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MASTER THESIS

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Generalized random tessellations, their properties, simulation and applications

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Abstract: Abstract.

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Contents

Possibly only refer to sections, not subsections?

1. Geometric preliminaries

Spell-check everything!

Chapter intros give overviews

Before diving into the mathematics of Gibbs-Laguerre-Delaunay tetrahedrization models, we must first lay out the fundamentals of their geometric and combinatorial structure. The key geometric components are the the circumball for Delaunay tetrahedrizations and characteristic point for Laguerre tetrahedrizations. We will first study their geometry and then analyze their structure in terms of hypergraphs.

Notation and basic terms

This text will predominantly focus on *marked* points in $\mathbb{R}^3$, that is elements of $\mathbb{R}^3 \times S$, where $S = [0, W], W > 0$ is the *mark set*. A great deal of care must be dedicated to clearly distinguish between *positions* of points (their projection to $\mathbb{R}^3$) and their *marks*[1] (projection to S). To this end, we adopt the following notation. A point $p \in \mathbb{R}^3 \times S$ has the position $p' \in \mathbb{R}^3$ and mark $p'' \in S$. Similarly, the notation of sets follows accordingly — the Borel σ-algebra on $\mathbb{R}^3 \times S$ will be denoted $\mathcal{B}$, its counterpart on $\mathbb{R}^3$ will be denoted $\mathcal{B}'$. The subset of $\mathcal{B}$ ($\mathcal{B}'$) containing only bounded sets is $\mathcal{B}_0$ ($\mathcal{B}'_0$).

A *configuration* is a set $\mathbf{x} \in \mathbf{N}_{lf}$, where

$$\mathbf{N}_{lf} = \{\mathbf{x} \subset \mathbb{R}^3 \times S : \operatorname{card}(\mathbf{x} \cap B) < \infty, B \in \mathcal{B}_0\}$$

be the set of locally finite sets on $\mathbb{R}^3 \times S$. Let $\mathbf{N}_f \subset \mathbf{N}_{lf}$ be the set of all finite sets on $\mathbb{R}^3 \times S$. Lastly, for $\Lambda \in \mathcal{B}'_0$, playing the role of the observation window, denote

$$\mathbf{N}_\Lambda = \{\mathbf{x} \in \mathbf{N}_f : \mathbf{x}' \subset \Lambda\}.$$

A subset of $\mathbf{x}$ will be denoted η. If $\operatorname{card}(\eta) = 4$, then η is *tetrahedral* or a *tetrahedron*. The symbols $\mathbf{x}' = \operatorname{pr}_{\mathbb{R}^3}(\mathbf{x}), \eta' = \operatorname{pr}_{\mathbb{R}^3}(\eta)$ again refer only to the positional part.

Probably comment here on the fact that $|\Lambda|$ will be assumed to be positive

1.1 Tetrahedrizations

The aim of this section is to introduce the geometric concepts necessary for the understanding of two types of tetrahedrizations: Delaunay and Laguerre. The main focus of this text lies on the Laguerre tetrahedrization and thus Delaunay tetrahedrization will receive significantly less attention and often will be treated only as a special case. Note that although this text focuses solely on the three dimensional case, most ideas remain valid for a triangulation in any dimension.

Reference some resources on Delaunay and Laguerre-Delaunay

We introduce the notion of (reinforced) general position, a traditional assumption on configurations.

[1] Marks will also be often called weights.

Definition 1. Let $\mathbf{x} \in \mathbf{N}_{lf}$. We say $\mathbf{x}$ is in **general position** if

$$\eta \subset \mathbf{x}, 2 \leq \operatorname{card}(\eta) \leq 3 \Rightarrow \eta' \text{ is affinely independent in } \mathbb{R}^3.$$

Denote $\mathbf{N}_{gp} \subset \mathbf{N}_{lf}$ the set of all locally finite configurations in general position.

Comment on the fact that we need a vector space with measurable inner product etc?

It's sufficient to check only subsets with $d+1$ points

Definition 2. Let $\mathbf{x} \in \mathbf{N}_{gp}$. We say $\mathbf{x}$ is in **reinforced general position** if

$$\eta \subset \mathbf{x}, 3 \leq \operatorname{card}(\eta) \leq 4 \Rightarrow \eta' \text{ is not cocircular.}$$

Denote $\mathbf{N}_{rgp}$ the set of all locally finite configurations in reinforced general position.

This definition is possibly not even needed

Again, only need to check $d+2$

1.1.1 Delaunay tetrahedrization

This section will shortly introduce the three dimensional equivalent of the well known Delaunay triangulation. While the configurations in this section are technically marked sets, none of the terms take marks into consideration, as the Delaunay tetrahedrization relies on positions only.

Add references to resources

Definition 3. Let $\mathbf{x} \in \mathbf{N}_{gp}$, $\eta \subset \mathbf{x}$. An open ball $B(\eta, \mathbf{x})$ such that $\eta' \subset \partial B(\eta, \mathbf{x})$ is called a *circumball of* η. The boundary $\partial B(\eta, \mathbf{x})$ is called a *circumsphere*. Let $\eta \subset \mathbf{x}$, $\operatorname{card}(\eta) = 4$, be a tetrahedron. Then we will denote its (uniquely defined) circumball by $B(\eta)$ as its definition does not depend on $\mathbf{x}$.

Definition 4. Let $\mathbf{x} \in \mathbf{N}_{gp}$ and $\eta \subset \mathbf{x}$. We say that $(\eta, \mathbf{x})$ satisfies the *empty ball property* if $B(\eta, x) \cap \mathbf{x}' = \emptyset$. For convenience, for $\mathbf{x} \in \mathbf{N}_{lf} \setminus \mathbf{N}_{gp}$, we define any $\eta \subset \mathbf{x}$ that does not satisfy the assumptions of general position as not satisfying the empty ball property.

Definition 5. Let $\mathbf{x} \in \mathbf{N}_{lf}$. Define the set

$$\mathcal{D}(\mathbf{x}) := \{\eta \subset \mathbf{x} : \eta \text{ satisfies the empty ball property }\}.$$

and its subsets

$$\mathcal{D}_k(\mathbf{x}) := \{\eta \in \mathcal{D}(\mathbf{x}) : \operatorname{card}(\eta) = k\}, \quad k = 1, \ldots, 4.$$

We then define the *Delaunay tetrahedrization of* $\mathbf{x}$ as the set $\mathcal{D}_4(\mathbf{x})$.

The set $\mathcal{D}_4$ contains the structure we would expect from the name tetrahedrization, namely it contains sets of 4-tuples of points whose convex hull are the tetrahedra forming the Delauany tetrahedrization. The fact that we've defined the set $\mathcal{D}_k(\mathbf{x})$ for any $k = 1, \ldots, 4$ reflects the hypergraph approach to these structures presented in Section 1.2.

Possibly remark on existence and uniqueness, although this is not that interesting under this definition

The following proposition shows one important property of the set $\mathcal{D}_2(\mathbf{x})$ for any $\mathbf{x} \in \mathbf{N}_{lf}$ — it contains the edges of the (undirected) nearest neighbor graph.

Proposition 1. *Define*

$$\mathrm{NNG}(\mathbf{x}) = \Big\{\{p,q\} \subset \mathbf{x}\times\mathbf{x} : p \neq q, \|p-q\| \leq \|p-s\|, s \in \mathbf{x}\setminus\{p\}\Big\}.$$

Then

$$\mathrm{NNG}(\mathbf{x}) \subset \mathcal{D}_2(\mathbf{x}).$$

Proof. Let $\mathbf{x} \in \mathbf{N}_{lf}$ and $\eta = \{p,q\} \in \mathrm{NNG}(\mathbf{x})$. WLOG assume that q is the nearest neighbor of p. Then $B(p,\|p-q\|) \cap \mathbf{x}' = \{p\}$. Then η satisfies the empty ball property with the circumball $B(\eta,\mathbf{x}) := B((p+q)/2, \|p-q\|/2) \subset B(p,\|p-q\|)$. □

$x \in B(\eta,\mathbf{x})$ implies $\|x-a\| < \mathrm{diam}(B(\eta,\mathbf{x})) = \|p-q\|/2$

Possibly remark on the relationship between individiual $\mathcal{D}_k$. It would be useful later.

1.1.2 Laguerre tetrahedrization

Short intro to Laguerre with some references

The key information to understanding the geometry of Laguerre tetrahedrizations is that a point $p = (p', p'') \in \mathbb{R}^3 \times S$ can be interpreted as an open ball $B(p', \sqrt{p''})$. We will call $B_p = B(p', \sqrt{p''})$ the *ball defined by* p. We define the sphere $S_p = \partial B_p$.

Definition 6. Define the *power distance* of the unmarked point $q' \in \mathbb{R}^3$ from the point $p = (p', p'') \in \mathbb{R}^3 \times S$ as

$$d(q',p) = \|q'-p'\|^2 - p''.$$

Much intuition can be gained from properly understanding the geometric interpretation of the power distance.

Remark 1 (Geometric interpretation of power distance). We split the interpretation into two cases.

- $d(q',p) \geq 0$. The point q' lies outside of B_p. The quantity $\sqrt{d(p,q')}$ can be understood as the length of the line segment from q' to the point of tangency with B_p [fig]. The power distance is equal to zero precisely when q' lies on the boundary B_p.

- $d(q',p) < 0$. The point q' lies inside of B_p. The quantity $\sqrt{d(p,q')}$ now describes the length of the segment $q's'$, where $s' \in S_p$ such that the triangle $\Delta p'q's'$ has a right angle $\angle p'q's'$.

This whole section really needs figures.

Definition 7. For two (marked) points $p = (p', p'')$ and $q = (q', q'')$, define their *power product*[2] by

$$\rho(p,q) = \|p'-q'\|^2 - p'' - q''.$$

Notice that $\rho(p,q) = d(p,q') - q'' = d(q,p') - p''$ and that $\rho(p,(q',0)) = d(p,q')$.

[2] The motivation for calling the quantity $\rho(p,q)$ a product is most fascinating. It was first introduced by G. Darboux in 1866 as a generalization of the power distance. However, it was later discovered that the spheres can be represented as vectors in a pseudo-Euclidean space where the power product plays the role of the quadratic form that defines the space, often called the inner product. The resulting space is then the Minkowski space — the setting in which the special theory of relativity is formulated. The positions of the sphere centres are then the positions in space, whereas the radius denotes a position in time. More can be found in e.g. Kocik [2007].

Similarly to the power distance, the power product has a geometric interpretation that is vital to the understanding of the geometry of Laguerre tessellations.

Remark 2 (Geometric interpretation of power product). Let $p, q \in \mathbb{R}^3 \times S$ be two points. The following observations follow immediately from the definiton.

- $B_p \cap B_q = \emptyset$. We obtain $\|p' - q'\|^2 \geq (\sqrt{p''} + \sqrt{q''})^2 = p'' + q'' + 2\sqrt{p''}\sqrt{q''}$ and thus $\rho(p,q) \geq 2\sqrt{p''q''}$.

- $B_p \subset B_q$. We obtain $\|p' - q'\| + \sqrt{p''} \leq \sqrt{q''}$. Squaring the inequality yields $\rho(p,q) \leq -2\sqrt{p''q''}$.

- $B_p \cap B_q \neq \emptyset$ and neither is a proper subset of the other. This case is the most important for us. In this case, the spheres S_p and S_q intersect and $S_p \cap S_q$ is a circle. Denote $a' \in S_p \cap S_q$ the point of their intersection (it does not matter which) and θ the angle $\angle p'a'q'$. We then obtain from the law of cosines.

  $$-2\sqrt{p''q''}\cos\theta = \|p' - q'\|^2 - p'' - q'' = \rho(p,q)$$

  Note that $\theta = \pi \Rightarrow \rho(p,q) = 0$.

Some diagram to visualise the proposition

The above observations allow us to interpret the power product as a kind of distance of two marked points. The case $\rho(p,q) = 0$ is crucial for the Laguerre geometry. If p and q satisfy this equality then they are said to be *orthogonal*.

We are now well-equiped to define the central terms necessary for the definition of the Laguerre tetrahedrization.

Definition 8. Let $\eta \in \mathbf{N}_{gp}$. Define the *characteristic point* of η as the point $p_\eta = (p'_\eta, p''_\eta) \in \mathbb{R}^3 \times \mathbb{R}$ which is orthogonal to every $p \in \eta$. If such point exists, we call η *Laguerre-cocircular*.

Visualise that there's no simple relationship between $B(\eta)$ and p''_η?

An alternative way to describe the characteristic point is by the equality

$$d(p'_\eta, p) = p''_\eta \text{ for each } p \in \eta. \tag{1.1}$$

Note that the mark of the characteristic point can be any real number and thus isn't limited to $S = [0, W]$ unlike the points of $\mathbf{x}$. If its weight is positive, the characteristic point can be interpreted as a sphere that intersects each sphere $S_p, p \in \eta$ at a right angle. If negative, Edelsbrunner and Shah [1996] has suggested p_η to be thought of as a sphere with an imaginary radius, though as far as we are aware, there is no further advantage to be gained from such interpretation.

The following proposition looks at the existence and uniqueness of the characteristic point.

Proposition 2 (Existence and uniqueness of the characteristic point). *Let $\eta \in \mathbf{N}_{gp}$. Then the following holds for the characteristic point p_η.*

1. *If* $\operatorname{card}(\eta) < 4$*, then the p_η exists and is not unique.*

2. *If* $\operatorname{card}(\eta) = 4$*, then the* p_η *exists and is unique.*

3. *If* $\operatorname{card}(\eta) > 4$*, then the* p_η *exists if and only if* η *is Laguerre-cocircular.*

Proof. .

Possibly rewrite this, or add a lemma that shows general position =¿ full row rank (for ≤ 4 rows)

We will look at the case $\operatorname{card}(\eta) = 4$, from which the rest will follow. Let $\eta = \{p_1, \ldots, p_4\}$ and denote the coordinates of p'_i as $x_i, y_i, z_i, i = 1, \ldots 4$. The characteristic point p_η must satisfy the set of equations

Not really follow, more like be directly observable

$$\|p'_\eta - p'_i\|^2 - p''_\eta - p''_i = 0 \quad i = 1, \ldots, 4$$

If we denote $\alpha = x_\eta^2 + y_\eta^2 + z_\eta^2 - p''_\eta$, where (x_η, y_η, z_η) are the coordinates of p'_η, we obtain the equations

$$\alpha - 2x_i x_\eta - 2y_i y_\eta - 2z_i z_\eta = w_i - x_i^2 - y_i^2 - z^2,$$

a system of equations which is linear with respect to $(\alpha, x_\eta, y_\eta, z_\eta)$. In an augmented matrix form, the system is written as

$$\left(\begin{array}{cccc|c} 1 & -2x_1 & -2y_1 & -2z_1 & p''_1 - x_1^2 - y_1^2 \\ 1 & -2x_2 & -2y_2 & -2z_2 & p''_2 - x_2^2 - y_2^2 \\ 1 & -2x_3 & -2y_3 & -2z_3 & p''_3 - x_3^2 - y_3^2 \\ 1 & -2x_4 & -2y_4 & -2z_4 & p''_4 - x_4^2 - y_4^2 \end{array}\right) \tag{1.2}$$

The fact that $\eta \in \mathbf{N}_{gp}$ implies that $p'_1, \ldots, p'_4$ are affinely independent, i.e. not coplanar. This means that the homogenous system of linear equations defined by the matrix

$$\begin{pmatrix} 1 & x_1 & y_1 & z_1 \\ 1 & x_2 & y_2 & z_2 \\ 1 & x_3 & y_3 & z_3 \\ 1 & x_4 & y_4 & z_4 \end{pmatrix} \tag{1.3}$$

does not have a solution, that is, the matrix has full rank. If it did, the points $p'_1, \ldots, p'_4$ would all satisfy the equation $Ax + By + Cz + D = 0$ for some $A, B, C, D \in \mathbb{R}$. The matrix 1.3 has the same column space as the left hand side of 1.2 and therefore the system has a unique solution.

If $\operatorname{card}(\eta) < 4$, we would obtain an underdetermined system, having either infinitely many or no solutions. Here, again, the general position property gives us full row rank of the left side of the augmented matrix, implying that there are infinitely many solutions. For $\operatorname{card}(\eta) = 2$, general position implies that the points are unequal. For $\operatorname{card}(\eta) = 3$, general position implies that the points are not collinear.

Write clearer later

If $\operatorname{card}(\eta) > 4$, the system is overdetermined and has no solution, unless the whole augmented matrix has rank 4. For e.g. $|\eta| = 5$, this means that the homogenous system given by the matrix

$$\begin{pmatrix} 1 & x_1 & y_1 & z_1 & x_1^2 + y_1^2 + z_1^2 - p''_1 \\ 1 & x_2 & y_2 & z_2 & x_2^2 + y_2^2 + z_2^2 - p''_2 \\ 1 & x_3 & y_3 & z_3 & x_3^2 + y_3^2 + z_3^2 - p''_3 \\ 1 & x_4 & y_4 & z_4 & x_4^2 + y_4^2 + z_4^2 - p''_4 \\ 1 & x_5 & y_5 & z_5 & x_5^2 + y_5^2 + z_5^2 - p''_5 \end{pmatrix}$$

has a solution. However, this is equivalent to saying that there exists p_η such that $\rho(p_\eta, p_i) = 0$, i.e. that η is Laguerre-cocircular. $\square$

Definition 9. Let $p, q \in \mathbb{R}^3 \times S$. We call the set

$$H(p,q) = \{x \in \mathbb{R}^3 : d(x,p) = d(x,q)\}$$

the *radical hyperplane* of p and q.

Proposition 3. *$H(p,q)$ is a hyperplane in $\mathbb{R}^3$ for any $p, q \in \mathbb{R}^3 \times S$. Let $\{p_1, \ldots, p_k\} = \eta \subset \mathbf{x} \in \mathbf{N}_{gp}$, $k = 2, 3, 4$. If*

$$p' \in \bigcap_{i,j=1,\ldots,4} H(p_i, p_j), \tag{1.4}$$

then p' is the position of the characteristic point of η. Lastly, if $|\eta| = 4$, then the uniquely defined characteristic point p_η is characterized by

$$p'_\eta = H(p_1,p_2) \cap H(p_1,p_3) \cap H(p_1,p_4). \tag{1.5}$$

Proof. By simple calculation we have

$$H(p,q) = \{x \in \mathbb{R}^3 : 2\langle q' - p', x\rangle = \|q'\|^2 - \|p'\|^2 - q'' + p''\}.$$

From 1.1 we obtain the characterization 1.4. For a tetrahedral η, we know from Proposition 2 that p_η is uniquely defined. To obtain 1.5, we only need to realize that three hyperplanes are sufficient to specify the set of points $x \in \mathbb{R}^3$ for which $d(x,p_i) = d(x,p_j), i,j = 1, \ldots, 4$. □

Notice that changing the weight of either of the points amounts to translation of the hyperplane.

We not introduce the equivalent of the empty sphere property for the Laguerre case.

Definition 10. Let $x \in \mathbf{N}_{gp}$ be a configuration, $\eta \subset \mathbf{x}$ and p_η its characteristic point. We say that the pair $(\eta, \mathbf{x})$ is *regular*, or that η is *regular in* $\mathbf{x}$, if $\rho(p_\eta, p) \geq 0$ for all $p \in \mathbf{x}$. For convenience, for $\mathbf{x} \in \mathbf{N}_{lf} \setminus \mathbf{N}_{gp}$, we define any $\eta \subset \mathbf{x}$ that does not satisfy the assumptions of general position as not regular.

The definition can also be equivalently stated as

$$\text{There is no point } q \in \mathbf{x} \text{ such that } d(p'_\eta, q) < p''_\eta.$$

The regularity property ensures that no point of $\mathbf{x}$ is closer to the characteristic point p_η in the power distance than the points of η. This is analogous to the empty ball property in Delaunay tetrahedrization, where the circumball plays the role of the characteristic point.

c.f. remark that comes later

Definition 11. Let $\mathbf{x} \in \mathbf{N}_{lf}$. Define the set

$$\mathcal{LD}(\mathbf{x}) := \{\eta \subset \mathbf{x} : \eta \text{ is regular}\}.$$

and its subsets

$$\mathcal{LD}_k(\mathbf{x}) := \{\eta \in \mathcal{LD}(\mathbf{x}) : \text{card}(\eta) = k\}, \quad k = 1, \ldots, 4.$$

We then define the *Laguerre tetrahedrization of* $\mathbf{x}$ as the set $\mathcal{LD}_4$.

