Persistent homology based goodness-of-fit tests for spatial tessellations

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ABSTRACT
Motivated by the rapidly increasing relevance of virtual material design in the domain of materials science, it has become essential to assess whether topological properties of stochastic models for a spatial tessellation are in accordance with a given dataset. Recently, tools from topological data analysis such as the persistence diagram have allowed to reach profound insights in a variety of application contexts. In this work, we establish the asymptotic normality of a variety of test statistics derived from a tessellation-adapted refinement of the persistence diagram. Since in applications, it is common to work with tessellation data subject to interactions, we establish our main results for Voronoi and Laguerre tessellations whose generators form a Gibbs point process. We elucidate how these conceptual results can be used to derive goodness of fit tests, and then investigate their power in a simulation study. Finally, we apply our testing methodology to a tessellation describing real foam data.

1. Introduction

The concept of spatial tessellations is of high importance in spatial statistics due to their appearance in a wide variety of disciplines including telecommunications, location planning, modelling of biological cells or microstructures in materials science. In particular, there is a pronounced need for goodness of fit tests involving spatial tessellations on specific random point patterns as null models. The challenge in this situation is that we want to use test statistics that can capture refined aspects of the tessellation structure while still being able to develop tests that are asymptotically exact. In this paper, we illustrate how such a goal can be achieved via tests that are based on the concept of persistent homology from topological data analysis. To provide the reader with a specific instance of this general challenge, we now elaborate on the importance of such tests in materials science as one of many prototypical application areas.

Accurate stochastic-geometry models for the microstructure of complex materials have become an indispensable tool in modern materials science, as they open the door towards
virtual material design. More precisely, by being able to rapidly generate plausible realisations of microstructures stemming from a large variety of production parameters, it is possible to reduce costly experiments to the most promising candidates for a desired functional property of the new material (Neumann et al. 2020; Redenbach et al. 2012; Westhoff et al. 2018).

Clearly, the success of virtual material design hinges on the question whether the chosen model provides a good fit to the considered dataset. If the model is too simple, then important characteristics of the dataset are missed. Hence, also the functional properties of the virtual realisations may differ substantially from the actual materials. On the other hand, extremely detailed models are at the risk of over-fitting the data. That is, realisations of such models may mimic certain particularities of the specific sample, and thereby fail to reflect accurately the true variability of microstructures seen in real data. In this setting, statistical hypothesis tests provide a scientifically sound methodology to decide whether at a given significance level a considered dataset is consistent with a null hypothesis formulated in advance.

The design of versatile test statistics is the key challenge in devising powerful statistical hypothesis tests for data involving stochastic morphologies. The difficulty lies in finding appropriate numerical characteristics that encapsulate the relevant complex topology of the dataset. In particular, different model classes from stochastic geometry, e.g. point processes, particle processes, line processes or random tessellations, come with different natural statistics. Here, we will restrict attention to random tessellations which are widely established as models for cellular and polycrystalline materials (Bourne et al. 2020; Redenbach 2009). The first natural step is to consider geometric properties of the tessellation cells such as edge lengths or cell surface areas (Vecchio et al. 2016). However, for detecting subtle morphological differences, more refined characteristics may deliver additional value. For instance, Arns et al. (2004) compute Minkowski functionals of morphologies resulting through continuous dilation of the original dataset.

More recently, topological data analysis (TDA) has emerged as a promising new idea to detect subtle differences in the shapes of complex morphologies. The key tool in TDA are persistence Betti numbers and the persistence diagram. The Betti numbers are classical invariants from algebraic topology counting the number of holes of a certain dimension in a topological space. Persistent Betti numbers refine this idea and are able to capture topological features at multiple scales from a dataset sampled on an unknown underlying topological space. Loosely speaking, the persistence diagram provides precise information about when topological features such as connected components, loops and cavities appear, and also when they disappear again. The statistical use of the persistence diagram is illustrated by an impressive number of studies in a wide variety of applications (Bendich et al. 2016; Hiraoka et al. 2016; Robinson and Turner 2017; Saadatfar et al. 2017).

We note that similarly as in Arns et al. (2004), the novel TDA approach studies the evolution of the morphology resulting from suitable dilation operations. Instead of the Minkowski functionals, TDA uses the toolkit of persistent homology from algebraic topology to detect structure changes after dilation. Hence, persistent homology is a characteristic, which by its design is a promising candidate when it comes to distinguishing structures with respect to their topological properties rather than their geometric ones.

To date, the widespread use of TDA in materials science is severely restricted since there is no tessellation-adapted version of the persistence diagram. More precisely, while the
Čech and Vietoris-Rips filtrations are highly popular tools to compute the persistence diagram on point clouds, these filtrations do not take into account the rich adjacency structure inherent in spatial random tessellations. The key contribution of our work is to propose two specific ways to devise a variant of the persistence diagram that is capable of reflecting the information that the vertices belong to a random spatial tessellation. This will lead to the edge-based persistence diagram and the M-localised persistence diagram that we discuss in further detail in Section 2 below. To illustrate that TDA-based testing of spatial tessellation models is feasible, we carry out an analysis in three directions.

First, we show that the persistent Betti numbers derived from the new persistence diagrams are asymptotically normal in large domains (for similar results see Bickel and Wichura 1971; Billingsley 1999; Davydov and Zitikis 2008; Divol and Polonik 2019; Fernández et al. 2001; Krebs and Hirsch 2022; Penrose and Yukich 2001). We stress that we derive this asymptotic normality in the form of a functional central limit theorem. This functional formulation is an decisive advantage as it allows us to consider not only the individual persistent Betti numbers but any test statistics that results as a continuous transformation from the persistence diagram. This is a key insight since it guarantees that for large sampling windows, asymptotically exact hypothesis tests can be constructed from the knowledge of means and variances in the null model. In the context of spatial random tessellations, arguably the most fundamental null model is that of a Poisson-Voronoi tessellation, corresponding to a tessellation obtained from a randomly scattered collection of indistinguishable cell centres. However, due to the complex physical phenomena governing the organisation of real microstructures, the Poisson-Voronoi tessellation is rarely considered as a serious contender for an appropriate null model. Therefore, we establish the asymptotic normality in the framework of Laguerre tessellations with generators forming a Gibbsian point process. This enables modelling of substantial variations in the tessellation cells as well as interactions between the cell centres.

