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AN ALGORITHM FOR RECOVERING UNKNOWN PROJECTION ORIENTATIONS AND SHIFTS IN 3-D TOMOGRAPHY

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Abstract. It is common for example in Cryo-electron microscopy of viruses, that the orientations at which the projections are acquired, are totally unknown. We introduce here a moment based algorithm for recovering them in the three-dimensional parallel beam tomography. In this context, there is likely to be also unknown shifts in the projections. They will be estimated simultaneously. Also stability properties of the algorithm are examined. Our considerations rely on recent results that guarantee a solution to be almost always unique. A similar analysis can also be done in the two-dimensional problem.

1. Introduction

In n-dimensional computerized tomography the objective is to construct an object in $\mathbb{R}^n$ from its measured $n-1$-dimensional projections. In applications usually $n=2$ or $n=3$. A projection is a function on $\mathbb{R}^{n-1}$, defined by line integrals taken from the density function of the object. It is supposed here that in each projection the integral lines are straight, mutually parallel and perpendicular to the projection plane/line (parallel beam tomography). For having relation to the density function, one needs to know the geometry of projection: its orientation and the origin of the coordinate system that also transfers to the origin of the projection plane/line. That belongs to the standard formulation of tomography and is usually satisfied by experimental design.

By a projection orientation we mean an orthogonal matrix that rotates the object with respect to a fixed $x_1x_2x_3/x_1x_2$-coordinate system before being projected to the x_1x_2-plane/x_1-line (cf. (5) below). This also includes that the origins, transfered to the projection planes/lines, need to be known. In the case of noiseless projection data they are readily determined because of the fact, that a projection keeps the mass center point. Applying both to 2-D and 3-D parallel beam tomography, we

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have recently demonstrated that under fairly general conditions the projection data actually determines also the projection orientations uniquely (up to an equivalence) [14, 13]. In the 2-D case quite similar uniqueness results have been presented also by S. Basu and Y. Bresler [1]. Particularly, in both dimensions there exists a system of polynomial equations that gives besides the desired orientations also some of object's geometric moments. We have shown that these systems almost always admit of an essentially unique solution. If they can be reliably numerically solved also in the presence of measurement noise, we have a practical method for determining the unknown orientations, and that would make possible to apply tomography to more difficult data collections. For instance, in magnetic resonance imaging (MRI) the projection orientations may be known only approximately due to involuntary motion of the patient, which can result in unknown shifts in the projections as well [11]. The three-dimensional problem arises for example in Cryo-electron microscopy of viruses, where the projection is taken from a large number of identical particles lying in medium randomly at unknown orientations. Then also the exact positions of particles are unknown, which results in unknown shifts in the projections.

In the literature several methods have been proposed for finding the unknown projection orientations (and shifts). In the model matching method a *finitely* parametrized object is fitted in the projection data. This can be relatively effective [4], particularly if the object has some *known* rotational symmetries, when appropriate basis functions can be applied. It even has been proposed estimation of the object statistically, without finding the orientations at all [5, 7, 18]. Indeed, many times they itself are not very interesting, but they have only instrumental value. Statistical estimation can be applicable particularly when the object is so symmetric, that one has to leave the methods recovering orientations out of account. In the so-called common line technique one determines the intersection lines of the projection planes [20, 9, 10, 8, 15]. It can be applied only in three dimensions ($n = 3$). Moment based methods have been examined for example in [14, 13, 1, 2, 9, 10, 8, 19]. Also the algorithm we present in this paper is such one: it is based - as we already pointed above - on solving a system of equations involving the orientations and some of object's moments. Into this system also the origins of projections can be quite readily added as unknown variables. We concentrate here on the three-dimensional problem only, because S. Basu and Y. Bresler have already examined the two-dimensional case in [2]. Like them, we emphasize the notion of stability in our algorithm: it forms an important part of reliability when working with real noisy measurements.

The paper is organized as follows. In the second section we formulate the problem and give the basic systems of equations, on which our algorithm of recovering the projection orientations and shifts relies. Some fundamental notions are introduced. Also in Section ii, non-uniqueness in solutions of the systems is removed by defining an appropriate subset for considered objects so that operation will mean no essential limitation, i.e. a representative inside an equivalence class is chosen. In the third section we define the notion of stability applied to solving a nonlinear least squares problem. Here we totally follow S. Basu and Y. Bresler [2, 3]. Also our main result is stated, by which the problem of recovering the unknown projection orientations and shifts from a projection data is almost always, besides uniquely solvable, also stable in the presence of noise (considered as a nonlinear least squares problem). In the fourth section we prove our stability result. Implementation of the recovery algorithm, its main features, are briefly sketched in the next section.

In the sixth section we consider simulation results, and the conclusion is drawn in the last section.

2. Problem Formulation

We consider the recovering problem only in 3-D tomography. Let $B = B(0,1)$ be the closed unit ball in $\mathbb{R}^3$. Denote by $L^1(B)$ the space of integrable functions $f : \mathbb{R}^3 \to \mathbb{R}$ with support in B. By the *object* we mean a function in $L^1(B)$. Its *(geometric) moments* are

$$m_{\boldsymbol{\alpha}}(f) = \int_{\mathbb{R}^3} \mathbf{x}^{\boldsymbol{\alpha}} f(\mathbf{x})\, d\mathbf{x} \in \mathbb{R}, \quad \boldsymbol{\alpha} \in \mathbb{N}^3, \tag{1}$$

where $\boldsymbol{\alpha} = (\alpha_1, \alpha_2, \alpha_3)$ is a multi-index. The integer $|\boldsymbol{\alpha}| = \alpha_1 + \alpha_2 + \alpha_3$ is the *order* of moment.

An *(projection) orientation* is a real orthogonal matrix

$$R = \begin{bmatrix} \mathbf{r}_1 & \mathbf{r}_2 & \mathbf{r}_3 \end{bmatrix} \in SO(3). \tag{2}$$

Here $SO(3)$ is the subgroup of $O(3)$ consisting of $R \in O(3)$ such that $\det R = 1$, and $O(3)$ is the group of real orthogonal 3×3-matrices. Let ϕ, θ and ψ be the Euler angles of the orientation R, given in operative order. Denote $\Psi = (\phi, \theta, \psi)$. Then

$$R(\Psi) = R(\phi, 0, 0) R(0, \theta, 0) R(0, 0, \psi) \tag{3}$$

For clarity we use for the *projection direction* a specific notation

$$\boldsymbol{\omega} = \boldsymbol{\omega}(R) = \mathbf{r}_3 \in S^2 \subset \mathbb{R}^3. \tag{4}$$

The *(parallel-beam line integral) projection* of object f at orientation R is the function $P(f; R) \in L^1(\mathbb{R}^2)$ defined almost everywhere by

$$P(f; R)(x_1, x_2) = \int_{\mathbb{R}} f(R\mathbf{x})\, dx_3, \quad (x_1, x_2) \in \mathbb{R}^2. \tag{5}$$

The *projection moments* are defined by

$$p_{(k,l)}(f; R) = \int_{\mathbb{R}^2} x_1^k x_2^l P(f; R)\, dx_1 dx_2, \quad k, l \in \mathbb{N}. \tag{6}$$

Let f be an object and $U \in O(3)$ be a real orthogonal matrix. The *transformed object* $f_U \in L^1(B)$ is defined by

$$f_U(\mathbf{x}) = f(U\mathbf{x}), \quad \mathbf{x} = (x_1, x_2, x_3) \in \mathbb{R}^3. \tag{7}$$

Then it holds that

$$p_{(k,l)}(f; R) = \int_{\mathbb{R}^2} x_1^k x_2^l \int_{\mathbb{R}} f(R\mathbf{x})\, dx_3 dx_1 dx_2 = m_{(k,l,0)}(f_R), \tag{8}$$

and further that (a form of the Helgason-Ludwig consistency conditions)

$$p_{(k,l)}(f;R) = m_{(k,l,0)}(f_R) = \sum_{\substack{|\boldsymbol{\alpha}|=k \\ |\boldsymbol{\beta}|=l}} \binom{k}{\boldsymbol{\alpha}} \binom{l}{\boldsymbol{\beta}} m_{\boldsymbol{\alpha}+\boldsymbol{\beta}}(f) \mathbf{r}_1^{\boldsymbol{\alpha}} \mathbf{r}_2^{\boldsymbol{\beta}} \quad k,l \in \mathbb{N}, \tag{9}$$

where

$$\binom{k}{\boldsymbol{\alpha}} = \frac{k!}{\alpha_1!\alpha_2!\alpha_3!}. \tag{10}$$

The projection data of our recovery problem is defined as follows: Let $f \in L^1(B)$ and $R_i = [\mathbf{r}(i)_1 \ \mathbf{r}(i)_2 \ \mathbf{r}(i)_3] \in SO(3)$, $i = 1, \cdots, n$, be unknown. The measured functions are either the projections $P(f;R_i)$, for clarity denoted by

$$pr(i;\mathbf{x}), \quad \mathbf{x} = (x_1, x_2) \in B_2, \quad i = 1, \cdots, n, \tag{11}$$

or - if the origin of the coordinate system has been lost, and thus the projections have unknown shifts - the shifted projections $\widehat{pr}(i;\mathbf{x})$, $i = 1, \cdots, n$, where

$$\widehat{pr}(i;\mathbf{x}) = pr(i;\mathbf{x} - \mathbf{x}_i), \quad \mathbf{x} \in \mathbb{R}^2, \quad i = 1, \cdots, n, \tag{12}$$

and $\mathbf{x}_i = (x(i)_1, x(i)_2) \in \mathbb{R}^2$ are unknown. In the terminology of S. Basu and Y. Bresler, the first case is referred to as the *Angle Recovery Problem* (ARP) and the latter case as the *Shift-Angle Recovery Problem* (SHARP) (angle refers here to the Euler angles).