It might be a good idea to characterize the relationsihp between individual $\mathcal{LD}_k$.

Remark 3 (Constructing Laguerre and Delaunay tetrahedrization). The proof of Proposition 2 also gives a hint on how to check whether η is regular. Gavrilova [1998]

TO BE DONE

Cocircular points do not create multiplicities in the cliques, since we're limiting k to max 4

Remark 4 (Invariance in weights). Let $w \in \mathbb{R}$. Denote $\mathbf{x}_w = \{(p', p'' + w) : (p', p'') \in \mathbf{x}\}$ be the set of points of $\mathbf{x}$ with added weight w. Notice that $\eta \subset \mathbf{x}_w$ is regular if and only if the corresponding $\eta \subset \mathbf{x}$ is regular. This implies that the Laguerre tetrahedrization is invariant under the map $\mathbf{x} \mapsto \mathbf{x}_w$ for any w such that the marks of $\mathbf{x}_w$ still lie in $[0, W]$.

Explain this more

Remark 5 (Delaunay as a special case of Laguerre). Let $\mathbf{x} \in \mathbf{N}_{lf}$ be a configuration where all points have mark 0. Then for any $\eta \subset \mathbf{x}, \operatorname{card}(\eta) = 4$ the ball B_{p_η} defined by the characteristic point of η becomes precisely $B(\eta)$, the circumball of η. Similarly η is regular if and only if η satisfies the empty ball property. Notice that by the previous remark, the same property must hold if we replace the mark 0 by any $w \in [0, W]$. Thus for a configuration $\mathbf{x}$ with equal marks we have

$$\mathcal{D}_4(\mathbf{x}) = \mathcal{LD}_4(\mathbf{x})$$

and the Delaunay tetrahedrization can be seen as merely a special case of Laguerre tetrahedrization, albeit very important.

Redundant points

A major difference in the Laguerre case from the Delaunay case is the fact that some points may not play any role in the resulting structure.

Definition 12. We call a point $p \in \mathbf{x}$ *redundant in* $\mathbf{x}$ if $\mathcal{LD}(\mathbf{x}) = \mathcal{LD}(\mathbf{x} \setminus \{p\})$.

To find more about redundant points, it is useful to introduce the notion of a Laguerre cell.

Definition 13. Let $p \in \mathbf{x}$. We then define the *Laguerre cell of* p *in* $\mathbf{x}$, denoted C_p, as the set

$$C_p := \{x' \in \mathbb{R}^3 : d(x', p) \leq d(x', q)\ \forall q \in \mathbf{x}\}.$$

Proposition 4. *A point* p *is redundant if and only if* $C_p = \emptyset$.

Proof. ($\Leftarrow$) Assume p is not redundant. That means there exists a regular $\eta \subset \mathbf{x}$ with a characteristic point p_η such that $\rho(q, p_\eta) = 0$ for all $q \in \eta$ and $\rho(q, p_\eta) \geq 0$ for all $q \in \mathbf{x}$. This however means that $d(p'_\eta, p) = p''_\eta \leq d(p'_\eta, q)$ for all $q \in \mathbf{x}$, implying $p'_\eta \in C_p$.
($\Rightarrow$) Assume $C_p \neq \emptyset$. There exist $x' \in C_p$ and $q \in \mathbf{x}, q \neq p$, such that $d(x', q) = d(x', p)$, due to continuity of the power distance. But this implies that the point $p_\eta = (x', d(x', p))$ is the characteristic point of $\eta = \{p, q\}$ and that η is regular. $\square$

Apart from the empty Laguerre cell, there is, to our knowledge, no simple geometric characterization of a redundant point. There is however a necessary condition.

Proposition 5. *If p is redundant in $\mathbf{x}$, then the sphere B_p is completely contained in the balls of other points in $\mathbf{x}$, that is*

$$B_p \subset \bigcup_{q \in \mathbf{x} \setminus \{p\}} B_q.$$

Proof. Assume there exists $x' \in B_p$ such that $x' \notin B_q$ for any $q \neq p$. Then $x' \in C_p$, since $d(x', p) \leq 0$, while $d(x', q) \geq 0$ for all $q \in \mathbf{x}, q \neq p$. $\square$

This definitely needs a figure + some comment on the fact that it's not an equivalence

From the above proposition we can also see why there cannot be any redundant points in $\mathcal{D}(\mathbf{x})$, since in the Delaunay case all balls have radius 0.

Do we need to restrict it on non-redundant points? Measurability?

Perhaps talk about lifting - additional intuition on how this stuff works

1.2 Hypergraph structures

Are graphs geometric? I mean, geometric graphs are geometric. But graphs in general? Are potentials part of this?

Both Delaunay and Laguerre tetrahedrizations can be seen as graphs where two points $p, q \in \mathbf{x}$ are joined if they are part of the same tetrahedron with the empty sphere property, or the regularity property. However, for the purposes of this text, a more natural structure will be the hypergraph.

1.2.1 Tetrihedrizations as hypergraphs

Here we already need to have defined the σ-algebras on $\mathbf{N}_{lf}$ and $\mathbf{N}_f$, which are defined in section 2.

Definition 14. A *hypergraph structure* is a measurable subset $\mathcal{E}$ of $(\mathbf{N}_f \times \mathbf{N}_{lf}, \mathcal{N}_f \otimes \mathcal{N}_{lf})$ such that $\eta \subset \mathbf{x}$ for all $(\eta, \mathbf{x}) \in \mathcal{E}$. We call η a *hyperedge* of $\mathbf{x}$ and write $\eta \in \mathcal{E}(\mathbf{x})$, where $\mathcal{E}(\mathbf{x}) = \{\eta : (\eta, \mathbf{x}) \in \mathcal{E}\}$. For a given $\mathbf{x} \in \mathbf{N}_{lf}$, the pair $(\mathbf{x}, \mathcal{E}(\mathbf{x}))$ is called a *hypergraph*.

A hypergraph is thus a generalization of a graph in the sense that edges are now allowed to "join" any number of points. A hypergraph structure can be thought of as a rule that turns a configuration $\mathbf{x}$ into the hypergraph $(\mathbf{x}, \mathcal{E}(\mathbf{x}))$. The subset $\eta \subset \mathbf{x}$ now plays the role of a hyperedge. e.g. a tetrahedron.

The beauty in this approach is that we do not need to impose any additional structure on $\mathcal{D}(\mathbf{x})$ or $\mathcal{LD}(\mathbf{x})$ — they already directly define a hypergraph structure!

Definition 15 (Delaunay and Laguerre-Delaunay hypergraph structures)**.** Define the hypergraph structues

- $\mathcal{D} = \{(\eta, \mathbf{x}) : \eta \in \mathcal{D}(\mathbf{x})\}$
- $\mathcal{D}_k = \{(\eta, \mathbf{x}) : \eta \in \mathcal{D}_k(\mathbf{x})\}, k = 1, \ldots, 4$
- $\mathcal{LD} = \{(\eta, \mathbf{x}) : \eta \in \mathcal{LD}(\mathbf{x})\}$
- $\mathcal{LD}_k = \{(\eta, \mathbf{x}) : \eta \in \mathcal{LD}(\mathbf{x})\}, k = 1, \ldots, 4$

The symbol $\mathcal{LD}$ only makes sense now, when it's Laguerre-Delaunay. Comment on it before or sth.

Hyperedge potentials

The set $\mathcal{E}$ defines the structure of the hypergraph. What we are ultimately interested in is assigning a numeric value to each hyperedge and thus to (a region of) the hypergraph. To this end, we define the *hyperedge potential*.

Definition 16. A *hyperedge potential* is a measurable function $\varphi : \mathcal{E} \to \mathbb{R} \cup \{+\infty\}$.
Hyperedge potential is *shift-invariant* if

$$(\vartheta_x \eta, \vartheta_x \mathbf{x}) \in \mathcal{E} \text{ and } \varphi(\vartheta_x \eta, \vartheta_x \mathbf{x}) = \varphi(\eta, \mathbf{x}) \text{ for all } (\eta, \mathbf{x}) \in \mathcal{E} \text{ and } x \in \mathbb{R},$$

where $\vartheta_x(\mathbf{x}) = \{(x', x'') \in \mathbb{R}^3 \times S : (x' + x, x'') \in \mathbf{x}\}$ is the translation of the positional part of the configurations by the vector $-x \in \mathbb{R}^3$.

For notational convenience, we set $\varphi = 0$ on $\mathcal{E}^c$.

The fact that the hyperedge potential contains $\mathbf{x}$ as a second argument suggests that it is allowed to depend on points of $\mathbf{x}$ other than those in η.
For the remainder of this text, we will always assume any hyperedge potential to be shift-invariant.

Define a proper Example environment with title and a possibility of a reference

Example. [Hyperedge potentials] The hyperedge potential can take various forms. As we will see later, its specification radically alters the distribution of the resulting Gibbs point process and thus it allows a great freedom in the types of hypergraphs we can obtain.
Volume of tetrahedron: For $\eta \in \mathcal{E}(\mathbf{x})$ on $\mathcal{D}_4$ or $\mathcal{LD}_4$ define

$$\varphi(\eta, \mathbf{x}) = |\text{conv}(\eta)|.$$

Where $\text{conv}(\eta)$ is the convex hull of η.
Hard-core exclusion: For $\eta \in \mathcal{E}(\mathbf{x})$ on $\mathcal{D}_4$ or $\mathcal{LD}_4$, $\alpha > 0$ define

$$\varphi(\eta, \mathbf{x}) = \delta(\eta) \quad \text{if } \delta(\eta) \leq \alpha$$

$$\varphi(\eta, \mathbf{x}) = \infty \quad \text{if } \delta(\eta) > \alpha$$

Where $\delta(\eta) = \text{diam} B(\eta)$ is the diameter of the circumscribed ball. Notice that this potential becomes infinite on tetrahedra with circumdiameter larger than α. As we will see later, this allows us to restrict the resulting tetrahedronization only those tetrahedra η for which $\varphi(\eta, \mathbf{x}) \leq \alpha$.
Laguerre cell interaction: For $\eta \in \mathcal{E}(x)$ on $\mathcal{LD}_2$ such that $\eta = \{p, q\}$ and $|C_p| < \infty, |C_q| < \infty$, $\theta \neq 0$, define

$$\varphi(\eta, \mathbf{x}) = \theta \left(\frac{\max(Vol(C_p), Vol(C_q))}{\min(Vol(C_p), Vol(C_q))} - 1 \right)$$

where the potential now depends on the size of neighboring Laguerre cells. Notice that θ can be negative, yielding a negative potential.
Tetrahedral interaction: In the present setting, we cannot specify interaction between tetrahedra in $\mathcal{D}_4$ or $\mathcal{LD}_4$ as easily as between Laguerre cells. This can be solved by for example defining a new hypergraph structure

$$\mathcal{LD}_4^2 = \{(\eta, \mathbf{x}) : \exists \eta_1, \eta_2 \in \mathcal{LD}_4(\mathbf{x}), \text{card}(\eta_1 \cap \eta_2) = 3, \eta = \eta_1 \cup \eta_2\}$$

Which contains the quintuples of points which form adjacent tetrahedra in $\mathcal{LD}_4(\mathbf{x})$. $\blacksquare$

This works, but it's not as simple this may suggest. η can create $2, 3$, or 4 tetrahedra and the hyperedge potential must take that into account.

Definition 17. A hyperedge potential ϕ is *unary* for the hypergraph structure $\mathcal{E}$ if there exists a measurable function $\hat{\varphi} : \mathbf{N}_{lf} \to \mathbb{R} \cup \{+\infty\}$ such that

$$\varphi(\eta, \mathbf{x}) = \hat{\varphi}(\eta) \text{ for } \eta \in \mathcal{E}(\mathbf{x}).$$

The value of an unary hyperedge potential depends only on the points from η, as long as $\eta \in \mathcal{E}(x)$. Recall however the convention $\varphi = 0$ on $\mathcal{E}^c$, thus the equality above cannot be extended to all $\eta \subset \mathbf{x}$. In example 1.2.1, only the first two potentials are unary. Broken reference

For a given hypergraph structure $\mathcal{E}$, the *energy function* of a finite configuration $\mathbf{x} \in \mathbf{N}_f$ is defined as the function[3]

$$H(\mathbf{x}) = \sum_{\eta \in \mathcal{E}(\mathbf{x})} \varphi(\eta, \mathbf{x}).$$

However, in our case, we will typically deal with $\mathbf{x} \in \mathbf{N}_{lf}$, for this such potentials would typically be equal to $\pm\infty$ or even be undefined. We will therefore be interested in the energy for only a bounded window $\Lambda \in \mathcal{B}'_0$. Currently, we don't have the necessary terms to describe such energy function precisely, thus we will postpose its definition to the next section.

The words *potential* and *energy* point to a connection with statistical mechanics, which gave rise to many of the concepts used in this text. Indeed, Gibbs measure and concepts related to them continue to be an area with a rich interplay between statistical mechanics and probability theory[4].

1.2.2 Hypergraph potentials and locality

Reformulate the intro

A natural question to ask is "How do the hyperedges of $\mathcal{E}(\mathbf{x})$ influence each other?". We have seen that there is a type of locality at play, for example the empty ball property of a tetrahedron $\eta \in \mathcal{D}_4(\mathbf{x})$ is dependent solely on presence of points of $\mathbf{x}$ inside $B(\eta)$. As we will see in Chapters 2 and 3, this locality is essential for the existence of our models and Gibbs measures in general. The question is also further complicated by the presence of the hyperedge potential. This section will refine our understanding of the question by defining different locality properties.

Definition 18. A set $\Delta \in \mathcal{B}'_0$ is a *finite horizon* for the pair $(\eta, \mathbf{x}) \in \mathcal{E}$ and the hyperedge potential φ if for all $\tilde{\mathbf{x}} \in \mathbf{N}_{lf}, \tilde{\mathbf{x}} = \mathbf{x}$ on $\Delta \times S$

$$(\eta, \tilde{\mathbf{x}}) \in \mathcal{E} \text{ and } \varphi(\eta, \tilde{\mathbf{x}}) = \varphi(\eta, \mathbf{x}).$$

The pair $(\mathcal{E}, \varphi)$ satisfies the *finite-horizon property* if each $(\eta, \mathbf{x}) \in \mathcal{E}$ has a finite horizon.

[3] The energy H is often also called *Hamiltonian* in statistical mechanics.

[4] In fact, Gibbs measures, named after Josiah Willard Gibbs, stood at the forefront of emergence of statistical mechanics — Gibbs, who coined the term "statistical mechanics" was one of the founders of the field.

The finite horizon of $(\eta, \mathbf{x})$ delineates the region outside which points can no longer violate the regularity (or the empty ball property) of η. Note also that for an unary potential, the finite horizon of $(\eta, \mathbf{x}) \in \mathcal{E}$ depends only on η.

Assume potentials are unary, since that's what I am talking about after this point

Remark 6 (Finite horizons for $\mathcal{D}$ and $\mathcal{LD}$). For $\mathcal{D}$, the closed circumball $\bar{B}(\eta, \mathbf{x})$ itself is a finite horizon for $(\eta, \mathbf{x})$.

For $\mathcal{LD}$, the situation is slightly more difficult. For one, $B(p'_\eta, \sqrt{p''_\eta})$ does not contain the points of η. To see this, take two points p, q with $p'', q'' > 0$ such that $\rho(p, q) = 0$. Then $q'' = d(q', p) < \|q' - p'\|^2$ and thus $\sqrt{q''} < \|q' - p'\|$. More importantly, however, any point s outside of $B(p'_\eta, \sqrt{p''_\eta})$ with a sufficiently large weight can violate the inequality $\rho(p_\eta, s) = \|p'_\eta - x'\|^2 - p''_\eta - s'' \geq 0$.

To obtain a finite horizon for $\mathcal{LD}$, we need to use the fact that the mark space is bounded, $S = [0, W]$. If $s'' \leq W$, then $\Delta = B(p'_\eta, \sqrt{p''_\eta + W})$ is sufficient as a horizon, since any point s outside Δ satisfies

$$\rho(p_\eta, s) = \|p'_\eta - s'\|^2 - p''_\eta - s'' \geq (\sqrt{p''_\eta + W})^2 - p''_\eta - W = 0.$$

From a practical perspective, the maximum weight W limits the resulting tessellation in the sense that the difference of weights can never be greater than W. Marks greater than W are not necessarily a problem, as we can always find an identical tessellation with marks bounded by W, as long as there are no two points p, q with $|p'' - q''| > W$ (see Remark 4).

This remark is probably more fitting for the simulation chapter

Let us now return again to the task of defining an energy function H that depends on the configuration in some bounded window $\Lambda \in \mathcal{B}'_0$. To that end, we must define the set of hyperedges for which the hyperedge potential depends on the configuration inside Λ.

Definition 19. Let $\Lambda \in \mathcal{B}'_0$. Define the set of

$$\mathcal{E}_\Lambda(\mathbf{x}) := \{\eta \in \mathcal{E}(\mathbf{x}) : \varphi(\eta, \zeta \cup \mathbf{x}_{\Lambda^c}) \neq \varphi(\eta, \mathbf{x}) \text{ for some } \zeta \in \mathbf{N}_\Lambda\}.$$

In the Laguerre case, we could also distinguish marks, but we won't do so, maybe comment on it

Recall that we have defined $\varphi = 0$ on $\mathcal{E}^c$. This means that for $\eta \in \mathcal{E}(\mathbf{x})$ such that $\varphi(\eta, \mathbf{x}) \neq 0$ we have

$$\eta \notin \mathcal{E}(\zeta \cup \mathbf{x}_{\Lambda^c}) \text{ for some } \zeta \in \mathbf{N}_\Lambda \Rightarrow \eta \in \mathcal{E}_\Lambda(\mathbf{x})$$

Notice that $\mathbf{x}_\Lambda$ does not play any role in the definition in the sense that $\mathcal{E}_\Lambda(\mathbf{x}) = \mathcal{E}_\Lambda(\zeta \cup \mathbf{x})$ for any $\zeta \in \mathbf{N}_\Lambda$. The configuration $\mathbf{x}$ thus only plays the role of a boundary condition.

To further characterize $\mathcal{E}_\Lambda(\mathbf{x})$, we present the following lemma.

Lemma 1. *Let $\eta \in \mathcal{E}(\mathbf{x})$ have the finite horizon Δ. Then*

$$\eta \in \mathcal{E}_\Lambda(\mathbf{x}) \Rightarrow \Delta \cap \Lambda \neq \emptyset$$

Proof.

$$\begin{aligned}
\eta \in \mathcal{E}_\Lambda(\mathbf{x}) &\iff \exists \zeta \in \mathbf{N}_\Lambda : \varphi(\eta, \mathbf{x}) \neq \varphi(\eta, \zeta \cup \mathbf{x}_{\Lambda^c}) \\
&\Rightarrow \exists \zeta \in \mathbf{N}_\Lambda : \zeta' \cap \Delta \neq \emptyset \\
&\Rightarrow \Lambda \cap \Delta \neq \emptyset
\end{aligned}$$

□

The fact that we don't have equivalence is a consequence of the fact that $\zeta \in \Delta$ does not imply that it changes η. But this fact is true the unary potentials, so comment on that.

With the definition of $\mathcal{E}_\Lambda(\mathbf{x})$, we are now ready for the desired definition of the energy function.

Definition 20. Let $\Lambda \in \mathcal{B}_0'$, $\zeta \in \mathbf{N}_\Lambda$. The *energy of* ζ *in* Λ *with boundary condition* $\mathbf{x}$ is given by the formula

$$H_{\Lambda,\mathbf{x}}(\zeta) = \sum_{\eta \in \mathcal{E}_\Lambda(\zeta \cup \mathbf{x}_{\Lambda^c})} \varphi(\eta, \zeta \cup \mathbf{x}_{\Lambda^C})$$

for $\zeta \in \mathbf{N}_\Lambda$, provided the sum is well-defined.
For the case $\zeta = \mathbf{x}_\Lambda$ we use the shortened notation $H_\Lambda(\mathbf{x}) := H_{\Lambda,\mathbf{x}}(\mathbf{x}_\Lambda)$.