Second, in a simulation study, we illustrate that the asymptotic normality becomes already accurate for moderately large sample sizes. We also give first indications of the power of the TDA-based test statistics and compare the testing power of these new test statistics to more elementary alternatives. Third, we apply the testing methodology to a specific dataset of an open cell foam from materials science.

We stress that the goal of our investigation is to develop a TDA-based framework for analysing tessellations that (1) has a rigorous statistical foundation, (2) is validated in a simulation study and (3) is applied to a challenging dataset from materials science. In particular, considered in itself, each of the three parts contains possibilities for further investigations. However, to strengthen the coherence between the different parts, we did not work out such refinements although they would be logical when considered in isolation within one of the parts. We believe that after having made the first steps in the present work, these could be exciting avenues for future research. We will elaborate on these possibilities in Section 5.

2. Model and main results

We develop goodness of fit tests for random spatial tessellations observed in the sampling window $W_n := [0, n]^p, p \geq 2$. Due to their central place in materials science, we focus on the pivotal model of Laguerre tessellations, which include Voronoi tessellations as a special
case (Redenbach 2009). Laguerre tessellations are obtained from a marked point process of cell centres through a deterministic construction rule.

More precisely, we assume that $\mathcal{X}_n = \{\tilde{X}_i\}_{i \geq 1} = \{(X_i, R_i)\}_{i \geq 1}$ is a marked point process on $W_n$, with locations $X_i \in W_n$, and marked by radii $R_i > 0$. Here, the marks may be continuous or discrete. Then, we let

$$C(\tilde{X}_i, \mathcal{X}_n) := \left\{ y \in \mathbb{R}^p : |y - X_i|^2 - R_i^2 \leq \min_{(x,r) \in \mathcal{X}_n} (|y - x|^2 - r^2) \right\}$$

denote the Laguerre cell associated with $\tilde{X}_i$. The collection $\mathcal{Z}_n := \mathcal{Z}(\mathcal{X}_n) := \{C(\tilde{X}_i, \mathcal{X}_n)\}_{X_i \in \mathcal{X}_n}$ of all Laguerre cells defines the Laguerre tessellation, and we write $\mathcal{Z}_n^{(q)}$ for the family of all $q$-faces of $\mathcal{Z}_n$.

Another approach would be to build the tessellation on a stationary point process $\mathcal{X}$, and then only restrict to the cells whose generator is contained in the window $W_n$. Although conceptually appealing, this approach has the disadvantage that the existing asymptotic theory for functionals on Gibbs point processes that will be used later is developed for functionals computed on $\mathcal{X}_n$ (Schreiber and Yukich 2013). It seems plausible that under suitable additional conditions on the process and the functional, the two approaches should become equivalent. However, already the verification of the standard conditions in Schreiber and Yukich (2013) is delicate. For the sake of attaining a more accessible presentation, we therefore decided to refrain from establishing this equivalence in the present work.

### 2.1. Edge-based $M$-bounded persistent Betti numbers

The permeability of an open cell foam is influenced by the size distribution of the windows between the foam cells (Föhst et al. 2022; Westhoff et al. 2018). Hence, when modelling the foam by a random tessellation, the distribution of face sizes has to be controlled. Suitable geometric characteristics are the area of faces or the face-inradius. Here, we propose to proceed in the vein of Arn et al. (2004) and consider the latter.

Fixing the dimension $p = 3$ and starting from the tessellation edges, the face inradius corresponds to the dilation radius at which a face gets completely covered by the edges forming its boundary. More precisely, we define the inradius $r(f)$ of a convex polygon $f$ bounded by the edges $\{e_1, \ldots, e_k\}$ as

$$r(f) := \max_{x \in f} \text{dist} \left( x, \bigcup_{j \leq k} e_j \right)$$

i.e. as the first level $r \geq 0$ where the $r$-dilated edge set covers the entire face. Due to edge effects, faces that are close to the boundary of the sampling window (and also some faces completely contained in the window) may be highly skewed and could therefore potentially influence the test statistics significantly.

To counter such effects, we will restrict our attention to faces with a bounded eccentricity: for a 2-face $f \in \mathcal{Z}_n^{(2)}$ shared by the cells centred at $P_1$ and $P_2$, we define $\text{ecc}(f) := \max_{y \in f, i \in \{1,2\}} |y - P_i|$. This ensures that both the face is not too far from the centres, and also that its diameter is small. Hence, for Voronoi tessellations, the eccentricity includes information on both, the size of a face and its distance to the generator points of the adjacent cells. For Laguerre tessellations based on independent radii with a highly skewed
distribution the interpretation is more involved. Indeed, for generators with small radius, it may happen that the generating point is not contained in the cell. Thus, in the Laguerre setting, the eccentricity also takes into account the degree of cell inhomogeneity.

Then, we introduce the edge-based persistent Betti number

$$\beta_{n,M,s} := \# \left\{ f \in \Xi_n^{(2)} : r(f) > s, \text{ecc}(f) \leq M \right\}$$

as the number of faces with inradius at least $s$ and eccentricity at most $M$. The reason for referring to this quantity as a Betti number is the following. We may use the inradius $r_I$ to define a filtration on the faces in $\Xi_n^{(2)}$. If we assume that all edges are present at time 0, then the value $r_I(f)$ corresponds to the death time obtained from adding the face $f$.

### 2.2. $M$-localised persistent Betti numbers

Face-inradii are very natural univariate functional characteristics associated with a tessellation. However, TDA draws its appeal from the ability to extract far more subtle bivariate quantities describing the times when topological features appear, and when they disappear again. This machinery relies on a suitable notion of filtrations of topological spaces. In the analysis of point patterns, the Čech- and the Vietoris-Rips filtrations have emerged as universally accepted choices. However, when dealing with tessellations there is no clear suggestion from the literature that one could build upon. In order to respect the inherent structure of the tessellation, we propose tessellation-adapted filtrations where entire lower-dimensional faces are added at filtration times that are given by their circumradii. In other words, a $q$-face $f \in \Xi_n^{(q)}$ defined by vertices $P_0, \ldots, P_m$ belongs to the filtration at a level $s > 0$ if and only if $r_C(f) \leq s$, where the circumradius $r_C(f)$ of $f$ is defined by

$$r_C(f) := \min_{y \in \mathbb{R}^p} \max_{i \leq m} |y - P_i|.$$ 

The circumradius of a $q$-face is always determined by the circumradii of its $q$-simplices in the sense that there exist $P_{j_0}, \ldots, P_{j_r}$ with $r_C(f) = r_C(\{P_{j_0}, \ldots, P_{j_r}\})$. We will refer to this as the tessellation-adapted filtration associated with the faces of the tessellation. Figure 1 illustrates the difference between the tessellation-adapted and the standard Čech filtration.

