EBSD data analysis with \textit{MathLAB toolbox} MTEX

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Challenges of texture analysis
Unique approach to texture analysis with integral or individual orientation measurements
A practical application
Conclusions
Challenges of texture analysis
Objective of texture analysis

Determination of an orientation probability density function,

1. which globally or locally explains experimental “integral” pole intensity data well, or

2. which is derived from individual orientation measurements, and its characteristics like

   - harmonic (Fourier) coefficients,
   - texture index,
   - entropy,
   - volume fractions around peaks or fibres
   - ...
   - ...
Orientation distribution within a single hematite crystal

Neutron diffraction pole figure data corresponding to a grid comprising 14,616 positions with a mean distance of 1.5 degree

Pole point plots corresponding to a total of 69,541 individual orientation measurements

Data courtesy Heinrich Siemes, RWTH Aachen
Comparison by numbers

<table>
<thead>
<tr>
<th>Neutron</th>
<th>((\alpha, \beta, \gamma))</th>
<th>(\int_{b(g_m;10)} f(g)dg)</th>
<th>(f(\alpha, \beta, \gamma))</th>
</tr>
</thead>
<tbody>
<tr>
<td>(g_M)  (black)</td>
<td>(155, 3, 53)</td>
<td>0.45</td>
<td>14,709</td>
</tr>
<tr>
<td>(g_{m1}) (blue)</td>
<td>(90, 65, 59)</td>
<td>0.09</td>
<td>675</td>
</tr>
<tr>
<td>(g_{m2}) (red)</td>
<td>(30, 115, 1)</td>
<td>0.18</td>
<td>750</td>
</tr>
<tr>
<td>(g_{m3}) (green)</td>
<td>(150, 115, 1)</td>
<td>0.09</td>
<td>545</td>
</tr>
<tr>
<td>sum</td>
<td>0.36</td>
<td></td>
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</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>EBSD</th>
<th>((\alpha, \beta, \gamma))</th>
<th>(\int_{b(g_m;10)} f(g)dg)</th>
<th>(f(\alpha, \beta, \gamma))</th>
</tr>
</thead>
<tbody>
<tr>
<td>(g_M)  (black)</td>
<td>(100, 178, 11)</td>
<td>0.45</td>
<td>12,251</td>
</tr>
<tr>
<td>(g_{m1}) (blue)</td>
<td>(90, 65, 59)</td>
<td>0.05</td>
<td>699</td>
</tr>
<tr>
<td>(g_{m2}) (red)</td>
<td>(30, 115, 1)</td>
<td>0.04</td>
<td>450</td>
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<tr>
<td>(g_{m3}) (green)</td>
<td>(150, 115, 1)</td>
<td>0.33</td>
<td>2,611</td>
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<tr>
<td>sum</td>
<td>0.42</td>
<td></td>
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</tbody>
</table>
Unique approach to texture analysis
with integral or individual orientation measurements
Examples of radially symmetric functions

**de la Vallée Poussin kernel**

\[
\psi_\kappa(\omega(\mathbf{g} \mathbf{g}_0^{-1})) = \frac{B\left(\frac{3}{2}, \frac{1}{2}\right)}{B\left(\frac{3}{2}, \kappa + \frac{1}{2}\right)} \cos^{2\kappa} \frac{\omega(\mathbf{g} \mathbf{g}_0^{-1})}{2},
\]

\[
\mathcal{R}\psi_\kappa(\mathbf{h}, \mathbf{r}) = (1 + \kappa) \cos^{2\kappa} \frac{\arccos(\mathbf{g}_0 \cdot \mathbf{r})}{2}
\]
Examples of radially symmetric functions

de la Vallée Poussin kernel

\[ \psi_\kappa(\omega(\mathbf{g}_0^{-1})) = \frac{B\left(\frac{3}{2}, \frac{1}{2}\right)}{B\left(\frac{3}{2}, \kappa + \frac{1}{2}\right)} \cos^2 \kappa \frac{\omega(\mathbf{g}_0^{-1})}{2}, \]

\[ \mathcal{R}\psi_\kappa(\mathbf{h}, \mathbf{r}) = (1 + \kappa) \cos^2 \kappa \frac{\arccos(\mathbf{g}_0 \cdot \mathbf{r})}{2} \]

von Mises–Fisher kernel

\[ \psi_\kappa(\omega(\mathbf{g})) = \frac{1}{\mathcal{I}_0(\kappa) - \mathcal{I}_1(\kappa)} e^{2\kappa \cos^2 \frac{\omega(\mathbf{g})}{2} - \kappa}, \]

