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MASTER THESIS

Daniel Jahn

Generalized Random Tessellations

Department of Probability and Mathematical Statistics

Supervisor of the master thesis:	prof. RNDr. Viktor Beneš, DrSc.
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Author: Daniel Jahn

Department: Department of Probability and Mathematical Statistics

Supervisor: prof. RNDr. Viktor Beneš, DrSc., Department of Probability and Mathematical Statistics

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Possibly only refer to sections, not subsections?

Introduction

1. Geometric preliminaries

Before diving into the mathematics of Gibbs-Laguerre-Delaunay tetrihedrization 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 bounded sets is $\mathcal{B}_0$ ($\mathcal{B}'_0$).

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

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

be the set of locally finite sets on $\mathbb{R}^3 \times S$. Let $N_f \subset N_{lf}$ 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

$$N_\Lambda = \{\mathbf{x} \in N_f : \mathbf{x}' \subset \Lambda\}.$$

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

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

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

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

[1] Marks will also be often called weights

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 $\mathbf{x} \in N_{gp}$. 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 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 tetrihedrization

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 $\mathbf{x} \in N_{gp}$, $\eta \subset \mathbf{x}$. 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 as $B(\eta)$ as its definition does not depend on $\mathbf{x}$.

Definition 4. Let $\mathbf{x} \in N_{gp}$ and $\eta \subset \mathbf{x}$. We say that $(\eta, \mathbf{x})$ satisfies the *empty ball property* if $B(\eta) \cap \mathbf{x}' = \emptyset$. For convenience, for $\mathbf{x} \in N_{lf} \setminus N_{gp}$, 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 $\mathbf{x} \in N_{lf}$. 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 tetrihedrization 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 tetrihedrization, namely it contains sets of 4-tuples of points whose convex hull are the tetrahedra forming the Delauany tetrihedrization. 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 $\mathbf{x} \in N_{lf}$ — it contains the edges of the (undirected) nearest neighbor graph.

Proposition 1. *Define*

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

Then

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

Proof. Let $\mathbf{x} \in N_{lf}$ 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 $\|x - a\| < \mathrm{diam}(B(\eta, \mathbf{x})) = \|p - q\|/2$

1.1.2 Laguerre tetrihedrization

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 $\rho(p, (q', 0)) = d(p, q')$.

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

[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].

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 tetrihedrization.

Definition 8. Let $\eta \in N_{gp}$. 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 $\eta \in N_{gp}$. Then the following holds for the characteristic point p_η.*

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

2. *If* $\mathrm{card}(\eta) = 4$*, 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 $\leq$ 4 rows)

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

Not really follow, more like be directly observable

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

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 augumented 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 $\eta \in N_{gp}$ implies that $p'_1, \dots, p'_4$ 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 $p'_1, \dots, p'_4$ 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 augumented 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 augumented 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 $\{p_1, \dots, p_k\} = \eta \subset \mathbf{x} \in N_{gp}$, $k = 2, 3, 4$. If*

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

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 $d(x, p_i) = d(x, p_j), i, j = 1, \dots, 4$. □

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 $x \in N_{gp}$ 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 $\mathbf{x} \in N_{lf} \setminus N_{gp}$, 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

There is no point $q \in \mathbf{x}$ 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 tetrihedrization, where the circumball plays the role of the characteristic point.

c.f. remark that comes later

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

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

and its subsets

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

We then define the *Laguerre tetrihedrization 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 tetrihedrization). 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 tetrihedrization 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 $\mathbf{x} \in N_{lf}$ be a configuration where all points have mark 0. Then for any $\eta \subset \mathbf{x}, \mathrm{card}(\eta) = 4$ 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 tetrihedrization can be seen as merely a special case of Laguerre tetrihedrization, 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

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

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 $\rho(q, p_\eta) \ge 0$ for all $q \in \mathbf{x}$. This however means that $d(p'_\eta, p) = p''_\eta \le d(p'_\eta, q)$ 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 tetrihedrizations 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 N_{lf} and N_f, which are defined in section 2.

Definition 14. A *hypergraph structure* is a measurable subset $\mathcal{E}$ of $(N_f \times N_{lf}, \mathcal{N}_f \otimes \mathcal{N}_{lf})$ 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 $\mathbf{x} \in N_{lf}$, 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.

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

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

Where $\mathrm{conv}(\eta)$ 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 $\delta(\eta) = \mathrm{diam} B(\eta)$ 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

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

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

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 $\hat{\varphi} : N_{lf} \to \mathbb{R} \cup \{+\infty\}$ 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 $\eta \in \mathcal{E}(x)$. Also the finite horizon for $(\eta, \mathbf{x}) \in \mathcal{E}$ depends only on η. 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 $\mathbf{x} \in N_f$ 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 $\mathbf{x} \in N_{lf}$, for this such potentials would typically be equal to $\pm\infty$. 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 definining 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 $\tilde{\mathbf{x}} \in N, \tilde{\mathbf{x}} = \mathbf{x}$ 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.

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.

[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.

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 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 $\Lambda \in \mathcal{B}'_0$

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

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

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

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 $\zeta \in N_\Lambda$. 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.

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

$\square$

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 this definition, we are now ready for the desired definition of the energy function.

Definition 20. Let $\Lambda \in \mathcal{B}_0'$, $\zeta \in N_\Lambda$. 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 $\zeta \in N_\Lambda$, 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 $\partial\Lambda(\mathbf{x}) \times S$, $\zeta \in N_\Lambda$ 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 $\mathcal{LD}$.

Remark 8 (Adding and removing points in $\mathcal{D}_4$ and $\mathcal{LD}_4$). Let $\mathbf{x} \in N_{lf}$ 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

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

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

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

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

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

2. Stochastic geometry

Ultimately we want to study the behaviour of hypergraph structures and hyperedge potentials under some probabilistic assumptions on the distribution of the configuration $\mathbf{x}$. This chapter introduces the theory of point processes and random tessellations, both examples of the area of stochastic geometry, the concepts that will allow us to introduce randomness into hypergraphs. 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 tesssellation, giving us a great freedom in the specification of our models.

