Modelling Polycrystalline Materials: An Application of Optimal Transport

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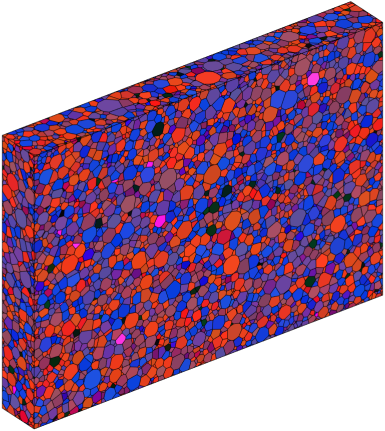
Microstructures

Using Optimal Transport; we can generate models of the microstructure of polycrystalline materials.



In particular, steel.

Microstructures

At the atomic level atoms in steel form lattices:

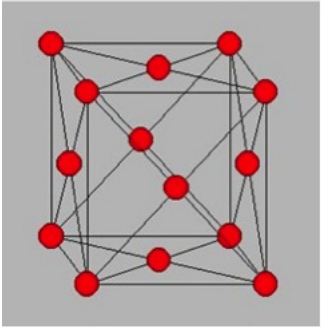
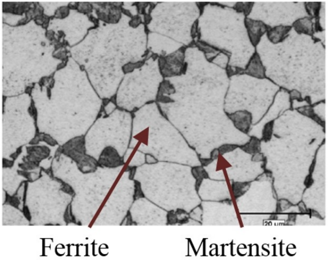
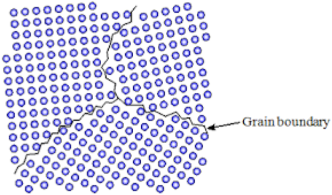


Figure: A Face-Centered Cubic lattice.

Microstructures

If we zoom out, the lattices are arranged in grains:





- The grains are regions of constant orientation and crystal structure.
- The size and orientation of these grains is a result of its composition and the way in which its made.
- This geometry has a large affect on the steels mechanical properties.

Representing Microstructures Mathematically

Given a domain $\Omega \subset \mathbb{R}^d$ and a set of seeds and weights, $(\mathbf{x}, \mathbf{w}) = \{x_i, w_i\}_{i=1}^n$ we define a Laguerre Tessellation of Ω generated by $(\mathbf{x}, \mathbf{w})$ to be the collection $\{L_i(\mathbf{x}, \mathbf{w})\}_{i=1}^n$ where:

$$L_i(\mathbf{x}, \mathbf{w}) = \{x \in \Omega : |x - x_i|^2 - w_i \leq |x - x_j|^2 - w_j \quad \text{for all } j\}$$

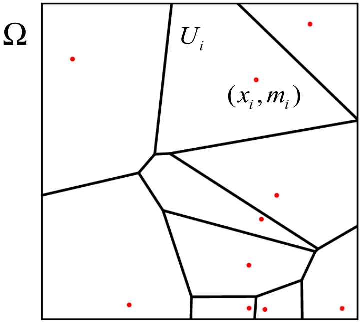


Figure: Laguerre Tessellation

Goals

Goals: Improve steel grades (alloys) and steel-forming processes by controlling the size and geometry of the grains.

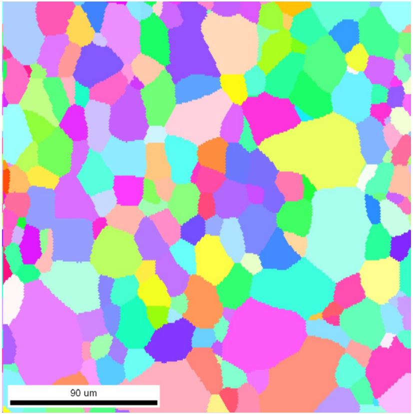
1. Geometric modelling: Use Laguerre Tessellations to model the structure of steel.
2. Computational Homogenisation: Assign mechanical properties to each grain. Simulate standard mechanical tests (uni-axial load, shear).

Today we will be concerned with the first goal.

Goals

Create models of steel (Laguerre Tessellations) with desirable properties such as:

- Volume Distribution.
- Spatial Distribution.
- Aspect ratio.



Goal 1

Goal (Objective)

Find $(\mathbf{x}, \mathbf{w})$ *such that,*

$$L_i(\mathbf{x}, \mathbf{w}) = v_i,$$

where $v_i > 0$ *is the desired volume of the ith cell.*

Question: When is this possible?