Remark 1. We can suppose without any loss of generality, the origin of the coordinate system is fixed to be the mass center point of object. Then the real origin of the coordinate system of the projection plane is analogously located at the mass center point of projection. However, this cannot be exactly determined, if the measurements are corrupted by noise. So one fix some coordinate systems in the projection planes, and then the real origins are represented as unknown variables $\mathbf{x}_i \in \mathbb{R}^2$, $i = 1, \cdots, n$. Instead arbitrary rotations of the plane coordinate systems are taken automatically into account as appropriate $\psi(i)$ in R_i.

In the ARP one can calculate from the data $\{pr(i;\mathbf{x}) \,|\, i = 1, \cdots, n\}$ projection moments $p_{(k,l)}(i) = \int_{\mathbb{R}^2} x_1^k x_2^l \, pr(i;\mathbf{x}) \, d\mathbf{x}$, $k,l \in \mathbb{N}$, $i = 1, \cdots, n$. We suppose to the rest of this paper almost always that

$$m_{100}(f) = m_{010}(f) = m_{001}(f) = 0, \tag{13}$$

i.e. the origin is set into the mass center point of object. By (9) then

$$p_{(1,0)}(i) = p_{(0,1)}(i) = 0, \quad i = 1, \cdots, n. \tag{14}$$

Using moments of order $0, 2, \cdots, c$ gives by (9) the system

$$\begin{gathered} p_{(k,l)}(i) = m_{(k,l,0)}(f_{R_i}) = \textstyle\sum_{|\boldsymbol{\alpha}|=k+l} a(R_i;k,l;\boldsymbol{\alpha}) \, m_{\boldsymbol{\alpha}}, \\ k+l = 0, 2, \cdots, c, \quad i = 1, \cdots, n, \end{gathered} \tag{15}$$

where

$$a(R_i;k,l;\boldsymbol{\alpha}) = \sum_{\substack{\boldsymbol{\beta}\le\boldsymbol{\alpha}\\ |\boldsymbol{\beta}|=k}} \binom{k}{\boldsymbol{\beta}}\binom{l}{\boldsymbol{\alpha}-\boldsymbol{\beta}}\mathbf{r}(i)_1^{\boldsymbol{\beta}}\mathbf{r}(i)_2^{\boldsymbol{\alpha}-\boldsymbol{\beta}}, \tag{16}$$

and unknowns are the moments $m_{\boldsymbol{\alpha}} = m_{\boldsymbol{\alpha}}(f)$, $|\boldsymbol{\alpha}| = 0, 2, \cdots, c$, and the orientations $R_i = [\mathbf{r}(i)_1\ \mathbf{r}(i)_2\ \mathbf{r}(i)_3]$, $i = 1, \cdots, n$. Additionally, $\boldsymbol{\beta} \le \boldsymbol{\alpha}$ means that $\beta_j \le \alpha_j$, $j = 1, 2, 3$.

Let $\mathbf{p}(k;i) = [p_{(k,0)}(i) \cdots p_{(0,k)}(i)]^T$ and $\mathbf{p}_c(i) = [\mathbf{p}(0;i)^T, 0, 0, \mathbf{p}(2;i)^T \cdots \mathbf{p}(c;i)^T]^T \in \mathbb{R}^p$, $p = (1/2)(c^2+3c+2)$. Let o_k be some order in the subset $\{\boldsymbol{\alpha} \in \mathbb{N}^3 \,|\, |\boldsymbol{\alpha}| = k\}$ of multi-indices. Let $\boldsymbol{m}(k)$ be a vector consisting of components $m_{\boldsymbol{\alpha}}$, $|\boldsymbol{\alpha}| = k$, ordered by o_k, and let $\boldsymbol{m}_c = [\boldsymbol{m}(0)^T\ \boldsymbol{m}(2)^T \cdots \boldsymbol{m}(c)^T]^T \in \mathbb{R}^r$, where $r = (1/6)(c+1)(c+2)(c+3) - 3$. Define for $k \in \mathbb{N} \setminus \{1\}$ matrices $A(k;\Psi) \in \mathbb{R}^{(k+1)\times r}$, $r = (1/2)(k^2+3k+2)$, by setting

$$A(k;\Psi)(l+1, o_k(\boldsymbol{\alpha})) = a(R(\Psi); k-l, l; \boldsymbol{\alpha}). \tag{17}$$

Define more "an almost block diagonal matrix" (two zero rows)

$$A_c(\Psi) = \begin{bmatrix} A(0;\Psi) & 0 & \cdots & \cdots & 0 \\ 0 & \cdots & \cdots & \cdots & 0 \\ 0 & \cdots & \cdots & \cdots & 0 \\ \mathbf{0} & A(2;\Psi) & \mathbf{0} & \cdots & \mathbf{0} \\ \cdots & \cdots & \cdots & \cdots & \cdots \\ \mathbf{0} & \cdots & \cdots & \mathbf{0} & A(c;\Psi) \end{bmatrix} \in \mathbb{R}^{p\times r}, \tag{18}$$

where $p = (1/2)(c^2+3c+2)$ and $r = (1/6)(c+1)(c+2)(c+3) - 3$. Then (15) can be rewritten as

$$\mathbf{p}_c(i) = A_c(\Psi_i)\,\boldsymbol{m}_c, \quad i = 1, \cdots, n. \tag{19}$$

Remark 2. The notation $\boldsymbol{m}_c$ has here a different sense as in [13].

For better understanding of our uniqueness results below, we give some definitions. Let $f \in L^1(B)$ and $\boldsymbol{\theta} \in S^2$. Define

$$Q_k(f;\boldsymbol{\theta}) = \int_{\mathbb{R}^3} (\boldsymbol{\theta}\cdot\mathbf{x})^n f(\mathbf{x})\,d\mathbf{x} = \sum_{|\boldsymbol{\alpha}|=k} \binom{k}{\boldsymbol{\alpha}} m_{\boldsymbol{\alpha}}(f)\,\boldsymbol{\theta}^{\boldsymbol{\alpha}}, \quad k \in \mathbb{N}. \tag{20}$$

It can interpret as the moment of order k of f at the direction $\boldsymbol{\theta}$.

Definition 2.1. Let $K \subset \mathbb{N}$. The set $\mathcal{O}_K$ consists of those objects $f \in L^1(B)$ ((13) not supposed), which satisfy the following condition: If $\boldsymbol{\theta}, \boldsymbol{\psi} \in S^2$ and $Q_k(f;\boldsymbol{\theta}) = Q_k(f;\boldsymbol{\psi})$ for all $k \in K$, then $\boldsymbol{\theta} = \boldsymbol{\psi}$.

Let $\boldsymbol{m}_K$ be a vector consisting of all moments of order $k \in K$ and let $n(K)$ be its dimension. Set more

$$\mathcal{M}_K = \left\{\boldsymbol{m}_K(f) \in \mathbb{R}^{n(K)} \,\middle|\, f \in \mathcal{O}_K\right\}. \tag{21}$$

Definition 2.2. Let $A \subset B \subset \mathbb{R}^m$, where B is of positive Lebesgue measure. The set A is *generic* in B, if $B \setminus A$ is of Lebesgue measure zero and nowhere dense in B.

The Lebesgue measure, na

Sets that can be assigned a Lebesgue measure are called Lebesgue-measurable; the measure of

In particular, define $H = \{2, 3, 5, 7, d\}$, $d \in \mathbb{N} \setminus \{0, 2, 3, 5, 7\}$. Then "almost all" objects belong to $\mathcal{O}_H$, which follows from the theorem that is a key result in [13]:

Theorem 2.3. *The set $\mathcal{M}_H$ is generic in $\mathbb{R}^{n(H)}$.*

Remark 3. The definition of the set $\mathcal{O}_H$ (influencing also to $\mathcal{M}_H$) does not precisely coincide with the given in [13], where also nontrivial *complex* solutions were refused. Significant is that the $\mathcal{O}_H$ defined here contains the version defined in [13], and it still works in Theorem 2.4 below.