Next, we construct the persistence diagram $\{(B_{i,n,q}, D_{i,n,q})\}_{i \geq 1}$ of birth times $B_{i,n,q}$ and death times $D_{i,n,q}$ of the $q$-features. For $p = 3$, a 0-feature is a connected component, a 1-feature is a circular hole (tunnel) and a 2-feature is a void (connected component of the complement). Based on the persistence diagram, we define the persistent Betti number for $b, d > 0$ as

$$\beta_{n,q}^{b,d} := \# \{ i \geq 1 : B_{i,n,q} \leq b, D_{i,n,q} \geq d \}.$$ (2)

the number of $q$-features born before time $b > 0$ and living past time $d > 0$.

Since it is highly delicate to derive the persistence diagram from a given point cloud, we need to implement some approximation and truncation steps in order to establish the asymptotic normality rigorously. First, we want to avoid very elongated faces with a small inradius, and therefore write $\Xi_{n,M}^{(q)}$ for the family of all $q$-faces in $\Xi_n$ of eccentricity at most $M$ and whose inradius is at least $M^{-1}$ for some (large) $M > 0$. An additional major difficulty arises through long-range correlations induced by very large features spanning
over large parts of the sampling window. More precisely, the methodology of Schreiber and Yukich (2013) uses the concept of exponential stabilisation to exclude long-range correlations. To deal with this issue, we restrict our attention to \( M \)-localised Betti numbers, which we now discuss in further detail. Loosely speaking, \( M \)-localised persistent Betti numbers first determine locally the contribution of features involving a \( q \)-face and then aggregate these contributions over all faces in the entire window. Fixing \( M > 0, b \leq d \), for each \( f \in \Xi_{n,M}^{q,(q)} \), we consider all cells contained in the sub-window \( z(f) + [-M, M]^p \) centred at the centroid \( z(f) \) of the face \( f \). More precisely, this means that when deciding whether a face is negative (definition below) and when computing the birth time of the associated feature, we look only at the cells in \( z(f) + [-M, M]^p \).

Figure 1. Top row: Snapshots at four time points illustrating the evolution of the standard Čech filtration for a cloud of four points. At time point 1, all four points are in separate connected components. At time point 2, a loop has appeared, thereby leading to the birth of a 1-feature. At time point 3 a second 1-feature is born. At time point 4 both 1-features die. Bottom row: Corresponding evolution of the tessellation-adapted filtration, where the four points are the vertices of a cell (in dashed lines). At time points 1 and 2 there is no difference to the standard Čech filtration. However, at time point 3 no new feature is born since the connecting edge is not part of the tessellation. At time point 4, the feature born at time point 1 dies.

Here, when computing the persistent Betti numbers, we rely on an incremental algorithm. We now explain loosely how this algorithm can be used to compute the birth times and death times of features, referring the reader to Boissonnat et al. (2018, Algorithm 11) for a detailed exposition. We start from a completely empty space, and then reconstruct the tessellation by adding the faces one after another in the order of increasing circumradius. When adding a face, one of two cases may occur. Either the addition of the face kills one of the existing features, in which case it is called negative. For instance, in dimension \( p = 3 \), the addition of a face can cause a loop to be contractible. Otherwise, the face is called positive as it will give rise to a new feature. In \( p = 3 \), this corresponds to the creation of a 3D cavity. If the face \( f \) is negative, then we write \( b(f) \) for the birth time and \( d(f) = r_c(f) \) for the death time of the feature killed by the addition of face \( f \). In the case where the feature-death is caused by the simultaneous addition of multiple faces, we can formally attach the feature to the face with the left-most circumcenter. Note that this case occurs with probability 0 for the considered random tessellations. The \( M \)-localised persistent Betti number \( \beta_{n,q}^{M,b,d} \) is
then defined as the total number of such features

\[ \beta_{n,q}^{M,b,d} := \# \left\{ f \in S_{n,M}^{(q)} : b(f) \leq b, \ d(f) \geq d \right\} . \]

### 2.3. Definition of the generating point process and conditions for the main result

Since tessellations appearing in materials science typically feature highly complex interactions between different cells, it is essential to work with classes of marked point processes that are flexible enough to reproduce such interaction patterns. Since Gibbsian point processes have been successfully used in a variety of application scenarios with complex dependencies, our investigations will be focussed on this class of point processes.

First, we recall the definition of Gibbs point processes from Schreiber and Yukich (2013, Equation (1.5)). Let \( \mathcal{P}_{\tau,Q} \) denote an independently marked Poisson point process on \( \mathbb{R}^p \) with intensity \( \tau > 0 \) and mark distribution \( Q \) whose support will be assumed to be contained in a bounded interval of the form \([0, \mu]\) for some \( \mu > 0 \). Second, let \( \Psi \) be a translation- and rotation-invariant nonnegative functional defined on finite point configurations, which we henceforth refer to as a Hamiltonian. For \( \alpha > 0 \), and any bounded open \( D \subseteq \mathbb{R}^p := \mathbb{R}^p \times [0, \mu] \), a marked point process \( X_D = X_D^\alpha \Psi \) is called Gibbs point process with Hamiltonian \( \alpha \Psi \), if the Radon-Nikodym density of the marked point process \( X_D \) with respect to the Poisson point process \( \mathcal{P}_{\tau,Q} \cap D \) is proportional to \( e^{-\alpha \Psi(\cdot)} \). That is, writing \( \mathcal{L} \) for the law of a point process, we have

\[ \frac{d\mathcal{L}(X_D)}{d\mathcal{L}(\mathcal{P}_{\tau,Q} \cap D)}(\varphi) = \frac{1}{Z_{\alpha,D}} e^{-\alpha \Psi(\varphi)} , \]

where \( \varphi \subseteq D \) is a finite configuration and \( Z_{\alpha,D} := \mathbb{E}(\exp(-\alpha \Psi(\mathcal{P}_{\tau,Q} \cap D))) \). If \( \alpha \) and \( \Psi \) are fixed, we will also use the abbreviation \( X_n := X_n^{\alpha \Psi} \).