2.1 Point processes

This section will develop the bare minimum of the theory necessary to define and use Gibbs point processes. For a comprehensive introductory text, we recommend Moller and Waagepetersen [2003], as it is the most relevant text.

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

Really? Check it

The main aim of this text is to build Gibbs point processes with interactions based on the Laguerre tetrihedrizaion. 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 $N_{lf}(E)$ the space of all locally finite counting measures on E. We equip the space $N_{lf}(E)$ with the σ-algebra

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

Finally we define the set $N_f(E) \subset N_{lf}(E)$ of finite measures on E by

Maybe pospone this to a later section?

$$N_f(E) = \{\nu \in N_{lf}(E) : \nu(E) < \infty\}$$

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

We use the shortened notation $N_{lf}(\mathbb{R}^3 \times S) := N_{lf}$. Similarly for the terms $N_f, \mathcal{N}_f, \mathcal{N}_{lf}, \mathcal{B}, \mathcal{B}_0$.

Remark 9 (Simple PP).

Remark 10 (Duality of locally finite counting measures and configurations). In chapter 1, we introduced the sets N_{lf} and 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. For details and a proof, see lemma 3.1.4. in Schneider [2008].

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

Do we need anything else?

Poisson point process

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

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

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 Y_i and we can write

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

However, similarly to chapter 1, not explicitely stating the positional and mark part leads to a cleaner notation.

Proposition 7. *Let $\Phi_n = \sum_{i=1}^{n} \delta_{X_i}$ be a binomial point process on $B \in \mathcal{B}_0(E)$. 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 $A_i \subset B, i = 1, \dots, k$ that

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

That is 2.1 for $f(x_1, \dots, x_k) = 1_{A_1}(x_1) \dots 1_{A_k}(x_k)$. 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

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

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

The $\mathcal{B}^k$ is weird there, considering that we kinda have $\mathcal{B}^3 = \mathcal{B}$ elsewhere

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^ν_B 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^z_B the distribution of marked Poisson point process with intensity ν restricted to Λ. For $z = 1$, we lose the z and denote the distribution simply Π_Λ.

Notice that the set Λ refers only to the positions of the points. This is because we will always work with the whole mark space S.

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 $\Gamma \in \mathcal{N}_{lf}$

$$\Pi^z_\Lambda(\Gamma) = P(\Phi \in \Gamma) = \sum_{k=0}^{\infty} P(\Phi \in \Gamma | \Phi(\Lambda) = k) P(\Phi(\Lambda) = k) \tag{2.2}$$

$$= \sum_{k=0}^{\infty} \frac{(z|\Lambda|)^k}{k!} e^{-z|\Lambda|} P(\Phi^{(k)} \in \Gamma) \tag{2.3}$$

$$= \sum_{k=0}^{\infty} \frac{z^k}{k!} e^{-z|\Lambda|} \int_{\Lambda \times S} \cdots \int_{\Lambda \times S} 1_\Gamma \left(\sum_{i=1}^{k} \delta_{X_i} \right) \nu(dx_1), \dots, \nu(dx_k) \tag{2.4}$$

$$\tag{2.5}$$

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 N_{gp} and N_{rpp}. Zessin [2008].

2.1.2 Finite point processes with density

Analogy with random variables, why Poisson is the best

Restriction to finite set? Define Nf properly. Other problems with this..? Define finite point processes?

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 $p : \mathcal{N}_f \to \mathbb{R}^+$ such that $\int p(\gamma)\Pi_\Lambda(\gamma) = 1$ and

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

These calculations are overly complicated now, make them clearer

Notice that using the calculations in 7 and 2.2 we have

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

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 $\Phi \sim \Pi^z_\Lambda$.

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

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

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

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

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

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

□

2.1.3 Gibbs Point Processes

This section is a mess, edit

This really doesn't work. Instead start with connecting energy to the energy in the last chapter. Asssume it to be hereditary and define fGPP already within a hypergraph structure, DLR, then simply define GPP (careful about cr or admissible energy) through DLR. Then talk about GNZ and say what happens in the non hereditary case

A large class of point processes are the Gibbs point processes, the main object of our study.

Definition 29. The *finite Gibbs measure* on Λ with activity $z > 0$ is the distribution P^z_Λ such that $P^z_\Lambda \ll \Pi_\Lambda$ with density

$$p(\gamma) = \frac{1}{Z^z_\Lambda} z^{\gamma(\Lambda)} e^{-H(\gamma)}.$$

where $Z^z_\Lambda = \int z^{N_\Lambda} e^{-H} \Pi_\Lambda$ is the normalizing constant, called *partition function.* The measurable function $H : N_f \to \mathbb{R} \cup \{+\infty\}$ such that $Z^z_\Lambda < \infty$.
Process with the distribution P^z_Λ is called the *finite Gibbs point process* (finite GPP).

Notation for N_Λ

Show DLR, since that's how infinite is later defined

Due to its defintion, the finite GPP favours 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, called *forbidden*. A configuration that is not forbidden is *allowed*.

Before we continue onto extending the definition to N_{lf}, we will turn to the properties and form of the energy function.

The energy function

Here we will connect the definition of the energy function from definition 29 with that from definition 20. 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 structure of $\mathcal{D}$ and $\mathcal{LD}$, see example 1.2.1. The energy function is where the power of Gibbs point processes lies, but also where some of the difficulties arise.

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

Make stationarity more explicit. Also connect this with the last chapter better

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

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

- **Hereditarity**: For any $\gamma \in N_f$ 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 $\gamma \in N_f$
$$H(\gamma) \geq c_S \cdot \gamma(\mathbb{R}^3 \times S).$$

Stability bounds the density function $p(\gamma) \propto z^{\gamma(\Lambda)} e^{-H(\gamma)} \leq (ze^{-c_S})^{\gamma(\Lambda)}$ and thus ensures $Z^z_\Lambda < \infty$. 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.

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. Removing a point can lead to emergence of a tetrahedron with a larger circumdiameter, thus resulting in a forbidden configuration.

