Stereological determination of particle size distributions for similar convex bodies

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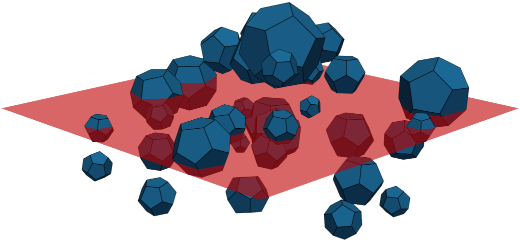
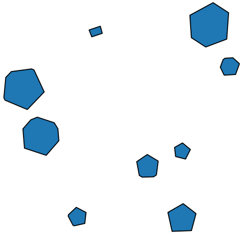
Introduction

- Fix a particle, a convex body $K \subset \mathbb{R}^3$. Instances of K of varying size are randomly positioned and oriented in $\mathbb{R}^3$. This isotropic system of particles is intersected with a plane.
- We wish to determine the particle size distribution given the distribution of observed section areas.
- Generalization of the classical Wicksell's corpuscle problem (Wicksell 1925).



(a) 3D objects



(b) 2D observations

Introduction

- The particles have random sizes, a particle of size λ is equal to λK up to rotation and translation. Let H denote the CDF of the size distribution.
- We assume:
$$\mathbb{E}(\Lambda) = \int_0^\infty \lambda \mathrm{d}H(\lambda) < \infty.$$
- The integral equation relating H to the CDF of observed section areas F_A have already been derived under various assumptions. See for example (Santaló and Kac 2004), (Ohser and Mücklich 2000), (Beneš and Rataj 2004).

Isotropic Uniformly Random (IUR) sections

- Let $[K]$ denote the set of all planes which intersect K. An IUR plane hitting K is a plane T chosen uniformly at random from $[K]$. The probability measure is the unique motion invariant measure on the space of all planes, restricted to $[K]$.
- Introduction of IUR planes: Davy and Miles 1977.
- Let T be an IUR plane hitting K, define the CDF:

$$G_K(z) := \mathbb{P}\left(\text{vol}_2(K \cap T) \leq z\right).$$

  We call G_K the section volume CDF.
- If a particle with size λ is hit by the plane, its random section area is equal in distribution to the area of an IUR section of λK.

Deriving the stereological integral equation

Lemma (Davy and Miles 1977)

Suppose that $Q \subset \mathbb{R}^3$ is a convex body and $K \subset Q$ is another convex body. Let T be an IUR plane hitting Q, then:

1. *Hitting probability:*

$$\mathbb{P}(T \cap K \neq \varnothing) = \frac{\bar{b}(K)}{\bar{b}(Q)}.$$

2. *Conditional property: Given that T hits K, i.e. $T \cap K \neq \varnothing$, T is an IUR plane hitting K.*

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- Suppose the particles are contained in $Q \in \mathcal{K}^3$. If $\lambda K \subset Q$ and T is an IUR plane hitting Q then:

$$\mathbb{P}(T \cap \lambda K \neq \varnothing) = \frac{\bar{b}(\lambda K)}{\bar{b}(Q)} = \lambda \frac{\bar{b}(K)}{\bar{b}(Q)}.$$

  The probability that a particle is sampled is proportional to its size.

The stereological integral equation

- Consider the following two facts:
  - H^b is the size distribution of particles hit by the section plane.

$$H^b(\lambda) = \frac{\int_0^\lambda x \mathrm{d}H(x)}{\int_0^\infty x \mathrm{d}H(x)}.$$

  - Given that a particle of size λ appears in the section plane, its area is distributed according to $G_{\lambda K}$.

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  - Given that a particle of size λ appears in the section plane, its area is distributed according to $G_{\lambda K}$.
- As a consequence:

$$F_A(a) = \int_0^\infty G_{\lambda K}(a) \mathrm{d}H^b(\lambda) = \frac{1}{\mathbb{E}(\Lambda)} \int_0^\infty G_{\lambda K}(a) \lambda \mathrm{d}H(\lambda).$$

- Note that $G_{\lambda K}(z) = G_K(z/\lambda^2)$. In other words, if $Z \sim G_K$, then $Z\lambda^2 \sim G_{\lambda K}$. Hence,

$$F_A(a) = \frac{1}{\mathbb{E}(\Lambda)} \int_0^\infty G_K\left(\frac{a}{\lambda^2}\right) \lambda \mathrm{d}H(\lambda).$$

Separating shape and size

Lemma (Jongbloed, Vittorietti, and TJ 2023b)

Consider a distribution function H with length-biased version H^b. Suppose $Z \sim G_K$ and $\Lambda_b \sim H^b$ with Z and Λ_b^2 independent. Set $A = Z\Lambda_b^2$. Then, $A \sim F_A$, and F_A, G_K and H^b are related via:

$$F_A(a) = \int_0^\infty G_K\left(\frac{a}{\lambda^2}\right) \mathrm{d}H^b(\lambda).$$

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Proof.