The topic of the present paper is the development of TDA-based hypothesis tests for spatial tessellations. To give a precise description of the testing framework, we now provide a formal statement of the null hypothesis and alternative. The null hypothesis is that the observed spatial tessellation comes from a realisation of the Voronoi/Laguerre tessellation of the (marked) Gibbs process \( X_n \) with a specified Hamiltonian. The alternative is that the observed spatial tessellation does not come from a realisation of such a tessellation.

In the following, we will prove asymptotic normality of test statistics based on the edge-based and \( M \)-localised persistent Betti numbers. Recently, establishing functional CLTs for Gibbs point patterns has become a vigorous research topic in spatial statistics. For instance, Biscio and Svane (2022) establish asymptotic normality for Ripley’s \( K \)-function. This quantity is an important characteristic in spatial statistics but only takes into account the distances between point pairs of the Gibbs process. The setting in the present paper is substantially more involved since we deal with topological functionals of 3D tessellations where the Gibbs point patterns are not the vertices but the generators of the cells. On the conceptual side, one of the major contributions of our work is to explain how the delicate moment bounds can be established in this complex setting. Similarly as in Biscio and Svane (2022), our proof crucially relies on the techniques from Schreiber and Yukich (2013) and Xia and Yukich (2015). Although, formally the framework there is stated for point processes without marks, the remark following Schreiber and Yukich (2013, Theorem 2.4)
stresses that the proof of the asymptotic normality also extends seamlessly to marked Gibbs point processes.

The asymptotic normality in Schreiber and Yukich (2013) and Xia and Yukich (2015) is established for a specific class $\Psi^*$ of translation- and rotation-invariant nonnegative Hamiltonians $\Psi$ defined on finite point configurations $\varphi \subseteq \mathbb{R}_p$: a Hamiltonian $\Psi$ belongs to the class $\Psi^*$ if (i) $\Psi(\varphi) \leq \Psi(\varphi')$ for $\varphi \subseteq \varphi'$, (ii) $\Psi(\varphi) < \infty$ whenever $\#\varphi \leq 1$ and (iii) $\Psi$ has a finite range $r_0 > 0$. We refer the reader to Xia and Yukich (2015, Section 1.1.1) for a more detailed discussion. For the rest of the present paper, the main implication is that the Hamiltonian of the Strauss process considered in Section 3 below belongs to the class $\Psi^*$.

### 2.4. Asymptotic normality

After having introduced the conditions in Section 2.3, we now state asymptotic normality of test statistics computed from edge-based and $M$-localised persistent Betti numbers. First, we consider statistics, which concern persistent Betti numbers for fixed values of the levels. To state our results precisely, we require an upper bound for the Poisson intensity which is given by

$$\tau_0(\Psi) := |B_1(o)|^{-1} \exp(\alpha m_0^\Psi(r_0 + 1)^{-p},$$

where $m_0^\Psi := \inf_{\varphi \text{finite}}(\Psi(\varphi \cup \{o\}) - \Psi(\varphi))$.

**Theorem 2.1 (Asymptotic normality at a fixed level):** For $n \geq 1$ let $X_n = X_n^{\alpha \Psi}$ be a marked Gibbs point process with Hamiltonian $\alpha \Psi$ of type $\Psi^*$ on $W_n$, and $\tau < \tau_0(\Psi)$.

(1) Let $s > 0$. Then,

$$\frac{\beta_n^{\Phi,M,s} - \mathbb{E}[\beta_n^{\Phi,M,s}]}{\sqrt{|W_n|}}$$

converges in distribution to a mean-zero normal random variable.

(2) Let $d \geq b \geq 0$. Then,

$$\frac{\beta_n^{M,h,d} - \mathbb{E}[\beta_n^{M,h,d}]}{\sqrt{|W_n|}}$$

converges in distribution to a mean-zero normal random variable.

It is possible to provide an integral expression for the variance of the limiting random variable, see Schreiber and Yukich (2013, Identity 2.11). However, since this integral is not amenable to an evaluation in closed form, we refrain from reproducing the precise expression. In the simulation study in Section 3 below, we determine the variance under the null model through simulations.

We note that Theorem 2.1 is an asymptotic result in the sense that the convergence to a Gaussian only holds in the limit of increasing windows. Later, in Figure 4 from Section 3, we illustrate that the approximate Gaussianity is already visible for moderately large datasets. More precisely, in that section, we consider a system of 300 points in $[0, 1]^3$. The strength of the asymptotic approach is that due to the asymptotic Gaussianity, the distribution of the test statistics is in fact understood better for larger windows. On the other hand, we
also stress that for small sample sizes the approximation by a Gaussian will not be accurate. However, the threshold from which the distribution may be assumed Gaussian will depend both on the null model and also on the degree to which the practitioner can accept a deviation from a normal distribution. Therefore, we refrain from providing a specific threshold for the system size from which on the Gaussianity holds.

Finally, we extend the fixed-level asymptotic normality from Theorem 2.1 to asymptotic normality on a functional level. That is, we consider $\beta_n^{e,M,s}$ as a function in $s$ and $\beta_n^{M,b,d}$ as a function in $b, d$. While for the fixed-level asymptotic normality, the main challenge is to control the long-range spatial dependence, the extension to the functional level also relies on continuity properties when varying the levels at which the persistence Betti numbers are computed. Establishing the required continuity properties is already delicate when dealing with point clouds described by a Poisson point process, and a direct extension to Gibbs-Laguerre tessellations seems out of reach. We now explain that these problems can be avoided by incorporating additional sources of noise into the original models.

More precisely, motivated by applications such as foams we assume that the tessellation edges are not just purely 1-dimensional links but come with a certain random thickness. That is, we assume that the process of edges $\{e_i\}_{i \geq 1}$ is independently marked with positive thicknesses $\{\rho_i\}_{i \geq 1}$. This model extension helps to ensure a higher degree of distributional smoothness on the conceptual side and also moves the model closer to real structures found in materials science.

