SINGULAR VALUE DECOMPOSITION OF THE ODF–PDF PROJECTION OPERATOR

SVD of PDF Projection

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Abstract

The simple relationship between harmonics for $SO(3)$ and harmonics for the unit sphere S^2 provided by the pole figure projection operator is represented as a system composed of nested matrices of simple form. This structure can be advantageously exploited to compute the singular value decomposition at small computational costs. Of the manifold applications of svd two are represented in this communication, experimental design to choose the subset of experimentally accessible pole figures imparting the most information with respect to the orientation distribution function to be reconstructed, and determination of high order harmonic coefficients from a given set of pole figures minimising the mean squared error.

Keywords: Singular value decomposition, ODF, PDF, measurement error, planning of experiments, reconstruction of high order harmonics

1 Singular value decomposition of the projection of the ODF onto a finite number of pole figures

Suppose a finite set $\{P_h : h \in H\}$ of pole figures has been measured.

$$P_h(y) = 4\pi \sum_{l=0}^{\infty} \sum_{\nu=1}^{N(l)} F_{lh}^{\nu} \, \dot{k}_l^{\nu}(y), \quad ODF(g) = \sum_{l=0}^{\infty} \sum_{\mu=1}^{M(l)} \sum_{\nu=1}^{N(l)} C_l^{\mu\nu} \, \ddot{T}_l^{\mu\nu}(g),$$

Assume the $\ddot{T}_l^{\mu\nu}(g)$ and $\dot{k}_l^{\nu}(y)$ to form a orthonormal system of functions in $L^2(SO_3)$ and $L^2(S^2)$. The structure of the projection operator in terms of C and F for $l = 1, \ldots, L$ may be represented in matrix notation as

$$\begin{pmatrix} A_1 & & & & \\ & A_2 & & & \\ & & A_3 & & \\ & & & \ddots & \\ & & & & A_L \end{pmatrix} \begin{pmatrix} C_1 \\ C_2 \\ C_3 \\ \vdots \\ C_L \end{pmatrix} = \begin{pmatrix} F_1 \\ F_2 \\ F_3 \\ \vdots \\ F_L \end{pmatrix} \quad \Leftrightarrow \quad A_l C_l = F_l \; \forall l$$

These components of the system of equations have the same structure

$$\begin{pmatrix} A_l^1 & & & \\ & A_l^2 & & \\ & & \ddots & \\ & & & A_l^{N(l)} \end{pmatrix} \begin{pmatrix} C_l^{1,\cdot} \\ C_l^{2,\cdot} \\ \vdots \\ C_l^{N(l),\cdot} \end{pmatrix} = \begin{pmatrix} F_l^1 \\ F_l^2 \\ \vdots \\ F_l^{N(l)} \end{pmatrix} \Leftrightarrow A_l^\nu C_l^{\nu,\cdot} = F_l^\nu \; \forall l, \forall \nu$$

where these components are defined by

$$A_l^\nu = \tilde{A}_l = \frac{1}{\sqrt{2l+1}} \left(\dot{k}_l^\mu (h_b) \right)_{b=1,\dots,|H|\;,\;\mu=1,\dots,M(l)}$$

Thus A_l^ν is independent of ν.

$$C_l^{\cdot,\nu} = (C_l^{\mu\nu})_{\mu=1,\dots,M(l)}, \quad F_l^\nu = \left(F_{lh_b}^\nu\right)_{b=1,\dots,|H|}$$

Let $\tilde{P}_l \tilde{D}_l \tilde{Q}_l = \tilde{A}_l$ be a singular value decomposition (svd) of the small matrix $\tilde{A}_l$ with orthonormal matrices $\tilde{P}_l \in \mathbb{R}^{|H| \times r}$ and $\tilde{Q}_l \in \mathbb{R}^{r_l \times M(l)}$, and diagonal matrix $\tilde{D}_l \in \mathbb{R}^{r_l \times r_l}$ of minimal frame size $r_l = \text{rank}\tilde{A}_l$. This decomposition can be computed very fast with a computer because the frame size of $\tilde{A}$ is small (i.e. $r \leq 2l+1 \ll 1000$). Then a singular value decomposition PDQ of A is given with matrices P, D, Q constituted of $\tilde{P}_l, \tilde{D}_l, \tilde{Q}_l$, respectively, in the form