The usage of e.g. $\mathcal{D}_\Lambda(\mathbf{x})$ should probably be commented upon

Remark 7 ($\mathcal{E}_\Lambda(\mathbf{x})$ for $\mathcal{D}$ and $\mathcal{LD}$). For $\mathcal{D}$, $\eta \in \mathcal{D}_\Lambda(\mathbf{x}) \iff B(\eta, \mathbf{x}) \cap \Lambda \neq \emptyset$.
For $\mathcal{LD}$, $\eta \in \mathcal{LD}_\Lambda(\mathbf{x}) \iff d(p_\eta', \Lambda) \leq \sqrt{p_\eta'' + W}$, where $d(p_\eta', \Lambda) = \inf\{\|p_\eta' - x\| : x \in \Lambda\}$ is the distance of p_η' from Λ.

Explain why

Confusing notation, d is reserved for the power distance

The final basic term again characterizes a type of finite-range property, this time as a property of the configuration $\mathbf{x}$.

Definition 21. Let $\Lambda \in \mathcal{B}_0'$ be given. We say a configuration $\mathbf{x} \in N$ *confines the range of* φ *from* Λ if there exists a set $\partial\Lambda(\mathbf{x}) \in \mathcal{B}_0'$ such that $\varphi(\eta, \zeta \cup \tilde{\mathbf{x}}_{\Lambda^c}) = \varphi(\eta, \zeta \cup \mathbf{x}_{\Lambda^c})$ whenever $\tilde{\mathbf{x}} = \mathbf{x}$ on $\partial\Lambda(\mathbf{x}) \times S$, $\zeta \in \mathbf{N}_\Lambda$ and $\eta \in \mathcal{E}_\Lambda(\zeta \cup \mathbf{x}_{\Lambda^c})$. In this case we write $\mathbf{x} \in N_{\mathrm{cr}}^\Lambda$. We denote $r_{\Lambda,\mathbf{x}}$ the smallest possible r such that $(\Lambda + B(0,r)) \setminus \Lambda$ satisfies the definition of $\partial\Lambda(\mathbf{x})$. We will use the abbreviation $\partial_\Lambda \mathbf{x} = \mathbf{x}_{\partial\Lambda(\mathbf{x})}$.

While the set $\mathcal{E}_\Lambda(\mathbf{x})$ contains hyperedges η which can be influenced by points in Λ, the set $\partial_\Lambda \mathbf{x}$ contains those points of $\mathbf{x}$ that influence the value of those η. This allows us to express $H_{\Lambda,\mathbf{x}}$ truly locally.

Proposition 6. *Let* $\mathbf{x} \in N_{\mathrm{cr}}^\Lambda$. *Then*

$$H_{\Lambda,\mathbf{x}}(\zeta) = \sum_{\eta \in \mathcal{E}_\Lambda(\zeta \cup \partial_\Lambda \mathbf{x})} \varphi(\eta, \zeta \cup \partial_\Lambda \mathbf{x}).$$

Proof. The definition of N_{cr}^Λ implies the hyperedge potential does not depend on the points $\mathbf{x} \setminus \partial_\Lambda \mathbf{x}$ and $\mathcal{E}_\Lambda(\mathbf{x})$ inherits this property by its definition through the hyperedge potential. □

Comment on the definition and what it means for $\mathcal{D}$ and $\mathcal{LD}$.

It probably is unclear that we're going to be talking about $\mathcal{D}_4$ afterwards, i.e. tetrahedrizations only

Remark 8. [Adding and removing points in $\mathcal{D}_4$ and $\mathcal{LD}_4$] Let $\mathbf{x} \in \mathbf{N}_{lf}$ be a configuration and $x \in (\mathbb{R}^3 \times S) \setminus \mathbf{x}$ a point outside the configuration. The question is: how does $\mathcal{LD}_4(\mathbf{x} \cup \{x\})$ differ from $\mathcal{LD}_4(\mathbf{x})$? First imagine we want to add the point x to $\mathbf{x}$. Denote the set

$$\mathcal{LD}_4^{\otimes}(x, \mathbf{x}) := \{\eta \in \mathcal{LD}_4(\mathbf{x}) : \rho(p_\eta, x) < 0\}.$$

Then this set contains precisely those tetrahedra, which cannot be present in $\mathcal{LD}_4(\mathbf{x} \cup \{x\})$, that is

$$\mathcal{LD}_4(\mathbf{x}) \setminus \mathcal{LD}_4(\mathbf{x} \cup \{x\}) = \mathcal{LD}_4^{\otimes}(x, \mathbf{x}).$$

Now take $\eta \in \mathcal{LD}_4(\mathbf{x} \cup \{x\})$ such that $x \notin \eta$. Then $\eta \notin \mathcal{LD}_4^{\otimes}(x, \mathbf{x})$ and thus $\eta \in \mathcal{LD}_4(\mathbf{x})$, yielding

$$\mathcal{LD}_4(\mathbf{x} \cup \{x\}) \setminus \mathcal{LD}_4(\mathbf{x}) = \{\eta \in \mathcal{LD}_4(\mathbf{x} \cup \{x\}) : x \in \eta\} =: \mathcal{LD}_4^{\ell}(x, \mathbf{x} \cup \{x\}).$$

Using the same logic we can now remove the point x from $\mathbf{x} \cup \{x\}$. This means we remove $\eta \in \mathcal{LD}_4^{\ell}(x, \mathbf{x} \cup \{x\})$ and add $\eta \in \mathcal{LD}_4^{\otimes}(x, \mathbf{x})$.

In $\mathcal{D}_4$, we obtain similar sets

$$\mathcal{D}_4^{\otimes}(x, \mathbf{x}) := \{\eta \in \mathcal{D}_4(\mathbf{x}) : x \in B(\eta)\},$$

$$\mathcal{D}_4^{\ell}(x, \mathbf{x}) := \{\eta \in \mathcal{D}_4(\mathbf{x}) : x \in \eta\}.$$

We note that the sets denoted by $\otimes$ stand for *conflicting* tetrahedra and the ℓ stands for tetrahedra *linked* to x.

2. Stochastic geometry

Rewrite the introduction

In the first chapter we have introduced tetrahedrizations as hypergraph structures and defined their energy in terms of the hyperedge potential. Ultimately we want to study their behaviour under some probabilistic assumptions on the distribution of the configuration $\mathbf{x}$.

This chapter introduces the theory of point processes which will allow us to add stochasticity to the hypergraph structures. The main goal of this chapter is to introduce the Gibbs-type tessellation, where the location of the points are allowed to interact with the geometric properties of the tessellation, giving us a great freedom in the specification of our models.

2.1 Point processes

In Chapter 1 we studied the behaviour of the hypergraph structures for a fixed configuration. In this section, we will shift the view from the configuration as fixed deterministic set to configuration as a particular realization of a ranom point process. We develop only the bare minimum of the theory of point processes necessary to define and use Gibbs point processes. For a comprehensive introductory text, we recommend Moller and Waagepetersen [2003], as it is most relevant to our case.

In general, we assume E to be a locally compact separable space. This is the setting in many texts, such as Schneider [2008].

The main aim of this text is to build Gibbs point processes with interactions based on the Laguerre tetrahedrizaion. As such, the focus is on marked points and the Delaunay case is treated as secondary. To avoid having a dual marked and unmarked theory, we will treat unmarked point as a special case of marked points in the following way.

- Marked case: We take $E = \mathbb{R}^3 \times S$ where $S = [0, W], W > 0$ is the space of marks. The measure on E is $z\lambda \otimes \mu$, where μ is a non-atomic probability distribution of marks, $z > 0$.
- Unmarked case: We use the same space, but the distribution of marks $\mu = \delta_0$ is now concentrated on 0.

2.1.1 Basic terms

Definition 22. Define a *counting measure* on E as a measure ν on E for which

$$\nu(B) \in \mathbb{N} \cup \{0, \infty\}, B \in \mathcal{B}_0(E) \quad \text{and} \quad \nu(\{x\}) \leq 1, x \in E.$$

We say a measure ν is *locally finite* if $\nu(B) < \infty$ for any $B \in \mathcal{B}_0(E)$. Denote $\mathbf{N}_{lf}(E)$ the space of all locally finite counting measures on E. We equip the space $\mathbf{N}_{lf}(E)$ with the σ-algebra

$$\mathcal{N}_{lf}(E) = \sigma(\{\nu \in \mathbf{N}_{lf}(E) : \nu(B) = n\} : B \in \mathcal{B}_0(E), n \in \mathbb{N}_0).$$

Finally we define the set $\mathbf{N}_f(E) \subset \mathbf{N}_{lf}(E)$ of finite measures on E by

$$\mathbf{N}_f(E) = \{\nu \in \mathbf{N}_{lf}(E) : \nu(E) < \infty\}$$

with the σ-algebra $\mathcal{N}_f$ defined as the trace σ-algebra of $\mathbf{N}_f(E)$ on $(\mathbf{N}_{lf}(E), \mathcal{N}_{lf}(E))$. ▌

Define $\mathbf{N}_\Lambda$

For the case $E = \mathbb{R}^3 \times S$, we use the shortened notation $\mathbf{N}_{lf}(\mathbb{R}^3 \times S) := \mathbf{N}_{lf}$. Similarly for the terms $\mathbf{N}_f, \mathcal{N}_f, \mathcal{N}_{lf}, \mathcal{B}, \mathcal{B}_0$.

I've dropped the dashed notation, but it's still useful. Use it?

Still not quite happy about the measure-set duality. Perhaps γ is always a set, ν a counting measure? Or just use γ always, but limit this chapter too treating it as a measure only?

Remark 9 (Duality of locally finite counting measures and configurations). In chapter 1, we introduced the sets $\mathbf{N}_{lf}$ and $\mathbf{N}_f$ as spaces of (finite) configurations — locally finite sets. This abuse of notation is justified by the fact that there is a measurable bijection between the space of locally finite counting measures (as defined here) and locally finite sets with the Borel σ-algebra on the Fell topology. For details, see lemma 3.1.4. in Schneider [2008].

Whether a configuration is treated as a set or a counting measure will be clear from the context. With this in mind, we introduce the notation

$$x \in \nu \text{ if } \nu(\{x\}) = 1, \quad \nu \in \mathbf{N}_{lf}.$$

Definition 23. A *point process* on E is a measurable mapping $\Phi : (\Omega, \mathcal{A}, P) \to (\mathbf{N}_{lf}(E), \mathcal{N}_{lf}(E))$.
A *marked point process* Φ_m is a point process on $\mathbb{R}^3 \times S$ for which the projection $\Phi_m(\cdot \times S)$ is a point process on $\mathbb{R}^3$.

Note that this definition requires the realizations of the projection of the marked point process to be locally finite counting measures in the sense of Definition 22.

Remark 10 (Simple point process). We have defined the counting measure to have values in $\{0, 1\}$. Such couting measures, as well as the point processes defined through them, are commonly called *simple*. We do not need this distinction here, therefore we do not use the term.

Do we need anything else? Intensity, Campbell?

Poisson point process

Perhaps the most important example of a point process is the Poisson point process which formalizes the notion of a complete spatial randomness. Before we define the Poisson point process, we first define a process closely related it.

Definition 24. Let ν be a measure on E, $B \in \mathcal{B}_0(E)$ such that $0 < \nu(B) < \infty$. For $n \in \mathbb{N}$ let $X_1, \ldots, X_n$ be independent and ν-uniformly distributed random variables on B, that is

$$P(X_i \in A) = \frac{\nu(A)}{\nu(B)}, \; A \in \mathcal{B}(E), A \subset B$$

Then we define the *binomial point process* of n points in B as

$$\Phi(n) = \sum_{i=1}^{n} \delta_{X_i}.$$

We use the convention $\sum_{i=1}^{0} \delta_{X_i} = \varnothing$, where $\varnothing(E) = 0$ is the *empty point process.*

In the marked case, $X_i = (X_i', M_i)$ where X_i' is the position and M_i the mark of X_i and we can write

$$\Phi(n) = \sum_{i=1}^{n} \delta_{(X_i', M_i)}.$$

However, similarly to chapter 1, we only specify the marks where needed, as this approach leads to a cleaner notation.

Improve the connnection of ν to the process

Proposition 7. *Let $\Phi_n = \sum_{i=1}^{n} \delta_{X_i}$ be a binomial point process on $B \in \mathcal{B}_0(E)$ with the measure ν. Then for a non-negative measurable f we have*

$$Ef(X_1, \ldots, X_k) = \frac{1}{\nu(B)^k} \int_B \cdots \int_B f(x_1, \ldots, x_k)\nu(dx_1) \cdots \nu(dx_k), \quad k = 1, \ldots, n \tag{2.1}$$

Proof. From the definition of Φ_n, we have for Borel $A_i \subset B, i = 1, \ldots, k$ that

$$\begin{aligned} P(X_1 \in A_1, \ldots, X_k \in A_k) &= P(X_1 \in A_1) \cdots P(X_k \in A_k) \\ &= \frac{1}{\nu(B)^k} \int_B \cdots \int_B 1_{A_1}(x_1) \cdots 1_{A_k}(x_k)\nu(dx_1) \cdots \nu(dx_k) \end{aligned}$$

That is 2.1 for $f(x_1, \ldots, x_k) = 1_{A_1}(x_1) \ldots 1_{A_k}(x_k)$. By a standard argument, we first extend this to a general set $C \in \mathcal{B}^k(E), C \subset B^k$ using the Dynkin system

$$\{C \in \mathcal{B}^k(E) : E1_C(x_1, \ldots, x_k) = \int \cdots \int 1_C(x_1, \ldots, x_k)dx_1 \cdots dx_k\}$$

and then from indicators to any non-negative measurable function. □

Definition 25. Let $\nu =$ be a measure on E. A point process Φ satisfying

1. $\Phi(B)$ has a Poisson distribution with parameter $\nu(B)$ for each $B \in \mathcal{B}_0(E)$,
2. Conditonally on $\Phi_B = n, n \in \mathbb{N}$, $\Phi|_B$ is the Binomial point process of n points in B, $B \in \mathcal{B}_0(E)$.

is a *Poisson process* on E with *intesity measure* ν. For $B \in \mathcal{B}_0(E)$, denote Π_B^ν the distribution of a Poisson point process with intensity measure ν restricted to B.

Definition 26. We define the *marked Poisson process* is a Poisson process on $\mathbb{R}^3 \times S$ with intensity measure $z\lambda \otimes \mu$. We call the parameter z the *intensity.* For $\Lambda \in \mathcal{B}_0(\mathbb{R}^3)$, denote Π_Λ^z the distribution of a marked Poisson point process with intensity $z\lambda \otimes \mu$ restricted to $\Lambda \times S$. For $z = 1$, we lose the z and denote the distribution simply Π_Λ.

We could also define Π_Λ as the marginal, without marks. Think this through

Note that thanks to 7 we have for a marked Poisson process Φ with intensity z and $\Gamma \in \mathcal{N}_{lf}$

$$\begin{aligned}\Pi^z_\Lambda(\Gamma) = P(\Phi \in \Gamma) &= \sum_{k=0}^{\infty} P(\Phi \in \Gamma | \Phi(\Lambda) = k) P(\Phi(\Lambda) = k) \\ &= \sum_{k=0}^{\infty} \frac{(z|\Lambda|)^k}{k!} e^{-z|\Lambda|} P(\Phi^{(k)} \in \Gamma) \\ &= \sum_{k=0}^{\infty} \frac{z^k}{k!} e^{-z|\Lambda|} \int_{\Lambda\times S} \cdots \int_{\Lambda\times S} 1_\Gamma \left(\sum_{i=1}^{k} \delta_{X_i} \right) \nu(dx_1), \ldots, \nu(dx_k)\end{aligned} \tag{2.2}$$

where $\Phi^{(k)} = \sum_{i=1}^{k} \delta_{(X_i, M_i)}$ denotes the Binomial point process of k points in C and $\nu = \lambda \otimes \mu$.

Remark 11 (Points in general position). In Section 1.1 we introduced the sets $\mathbf{N}_{gp}$ and $\mathbf{N}_{rgp}$. In Zessin [2008], it is proved[1] that these sets are measurable and that for $\Lambda \in \mathcal{B}_0(\mathbb{R}^3)$

$$\Pi^z_\Lambda(\mathbf{N}_{gp}) = \Pi^z_\Lambda(\mathbf{N}_{rgp}) = 0.$$

2.1.2 Finite point processes with density

Maybe we should use $\mathbf{N}_\Lambda$ instead of $\mathbf{N}_f$. Check this

A standard approach in probability theory is to define random variables with distributions absolutely continuous with respect to some reference measure. In Euclidean spaces, the reference measure is typically the Lebesgue or counting measure. In the space $(\mathbf{N}_{lf}, \mathcal{N}_{lf})$ the convenient properties of the Poisson point process make it the perfect candidate for the reference measure. In this chapter, we will restrict ourselves only to the space $(\mathbf{N}_f, \mathcal{N}_f)$ of finite counting measures.

Why Poisson is the best

In this chapter, we limit ourselves entirely to the case $E = \mathbb{R}^3 \times S$. At the same time, we will stop using the term “marked” where we deem it redundant.

Definition 27. We say that a point process Ψ on $\mathbb{R}^3 \times S$ *has the density* p with respect to the Poisson process if its distribution is absolutely continuous w.r.t. Π_Λ with density function p. That is there exists a measurable function $p : \mathbf{N}_f \to \mathbb{R}^+$ such that $\int p(\gamma)\Pi_\Lambda(\gamma) = 1$ and

$$P(\Psi \in \Gamma) = \int_\Gamma p(\gamma) \Pi_\Lambda(d\gamma), \ \Gamma \in \mathcal{N}_f$$

Make the calculations clearer, they're a bit scattered now

Notice that using the calculations in Proposition 7 and 2.2 we have

$$P(\Psi \in \Gamma) = \sum_{k=0}^{\infty} \frac{1}{k!} e^{-|\Lambda|} \int_{\Lambda\times S} \cdots \int_{\Lambda\times S} 1_\Gamma \left(\sum_{i=1}^{k} \delta_{X_i} \right) p \left(\sum_{i=1}^{k} \delta_{X_i} \right) \nu(dx_1) \ldots \nu(dx_k)$$

[1] This fact seems to have been generally accepted as true in the literature for decades, yet — as far as we are aware — no formal proof was ever published until 2008.

where $\nu = \lambda \otimes \mu$. The equation above is a special case of

$$Eh(\Psi) = Eh(\Phi)p(\Phi)$$

for Π_Λ-measurable function h, where $\Phi \sim \Pi_\Lambda$.

A useful function for dealing with point processes with density is the Papangelou conditional intensity.

Definition 28. For a point process Φ with density p we define the *Papangelou conditonal intensity* as

$$\lambda^*(x,\gamma) = \frac{p(\gamma+\delta_x)}{p(\gamma)},\ x \in \mathbb{R}^3 \times S, \gamma \in \mathbf{N}_f : p(\gamma) > 0.$$

An example of a point process with a density, albeit uninteresting, is the Poisson process with intensity z.
Denote the *counting function* for $\Lambda \in \mathcal{B}_0(\mathbb{R}^3)$ and $\gamma \in \mathbf{N}_{lf}$:

$$N_\Lambda(\gamma) = \gamma(\Lambda \times S)$$

Proposition 8. $\Pi^z_\Lambda \ll \Pi_\Lambda$ *with density* $p(\gamma) = z^{N_\Lambda(\gamma)} \exp(|\Lambda|(1-z))$, $\gamma \in N_\Lambda$.

Proof. Denote $\Phi \sim \Pi_\Lambda$, we have for $\Gamma \in \mathcal{N}_f$, using Proposition 7 and 2.2

$$\Pi^z_\Lambda(\Gamma) = E(1_\Gamma(\Phi) z^{|\Phi|} e^{|\Lambda|} e^{-z|\Lambda|})$$

□

2.1.3 Gibbs Point Processes

This section is underdeveloped

At the end of the last section we have found that $\Pi^z_\Lambda \ll \Pi_\Lambda$ with the density $p(\gamma) \propto z^{N_\Lambda(\gamma)}$. The introduction of the Gibbs point process is outwardly simple, since we merely add an additional term containing the energy function from Definition 20, so that the density is proportional to the expression

$$z^{N_\Lambda(\gamma)} e^{-H_\Lambda(\gamma)}. \tag{2.3}$$

By this seemingly small alteration we introduce a great complexity into the structure of the resulting process. Before we proceed with the formal definition of (finite) Gibbs point processes, we must impose some additional assumptions on the energy function.