In the case of the $M$-localised persistent Betti numbers, we assume that extracting the location of the tessellation vertices from data comes with a certain measurement error (Cheng et al. 2019). We incorporate this constraint by considering iid noise vectors $\{\eta_i\}_{i \geq 1}$ that are uniformly distributed in a ball $B_{h_0}$ for some small $h_0 > 0$. Then, we set the measured locations as $P_i + \eta_i$, which will replace $P_i$ when determining the circumradius in the tessellation-adapted filtration.

Theorem 2.2 (Functional asymptotic normality): Let $S > 0$ and for $n \geq 1$ let $X_n = X_n^{\alpha,\Psi}$ be a marked Gibbs point process with Hamiltonian $\alpha \Psi$ of type $\Psi^*$ on $W_n$ and $\tau < \tau_0(\Psi)$.

1. Assume that the process of edges $\{e_i\}_{i \geq 1}$ is independently marked with positive thicknesses $\{\rho_i\}_{i \geq 1}$. When considered as a process in $s \leq S$, the process

$$\left( |W_n|^{-1/2}(\beta_n^{e,M,s} - E[\beta_n^{e,M,s}]) \right)_{s \leq S}$$

converges in the Skorokhod topology to a centred Gaussian process.

2. Assume that we set the measured locations as $P_i + \eta_i$ where the iid noise vectors $\{\eta_i\}_{i \geq 1}$ are uniformly distributed in a ball $B_{h_0}$ for some small $h_0 > 0$. When considered as a process in $b, d \leq S$, the process

$$\left( |W_n|^{-1/2}(\beta_n^{M,b,d} - E[\beta_n^{M,b,d}]) \right)_{b,d \leq S}$$

converges in the Skorokhod topology to a centred Gaussian process.

We note that for the $M$-localised persistent Betti numbers, Theorems 2.1 and 2.2 could also be shown for $\beta_n^{p-1}$ instead of $\beta_n^{p-2}$ when associating a feature with the face causing its birth (instead of the death). Moreover, the restriction to $M$-localised features can
be avoided when replacing the persistent Betti numbers by the Euler characteristic curve. While we do not provide the detailed arguments here, we refer to Krebs et al. (2021) for a similar situation. Although the latter is a coarser characteristic, it may still deliver interesting topological insights.

3. Simulation study

In this section, we present a simulation study analysing goodness-of-fit tests derived from the asymptotic normality established in Theorems 2.1 and 2.2. To that end, we consider six tessellation models on the 3D unit cube $[0, 1]^3$, where to compensate for edge effects, we work with periodic boundary conditions. The first three models correspond to Voronoi tessellations formed on configurations of 300 generators in the unit cube. In the simplest model, the 300 generators are scattered independently at random in $[0, 1]^3$. In the second model, the 300 generator points are distributed according to a Strauss process, which is a Gibbs point process featuring a repulsive interaction between points. While the general limit theory developed in Section 2 concerns Gibbs point processes with a variable number of points, for the simulation study, we have decided to rely on a variant where the number of points is held constant at 300. This model choice enables a cleaner comparison of the refined topological properties of the different tessellation models. We recall that the Strauss process is a Gibbsian point process whose unnormalised density with respect to a Binomial point process is given by $f(x) := \gamma^{s_{r_0}(x)}$, for certain parameters $r_0 > 0$ and $\gamma \in [0, 1]$. Here, $s_{r_0}(x)$ is the number of point pairs at distance at most $r_0$. In particular, the inverse temperature $\alpha$ from Section 2.3 and the parameter $\gamma$ are related through $\alpha = -\log(\gamma)$.

Although Strauss processes are a popular choice for modelling repulsive point patterns, they are most useful for scenarios with a relatively low regularity. Therefore, we now explain more precisely how to create more regular point patterns. One of the most popular approaches is to construct random sphere packings via collective rearrangement, e.g. the force-biased algorithm. Such algorithms first start from a configuration of potentially overlapping spheres. Then, colliding spheres are iteratively pushed into the vacant space, and this procedure is repeated until a hard-core configuration is obtained (Mosinski et al. 1989). Such point patterns form the third model considered in our simulation study. We now summarise again the three models and provide the specific parameter choices.

(1) A **Binomial-Voronoi tessellation;** short **Bin-Vor.** The Voronoi tessellation is constructed on 300 generator points that are scattered independently uniformly in $[0, 1]^3$.

(2) A **Voronoi tessellation** based on a **Strauss process;** short **St-Vor.** The interaction parameter $\gamma$ of the Strauss process is set to $\gamma = 0.01$, and the interaction range $r_0$ is fixed as $r_0 = 0.14$. When interpreting the point configuration as a set of non-overlapping balls of radius $r_0/2 = 0.07$, this corresponds to a volume fraction of 43%. We note that larger choices of $r_0$ caused serious convergence issues of the MCMC sampler.

(3) A **Voronoi tessellation** based on a **force-biased sphere packing** with a constant sphere radius of $r = 0.07816$ resulting in a volume fraction of 60%; short **Fb-Vor.**
As a further refinement of the above setting, we replace the simplistic Voronoi model by a more refined Laguerre model with random radii. We note that to achieve on average 300 cells in the Laguerre tessellations, a substantially higher initial number of generator points is needed in order to compensate for empty cells. More precisely, the initial number of the generators was chosen as 325 for the Binomial process and 324 for the Strauss process. Since the spheres in the force-biased algorithm are disjoint by construction, no correction is needed in this example.

(4) A Laguerre tessellation based on a Binomial point process; short Bin-Lag. The volume of the balls associated with the Laguerre tessellation follows a lognormal-distribution with parameters $\mu = -6.3262$ and $\sigma = 0.47238$. This corresponds to a coefficient of variation of 0.5.

(5) A Laguerre tessellation based on a Strauss process; short St-Lag. The interaction parameter $\gamma$ of the Strauss process is set to $\gamma = 0.01$, and the interaction radius $r_0$ is fixed as $r_0 = 0.14$. The Laguerre radius distribution is the same as before.

(6) A Laguerre tessellation based on a force-biased sphere packing; short Fb-Vor. The Laguerre radius distribution is the same as before and the volume fraction is 60%.

In Figure 2, we illustrate 2D sections for realisations from each of the six tessellation models.