Let X, Y, Z be non-negative random variables, with CDF F_X, F_Y and F_Z respectively. If $X = YZ$ with Y and Z independent, then their distribution functions are related via:

$$F_X(x) = \int_0^\infty F_Y\left(\frac{x}{z}\right) \mathrm{d}F_Z(z).$$

Substituting $\mathbb{P}(\Lambda_b^2 \leq \lambda)$ for $H^b(\lambda) = \mathbb{P}(\Lambda_b \leq \lambda)$ yields the result. $\square$

The Mellin-Stieltjes transform

Definition (Mellin-Stieltjes transform)

Given a non-negative random variable X, with CDF F, the Mellin-Stieltjes transform of X is defined as:

$$\mathcal{M}_X(s) = \mathbb{E}(X^{s-1}) = \int_0^\infty x^{s-1} \mathrm{d}F(x),$$

for $s \in \mathbb{C}$, whenever the integral is absolutely convergent.

- Note, for non-negative independent random variables X and Y:

  $$\mathcal{M}_{XY}(s) = \mathbb{E}\left((XY)^{s-1}\right) = \mathcal{M}_X(s)\mathcal{M}_Y(s),$$

  whenever these expressions are finite.
- If $\int x^{c-1} \mathrm{d}F(x) < \infty$ for $c \in \mathbb{R}$, then $\mathcal{M}_X(c + it) < \infty$ for all $t \in \mathbb{R}$.

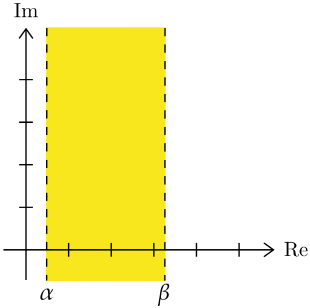
The strip of analyticity

- Define:

$$\mathrm{St}(\alpha, \beta) := \{s \in \mathbb{C} : \alpha < \Re(s) < \beta\}$$

$$\mathrm{St}[\alpha, \beta] := \{s \in \mathbb{C} : \alpha \leq \Re(s) \leq \beta\}.$$

- If we find $\alpha < \beta$ such that the Mellin transform of X converges absolutely on $\mathrm{St}[\alpha, \beta]$, then $\mathcal{M}_X$ is analytic on $\mathrm{St}(\alpha, \beta)$



Identifiability and inversion formula

Theorem (Jongbloed, Vittorietti, and TJ 2023b)

Suppose there is a CDF H such that F_A, G_K and H are related via:

$$F_A(a) = \frac{1}{\mathbb{E}(\Lambda)} \int_0^\infty G_K\left(\frac{a}{\lambda^2}\right) \mathrm{d}H(\lambda). \tag{1}$$

1. *If $\int_0^\infty z^{-\alpha} \mathrm{d}G_K(z) < \infty$ for some $\alpha > 0$, then there is only one distribution function H on $(0, \infty)$ satisfying (1).*
2. *Assume $\int_0^\infty x^{1+\delta} \mathrm{d}H(x) < \infty$, for some $\delta > 0$. Then, there is only one such distribution function H on $(0, \infty)$ satisfying (1).*

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- Let $Z \sim G_K$ and $A \sim F_A$. If one of the conditions is satisfied and H^b is continuous, there exists a $c \in \mathbb{R}$ such that:

$$H^b\left(\sqrt{x}\right) = \lim_{T \to \infty} \frac{1}{2\pi i} \int_{c-iT}^{c+iT} -\frac{\mathcal{M}_A(s)}{\mathcal{M}_Z(s)} \frac{x^{-s+1}}{s} \mathrm{d}s, \;\; x \geq 0.$$

Inversion formula proof sketch

- Recall, letting $A \sim F_A$, $Z \sim G_K$ and $\Lambda_b \sim H^b$ with Z and Λ_b independent we have:
$$A \stackrel{d}{=} Z\Lambda_b^2.$$
- Due to the moment conditions we have for $s \in \mathrm{St}(\max\{1-\alpha, 1\}, 1)$:
$$\mathcal{M}_A(s) = \mathcal{M}_Z(s)\mathcal{M}_{\Lambda_b^2}(s).$$
- Let $c \in (\max\{1-\alpha, 1\}, 1)$. Since analytic functions only have isolated zeros, $\mathcal{M}_{\Lambda_b^2}(c+it) = \mathcal{M}_A(c+it)/\mathcal{M}_Z(c+it)$ for almost all $t \in \mathbb{R}$.