The following theorem can also be found in [13] ($\mathbb{P}^2$ is the 2-D projective space):

Theorem 2.4. *Let $H = \{2, 3, 5, 7, d\} \subset K \subset \mathbb{N}$, where $d \in \mathbb{N} \setminus \{0, 2, 3, 5, 7\}$ and K are arbitrary, and $f, g \in L^1(B)$. Let $(R_i)_{i\in I}$ and $(\widehat{R}_i)_{i\in I}$ be sequences of orientations with $R_i = [\mathbf{r}(i)_1\ \mathbf{r}(i)_2\ \boldsymbol{\omega}(i)]$.*

Suppose $f \in \mathcal{O}_H$ and $\{\boldsymbol{\omega}(i) \,|\, i \in I\}$ satisfies the following conditions:
(i) It contains a linearly independent triplet.
(ii) $\#\{\boldsymbol{\omega}(i) \in \mathbb{P}^2 \,|\, i \in I\} \geq \sup K + 1$.

Then it holds that

$$m_{(k,l,0)}(f_{R_i}) = m_{(k,l,0)}(g_{\widehat{R}_i}) \text{ for all } k + l \in K,\ i \in I, \tag{22}$$

if and only if there exists an orthogonal matrix $U \in O(3)$ such that $\boldsymbol{m}_K(g) = \boldsymbol{m}_K(f_U)$ and $\widehat{R}_i = U^T R_i$ for all $i \in I$ or $\widehat{R}_i = U^T R_i T$ for all $i \in I$, where T is the reflection

$$T = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & -1 \end{bmatrix} \in O(3). \tag{23}$$

Actually, the set $\mathcal{O}_H$ can be replaced by $\mathcal{O}_K$ in Theorem 2.4. Note that all vectors $\boldsymbol{m}_K \in \mathbb{R}^{n(K)}$ are moment vectors and thus under consideration in this theorem: for a finite $K \subset N$ all points $\boldsymbol{m}_K \in \mathbb{R}^{n(K)}$ have a representation $\boldsymbol{m}_K = \boldsymbol{m}_K(f)$ for some $f \in L^1(B)$ ([13], Lemma 2.1). Theorem 2.4 guarantees an essentially unique solvability of system (15)=(19), if $n > c \geq 7$ (with mild assumptions concerning projection directions) and the object that has created the data, i.e. $p_{(k,l)}(i)$:s, belongs to $\mathcal{O}_H$ ($\mathcal{O}_K$). Thus, one can say that system (19) almost always has an essentially unique solution, if $n > c \geq 7$. It is readily seen that the solution is entirely uniquely determined, if one orientation is fixed to be the identity matrix and the sign of $\sum_{\boldsymbol{\alpha}, \alpha_3 = odd} \boldsymbol{m}_{\boldsymbol{\alpha}}$ is also fixed (choosing between an object f and its reflective image f_T, since $m_{\boldsymbol{\alpha}}(f_T) = (-1)^{\alpha_3} m_{\boldsymbol{\alpha}}(f)$). Actually, the fixed orientation could be chosen arbitrarily, but then the reflection that remains to be possible, would be more complicated than T leading also to a more complicated rule than our sign rule is.

Definition 2.5. Let $\Psi_i = (\phi(i), \theta(i), \psi(i))$, $0 \leq \theta(i) \leq \pi$, $0 \leq \phi(i), \psi(i) < 2\pi$, $i = 1, \cdots, n$. Set

$$\Omega_n = \left\{ \boldsymbol{\Psi} = (\Psi_1, \cdots, \Psi_n) \,\middle|\, \Psi_1 = (0, 0, 0) \right\}. \tag{24}$$

Let $n > c$. Define more the subset $\Omega_{n,c} \subset \Omega_n$ to be consisting of those $\boldsymbol{\Psi} \in \Omega_n$, which satisfy the following conditions:

(i) $\{\boldsymbol{\omega}(i) = \boldsymbol{\omega}(R(\Psi_i)) \,|\, i = 1, \cdots, n\}$ contains a linearly independent triplet.
(ii) $\#\{\boldsymbol{\omega}(i) \in \mathbb{P}^2 \,|\, i = 1, \cdots, n\} \geq c + 1$.
(iii) $\theta(i) \neq 0, \pi$, $i = 2, \cdots, n$.

Remark 4. (iii): We need that not only the orientations $R_i = R(\Psi_i)$, but also the Euler angles Ψ_i are uniquely determined. If $\theta = 0$ or π, this does not happen.

Definition 2.6. Let $\mathcal{R}_c$ be the closed half space

$$\mathcal{R}_c = \big\{\boldsymbol{m}_c \in \mathbb{R}^r \,\big|\, \sum_{\substack{\boldsymbol{\alpha} \\ \alpha_3 = odd}} \boldsymbol{m}_{\boldsymbol{\alpha}} \geq 0\big\}, \tag{25}$$

where $r = (1/6)(c+1)(c+2)(c+3) - 3$. Define more

$$\mathcal{M}_c = \big\{\boldsymbol{m}_c(f) \in \mathbb{R}^r \,\big|\, f \in \mathcal{O}_{\{2,\cdots,c\}}\big\} \tag{26}$$

and $\mathcal{S}_c = \mathcal{M}_c \cap \mathcal{R}_c^\circ$, where $\mathcal{R}_c^\circ$ is the interior of $\mathcal{R}_c$.

It is no limitation to suppose the projection data is acquired at $(\boldsymbol{m}_c, \boldsymbol{\Psi}) \in \mathcal{R}_c \times \Omega_n$. If $c \geq 7$, then by Theorem 2.3 the set $\mathcal{M}_c$ is generic in $\mathbb{R}^r$, and thus $\mathcal{S}_c$ is clearly generic in $\mathcal{R}_c$. Obviously also $\Omega_{n,c}$ is generic in Ω_n.

Definition 2.7. Let $A \subset \mathbb{R}^m$, $F : A \to \mathbb{R}^l$ be a mapping and $\mathbf{z}_0 \in A$. Then we call $\mathbf{z}_0$ *identifiable* in A by the system

$$F(\mathbf{z}_0) = F(\mathbf{z}), \tag{27}$$

if $\mathbf{z} = \mathbf{z}_0$ is the only solution in A to system (27).

Theorem 2.8 (Uniqueness of the ARP). *Suppose $n > c \geq 7$. Then all $(\boldsymbol{m}_c^0, \boldsymbol{\Psi}^0) \in \mathcal{S}_c \times \Omega_{n,c}$ are identifiable in $\mathcal{R}_c \times \Omega_n$ by the system*

$$A_c(\Psi_i^0)\, \boldsymbol{m}_c^0 = A_c(\Psi_i)\, \boldsymbol{m}_c, \quad i = 1, \cdots, n. \tag{28}$$

In addition, $\mathcal{S}_c$ is generic in $\mathcal{R}_c$ and $\Omega_{n,c}$ in Ω_n.

In the SHARP the data is $\{\widehat{pr}(i;\mathbf{x}) \,|\, i = 1, \cdots, n\}$, where $\widehat{pr}(i;\mathbf{x}) = pr(i;\mathbf{x} - \mathbf{x}_i)$ and $\mathbf{x}_i = (x(i)_1, x(i)_2) \in \mathbb{R}^2$ are unknown (representing unknown shifts). So, the moments that can be calculated are

$$\hat{p}_{(k,l)}(i) = \int_{\mathbb{R}^2} x_1^k x_2^l\, \widehat{pr}(i;\mathbf{x})\, dx_1 dx_2 = \sum_{s=0}^{k} \sum_{t=0}^{l} \binom{k}{s} \binom{l}{t} x(i)_1^{k-s} x(i)_2^{l-t}\, p_{(k,l)}(i). \tag{29}$$

We define the vectors $\hat{\mathbf{p}}_c(i) \in \mathbb{R}^p$, $i = 1, \cdots, n$, $p = (1/2)(c^2 + 3c + 2)$, otherwise analogously to $\mathbf{p}_c(i)$, but including $\hat{\mathbf{p}}(1;i) = [\hat{p}_{(1,0)}(i)\ \hat{p}_{(0,1)}(i)]^T$ too (whereas by (14) $\mathbf{p}(1;i) = [0\ 0]^T$). Then by (29)

$$\hat{\mathbf{p}}_c(i) = O(\mathbf{x}_i)\, \mathbf{p}_c(i), \quad i = 1, \cdots, n, \tag{30}$$

where $O(\mathbf{x}) \in \mathbb{R}^{p \times p}$ is a regular lower triangular matrix with

$$O(\mathbf{x})(i,j) = \begin{cases} \binom{k}{s}\binom{l}{t} x_1^{k-s} x_2^{l-t}, & \text{if } i = (1/2)(k+l)(k+l+1)+l+1 \text{ and} \\ & j = (1/2)\cdot(s+t)(s+t+1)+t+1, \\ & s = 0,\cdots,k,\ t = 0,\cdots,l, \\ 0 & \text{otherwise.} \end{cases} \tag{31}$$

By (19) and (30) we get the following system for the SHARP:

$$\hat{\mathbf{p}}_c(i) = O(\mathbf{x}_i) A_c(\Psi_i)\, \boldsymbol{m}_c, \quad i = 1,\cdots,n, \tag{32}$$

where the unknowns are $\boldsymbol{m}_c$, $\boldsymbol{\Psi}$ and $\underline{\mathbf{x}} = (\mathbf{x}_1,\cdots,\mathbf{x}_n)$. The following lemmas result in uniqueness of the SHARP; proofs of them are straightforward.

