Estimating Particle Shape and Orientation Using Volume Tensors

Johanna F. Ziegel

University of Bern, Switzerland

joint work with
Eva B. Vedel Jensen, Markus Kiderlen, Astrid Kousholt, Jens R. Nyengaard and Ali H. Rafati

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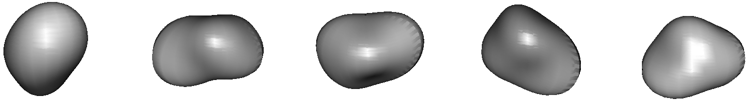
Some particles



Introduction

- Goal: Define a framework to analyze the size, shape and orientation of particle populations.
- Impose minimal shape assumptions.
- Approach should be sophisticated enough to distinguish important characteristics, but simple enough to allow comparisons between populations.
- Minkowski tensors have been used to accomplish this in material science.
- We use local stereology to estimate volume tensors of particle populations.

Volume tensors

Let $K \subset \mathbb{R}^3$ be a compact set.

Volume tensor of rank $r \in \mathbb{N}_0$

$$\Phi_r(K) = \frac{1}{r!} \int_K x^r \, \mathrm{d}x$$

x^r: Symmetric tensor product of rank r.

$x^0 = 1$, $x^1 = x$, $x^2 = (x_i x_j)_{ij} = xx^\top$.

Volume tensors are a special case of Minkowski tensors ($\Phi_r = \Phi_{3,r,0}$) which in turn are natural generalization of intrinsic volumes.

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Important special cases

$r = 0$
$\Phi_0(K) = V(K), \quad$ the volume of K,

$r = 1$
$\Phi_1(K)/\Phi_0(K) = c(K), \quad$ the centre of gravity.

$r = 2$: Shape and orientation information

Let

$$\bar{K} = (K - c(K))/V(K)^{1/3},$$

then

$$\Phi_2(\bar{K}) = \frac{1}{\Phi_0(K)^{5/3}}\left(\Phi_2(K) - \frac{\Phi_1(K)^2}{2\Phi_0(K)}\right).$$

If K is an ellipsoid (or a cuboid or ....), then $\Phi_2(\bar{K})$ determines it uniquely (up to scale and location).

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Volume tensors of particle populations

The particle process X

- Stationary marked point process

$$\{[x(K); K - x(K)] \mid K \in X\}.$$

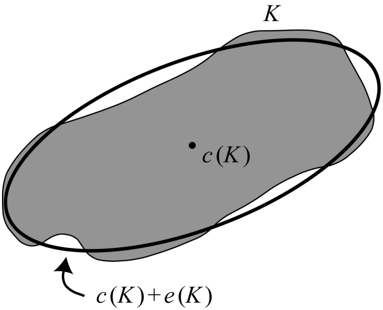
- $x(K)$ is the reference point of the particle $K \in X$.
- Particle (mark) distribution is denoted by $\mathbb{Q}$.
- Typical particle: $\mathbf{K}_0 \sim \mathbb{Q}$.
- Illustrate shape of the particle population by an ellipsoidal approximation.

Illustration of an ellipsoidal approximation

Miles ellipsoid

$e(X)$: ellipsoid with $V(e(X)) = \mathbb{E}V(\mathbf{K}_0)$,

$$\Phi_2(e(X)) = \mathbb{E}\Phi_2(\mathbf{K}_0) - (\mathbb{E}\Phi_1(\mathbf{K}_0))^2/(2\mathbb{E}\Phi(\mathbf{K}_0))$$



Motivation of the Miles ellipsoid

Particle cover density

$$f_{\mathbf{K}_0}(x) = \frac{\mathbb{P}(x \in \mathbf{K}_0)}{\mathbb{E}V(\mathbf{K}_0)}, \quad x \in \mathbb{R}^3.$$

The Miles ellipsoid $e(X)$ is the uniquely determined centered ellipsoid such that a particle process with a deterministic ellipsoidal mark has the same expected volume and covariance of the cover density as X.