The energy function

Thanks to the energy function, we can force the realizations of the finite GPP to obey a diverse set of geometrical properties. In our case those geometrical properties come through the hypegraph structures $\mathcal{D}$ and $\mathcal{LD}$, see Example 1.2.1.

In the following, we restrict ourselves to $\mathbf{N}_f$ and for $\gamma \in \mathbf{N}_f$ we denote $H(\gamma) := H_{\mathbb{R}^3}(\gamma)$.

Traditionally, the energy function is required to satisfy some assumptions. Here we list those from Dereudre [2017].

- **Non-degeneracy**:
$$H(\varnothing) < +\infty.$$

I don't really understand the role of $\emptyset$ in Gibbs theory.

- **Hereditarity**: For any $\gamma \in \mathbf{N}_f$ and $x \in \gamma$
$$H(\gamma) < +\infty \Rightarrow H(\gamma - \delta_x) < +\infty.$$

- **Stability**: there exists a constant $c_S \geq 0$ such that for any $\gamma \in \mathbf{N}_f$
$$H(\gamma) \geq c_S \cdot N_{\mathbb{R}^3}(\gamma).$$

Recall also that we assumed all potentials to be shift-invariant and thus any energy function inherits this property.

Stability bounds the density function $p(\gamma) \propto z^{N_\Lambda(\gamma)} e^{-H(\gamma)} \leq (ze^{-c_S})^{N_\Lambda(\gamma)}$ and thus ensures $Z_\Lambda^z < \infty$. Integrability of the density is obviously a necessary assumption and thus some form of stability cannot be avoided. Non-degeneracy, when paired with hereditarity, is a very natural assumption; without it, hereditarity would imply that the energy is always infinite.

The form 2.3 of the density function suggests that the resulting distitribution will favor configurations with low energy. Configurations with high energy are unlikely to happen and an infinite energy means that the configuration is not possible under the distribution. We call such a configuration *forbidden*. A configuration that is not forbidden is *permissible*.

Hereditarity ensures that removing a point will not result in a forbidden configuration. Equivalently it ensures that adding a point to a forbidden configuration will not result in an allowed configuration. This assumption is, however, not necessarily satisfied by our models. Take for example the hard-core exclusion potential from 1.2.1. Removing a point can lead to appearance of a tetrahedron with a larger circumdiameter, thus resulting in a forbidden configuration.

Unlike non-degeneracy or hereditarity, it is not immediately clear what the role of hereditarity is. Luckily for us, it means that we can define Gibbs point processes without the assumption and only then explore its function.

Finite volume Gibbs measures

Definition 29. Let $\mathcal{E}$ be a hypergraph structure and H an energy function on $\mathcal{E}$ such that H is non-degenerate and stable. The *finite Gibbs measure* on $\Lambda \in \mathcal{B}_0(\mathbb{R}^3)$ with activity $z > 0$ is the distribution P_Λ^z such that $P_\Lambda^z \ll \Pi_\Lambda$ with density
$$p(\gamma) = \frac{1}{Z_\Lambda^z} z^{\gamma(\Lambda)} e^{-H(\gamma)}, \quad \gamma \in \mathbf{N}_f,$$

where $Z_\Lambda^z = \int z^{N_\Lambda} e^{-H} \Pi_\Lambda$ is the normalizing constant, called *partition function*. The point process with the distribution P_Λ^z is called the *finite Gibbs point process* (finite GPP).

An important characterization are the **Dobrushin-Lanford-Ruelle** (**DLR**) **equations**.

Proposition 9. *Let $\Delta, \Lambda \in \mathcal{B}_0(\mathbb{R}^3)$ with $\Delta \subset \Lambda$. Then for P^z_Λ-a.s. all γ_{Δ^c}*

$$P^z_\Lambda(d\gamma_\Delta | \gamma_{\Delta^c}) = \frac{1}{Z^z_\Delta(\gamma_{\Delta^c})} z^{N_\Delta(\gamma)} e^{-H_\Delta(\gamma)} \Pi_\Delta(d\gamma_\Delta),$$

where $Z^z_\Delta(\gamma_{\Delta^c}) = \int z^{N_\Delta(\gamma)} e^{-H_\Delta(\gamma)} \Pi_\Delta(d\gamma_\Delta)$ is the normalizing constant.

Proof. .

As of now, this is **not** the same as Dereudre [2017], since we have a different local energy. However, we can probably adapt the proof using Lemma 2. Do so later.

□

The DLR equations express the conditional probability of configurations inside the window Δ, given the configuration outside it.

Comment on DLR. Condtiional probability. Normalizing constant. Possibly integral form?

Infinite volume Gibbs measures

As noted in section 1.2, without extra assumptions on γ, such as the range confinement, the energy H may not be well-defined. We will therefore restrict our definition of infinite volume Gibbs measures, or simply Gibbs measures, only to configurations γ such that $\gamma \in N^\Lambda_{cr}$ for every $\Lambda \in \mathcal{B}_0(\mathbb{R}^3)$. We will learn in Proposition 13 that this restriction does not limit us in any way.

First, we define $\Theta = (\vartheta_x)_{x \in \mathbb{R}^3}$ be the translation group define by the translations ϑ_x from Definition 16. Let $\mathcal{P}_\Theta$ denote the set of all Θ-invariant probability measures on $(\mathbf{N}_{lf}, \mathcal{N}_{lf})$ with $\int N_{[0,1]^3 \times S} dP < \infty$.

maybe connect this to intensity, i.e. define intensity etc

Definition 30. Let $\mathcal{E}$ be a hypergraph structure and H an energy function on $\mathcal{E}$ such that H is non-degenerate and stable. A probability measure $P \in \mathcal{P}_\Theta$ on $(\mathbf{N}_{lf}, \mathcal{N}_{lf})$ is the *Gibbs measure* with activity $z > 0$ if $P(\mathbf{N}^\Lambda_{cr}) = 1$ and

$$\int f dP = \int_{\mathbf{N}^\Lambda_{cr}} \frac{1}{Z^z_\Lambda(\gamma)} \int_{\mathbf{N}_\Lambda} f(\zeta \cup \gamma_{\Lambda^c}) e^{H_{\Lambda,\gamma}(\zeta)} \Pi^z_\Lambda(d\zeta) P(d\gamma)$$

for every $\Lambda \in \mathcal{B}_0(\mathbb{R}^3)$ and every measurable $f : \mathbf{N}_{lf} \to [0, \infty)$.

The definition is a direct analogue of the DLR equations for finite GPP. In fact it is the same relationship, only expressed in integral form

Actually explain this

While defining the Gibbs measure is relative straight-forward, proving its existence is not. The existence and uniqueness of Gibbs measures is an active field of research and one where we still currently do not know much, particularly in case of uniqueness. The non-uniqueness is a consequence of the fact that the existence of a Gibbs measure is typically proven only through proving tightness of a sequence of finite Gibbs measures, thus yielding only a convergent subsequence. We will not delve into the topic any further here and we refer the reader to an introductory text Dereudre [2017] and the paper on which we base the proof of existence for our models, Dereudre et al. [2012]. We also recommend reading the introduction to Georgii [2011 (2nd ed.] — although the book is about Gibbs random fields rather than point processes, the introduction gives an intuitive explanation for the form of the density and in particular the connection of the non-uniqueness with phase transitions.

Hereditary GPP

One of the disadvantages of the characterization through DLR equations is the presence of the normalization constant, as it is, in most cases, unknown. This is where the use of the hereditarity assumption comes in.

For $\gamma \in \mathbf{N}_f$ and $x \in \mathbb{R}^3 \times S$, define the *local energy* of x in γ as

$$h(x, \gamma) = H(\gamma + \delta_x) - H(\gamma),$$

with the convention $+\infty - (+\infty) = 0$. Notice that for $\gamma \in \mathbf{N}_f$ such that $p(\gamma) > 0$, where p is now the density of a finite GPP, we have

$$\lambda^*(x, \gamma) = z \cdot e^{-h(x,\gamma)}.$$

Talk about the fact that it's well-defined thanks to range confinement

We then obtain the following result, known as the **Georgii-Nguyen-Zessin (GNZ)equations**.

Proposition 10. *Let P be a Gibbs measure and $\Lambda \in \mathcal{B}(\mathbb{R}^3)$ such that $|\Lambda| > 0$. For any non-negative measurable function f from $(\mathbb{R}^3 \times S) \times \mathbf{N}_{lf}$ to $\mathbb{R}$,*

$$\int \sum_{x \in \gamma} f(x, \gamma - \delta_x) P(d\gamma) = z \int \int_{\Lambda \times S} f(x, \gamma) e^{-h(x,\gamma)} dx P(d\gamma). \tag{2.4}$$

Furthermore P^z_Λ is uniquely defined by 2.4 in the sense that if a probability measure P on $\mathbf{N}_f$ satisfies 2.4, then $P = P^z_\Lambda$.

Proof. Adapt theorem 2 in sectino 2.5. from Dereudre [2017]?

□

Fix use of P in the above proposition

Check whether the usage of marks is okay here. I think I am forgetting the mark distribution..

Hereditarity thus gives us a powerful characterization of the finite Gibbs measure. Possibly even more important is that a number of estimation techniques (maximum pseudolikelihood used here being one of them) make use the Papangelou conditional intensity and GNZ equations, thus the presence of non-hereditarity provides a direct obstacle to estimation.

Luckily, the approach in Dereudre and Lavancier [2009] allows us to directly use GNZ equations even for the non-hereditary case.

Possibly cite the later edition? What's the approach here?

Non-hereditary

Having defined the Gibbs measure, we can now continue to present the approach of Dereudre and Lavancier [2009] extending the GNZ equations to Gibbs point processes with non-hereditary energy functions.

First define

$$\mathbf{N}_\infty = \{\mathbf{x} \in \mathbf{N}_{lf} : \forall \Lambda \in B_0(\mathbb{R}^3) : H_\Lambda(\mathbf{x}) < \infty\},$$

the set of all permissible configurations.

Measurability?

Definition 31. Let $\gamma \in \mathbf{N}_\infty$. We say $x \in \gamma$ is *removable* if

$$\text{there exist } \Lambda \in \mathcal{B}(\mathbb{R}^3) \text{ such that } x \in \Lambda \text{ and } H_\Lambda(\gamma - \delta_x) < \infty$$

Lemma 2. *There exists a measurable function* $\psi_{\Delta,\Lambda} : \mathbf{N}_{lf} \to \mathbb{R} \cup \{+\infty\}$ *such that*

$$\forall \gamma \in \mathbf{N}_{lf}, \quad H_\Lambda(\gamma) = H_\Delta(\gamma) + \psi_{\Delta,\Lambda}(\gamma_{\Delta^c})$$

Proof. To find such function, we only need to realize that

$$H_\Lambda(\gamma) - H_\Delta(\gamma) = \sum_{\eta \in \mathcal{E}_\Lambda(\gamma) \setminus \mathcal{E}_\Delta(\gamma)} \varphi(\eta, \gamma)$$

depends only on γ_{Δ^c}. As noted below the Definition 19, both $\mathcal{E}_\Delta(\gamma)$ and $\mathcal{E}_\Lambda(\gamma)$ depend only on γ outside the window Λ and Δ respectivelly.By $\eta \notin \mathcal{E}_\Delta(\gamma)$ we have that $\forall \zeta \in \mathbf{N}_\Delta : \varphi(\eta, \gamma) = \varphi(\eta, \zeta \cup \gamma_{\Delta^c})$ and thus we can set

$$\psi_{\Delta,\Lambda}(\gamma_{\Delta^c}) = \sum_{\eta \in \mathcal{E}_\Lambda(\gamma_{\Delta^c}) \setminus \mathcal{E}_\Delta(\gamma_{\Delta^c})} \varphi(\eta, \gamma_{\Delta^c}).$$

□

Say what the set is equal to for us

Proposition 11. *Let* $\gamma \in \mathbf{N}_\infty$, *then* $x \in \gamma$ *is removable if and only if* $\gamma - \delta_x \in \mathbf{N}_\infty$.

Proof. Follows from Lemma 2 above and Proposition 1 in Dereudre and Lavancier [2009]. □

Definition 32. Let x be a removable point in a configuration γ in N. The local energy of x in $\gamma - \delta_x$ is defined as

$$h(x, \gamma - \delta_x) = H_\Lambda(\gamma) - H_\Lambda(\gamma - \delta_x)$$

where $\Lambda \in \mathcal{B}_0(\mathbb{R}^3)$

Let us remark that such set always exists by definition and that the value of $h(x, \gamma - \delta_x)$ does not depend on the choice of Λ as a consequence of 2.

Proposition 12. *Let P be a stationary Gibbs measure. For every bounded non-negative measurable* $f : (\mathbb{R}^3 \times S) \times \mathbf{N}_{lf} \to \mathbb{R}$ *we have*

$$\int 1_{\mathbf{N}_\infty}(\gamma) \sum_{x \in \gamma} f(x, \gamma - \delta_x) P(d\gamma) = z \int \int f(x, \gamma) e^{-h(x,\gamma)} dx P(d\gamma).$$

Proof. See Proposition 2 in Dereudre and Lavancier [2009]. □

But what about marks, does it work?

Note that we lose the converse implication. That is the GNZ equations no longer characterize Gibbs point process with non-hereditary energy function. Imagine a measure P under which γ a.s. does not contain any removable points. The equation then becomes the trivial equation $0 = 0$.

Measurability!

2.2 Random tessellations

Is there any use for this section? We power the tessellations entirely through the point generators and we don't make use of any facts from stochastic geometry.

3. Existence of Gibbs-type models

In this chapter, the theorem from Dereudre et al. [2012] will be presented and then we will proceed to verify its assumptions for our models.

3.1 Existence theorem

In this section we first state the two existence theorems from Dereudre et al. [2012] and then proceed to introduce its assumptions.

Theorem 1. *For every hypergraph structure $\mathcal{E}$, hyperedge potential φ and activity $z > 0$ satisfying **(S)**, **(R)** and **(U)** there exists at least one Gibbs measure.*

Theorem 2. *For every hypergraph structure $\mathcal{E}$, hyperedge potential φ and activity $z > 0$ satisfying **(S)**, **(R)** and **($\hat{\mathbf{U}}$)** there exists at least one Gibbs measure.*

Proofs of both theorems can be found in Dereudre et al. [2012], see also remark 3.7. in the same paper about the marked case.

3.1.1 Stability

A standard assumption without which it is impossible to define the Gibbs measure is the stability assumption.

(S) *Stability.* The energy function H is called *stable* if there exists a constant $c_S \geq 0$ such that

$$H_{\Lambda,\mathbf{x}}(\zeta) \geq -c_S \cdot \mathrm{card}(\zeta \cup \partial_\Lambda \mathbf{x})$$

for all $\Lambda \in \mathcal{B}_0, \zeta \in \mathbf{N}_\Lambda, \mathbf{x} \in N_{\mathrm{cr}}^{\Lambda}$.

The first thing to note that when φ is non-negative, then we can simply choose $c_S = 0$. The interesting cases therefore is when φ can attain negative values.

Stability in $\mathbb{R}^2$

TO BE DONE

Stability in $\mathbb{R}^3$

TO BE DONE

Possibly move the discussion to an appendix

Could we at least use spread for gibbs with limited distance between points?

Assumption 1: All hyperedge potentials in the remained of this text are assumed to be non-negative.

3.1.2 Range condition

As stated previously, the fact that the hyergraph structures posses a type of locality property is crucial for the existence of Gibbs measures. The simplest such assumption is the *finite range* assumption, see Definition 7 in Dereudre [2017], which roughly states that there exists $R > 0$ such that the energy of $\mathbf{x}$ in Λ only depends on points in $\Lambda + b(0, R)$. This is a strong assumption and one that is not fulfilled by our models.

This is reflected in part in the range condition introduced here and later in the uniform confinement condition 3.1.

(R) *Range condition.* There exist constants $\ell_R, n_R \in \mathbb{N}$ and $\delta_R < \infty$ such that for all $(\eta, \mathbf{x}) \in \mathcal{E}$ there exists a finite horizon Δ satisfying: For every $x, y \in \Delta$ there exist ℓ open balls $B_1, \ldots, B_\ell$ (with $\ell \leq \ell_R$) such that

- the set $\cup_{i=1}^{\ell} \bar{B}_i$ is connected and contains x and y, and
- for each i, either $\mathrm{diam} B_i \leq \delta_R$ or $N_{B_i}(\mathbf{x}) \leq n_R$.

Apart from being one of the assumptions necessary for the existence, the range condition also gives us the following crucial result we used in the definition of GPP.

Proposition 13. *Let $\Lambda \in \mathcal{B}_0(\mathbb{R}^3)$. Under the assumption 3.1.2, there exists a set $\hat{\mathbf{N}}_{cr}^{\Lambda} \in \mathbf{N}_{\Lambda^c}$ such that $\hat{\mathbf{N}}_{cr}^{\Lambda} \subset \mathbf{N}_{cr}^{\Lambda}$ and $P(\hat{\mathbf{N}}_{cr}^{\Lambda}) = 1$ for all $P \in \mathcal{P}_\Theta$ with $P(\varnothing) = 0$.*

Proof. Can be found in Theorem 5.4. in Dereudre et al. [2012]. See also remark 3.7. in connection to the marked case. □

This is wrong, since we're using the wrong set $\mathbf{N}_\Lambda$

The proposition shows that any Θ-invariant probability measure on $(\mathbf{N}_{lf}, \mathcal{N}_{lf})$ is concentrated on the set $\mathbf{N}_{cr}^{\Lambda}$ for any $\Lambda \in \mathcal{B}_0(\mathbb{R}^3)$.

3.1.3 Upper regularity

In order to present the upper regularity conditions, we introduce the notion of *pseudo-periodic* configurations.

Let $M \in \mathbb{R}^{3\times 3}$ be an invertible 3×3 matrix with column vectors (M_1, M_2, M_3). For each $k \in \mathbb{Z}^3$ define the cell

$$C(k) = \{Mx \in \mathbb{R}^3 : x - k \in [-1/2, 1/2)^3\}.$$

These cells partition $\mathbb{R}$ into parallelepipeds. We write $C = C(0)$. Let $\Gamma \in \mathcal{N}_C'$ be non-empty. Then we define the *pseudo-periodic* configurations $\bar{\Gamma}$ as

Again, need to define these sets

$$\bar{\Gamma} = \{\mathbf{x} \in \mathbf{N}_{lf} : \vartheta_{Mk}(\mathbf{x}_{C(k)}) \in \Gamma \text{ for all } k \in \mathbb{Z}^3\},$$

the set of all configurations whose restriction to $C(k)$, when shifted back to C, belongs to Γ. The prefix pseudo- refers to the fact that the configuration itself does not need to be identical in all $C(k)$, it merely needs to belong to the same class of configurations.

(U) *Upper regularity.* M and Γ can be chosen so that the following holds.

(U1) *Uniform confinement*: $\bar{\Gamma} \subset N_{\text{cr}}^{\Lambda}$ for all $\Lambda \in \mathcal{B}_0$ and

$$r_\Gamma := \sup_{\Lambda \in \mathcal{B}_0} \sup_{\mathbf{x} \in \bar{\Gamma}} r_{\Lambda,\mathbf{x}} < \infty \tag{3.1}$$

(U2) *Uniform summability*:

$$c_\Gamma^+ := \sup_{\mathbf{x} \in \bar{\Gamma}} \sum_{\eta \in \mathcal{E}(\mathbf{x}) : \eta \cap C \neq \emptyset} \frac{\varphi^+(\eta, \mathbf{x})}{\#(\hat{\eta})} < \infty,$$

where $\hat{\eta} := \{k \in \mathbb{Z}^3 : \eta \cap C(k) \neq \emptyset\}$ and $\varphi^+ = \max(\varphi, 0)$ is the positive part of φ.

(U3) *Strong non-rigidity*: $e^{z|C|}\Pi_C^z(\Gamma) > e^{c_\Gamma}$, where c_Γ is defined as in (U2) with φ in place of φ^+.

Notice that (U1) is very close to the classic finite range property mentioned at the beginning of Section 3.1.2. The major difference is that here the property is only required of the pseudo-periodic configuration.