Most of the simulations were carried out using python. In particular, the tess-package was used for the generation of the tessellations. The simulations of the Strauss process were carried out in R where we used the rstrauss package.
3.1. Section overview

First, Section 3.2 reveals how geometric and topological properties of the different models are reflected by suitable test statistics. Then, Section 3.3 illustrates to which extent the approximate asymptotic normality is accurate in bounded sampling windows and for models that go beyond those covered by the sufficient conditions in Theorems 2.1 and 2.2. Finally, Section 3.4 compares the power of goodness-of-fit tests for the statistics considered in Sections 3.2 and 3.3.

3.2. Exploratory analysis

In this section, we illustrate how different test statistics behave for the six tessellation models described in Section 3. We illustrate in the kernel-density estimates in Figure 3 three prototypical examples of model characteristics, namely face areas, face inradii and vertex-based persistences.

To begin with, we consider the distribution of the face areas in the six models. Due to the higher variability, faces with a very small area occur far more often in the Binomial than in the Strauss models. This difference becomes even more pronounced when focussing on exceptionally large cells. Moreover, in the force-biased models the histograms have a clear peak corresponding to an area that is substantially bounded away from 0. Qualitatively, we can make similar observations for the persistence (i.e. lifetime) of features in the vertex-based filtration from Section 2.2. In particular, the kernel-density estimates in Figure 3 illustrate that long lifetimes of features are common in the force-biased model. For the face-inradii from Section 2.1, the differences between the models are far less pronounced. Moreover, we observe that in all cases, the histograms corresponding to the Voronoi and to the Laguerre model are very similar.

3.3. Asymptotic normality

The exploratory analysis in Section 3.2 already revealed that suitable geometric and topological statistics can uncover substantial differences between considered models. In the next step, we use these summary statistics to devise goodness-of-fit tests. We have experimented with different forms of statistics and in general found the ones concentrating on...
the upper tails to have the highest testing power. Hence, we will use the following three statistics.

(1) **Face areas.** The statistic

$$T_{\text{Area}} := \# \{ f \in \mathbb{S}_n^{(2)} : |f| > a_{\text{Area}} \}$$

counts the number of tessellation faces $f$ with area $|f|$ exceeding a given threshold $a_{\text{Area}} > 0$.

(2) **Face inradii.** The statistic

$$T_I := \# \{ f \in \mathbb{S}_n^{(2)} : \eta(f) > a_I \}$$

counts the number of tessellation faces $f$ with face-inradii time $\eta(f)$ exceeding a given threshold $a_I > 0$.

(3) **Persistence in tessellation-adapted filtrations.** The statistic

$$T_{\text{Pers}} := \# \{ j : D_j - B_j > a_{\text{Pers}} \}$$

counts the number of features in the tessellation-adapted persistence diagram from Section 2.2 with lifetime exceeding a given threshold $a_{\text{Pers}} > 0$.

For selecting critical values of the tests, we rely on the approximate normality in large domains. We will first discuss why asymptotic normality is plausible from a conceptual viewpoint (especially in light of Theorems 2.1 and 2.2), before providing numerical evidence that the normal approximation is already accurate in the considered sampling windows.

First, we note that the number of tessellation faces whose inradius exceeds a fixed threshold corresponds to the edge-based persistent Betti numbers $\beta_{\text{e},M,s}^n$, where to simplify the implementation, we have not enforced the technical restriction to faces with eccentricity at most $M$. As we will discuss in the following paragraph, although some of the technical assumptions needed in the proof of Theorem 2.1 are not satisfied in our simulation study, the numerical evidence provided in Figure 4 illustrates convincingly that the asymptotic normality remains plausible in this more general setting.

For Poisson-Voronoi and Laguerre tessellations, Flimmel et al. (2020, Theorem 2.3) show asymptotic normality of geometric functionals of cells subject to certain stabilisation and moment conditions. In particular, the distribution function of the cell volume and the aggregated cell surface area are provided as specific examples. It is plausible that the methods can be extended to yield asymptotic normality of more complicated statistics on the face areas, and also when suitable Gibbs processes are used as generators. Again, our numerical results will make this belief credible.

Finally, we move to the $M$-localised persistent Betti numbers. Here, we recall that for fixed $d \geq b \geq 0$ the test statistic $\beta_{n,1}^{M,b,d}$ counts the number of $1$-features that are born before time $b$ and die after time $d$. However, to recover the number of features exceeding a given lifetime a single test statistic $\beta_{n,1}^{M,b,d}$ does not suffice. This is similar to the situation considered in Biscio et al. (2020). There, it was shown that the sum of all lifetimes is a continuous functional in $\beta_{n,1}^{M,b,d}$, when considered as a 2-parameter process in the entries $b, d \geq 0$. This
Figure 4. Standardised distributions of $T_{\text{Area}}$, $T_{t}$, and $T_{\text{Pers}}$ (top, middle and bottom). From left to right, each row shows the Binomial-Voronoi, Strauss-Voronoi, force-biased Voronoi, Binomial-Laguerre, Strauss-Laguerre and force-biased Laguerre model.

stresses the importance of functional limit theorems (such as Theorem 2.2), since then the classical continuous mapping theorem makes it possible to derive the asymptotic normality for persistence-based test statistics that go beyond simple linear combinations of individual persistent Betti numbers.

In Theorems 2.1 and 2.2, the normality of the considered test statistics is established only in the limit of unboundedly large windows, this leaves the question to what extent the normal distribution is already appropriate for bounded sampling windows. Moreover, as mentioned above, some of the models described in Section 3 do not satisfy all of the technical conditions that we imposed in order to be able to prove Theorems 2.1 and 2.2 rigorously, namely:

1. the number of cells is fixed in the Voronoi case.
2. the tessellation edges have no thickness;
3. the tessellation vertices are not perturbed;
4. the inequality $\tau \leq |B_1(o)|^{-1} \exp(\beta m_{0}^{\Psi})(r_0 + 1)^{-p}$ is violated;
5. the support of the mark distribution $\mathcal{Q}$ may be unbounded;
6. the restriction of considering only $M$-localised features is dropped;
7. the restrictions on $\text{size}(f)$ are dropped;
8. the tessellation-adapted filtration is formed with respect to the alpha complex rather than the Čech complex.
We stress that we are confident that the asymptotic normality of Betti numbers holds under less restrictive conditions than the ones described in Theorems 2.1 and 2.2. As we will elaborate in further detail below, numerical evidence for this hypothesis is one of the major contributions from our simulation study.