To see the usefulness of hereditarity, we first assume H is hereditary. For $\gamma \in N_f$ and $x \in \mathbb{R}^3 \times S$, define

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

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

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

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

Define supp or say we will treat them as sets

Proposition 9. *Let $\Lambda \in \mathcal{B}(\mathbb{R}^3)$ such that $|B| > 0$. For any non-negative measurable function f from $(\mathbb{R}^3 \times S) \times N_f$ to $\mathbb{R}$,*

$$\int \sum_{x \in \gamma} f(x, \gamma - \delta_x) P^z_\Lambda(d\gamma) = z \int \int_{\Lambda \times S} f(x, \gamma) e^{-h(x,\gamma)} dx P^z_\Lambda(d\gamma). \tag{2.6}$$

Furthermore P^z_Λ is uniquely defined by 2.6 in the sense that if a probability measure P on N_f satisfies 2.6, then $P = P^z_\Lambda$.

Proof. Direct adaption of propositions 4 and 5 from Dereudre [2017], where we take $d = 4$, use the last dimension as the space of marks concentrated on $[0, W]$ and then continue the proof using 7. ☐

Also need to refer on marked Slivnya-Mecke or sth

Hereditarity thus gives us a powerful characterization of the finite Gibbs measure. This characterization remains true even for (infinite) Gibbs measures, see theorem 2 in section 2.5 in Dereudre [2017]. 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.

Luckily, the approach in Dereudre and Lavancier [2007] allows us to directly use GNZ equations even for the non-hereditary case. Before we present the solution, we must first extend the definition of GPP to N_{lf}. Here we will diverge from Dereudre [2017], which requires a strong finite range property which our models do not satisfy, and take the approach of Dereudre et al. [2012], which uses the weaker range confinement property defined in definition 21.

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

Infinite volume Gibbs measures

maybe connect this with the discussion already writte in the energy section - it doesn't make sense for infinite sets etc

Perhaps instead of saying all this, just assume $\gamma \in N^\Lambda_{cr}$ and say it will be clarified later

First, define $\Theta = (\vartheta_x)_{x \in \mathbb{R}^3}$ be a group of translations ϑ_x defined in definition . The set $\mathcal{P}_\Theta$ denotes the set of all Θ-invariant probability measures on $(N_{lf}, \mathcal{N}_{lf})$ with $\int N_{[0,1]^3 \times S} dP < \infty$. Under an additional assumption presented in the next chapter, we then obtain that Θ-invariant measures are already concentrated on N^Λ_{cr}.

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

The set Λ should probably always have positive measure. Check this and write it somewhere

References to assumptions clear

Proposition 10. *Let $\Lambda \in \mathcal{B}_0(\mathbb{R}^3)$. Under the assumption 3.1.2, there exists a set $\hat{N}^{\Lambda}_{cr} \in N_{\Lambda^c}$ such that $\hat{N}^{\Lambda}_{cr} \subset N^{\Lambda}_{cr}$ and $P(\hat{N}^{\Lambda}_{cr}) = 1$ for all $P \in \mathcal{P}_{\Theta}$ with $P(\varnothing) = 0$.*

Define N_Λ

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

Thanks to this fact we can now use the form of the energy function in proposition 6 and define the (infinite volume) Gibbs measure and Gibbs point process.

Definition 30.

While the definition is simple and analogous to the finite case, proving the 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 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.

Having defined the Gibbs measure, we can now continue to present the approach of Dereudre and Lavancier [2007] extending the GNZ equations to Gibbs point processes with non-hereditary energy functions.

Define N_∞

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

Measurability?

Definition 31. Let $\gamma \in N_\infty$. 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 $\psi_{\Delta,\Lambda} : N_{lf} \to \mathbb{R} \cup \{+\infty\}$ such that*

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

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 $\forall \zeta \in N_\Delta : \varphi(\eta, \gamma) = \varphi(\eta, \zeta \cup \gamma_{\Delta^c})$ 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 $\gamma \in N_\infty$, then $x \in \gamma$ is removable if and only if $\gamma - \delta_x \in N_\infty$.*

Proof. Follows from lemma 2 above and proposition 1 in Dereudre and Lavancier [2007]. □

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 $f : (\mathbb{R}^3 \times S) \times N_{lf} \to \mathbb{R}$ we have*

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

Proof. See proposition 2 in Dereudre and Lavancier [2007]. □

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!

Any use in mentioning Markov processes and such

2.2 Random tessellations

Is there any use for this chapter?

3. Existence of Gibbs-type models

In this chapter, the theorem from **?** 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 **?** 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 **?**.

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

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

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

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

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

Assumption 1: All hyperedge potentials in the following are 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 Δ only depends on points in $\Delta + b(0, R)$. 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 $\operatorname{diam} B_i \leq \delta_R$ or $|\mathbf{x}_{B_i}| \leq n_R$.

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

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

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

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

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*: $e^{z|C|}\Pi^z_C(\Gamma) > e^{c_\Gamma}$, 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.

Check how I treat PP and random sets. Maybe use the duality between them?

As long as $\Pi^z_C(\Gamma) > 0$, (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

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

which can be derived using proposition 7. Indeed, let $\Phi \sim \Gamma^z_C$ be a Poisson point process with intensity z, restricted to C, we then have

$$\begin{aligned}
\Pi^z_C(\Gamma) = P(\Phi \in \Gamma) &= \sum_{k=0}^{\infty} P(\Phi \in \Gamma | \Phi(C) = k) P(\Phi(C) = k) \\
&= \sum_{k=0}^{\infty} \frac{(z|C|)^k}{k!} e^{-z|C|} P(\Phi^{(k)} \in \Gamma) \\
&= \sum_{k=0}^{\infty} \frac{z^k}{k!} e^{-z|C|} \int_C \cdots \int_C 1_\Gamma \left(\sum_{i=1}^{k} \delta_{X_i} \right) dx_1, \ldots, dx_k
\end{aligned}$$

where $\Phi^{(k)} = \sum_{i=1}^{k} \delta_{X_i}$ denotes the Binomial point process of k points in C and $\Phi^{(0)} = \delta_\emptyset$.

Remark about U3 monotonicity, possibly some other remarks about the assumptions

Get 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 $\#(\zeta) \geq c|\Lambda| - d$ whenever $\zeta \in N_f \cap N_\Lambda$ 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*: $\Pi^z_C(\Gamma) > 0$.