\[ \mathcal{R}\psi_\kappa(\mathbf{h}, \mathbf{r}) = \frac{\mathcal{I}_0(\kappa \cos 2\angle(\mathbf{h}, \mathbf{r}))}{\mathcal{I}_0(\kappa) - \mathcal{I}_1(\kappa)} e^{\kappa \frac{\mathbf{h} \cdot \mathbf{r} - 1}{2}} \]
The odf is modelled as a positive linear combination

\[ f(\mathbf{g}) = \sum_{m=1}^{M} c_m \psi_\kappa(\omega(\mathbf{g}^{-1} \mathbf{g}_m)) \]

of non-negative radially symmetric kernels \( \psi_\kappa(\omega(\mathbf{g}^{-1} \mathbf{g}_m)) \) centered at grid nodes \( \mathbf{g}_m \) resulting in

\[ \mathcal{X} f(\mathbf{h}, \mathbf{r}) = \sum_{m=1}^{M} c_m \left( \mathcal{R} \psi_\kappa(\mathbf{g}_m \mathbf{h}, \mathbf{r}) + \mathcal{R} \psi_\kappa(-\mathbf{g}_m \mathbf{h}, \mathbf{r}) \right) \]

modelling the diffraction pole intensities, where \( \mathcal{R} \) denotes the Radon transform.
Then the non-linear problem to be solved reads

\[
\hat{c} = \arg\min \sum_{i=1}^{N} \sum_{j_i=1}^{N_i} \left( \sum_{m=1}^{M} a(h_i) c_m \chi_\psi_{\kappa}(g_m h_i, r_{j_i}) + l_{ij} - l_{ij}^b \right)^2 \\
+ \lambda \left\| \sum_{m=1}^{M} c_m \psi_{\kappa}(\circ g_m^{-1}) \right\|^2_{\mathcal{H}(SO(3))},
\]

where \(\lambda\) is the parameter of regularization weighting the penalty term.
Kernel density estimation of individual orientation measurements

Kernel density estimator and its Radon transform

The odf is modelled as a positive linear combination

\[ \hat{f}_κ(\mathbf{g}; \mathbf{g}_1, \ldots, \mathbf{g}_n) = \frac{1}{n} \sum_{i=1}^{n} \psi_κ(\omega(\mathbf{g}_i^{-1})) \]

of non–negative radially symmetric kernels \( \psi_κ(\omega(\mathbf{g}_i^{-1})) \) centered at observed individual orientations \( \mathbf{g}_i \) resulting in corresponding pdfs

\[ X[\hat{f}_κ(\mathbf{circ}; \mathbf{g}_1, \ldots, \mathbf{g}_n)](\mathbf{h}, \mathbf{r}) = \frac{1}{n} \sum_{i=1}^{n} \left( R\psi_κ(\mathbf{g}_i \mathbf{h} \cdot \mathbf{r}) + R\psi_κ(-\mathbf{g}_i \mathbf{h} \cdot \mathbf{r}) \right). \]
Unbiased estimator \( \hat{C}_{\ell}^{kk'} \)

\[
\hat{C}_{\ell}^{kk'}(g_1, \ldots, g_n) = \frac{1}{n} \sum_{i=1}^{n} T_{\ell}^{kk'}(g_i), \quad \ell = 1, \ldots, L
\]
Estimation of $C_{\ell}^{kk'}$

**Dirichlet kernel**

\[
\psi_L(\omega(g^{-1}g_0)) = \sum_{\ell=0}^{L} \sum_{k,k'=-\ell}^{\ell} (2\ell + 1) T_{L}^{kk'}(g) T_{L}^{kk'}(g_0)
\]

\[
= \sum_{\ell=0}^{L} (2\ell + 1) \frac{\sin((2\ell + 1)\omega(g^{-1}g_0)/2)}{\sin(\omega(g^{-1}g_0)/2)}
\]

\[
= \sum_{\ell=0}^{L} (2\ell + 1) U_{2\ell} \left( \cos \frac{\omega(g^{-1}g_0)}{2} \right)
\]

Spatial domain \hspace{1cm} Frequency domain
Harmonic coefficients of Dirichlet kernel density estimator

With the Dirichlet kernel we get

$$\hat{f}_{DL}(g_1, g_2, \ldots, g_n) = \frac{1}{n} \sum_{i=1}^{n} \sum_{\ell=0}^{L} (2\ell + 1) U_{2\ell} \left( \cos \frac{\omega(g_{i-1})}{2} \right)$$

with

$$C_{\ell kk'}(\hat{f}_{DL}) = \begin{cases} \hat{C}_{\ell kk'}(g_1, \ldots, g_n), & \text{if } \ell \leq L \\ 0, & \text{otherwise} \end{cases}$$

which is the

Unbiased estimator $\hat{C}_{\ell kk'}$

$$\hat{C}_{\ell kk'}(g_1, \ldots, g_n) = \frac{1}{n} \sum_{i=1}^{n} T_{\ell kk'}(g_i), \ \ell = 1, \ldots, L.$$
Simulated EBSD data