In accordance with the tests to be derived in Section 3.4, we fix the thresholds $a_{\text{Area}}$, $a_{1}$ and $a_{\text{Pers}}$ as the 40%, 60% and 70% quantiles of the corresponding test statistics under the considered null model. To fix the specific threshold levels, we used several pilot runs to determine which values have the potential to lead to promising goodness-of-fit tests.

Figure 4 compares the density of the standard normal distribution with the standardised test statistics based on 1,000 simulation runs. On a very general level, we draw the conclusion that the asymptotic normality is already reasonably accurate in moderately large windows.

### 3.4. Power analysis

Now, we analyse the power of goodness-of-fit tests derived from the statistics $T_{\text{Area}}$, $T_{1}$ and $T_{\text{Pers}}$ for the six models introduced in the beginning of Section 3. To that end, we proceed as follows. First, we generate 1,000 realisations from each of the six models to determine the distribution of the test statistics under the respective null hypotheses.

That is, for each test statistic $T$ and null model, we compute the empirical mean and variance from these realisations. Assuming a normal distribution, we can construct asymptotic confidence intervals that yield the acceptance region of the tests. For evaluating the powers of the test, we generate a new set of 1,000 realisations per model. The hypothesis that one of these realisations is generated by a tessellation model $M_{0}$ is rejected, if the test statistic $T$ for the data falls outside the confidence interval of $T$ under model $M_{0}$. The power of the test is then obtained as the proportion of simulations where the null hypothesis is rejected.

Table 1 summarises these findings. First, we observe that the rejection rates along the diagonal are mostly fairly close to the nominal 5%-level. Second, although the face areas are a relatively elementary characteristic of the data, we see that the test $T_{\text{Area}}$ is already quite powerful in a variety of testing scenarios. This is most clearly seen when distinguishing between the models Bin-Vor and St-Lag, and between the models St-Vor and St-Lag. Although, in many cases the inradii- and persistence-based statistics $T_{1}$ and $T_{\text{Pers}}$ lead to lower rejection rates, we see a substantial improvement for the cases where Bin-Lag and St-Lag are the null models and Bin-Vor and St-Vor are the alternatives, respectively. This already gives an indication that these new statistics can provide additional insights in settings where the traditional approaches fail. In the real data example in Section 4 below, we will see an additional example for the added value of the persistence-based characteristics.

We also note that in general $T_{\text{Area}}$ seems quite powerful. However, the low rejection rate for St-Lag against St-Vor is remarkable. Looking closer on the simulated data, we have found the following tentative explanation, which should be taken with caution. The mean values for St-Lag and St-Vor are very close (2737.48 versus 2752.046), whereas the variance for St-Lag is considerably larger than for St-Vor (41 versus 30). A similar effect can be observed for Bin-Lag and Bin-Vor (with variances 46 versus 30). We hypothesise that the higher variance for St-Lag is caused by the additional randomness induced by the random radii. Note that we consider only large facets and that the marking is carried out independently. In the Voronoi tessellation, facet sizes are mainly governed by the distances between the
Table 1. Rejection rates in percentage points for the goodness-of-fit tests based on $T_{\text{Area}}$, $T_{\text{I}}$ and $T_{\text{Pers}}$. Each row describes the null model that is used to compute the mean and variance for the test based on asymptotic normality; each column corresponds to the alternative for which the test statistic is computed.

| $H_0 \setminus H_1$ | $T_{\text{Area}}$ | $T_{\text{I}}$ | $T_{\text{Pers}}$ |
|---------------------|-------------------|----------------|------------------|
|                     | Bin--Vor | St--Vor | Fb--Vor | Bin--Lag | St--Lag | Fb--Lag | Bin--Vor | St--Vor | Fb--Vor | Bin--Lag | St--Lag | Fb--Lag | Bin--Vor | St--Vor | Fb--Vor | Bin--Lag | St--Lag | Fb--Lag |
| Bin--Vor            | 4.7      | 98.7    | 100.0   | 22.8     | 92.1    | 100.0   | 5.8      | 4.6     | 84.3    | 16.0     | 12.4    | 99.2    |
| St--Vor             | 99.0     | 5.5     | 100.0   | 97.5     | 15.1    | 100.0   | 49.4     | 4.6     | 80.1    | 14.3     | 10.7    | 98.9    |
| Fb--Vor             | 100.0    | 100.0   | 5.5     | 100.0    | 100.0   | 99.9    | 75.4     | 72.4    | 4.0     | 55.9     | 63.0    | 12.5    |
| Bin--Lag            | 0.5      | 86.4    | 100.0   | 6.4      | 74.3    | 100.0   | 3.0      | 1.5     | 56.3    | 5.1      | 4.6     | 92.3    |
| St--Lag             | 89.7     | 1.3     | 100.0   | 86.9     | 3.4     | 100.0   | 3.0      | 1.6     | 61.4    | 5.9      | 5.5     | 93.9    |
| Fb--Lag             | 100.0    | 100.0   | 97.2    | 100.0    | 100.0   | 5.5     | 99.0     | 99.1    | 27.7    | 92.5     | 95.9    | 5.3     |

points. In the Laguerre tessellation, quite different facet systems can be generated from the same point configuration when modifying the weights.

In order to assess the robustness of this finding, we have carried out a further simulation: we considered a Laguerre tessellation, where the $\sigma$-parameter of the lognormal distribution was increased from 0.47 to 1. The $\mu$-parameter was chosen such that mean volume remains the same. As expected, the variance of the face areas increases drastically compared to the Voronoi case, namely from 41 to 82. We also still obtain a very low rejection rate for St-Lag against St-Vor, namely 7.2%. Note that this is a bit higher than in the previous simulation, which can be explained by the fact that for the new simulation the two mean values are a bit further apart.

4. Application to foam data

We now apply the testing methodology to a dataset describing the structure of an open aluminium alloy foam. A cubic sample of edge length 40 mm is spatially imaged by micro computed tomography at voxel size 29.44 $\mu$m. The foam cells show an elongation in $y$-direction (Jung et al. 2022). Hence, we consider a rescaled version of the image to obtain an isotropic cell system. Cells are reconstructed by using the watershed transform, see Jung et al. (2022) for details. The resulting dataset consists of 962 cells in a $[1,657] \times$
Figure 5. 2D section of the original foam data (left) and the fitted Laguerre model (right).

\[ [1, 533] \times [1, 642] \] voxel sampling window. To represent this dataset in the form of a tessellation, we compute a Laguerre approximation by the method from Šedivý et al. (2016). Figure 5 shows a 2D section of the original dataset and the corresponding section in the Laguerre tessellation. This comparison illustrates that the Laguerre approximation gives a good representation of the original dataset.