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

$$\Gamma^A = \{\zeta \in N_C : \zeta = \{p\}, p \in A\},$$

the set of configurations consisting of exactly one point in the set A. The set of pseudo-periodic configurations $\tilde{\Gamma}$ 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 $b \leq \rho_0 a$ for some sufficiently small $\rho_0 > 0$.

The vagueness about ρ_0 is not satisfactory, though it's the way DDG did it. If possible, change this

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 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 spheres being fully contained in their neighboring spheres, 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_0, the minimum distance between individual points is $a - 2\rho_0 a = a(1 - 2\rho_0)$. For $\mathcal{LD}$ models we therefore choose

$$A = B(0, b) \times \left[0, \sqrt{\frac{a}{2}(1 - 2\rho_0)}\right]$$

in order for spheres 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 $\#(\hat{\eta}) = |\eta|$, 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 $A = B(0, \rho_0 a) \times [0, \sqrt{\frac{a}{2}(1 - 2\rho_0)}]$ for $\mathcal{LD}$, we have

$$|A| = \frac{4}{3}\pi(\rho_0 a)^3 \cdot \sqrt{\frac{a}{2}(1 - 2\rho_0)} = \frac{4\pi}{3\sqrt{2}} \cdot \rho_0^3 \sqrt{1 - 2\rho_0} \cdot a^{7/2}$$

3.2.2 Geometrical structure of the tetrihedrizations defined by Γ^A and M

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

The advantage of the choice of M and A is that the tetrihedrizations formed by the configurations in $\tilde{\Gamma}^A$ can be described relatively simply. In particular, a sufficiently small ρ_0 ensures that the structure of the tetrihedrization does not change a lot and avoids degenerate cases of points not in general position.

For exmaple, in the $\mathbb{R}^2$ case, the two column vectors with angle $\pi/3$ define a triangulation made of equilateral triangles. Depending on the bound for ρ_0, the points never become collinear ($\sqrt{3}/6$) or even always generate the same triangultaion ($(\sqrt{3}-1)/4$) up to the movement of points within their respective set A.

Before we investigate the structure of the resulting tetrihedrizations, we list the properties we are interested in obtaining.

1. The number of tetrahedra incident to the point in C,

$$n_T := \#\{\eta \in \mathcal{E}(\mathbf{x}) : \eta \cap C \neq \emptyset\}.$$

2. The behaviour of the hyperedge potentials

Make precise later

3. The position of points with respect to the (reinforced) general position.

4. Boundedness of the weight of the characteristic points, i.e.

There's now a double use of the word regular. Do something about this. Perhaps call them Platonic

As noted previously, the using an analogous definition in $\mathbb{R}^2$ forms a triangulation containing equilateral triangles. Sadly, the three dimensional case is not as simple[1]. To better understand the structure of the resulting tetrahedrizations, we choose a particular example of a configuration from $\tilde{\Gamma}^a$.

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

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

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

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 tetrihedrization.

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

It's unclear what p_i are

[1]And it couldn't be, because the analogue of the two-dimensional equilateral triangle, the regular tetrahedron, does not tessellate, as Aristotle famously wrongly claimed Lagarias and Zong [2012]

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

To obtain the tetrihedrization of the parallelohedron formed by $\mathbb{p}_0$, we could mechanically perform the INCIRCLE test on all quintuples of points in $\mathbb{p}_0$ (see remark 3). We can also use our knowledge of the Delaunay tetrahedrization and geometry to deduce the structure of the tetrihedrization.

Format this section so that it's not just a wall of text

Comment on why the distances are what they are

We know (proposition 1) that $\mathrm{NNG}(\mathbb{p}_0) \subset \mathcal{D}_2(\mathbb{p}_0)$. $\mathrm{NNG}(\mathbb{p}_0)$ 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 $\{p_2, \dots, p_7\}$. Their regularity comes from the fact that all edges are of length 1. This polyhedral configuration is well known to tessellate[2].

To obtain the Delaunay tetrohedronization, we need to tetrahedronize the regular octahedron $O = \{p_2, \dots, p_7\}$. A regular octahedron is a Platonic solid and as such all of its vertices are cocircular [ref]. Furthermore it contains three quadruples of points that are coplanar [ref]. This configuration produces $\binom{6}{4} - 3 = 12$ tetrahedra, many of which intersect each other, a degeneracy that is nevertheless allowed in our definition of $\mathcal{D}_4$. In most (in fact almost surely w.r.t. Π^z) configurations in $\tilde{\Gamma}^A$ this won't be the case as the octahedron won't be regular. However, since we're interested in the supremum, we must consider this extreme case.

Try to show that we really only need almost all $\omega \in \tilde{\Gamma}$

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

Now we turn to the combinatorial structure of $\mathcal{D}(\mathbf{x})$. 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

[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].

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 $\mathbf{x} \in \tilde{\Gamma}$.

Proposition 13. *$\mathcal{D}_4(\mathbf{x}_0)$ 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. We know that $\mathrm{NNG}(\mathbb{p}_0)$ is composed of two regular tetrahedra and one regular octahedron O with all edge lengths equal to a. 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 $\mathcal{D}_4(\mathbb{p}_0)$ translated by vectors $k \in \mathbb{Z}^3$, we have fully characterized the tetrahedra of $\mathcal{D}_4(\mathbf{x}_0)$. □

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

With this knowledge we are ready to investigate the

Proposition 14. *Let $\mathbf{x} \in \tilde{\Gamma}^A$. Then 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 proposition 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 proposition **??**). Given the fact that weights are bounded, $S = [0, W]$, we find that there exists $B_{\eta'} > 0$ such that for given positions η', we have $p''_\eta \leq B_{\eta'}$ regardless of the weights. It remains to prove that $\sup_{\eta'} B_{\eta'} < \infty$, i.e. changing the points' positions can produce only bounded p''_η. This ammounts 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. □

3.2.3 Existence propositions

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

We can do more, but for the first draft use this

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 3. *Let $\Gamma \subset N_{lf}$ be a class of configurations. If there exists $d_{max} > 0$ such that* $\mathrm{diam}\Delta < d_{max}$ *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. □

Proposition 15. *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 **??**.