Lemma 2.9. *Suppose $(\boldsymbol{m}_c^0, \boldsymbol{\Psi}^0)$ is identifiable in $\mathcal{R}_c \times \Omega_n$ by system (28) and $m_{000}^0 \neq 0$. Then $(\boldsymbol{m}_c^0, \boldsymbol{\Psi}^0, \underline{0})$ is identifiable in $\mathcal{R}_c \times \Omega_n \times \mathbb{R}^{2n}$ by the system*

$$A_c(\Psi_i^0)\, \boldsymbol{m}_c^0 = O(\mathbf{x}_i) A_c(\Psi_i)\, \boldsymbol{m}_c, \quad i = 1,\cdots,n. \tag{33}$$

Lemma 2.10. *For all $\mathbf{x}, \mathbf{y} \in \mathbb{R}^2$ it holds that*

$$O(\mathbf{x})O(\mathbf{y}) = O(\mathbf{x}+\mathbf{y}) = O(\mathbf{y})O(\mathbf{x}). \tag{34}$$

Lemma 2.11. *Suppose $(\boldsymbol{m}_c^0, \boldsymbol{\Psi}^0)$ is identifiable in $\mathcal{R}_c \times \Omega_n$ by system (28) and $m_{000}^0 \neq 0$. Let $\underline{\mathbf{x}}^0 \in \mathbb{R}^{2n}$ be arbitrary. Then $(\boldsymbol{m}_c^0, \boldsymbol{\Psi}^0, \underline{\mathbf{x}}^0)$ is identifiable in $\mathcal{R}_c \times \Omega_n \times \mathbb{R}^{2n}$ by the system*

$$O(\mathbf{x}_i^0) A_c(\Psi_i^0)\, \boldsymbol{m}_c^0 = O(\mathbf{x}_i) A_c(\Psi_i)\, \boldsymbol{m}_c, \quad i = 1,\cdots,n. \tag{35}$$

Theorem 2.12 (Uniqueness of the SHARP)**.** *Suppose $n > c \geq 7$ and set $\mathcal{S}_c' = \mathcal{S}_c \cap \{\boldsymbol{m}_c \,|\, m_{000} \neq 0\}$. Then all $(\boldsymbol{m}_c^0, \boldsymbol{\Psi}^0, \underline{\mathbf{x}}^0) \in \mathcal{S}_c' \times \Omega_{n,c} \times \mathbb{R}^{2n}$ are identifiable in $\mathcal{R}_c \times \Omega_n \times \mathbb{R}^{2n}$ by the system*

$$O(\mathbf{x}_i^0) A_c(\Psi_i^0)\, \boldsymbol{m}_c^0 = O(\mathbf{x}_i) A_c(\Psi_i)\, \boldsymbol{m}_c, \quad i = 1,\cdots,n. \tag{36}$$

In addition, $\mathcal{S}_c'$ is generic in $\mathcal{R}_c$.

3. Main Results on Stability

In the previous section we analyzed the ARP and SHARP supposing noiseless projection data: projection moments $p_{(k,l)}(i)$ were exact, perfectly acquired at some $(\boldsymbol{m}_c^0, \boldsymbol{\Psi}^0) \in \mathcal{R}_c \times \Omega_n$ (that represents some object $f \in L^1(B)$ and orientations $R_i \in SO(3)$). Throughout this and the next sections we suppose the data is corrupted by additive noise $n(i;\mathbf{x})$. We focus on the SHARP, since it actually includes the ARP and is perhaps more present in applications. In the SHARP available projections are

$$\widetilde{\widehat{pr}}(i;\mathbf{x}) = \widehat{pr}(i;\mathbf{x}) + n(i;\mathbf{x}), \quad i = 1,\cdots,n. \tag{37}$$

Naturally, in applications projections (37), since being measured, are known only on some finite sets of points. Noise $n(i;\mathbf{x})$ is usually modeled as a random field such as white Gaussian noise, or the whole projection is modeled for example as a Poisson

process with the exact projection as a mean (having a random field $n(i;\mathbf{x})$ as a consequence). However, integration by some quadrature yields corrupted projection moments

$$\tilde{\hat{p}}_{(k,l)}(i) = \hat{p}_{(k,l)}(i) + n_{(k,l)}(i), \quad k,l \in \mathbb{N}. \tag{38}$$

Let $\mathbf{n}_c(i)$ and $\tilde{\hat{\mathbf{p}}}_c(i)$ be random vectors defined analogously to $\hat{\mathbf{p}}_c(i)$ (consisting of $n_{(k,l)}(i)$ and $\tilde{\hat{p}}_{(k,l)}(i)$). If supposing for instance a white Gaussian noise process, independent in each projection, then $\mathbf{n}_c(i)$ and $\mathbf{n}_c(j)$, $i \neq j$, are independent Gaussian random vectors with zero as means. In addition, the covariance matrix $Cov(\mathbf{n}_c(i))$, $i = 1, \cdots, n$, is then approximately in proportion to $\Sigma \in \mathbb{R}^{p\times p}$, where $p = (1/2)(c^2 + 3c + 2)$ and (B_2 is the unit disk)

$$\Sigma\big((k,l),(s,t)\big) = \int_{B_2} x_1^{k+s} x_2^{l+t}\, dx. \tag{39}$$

So, it is natural to solve system (32) as a (partly) nonlinear least squares problem by minimizing

$$\widehat{S}_{\Sigma^{-1}}(\boldsymbol{m}_c, \boldsymbol{\Psi}, \underline{\mathbf{x}}) = \sum_{i=1}^{n} \big(\tilde{\hat{\mathbf{p}}}_c(i) - O(\mathbf{x}_i)A_c(\Psi_i)\,\boldsymbol{m}_c\big)^T \Sigma^{-1} \big(\tilde{\hat{\mathbf{p}}}_c(i) - O(\mathbf{x}_i)A_c(\Psi_i)\,\boldsymbol{m}_c\big) \tag{40}$$

in the set $\mathcal{R}_c \times \Omega_n \times \mathbb{R}^{2n}$.

Remark 5. Σ^{-1} in (40) actually corresponds with changing from geometric to orthogonal moments in least squares. If supposing $\mathbf{n}_c(i) \sim \mathcal{N}(0,\Sigma)$, a minimizer of (40) is a maximum likelihood estimate as well. Supposing a more complicated model can yield another covariance matrix than Σ above. If being reasonably estimated, it should be used in (40). An example about that is modeling projections $\widetilde{\hat{pr}}(i;\mathbf{x})$ as a process $Poisson(\hat{pr}(i;\mathbf{x}))$.

We have come to problem (40)), which is a special case of the following general nonlinear least squares (NLS) problem:

Let $A \subset \mathbb{R}^m$, $F : A \to \mathbb{R}^l$ be a mapping, $C \in \mathbb{R}^{l\times l}$ be a symmetric, positive definite matrix and $\mathbf{y} \in \mathbb{R}^l$. Minimize in A with respect to $\mathbf{z}$ the function

$$S_C(\mathbf{y};\mathbf{z}) = \big(\mathbf{y} - F(\mathbf{z})\big)^T C\big(\mathbf{y} - F(\mathbf{z})\big). \tag{41}$$

Note that, if (41) is applied to (40), then C is defined as a block diagonal matrix with blocks Σ^{-1}. We utilize known stability results of NLS problem (41) considering only main features of the issue; for proofs and more details we refer to [3, 6].

Definition 3.1 (Deterministic Stability)**.** Let $B(0;\delta) = \{\mathbf{y} \,|\, \|\mathbf{y}\| < \delta\}$ be an open ball in $\mathbb{R}^l$, centered at the origin. NLS problem (41) is called *deterministically stable* at $\mathbf{z}_0 \in A$, if there exist $\delta > 0$ and a continuously differentiable function $\phi : B(0;\delta) \to A$ such that $\phi(\mathbf{n})$ is for all (fixed) $\mathbf{n} \in B(0;\delta)$ a strict global minimizer in A with respect to $\mathbf{z}$ to

$$S_C(\mathbf{z}_0,\mathbf{n};\mathbf{z}) = \big(F(\mathbf{z}_0) + \mathbf{n} - F(\mathbf{z})\big)^T C\big(F(\mathbf{z}_0) + \mathbf{n} - F(\mathbf{z})\big). \tag{42}$$

Note that stability at $\mathbf{z}_0$ necessarily implies $\phi(0) = \mathbf{z}_0$ and that $\mathbf{z}_0$ is identifiable in A by the system $F(\mathbf{z}_0) = F(\mathbf{z})$.

We can consider stability also in a stochastic sense, in the context of the nonlinear parameter estimation problem of the form

$$\mathbf{y} = F(\mathbf{z}) + \mathbf{n}, \tag{43}$$

where noise $\mathbf{n}$ is modeled as a random vector with a known distribution. Suppose $\mathbf{n} \sim \mathcal{N}(0, C^{-1})$. Then a minimizer of (41) is the MLE for estimation problem (43). Let $d(\mathbf{y} \,|\, \mathbf{z})$ be the conditional density of the observation $\mathbf{y}$ for a given value of the parameter $\mathbf{z}$. Then the *Fisher information matrix* (FIM) [21] at $\mathbf{z}_0 \in A$, if exists, is defined as an expectation (with respect to $d(\mathbf{y} \,|\, \mathbf{z}_0)$)

$$\mathrm{FIM}(\mathbf{z}_0) = E\big\{(\nabla_{\mathbf{z}} \log d(\mathbf{y} \,|\, \mathbf{z}_0))(\nabla_{\mathbf{z}} \log d(\mathbf{y} \,|\, \mathbf{z}_0))^T\big\}. \tag{44}$$

Note that the gradient $\nabla_{\mathbf{z}}$ requires that $\mathbf{z}_0$ belongs to the interior of A: $\mathbf{z}_0 \in A^\circ$.

