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MASTER THESIS

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Generalized Random Tessellations

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Abstract: Abstract.

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Contents

Introduction

An achievement is also the first chapter Creating a standalone text about Laguerre tetrihedrization that does utilize the duality to Laguerre tessellatino, which is the usual approach in many texts.

1. Geometric preliminaries

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

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 component is the empty ball property [...] which determines the edge structure, which is in turn analyzed in terms of hypergraphs.

$\mathcal{F}$ or $\mathcal{N}$

Let $\mathcal{F}_{lf}$ be the set of locally finite sets on $\mathbb{R}^3$, and $\mathcal{F}_f \subset \mathcal{F}_{lf}$ the set of all finite sets on $\mathbb{R}^3$. An elements of F_{lf} will be usually denoted $\mathbb{x}$ and called a *configuration* and its subset η. If $|\eta| = 4$, as will be the case for the majority of this text, then η will be called *tetrahedron*.

Possibly define notation for spheres and then use it, it might be useful

1.1 Tetrahedrizations

The aim of this section is to introduce the geometric concepts necessary for the definition of the hypergraph structures in the following section. Definitions might be postponed. Note that although this text focuses solely on the three dimensional case, most ideas remain valid for a triangulation in any dimension. Furthermore, many facts have an analogous result in the case of Delaunay and Laguerre tessellations. This text is concerned with two types of tetrihedrizations.

Say this better and reference where to read about them

We introduce the notion of (reinforced) general position. This requirement will be later relaxed.

Definition 1. Let $\mathbb{x} \in \mathcal{F}_{lf}$. We say $\mathbb{x}$ is in **general position** if

$$\eta \subset \mathbb{x}, 2 \leq |\eta| \leq 3 \Rightarrow \eta \text{ is affinely independent.}$$

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

Commment on measurability of the set of locally finite sets in general position. This comes from cite[Zessin2008] and the $\mathcal{F}$ $\mathcal{M}$ equivalence?

Also 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 $\mathbb{x} \in \mathcal{F}_{gp}$. We say $\mathbb{x}$ is in **reinforced general position** if

$$\eta \subset \mathbb{x}, 3 \leq |\eta| \leq 4 \Rightarrow \eta \text{ is not cocircular.}$$

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

Define cocircular in general

Again, only need to check $d + 2$

1.1.1 Delaunay tetrihedrization

This section will shortly introduce the well known Delaunay tetrihedrization. There is vast literature on the topic, e.g. [ref].

Marks..

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

Note that the circumball is uniquely defined by η.

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

Definition 5. Let $\mathbb{x} \in \mathcal{F}_{lf}$. Define the set

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

and its subsets

$$\mathcal{D}_k(\mathbb{x}) := \{\eta \in \mathcal{D}(\mathbb{x}) : |\eta| = k\}, \quad k = 1, \dots, 4.$$

We then define the *Delaunay tetrihedrization of* $\mathbb{x}$ as the set $\mathcal{D}_4$.

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. It will however be useful to also consider subsets with a different number of points.

Talk about how we defined it, cause this ain't normal, man

Existence and uniqueness

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

Proposition 1. *Define*

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

Then

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

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

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

1.1.2 Laguerre tetrihedrization

A point $p = (p', p'') \in \mathbb{R}^3 \times S$ can be seen 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 $S_p = \partial B_p$.

Probably link to credenbach or something for the properties of this

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 the power distance). We split the interpretation into two cases and use the Pythagorean theorem.

- $d(q', p) \geq 0$. 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 .

Describe using a fig

Figures

Definition 7. For two (marked) points $p = (p', p'')$ and $q = (q', q'')$, define their *power product*[1] 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.

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 $\rho(p, q) \leq -2\sqrt{p''q''}$.

[1] 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. 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].

- $B_p \cap B_q \neq \emptyset$ 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 at two points. Denote a' the point of their intersection (it does not matter which one) and θ the angle $\angle p'a'q'$. We then obtain from the law of cosines.