Moments of the cover density

$$\frac{\mathbb{E}\Phi_r(\mathbf{K}_0)}{\mathbb{E}V(\mathbf{K}_0)} = \frac{1}{r!}\int_{\mathbb{R}^3} x^r f_{\mathbf{K}_0}(x)\,\mathrm{d}x$$

Estimating expected volume tensors

Aim: Estimate

$$\mathbb{E}\Phi_r(\mathbf{K}_0)$$

based on a sample

$$\{K \in X \mid x(K) \in W\}.$$

The estimator

$$\frac{\mathbb{E}\sum_{K \in X, x(K) \in W} \Phi_r(K - x(K))}{N(W)}$$

is ratio-unbiased for $\mathbb{E}\Phi_r(\mathbf{K}_0)$ and it is consistent under suitable assumptions in an expanding window regime.

- If we have a 3D image of each particle (with sufficient resolution), we can calculate the volume tensors (up to very small errors).
- If complete access to the sampled particles is not possible: Stereological estimators of volume tensors.

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Estimating expected volume tensors

Suppose that $\widehat{\Phi}(K)$ is a design-unbiased estimator of $\Phi(K)$. Then,

$$\widehat{\Phi}_r^{N(W)} := \frac{\mathbb{E} \sum_{K \in X, x(K) \in W} \widehat{\Phi}_r(K - x(K))}{N(W)}$$

is ratio-unbiased for $\mathbb{E}\Phi_r(\mathbf{K}_0)$ and it is consistent under suitable assumptions in an expanding window regime.

Isotropy assumptions

No isotropy assumption

- Slice estimators $\widehat{\Phi}$

Restricted isotropy

$\mathbb{Q}$ is invariant under rotations around a fixed axis L_1

- Slice estimators $\widehat{\Phi}$
- Section estimators $\widetilde{\Phi}$

Rotation invariance

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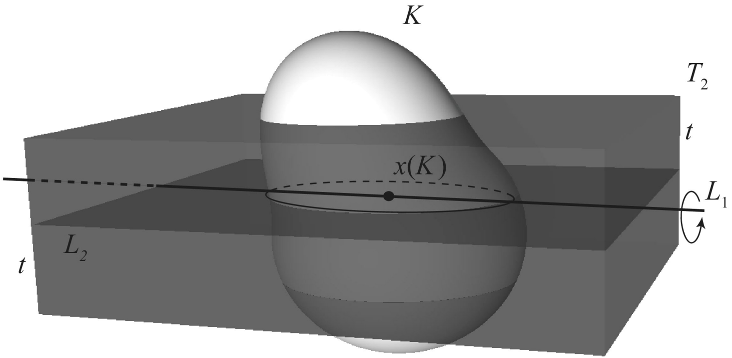
Local stereology

- Design-based approaches.
- Sampling designs based on sections/slices containing a fixed point or line.
- Many biological structures are naturally centered around a point of reference.
  Example: Nucleus of a cell.
- Convenient in microscopy because it avoids problems with overprojection.

Slice estimators: The optical rotator design



Slice estimators for volume tensors

- L_2 is a randomly rotated plane containing the vertical axis L_1.
- $T_2 = L_2 + B(O, t)$ is a vertical random slice.
- Let $x \in \mathbb{R}^3$. Then

$$\mathbb{P}(x \in T_2) = \frac{2}{\pi} \arcsin\left(\frac{t}{d(x, L_1)}\right).$$

- Design-unbiased estimator of $\Phi_r(K)$:

$$\hat{\Phi}_r(K) = \frac{1}{r!} \int_{K \cap T_2} x^r \, \mathbb{P}(x \in T_2)^{-1} \, \mathrm{d}x.$$

- Usually, the slice T_2 is subsampled further.
- Final sample of the particle consists of approx. 12 points on the boundary.