(U1) We know from [ref] that the exists $d_{max} > 0$ such that $\mathrm{diam} B(\eta) \leq d_{max}$. By lemma 3 $r_\Gamma \leq d_{max}$.

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

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

$$c_{\Gamma^A} \leq \frac{a}{4}(8 \cdot \delta_1 + 48 \cdot \delta_2)$$

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

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

□

Proposition 16. *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 **??**.

(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 [ref], 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.

□

Proposition 17. *There exists at least one Gibbs measure for the model* $(\mathcal{LD}_4, \varphi_S)$ *and every activity*

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

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 **??**.

(U1) By proposition 14 there is $C > 0$ such that $p''_\eta \leq C$ for all $\eta \in \mathcal{LD}_4(\mathbf{x}), \mathbf{x} \in \tilde{\Gamma}^A$. By lemma 3 we have $r_\Gamma \leq \sqrt{C + W}$.

(U2) is trivial since $n_T < 56$ and φ_S is bounded by [ref].

(U3) We proceed similarly as in 15 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

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

□

Proposition 18. *There exists at least one Gibbs measure for the model* $(\mathcal{D}_4, \varphi_S)$ *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 proposition 3.

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 **??**.

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

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

(U3) $\Pi_\Lambda^z(\Gamma) > 0$ 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.

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. 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^z_Λ. To that end, we emply Money Chain Markov Carlo (MCMC) techniques.

4.1 Monte Chain Markov Carlo

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 respect to point processes with density, see chapter 7 in Moller and Waagepetersen [2003]. For a more comprehensive text, we refer to Meyn and Tweedie [1993].

TO BE DONE

4.2 Simulating Gibbs-Laguerre-Delaunay tessellations

4.2.1 Birth-Death-Move Metropolis-Hastings algorithm

General description of the algorithm

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

Use in our models

4.2.2 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.

Birth step **??** then becomes:

$$\begin{aligned}\frac{f(\gamma_0+\delta_x)}{f(\gamma_0)} &= \exp\left(\sum_{\eta\in\mathcal{E}_\Lambda(\gamma_0+\delta_x)} V_1(T) - \sum_{\eta\in\mathcal{E}_\Lambda(\gamma_0)} V_1(T)\right)\\ &= \exp\left(\sum_{T\in\mathrm{DT}^{\otimes}(x,\gamma_0)} V_1(T) - \sum_{T\in\mathrm{DT}^{\ell}(x,\gamma_0\cup\{x\})} V_1(T)\right)\end{aligned}$$

Death step **??** becomes:

$$\frac{f(\gamma_0-\delta_x)}{f(\gamma_0)} = \exp\left(\sum_{\eta\in\mathcal{E}_\Lambda(\gamma-\delta_x)} V_1(T) - \sum_{\eta\in\mathcal{E}_\Lambda(\gamma)} V_1(T)\right)$$
$$= \exp\left(\sum_{T\in \mathrm{DT}^\ell(x,\gamma_0)} V_1(T) - \sum_{T\in \mathrm{DT}^\otimes(x,\gamma_0\setminus\{x\})} V_1(T)\right)$$

Move step **??** becomes:

$$\frac{f(\gamma_0-\delta_x+\delta_y)}{f(\gamma_0)} = \frac{f(\gamma_0\setminus\{x\}\cup\{y\})}{f(\gamma_0\setminus\{x\})}\frac{f(\gamma_0\setminus\{x\})}{f(\gamma_0)}$$
$$= \exp\left(\sum_{T\in \mathrm{DT}^\otimes(x,\gamma_0\setminus\{x\})} V_1(T) - \sum_{T\in \mathrm{DT}^\ell(x,\gamma_0\setminus\{x\}\cup\{y\})} V_1(T)\right.$$
$$\left.+ \sum_{T\in \mathrm{DT}^\ell(x,\gamma_0)} V_1(T) - \sum_{T\in \mathrm{DT}^\otimes(x,\gamma_0\setminus\{x\})} V_1(T)\right)$$

These expressions simplify the energy calculation immensely. Whereas calculating the energy for the whole tessellation requires all the tetrahedra, and thus depends on card$(\gamma\cap\Lambda)$, the final expressions only contain the tetrahedra local to x, and thus the energy can be calculated in constant time.

4.2.3 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 α and ϵ.

4.2.4 Irreducibility

TO BE DONE

5. Estimation

5.1 Maximum pseudolikelihood

Assume now that we obtain the point configuration γ on the observation window $\Lambda_n = [-n, n]^3 \times W$ and wish to estimate the model parameters.

Boundary problems. Do they simply exist because we're assuming to *only* know the configuration on Λ_n?

The estimation procedure closely follows that from **?**. That is a two-step approach, first estimating the hardcore parameters $\beta = (\epsilon, \alpha)$ and then using the estimates to obtain the estimate of θ through maximum pseudolikelihood (MPLE).

What exactly is the role of the growing window in **??**

5.1.1 Estimation of the hardcore parameters

Thanks to the fact that the hardcore parameter ϵ satisfies

? has this the other way around?

$$\text{if } \epsilon > \epsilon' \text{ then } \forall \Lambda,\ E_{\Lambda}^{\epsilon,\alpha,\theta}(\gamma_{\Lambda}, \gamma_{\Lambda^c}) < \infty \Rightarrow E_{\Lambda}^{\epsilon',\alpha,\theta}(\gamma_{\Lambda}, \gamma_{\Lambda^c}) < \infty,$$

and the hardcore parameter α satisfies

$$\text{if } \alpha < \alpha' \text{ then } \forall \Lambda,\ E_{\Lambda}^{\epsilon,\alpha,\theta}(\gamma_{\Lambda}, \gamma_{\Lambda^c}) < \infty \Rightarrow E_{\Lambda}^{\epsilon,\alpha',\theta}(\gamma_{\Lambda}, \gamma_{\Lambda^c}) < \infty,$$

their consistent estimators are:

$$\hat{\epsilon} = \inf\{\epsilon > 0, E_{\Lambda}(\gamma_{\Lambda}, \gamma_{\Lambda}^c) < \infty\},$$

$$\hat{\alpha} = \sup\{\alpha > 0, E_{\Lambda}(\gamma_{\Lambda}, \gamma_{\Lambda}^c) < \infty\}.$$

In practice, the parameters are estimated as

Are these consistent? Why?

$$\hat{\epsilon} = \min\{a(T), T \in Del_{\Lambda}(\gamma)\},$$

$$\hat{\alpha} = \max\{r(T), T \in Del_{\Lambda}(\gamma)\}.$$

The estimate $\hat{\beta} = (\hat{\epsilon}, \hat{\alpha})$ is then used in the pseudo-likelihood function in the second estimation step.