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

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 $\eta \in \mathcal{F}_{gp}$. 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-coocircular.*

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 $S = [0, W]$ as the points of $\mathbb{x}$.

But it doesn't exist if it lies inside any of the spheres - it would require a negative weight / imaginary radius

Possibly add the characterization through power distance

If its weight is positive, the characteristic point can thus be interpreted as a sphere that intersects each sphere $S_p, p \in \eta$ at a right angle. If negative, [ref] 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. Its proof is crucial.

Existence and uniqueness

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

1. *If $|\eta| < 4$, then the p_η exists and is not unique.*
2. *If $|\eta| = 4$, then the p_η exists and is unique.*
3. *If $|\eta| > 4$, then the p_η exists if and only if η is Laguerre-cocircular.*

define the term

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

Not really follow, more like be directly observable

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

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

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

a system of equations which is linear with respect to $(\alpha, x_\eta, y_\eta, z_\eta)$. In an 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 $\eta \in \mathcal{F}_{gp}$ implies that $p'_1, \ldots, p'_4$ are affinely independent, i.e. not coplanar. This means that the homogenous system of linear equations defined by the matrix

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

does not have a solution, that is, the matrix has full rank. If it did, the points $p'_1, \ldots, p'_4$ would all satisfy the equation $Ax + By + Cz + D = 0$ for some $A, B, C, D \in \mathbb{R}$. The matrix 1.1.2 has the same column space as the left hand side of 1.2 and therefore the system has a unique solution.

If $|\eta| < 4$, 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 $|\eta| = 2$, general position implies that the points are unequal. For $|\eta| = 3$, general position implies that the points are not collinear.

Write better later

If $|\eta| > 4$, 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

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

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. $\square$

Connect this to incircle?

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.*

Proposition 3. *Let $p, q \in \mathbb{R}^3 \times S$. $H(p,q)$ is a hyperplane in $\mathbb{R}^3$.*

Proof. By simple calculation we have

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

$\square$

Notice that changing the weight of either of the points ammounts to translation of the hyperplane. Notice also that the characteristic point p_η of η, by 1.1, lies on the intersection of the hyperplanes

$$\bigcap_{p,q\in\eta} H(p,q).$$

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

The definition can also be equivalently stated as

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

The regularity property ensures that no point of $\mathbb{x}$ 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 $\mathbb{x} \in \mathcal{F}_{lf}$. Define the set

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

and its subsets

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

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

Remark 2 (Constructing Laguerre and Delaunay tetrihedrization). The proof of proposition 2 also gives a hint on how to check whether η is regular. [ref: gavrilova] **TO BE DONE**

Talk about how cocircular points create multiplicities in the cliques - no they don't, since we're limiting k to max 4

Remark 3 (Invariance in weights). Notice that adding or subtracting weights to all points in $\mathbb{x}$ does not change regularity of any $\eta \subset \mathbb{x}$. This implies that the Laguere tetrihedrization is invariant under this operation.

Why? Also write a bit more

Remark 4 (Delaunay as a special case of Laguerre). **TO BE DONE**

Redundant points

A major difference of the Laguerre tetrihedrization is the fact that some points may not play any role in the resulting structure.

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

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

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

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

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 $\eta \subset \mathbb{x}$ with a characteristic point p_η such that $\rho(q, p_\eta) = 0$ for all $q \in \eta$ and $\rho(q, p_\eta) \geq 0$ for all $q \in \mathbb{x}$. This however means that $d(p'_\eta, p) = p''_\eta \leq d(p'_\eta, q)$ for all $q \in \mathbb{x}$, implying $p'_\eta \in C_p$.
($\Rightarrow$) Assume $C_p \neq \emptyset$. There exist $x' \in C_p$ and $q \in \mathbb{x}, q \neq p$, 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* $\mathbb{x}$*, then the sphere* B_p *is completely contained in the balls of other points in* $\mathbb{x}$*, that is*

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

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 $q \in \mathbb{x}, q \neq p$. $\square$

To interpret this fact intuitively see fig. [fig].