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Section estimators for volume tensors

- L_2 is a randomly rotated plane containing the vertical axis L_1.
- Restricted isotropy implies

$$\mathbb{E}\Phi_r(\mathbf{K}_0) = \mathbb{E}\int_{\mathcal{M}} \Phi_r(R\mathbf{K}_0)\,\mathrm{d}\nu(R) = \mathbb{E}\overline{\Phi}_r(\mathbf{K}_0)$$

  where $\mathcal{M}$ is the set of all rotations around L_1, and ν is the uniform probability measure on $\mathcal{M}$.
- Design-unbiased estimator $\widetilde{\Phi}_r(K)$ of $\overline{\Phi}_r(K)$ based on observations in L_2 is possible.
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Comments on the construction of the estimators

- Slice estimators
  - Rotational integral formula for volume tensors is used.
  - Purely design-based estimator for $\Phi_r(K)$.
  - Under restricted isotropy, estimators may not "reflect" this property.
- Section estimators
  - Restricted isotropy assumption is used at the population level.
  - Rotational integral formula for auxiliary quantity $\overline{\Phi}_r$ which is not a volume tensor.
  - Estimators "reflect" restricted isotropy (if it holds or not).
- Section estimators are also possible without the restricted isotropy assumption
- Slice estimators should also be possible under restricted isotropy, smaller variance?

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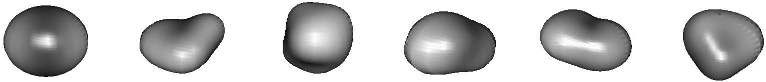
Simulation comparison of slice and section estimators

Lévy particle model

Random deformations and translation of a prolate ellipsoid



- Model fulfils the restricted isotropy assumption
- 500'000 simulated particles
- Volume tensors estimated from n=10,20,50,100 particles in 500'000/n samples
- Slice estimator: approx. 12 points per particle
- Section estimator: approx. 4 points per particle

Simulation results: mean (CV)

Slice estimators

n	10	20	50	100
v	606.86 (0.151)	606.86 (0.095)	606.86 (0.067)	606.86 (0.047)
z	-0.073 (6.162)	-0.074 (4.021)	-0.074 (2.867)	-0.074 (2.034)
a	5.821 (0.082)	5.841 (0.054)	5.848 (0.039)	5.852 (0.028)
b	4.981 (0.068)	4.977 (0.044)	4.976 (0.031)	4.975 (0.022)

Section estimators

n	10	20	50	100
v	606.33 (0.152)	606.33 (0.096)	606.33 (0.068)	606.33 (0.048)
z	-0.069 (7.057)	-0.069 (4.56)	-0.069 (3.258)	-0.069 (2.337)
a	5.797 (0.098)	5.832 (0.064)	5.844 (0.047)	5.85 (0.033)
b	4.992 (0.07)	4.981 (0.044)	4.976 (0.032)	4.974 (0.022)

True values

$v = 606.55,\ z = -0.073,\ a = 5.857,\ b = 4.972$

Side note on the slice estimator for Φ_2

Restricted isotropy

If $\mathbb{Q}$ is invariant under rotations around an axis L_1, then

- $$\mathbb{E}\Phi_1(\mathbf{K}_0) \in L_1$$

  Project $\widehat{\Phi}_1^n$ onto L_1.

- $$\mathbb{E}\Phi_2(\mathbf{K}_0) = B\Lambda B^\top, \quad \Lambda = \mathrm{diag}(\eta_1, \eta_2, \eta_2).$$

  Estimate $\mathbb{E}\Phi_2(\mathbf{K}_0)$ as the minimizer of the Frobenius norm of

  $$\widehat{\Phi}_2^n - B\tilde{\Lambda}B^\top, \quad \tilde{\Lambda} = \mathrm{diag}(\beta_1, \beta_2, \beta_2).$$

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Statistical tests for isotropy

Based on the slice estimator

Under rotation invariance of $\mathbb{Q}$ it holds that

$$\mathbb{E}\Phi_2(\mathbf{K}_0) = (\phi_{ij})_{i,j=1,2,3} = \sigma^2 I_3$$

for some $\sigma > 0$.

