + \delta^{ij} \delta^{kl} \delta_{ps} \delta_{qr} \\ & + \delta^{ik} \delta^{jl} \delta_{pq} \delta_{rs} + \delta^{ik} \delta^{jl} \delta_{ps} \delta_{qr} + \delta^{il} \delta^{jk} \delta_{pq} \delta_{rs} + \delta^{il} \delta^{jk} \delta_{pr} \delta_{qs}). \end{aligned} \quad (\text{A.6})$$

The reduction to two undetermined constants made use of permutation symmetries. Contracting indices k and l in (A.5) gives our previous result for (A.1) multiplied by δ_{rs} , which can then be compared with the result of contracting the same pair of indices in (A.6). Consistency yields two equations with the solutions

$$a_1 = \frac{N+1}{(N-1)N(N+2)} \quad (\text{A.7})$$

$$a_2 = \frac{-1}{(N-1)N(N+2)}. \quad (\text{A.8})$$

The random matrix averages of the traces of products of projections are obtained by contracting the tensor expressions (A.3) and (A.6) with the projections P_1 and P_2 :

$$\langle \text{Tr } P_1 O^T P_2 O \rangle = a (\text{Tr } P_1) (\text{Tr } P_2) \quad (\text{A.9})$$

$$\begin{aligned} \langle \text{Tr } P_1 O^T P_2 O P_1 O^T P_2 O \rangle = & a_1 (\text{Tr } P_1) (\text{Tr } P_2) (1 + \text{Tr } P_1 + \text{Tr } P_2) \\ & + a_2 (\text{Tr } P_1) (\text{Tr } P_2) (3 + \text{Tr } P_1 + \text{Tr } P_2 + (\text{Tr } P_1) (\text{Tr } P_2)). \end{aligned} \quad (\text{A.10})$$

After taking the limit $N \rightarrow \infty$ in (A.10) we obtain the results quoted in section 5.

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