Perhaps talk a bit more about the interpretation, e.g. why it's not sufficient

Restrict on non-redundant points? Measurability?

Talk about lifting - additional intuition on how this stuff works

1.2 Hypergraph structures

Both Delaunay and Laguerre tetrihedrizations can be seen as graphs where two points $p, q \in \mathbb{x}$ are joined if they are part of the same tetrahedron. For the purposes of this text, a more natural structure will be the hypergraph.

satisfying ESP or sth

1.2.1 Tetrihedrizations as hypergraphs

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

The subset $\eta \subset \mathbb{x}$ now plays the role of a hyperedge. e.g. tetrahedron.

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

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

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

$\mathcal{LD}$ 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 interest 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.* kkk

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

Hyperedge potential is *shift-invariant* if

Define ϑ_x

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

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

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

The fact that the hyperedge potential contains $\mathbb{x}$ as a second argument suggests that it is allowed to depend on points of $\mathbb{x}$ other than those in η.

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 measure thus alowing a great freedom in the types of hypergraphs we can obtain.

Volume of tetrahedron: $\eta \in \mathcal{E}(\mathbb{x})$ on $\mathcal{D}_4$ or $\mathcal{LD}_4$

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

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

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

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

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

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

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

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

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

Yeah but what if the 5 points actually describe 3 tetrahedra, as can be the case? This needs improving

For a given hypergraph structure $\mathcal{E}$, the *energy* of a finite configuration $\mathbb{x} \in \mathcal{F}_f$ is defined as the function[2]

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

However, in our case, we will typically deal with $\mathbb{x} \in \mathcal{F}_{lf}$, for this such potentials would typically be equal to $\pm\infty$. We will therefore be interested in the energy for only a bounded window $\Delta \in \mathcal{B}_0$. 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* suggest a connection with statistical mechanics, which gave rise to many of the concepts used in this text. Gibbs measure and concepts related to them continue to be an area with a rich interplay between statistical mechanics and probability theory. [3].

1.2.2 Hypergraph potentials and locality

A natural question to ask is "How do the points of $\mathbb{x}$ influence each other?". We've seen that there is a type of locality at play, for example in $\mathcal{D}_4$ the empty ball

[2]The letter H is often used for the energy in statistical mechanics, possibly stemming from the fact that it is also often called the Hamiltonian

[3]In fact, Gibbs measures beginning of statistical mechanics -, name after Josiah Willard Gibbs, who coined the term statistical mechanics

property of a tetrahedron η is dependent solely on presence of points of $\mathbb{x}$ inside $B(\eta)$. The question is further complicated by the presence of the hyperedge potential. This section will refine the question by definining different locality properties.

As we will see in chapter [ref], this locality is essential for the existence of our models and Gibbs measures in general.

Definition 17. A set $\Delta \in \mathcal{B}_0$ is a *finite horizon* for the pair $(\eta, \mathbb{x}) \in \mathcal{E}$ and the hyperedge potential φ if for all $\tilde{\mathbb{x}} \in N, \tilde{\mathbb{x}} = \mathbb{x}$ on $\Delta \times S$

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

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

The finite horizon of $(\eta, \mathbb{x})$ delineates the region outside which points can no longer violate the regularity (or the empty ball property) of η.

Remark 5 (Finite horizons for $\mathcal{D}$ and $\mathcal{LD}$). For $\mathcal{D}$, the closed circumball $\bar{B}(\eta, \mathbb{x})$ itself is a finite horizon for $(\eta, \mathbb{x})$.

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 on invariance).

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 18.

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

Later in the text, these are exactly the sets of tetrahedra used for the calculation, connect those two

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

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

Notice that $\mathbb{x}_\Lambda$ does not play any role in the definition. The configuration $\mathbb{x}$ thus only plays the role of a boundary condition.

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

Definition 19. The *energy of* ζ *in* Λ *with boundary condition* $\mathbb{x}$ is given by the formula

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

for $\zeta \in \mathcal{F}_\Lambda$, provided the sum is well-defined.