Other possibilities (mostly unexplored)

- Compare slice estimator to restricted isotropy slice estimator
- Compare (unrestricted) section estimator to restricted isotropy section estimator
- The same is possible for testing isotropy under the assumption of restricted isotropy
- Tests for isotropy based on the characteristic function of the cover density of the particle process

A non-parametric test for isotropy

We want to test the hypothesis

$$H_0: \quad \phi_{ii} = \sigma^2 > 0, \quad \phi_{ij} = 0,\ i \neq j.$$

Approximate the distribution of

$$(\hat{\phi}_{11}, \hat{\phi}_{22}, \hat{\phi}_{33}, \hat{\phi}_{12}, \hat{\phi}_{13}, \hat{\phi}_{23})$$

by a six-dimensional normal distribution (delta method for n large enough) and derive a χ^2-statistic.

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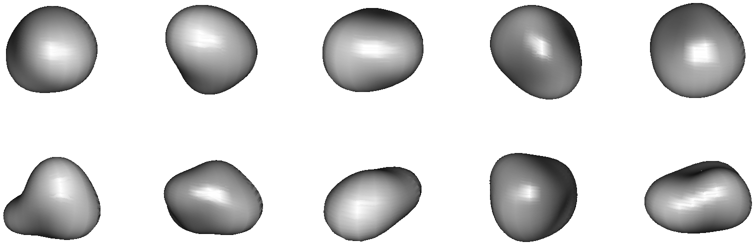
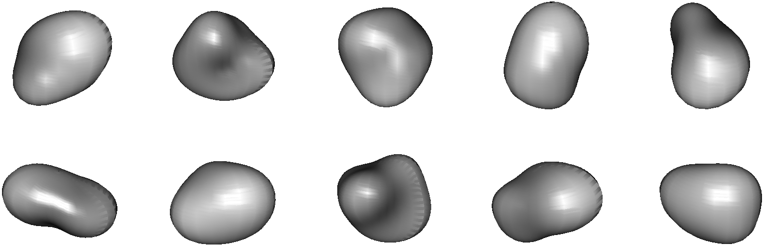
Empirical level of the test



Empirical level of the test

n	First model 0.01	First model 0.05	First model 0.1	Second model 0.01	Second model 0.05	Second model 0.1	n_{simu}
25	0.003	0.042	0.100	0.001	0.026	0.082	4200
50	0.012	0.056	0.112	0.008	0.048	0.109	2100
100	0.012	0.070	0.127	0.012	0.056	0.111	1050
150	0.006	0.051	0.106	0.011	0.049	0.104	700
200	0.013	0.067	0.124	0.006	0.044	0.101	525

Empirical power of the test



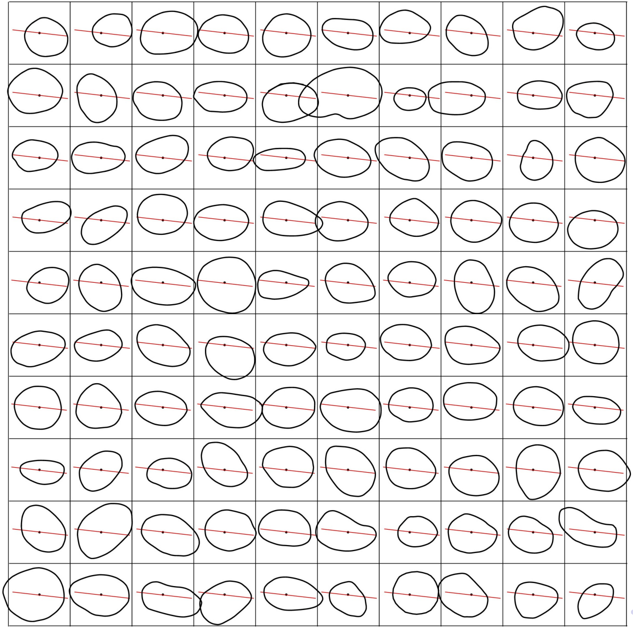
Empirical power of the test

n	First model				Second model			
	0.01	0.05	0.1	n_{simu}	0.01	0.05	0.1	n_{simu}
25	0.003	0.048	0.139	3840	0.018	0.252	0.500	2240
50	0.026	0.146	0.262	1920	0.355	0.733	0.871	1120
100	0.096	0.293	0.473	960	0.893	0.980	0.998	560
150	0.219	0.489	0.628	640	0.995	0.997	1	373
200	0.365	0.654	0.796	480	1	1	1	280