Definition 3.2 (Stochastic Stability)**.** Parameter estimation problem (43) is called *stochastically stable* at $\mathbf{z}_0 \in A^\circ$, if $\mathrm{FIM}(\mathbf{z}_0)$ exists and is positive definite.

The definition is justified by what follows: $\mathrm{FIM}(\mathbf{z}_0)$ is always positive semidefinite. If it is positive definite, the variances of any unbiased estimator $\hat{\mathbf{z}}(\mathbf{y}) = (\hat{z}_1(\mathbf{y}), \cdots, \hat{z}_m(\mathbf{y}))$ of $\mathbf{z}_0$ are bounded below by the *information inequality*, referred also to as the *Cramér-Rao bound* (CRB) [21, 16],

$$Var(\hat{z}_k(\mathbf{y})) \geq J(\mathbf{z}_0)(k,k), \quad k = 1, \cdots, m, \tag{45}$$

where $J(\mathbf{z}) = \mathrm{FIM}(\mathbf{z})^{-1}$. Additionally, if an estimator satisfies the equalities in (45), it necessarily is the MLE.

Let $F = (F_1, \cdots, F_l)$ be differentiable at $\mathbf{z}_0 \in A^\circ$, and let $D(\mathbf{z}_0) \in \mathbb{R}^{l \times m}$ be its derivative matrix at $\mathbf{z}_0$. If $\mathbf{n} \sim \mathcal{N}(0, C^{-1})$, it is readily seen that

$$\mathrm{FIM}(\mathbf{z}_0) = D(\mathbf{z}_0)^T C D(\mathbf{z}_0). \tag{46}$$

Define $M(\mathbf{z}_0, \mathbf{n}) \subset A$ to be the set of global minimizers in A of (42). The next theorem is a key result in stability considerations.

Theorem 3.3. *Let $A \subset \mathbb{R}^m$, $F : A \to \mathbb{R}^l$ be a continuous mapping and $C \in \mathbb{R}^{l \times l}$ be symmetric and positive definite. Suppose F is twice continuously differentiable in a neighborhood of $\mathbf{z}_0 \in A^\circ$, and $\mathbf{z}_0$ is identifiable in A by the system $F(\mathbf{z}_0) = F(\mathbf{z})$. Suppose more there exists $\delta > 0$ such that $M(\mathbf{z}_0, \mathbf{n}) \neq \emptyset$ for all $\mathbf{n} \in B(0, \delta)$ and the set $\cup_{\mathbf{n} \in B(0,\delta)} M(\mathbf{z}_0, \mathbf{n})$ is bounded. Then the following items are equivalent:*
(i) The derivative matrix $D(\mathbf{z}_0) \in \mathbb{R}^{l \times m}$ of F is of full column rank.
(ii) Nonlinear least squares problem (41) is deterministically stable at $\mathbf{z}_0$.
(iii) Nonlinear parameter estimation problem (43) is stochastically stable at $\mathbf{z}_0$ for Gaussian noise.

The proof of Theorem 3.3 can be found in [3]. Note that the last assumption concerning $M(\mathbf{z}_0, \mathbf{n})$, which we have added to the version presented here, or some counterpart of it is necessary (for example for Lemma 7 in [3]). This extra condition is automatically satisfied, if A is for instance compact. We find that S. Basu and Y. Bresler have implicitly set this assumption. Indeed, minimizing can be restricted

to compact, explicitly known sets in problem (40): If we suppose that objects f are nonnegative, then $|m_{\boldsymbol{\alpha}}(f)| \leq m_{000}(f) = p_{0,0)}(i)$ for all $\boldsymbol{\alpha}$, since f is supported in $B = B(0,1)$. In the same results also a common, known bound for the L^1-norms of objects. For $\Psi_i = (\phi(i), \theta(i), \psi(i))$ we can set $0 \leq \phi(i), \psi(i) \leq 2\pi$, and obviously the variables $\mathbf{x}_i \in \mathbb{R}^2$ can be restricted to compact (known) sets too.

Our main result on stability is the following theorem.

Theorem 3.4 (Stability of the SHARP)**.** *Let $W_{n,c}$ be a subset of $\mathcal{S}'_c \times \Omega_{n,c}$ such that nonlinear least squares problem (40) is stable in $W_{n,c} \times \mathbb{R}^{2n}$ by means of Theorem 3.3.*
(i) Suppose $n > c \geq 7$. Then $W_{n,c}$ is generic in $\mathcal{R}_c \times \Omega_n$.
(ii) If $c \geq n$, problem (40) is not stable.

The proof of this theorem is postponed until the next section.

4. Stability of the SHARP

In this section we proof Theorem 3.4. The proofs rely on Theorem 3.3, by which we have to consider column rank of the derivative matrix of the mapping that defines the least squares problem. As presented just below Theorem 3.3, we can restrict our considerations in problem (40) to a compact set $A \subset \mathcal{R}_c \times \Omega_n$ (where Ω_n interpreted as compact) and its inner points $(\boldsymbol{m}_c^0, \boldsymbol{\Psi}^0) \in A^\circ$. If supposing $(\boldsymbol{m}_c^0, \boldsymbol{\Psi}^0)$ belongs to $\mathcal{S}'_c \times \Omega_{n,c}$ (and $n > c \geq 7$), then Theorem 2.12 is valid. Then all conditions of Theorem 3.3 are satisfied for $\mathbf{z}_0 = (\boldsymbol{m}_c^0, \boldsymbol{\Psi}^0, \underline{\mathbf{x}}^0)$. So it is sufficient to consider the derivative matrix at such $\mathbf{z}_0$.

Define

$$B_c(n) = B_c(\Psi_1, \cdots, \Psi_n) = \begin{bmatrix} A_c(\Psi_1) \\ \vdots \\ A_c(\Psi_n) \end{bmatrix} \tag{47}$$

and consider the mapping $B_c(n)\, \boldsymbol{m}_c$ of the variable $(\boldsymbol{m}_c, \boldsymbol{\Psi})$. Its derivative matrix is

$$\begin{aligned} D_c(n) &= D_c(\boldsymbol{m}_c; \Psi_1, \cdots, \Psi_n) = \big[B_c(n) \,|\, E_c(n)\big] \\ &= \begin{bmatrix} A_c(\Psi_1) & \mathbf{0} & \cdots & \cdots & \mathbf{0} \\ A_c(\Psi_2) & \frac{\partial A_c}{\partial \Psi}(\boldsymbol{m}_c; \Psi_2) & \mathbf{0} & \cdots & \mathbf{0} \\ A_c(\Psi_3) & \mathbf{0} & \frac{\partial A_c}{\partial \Psi}(\boldsymbol{m}_c; \Psi_3) & \cdots & \mathbf{0} \\ \cdots & \cdots & \cdots & \cdots & \cdots \\ A_c(\Psi_n) & \mathbf{0} & \cdots & \mathbf{0} & \frac{\partial A_c}{\partial \Psi}(\boldsymbol{m}_c; \Psi_n) \end{bmatrix} \in \mathbb{R}^{p \times r}, \end{aligned} \tag{48}$$

where $p = (n/2)(c^2 + 3c + 2)$, $r = (1/6)(c+1)(c+2)(c+3) + 3(n-2)$ and

$$\frac{\partial A_c}{\partial \Psi}(\boldsymbol{m}_c; \Psi) = \left[\frac{\partial A_c(\Psi)}{\partial \phi}\, \boldsymbol{m}_c \quad \frac{\partial A_c(\Psi)}{\partial \theta}\, \boldsymbol{m}_c \quad \frac{\partial A_c(\Psi)}{\partial \psi}\, \boldsymbol{m}_c\right] \in \mathbb{R}^{p \times r}, \tag{49}$$

$p = (1/2)(c^2 + 3c + 2)$ and $r = 3$ (note that $\Psi_1 = (0,0,0)$ is a constant).

Lemma 4.1. *Let $M \in \mathbb{R}^{m \times l}$, where $m \geq l$. The matrix M is of full column rank, if and only if some $l \times l$-subdeterminant of it is nonzero.*

Proof. Define $\widehat{M} = [M \ \mathbf{s}_{l+1} \ \cdots \ \mathbf{s}_m] \in \mathbb{R}^{m\times m}$, where $\mathbf{s}_i \in \mathbb{R}^m$, $i = l+1, \cdots, m$, are arbitrary. M is not of full column rank precisely if $\widehat{M}$ is not that, equivalently $\det \widehat{M} = 0$ for all $\mathbf{s}_i$.