As long as $\Pi_C^z(\Gamma) > 0$, (U3) will always hold for all z exceeding some threshold $z_0 \geq 0$. This is because the left hand side is an increasing function of z, as can be seen from the equality

$$e^{z|C|}\Pi_C^z(\Gamma) = \sum_{k=1}^{\infty} \frac{z^k}{k!} \int_C \cdots \int_C 1_\Gamma \left(\sum_{i=1}^{k} \delta_{X_i} \right) dx_1, \ldots, dx_k,$$

which can be derived using 2.2.

Add more intuition about U3 and comment on why Û is useful

For some models it is possible to replace the upper regularity assumptions by their alternative and prove the existence for all $z > 0$.

(**Û**) *Alternative upper regularity.* M and Γ can be chosen so that the following holds.

(Û1) *Lower density bound*: There exist constants $c, d > 0$ such that $\text{card}(\zeta) \geq c|\Lambda| - d$ whenever $\zeta \in \mathbf{N}_f \cap \mathbf{N}_\Lambda$ is such that $H_{\Lambda,\mathbf{x}}(\zeta) < \infty$ for some $\Lambda \in \mathcal{B}_0$ and some $\mathbf{x} \in \bar{\Gamma}$.

(Û2) = (U2) *Uniform summability.*

(Û3) *Weak non-rigidity*: $\Pi_C^z(\Gamma) > 0$.

3.2 Verifying the assumptions

3.2.1 The choice of Γ and M for Laguerre-Delaunay models

Fix some $A \subset C \times S$ and define

$$\Gamma^A = \{\zeta \in \mathbf{N}_C : \zeta = \{p\}, p \in A\},$$

the set of configurations consisting of exactly one point in the set A. The set of pseudo-periodic configurations $\bar{\Gamma}$ thus contains only one point in each $C(k), k \in \mathbb{Z}^3$.

Let M be such that $|M_i| = a > 0$ for $i = 1, 2, 3$ and $\angle(M_i, M_j) = \pi/3$ for $i \neq j$.

Choice of the set A

In Dereudre et al. [2012], A is chosen to be $B(0,b)$ for $b \leq \rho a$ for some sufficiently small $\rho > 0$.

We will use this form for the positions of the points as well — the question, however, is how to choose the mark set. For Delaunay models, we choose $A = B(0,b) \times \{0\}$. It would be convenient to do this in the Laguerre case and only deal with the Delaunay tetrahedronization. However, for Laguerre-Delaunay models, this would mean that $\Pi^z_C(\Gamma) = 0$, conflicting with both $(U3)$ and $(\hat{U}3)$. The choice $A = B(0,b) \times S$ could, for a small enough a, result in some balls being fully contained in their neighboring balls, possibly resulting in redundant points, thus changing the desired properties of Γ. It is thus necessary to choose the mark space dependent on a. For given a, ρ, the minimum distance between individual points, is $a - 2\rho a = a(1-2\rho)$. For $\mathcal{LD}$ models we therefore choose

$$A = B(0,b) \times \left[0, \sqrt{\frac{a}{2}(1-2\rho)}\right]$$

in order for balls to never overlap .

This is perhaps unnecessarily conservative, we could widen it

Remark 12 (Simplification of (U2) and (U3)). Using the set Γ^A, we can simplify the assumptions (U2) and (U3).

(U2) We now have $\#(\hat{\eta}) = \mathrm{card}(\eta)$, since now each point of η is necessarily in a different set $C(k)$.

Check how I am using $|\cdot|$ and $\#$

(U2) $\Pi^z_C(\Gamma)$ can now be directly calculated.

$$\begin{aligned}\Pi^z_C(\Gamma) &= \Pi^z_C(\{\zeta \in N_C : \zeta = \{p\}, p \in A\}) \\ &= e^{-z|A|} z|A| e^{-z|C \setminus A|} \\ &= e^{-z|C|} z|A|,\end{aligned}$$

and thus (U3) becomes

$$z|A| > e^{c_A},$$

where $c_A := c_{\Gamma^A}$.

In the case $A = B(0,\rho a) \times [0, \sqrt{\frac{a}{2}(1-2\rho)}]$ for $\mathcal{LD}$, we have

$$|A| = \frac{4}{3}\pi(\rho a)^3 \cdot \sqrt{\frac{a}{2}(1-2\rho)} = \frac{4\pi}{3\sqrt{2}} \cdot \rho^3 \sqrt{1-2\rho} \cdot a^{7/2}$$

3.2.2 Geometric properties of the tetrahedrizations defined by Γ^A and M

Am I talking about tetrahedrization or hypergraph? Check and unify this

To understand the advantage of the particular choice of M and Γ^A we first turn to the two-dimensional case. For $\mathbb{R}^2$, the two column vectors with angle $\pi/3$ define a triangulation made of equilateral triangles. Depending on the bound for ρ, the points never become collinear $(\sqrt{3}/4)$, have a bound for the circumradius that is linear in ρ $(\sqrt{3}/6)$ or even always generate the same triangultaion $((\sqrt{3}-1)/4)$ up to the movement of points within their respective set A. Thus the resulting triangulation has many desirable properties.

It is not however obvious that the desirable properties carry over to $\mathbb{R}^3$. Before we investigate the structure of the resulting tetrahedrizations, we list the properties we are interested in obtaining.

1. A description of the tetrahedra present in the tetrahedrization.
2. The number of tetrahedra incident to the point in C,
$$n_T := \operatorname{card}\{\eta \in \mathcal{E}(\mathbf{x}) : \eta' \cap C \neq \emptyset\}.$$
3. Bounds for circumdiameters of the tetrahedra.
4. The position of points with respect to the (reinforced) general position.
5. Boundedness of the weight of the characteristic points.

There's now a double use of the word regular.

As noted previously, using an analogous definition of M in $\mathbb{R}^2$ forms a triangulation containing equilateral triangles. Sadly, the three-dimensional case is not as simple[1].

The structure of the tetrahedrization formed by $\bar{\Gamma}^A$

To better understand the structure of the resulting tetrahedrizations, we choose a particular example of a configuration from $\bar{\Gamma}^A$.

$$\mathbf{x}_0 = \{(M_a k, 0) \in \mathbb{R}^3 \times S : k \in \mathbb{Z}^3\} \in \bar{\Gamma},$$

the set of zero-weight points lying in the center of their respective cells $C(k)$, where

$$M_a := a \begin{pmatrix} 1 & \frac{1}{2} & \frac{1}{2} \\ 0 & \frac{\sqrt{3}}{2} & \frac{1}{2\sqrt{3}} \\ 0 & 0 & \sqrt{\frac{2}{3}} \end{pmatrix}$$

is a particular example of the matrix M.

From Remark 5 we know that $\mathcal{LD}_4(\mathbf{x}_0) = \mathcal{D}_4(\mathbf{x}_0)$, therefore we can work with its Delaunay tetrahedrization.

Again we're not using marks without comment

To further simplify the line of reasoning, we will look at only a subset $\mathbf{x}_1 \subset \mathbf{x}_0$ of the points whose preimage under M_a are the boundary points of the unit cube $[0,1]^3$. The points of $\mathbf{x}_1$, denoted $p_1, \dots, p_8$ then are:

It's unclear what p_i are

[1] And it could not be, because the analogue of the two-dimensional equilateral triangle, the regular tetrahedron, does not tessellate, as Aristotle famously wrongly claimed, see e.g. Lagarias and Zong [2012]

$$
\begin{array}{rccc}
p_1: & (0,0,0) & \longmapsto & a(0,0,0) \\
p_2: & (1,0,0) & \longmapsto & a(1,0,0) \\
p_3: & (0,1,0) & \longmapsto & a(1/2,\sqrt{3}/2,0) \\
p_4: & (1,1,0) & \longmapsto & a(3/2,\sqrt{3}/2,0) \\
p_5: & (0,0,1) & \longmapsto & a(1/2,1/(2\sqrt{3}),\sqrt{2/3}) \\
p_6: & (1,0,1) & \longmapsto & a(3/2,1/(2\sqrt{3}),\sqrt{2/3}) \\
p_7: & (0,1,1) & \longmapsto & a(1,2/\sqrt{3},\sqrt{2/3}) \\
p_8: & (1,1,1) & \longmapsto & a(2,2/\sqrt{3},\sqrt{2/3})
\end{array}
$$

To obtain the tetrahedrization of the parallelepiped formed by $\mathbf{x}_1$, we could mechanically perform the INCIRCLE test on all quintuples of points in $\mathbf{x}_1$ (see Remark 3). Such approach is lengthy and ultimately not very illuminative. We will therefore derive its structure through a few geometric observations.

These lemmas are almost impossible to follow without figures

Lemma 3. NNG($\mathbf{x}_1$) *is formed by two regular tetrahedra,* $\{p_1, p_2, p_3, p_5\}$ *and* $\{p_4, p_6, p_7, p_8\}$*, and an regular octahedron* $\{p_2, \dots, p_7\}$*.*

Proof. Any invertible linear transformation maps a parallelepiped onto a parallelepiped. Since $\|p_2 - p_1\| = \|p_3 - p_1\| = \|p_5 - p_1\| = a$ by definition of M, we obtain that all the edges of the parallelepiped $\{p_1, \dots, p_8\}$ have length a. Furthermore, each face of the parallelepiped can be split into two equilateral triangles, e.g. $\|p_3 - p_2\| = a$. Consequently $\{p_1, p_2, p_3, p_5\}$ and $\{p_4, p_6, p_7, p_8\}$ are regular tetrahedra, the regularity coming from the fact that all edges have length a. Similarly, the sextuple $\{p_2, \dots, p_7\}$ is a regular octahedron, as all its edges have length a. $\square$

This polyhedral configuration is well known to tessellate[2]. The knowledge of NNG($\mathbf{x}_1$) allows us to fully categorize the tetrahedra in $\mathcal{D}_4(\mathbf{x}_0)$.

Proposition 14. $\mathcal{D}_4(\mathbf{x}_0)$ *contains two types of tetrahedra,* T_1 *and* T_2*, with edge lengths*

$$T_1 : (a, a, a, a, a, a) \quad T_2 : (a, a, a, a, a, \sqrt{2}a)$$

Proof. From Theorem 1 we know that NNG($\mathbf{x}_1$) $\subset \mathcal{D}_2(\mathbf{x}_1)$.

We know that NNG($\mathbf{x}_1$) is composed of two regular tetrahedra and one regular octahedron O with all edge lengths equal to a. Therefore all that remains to be done is to tetrahedronize the octahedron. By the symmetry of the regular octahedron, all the tetrahedra inside O must be the same up to rotation. Each tetrahedron has five out of six edge lengths equal to a, therefore we only need to determine the remaining edge length. We can take e.g. any four points forming a square with side lengths a to see that the remaining edge length is $\sqrt{2}a$.

Since $\mathcal{D}_4(\mathbf{x}_0)$ is tessellated by copies of $\mathcal{D}_4(\mathbf{x}_1)$ translated by vectors $k \in \mathbb{Z}^3$, we have fully characterized the tetrahedra of $\mathcal{D}_4(\mathbf{x}_0)$. $\square$

[2] The tessellation is of great importance to many fields and thus is known under many names. In mathematics, it is most commonly called the *tetrahedral-octahedral honeycomb*, or the *alternated cubic honeycomb*. In structural engineering, it is known as the *octet truss*, as named by Buckminster Fuller, or the *isotropic vector matrix*. It is stored as *fcu* in the Reticular Chemistry Structure ResourceO'Keeffe et al. [2008]. It is also the nearest-neighbor-graph of the face-centered cubic (fcc) crystal in crystallographyGabbrielli et al. [2012].

We note that the circumradii of the tetrahedra can be calculated using the Cayley-Menger determinant (see Appendix A) and are $\sqrt{6}/4 \cdot a$ for T_1 and $1/\sqrt{2} \cdot a$ for T_2.

Combinatorial structure of $\mathcal{D}_4(\mathbf{x}_0)$

Now we turn to the combinatorial structure of $\mathcal{D}_4(\mathbf{x}_0)$. In the tetrahedronized regular octahedron, each vertex is incident to $\binom{5}{3} - 2 = 8$ tetrahedra. In the tetrahedron-octahedron tessellation, each vertex is incident to eight regular tetrahedra and six regular octahedra. This gives us $n_T = 8 + 6 \cdot 8 = 56$. While still large, this is less than quarter of $8 \cdot \binom{7}{3} = 280$ for the case of regular cube tessellation induced by the choice $M = aE$. Note that n_T is much smaller for the non-degenerate case, when O contains only 4 tetrahedra and its vertices are incident either to 2 or 4 tetrahedra. In this case, $n_T \leq 8 + 6 \cdot 4 = 32$.

Reference, possibly using Schlafli symbols

Overcounting degenerate cases

Make it clear that the whole thing is proved in appendix. Also, make this whole thing clearer.

Circumdiameter and characteristic point weight

The bound on circumdiameters of the circumballs and characteristic point weights is crucial for the assumption (U1) as well as (U2) and (U3) for potentials that include them. Without such a bound, we have no uniform confinement and the hyperege potential can grow to infinity. We therefore have to investigate the shape of the tetrahedra that are possible with $\mathbf{x} \in \bar{\Gamma}$.

Proposition 15. *Let $\mathbf{x} \in \bar{\Gamma}^A$ with $\rho < 1/4$. Then the weight of the characteristic point is uniformly bounded. That is there exists $C > 0$ such that $p''_\eta \leq C$ for all $\eta \in \mathcal{LD}_4(\mathbf{x})$.*

Proof. Denote $\eta = \{p_1, p_2, p_3, p_4\}$, denote their positions η' and weights η''. From Theorem 3 and the remark below it, we know that $p'_\eta = H(p_1, p_2) \cap H(p_1, p_3) \cap H(p_1, p_4)$.

Fix the positions η'. Changing any of the points' weights ammounts to translation of the radical hyperplanes defined by that point (see note after Theorem 3). Given the fact that weights are bounded, $S = [0, W]$, we find that for given positions η' there exists $W_{\eta'} > 0$ such that , we have $p''_\eta \leq W_{\eta'}$ regardless of the weights.

It remains to prove that $\sup_{\eta'} W_{\eta'} < \infty$, i.e. changing the points' positions can produce only bounded p''_η. This amounts to proving that the points of η are not allowed to come arbitrarily close to (or even attain) a non-general position. This is equivalent with boundedness of the circumsphere of η', which is proved for $\rho < 1/4$ in the Appendix A. $\square$

Improve references to appendix

3.2.3 Existence theorems

Specify these things as “models” of the form $(\mathcal{D}_4, \varphi_S)$.Specify the measure μ in there, too

In this section, we will verify the assumptions for the existence of Gibbs measures with the energy function defined on the hypergraphs $\mathcal{D}_4$ and $\mathcal{LD}_4$. We use the general letter $\mathcal{E}$ when we mean either $\mathcal{D}$ or $\mathcal{LD}$. Two potentials will be considered

Smooth interaction: For $\eta \in \mathcal{E}_4(\mathbf{x})$ define the potential φ_S as an unary potential such that

$$\varphi_S(\eta, \mathbf{x}) \leq K_0 + K_1 \delta(\eta)^\alpha$$

for some $K_0, K_1 \geq 0, \alpha > 0$

Hard-core interaction: For $\eta \in \mathcal{E}_4(\mathbf{x})$ define the potential φ_{HC} as an unary potential such that

$$\sup_{\eta : d_0 \leq \delta(\eta) \leq d_1} \varphi_{HC}(\eta, \mathbf{x}) < \infty \text{ and } \varphi_{HC}(\eta, \mathbf{x}) = \infty \text{ if } \delta(\eta) > \alpha.$$

for some $0 \leq d_0 < d_1 \leq \alpha$ How exactly does this look? Why?

We assume by Assumption 1 that $\varphi_S, \varphi_{HC} \geq 0$.

We first present a general lemma. Recall the definition of r_Γ from (U1).

Lemma 4. *Let $\Gamma \subset N_{lf}$ be a class of configurations. If there exists $d_{max} > 0$ such that* $\text{diam}\Delta < d_{max}$ *for the horizon Δ of any $(\eta, \mathbf{x}), \eta \in \mathcal{E}(\mathbf{x}), \mathbf{x} \in \Gamma$, then*

$$r_\Gamma < d_{max}.$$

Proof. Choose $\Lambda \in \mathcal{B}_0$ and $\mathbf{x} \in \Gamma$. Let $\zeta \in N_\Lambda$ and $\eta \in \mathcal{E}_\Lambda(\zeta \cup \mathbf{x}_{\Lambda^c})$ and denote Δ the finite horizon of $(\eta, \mathbf{x})$. From lemma 1 we obtain $\Delta \cap \Lambda \neq \emptyset$. Then $\Delta \subset \Lambda + B(0, d_max)$. If we take $\tilde{\mathbf{x}} \in \Gamma$ such that $\tilde{\mathbf{x}} = \mathbf{x}$ on $\partial\Lambda(\mathbf{x})$ then $\varphi(\eta, \zeta \cup \mathbf{x}_{\Lambda^c}) = \varphi(\eta, \zeta \cup \tilde{\mathbf{x}}_{\Lambda^c})$ since $\zeta \cup \mathbf{x}_{\Lambda^c}$ and $\zeta \cup \tilde{\mathbf{x}}_{\Lambda^c}$ differ only on Δ^c. □

Theorem 3. *There exists at least one Gibbs measure for the model $(\mathcal{D}_4, \varphi_S)$ and every activity*

$$z > \frac{3}{4\pi} e^{14K_0} (2K_1 \alpha e^3/3)^{1/\alpha} \frac{(\delta_1(\rho)^\alpha + \delta_2(\rho)^\alpha)^{1/\alpha}}{\rho^3}.$$

Proof. **(R)** The finite-horizon $\Lambda = \bar{B}(\eta, \mathbf{x})$ with $\ell_R = 1, n_R = 0$ and δ_R arbitrary can be used. This is because it itself contains no points of $\mathbf{x}$ by definition of $\mathcal{D}$ and acts as the open ball from the definition of the range condition.

(S) Stability is satisfied because of φ is non-negative.

(U) We choose M and Γ as in section 3.2.1.

(U1) We know from 7 that the exists $d_{max} > 0$ such that $\text{diam}B(\eta) \leq d_{max}$. By lemma 4 $r_\Gamma \leq d_{max}$.

(U2) is trivially satisfied since $n_T < 58$ and φ_S is bounded by 7.

(U3) By remark 12 we want to find z as small as possible such that $z|A| > e^{c_A}$. We know from 3.2.2 that there are 8 T_1 and 48 T_2 tetrahedra intersecting C, therefore from 7

$$c_A \leq \frac{a}{4}(8 \cdot \delta_1 + 48 \cdot \delta_2)$$

This yield the bound

$$\begin{aligned} z &> \frac{4\pi\rho^3}{3} e^{2(K_0 + K_1(a\delta_1)^\alpha) + 12(K_0 + K_1(a\delta_2)^\alpha)} / a^3 \\ &= C_0 e^{C_1 a^\alpha} / a^3 \end{aligned}$$

where $C_0 = 3e^{14K_0}/(4\pi\rho^3), C_1 = 2k_1(\delta_1^\alpha + 6\delta_2^\alpha)$.

We now choose a to minize the expression above. By optimizing over a we obtain $a = (3/(C_1\alpha))^{1/\alpha}$ which yields the bound

$$z > C_0(C_1\alpha e^3/3)^{1/\alpha}.$$

□

Theorem 4. *There exists at least one Gibbs measure for the model* $(\mathcal{D}_4, \varphi_{HC})$ *and every activity* $z > 0$.

Proof. **(R)** Again, $\Lambda = \bar{B}(\eta, \mathbf{x})$ with $\ell_R = 1, n_R = 0$. Because of the hard-core condition, we can also take $\delta_R = 2\alpha$.

(S) Stability is satisfied because of φ is non-negative.

(Û) We choose M and Γ as in section 3.2.1.

(Û1) For all $\eta \in \mathcal{D}_4(\mathbf{x})$ for $\mathbf{x} \in \Gamma^A$ such that $H_\Lambda(\mathbf{x}) < \infty$ we have $\delta(\eta) < \alpha$. This imposes a minimum density of points, since e.g. no ball with diameter α can be empty.

(Û2) We have $n_T < 56$ and thus the only quantity in question is φ_{HC}. By 7, we have $\delta(\eta) \leq a\delta_2^{max}(\rho)$, thus we only need to choose a such that $\delta_2^{max}(\rho) \leq \alpha/a$.

(Û3) $\Pi_\Lambda^z(\Gamma) > 0$ by remark 12.