5.1.2 Estimation of the smooth interaction parameters

Equation references

The classical version of MPLE requires hereditarity of the interactions. Hereditarity means that for every permissible γ, the point pattern $\gamma \setminus \{x\}$ remains permissible for every $x \in \gamma$, that is any point can be removed from the point pattern. The hardcore interaction in the model **??** does not satisfy this condition. However, **?** extends MPLE to the non-hereditary case.

How does it relate to my case, exactly?

Since some points cannot be removed from the tessellation, we need to introduce the notion of a removable points. A point $x \in \gamma$ is removable in γ iff $\gamma \setminus \{x\}$ is permissible. We denote $\mathcal{R}^{\beta}(\gamma)$ the set of removable points of γ. Similarly the

The definition in **?** is actually different and this is given notion of an addable point will be useful. A point $x \in \gamma$ is addable in γ iff $\gamma \cup \{x\}$ is permissible.

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

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

where Λ_n' is the set of all addable points in Λ_n and $h^{\beta,\theta}(x, \gamma \setminus \{x\})$ 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

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

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

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

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

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

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

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

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

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

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

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

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.

5.1.3 Consistency

TO BE DONE

6. Numerical Results

Conclusion

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A. Appendix: Geometry

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

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].

$$-9216A^2 = \begin{vmatrix} 0 & 1 & 1 & 1 & 1 & 1 \\ 1 & 0 & d_{12}^2 & d_{13}^2 & d_{14}^2 & d_{15}^2 \\ 1 & d_{21}^2 & 0 & d_{23}^2 & d_{24}^2 & d_{25}^2 \\ 1 & d_{31}^2 & d_{32}^2 & 0 & d_{34}^2 & d_{35}^2 \\ 1 & d_{41}^2 & d_{42}^2 & d_{43}^2 & 0 & d_{44}^2 \\ 1 & d_{51}^2 & d_{52}^2 & d_{53}^2 & d_{54}^2 & 0 \end{vmatrix}$$

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 $\|c - p_i\| = r \forall i = 1, \ldots, 4$ $d \in \mathbb{R}$. 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 obtain by the Cayley-Menger determinant, because $p_1, \ldots, p_4, c$ now form a 4-dimensional simplex of volume 0. We therefore have

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

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

It would be possible to solve this as an equation of r. We can however do better. We can subtract r^2 times the first row from last and subtract r^2 of the first column from the last to obtain the determinant.

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

and expand by the last row, to 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

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

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

A.2 Bounding the circumdiameter hyperedge potential

We have the following optimization problems.

For the regular tetrahedron, the problem is

$$\begin{aligned} \underset{p_1,p_2,p_3,p_4 \in \mathbb{R}^3}{\text{maximize}} \quad & \delta(\{p_1, p_2, p_3, p_4\}) \\ \text{subject to} \quad & \|p_i - t_i\| \leq \rho_0 a, t_i \in \mathbb{R}^3 i = 1, 2, 3, 4, \\ & \|t_i - t_j\| = a, i = 1, 2, 3, 4. \end{aligned} \tag{A.2}$$

To state the second problem, first denote

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

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

$$\begin{aligned} \underset{p_1,p_2,p_3,p_4 \in \mathbb{R}^3}{\text{maximize}} \quad & \delta(\{p_1, p_2, p_3, p_4\}) \\ \text{subject to} \quad & p_i \in \bar{B}(t_i, \rho_0 a), t_i \in \mathbb{R}^3 i = 1, 2, 3, 4, \\ & \|t_i - t_j\| = d_{ij}, i, j = 1, 2, 3, 4. \end{aligned} \tag{A.3}$$

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

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 $c(p)$.

Lemma 4. *$c(p)$ is continuous, has a global minimum $c_{min} := \delta(\{p_1, p_2, p_3\})$ and*

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

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

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

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 **??** 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's a polynomial function. Thus $c(p)$ is continuous.

The we can rewrite L_a as

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

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 diameter a. Define the hyperplanes

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

Then their 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 a line at a given distance from the point. This proves that there are at most two spheres satisfying the definition of S.

Using 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 we have $c(p_{min}) = \delta(\{p_1, p_2, p_3\})$.

Improve the last bit, possibly simplify

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 and centre 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 the case $S_{a1} = S_{a2}$ is precisely when $a = c_{min}$.

Proposition 19. *Any solution* (p_1, p_2, p_3, p_4) *of the problem A.2 will lie on a sphere* S *that is (internally or externally) tangent to the spheres* $\partial B(t_i, \rho_0 a), i = 1, 2, 3, 4.$

Proof. Denote $c(p_1) = \delta(\{p_1, p_2, p_3, p_4\}) = c$ and S the sphere such that $\{p_1, \ldots, p_4\}$. First, WLOG assume that $p_1 \in B(t_1, \rho_0 a)$ 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.

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 $p_1 \in \partial B(t_1, \rho_0 a) =: S_1$. We now choose p_I and p_O with the additional requirement that they must both lie on $\partial B(t_1, \rho_0 a)$. This fails 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

We have found that the solutions to A.2 and A.3 must lie on a sphere that tangent to the spheres within which points can move. This is a major improvement. The space of possible solution narrows down to just $2^4 = 16$ possible quadruples of points (and even less beacause of symmetries), which are all the solution of a three-dimensional equivalent of the famous **Apollonius problem**.

First note that if 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, 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.