By the Cramer's rule $\det \widehat{M}$ is a homogeneous polynomial in $\mathbf{s}_i$, $i = l+1, \cdots, m$, the coefficients of which are the $l \times l$-subdeterminants of M. □

The subdeterminants of $D_c(n)$, as in Lemma 4.1, are trigonometric polynomials in Ψ_i, $i = 2, \cdots, n$, the coefficients of which are homogeneous polynomials in $\boldsymbol{m}_c$, i.e. they are real analytic functions.

Theorem 4.2. *Let $\xi : \mathbb{R}^m \to \mathbb{R}$ be a nonzero real analytic function. Then the complement of its zero set is generic in $\mathbb{R}^m$.*

Proof. Suppose ξ is a nonzero real analytic function and let $A = \{\mathbf{z} \in \mathbb{R}^m \,|\, \xi(\mathbf{z}) = 0\}$ be its zero set. That A is of Lebesgue measure zero, is quite easily seen by using induction with respect to m [12], p. 67. Indeed, let first $m = 1$ and suppose A has an accumulation point z_0 in $\mathbb{R}$. Since being real analytic, ξ has a Taylor series that converges round z_0. It is readily seen that the coefficients of that series are zero. Thus ξ is locally and so, as a real analytic function, globally zero.

Suppose the zero set of a nonzero real analytic function is of Lebesgue measure zero for $m = k \in \mathbb{N}_+$. Let then $m = k+1$ and $z \in \mathbb{R}$. The set $A_z = \{(z_1, \cdots, z_k) \in \mathbb{R}^k \,|\, (z_1, \cdots, z_k, z) \in A\}$ is the zero set of a real analytic function $\xi_z : \mathbb{R}^k \to \mathbb{R}$, $\xi_z(z_1, \cdots, z_k) = \xi(z_1, \cdots, z_k, z)$. So it is either of Lebesgue measure zero in $\mathbb{R}^k$ (whenever ξ_z is nonzero) or ξ_z is a zero function. Suppose the set Z of those z that satisfy the latter case, has an accumulation point in $\mathbb{R}$. Let $(z_1, \cdots, z_k) \in \mathbb{R}^k$. The function $\xi_{(z_1,\cdots,z_k)} : \mathbb{R} \to \mathbb{R}$, $\xi_{(z_1,\cdots,z_k)}(z) = \xi(z_1, \cdots, z_k, z)$, is real analytic, and additionally it vanishes on a set containing Z. By what we have shown first, $\xi_{(z_1,\cdots,z_k)}$ is a zero function. Since that happens for all $(z_1, \cdots, z_k)$, also ξ is zero, a contradiction. Hence A_z is of Lebesgue measure zero for almost all $z \in \mathbb{R}$.

Let μ_k be the Lebesgue measure in $\mathbb{R}^k$. We can apply the Fubini's theorem to the closed set A and its characteristic function χ_A:

$$\mu_m(A) = \int_{\mathbb{R}^{k+1}} \chi_A(\mathbf{z})\, d\mu_{k+1}(\mathbf{z}) = \int_{\mathbb{R}} \int_{A_z} 1\, d\mu_k(z_1, \cdots, z_k)\, d\mu_1(z) = \int_{\mathbb{R}} 0\, d\mu_1(z) = 0. \tag{50}$$

Secondly we show that A is nowhere dense. Let U be an open subset of $\mathbb{R}^m$ such that $U \subset \bar{A}$ (the bar denotes the closure). Since A is closed, $U \subset A$. Thus ξ is zero in the open set U. It means that either ξ is identically zero or $U = \emptyset$. Hence $U = \emptyset$, which proves the last part. □

As studying column rank, $D_3(4) \in \mathbb{R}^{40\times 26}$ can be simplified to a matrix $\widehat{D}_3(4) \in \mathbb{R}^{21\times 18}$ by taking into account $\Psi_1 = (0,0,0)$ and removing irrelevant rows and columns. That leaves over $\binom{21}{18} = 1330$ subdeterminants. We have demonstrated numerically, that they are not all zero functions (which is quite obvious but not self-evident: for instance, if $\phi(2) = \phi(3)$ and $\theta(2) = \theta(3)$, by Lemma 4.4 (ii) they are all identically zero). Thus, $D_3(4) = D_3(\boldsymbol{m}_3; \Psi_1, \cdots, \Psi_4)$ is by Theorem 4.2 and Lemma 4.1 of full column rank for $(\boldsymbol{m}_3; \Psi_1, \cdots, \Psi_4)$ in a generic set. At the same time we note by (48) that also $\frac{\partial A_3}{\partial \Psi}(\boldsymbol{m}_3; \Psi) \in \mathbb{R}^{10\times 3}$ is of full column rank for $(\boldsymbol{m}_3; \Psi)$ in a generic set. We omit most (straightforward) proofs of the following lemmas.

Lemma 4.3. *Let $\Psi_{n+1} = (\phi(n+1), \theta(n+1), \psi(n+1))$. Suppose $D_c(n) = D_c(\boldsymbol{m}_c; \Psi_1, \cdots, \Psi_n)$ and $\frac{\partial A_c}{\partial \Psi}(\boldsymbol{m}_c; \Psi_{n+1})$ are of full column rank. Then*

(51)
$$D_c(n+1) = D_c(\boldsymbol{m}_c; \Psi_1, \cdots, \Psi_{n+1}) = \begin{bmatrix} D_c(n) & \cdots & \cdots & \mathbf{0} \\ A_c(\Psi_{n+1}) & \mathbf{0} & \cdots & \frac{\partial A_c}{\partial \Psi}(\boldsymbol{m}_c; \Psi_{n+1}) \end{bmatrix}$$

is of full column rank, too.

Lemma 4.4. *(i) Suppose $n > 7$ and $\boldsymbol{\Psi} = (\Psi_1, \cdots, \Psi_n) \in \Omega_{n,n-1}$ (particularly $\#\{\boldsymbol{\omega}(i) \in \mathbb{P}^2 \,|\, i = 1, \cdots, n\} = n$). Then $B_c(\Psi_1, \cdots, \Psi_n)$, as defined in (47), is of full column rank for all $c < n$.*

(ii) Let Ψ_i, $i = 1, \cdots, n$, be arbitrary. Then $B_c(n)$ is not of full column rank for any $c \geq n$.

Proof. (i) Suppose $7 \leq c < n$. By uniqueness Theorems 2.3 and 2.4 there exists $\boldsymbol{m}_c \in \mathbb{R}^r$ such that, if $\widehat{\boldsymbol{m}}_c \in \mathbb{R}^r$ and $B_c(n)\, \widehat{\boldsymbol{m}}_c = B_c(n)\, \boldsymbol{m}_c$, then $\widehat{\boldsymbol{m}}_c = \boldsymbol{m}_c$ (actually almost all $\boldsymbol{m}_c$ satisfy that). Thus the null space of $B_c(n)$ is zero. Because of the block structure of $B_c(n)$ this holds also for $c < 7$.

(ii) Define $\boldsymbol{m}_n = \boldsymbol{m}_n(f)$, $f \in L^1(B)$, by setting $m_{\boldsymbol{\alpha}} = 0$, whenever $|\boldsymbol{\alpha}| < n$, and

$$Q_n(f; \mathbf{x}) = \sum_{|\boldsymbol{\alpha}|=n} \binom{n}{\boldsymbol{\alpha}} m_{\boldsymbol{\alpha}}\, \mathbf{x}^{\boldsymbol{\alpha}} = \prod_{i=1}^{n} (\boldsymbol{\omega}(i) \cdot \mathbf{x}). \tag{52}$$

Then $Q_k(f; \mathbf{x}) = 0$ for all $\mathbf{x} \in \boldsymbol{\omega}(i)^{\perp}$, $k = 0, \cdots, n$, and $i = 1, \cdots, n$. By what we have shown in [13], particularly identity (19) there, we get that $m_{(k,l,0)}(f_{R(\Psi_i)}) = 0$ for all $0 \leq k + l \leq n$ and $i = 1, \cdots, n$. By (15), (19) and (47) equivalently $B_n(n)\, \boldsymbol{m}_n = 0$. Certainly $\boldsymbol{m}_n \neq 0$. For $c > n$ the assertion follows from the block structure of $B_c(n)$. □

Lemma 4.5. *Suppose $\boldsymbol{\Psi} = (\Psi_1, \cdots, \Psi_n) \in \Omega_{n,n-1}$ and $n > \max\{7, c+1\}$. Suppose more $D_c(n) = D_c(\boldsymbol{m}_c; \Psi_1, \cdots, \Psi_n)$ is of full column rank. Then $D_{c+1}(n) = D_{c+1}(\boldsymbol{m}_{c+1}; \Psi_1, \cdots, \Psi_n)$ is of full column rank too.*

Lemma 4.6. *Suppose $n > 7$ and $3 \leq c < n$. Then the matrix $D_c(n) = D_c(\boldsymbol{m}_c; \Psi_1, \cdots, \Psi_n)$ is of full column rank for $(\boldsymbol{m}_c, \boldsymbol{\Psi})$ in a generic set.*