□

Theorem 5. *There exists at least one Gibbs measure for the model* $(\mathcal{LD}_4, \varphi_S)$ *and every activity*

$$z > \frac{3\sqrt{2}}{4\pi} e^{14K_0}(4K_1\alpha e^{7/2}/7)^{1/\alpha} \frac{(\delta_1(\rho)^\alpha + \delta_2(\rho)^\alpha)^{1/\alpha}}{\rho^3\sqrt{1-2\rho}}.$$

Proof. **(R)** Take the horizon set $\Delta = B(p'_\eta, \sqrt{p''_\eta + W})$. Δ can be decomposed into the sphere p_η and $\Delta \setminus p_\eta$, a 3-dimensional annulus with width $\sqrt{p''_\eta + W} - \sqrt{p''_\eta} = W/(\sqrt{p''_\eta + W} + \sqrt{p''_\eta})$. By definition of $\mathcal{LD}$ and remark, p_η cannot contain any points of $\mathbf{x}$. Although the annulus $\Delta \setminus p_\eta$ does not have any bound on the number of points, its width is bounded by $\sqrt{W} \geq W/(\sqrt{p''_\eta + W} + \sqrt{p''_\eta})$. This means that any $x, y \in \Delta$ can be connected by the spheres $B(x, \sqrt{W}), p_\eta, B(y, \sqrt{W})$, yielding the parameters $\ell_R = 3, n_R = 0, \delta_R = 2\sqrt{W}$.

Ugly line placements, improve

(S) Stability is satisfied because of φ is non-negative.

(U) We choose M and Γ as in section 3.2.1.

(U1) By Theorem 15 there is $C > 0$ such that $p''_\eta \leq C$ for all $\eta \in \mathcal{LD}_4(\mathbf{x}), \mathbf{x} \in \bar{\Gamma}^A$. By lemma 4 we have $r_\Gamma \leq \sqrt{C + W}$.

(U2) is trivial since $n_T < 56$ and φ_S is bounded by 3.2.2.

(U3) We proceed similarly as in 3 and obtain

$$z > C_0 e^{C_1 a^\alpha}/a^{7/2}$$

where $C_0 = 3\sqrt{2}e^{14K_0}/(4\pi\rho^2\sqrt{1-2\rho})$, $C_1 = 2K_1(\delta_1^\alpha + 6\delta_2^\alpha)$. Optimizing over a we obtain $a = (7/(2C_1\alpha))^{1/\alpha}$ arriving at the bound

$$z > C_0(C_1\alpha e^{7/2}/(7/2))^{1/\alpha}.$$

□

Theorem 6. *There exists at least one Gibbs measure for the model $(\mathcal{LD}_4, \varphi_{HC})$ and every activity*

$$z > 0.$$

Proof. **(R)** The horizon set is $\Delta = B(p'_\eta, \sqrt{p''_\eta + W})$. Parameters can be chosen as in Theorem 5.

Is it a problem that there's no n_R circle? Cause the proof suggested something like that?

(S) Stability is satisfied because of φ is non-negative.

(U) We choose M and Γ as in section 3.2.1.

(U1) Same as in Theorem 4. Although the underlying structure is different, the potential still depends on $\delta(\eta)$ and ($\hat{\text{U}}$1) requires the configuration to have non-infinite energy.

(U2) Same as in Theorem 4, $n_T < 56$ and we choose an appropriate a.

(U3) $\Pi^z_\Lambda(\Gamma) > 0$ by remark 12

□

Remark 13 (Extending to other potentials). .

Directly obtainable results: 1) Smooth interaction for other unary potentials such as k-facet volume (use Hadamard inequality to bound them). 2) Adding additional constraints to hardcore models as long as we can find a to satisfy the constraints.

Remark 14 (Concrete values of z). **TO BE DONE**

4. Simulation

The Gibbs point process allows us a great flexibility in specifying the energy function. One of the disadvantages is that both simulating the GPP and estimating its parameters is computationally demanding. This chapter outlines the approach taken in simulating the GPP.

This (and the following chapter) is a direct extension of Dereudre and Lavancier [2010] to the Laguerre case in three dimensions. The principal issue in simulating GPP is that we do not know the value of the partition function Z_Λ^z. To that end, we emply Monte Chain Markov Carlo (MCMC) techniques.

4.1 Monte Chain Markov Carlo

If there's time left, revisit this chapter and properly understand the stuff

Before formulating the algorithm used to simulate our models, we first present some basic theory of Markov chains and their use in Monte Carlo techniques. For an introduction to these techniques with point processes with density in mind, see chapter 7 in Moller and Waagepetersen [2003]. For a more general and comprehensive text, we refer to Robert and Casella [2004] or Meyn and Tweedie [1993].

4.1.1 Basic notions

We first define the basic terms to do with general state-space Markov chains.

Definition 33. A measurable mapping $P : \Omega \times \mathcal{A} \to [0,1]$ such that

1. for each $B \in \mathcal{A}$, $P(\cdot, B)$ is a non-negative measurable function on Ω,
2. for each $x \in \Omega$, $P(x, \cdot)$ is a probability measure on Ω

is called a *probability kernel* on $(\Omega, \mathcal{A})$.

Definition 34. A stochastic process $Y = \{Y_n, n \in \mathbb{N}_0\}$ defined on $(\Omega, \mathcal{A})$ is called a *time-homogenous Markov chain* with *initial distribution* μ and *transition probability kernel* $P(x, A), x \in \Omega, A \in \mathcal{A}$, if for any $n \in \mathbb{N}_0$ and any sets $A_0, \dots, A_n$ we have

$$P_\mu(Y_0 \in A_0, \dots, Y_n \in A_n) = \int_{A_0} \cdots \int_{A_{n-1}} P(y_{n-1}, A_n) P(y_{n-2}, dy_{n-1}) \cdots P(y_0, dy_1) \mu(dy_0)$$

where $P_\mu(B), B \in \bigotimes_{n=0}^{\infty} \mathcal{A}$ is the probability of the event $[Y \in B]$.

Such process exists by Theorem 3.4.1 in Meyn and Tweedie [1993] if $\mathcal{A}$ is generated by a countable collection of sets. This is true for $\mathcal{N}_{lf}$, see Proposition B.1 in Moller and Waagepetersen [2003].

The definition suggests that the probability kernel $P(x, A)$ can be interpreted as a the probability that $Y_{m+1} \in A$ given that $Y_m = x$. Note that the probability is independent of m, which motivates the name *time-homogenous*.

Next we iteratively define the *m-step transition probability.* Set $P^0(x,A) = \delta_x(A)$ and for $n \geq 1$ define

$$P^m(x,A) = \int_\Omega P(y,A)P^{m-1}(x,dy)$$

In the following, let $Y = \{Y_n, n \in \mathbb{N}_0\}$ always be a Markov chain and π a probability distribution on $(\Omega, \mathcal{A})$.

Definition 35. A Markov chain $\{Y_n, n \in \mathbb{N}_0\}$

1. has an *invariant distribution* π if $Y_m \sim \pi$ implies $Y_{m+1} \sim \pi$. In the integral form,
$$\int_\Omega P(x,A)\pi(dx) = \int_A \pi(dx), \quad A \in \mathcal{A}.$$
2. is *reversible* with respect to the distribution π if $Y_m \sim \pi$ then (Y_m, Y_{m+1}) and (Y_{m+1}, Y_m) are identically distributed. In the integral form,
$$\int_B P(x,A)\pi(dx) = \int_A P(x,B)\pi(dx), \quad A, B \in \mathcal{A}.$$
3. is *irreducible*, or $\psi-$*irreducible* if ther exists a nonzero measure ψ such that for any $x \in \Omega, A \in \mathcal{A}$ with $\psi(A) > 0$ we have $P^m(x,A) > 0$ for some $m \in \mathbb{N}_0$.

From the definition it is immediately observable that if Y is reversible with respect to π, then π is also its invariant distribution.

Definition 36. Let Y be /*psi*-irreducible. Then we call Y *periodic* if there exists a partitioning $D_0, \ldots, D_{d-1}, A$ of Ω such that $\psi(A) = 0$ and

$$P(x, D_j) = 1, \; x \in D_i \; j = (i+1) \bmod d$$

with $d > 1$. In the opposite case Y is *aperiodic*

The partitioning always exists for an irreducible Markov chain Y by Theorem 5.4.4 in Meyn and Tweedie [1993].

There needs to be more about periodicity, 129 in MW

To measure the distance between two probability distribution, we recall the definition of the total variation norm.

Definition 37. Let μ, ν be two probability distributions on Ω. Then we define the *total variation norm* by

$$\|\mu - \nu\|_{TV} = \sup_{F \subset \Omega} |\mu(F) - \nu(G)|$$

Some notes, in particular implication of weak convergence

Definition 38. We say that π is a *limiting distribution* of Y if there exists $A \in \mathcal{A}, \pi(A) = 0$ such that

$$\lim_{m \to \infty} \|P^m(x, \cdot) - \pi\|_{TV} = 0$$

for all $x \in \Omega \setminus A$.

Proposition 16. *Let Y be irreducible and π its invariant distribution. Then π is the unique invariant distribution (up to null sets).*

Proof. Proposition 7.2 in Moller and Waagepetersen [2003] □

Proposition 17. *Let Y be irreducible and aperiodic and π its invariant distribution. Then π is also the limiting distribution of Y.*

Proof. Proposition 7.7 in Moller and Waagepetersen [2003]. □

Consider a probability distribution π on some measurable space $(\Omega, \mathcal{A})$. We wish to construct a Markov Chain Y on Ω with its stationary distribution equal to π. By the theory introduced in this section, we must construct a irreducible and aperiodic Markov chain reversible with respect to π. Then π is also the unique invariant distribution and thus the limiting distribution. Since convergence in total variation implies weak convergence, our task is complete. unique?

The question, however, is how to build such a Markov chain. The next sections answers that question.

4.1.2 Birth-Death-Move Metropolis-Hastings algorithm

In the last section we outlined how Markov chains may be used to sample from a distribution in general. In this section we introduce a variation of the Metropolis-Hastings algorithm for points processes with a density, the algorithm used to construct a Markov chain with the required properties.

We first describe the algorithm in general, adapted from Moller and Waagepetersen [2003].

Let $\Omega \subset \mathbf{N}_f$ be the state space. A natural choice is

$$\Omega = \{\gamma \in \mathbf{N}_f : f(\gamma) > 0\} = \mathbf{N}_f \cap \mathbf{N}_\infty$$

We first introduce the quantities to be used in the algorithm. Let $\gamma = \{x_1, \ldots, x_n\} \in \Omega$ be the current state and denote $\bar{\gamma} = (x_1, \ldots, x_n)$ the current state represented as a vector. We further denote

Instead of introducing f in the table, introduce it beforehand as the setting for this chapter.

$f(\cdot)$	Density of the point process with respect to Π_Λ.
$p(\gamma)$	Probability of birth proposal if the current state is γ.
$q_i(\bar{\gamma}, \cdot)$	Density for the location of the point replacing the point x_i.
$q_b(\gamma, \cdot)$	Density for the location of the point at birth proposal.
$q_d(\gamma, \cdot)$	Density for the selection of the point at death proposal.

Finally we introduce the so called *Hasting ratios*

$$r_i(\bar{\gamma}, y) = \frac{f(\gamma \setminus \{x_i\} \cup \{y\}) q_i((x_1, \ldots, x_{i-1}, y, x_{i+1}, \ldots, x_n), x_i)}{f(\gamma) q_i(\bar{\gamma}, y)},$$

$$r_b(\gamma, x) = \frac{f(\gamma \cup \{x\})(1 - p(\gamma \cup \{x\})) q_d(\gamma \cup \{x\}, \{x\})}{f(\gamma) p(\gamma) q_b(\gamma, x)},$$

$$r_d(\gamma, x) = \frac{f(\gamma \setminus \{x\}) p(\gamma \setminus \{x\}) q_b(\gamma \setminus \{x\}, x)}{f(\gamma)(1 - p(\gamma)) q_d(\gamma, x)},$$

with the convention $a/0 = 1$ for $a \geq 0$.

Algorithm A
Let $\gamma_0 \in \Omega$ be an initial configuration. For $m = 0, 1, \ldots,$ given $\gamma_m \in N_f$, generate γ_{m+1} as follows

1. Generate b and r_m independently and uniformly on $[0, 1]$.

2. If $r_m \leq q$, then set $\bar{\gamma}_m = (x_1, \ldots, x_n)$, generate i uniformly on $\{1, \ldots, n\}$, generate $y \sim q_i(\bar{\gamma}_m, \cdot)$ and set

$$\gamma_{m+1} = \begin{cases} \gamma_m \setminus \{x_i\} \cup \{y\} & \text{if } b < r_i(\bar{\gamma}_m, y) \\ \gamma_m & \text{otherwise.} \end{cases} \tag{4.1}$$

3. If $r_m > q$, perform the birth/deah step.

   (a) Generate r_b uniformly on $[0, 1]$.

   (b) If $r_b \leq p(\gamma_m)$, then generate $x \sim q_b(\gamma_m, \cdot)$ and set

   $$\gamma_{m+1} = \begin{cases} \gamma_m \cup \{x\} & \text{if } b < r_b(\gamma_m, x) \\ \gamma_m & \text{otherwise.} \end{cases} \tag{4.2}$$

   (c) If $r_b > p(\gamma_m)$ and $\gamma_m = \emptyset$ then set $\gamma_{m+1} = \emptyset$. Else if $\gamma_m \neq \emptyset$ generate $x \sim q_d(\gamma_m, \cdot)$ and set

   $$\gamma_{m+1} = \begin{cases} \gamma_m \setminus \{x\} & \text{if } b < r_d(\gamma_m, x) \\ \gamma_m & \text{otherwise.} \end{cases} \tag{4.3}$$

The correctness of this approach is guaranteed by the following proposition.

Proposition 18. *The Markov chain generated by Algorithm A is*

1. *reversible with respect to h,*

2. *Ψ-irreducible and aperiodic*

if the following conditions are satisfied

(i) $p(\emptyset) < 1$,

(ii) for all $\gamma \in E, \gamma \neq \emptyset$ exists $x \in \gamma$ such that

$$(1 - p(\gamma))q_d(\gamma, x) > 0 \textit{ and } f(\gamma \setminus \{x\})p(\gamma \setminus \{x\})q_b(\gamma \setminus \{x\}, x) > 0.$$

Proof. Proposition 7.15 in Moller and Waagepetersen [2003]. □

Condition (i) ensures that the chain can remain in $\emptyset$. Condition (ii) ensures that a point can always be deleted and thus the chain can move from γ to $\emptyset$ in $N_\Lambda(\gamma)$ steps.

4.2 Simulating Gibbs-Laguerre-Delaunay tessellations

4.2.1 Definition of the models

Our goal is to simulate examples of both smooth-interaction and hardcore-interaction potentials defined in Section 3.2.3 on $\mathcal{D}$ and $\mathcal{LD}$ models. To that end, we choose a particular form of the potentials.

$$\varphi_{HC}^{\theta,\alpha}(\eta,\mathbf{x}) = \begin{cases} \infty & \text{if } \delta(\eta) > \alpha, \\ \theta \mathrm{Sur}(\eta) & \text{otherwise,} \end{cases} \tag{4.4}$$

$$\varphi_{S}^{\theta}(\eta,\mathbf{x}) = \theta \mathrm{Sur}(\eta) \tag{4.5}$$

where $\mathrm{Sur}(\eta)$ is the surface area of $\mathrm{conv}(\eta)$, $\alpha > 0$, $\theta \in \mathbb{R}$. We then consider the models $(\mathcal{D}_4, \varphi_{HC}^{\theta,\alpha})$, $(\mathcal{D}_4, \varphi_S^{\theta})$, $(\mathcal{LD}_4, \varphi_{HC}^{\theta,\alpha})$ and $(\mathcal{LD}_4, \varphi_S^{\theta})$.

4.2.2 Simulation algorithm

We now present the variations of Algorithm A for our setting.

The first algorithm simulates the Delaunay tetrahedrization. All unmarked points formally represent marked points with marks set to 0. The state space thus is

$$\Omega = \{\gamma \in \mathbf{N}_f : f(\gamma) > 0, \gamma \subset \Lambda \times \{0\}\}$$

.

I really need to revisit the marked x unmarked formalism and improve it

Probably remind the reader what permissible means

Algorithm A-$\mathcal{D}$
First, start from a permissible initial configuration γ_0.

1. Let $n = N_\Lambda(\gamma)$.

2. Draw independently r and b uniformly on $[0,1]$.

3. If $r < 1/3$, then generate x uniformly on $[0,1]^3$ and set

$$\gamma_1 = \begin{cases} \gamma_0 \cup \{x\} & \text{if } b < \frac{zf(\gamma_0 \cup \{x\})}{(n+1)f(\gamma_0)}, \\ \gamma_0 & \text{otherwise.} \end{cases} \tag{4.6}$$

4. If $r > 2/3$, then generate x uniformly on γ_0 and set

$$\gamma_1 = \begin{cases} \gamma_0 \setminus \{x\} & \text{if } b < \frac{nf(\gamma_0 \setminus \{x\})}{zf(\gamma_0)}, \\ \gamma_0 & \text{otherwise.} \end{cases} \tag{4.7}$$

5. If $1/3 < r < 2/3$, then generate x uniformly on γ_0, generate $y \sim \mathcal{N}(x, \sigma^2 I)$ such that $y \in [0,1]^3$ and set

$$\gamma_1 = \begin{cases} \gamma_0 \setminus \{x\} \cup \{y\} & \text{if } b < \frac{f(\gamma_0 \setminus \{x\} \cup \{y\})}{f(\gamma_0)}, \\ \gamma_0 & \text{otherwise.} \end{cases} \tag{4.8}$$

6. Set $\gamma_0 \leftarrow \gamma_1$ and go to 1.

The second algorithm is for the simulation for the Laguerre tetrahedrization. The algorithm functions the same with one significant difference. In section 1.1.2 we introduced the notion of redundant points. It would be inconvenient to have a newly added point render other points redundant and vice versa. To prevent that, we define the set of point configurations producing Laguerre-Delaunay hypergraph structures with no redundant points,

$$\mathbf{N}_{nr} = \{\gamma \in \mathbf{N}_{lf} : \mathcal{LD}(\gamma) \text{ does not contain redundant points } \}.$$

Note that $\mathbf{N}_{nr}$ is measurable in $(\mathbf{N}_{lf}, \mathcal{N}_{lf})$ due to measurability of the hypergraph structures. Using this set, we set the state space of the chain to check this

$$\Omega = \mathbf{N}_f \cap \mathbf{N}_\infty \cap \mathbf{N}_{nr}.$$

We further denote the set

$$A_\gamma = \{x \in \Lambda \times S : \gamma \cup \{x\} \in N_{nr}\},$$

the set of points which we can propose if the chain is in the state γ. Generation of points in A_γ is done through rejection sampling.

Λ is basically undefined here

Algorithm A-$\mathcal{LD}$
First, start from a permissible initial configuration γ_0.

1. Let $n = N_\Lambda(\gamma)$.

2. Draw independently r and b uniformly on $[0, 1]$.

3. If $r < 1/3$, then generate x uniformly on A_γ and set

$$\gamma_1 = \begin{cases} \gamma_0 \cup \{x\} & \text{if } b < \frac{zf(\gamma_0 \cup \{x\})}{(n+1)f(\gamma_0)}, \\ \gamma_0 & \text{otherwise.} \end{cases} \tag{4.9}$$

4. If $r > 2/3$, then generate x uniformly on γ_0 and set

$$\gamma_1 = \begin{cases} \gamma_0 \setminus \{x\} & \text{if } b < \frac{nf(\gamma_0 \setminus \{x\})}{zf(\gamma_0)}, \\ \gamma_0 & \text{otherwise.} \end{cases} \tag{4.10}$$

5. If $1/3 < r < 2/3$, then generate x uniformly on γ_0, generate $y' \sim \mathcal{N}(x, \sigma^2 I)$ and y'' uniformly on S such that $y = (y', y'') \in A_{\gamma \setminus \{x\}}$ and set

$$\gamma_1 = \begin{cases} \gamma_0 \setminus \{x\} \cup \{y\} & \text{if } b < \frac{f(\gamma_0 \setminus \{x\} \cup \{y\})}{f(\gamma_0)}, \\ \gamma_0 & \text{otherwise.} \end{cases} \tag{4.11}$$

6. Set $\gamma_0 \leftarrow \gamma_1$ and go to 1.

This is not true at the moment, currently the algorithm just skips points in conflict with other points.