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

$$\begin{aligned}
(x_1 - x)^2 + (y_1 - y)^2 + (z_1 - z)^2 &= (r_1 \pm r)^2 \\
(x_2 - x)^2 + (y_2 - y)^2 + (z_2 - z)^2 &= (r_2 \pm r)^2 \\
(x_3 - x)^2 + (y_3 - y)^2 + (z_3 - z)^2 &= (r_3 \pm r)^2 \\
(x_4 - x)^2 + (y_4 - y)^2 + (z_4 - z)^2 &= (r_4 \pm r)^2
\end{aligned} \tag{A.4}$$

where we can take any combination of $+$ or $-$, yielding altogether 16 possible solutions. This excludes degenerate cases, which are not relevant in our case. 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.

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

First, for clarity, we define the variables $s_i \in \{+1, -1\}, i = 1, \dots, 4$ 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:

$$-2(x_1-x_i)x-2(y_1-y_i)y-2(z_1-z_i)z-2(s_1r_1-s_2r_2)r+x_1^2-x_i^2+y_1^2-y_i^2+z_1^2-z_i^2-r_1^2+r_i^2 = 0, \quad i = 2$$

This system can be solved to obtain expression of x, y, z in terms of r. We then substitute those expression into A.4 to obtain r.

Note that exact solutions of x, y, z, which we are not interested in, could then by obtained through the linear system.

All the solutions can be seen in 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 $\rho = 1/(2\sqrt{6})$. We will therefore assume $\rho < 1/(2\sqrt{6})$ and thus the solution to problem is $a(\sqrt{6}/4 + \rho)$. The simple linear form of the solution is not actually surprising — 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. Indeed the solution, for $\rho < 1/4$, is

$$a\frac{2\rho + \sqrt{2 - 32\rho^2 + 64\rho^4}}{2 - 32\rho^2}$$

Denote

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

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

From the form of the solutions one can also obtain the necessary bound for points to remain in general position. The bound is $\rho < 1/4$.

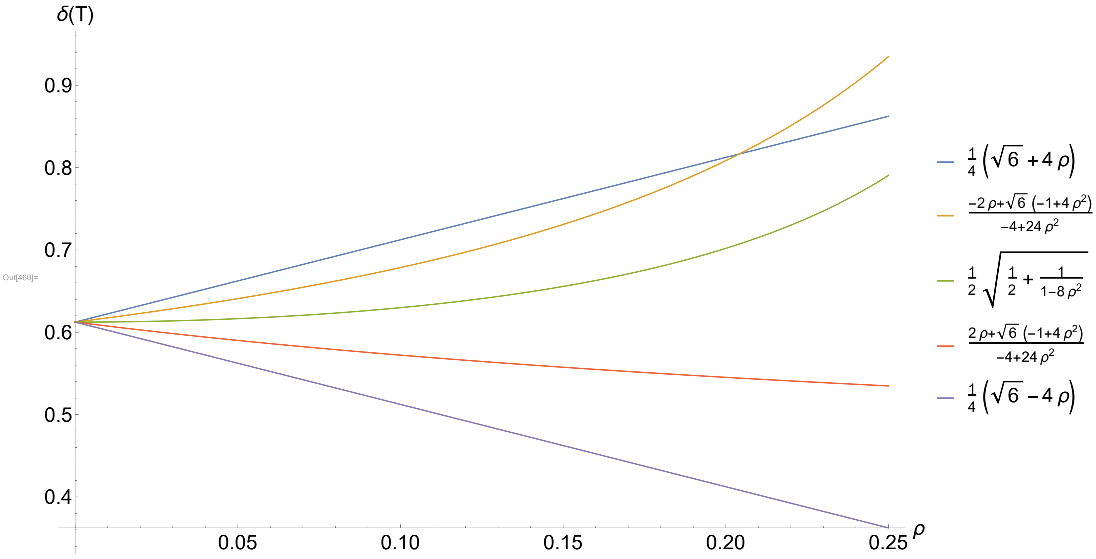

Figure A.1: All solutions to Apollonius problem with T_1, $a = 1$.