Using the test statistics presented in Section 3, we want to perform goodness-of-fit tests for several tessellation models for the foam structure. More precisely, we will investigate the face areas, face inradii as well as the persistences based on the tessellation-adapted filtration. In order to avoid edge effects, we restrict our analysis to the 356 cells that are entirely contained in the sampling window.

We compare characteristics of the foam dataset to those of four different stochastic models of increasing complexity. In the first two models, we consider two standard tessellation models from stochastic geometry, namely Binomial- and Strauss-Voronoï tessellations. As a prototypical example, we consider a highly repulsive point process with \( \gamma = 0.01 \) and \( R = 60 \). We first construct the stochastic models by using periodic boundary conditions, and then only retain the cells contained entirely in the sampling window. We choose the intensities of tessellation models so as to give in expectation 356 remaining cells. As more refined models, we consider a Laguerre tessellation based on a forced-biased sphere packing and its relaxation by the Surface Evolver (Brakke 1992). Both models are fitted to first and second moments of geometric characteristics of the foam cells, see Jung et al. (2022) for details.

4.1. Exploratory analysis

In a first step, in Figure 6 (left), we compare the face-area distributions of the model and of the data. We observe a clear difference between the two point-process based Voronoï models and the data. Both the Binomial-Voronoï and the Strauss-Voronoï tessellations exhibit a high variance: a substantial proportion of faces may exhibit a very small or a very large area. The main differences between the dataset and the force biased model are that the model still has too many faces with very small areas, and is also too sharply concentrated...
around the mode. We also see that in the current example, the relaxation through the Surface Evolver is slightly too aggressive in the sense that small face areas are removed entirely in this configuration, whereas there are still some faces with small areas in the dataset.

A similar effect is also visible for the face inradii as shown in Figure 6 (middle). Here, the Binomial-Voronoi and Strauss-Voronoi models exhibit a larger variability of the face inradii than the foam dataset. The sphere packing and surface evolver models lead to inradii distributions that are far more similar to the one observed in the data. However, in both models the concentration around the mode is a bit more pronounced than what we observe in the data.

Finally, in Figure 6 (right), we consider the total persistences. Again, we see that the Voronoi and Strauss models produce substantially too many small values. In contrast, the surface evolver model essentially removes all small persistences, whereas there are still some in the foam dataset. When considering just the persistences, the sphere packing model results in a good approximation to the foam data.

Here, we decided to rely on the widely used python-package seaborn for generating the kernel-density estimates. The bandwidth was computed with Scott’s rule of thumb. We note that seaborn does not implement boundary corrections. Hence, we applied a simple boundary correction for a positive-valued sample: we first transform the data to a log-scale, then compute the KDE with the log-transformed sample and, to get an estimator of the original density in a fixed point $x$, we divide the estimate for the transformed sample by $x$.

Finally, we proceed to the persistence diagram on the tessellation-adapted filtration. In comparison to the face inradii, now a slightly more sophisticated analysis is needed, since the features with respect to this filtration have both non-zero birth- and death times. Nevertheless, Figure 7 reinforces the previous observations: whereas the data is strongly concentrated, both the Voronoi and the Strauss model exhibit substantial fluctuations and noise. We also see that the evolver model produces fewer small persistences than observed in the foam dataset.

4.2. Goodness of fit tests

Finally, we apply the goodness-of-fit tests from Section 3.3 to the present datasets. To that end, we are guided by the exploratory analysis from Section 4.1, and choose the thresholds $a_{\text{Area}}, a_I, a_{\text{Pers}}$ to be the 40%, 60% and 70% quantiles of the test statistics $T_{\text{Area}}, T_I$ and $T_{\text{Pers}}$ under the null model. To compute the mean and variance under the Binomial and Strauss models we generated 1,000 realisations. Due to the high computational costs, for
the sphere packings we used only 100 realisations. In Table 2, we present the z-scores for the goodness of fit test of the considered null models to the specific dataset.

First, we see that the null-models of a Binomial-Voronoi or a Strauss-Voronoi tessellation are clearly rejected for all tests. Moreover, we stress that the highest z-scores occur for the persistence-based test statistic. This hints at the potential of TDA-based methods to assess the fit of classical random spatial tessellation models to data from materials science. Moreover, we see that the more advanced sphere-packing and evolver models lead to much lower z-scores, indicating by relying on such models it is possible to obtain substantially more realistic representations of the data set in contrast to the traditional standard models from stochastic geometry. As observed in Section 4.1 for the specific example, the removal of the small surfaces in the surface evolver is too aggressive, thereby leading to higher rejection rates than for the standard sphere packing.

5. Concluding remarks

In this article, we have developed a statistical methodology to test the goodness of fit of Gibbs-based Voronoi and Laguerre tessellations based on statistics derived from a tessellation-adapted form of persistent homology. We analysed the validity and performance of such tests for finite sample sizes in a simulation study. Finally, we illustrated how to apply our methods to a spatial tessellation originating from real foam data.

Our simulation study strongly suggests that the asymptotic normality of the test statistics should hold under substantially less restrictive assumptions than the ones imposed at the moment. In particular, it would be attractive to treat Gibbs processes with a fixed number of generators, to loosen the intensity constraint, and to allow for more flexible boundary conditions as well as possibly unbounded Laguerre marks. Furthermore, we believe that the constraint to the approximate $M$-bounded and $M$-localised Betti numbers is an artefact of our proofs and should not be needed from a conceptual perspective. Moreover, we believe that many of our methods can be generalised to other tessellation models such as Johnson-Mehl tessellations.
Concerning the simulation and data study, we have so far not attempted to search for the most powerful test statistic. We have also not yet developed a clear heuristic, which test statistic is the most suitable for a given dataset. Moreover, for the dataset studied in Section 4, all of the test statistics clearly reject inappropriate null models. It would be interesting, to consider also datasets where the topological discrepancies from the null model are more subtle so that the refined persistence-based methods can unfold their full potential.

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