Why does this work? Can we choose different proposal density to improve the convergence?

During the move step, the moved point might fall outside of $[0, 1]^3$. In Dereudre and Lavancier [2010], the point would be replaced by the periodic property. We do not use the periodic configuration (Section 4.2.4) and this approach would not be in line with the idea that a small perturbation to the point's position should not result in a radically different position. In our case the point is reflected back inside $[0, 1]^3$, as if it was 'bounced back' from the boundary of $[0, 1]^3$.

Is this a good approach? I makes the density of moved points next to

4.2.3 Simplified form of proposal densities

The Hastings ratios require us to calculate a ratio of densities f both containing the energy function. Such calculation would be lengthy and would render the whole approach infeasible. However, here again the locality of the tetrahedrization allows us to express the Hastings ratios with only those tetrahedra which are affected by the added, removed, or moved point. If we recall Remark 8, we obtain the following simplifications for the ratios in Algorithm A-$\mathcal{LD}$.

The ratio of densities in birth step 4.9 then becomes:

$$\begin{aligned}\frac{f(\gamma_0 \cup \{x\})}{f(\gamma_0)} &= \exp\left(\sum_{\eta \in \mathcal{E}_\Lambda(\gamma_0 \cup \{x\})} \varphi(\eta, \gamma_0 \cup \{x\}) - \sum_{\eta \in \mathcal{E}_\Lambda(\gamma_0)} \varphi(\eta, \gamma_0)\right) \\ &= \exp\left(\sum_{T \in \mathcal{LD}^{\otimes}(x, \gamma_0)} \varphi(\eta, \gamma_0) - \sum_{T \in \mathcal{LD}^{\ell}(x, \gamma_0 \cup \{x\})} \varphi(\eta, \gamma_0 \cup \{x\})\right)\end{aligned}$$

Ratio for death step 4.10 becomes:

$$\begin{aligned}\frac{f(\gamma_0 \setminus \{x\})}{f(\gamma_0)} &= \exp\left(\sum_{\eta \in \mathcal{E}_\Lambda(\gamma_0 \setminus \{x\})} \varphi(\eta, \gamma_0 \setminus \{x\}) - \sum_{\eta \in \mathcal{E}_\Lambda(\gamma_0)} \varphi(\eta, \gamma_0)\right) \\ &= \exp\left(\sum_{T \in \mathcal{LD}^{\ell}(x, \gamma_0)} \varphi(\eta, \gamma_0) - \sum_{T \in \mathcal{LD}^{\otimes}(x, \gamma_0 \setminus \{x\})} \varphi(\eta, \gamma_0 \setminus \{x\})\right)\end{aligned}$$

Ratio for move step 4.11 becomes:

$$\begin{aligned}&\frac{f(\gamma_0 \setminus \{x\} \cup \{y\})}{f(\gamma_0)} = \frac{f(\gamma_0 \setminus \{x\} \cup \{y\})}{f(\gamma_0 \setminus \{x\})} \frac{f(\gamma_0 \setminus \{x\})}{f(\gamma_0)} \\ &= \exp\left(\sum_{T \in \mathcal{LD}^{\otimes}(y, \gamma_0 \setminus \{x\})} \varphi(\eta, \gamma_0 \setminus \{x\}) - \sum_{T \in \mathcal{LD}^{\ell}(y, \gamma_0 \setminus \{x\} \cup \{y\})} \varphi(\eta, \gamma_0 \setminus \{x\} \cup \{y\}) \right. \\ &\left. + \sum_{T \in \mathcal{LD}^{\ell}(x, \gamma_0)} \varphi(\eta, \gamma_0) - \sum_{T \in \mathcal{LD}^{\otimes}(x, \gamma_0 \setminus \{x\})} \varphi(\eta, \gamma_0 \setminus \{x\})\right)\end{aligned}$$

These expressions simplify the energy calculation immensely. Whereas calculating the energy for the whole tessellation requires all the tetrahedra, and thus depends on the complexity of the sets $\mathcal{E}_\Lambda$, the final expressions only contain the tetrahedra local to x through the sets of type $\mathcal{LD}^{\otimes}$ and $\mathcal{LD}^{\ell}$, and thus the energy can be calculated in constant time.

We have presented the simplified ratios for Algorithm A-$\mathcal{LD}$. The case for Algorithm A-$\mathcal{D}$ is analogous, see Remark 8.

4.2.4 Practical implementation

All simulations were done in C++ using CGAL The CGAL Project [2018],Jamin et al. [2018]. More details can be found in appendix B.

Definitely sell this more later

Initial configuration

In Dereudre and Lavancier [2010], three options for the initial configuration are suggested: the empty configuration, a specific fixed outside configuration, and periodic configuration. We ruled out periodic configuration since the CGAL implementation of 3d periodic triangulations Caroli et al. [2018] has a much longer running time than in the non-periodic case. Dereudre and Lavancier [2010] rejects the empty configuration on the basis that it ”produces non bounded Delaunay-Voronoi cells”. While this is true for a Voronoi diagram, it does not hold for the Delaunay or Laguerre case and so such configuration would in fact be possible in our case. However, the method chosen was to fix a regular grid of points in and out of Λ such that the resulting tessellation fulfills the hardcore conditions. This does mean that the initial configuration is dependent on the values of the hardcore parameter α.

4.2.5 Convergence of the algorithm

TO BE DONE

5. Estimation

Assume now that we obtain the point configuration γ from model $(\varphi_{HC}^{\theta,\alpha}, \mathcal{LD}_4)$ on the observation window $\Lambda_n = [-n, n]^3$ and wish to estimate the model parameters (θ, α).

The estimation procedure closely follows that from Dereudre and Lavancier [2010]. That is a two-step approach, first estimating the hardcore parameter α and then using the estimates to obtain the estimate of θ through maximum pseudolikelihood (MPLE).

To underscore the dependence on the maximum circumdiameter α and smooth interaction parameter θ, we now denote the energy $H^{\theta,\alpha}$.

5.1 Estimation of the hardcore parameter

In the first step we estimate the hardcore parameter α. Thanks to the fact that the hardcore parameter α satisfies

$$\text{if } \alpha < \alpha' \text{ then } \forall \Lambda \in \mathcal{B}_0(\mathbb{R}^3),\ H_\Lambda^{\theta,\alpha}(\gamma) < \infty \Rightarrow H_\Lambda^{\theta,\alpha'}(\gamma) < \infty,$$

we can estimate it as

$$\hat{\alpha} = \sup\{\alpha > 0, H_\Lambda^{\theta,\alpha}(\gamma) < \infty\}.$$

In practice, the parameter can be estimated as

Are these consistent? Why?

$$\hat{\alpha} = \max\{\delta(\eta), \eta \in \mathcal{LD}_{4\Lambda}(\gamma)\}.$$

The estimate $\hat{\alpha}$ is then used in the pseudo-likelihood function in the second estimation step.

5.2 Estimation of the smooth interaction parameters

In the second step we estimate the smooth interaction parameters through maximum pseudolikelihood.

Improve handling of the Models - as of now they're sort of scattered

Equation references

The classical version of MPLE requires hereditarity of the energy function. Hereditarity means that for every permissible γ, the point pattern $\gamma \setminus \{x\}$ remains permissible for every $x \in \gamma$, see Section 2.1.3 for definition and discussion. The hardcore interaction in the model $(\mathcal{LD}_4, \varphi_H C)$ does not satisfy this condition. For that purpose, Section **??** presented the extension to the non-hereditary case from Dereudre and Lavancier [2009].

again, references, clear model definitions,..

Recall that a point $x \in \gamma$ is removable in a configuration $\gamma \in \mathbf{N}_{lf}$ if $\gamma \setminus \{x\}$ is permissible. We denote $\mathcal{R}^\alpha(\gamma)$ the set of removable points of γ. Similarly the notion of an addable point will be useful. A point $x \in \gamma$ is *addable* in γ if $\gamma \cup \{x\}$ is permissible and we denote $\mathcal{A}^\alpha(\gamma)$.

In the non-hereditary case, the pseudo-likelihood function then becomes:

$$PLL_{\Lambda_n}(\gamma, z, \theta, \alpha) = \int_{\Lambda_n \times S} 1_{\mathcal{A}^{\alpha}(\gamma)} z \exp(-h^{\theta,\alpha}(x,\gamma))dx + \sum_{x \in \mathcal{R}^{\beta}(\gamma) \cap (\Lambda_n \times S)} \Big(h^{\theta,\alpha}(x, \gamma \backslash \{x\}) - \ln(z)\Big), \tag{5.1}$$

where Λ_n' is the set of all addable points in Λ_n and $h^{\theta,\alpha}(x, \gamma \setminus \{x\})$ is local energy of x in γ defined for every $x \in \mathcal{R}^{\beta}(\gamma)$ by:

Connection between this and Papangelou could be useful

$$h^{\theta,\alpha}(x, \gamma \setminus \{x\}) = E_{\Lambda}^{\theta,\alpha}(\gamma_{\Lambda}, \gamma_{\Lambda^c}) - E_{\Lambda}^{\theta,\alpha}(\gamma_{\Lambda} \setminus \{x\}, \gamma_{\Lambda^c}).$$

The estimates $\hat{\theta}$ and $\hat{z}$ are obtained through minimizing the PLL_{Λ_n} function 5.1:

$$(\hat{z}, \hat{\theta}) = \operatorname{argmin}_{z,\theta} PLL_{\Lambda_n}(\gamma, z, \hat{\beta}, \theta).$$

By differentiating the PLL function 5.1 with respect to z, respectivelly θ, and setting them equal to zero, we obtain the estimate for $\hat{z}$,

$$\hat{z} = \frac{\operatorname{card}(\mathcal{R}^{\beta}(\gamma) \cap \Lambda_n)}{\int_{\Lambda_n} \exp\left(-h^{\hat{\beta},\theta}(x,\gamma)\right) dx}, \tag{5.2}$$

and the estimate $\hat{\theta}$ as the solution of

$$z \int_{\Lambda_n'} (h^{\hat{\beta},1}(x,\gamma) \exp\left(-h^{\hat{\beta},\theta}(x,\gamma)\right)) dx = \sum_{x \in \mathcal{R}^{\hat{\beta}}(\gamma) \cap \Lambda_n} h^{\hat{\beta},1}(x, \gamma \setminus \{x\}), \tag{5.3}$$

where we have used the fact that the local energy depends on θ linearly, yielding

$$\frac{\partial h^{\hat{\beta},\theta}}{\partial \theta}(x,\gamma) = h^{\hat{\beta},1}(x,\gamma).$$

5.2.1 Practical implementation

We obtain the estimate of θ by substituting the expression for $\hat{z}$ 5.2 into 5.3. This leads to the equation

$$\frac{\int_{\Lambda_n'} (h^{\hat{\beta},1}(x,\gamma) \exp\left(-h^{\hat{\beta},\theta}(x,\gamma)\right)) dx}{\int_{\Lambda_n} \exp\left(-h^{\hat{\beta},\theta}(x,\gamma)\right) dx} = \frac{\sum_{x \in \mathcal{R}^{\hat{\beta}}(\gamma) \cap \Lambda_n} h^{\hat{\beta},1}(x, \gamma \setminus \{x\})}{\operatorname{card}(\mathcal{R}^{\beta}(\gamma) \cap \Lambda_n)}.$$

In order to simplify the estimation of θ, we can simplify this equation further. First, we denote the righ-hand-side of the equation as c as it is constant with respect to θ. Second, we note that $x \notin \Lambda_n' \Rightarrow \exp\left(-h^{\hat{\beta},\theta}(x,\gamma)\right) = 0$ which enables us to integrate over Λ_n' instead of the whole Λ_n. Lastly we denote the local energy $h^{\hat{\beta},1}(x,\gamma) =: h(x)$, yielding the expression

$$\int_{\Lambda_n'} h(x) \exp\left(-\theta h(x)\right) dx = c \int_{\Lambda_n'} \exp\left(-\theta h(x)\right),$$

leading into the final expression

$$\int_{\Lambda_n'} \exp\left(-\theta h(x)\right)(h(x) - c) dx. \tag{5.4}$$

The integral 5.4 is estimated using Monte-Carlo integration, i.e. is approximately equal to

$$\frac{1}{N}\sum_{i=0}^{N} 1_{\Lambda_n'}(x_i)\exp(-\theta h_i)(h_i - c)dx$$

where $h_i = h^{\hat{\beta},1}(x_i, \gamma)$ and $x_1, \ldots, x_N$ is a random sample from the uniform distribution on Λ_n'

Do we need the indicator function if we're only sampling from Λ_n' ?

After $\hat{\theta}$ is estimated, we then obtain the estimate $\hat{z}$ with $\hat{\theta}$ instead of θ and the integral replaced by a MC-integration approximation.

5.3 Consistency

TO BE DONE

6. Numerical Results

Conclusion

Bibliography

Manuel Caroli, Aymeric Pellé, Mael Rouxel-Labbé, and Monique Teillaud. 3D periodic triangulations. In *CGAL User and Reference Manual*. CGAL Editorial Board, 4.12 edition, 2018. URL `https://doc.cgal.org/4.12/Manual/packages.html#PkgPeriodic3Triangulation3Summary`.

A. Cayley. On a theorem in the geometry of positions. *Cambridge Math*, 2: 267–271, 1841.

D. Dereudre. Introduction to the theory of Gibbs point processes. *ArXiv 1701.08105 [math.PR]*, January 2017.

D. Dereudre and F. Lavancier. Campbell equilibrium equation and pseudo-likelihood estimation for non-hereditary Gibbs point processes. *Bernoulli*, 15 (4):1368–1396, 2009.

D. Dereudre and F. Lavancier. Practical simulation and estimation for Gibbs Delaunay-Voronoi tessellations with geometric hardcore interaction. *Computational Statistics and Data Analaysis*, 55(1):498–519, 2010.

David Dereudre, Remy Drouilhet, and Hans-Otto Georgii. Existence of gibbsian point processes with geometry-dependent interactions. *Probability Theory and Related Fields*, 153(3):643–670, 2012.

H. Edelsbrunner and N. R. Shah. Incremental topological flipping works for regular triangulations. *Algorithmica*, 15(3):223–241, 1996.

Ruggero Gabbrielli, Yang Jiao, and Salvatore Torquato. Families of tessellations of space by elementary polyhedra via retessellations of face-centered-cubic and related tilings. *Phys. Rev. E*, 86:041141, 2012.

M Gavrilova. *Proximity and Applications in GeneraI Metrics*. PhD thesis, The University of Calgary, 1998.

H.O. Georgii. *Gibbs Measures and Phase Transitions*. De Gruyter Studies in Mathematics 9. Walter de Gruyter Inc, 2011 (2nd ed.).

Wolfram Research, Inc. Mathematica, Version 11.3. Champaign, IL, 2018.

Clément Jamin, Sylvain Pion, and Monique Teillaud. 3D triangulations. In *CGAL User and Reference Manual*. CGAL Editorial Board, 4.12 edition, 2018. URL `https://doc.cgal.org/4.12/Manual/packages.html#PkgTriangulation3Summary`.

Jerzy Kocik. A theorem on circle configurations, 2007.

Jeffrey C. Lagarias and Chuanming Zong. Mysteries in packing regular tetrahedra. *Notices of the American Mathematical Society*, 59(11):1392, dec 2012.

K. Menger. Untersuchungen uber allgemeine metrik. *Mathematische Annalen*, 100:120,133, 1928. URL `http://eudml.org/doc/159284`.

Sean P. Meyn and Richard L. Tweedie. *Markov Chains and Stochastic Stability*. Springer London, 1993.

J. Moller and R.P. Waagepetersen. *Statistical Inference and Simulation for Spatial Point Processes*. Chapman & Hall/CRC Monographs on Statistics & Applied Probability. CRC Press, 2003. URL `https://books.google.cz/books?id=dBNOHvElXZ4C`.

Michael O'Keeffe, Maxim A. Peskov, Stuart J. Ramsden, and Omar M. Yaghi. The reticular chemistry structure resource (rcsr) database of, and symbols for, crystal nets. *Accounts of Chemical Research*, 41(12):1782–1789, 2008.

Christian P. Robert and George Casella. *Monte Carlo Statistical Methods*. Springer New York, 2004.

W. Schneider, R. Weil. *Stochastic and Integral Geometry*. Probability and Its Applications. Springer-Verlag Berlin Heidelberg, 2008. URL `https://books.google.cz/books?id=dBNOHvElXZ4C`.

The CGAL Project. *CGAL User and Reference Manual*. CGAL Editorial Board, 4.12 edition, 2018. URL `https://doc.cgal.org/4.12/Manual/packages.html`.

J. V. Uspensky. *Theory of equations*. McGraw-Hill, 1948.

H. Zessin. Point processes in general position. *Journal of Contemporary Mathematical Analysis*, 43(1):59–65, Feb 2008. ISSN 1934-9416.

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A. Appendix: Geometry

This appendix investigates some facts and proposition about geometry in $\mathbb{R}^3$. Since marked points are not present here, the dashed notation introduced in Chapter 1 will be dropped.

This chapter needs better notation. E.g. $S(p_1, p_2, p_3, p_4)$ for a sphere defined by those points, etc.

A.1 Calculating the circumdiameter

Check circumdiameter x circumradius, it's a bit confusing in many places

Here we describe how to calculate the circumdiameter of a $3-$simplex through the Cayley-Menger determinantCayley [1841], Menger [1928], Uspensky [1948] .

Improve the references (chapter, placement,..)

Consider the points $p_1, \ldots, p_5 \in \mathbb{R}^4$ which form a 4-simplex. Denote $d_{ij} = \|p_i - p_j\|, i, j = 1, \ldots, 5$. Then its area A is given by the **Cayley-Menger determinant**[ref sommervile].

$$-9216A^2 = \begin{vmatrix} 0 & 1 & 1 & 1 & 1 & 1 \\ 1 & 0 & d_{12}^2 & d_{13}^2 & d_{14}^2 & d_{15}^2 \\ 1 & d_{21}^2 & 0 & d_{23}^2 & d_{24}^2 & d_{25}^2 \\ 1 & d_{31}^2 & d_{32}^2 & 0 & d_{34}^2 & d_{35}^2 \\ 1 & d_{41}^2 & d_{42}^2 & d_{43}^2 & 0 & d_{45}^2 \\ 1 & d_{51}^2 & d_{52}^2 & d_{53}^2 & d_{54}^2 & 0 \end{vmatrix}$$

Now consider non-coplanar points $p_1, \ldots, p_4 \in \mathbb{R}^3$ forming a 3-simplex, i.e. a tetrahedron. To obtain the circumradius of this tetrahedron, we imagine $p_1, \ldots, p_4$ to lie on a 3-dimensional hyperplane H in $\mathbb{R}^4$ and we consider the point $c \in H$ such that $\|c - p_i\| = r \; \forall i = 1, \ldots, 4 \; r \in \mathbb{R}$. The point c is, by definition, the center of the circumsphere of $p_1, \ldots, p_4$ and d is the circumradius. The circumradius r can be obtained using the Cayley-Menger determinant, since $p_1, \ldots, p_4, c$ now form a 4-dimensional simplex of volume 0. We therefore have

$$0 = \begin{vmatrix} 0 & 1 & 1 & 1 & 1 & 1 \\ 1 & 0 & d_{12}^2 & d_{13}^2 & d_{14}^2 & r^2 \\ 1 & d_{21}^2 & 0 & d_{23}^2 & d_{24}^2 & r^2 \\ 1 & d_{31}^2 & d_{32}^2 & 0 & d_{34}^2 & r^2 \\ 1 & d_{41}^2 & d_{42}^2 & d_{43}^2 & 0 & r^2 \\ 1 & r^2 & r^2 & r^2 & r^2 & 0 \end{vmatrix}, \tag{A.1}$$

where we again have $d_{ij} = \|p_i - p_j\|, i, j = 1, \ldots, 4$.