$$P = \begin{pmatrix} \begin{bmatrix} \tilde{P}_1 & & \\ & \ddots & \\ & & \tilde{P}_1 \end{bmatrix} & & \\ & \ddots & \\ & & \begin{bmatrix} \tilde{P}_L & & \\ & \ddots & \\ & & \tilde{P}_L \end{bmatrix} \end{pmatrix}$$

$$D = \begin{pmatrix} \begin{bmatrix} \tilde{D}_1 & & \\ & \ddots & \\ & & \tilde{D}_1 \end{bmatrix} & & \\ & \ddots & \\ & & \begin{bmatrix} \tilde{D}_L & & \\ & \ddots & \\ & & \tilde{D}_L \end{bmatrix} \end{pmatrix}$$

$$Q = \begin{pmatrix} \begin{bmatrix} \tilde{Q}_1 & & \\ & \ddots & \\ & & \tilde{Q}_1 \end{bmatrix} & & \\ & \ddots & \\ & & \begin{bmatrix} \tilde{Q}_L & & \\ & \ddots & \\ & & \tilde{Q}_L \end{bmatrix} \end{pmatrix}$$

Thus, the singular value decomposition of this ODF–PDF projection can be computed at small computational cost. In the next section it will be shown how this decomposition can be applied in practical texture analysis.

2 Practical application of the SVD

The singular value decomposition immediately provides the least squared error back transformation matrix and its singular value decomposition without additional computational effort, it is the Moore–Penrose inverse of the projection matrix, and in fact of the projection operator:

$$A^- := Q^t D^{-1} P^t, \text{where } D \text{ is a diagonal matrix} \quad \textbf{(1)}$$

with nonzero singular values

$$\lambda_{lk} = 1/\tilde{D}_{l,kk},\ l = 1, \dots, L, k = 1, \dots, r_l$$

of multiplicity given by $N(l)$.

Since the inverse A^- is independent of the measured intensities, it is sufficient to compute it once and use it for all experiments with measured pole figures of the same set H of crystal forms.

Given the variance–covariance matrix Σ_F of the measurement error of the experimental coefficients $\hat{F}^{\nu}_{lh}$, the variance–covariance matrix σ_C of the measurement error of the $C^{\mu\nu}_l$ coefficients may be computed according to

$$\Sigma_C = A^- \Sigma_F A^{-t} \quad \textbf{(2)}$$

In the next sections it will be shown how to use this relation, but first a modified decomposition will be considered which simplifies relation (2) and yields results with smaller estimation error.

3 Taking different measurement errors into account

Some pole figures can be measured with better accuracy than others. Therefore, they have different standard errors of the experimental coefficients of their series expansion. The normalisation condition

$$\oint \left(\alpha^{-1}\,\dot{k}_l^{\nu}(y)\right)^2 dy = \alpha^{-2}$$

can be used to deal with objects of different statistical measurement errors. If the random variables F_{lh}^{ν} are replaced by $\tilde{F}_{lh}^{\mu} = \alpha_{lh}^{\nu} F_{lh}^{\nu}$ such that $\mathrm{Var}\left[\tilde{F}_{lh}^{\nu}\right] = {\alpha_{lh}^{\nu}}^2 \mathrm{Var}\left[F_{lh}^{\nu}\right] = 1,\ \forall h \in H$, using constants $\alpha_{lh}^{\nu} := (\mathrm{Var}[F_l^{\nu,h}])^{-0.5}$ to represent how well a harmonic of order l can be determined using the h pole figure, depending on the the reflex and on the sampling grid. The variances can be found by repeated measurements on appropriate test samples.

Assuming that the variance only depends on l and μ these two parameters this renormalisation does not change the structure of the singular value decomposition. But it will change the svd itself. If the variance will also depend on ν, not only on l and h the block structure of the projection matrix A will be preserved, but the $A_l^{\nu}{}'$ will then depend on ν. This will only cost more computer time, but the theory is unaffected by this:

$$(A_l^{nu\prime})_{b\mu} = (1/\alpha_{lh_b}^{\nu})(A_l^{nu})_{b\mu}$$

Applying the singular value decomposition of the operator A' projecting the $C_l^{\mu\nu}$ to these modified $\tilde{F}$ to compute its Moore–Penrose inverse using formula (1) yields $\hat{C}_l^{\mu\nu}$ with minimal measurement error variance. This follows from the theory of optimum weighted least squares regression.

4 Design of experiments

Let H be a set of experimentally accessible pole figures with independent standard measurement errors σ_{hlm} for the experimental coefficients F_{lh}^{ν} of the h pole figure. Let PDQ denote the associated singular value decomposition.