Inversion formula proof sketch

- Assuming H^b is continuous, the Mellin inversion theorem (Kawata 1972) yields:

$$H^b\left(\sqrt{x}\right) = \mathbb{P}\left(\Lambda_b^2 \leq x\right) = \lim_{T\to\infty} \frac{1}{2\pi i} \int_{c-iT}^{c+iT} -\mathcal{M}_{\Lambda_b^2}(s) \frac{x^{-s+1}}{s} \mathrm{d}s$$
$$= \lim_{T\to\infty} \frac{1}{2\pi i} \int_{c-iT}^{c+iT} -\frac{\mathcal{M}_A(s)}{\mathcal{M}_Z(s)} \frac{x^{-s+1}}{s} \mathrm{d}s$$

  for $x \geq 0$.

- H can be retrieved via:

$$H(\lambda) = \frac{\int_0^\lambda \frac{1}{x} \mathrm{d}H^b(x)}{\int_0^\infty \frac{1}{x} \mathrm{d}H^b(x)}.$$

Absolute continuity of G_K

- Let T be an IUR plane hitting K, G_K is given by:

$$G_K(z) := \mathbb{P}\left(\mathrm{vol}_2(K \cap T) \le z\right).$$

- Suppose G_K has a Lebesgue density g_K, supported on $(0, a_{\max})$. Then, F_A is absolutely continuous with density:

$$f_A(a) = \frac{1}{\mathbb{E}(\Lambda)} \int_{\sqrt{\frac{a}{a_{\max}}}}^{\infty} g_K\left(\frac{a}{\lambda^2}\right) \frac{1}{\lambda} \mathrm{d}H(\lambda).$$

- Relevance for statistical inference: the likelihood is well-defined.

Parameterization of IUR planes

$$S_+^{n-1} = \{(x_1, \dots, x_n) \in \mathbb{R}^n : \|x\| = 1, x_n \geq 0\}.$$

$$T_{\theta,s} = \{x \in \mathbb{R}^n : \langle x, \theta \rangle = s\}, \tag{2}$$

Definition (IUR plane)

An IUR plane T hitting a fixed $K \in \mathcal{K}^n$, $n \geq 2$, is defined as $T = T_{\Theta,S}$ where (Θ, S) has joint probability density, $f_K : S_+^{n-1} \times \mathbb{R} \to [0, \infty)$ given by:

$$f_K(\theta, s) = \begin{cases} \frac{1}{\mu([K])} & \text{if } K \cap T_{\theta,s} \neq \varnothing \\ 0 & \text{otherwise,} \end{cases}$$

with $T_{\theta,s}$ as in Eq. (2) and

$$\mu([K]) = \int_{S_+^{n-1}} \int_{-\infty}^{\infty} \mathbb{1}\{K \cap T_{\theta,s} \neq \varnothing\} \mathrm{d}s \mathrm{d}\theta = \sigma_{n-1}\left(S_+^{n-1}\right) \bar{b}(K).$$

Brunn's theorem

- Recall the following classical result:

Theorem (Brunn)

Let $K \subset \mathbb{R}^n$ be a convex body, $n \geq 2$. Fix $\theta \in S^{n-1}$. The function $f_\theta : \mathbb{R} \to [0, \infty)$ given by:

$$f_\theta(s) = \mathrm{vol}_{n-1}(K \cap T_{\theta,s})^{\frac{1}{n-1}},$$

is concave on its support.

Absolute continuity of G_K

Theorem (Jongbloed, Vittorietti, and TJ 2023a)

Let $K \subset \mathbb{R}^n$ be a convex body, $n \geq 2$. For $\theta \in S_+^{n-1}$, define the function $f_\theta : \mathbb{R} \to [0, \infty)$ by:

$$f_\theta(s) = \mathrm{vol}_{n-1}(K \cap T_{\theta,s})^{\frac{1}{n-1}}.$$

If f_θ has a unique maximum and is continuous on $\mathbb{R}$ for almost all $\theta \in S_+^{n-1}$, then G_K is absolutely continuous with respect to Lebesgue measure.