900 simulated spatially indexed individual orientations according to Bingham quaternion distribution

Pole point plots for crystal forms \{100\}, \{110\}, \{111\}, and \{113\}
Grain 40 with 3068 spatially indexed individual orientations

Pole point plots of grain 40 for crystal forms \{100\}, \{110\}, \{111\}, and \{113\}
Grain 147 with 4324 spatially indexed individual orientations

Pole point plots of grain 147 for crystal forms \{100\}, \{110\}, \{111\}, and \{113\}
Single crystal EBSD data (courtesy W. Pantleon, Risø)

Grain 109 with 2253 spatially indexed individual orientations

Pole point plots of grain 109 for crystal forms \{100\}, \{110\}, \{111\}, and \{113\}
Single crystal EBSD data (courtesy W. Pantleon, Risø)
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The key statistics of orientation data is the “orientation tensor”

\[ T = \frac{1}{n} \sum_{\ell=1}^{n} q_\ell q_\ell^T \]

and its spectral decomposition, where the set of eigenvectors \( a_1, \ldots, a_4 \) provides a measure of location and the set of corresponding eigenvalues \( \lambda_1, \ldots, \lambda_4 \) provides a corresponding measure of dispersion. Since the orientation tensor \( T \) and the tensor of inertia \( I \) are related by

\[ I = E - T \]

the eigenvectors of \( T \) provide the principal axes of inertia and the eigenvalues of \( T \) provide the principal moments of inertia.

In general, a single eigenvector and its eigenvalue do not provide a reasonable characterization of the data. Therefore, often the ratios of the eigenvalues are being analyzed and interpreted.
The spectral analyses of the orientation matrices $T$ are numerically summarized in the following table.

<table>
<thead>
<tr>
<th></th>
<th>simIOM</th>
<th>grain 40</th>
<th>grain 147</th>
<th>grain 109</th>
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</thead>
<tbody>
<tr>
<td>sample size</td>
<td>900</td>
<td>3068</td>
<td>4324</td>
<td>2253</td>
</tr>
<tr>
<td>texture index</td>
<td>61.2971</td>
<td>337.7395</td>
<td>308.9108</td>
<td>178.4238</td>
</tr>
<tr>
<td>entropy</td>
<td>-3.6491</td>
<td>-5.3425</td>
<td>-5.1136</td>
<td>-4.7782</td>
</tr>
<tr>
<td>$\lambda_1$</td>
<td>0.9954</td>
<td>0.9965</td>
<td>0.9983</td>
<td>0.9956</td>
</tr>
<tr>
<td>$\lambda_2$</td>
<td>0.0016</td>
<td>0.0029</td>
<td>0.0009</td>
<td>0.0022</td>
</tr>
<tr>
<td>$\lambda_3$</td>
<td>0.0015</td>
<td>0.0003</td>
<td>0.0005</td>
<td>0.0019</td>
</tr>
<tr>
<td>$\lambda_4$</td>
<td>0.0014</td>
<td>0.0003</td>
<td>0.0004</td>
<td>0.0003</td>
</tr>
<tr>
<td>$\lambda_2/\lambda_3$</td>
<td>1.1043</td>
<td>9.7599</td>
<td>1.7465</td>
<td>1.1364</td>
</tr>
<tr>
<td>$\lambda_3/\lambda_4$</td>
<td>1.0517</td>
<td>1.1345</td>
<td>1.4199</td>
<td>6.1100</td>
</tr>
<tr>
<td>interpretation by inspection</td>
<td>spherical</td>
<td>prolate</td>
<td>spherical</td>
<td>oblate</td>
</tr>
</tbody>
</table>
Our novel approach matches the challenges and requirements of modern texture analysis to a large extent.
Conclusions: An Appreciation of Modern Numerics

Our novel approach matches the challenges and requirements of modern texture analysis to a large extent.

The method applies to
- any crystal symmetry, superpositions of crystal directions,
- arbitrarily scattered specimen directions, e.g., area detector data,
- high resolution or locally refined pole figure data,
- sharp textures,
- $C$–coefficients, volume portions, texture index, entropy, etc.
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Unique approach to analyse integral and individual orientation measurements.
MTEX Software

For the free and open-source Matlab toolbox MTEX see

http://code.google.com/p/mtex/

Accompanying publication

Hielscher, R., Schaeben, H., 2008,
A novel pole figure inversion method:
Specification of the MTEX algorithm:
Journal of Applied Crystallography 41, 1024-1037
Thank you for your attention.

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