Proof. Since $D_3(4)$ and $\frac{\partial A_3}{\partial \Psi}(\boldsymbol{m}_3; \Psi)$ are of full column rank in generic sets, as presented below Theorem 4.2, by Lemmas 4.3, 4.5 and 4.1 the subdeterminants of $D_c(n)$ are not all identically zero. The assertion follows now from Theorem 4.2 and Lemma 4.1. □

Lemma 4.7. *Problem (40) is stable at $(\boldsymbol{m}_c^0, \boldsymbol{\Psi}^0, \underline{\mathbf{x}}^0)$ both in the deterministic and stochastic sense, if and only if the NLS problem of minimizing*

$$\begin{gathered} \widehat{S}_{\Sigma^{-1}}(\boldsymbol{m}_c, \boldsymbol{\Psi}, \underline{\mathbf{y}} + \underline{\mathbf{x}}^0) = \\ \textstyle\sum_{i=1}^{n} \left(A_c(\Psi_i^0)\, \boldsymbol{m}_c^0 - O(\mathbf{y}_i) A_c(\Psi_i)\, \boldsymbol{m}_c\right)^T \times \\ O(\mathbf{x}_i^0)^T \Sigma^{-1} O(\mathbf{x}_i^0) \times \\ \left(A_c(\Psi_i^0)\, \boldsymbol{m}_c^0 - O(\mathbf{y}_i) A_c(\Psi_i)\, \boldsymbol{m}_c\right) \end{gathered} \tag{53}$$

in $\mathcal{R}_c \times \Omega_n \times \mathbb{R}^{2n}$ is stable at $(\boldsymbol{m}_c^0, \boldsymbol{\Psi}^0, \underline{0})$.

Recall (31) for the definition of $O(\mathbf{x}) \in \mathbb{R}^{p\times p}$. Define

$$\frac{\partial O}{\partial \mathbf{x}}(\boldsymbol{m}_c;\Psi;\mathbf{x}) = \left[\frac{\partial O(\mathbf{x})}{\partial x_1}A_c(\Psi)\,\boldsymbol{m}_c \quad \frac{\partial O(\mathbf{x})}{\partial x_2}A_c(\Psi)\,\boldsymbol{m}_c\right] \in \mathbb{R}^{p\times 2}, \tag{54}$$

where $\mathbf{x} = (x_1, x_2) \in \mathbb{R}^2$ and $p = (1/2)(c^2+3c+2)$, and

$$\begin{aligned} F_c(n) &= F_c(\boldsymbol{m}_c;\Psi_1,\cdots,\Psi_n;\underline{0}) \\ &= \begin{bmatrix} \frac{\partial O}{\partial \mathbf{x}}(\boldsymbol{m}_c;\Psi_1;0) & \mathbf{0} & \cdots & \mathbf{0} \\ \mathbf{0} & \frac{\partial O}{\partial \mathbf{x}}(\boldsymbol{m}_c;\Psi_2;0) & \cdots & \mathbf{0} \\ \cdots & \cdots & \cdots & \cdots \\ \mathbf{0} & \mathbf{0} & \cdots & \frac{\partial O}{\partial \mathbf{x}}(\boldsymbol{m}_c;\Psi_n;0) \end{bmatrix} \in \mathbb{R}^{p\times r}, \end{aligned} \tag{55}$$

where $p = (n/2)(c^2+3c+2)$ and $r = 2n$. Additionally we have

$$\frac{\partial O(0)}{\partial x_1}(i,j) = \begin{cases} k, & \text{if } i = (1/2)(k+l)(k+l+1)+l+1 \text{ and } j = (1/2) \\ & \cdot(k+l-1)(k+l)+l+1, \quad 1\le k\le c,\ 0\le l\le c, \\ 0 & \text{otherwise} \end{cases} \tag{56}$$

and

$$\frac{\partial O(0)}{\partial x_2}(i,j) = \begin{cases} l, & \text{if } i = (1/2)(k+l)(k+l+1)+l+1 \text{ and } j = (1/2) \\ & \cdot(k+l-1)(k+l)+l, \quad 0\le k\le c,\ 1\le l\le c, \\ 0 & \text{otherwise.} \end{cases} \tag{57}$$

Then the derivative matrix at $(\boldsymbol{m}_c, \boldsymbol{\Psi}, \underline{0})$, related to NLS problem (53), is

$$G_c(n) = G_c(\boldsymbol{m}_c;\Psi_1,\cdots,\Psi_n;\underline{0}) = \left[D_c(n)\,|\,F_c(n)\right] = \left[B_c(n)\,|\,E_c(n)\,|\,F_c(n)\right] \in \mathbb{R}^{p\times r}, \tag{58}$$

where $p = (n/2)(c^2+3c+2)$ and $r = (1/6)(c+1)(c+2)(c+3)+5n-6$.

Lemma 4.8. *Suppose $m_{000} \neq 0$. Then $G_c(n) = G_c(\boldsymbol{m}_c;\Psi_1,\cdots,\Psi_n;\underline{0})$ is of full column rank, if and only if $D_c(n) = D_c(\boldsymbol{m}_c;\Psi_1,\cdots,\Psi_n)$ is of full column rank.*

Now we are able to demonstrate stability of the SHARP.

Proof of Theorem 3.4. Follows from Theorems 2.12 and 3.3, and Lemmas 4.7, 4.8 and 4.6. The last statement follows from Lemma 4.4 (ii). □

5. Implementation

NLS: non least square

Our algorithm for recovering the orientations is simply a procedure of solving NLS problem (40) in the SHARP. At first we have to calculate the projection moments $\tilde{p}_{(k,l)}(i)$, $0\le k,l\le c$, $i = 1,\cdots,n$, by an integration quadrature. We set the origins of coordinate systems of projections at the mass center points of projections. They are not the correct origins, since projections are perturbed. Then we fit a two-dimensional smoothing spline to every projection and integrate relevant monomials against these splines. That kind of procedure is extensively suggested as considering integration of noisy data [22].

A troublesome task in the procedure is to handle optimization (40) in practice, although we can restrict the variable into a compact set. By large and even by

moderate n, globally convergent methods like simulated annealing tend to cost too much in time. So we prefer in optimization classical Newtonian or quasi-Newtonian methods: we use the Broyden-Fletcher-Goldfarb-Shanno (BFGS) algorithm, which belongs to the quasi-Newtonian family. It still requires using quite a good initial value for to converge towards a global minimum, and nothing guarantees that an attained minimum is not just a local one. Also S. Basu and Y. Bresler state this difficulty in connection of the two-dimensional recovery problem. Their solution is the so-called SNNI algorithm [2] (that works only in a special case). Our idea is to connect optimization (40), i.e. a moment based method, with the common line technique [20], which is available only in the three-dimensional problem. We calculate an initial value by it.That technique in turn can be based on the projection moments (already calculated), as we have shown in [13]: Let the data be created by an object $f \in \mathcal{O}_H$, i.e. $p_{(k,l)}(i) = m_{(k,l,0)}(f_{R_i})$, $k, l \in \mathbb{N}$, $i = 1, \cdots, n$, where $R_i = [\mathbf{r}(i)_1 \ \mathbf{r}(i)_2 \ \boldsymbol{\omega}(i)]$ are the used orientations. Then the system (where $i \neq j$)

$$\sum_{l=0}^{k} \binom{k}{l} p_{(l,k-l)}(i) \cos^l\theta \sin^{k-l}\theta = \sum_{l=0}^{k} \binom{k}{l} p_{(l,k-l)}(j) \cos^l\psi \sin^{k-l}\psi, \quad k = 0, \cdots, c, \tag{59}$$

of $(\theta, \psi) \in \mathbb{R}^2$ is essentially uniquely solvable (see equation (89) in [13]). Necessarily $\mathbf{r}(i)_1 \cos\theta + \mathbf{r}(i)_2 \sin\theta = \mathbf{r}(j)_1 \cos\psi + \mathbf{r}(j)_2 \sin\psi$ holds for that solution. So it tells where the common line of the projection planes $\boldsymbol{\omega}(i)^{\perp}$ and $\boldsymbol{\omega}(j)^{\perp}$ is outlined on those planes (giving " a hinge"). Naturally, we have to be content with corrupted moments $\tilde{\hat{p}}_{(k,l)}(i)$ in (59). Additionally, it is practical to solve (59) by means of least squares.

The common line orientation solutions are found by solving initially a triplet and then the rest of orientations by relying on those three ones. Using the common line technique leads to a common problem in computer vision, which is well studied [17]: Let S_i and T_i be 3×3-matrices with columns $[\cos\theta \ \sin\theta \ 0]^T$ and $\mathbf{r}(j)_1 \cos\psi + \mathbf{r}(j)_2 \sin\psi$, respectively, where (θ, ψ):s are solutions to (59), when j runs over the indices of the triplet (R_j:s are already known). The matrix R_i can be solved from the equation $R_i S_i = T_i$, a solution to which, in the set $SO(3)$ and by means of least squares, can be obtained by using the singular value decomposition $U\Lambda V^T = T_i S_i^T$. The optimal solution is then $R_i = UV^T \in SO(3)$.