An experimental design is a subset of these crystal forms. The general idea is to look for the best subset out of some sensible subsets and measure only the pole figures belonging to this subset.

4.1 Optimality criteria

Different optimality criteria are often used in experimental design (Pukelsheim 1993):

- Determinant optimality (D-optimality): Minimize the determinant of the variance matrix.
- Average optimality (A-optimality): Minimize the mean estimation variance.
- Eigenvalue optimality (E-optimality): Minimize the largest eigenvalue of the variance matrix.
- Trace optimality (T-optimality): Maximize the trace of the information matrix (which is the inverse of the estimation variance matrix).

These entities can be calculated form the singular value decomposition by the following formulae if the stochastic errors of $\alpha_l^{h_b} F_{lh_b}^{\mu}$ are independent and every single variance is rescaled to unity

$$\mathrm{D} = \left(\prod_{l=1}^{L} (\det \tilde{D}_l)^{N(l)} \right)^{-2} \qquad \mathrm{A} = \sum_{l=1}^{L} N(l) \mathrm{trace} \tilde{D}_l^{-2}$$

$$\mathrm{E} = (\min_{l,k} \tilde{D}_{l,kk})^{-2} \qquad \mathrm{T} = \sum_{l=1}^{L} N(l) \mathrm{trace} \tilde{D}_l^{2}$$

All these formulae can be evaluated with a computer very fast. Therefore, these criteria may be evaluated for all feasible sets of pole figures which in turn may be ranked according to the amount of information they provide. The average criterion is equivalent to best approximation of the ODF in mean squared error in the space of functions $L^2(SO_3)$.

4.2 Optimality in case of dependent measurement errors

Unfortunately, the assumption of independent measurement errors may not be realistic, and they have to be treated as dependent. Therefore, the assumption is relaxed that the measurement errors of F_{lh}^{ν} are uncorrelated for different h only. Then for the average criterion the theory remains exactly true because only the diagonal elements of the matrix $(Q^t D^{-1} P^t)\Sigma_F(PD^{-1}Q)$ are relevant. These depend only on the diagonal blocks of Σ_F because of the special block structure of $PD^{-1}Q$. These diagonal blocks of Σ_F are diagonal themselves. Therefore the the non diagonal elements of Σ_F do not influent the results. For the other criteria this is only true approximately. Thus the A-optimality criterion seems favourable as it is also equivalent to optimum approximation of the ODF as already mentioned above.

This kind of dependence is e.g. also introduced in case the normalisation must be calculated from the measurements as usual.

5 Extracting information of high order

The singular value decomposition also answers a question which seems to have slipped the attention: What do pole figures tell about the harmonic terms $C_l^{\mu\nu}$of degree $l > L = max_L \{L : N(L) \leq |H|\}$?

The conventional harmonic method reconstructs an ODF by first constraining the possible results to a subspace of functions represented by a finite harmonic series expansion of degree L, and then exactly calculates the projection of the true ODF to this subspace.

The singular value decomposition provides an orthogonal subspace of harmonic functions of any order l, for which the orthogonal projection of the ODF can be calculated. It is the subspace $\mathrm{im} Q_l^t$, where Q_l only consists of a minimum number of rows (this means the frame size of D_l is chosen to be minimum).

For these reconstructions it can be shown that

Proposition 1: If the pole figures $P_h(y)$ are compatible, then for the system

$$\hat{ODF}(g) = \sum_{l=1}^{\infty} \sum_{\nu=1}^{N(l)} \sum_{k=1}^{\mathrm{rank}\tilde{D}_l} \left(\tilde{D}_{l,kk}^{-1} \sum_{b=1}^{|H|} P_{l,bk} F_{lh_b}^{\nu} \right) \sum_{\mu=1}^{M(l)} Q_{l,k\mu} \ddot{T}_l^{\mu\nu}(g)$$

it holds

$$P_h[\hat{ODF}] = P_h, \ \forall h \in H$$

which means that the pole figures are reproduced exactly. If the pole figures are not compatible, then this solution minimizes the mean squared error under all functions

$$\sum_{b \in B} \int_{S^2} \left(P_{h_b}[\hat{ODF}](y) - \tilde{P}_{h_b}(y) \right)^2 dS(y) \longrightarrow \min$$

In both cases it is the function with minimum L^2 norm that satisfies the criterion. Since it is a projection, the coefficients of all basis vectors in the image space of the reconstruction are identifiable. □

Thus, pole figures can be reproduced exactly up to any order of their harmonic series expansion.

6 References

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