It would be possible to solve A.1 as an equation of r. A better approach is to subtract r^2 times the first row from last and subtract r^2 times the first column from the last to obtain the determinant

$$\begin{vmatrix} 0 & 1 & 1 & 1 & 1 & 1 \\ 1 & 0 & d_{12}^2 & d_{13}^2 & d_{14}^2 & 0 \\ 1 & d_{21}^2 & 0 & d_{23}^2 & d_{24}^2 & 0 \\ 1 & d_{31}^2 & d_{32}^2 & 0 & d_{34}^2 & 0 \\ 1 & d_{41}^2 & d_{42}^2 & d_{43}^2 & 0 & 0 \\ 1 & 0 & 0 & 0 & 0 & -2r^2 \end{vmatrix}.$$

By expanding by the last row, we obtain the equation

$$2r^2 \begin{vmatrix} 0 & 1 & 1 & 1 & 1 \\ 1 & 0 & d_{12}^2 & d_{13}^2 & d_{14}^2 \\ 1 & d_{21}^2 & 0 & d_{23}^2 & d_{24}^2 \\ 1 & d_{31}^2 & d_{32}^2 & 0 & d_{34}^2 \\ 1 & d_{41}^2 & d_{42}^2 & d_{43}^2 & 0 \end{vmatrix} - \begin{vmatrix} 1 & 1 & 1 & 1 & 1 \\ 0 & d_{12}^2 & d_{13}^2 & d_{14}^2 & 0 \\ d_{21}^2 & 0 & d_{23}^2 & d_{24}^2 & 0 \\ d_{31}^2 & d_{32}^2 & 0 & d_{34}^2 & 0 \\ d_{41}^2 & d_{42}^2 & d_{43}^2 & 0 & 0 \end{vmatrix} = 0,$$

from which r^2 is directly expressible.

$$r^2 = \frac{\begin{vmatrix} 1 & 1 & 1 & 1 & 1 \\ 0 & d_{12}^2 & d_{13}^2 & d_{14}^2 & 0 \\ d_{21}^2 & 0 & d_{23}^2 & d_{24}^2 & 0 \\ d_{31}^2 & d_{32}^2 & 0 & d_{34}^2 & 0 \\ d_{41}^2 & d_{42}^2 & d_{43}^2 & 0 & 0 \end{vmatrix}}{2\begin{vmatrix} 0 & 1 & 1 & 1 & 1 \\ 1 & 0 & d_{12}^2 & d_{13}^2 & d_{14}^2 \\ 1 & d_{21}^2 & 0 & d_{23}^2 & d_{24}^2 \\ 1 & d_{31}^2 & d_{32}^2 & 0 & d_{34}^2 \\ 1 & d_{41}^2 & d_{42}^2 & d_{43}^2 & 0 \end{vmatrix}}. \tag{A.2}$$

It is worth noting that the determinant in the quotient cannot equal zero, since it is again a Cayley-Menger determinant and we assumed $p_1, \dots, p_4$ to be non-coplanar.

A.2 Bounding the circumdiameter

Say a bit more about what this is

This section proves the bound used in Theorems 3 4 5 6 and Proposition 15.

A.2.1 Statement of the problem

The problem of founding the bounds can be stated as the following two optimization problems.

For the tetrahedron T_1, the problem is

$$\begin{aligned} \underset{p_1,p_2,p_3,p_4\in\mathbb{R}^3}{\text{maximize}} \quad & \delta(\{p_1,p_2,p_3,p_4\}) \\ \text{subject to} \quad & \|p_i - t_i\| \le \rho a, t_i \in \mathbb{R}^3, i = 1,2,3,4, \\ & \|t_i - t_j\| = a, i = 1,2,3,4. \end{aligned} \tag{A.3}$$

To state the problem for the tetrahedron T_2, first denote

$$D = \begin{pmatrix} 0 & \sqrt{2}a & a & a \\ \sqrt{2}a & 0 & a & a \\ a & a & 0 & a \\ a & a & a & 0 \end{pmatrix},$$

and denote the entries of matrix D as $d_{ij}, i, j = 1, 2, 3, 4$. Then the statement is:

$$\begin{aligned} &\underset{p_1,p_2,p_3,p_4 \in \mathbb{R}^3}{\text{maximize}} && \delta(\{p_1, p_2, p_3, p_4\}) \\ &\text{subject to} && \|p_i - t_i\| \leq \rho a, t_i \in \mathbb{R}^3, i = 1, 2, 3, 4, \\ & && \|t_i - t_j\| = d_{ij}, i, j = 1, 2, 3, 4. \end{aligned} \tag{A.4}$$

This is a non-linear optimization problem. We can arrive at its solution through some careful geometric arguments.

A.2.2 Solution to the problem

First, define the *circumdiameter function* of point $p \in \mathbb{R}^3$ with respect to non-collinear points $p_1, p_2, p_3 \in \mathbb{R}^3$:

$$c(p) = \delta(\{p, p_1, p_2, p_3\}).$$

Denote (x_i, y_i, z_i) the coordinates of $p_i, i = 1, \ldots, 3$. The following lemma describes the properties of $c(p)$.

Define δ for triangles, too

Lemma 5. *$c(p)$ is continuous, has a global minimum $c_{min} := \delta(\{p_1, p_2, p_3\})$ and level sets*

$$L_a := \{p \in \mathbb{R}^3 : c(p) = a\} = S_{a1} \cup S_{a2}, \quad a \geq c_{min},$$

where S_{a1} and S_{a2} are two spheres with diameter a such that $p_1, p_2, p_3 \in S_{a1} \cap S_{a2}$. Furthermore, the centers c_1, c_2 of S_{a1}, S_{a2} respectivelly, lie in the halfspaces Improve the wording

$$H_+ = \{x \in \mathbb{R}^3 : Ax \geq 0\}, \; H_- = \{x \in \mathbb{R}^3 : Ax \leq 0\},$$

where A defines the hyperplane $H = \{x \in \mathbb{R}^3 : Ax = 0\}$ on which p_1, p_2, p_3 lie.

Proof. Continuity: From A.2 we see that $c(p)$ can be seen as a composition of a norm, determinants and division. Determinant is continuous as a function of elements of the matrix since it is a polynomial function. Thus $c(p)$ is continuous.

We can rewrite L_a as

$$\{p \in \mathbb{R}^3 : \exists \text{ sphere } S \text{ s.t. } p_1, p_2, p_3, p \in S \text{ and diam} S = a\}.$$

We must therefore find the number of spheres going through the points p_1, p_2, p_3 with the diameter a. Denote S a sphere such that $\{p_1, p_2, p_3\} \subset S$ with $\text{diam}(S) = a$. Define the hyperplanes

$$H_{12} = \{x \in \mathbb{R}^3 : \|x - p_1\| = \|x - p_2\|\}, \quad H_{23} = \{x \in \mathbb{R}^3 : \|x - p_2\| = \|x - p_3\|\}.$$

The intersection $H_{12} \cap H_{23}$ is a line L, as p_1, p_2, p_3 are non-collinear. The center of S is at distance $a/2$ from all three points and thus lies on L. For any point, there are at most two points on the line L at a given distance from the point. This proves that there are at most two spheres satisfying the definition of S.

Using the line L, we can also deduce the rest of the proposition. The point on L at a minimum distance to p_1, p_2, p_3 is the point $p_{min} := L \cap H$. We know that p_{min} is equidistant from p_1, p_2, p_3 and that it lies on the hyperplane H, therefore it is the circmradius of the triangle defined by p_1, p_2, p_3 and we have $c(p_{min}) = \delta(\{p_1, p_2, p_3\})$.

If possible, simplify this argument

To see that c_1 and c_2 must be (non-strictly) separated by the hyperplane H, assume WLOG $\{c_1, c_2\} \subset H_+, c_1 \neq c_2$. Let $p \in S_{a1}$ and let $p_R \in \mathbb{R}^3$ be the reflection of p through the hyperplane H. The tetrahedron p_1, p_2, p_3, p_R then is a reflection of the tetrahedron $p_1, p_2, \ldots, p$ and therefore its circumsphere has diameter a. However, its centre lies in H_-, which is a contradiction. □

Note that S_{a1} and S_{a2} are not necessarily distinct. In fact, we can see from the proof that $S_{a1} = S_{a2}$ precisely when $a = c_{min}$.

We are now ready to characterize the set of solutions to A.3 and A.4. For the next proposition, we say a point lies "inside" or "outside" of the sphere S if the the point lies in B or in B^c respectivelly, where B is the closed ball such that $\partial B = S$.

Proposition 19. *Any solution (p_1, p_2, p_3, p_4) of the problem A.3 will lie on a sphere S that is (internally or externally) tangent to the spheres $\partial B(t_i, \rho a), i =$ 1, 2, 3, 4.*

Proof. Let (p_1, p_2, p_3, p_4) be a solution of A.3. Denote $c(p_1) = \delta(\{p_1, p_2, p_3, p_4\}) = c$ and S the circumshphere of $\{p_1, \ldots, p_4\} \subset S$. First, WLOG assume that $p_1 \in B(t_1, \rho a)$. Because p_1 maximizes the function $c(p)$, we have $c(p_1) \geq c(p), p \in U$, where U is some small neighborhood of p_1. Choose two points, $p_O, p_I \in U \setminus S$ such that

1. $c(p_O) = c(p_I) = b$,
2. p_I is on the inside of S and p_0 on the outside of S
3. $S(p_I, p_2, p_3, p_4)$ and $S(p_O, p_2, p_3, p_4)$ do not equal and their centers lie on the same halfspace (H_+ or H_-) as S.

Define this notation

Such choice is possible due to continuity of $c(p)$. Yet we arrive at a contradiction, as the level set L_b now contains two distinct spheres with centres in the same halfspace.

Assume now that $p_1 \in \partial B(t_1, \rho a) =: S_1$. We now choose p_I and p_O with the additional requirement that they must both lie on $\partial B(t_1, \rho a)$. Such choise is not possible precisely when S_1 and S are tangent, since then S_1 lies either completely inside or outside S and it is no longer possible to choose points both outside and inside. □

Make sure "inside" a sphere has a clear meaning

Note that Proposition 19 is formulated for problem A.3. However, we could re-

Is this a good way of proceeding?

peat the same exact argument for A.4 and thus the same holds for both problems.

We have found that the solutions to A.3 and A.4 must lie on a sphere that tangent to the spheres within which points can move. This is a dramatic improvement — we have narrowed the previously infinite space of possible solutions down to just $2^4 = 16$ possible quadruples of points (and even less beacause of symmetries). We also note that the set of solutions to our problem is precisely the set of solutions of a three-dimensional equivalent of the more than two thousand years old **Apollonius problem**

Encoding problem

A.2.3 Apollonius problem in $\mathbb{R}^3$

We want to find all the spheres that are externally or internally tangent to the spheres $\partial B(t_i, \rho a), i = 2, 3, 4$ as defined in problems A.3 and A.4.

First note that two externally tangent spheres $S_1 = ((x_1, y_1, z_1), r_1), S_2 = ((x_2, y_2, z_2), r_2)$ satisfy

$$\|(x_1, y_1, z_1) - (x_2, y_2, z_2)\| = r_1 + r_2.$$

Similarly, two externally tangent spheres satisfy

$$\|(x_1, y_1, z_1) - (x_2, y_2, z_2)\| = |r_1 - r_2|.$$

By squaring both equations, we obtain the equality

$$(x_1 - x_2)^2 + (y_1 - y_2)^2 + (z_1 - z_2)^2 = (r_1 \pm r_2)^2$$

Where we use $+$ for externally and $-$ for internally tangent spheres.

The Apollonius problem for spheres S_1, S_2, S_3, S_4 is therefore solved by any $S = ((x, y, z), r)$ such that

$$\begin{aligned}
(x_1 - x)^2 + (y_1 - y)^2 + (z_1 - z)^2 &= (r_1 \pm r)^2 \\
(x_2 - x)^2 + (y_2 - y)^2 + (z_2 - z)^2 &= (r_2 \pm r)^2 \\
(x_3 - x)^2 + (y_3 - y)^2 + (z_3 - z)^2 &= (r_3 \pm r)^2 \\
(x_4 - x)^2 + (y_4 - y)^2 + (z_4 - z)^2 &= (r_4 \pm r)^2,
\end{aligned} \tag{A.5}$$

where we can take any combination of $+$ or $-$, yielding altogether 16 possible solutions. We do not consider degenerate cases as they cannot happen in our setting.

As noted previously, the number of solutions for both T_1 and T_2 will reduce significantly. For T_1, the spheres are completely interchangeable and thus only solutions with different number of $+$ will differ. This yields 5 possible solutions. Geometrically the number of $+$ can be seen as the number of spheres the solution is externally tangent to. For T_2 the situation is more complex, as the problem isn't entirely symmetric with respect to the four points. Still, symmetries do exist and the number of solution will be reduced.

Sadly, for most choices of $+$ and $-$, these equations still seem to be too complex for Mathematica to solve. Luckily, we can simplify them further.

Solving the equations A.5 by linearizing

We formulate the solution as a theorem.

Theorem 7. *For $\rho < 1/(2\sqrt{6})$, the maximum in A.3 is*

$$\delta_1 := 2a(\sqrt{6}/4 + \rho).$$

For $\rho < 1/4$, the maximum in A.4 is

$$\delta_2 := 2a\frac{2\rho + \sqrt{2 - 32\rho^2 + 64\rho^4}}{2 - 32\rho^2}.$$

Proof. Recall that the solution must lie on a sphere solving the equations A.5. We must therefore solve them and find the solution with the largest circumdiameter.

First, for clarity, we define the variables $s_i \in \{+1, -1\}, i = 1, \ldots, 4$ instead of relying on the notation $\pm$. We begin by expanding the parentheses to obtain the equations

$$x^2+y^2+z^2+x_i^2+y_i^2+z_i^2-2xx_i-2yy_i-2zz_i = r^2+r_i^2+2(s_1r_1-s_2r_2)r, \quad i = 1, 2, 3, 4$$

By subtracting the $2, 3, 4$-th equation from the first, we get rid of the quadratic terms and obtain a system of linear equations with four variables and three equations:

$$\begin{aligned} &-2(x_1 - x_i)x - 2(y_1 - y_i)y - 2(z_1 - z_i)z - 2(s_1r_1 - s_2r_2)r \\ &\quad + x_1^2 - x_i^2 + y_1^2 - y_i^2 + z_1^2 - z_i^2 - r_1^2 + r_i^2 = 0, \quad i = 2, 3, 4 \end{aligned}$$

This system can be solved to obtain expression of x, y, z in terms of r. We then substitute those expression into A.5 to obtain r[1].

We have used Wolfram Mathematica Inc. to find the solutions. The full implementation can be found in the file `ApolloniusProblem.nb`. By comparing the circumdiameters of the solutions, we obtain the proposition.

□

All the solutions for the choice $a = 1$ can be seen in Figures A.1 and A.2. We can see that for $T_1, \rho < 1/\sqrt{6}$, we have the two solutions

$$a(\sqrt{6}/4 + \rho), a\frac{\rho - \sqrt{6}(4\rho^2 - 1)}{4 - 24\rho^2}$$

which itersect at $\rho = 1/(2\sqrt{6})$.

Notice the simple linear form of the first solution — it is precisely the sphere which is internally tangent to all four spheres. This sphere has the same center as the circumsphere of tetrahedron $\{t_1, t_2, t_3, t_4\}$. Thus the solution is a sum of circumradius of the tetrahedron, $\sqrt{6}/4$, and the radius of the four spheres, ρ. We can see similar behaviour in the solution that is externally tangent to all four spheres.

For T_2, the linear solution will no longer be the largest, as now we obtain a larger circumradius by using a sphere that is externally tangent to some of the spheres.

[1] Note that exact solutions of x, y, z, which we are not interested in, could then by obtained through substituting r back into the linear system.

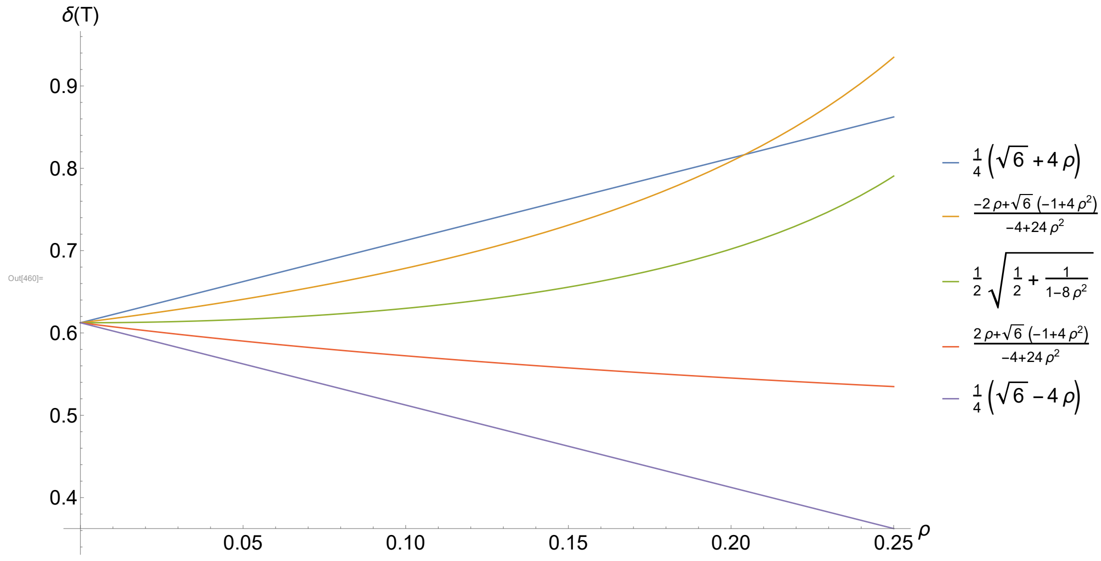

Figure A.1: All solutions to Apollonius problem with T_1, $a = 1$.

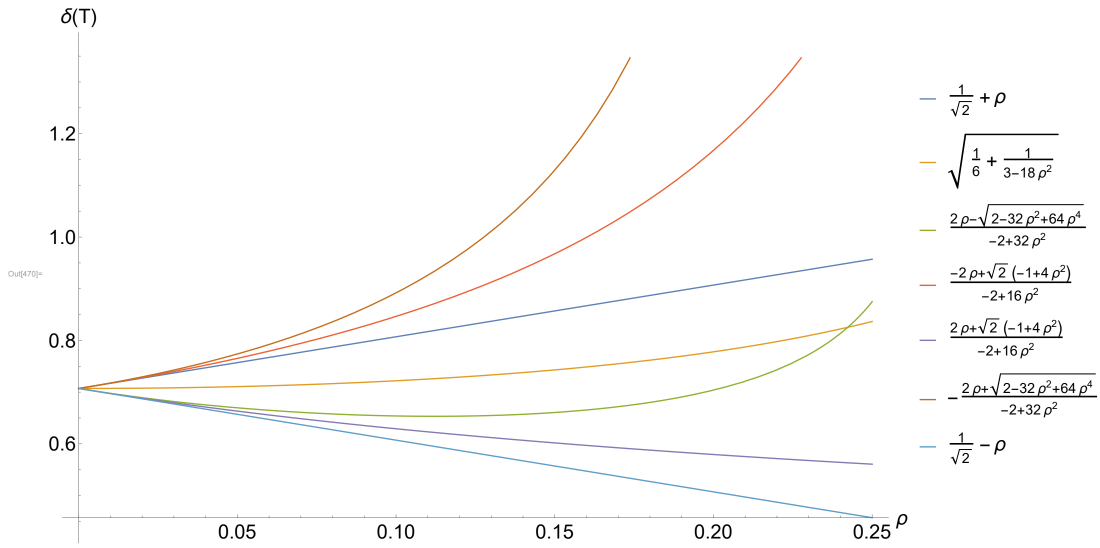

Figure A.2: All solutions to Apollonius problem with T_2, $a = 1$

Remark 15. [General position] From the form of the solutions one can also obtain the necessary bounds for ρ for the points to remain in general position. The points cease to be in general position precisely when any one of the solutions becomes infinite. This gives us $\rho < 1/(2\sqrt{6})$ for T_1 and $\rho < 1/4$ for T_2. Since we must control the circumdiamteter for all tetrahedra, we must assume $\rho < 1/4$.

B. Appendix: Implementation details

The latest version is available at `https://github.com/DahnJ/Gibbs-Delaunay`. Actually, change the url to reflect the Laguere case

B.1 C++ and CGAL

TO BE DONE

B.2 Python analysis

TO BE DONE

B.3 Wolfram Mathematica

TO BE DONE

Glossary of terms and abbreviations