Suppose we have a large number of projections waiting their orientation. One possibility is to solve the problem first for a moderate subset, still large enough that the moments of object will be determined very well. Then extra projections can be easily added to the collection of orientations that are already known, at least in first approximation, since for a known $\boldsymbol{m}_c$ any orientation can be separately solved in system (40). The procedure can be carried on iteratively: a collection of so calculated values gives initial values for an updating, larger NLS problem (40); n can be increased step by step.

A relevant factor in the procedure is the problem, how to choose c in relation to n. By Theorem 3.4, especially by its item (ii), a reasonable choice is bounded by $7 \leq c < n$. Suppose a Gaussian error distribution in the moments: $\mathbf{n} \sim \mathcal{N}(0, C^{-1})$ (recall equations (42) and (43)). By (46) the information matrix at $(\boldsymbol{m}_c, \boldsymbol{\Psi}, \underline{0})$ of the SHARP (also of problem (53); they have distinct C:s) is then

$$\mathrm{FIM}(\boldsymbol{m}_c, \boldsymbol{\Psi}, \underline{0}) = G_c(\boldsymbol{m}_c; \Psi_1, \cdots, \Psi_n; \underline{0})^T C G_c(\boldsymbol{m}_c; \Psi_1, \cdots, \Psi_n; \underline{0}). \tag{60}$$

Thus the Cramér-Rao bound concerning the whole variable $(\boldsymbol{m}_c, \boldsymbol{\Psi}, \underline{\mathbf{x}})$ is

$$J(\boldsymbol{m}_c, \boldsymbol{\Psi}, \underline{0}) = \left(G_c(n)^T C G_c(n)\right)^{-1}. \tag{61}$$

We are mostly interested in the variable $\boldsymbol{\Psi}$ only. Since the error $\mathbf{n}$ is Gaussian, we have a good reason to define the Cramér-Rao bound of $\boldsymbol{\Psi}$ to be the block $J_{\boldsymbol{\Psi}}$ of (61), which is associated with $\boldsymbol{\Psi}$ only.

Remark 6. Using $(\boldsymbol{m}_c, \boldsymbol{\Psi}, \underline{0})$, i.e. $\underline{0}$ for $\underline{\mathbf{x}}$, means using form (53) of the NLS problem. Thus C is precisely a block diagonal matrix with blocks $O(\mathbf{x}_i^0)^T \Sigma^{-1} O(\mathbf{x}_i^0)$, where $\mathbf{x}_i^0$:s are unknown. We suppose they are small, and thus the blocks can be approximated by Σ^{-1}.

The next figure shows a behavior of diagonal entries of $J_{\boldsymbol{\Psi}}$ as a function of c. From it we can see that for a moderate n, 10-14 is a reasonable upper bound for c.

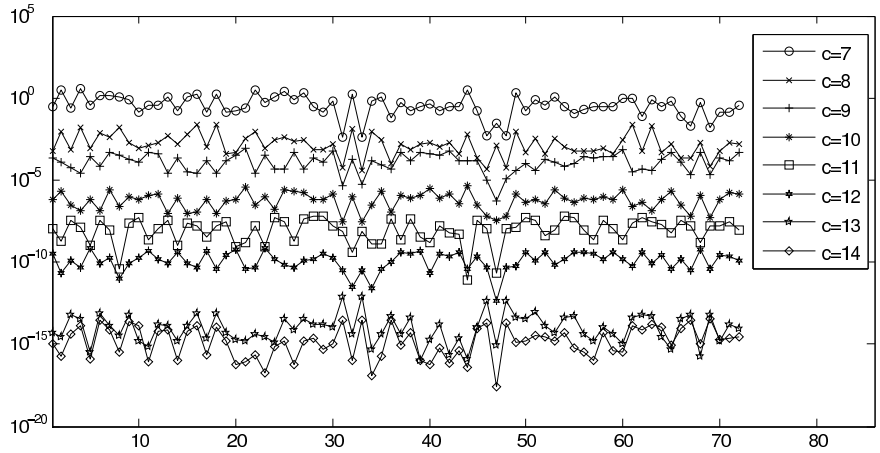

FIGURE 1. The diagonal entries of $J_{\boldsymbol{\Psi}}$ that are related to the Euler angles $(\phi_2, \theta_2, \psi_2, \cdots, \phi_{25}, \theta_{25}, \psi_{25})$ as a function of c $(n = 25)$.

6. SIMULATIONS

The simulations were performed with various levels and types of noise added to the simulated projections, which were calculated with various resolutions. Simulations were realized in three separate steps: data generation, finding an initial value and optimizing (40).

We demonstrate here an example, were the object and data are (partly) presented in Figure 2. Particularly, noise level was 25 per cent, and in the first stage we had $n = 12$. Initial values for orientations were calculated by using the moment based common line method as demonstrated in the previous section. Moments of orders $0, 1, 2, \cdots, 9$ were used. The basic triplet of orientations was chosen to be mutually as orthogonal as possible. All the rest of orientations were solved by determining their relation to the basic triplet.

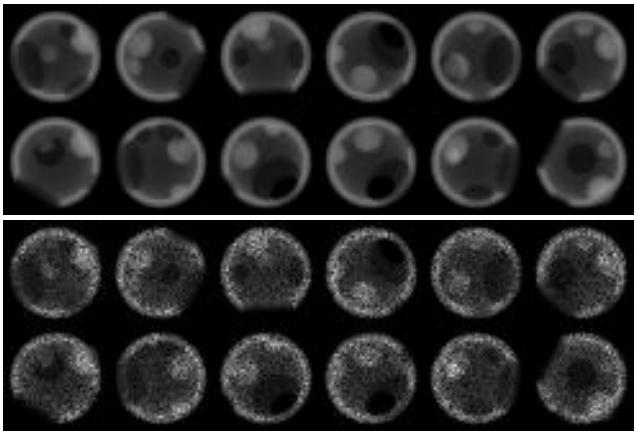

FIGURE 2. Set of 12 projections with 0% and with 25% Gaussian noise with resolution 41×41 pixels.

i	1	2	3	4	5	6	7	8	9	10	11	12
$\arccos(\mathbf{r}_1^{\text{est}} \cdot \mathbf{r}_1^{\text{cor}})$	7.53	11.8	9.40	6.44	2.65	5.23	5.04	9.58	2.05	3.06	20.2	19.6
$\arccos(\mathbf{r}_2^{\text{est}} \cdot \mathbf{r}_2^{\text{cor}})$	1.10	1.92	5.39	3.36	10.3	3.97	7.00	10.3	12.1	10.6	5.99	2.56
$\arccos(\mathbf{r}_3^{\text{est}} \cdot \mathbf{r}_3^{\text{cor}})$	7.55	11.9	10.8	5.54	10.0	5.59	5.20	9.20	12.3	10.4	19.3	19.7

TABLE 1. Errors in degrees between estimated and correct orientations by using the common line method for the projections in Figure 2.

The values obtained above were used as initial values for orientations, and additionally, the mass center points of projections were used as initial values for projection origins. Then these values were optimized by minimizing (40).

i	1	2	3	4	5	6	7	8	9	10	11	12
$\arccos(\mathbf{r}_1^{\text{est}} \cdot \mathbf{r}_1^{\text{cor}})$	1.38	0.58	2.45	0.31	0.73	1.01	0.98	1.29	1.60	3.21	1.42	1.34
$\arccos(\mathbf{r}_2^{\text{est}} \cdot \mathbf{r}_2^{\text{cor}})$	1.93	0.29	3.41	0.62	1.13	1.68	1.42	1.09	0.71	0.18	0.86	3.16
$\arccos(\mathbf{r}_3^{\text{est}} \cdot \mathbf{r}_3^{\text{cor}})$	2.36	0.56	3.29	0.53	0.91	1.88	1.09	1.49	1.75	3.21	1.45	3.35

TABLE 2. Final errors in degrees between estimated and correct orientations by using minimization (40) for the same projections as above.

After solving 12 projections (including object's moments), we were able to solve easily new extra projections by minimizing (40) with the (approximately) known and fixed $\boldsymbol{m}_c$ (so there were only five variables per a projection). In this example the relative error between the vectors of correct and estimated geometric moments was 7.4 per cent (in the Euclidean norm). Anyway this accuracy was sufficient for approximately determining new orientations. Carrying on iteratively we increased n step by step to the value $n = 100$. In the final result the mean errors in directions of column vectors were 4.21, 2.26 and 5.07 in degrees (1.34, 1.39 and 1.70 without projections 31, 35, 65, 76 and 100). The standard deviations were 19.1, 5.2 and 19.9 (1.55, 1.61 and 1.92), respectively. In summary, estimation went clearly wrong in a

few per cent of orientations, otherwise accuracy was quite good. Those poor cases can perhaps be removed from the used data by partly overlapping sub-collections of projections, so that every orientation will be calculated at least twice. Finally, estimation of the shifts succeeded precisely in every respect.

7. Conclusion

Our algorithm seems to work very well at least up to a moderate noise level, if measurement errors can be expected to be independent. We want to emphasize, we have introduced just a short scenario, no way a complete algorithm. It remains to be seen, whether it can be developed to tolerate such a high noise level that occurs for example in Cryo-electron microscopy of viruses.

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