Remark 6 ($\mathcal{E}_\Lambda(\mathbb{x})$ for $\mathcal{D}$ and $\mathcal{LD}$). For $\mathcal{D}$, $\eta \in \mathcal{D}_\Lambda(\mathbb{x}) \iff B(\eta, \mathbb{x}) \cap \Lambda \neq \emptyset$. For $\mathcal{LD}$, $\eta \in \mathcal{LD}_\Lambda(\mathbb{x}) \iff d(p'_\eta, \Lambda) \leq \sqrt{p''_\eta + W}$, 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 $\mathbb{x}$.

Definition 20. Let $\Lambda \in \mathcal{B}_0$ be given. We say a configuration $\mathbb{x} \in N$ *confines the range of* φ *from* Λ if there exists a set $\partial\Lambda(\mathbb{x}) \in \mathcal{B}_0$ such that $\varphi(\eta, \zeta \cup \tilde{\mathbb{x}}_{\Lambda^c}) = \varphi(\eta, \zeta \cup \mathbb{x}_{\Lambda^c})$ whenever $\tilde{\mathbb{x}} = \mathbb{x}$ on $\partial\Lambda(\mathbb{x}) \times S$, $\zeta \in N_\Lambda$ and $\eta \in \mathcal{E}_\Lambda(\zeta \cup \mathbb{x}_{\Lambda^c})$. In this case we write $\mathbb{x} \in N^\Lambda_{\mathrm{cr}}$. We denote $r_{\Lambda,\mathbb{x}}$ the smallest possible r such that $(\Lambda + B(0,r)) \setminus \Lambda$ satisfies the definition of $\partial\Lambda(\mathbb{x})$. We will use the abbreviation $\partial_\Lambda \mathbb{x} = \mathbb{x}_{\partial\Lambda(\mathbb{x})}$.

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

Proposition 6. *Let* $\mathbb{x} \in N^\Lambda_{cr}$. *Then*

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

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

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

Measurability

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 $\mathbb{x}$. 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

Follow Schneider and Weil. Introduce basic concepts and theorems as well as point out useful calculation techniques.

2.1.1 Random measures and point processes

Random measure, σ-algebra, point process, σ-algebra, introduce simple pp as configurations by abuse of notation, comment on $\mathcal{N}_{gp}$ (zessin), Intensity, factorial measure,..

Introduce some basic theorems and relations so we can function, e.g. rewriting campbell-like stuff

Poisson point process

Poisson process and basic properties, mainly connection to binomial pp and the way we can use it to calculate

Before we define the Poisson point process, we first define a process closely related it.

Definition 21. Let $B \in \mathcal{B}_0$. For $n \in \mathbb{N}$ let $X_1, \ldots, X_n$ be independent and uniformly distributed random variables on B, that is

$$P(X_i \in A) = \frac{|A|}{|B|}.$$

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

$$\Phi_n = \sum_{i=1}^{n} \delta_{X_i}.$$

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

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

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

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

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 $C \in \mathcal{B}^k, C \subset B^k$ using the Dynkin system

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

and then from indicators to any non-negative measurable function. $\square$

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

Definition 22. Let ν be a diffuse measure on E. A point process Φ satisfying

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

Specially if $\nu = z|\cdot|$, then we call the Poisson point process *homogenous*.

2.1.2 Point processes with density

Analogy with random variables, why Poisson is the best, stability

Gibbs measure and Gibss point process

Talk about hereditarity too, mention Markov processes and connection maybe.

2.2 Random tessellations

In general x Gibbs-type

3. Existence of Gibbs-type models

In this chapter, the theorem from Dereudre and Lavancier [2007] will be presented and then we will proceed to check its assumptions for our models.

3.1 Existence theorem

In this section we first state the two existence theorems from Dereudre and Lavancier [2007] and then proceed to introduce its assumptions.

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

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

Proofs of both theorems can be found in Dereudre and Lavancier [2007].