- Condition is satisfied for strictly convex bodies.

Main idea

- Writing G_K as a mixture distribution, conditioning on a fixed direction $\Theta = \theta$. With $(\Theta, S) \sim f_K$ and f_Θ the marginal density of Θ.

$$
\begin{aligned}
G_K\left(z^{n-1}\right) &= \mathbb{P}\left(\mathrm{vol}_{n-1}(K \cap T_{\Theta,S})\right)^{\frac{1}{n-1}} \leq z\Big) \\
&= \int_{S_+^{n-1}} \mathbb{P}\left(f_\theta(S) \leq z \middle| \Theta = \theta\right) f_\Theta(\theta) \mathrm{d}\theta.
\end{aligned}
$$

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$$G_K\left(z^{n-1}\right) = \mathbb{P}\left(\mathrm{vol}_{n-1}(K \cap T_{\Theta,S}))^{\frac{1}{n-1}} \le z\right)$$
$$= \int_{S_+^{n-1}} \mathbb{P}\left(f_\theta(S) \le z \middle| \Theta = \theta\right) f_\Theta(\theta)\mathrm{d}\theta.$$

- Conditional on $\Theta = \theta$ we have $S \sim \mathcal{U}(-h_K(-\theta), h_K(\theta))$.
- For almost all $\theta \in S_+^{n-1}$, the CDF

$$z \mapsto \mathbb{P}\left(\mathrm{vol}_{n-1}(K \cap T_{\Theta,S})^{\frac{1}{n-1}} \le z \middle| \Theta = \theta\right).$$

  is continuous on $\mathbb{R}$ and convex on its support.
- Fubini's theorem yields the desired result.

Convex polytopes

- For convex polytopes the function f_θ does not in general have a unique maximum.

Lemma

Let $P \subset \mathbb{R}^n$ be a full-dimensional convex polytope, $n \geq 2$. Fix $\theta \in S_+^{n-1}$ and define the function $f_\theta : \mathbb{R} \to [0, \infty)$ by:

$$f_\theta(s) = \mathrm{vol}_{n-1}(P \cap T_{\theta,s})^{\frac{1}{n-1}}.$$

Suppose f_θ attains its maximum on the entire interval $[s_-, s_+]$, with $s_- < s_+$. Then, any plane $T_{\theta,s}$ with $s \in [s_-, s_+]$ intersects the same edges of P and these edges are parallel.

Convex polytopes

- For convex polytopes the function f_θ does not in general have a unique maximum.

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Theorem (Jongbloed, Vittorietti, and TJ 2023a)

Let $P \subset \mathbb{R}^n$ be a full-dimensional convex polytope, $n \geq 2$. Let G_P be its section volume CDF. Then, G_P is absolutely continuous.

Main idea of proof

- For "non-maximal" sections we proceed as before.
- In general, f_θ attains its maximum in the entire interval $[s_-(\theta), s_+(\theta)]$, possibly with $s_-(\theta) = s_+(\theta)$. Define:

$$D := \left\{\theta \in S_+^{n-1} : s_+(\theta) > s_-(\theta)\right\}.$$

- D may be written as a disjoint union: $D = \bigcup_{i=1}^{k} D_i$.
  For any $\theta \in D_i$ any plane $T_{\theta,s}$ with $s \in [s_-(\theta), s_+(\theta)]$ intersects the same parallel edges of P.

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  For any $\theta \in D_i$ any plane $T_{\theta,s}$ with $s \in [s_-(\theta), s_+(\theta)]$ intersects the same parallel edges of P.
- Take $\phi_i \in S_+^{n-1}$ collinear to the edge directions corresponding to D_i.
  For $\theta \in D_i$ there exists a $v_i > 0$ such that:

$$\mathrm{vol}_{n-1}(P \cap T_{\theta,s}) = \max_{t \in \mathbb{R}} \mathrm{vol}_{n-1}(P \cap T_{\theta,t}) = \frac{v_i}{|\langle \theta, \phi_i \rangle|}.$$

- If we draw $\Theta \sim \mathcal{U}(S^{n-1})$, then the random variable $|\langle \Theta, \phi_i \rangle|$ has a Lebesgue density.

Final remark

- Statistical results: the identifiability result as well as the absolute continuity of G_K for a large class of convex bodies was used to define a non-parametric maximum likelihood estimator of H^b, which is proven to be strongly consistent. More details in Jongbloed, Vittorietti, and TJ 2023b

Thank you for your attention!

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