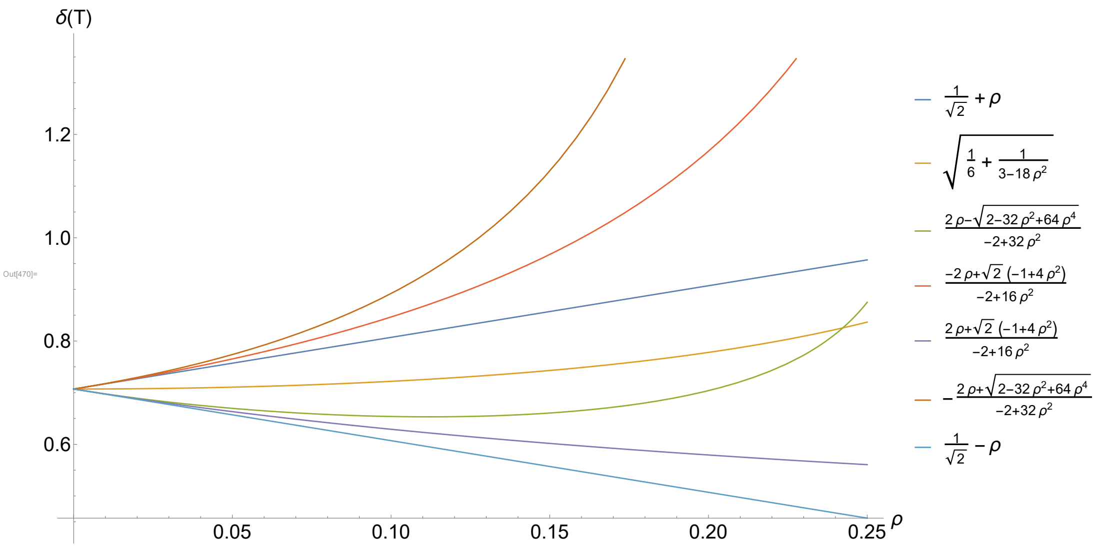

Figure A.2: All solutions to Apollonius problem with T_2,$a = 1$

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

List of Abbreviations

Todo list

Possibly only refer to sections, not subsections? . . . 2
Probably comment here on the fact that $|\Lambda|$ will be assumed to be positive 4
Reference some resources on Delaunay and Laguerre-Delaunay . . . 4
Comment on the fact that we need a vector space with measurable inner product etc? . . . 5
It's sufficient to check only subsets with $d+1$ points . . . 5
This definition is possibly not even needed . . . 5
Again, only need to check $d+2$ . . . 5
Add references to resources . . . 5
Possibly remark on existence and uniqueness, although this is not that interesting under this definition . . . 5
$x \in B(\eta, \mathbf{x})$ implies $\|x - a\| < \mathrm{diam}(B(\eta, \mathbf{x})) = \|p - q\|/2$ . . . 6
Short intro to Laguerre with some references . . . 6
This whole section really needs figures. . . . 6
Some diagram to visualise the proposition . . . 7
Visualise that there's no simple relationship between $B(\eta)$ and p''_η? . . . 7
Possibly rewrite this, or add a lemma that shows general position =¿ full row rank (for ≤ 4 rows) . . . 8
Not really follow, more like be directly observable . . . 8
Write clearer later . . . 8
c.f. remark that comes later . . . 9
It might be a good idea to characterize the relationsihp between individual $\mathcal{LD}_k$. . . . 10
Cocircular points do not create multiplicities in the cliques, since we're limiting k to max 4 . . . 10
Explain this more . . . 10
This definitely needs a figure + some comment on the fact that it's not an equivalence . . . 11
Do we need to restrict it on non-redundant points? Measurability? . . . 11
Perhaps talk about lifting - additional intuition on how this stuff works 11
Are graphs geometric? I mean, geometric graphs are geometric. But graphs in general? Are potentials part of this? . . . 11
Here we already need to have defined the σ-algebras on N_{lf} and N_f, which are defined in section 2. . . . 11
The symbol $\mathcal{LD}$ only makes sense now, when it's Laguerre-Delaunay. Comment on it before or sth. . . . 11
Define a proper Example environment with title and a possibility of a reference . . . 12
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. 12
Broken reference . . . 13
Reformulate the intro . . . 13
This remark is probably more fitting for the simulation chapter . . . 14
In the Laguerre case, we could also distinguish marks, but we won't do so, maybe comment on it . . . 14

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. 15
The usage of e.g. $\mathcal{D}_\Lambda(\mathbf{x})$ should probably be commented upon 15
Explain why 15
Confusing notation, d is reserved for the power distance 15
Comment on the definition and what it means for $\mathcal{D}$ and $\mathcal{LD}$. 15
Really? Check it 17
Maybe pospone this to a later section? 17
Do we need anything else? 18
The $\mathcal{B}^k$ is weird there, considering that we kinda have $\mathcal{B}^3 = \mathcal{B}$ elsewhere 19
We could also define Π_Λ as the marginal, without marks. Think this through 19
Analogy with random variables, why Poisson is the best 20
Restriction to finite set? Define Nf properly. Other problems with this..? Define finite point processes? 20
These calculations are overly complicated now, make them clearer . . . 20
This section is a mess, edit 20
This really doesn't work. Instead start with connecting energy to the energy in the last chapter. Asssume it to be hereditary and define fGPP already within a hypergraph structure, DLR, then simply define GPP (careful about cr or admissible energy) through DLR. Then talk about GNZ and say what happens in the non hereditary case 20
Notation for N_Λ 21
Show DLR, since that's how infinite is later defined 21
Make stationarity more explicit. Also connect this with the last chapter better 21
I don't really understand the role of $\emptyset$ in Gibbs theory. 21
Define supp or say we will treat them as sets 22
Also need to refer on marked Slivnya-Mecke or sth 22
Possibly cite the later edition? What's the approach here? 22
maybe connect this with the discussion already writte in the energy section - it doesn't make sense for infinite sets etc 22
Perhaps instead of saying all this, just assume $\gamma \in N_{cr}^\Lambda$ and say it will be clarified later 22
maybe connect this to intensity, i.e. define intensity etc 22
The set Λ should probably always have positive measure. Check this and write it somewhere 22
References to assumptions clear 22
Define N_Λ 23
Measurability? 23
Say what the set is equal to for us 24
But what about marks, does it work? 24
Measurability! 24
Any use in mentioning Markov processes and such 24
Is there any use for this chapter? 24
Could we at least use spread for gibbs with limited distance between points? 25

Check how I treat PP and random sets. Maybe use the duality between them? . . . 27
Remark about U3 monotonicity, possibly some other remarks about the assumptions . . . 27
Get more intuition about U3 and comment on why $\hat{\text{U}}$ is useful . . . 27
The vagueness about ρ_0 is not satisfactory, though it's the way DDG did it. If possible, change this . . . 28
This is perhaps unnecessarily conservative, we could widen it . . . 28
Check how I am using $|\cdot|$ and # . . . 28
Am I talking about tetrihedrization or hypergraph? Check and unify this 28
Make precise later . . . 29
There's now a double use of the word regular. Do something about this. Perhaps call them Platonic . . . 29
It's unclear what p_i are . . . 29
Format this section so that it's not just a wall of text . . . 30
Comment on why the distances are what they are . . . 30
Try to show that we really only need almost all $\omega \in \tilde{\Gamma}$ . . . 30
Reference, possibly using Schlafli symbols . . . 30
Overcounting degenerate cases . . . 30
Specify these things as "models" of the form $(\mathcal{D}_4, \varphi_S)$.Specify the measure μ in there, too . . . 31
We can do more, but for the first draft use this . . . 31
How exactly does this look? Why? . . . 32
Ugly line placements, improve . . . 33
Is it a problem that there's no n_R circle? Cause the proof suggested something like that? . . . 34
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. . . . 34
Definitely sell this more later . . . 36
Boundary problems. Do they simply exist because we're assuming to *only* know the configuration on Λ_n? . . . 37
What exactly is the role of the growing window in **??** . . . 37
? has this the other way around? . . . 37
Are these consistent? Why? . . . 37
Equation references . . . 37
How does it relate to my case, exactly? . . . 37
The definition in **?** is actually different and this is given as a proposition. 37
Is there any reason to define it the way **?** does? . . . 37
Connection between this and Papangelou could be useful . . . 38
Do we need the indicator function if we're only sampling from Λ'_n ? . . . 39
This chapter needs better notation. E.g. $S(p_1, p_2, p_3, p_4)$ for a sphere defined by those points, etc. . . . 46
Improve the last bit, possibly simplify . . . 48
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