3.1.1 Stability

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

(S) *Stability.* The hyperedge potential φ is called *stable* if there exists a constant $c_S \geq 0$ such that

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

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

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

Stability in $\mathbb{R}^2$

TO BE DONE

Stability in $\mathbb{R}^3$

TO BE DONE

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

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 e.g. [intro def7], which roughly states that there exists $R > 0$ such that the energy of $\mathbb{x}$ 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 [ref].

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

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

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

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

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*: $\bar{\Gamma} \subset N_{\mathrm{cr}}^{\Lambda}$ for all $\Lambda \in \mathcal{B}_0$ and

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

(U2) *Uniform summability*:

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

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

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

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

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

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

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

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

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

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 $H_{\Lambda,\mathbb{x}}(\zeta) < \infty$ for some $\Lambda \in \mathcal{B}_0$ and some $\mathbb{x} \in \bar{\Gamma}$.
- (Û2) = (U2) *Uniform summability.*
- (Û3) *Weak non-rigidity*: $\Pi_C^z(\Gamma) > 0$.

3.2 Checking 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. It would be convenient to choose $A = B(0, b) \times \{w\}$ for some $w \in S$ and then only deal with a Delaunay triangulation, but 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 $a - 2\rho_0 a = a(1 - 2\rho_0)$. We therefore choose

Only true if μ is non-atomic. But we could use an atomic μ for working with Delaunay.

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

in order for spheres to never overlap.

This is perhaps unnecessarily conservative, we could widen it

Remark 7 (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 $A = B(0, \rho_0 a) \times [0, \sqrt{\frac{a}{2}(1 - 2\rho_0)}]$, 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,

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

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 $\tilde{\Gamma}^a$.

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

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 4 we know that $\mathcal{LD}_4(\mathbb{x}_0) = \mathcal{D}_4(\mathbb{x}_0)$, 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 $\mathbb{x}_0$ 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 Archimedes famously wrongly claimed [ref]

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

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 2). 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 $\{p_2, \ldots, p_7\}$. 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 $O = \{p_2, \ldots, p_7\}$. 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 $\mathcal{D}(\mathbb{x}_0)$

Now we turn to the combinatorial structure of $\mathcal{D}(\mathbb{x})$. 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 $\mathbb{x} \in \tilde{\Gamma}$.

Proposition 8. *$\mathcal{D}_4(\mathbb{x}_0)$ 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 $\sqrt{a}$. Since $\mathcal{D}_4(\mathbb{x}_0)$ 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 $\mathcal{D}_4(\mathbb{x}_0)$. $\square$

With this knowledge we are ready to investigate the

4. Simulation

4.1 MCMC

4.2 Practical implementation

4.3 Results

5. Estimation

5.1 Results

Conclusion

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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. Appendix

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-coplanar 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 1. *$c(p)$ 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 $\{p_1, p_2, p_3\} \subset S$. Then $S \cap H = C$ where C is the (uniquely defined) circumcircle of p_1, p_2, p_3. **TO BE DONE**

Minimum: the smallest sphere containing p_1, p_2, p_3 has a great circle equal to the circumcircle of p_1, p_2, p_3.

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, the case $S_{a1} = S_{a2}$ is precisely when a is the global minimum of $c(p)$. Then the centre of S_{a1} lies on the hyperplane H.

Proposition 9. *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. One, because now the space of possible solution narrows down to just $2^4 = 16$ possible quadruples of points (and even less beacause of symmetries), and two, because the two-dimensional equivalent of this problem is a well known **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

$$(x_1 - x)^2 + (y_1 - y)^2 + (z_1 - z)^2 = (r_1 \pm r)^2 \tag{A.4}$$
$$(x_2 - x)^2 + (y_2 - y)^2 + (z_2 - z)^2 = (r_2 \pm r)^2 \tag{A.5}$$
$$(x_3 - x)^2 + (y_3 - y)^2 + (z_3 - z)^2 = (r_3 \pm r)^2 \tag{A.6}$$
$$(x_4 - x)^2 + (y_4 - y)^2 + (z_4 - z)^2 = (r_4 \pm r)^2 \tag{A.7}$$

List of Abbreviations

Todo list