Data example of the slice estimators

- Data collected from a histological slab of $140\mu m$ through the human brain cortex.
- Slab has been taken perpendicular to the brain surface with a random rotation around the normal to the brain surface.
- Interest: Nuclei of pyramidal neurons
- Question: Are the nuclei elongated perpendicular to the brain surface like the pyramidal neurons?
- Data: $n = 100$ neuron nuclei, nucleolus as reference point.

Results



Results – cont'd

- Assumption: Restricted isotropy, because we only have one rotated slice.
- Miles ellipsoid under restricted isotropy:
  Prolate ellipsoid with rotation axis perpendicular to the brain surface and semi axis 5.866 in this direction; other half-axis lengths are 4.968.
- Miles ellipsoid under isotropy: Sphere with radius 5.251.
- Null hypothesis of isotropy is rejected at level $\alpha = 0.05$.

Summary

- Volume tensors provide descriptors of size, location, shape and orientation of particles.
- In biological applications it is often not possible to observe the entire boundary of particles of interest.
- We use local stereological estimators for volume tensors in a combination of a model- and design-based approach.
- Volume tensors allow for easy interpretation of anisotropy through the Miles ellipsoid.

Outlook

- Two sample test for differences in shape and orientation.
- Minkowski tensors are natural extensions of intrinsic volumes.
- Is there interesting shape information that can be gathered by estimating other Minkowski tensors than volume tensors? (Local stereological estimators are available.)
- It is possible to estimate the characteristic function of the cover density. This can also be used for inference and testing. (Work in progress.)

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References

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The characteristic function of the cover density

Characteristic function of the cover density

$$\varphi_{K_0}(s) = \int_{\mathbb{R}^3} e^{i\langle s,x\rangle} f_{K_0}(x)\,\mathrm{d}x, \quad s \in \mathbb{R}^3.$$

We define the empirical characteristic function of the typical particle K_0

$$\widetilde{\varphi}_{K_0}(s) = \int_{K_0} e^{i\langle s,x\rangle}\,\mathrm{d}x,$$

because

$$\frac{\mathbb{E}\widetilde{\varphi}_{K_0}(s)}{\mathbb{E}V(K_0)} = \varphi_{K_0}(s).$$

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The isotropic characteristic function

If $\mathbb{Q}$ is rotation invariant, then there is $\psi_{K_0} : [0, \infty) \to \mathbb{C}$ with

$$\varphi_{K_0}(s) = \psi_{K_0}(\|s\|).$$

We can always define the isotropic characteristic function of f_{K_0} by

$$\psi_{K_0}(r) = \frac{1}{4\pi r^2} \int_{\partial B_r(0)} \varphi_{K_0}(s)\, \mathrm{d}s = \int_{\mathbb{R}^3} \frac{\sin(r\|x\|)}{r\|x\|} f_{K_0}(x)\, \mathrm{d}x$$

and the empirical isotropic characteristic function by

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Testing for (restricted) isotropy

We are interested in testing one of the following hypothesis:

$$H_0: \quad \varphi_{K_0}(s) = \psi_{K_0}(\|s\|), \quad s \in \mathbb{R}^3,$$

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- Easy to derive a test also for restricted isotropy.
- Distribution under the null is more complicated as we have a condition for all $s \in \mathbb{R}^3$ or $r \in [0, \infty)$.
- Possibilities:
  - Test on a grid of points.
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