Answer Thankfully always! We just need to solve the transport problem between two suitably chosen measures.

Link to Semi-Discrete Optimal Transport

Fitting the volumes

The OT problem can be solved (for any collection $\mathbf{x} = (x_i)_{i=1}^n$!) furthermore the optimal map T can be expressed as following form:

$$T(x) = \text{argmin} \ |x - x_i|^2 - w_i^*.$$

for some $\mathbf{w}^* = (w_i^*)_{i=1}^n \in \mathbb{R}^n$. The solution is a Laguerre Tesselation with the desired volumes.

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The weights can be found by maximising the dual function:

$$\mathcal{K}(w_1, ..., w_n) = \sum_{i=1}^n \int_{L_i} |x - x_i|^2 - w_i \, \mathrm{d}x + \sum_{i=1}^n w_i v_i$$

This is usually done using a damped Newton method. [Kitigawa, Mergiot, Thibert, 2017]

Selecting the seeds: LLoyds Algorithm

The problem then becomes how do we choose the seeds? One approach is to use Lloyd's algorithm which produces regularised Laguerre Tessellations:

1. Chose or randomise $x_1^{(0)}, ..., x_1^{(0)}$

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1. Chose or randomise $x_1^{(0)}, \dots, x_1^{(0)}$
2. Initialisation: Let $x_i^{(k)}$ be the centroid of the previous Laguerre cell:

$$x_i^{(k)} = \frac{1}{\mathcal{L}(L_i^{(k-1)})} \int_{L_i^{(k-1)}} x \, \mathrm{d}x$$

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3. Optimisation: Find $w_1, \ldots, w_n$ which maximise $\mathcal{K}$ (up to a tolerance).

Repeat (2)+(3) until $k = K$.

Lloyd's Algorithm

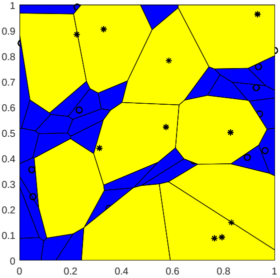


Figure: Initial Tesselation

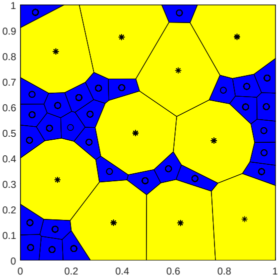
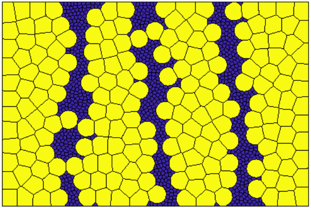


Figure: 20 Iterations

Lloyd's Algorithm



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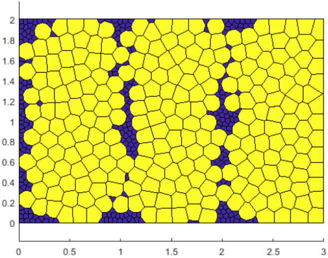

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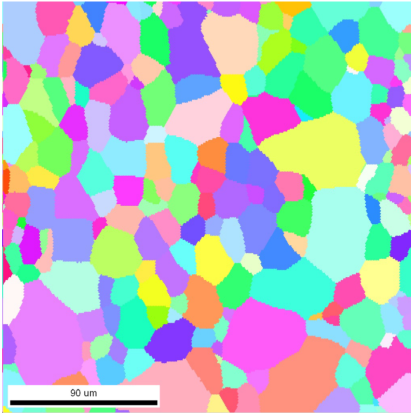

Spatial Distribution

Goal (Objective)

Given $\mathcal{D} = \{\mathbf{v}, \mathbf{b}\}$ *where* $\mathbf{v} = (v_i)_{i=1}^n \in \mathbb{R}_+^n$ *and* $\mathbf{b} = (b_i)_{i=1}^n \in \Omega^n$ *such that:*

$$\sum_{i=1}^n v_i = v_\Omega,$$

$$\sum_{i=1}^n v_i b_i = v_\Omega b_\Omega,$$

find

$$\mathbf{x} \in \operatorname{argmin} \sum_{i=1}^n |v_i(c_i(\mathbf{x}\ \mathbf{v}) - b_i)|^2$$

Which is a non-linear-least-squares problem. Thankfully this problem is linked to a concave optimisation problem.

From NLLS to concave optimisation

If we define,

$$H(\mathbf{x};\mathbf{v}) = \frac{1}{2}W_2^2(\mathcal{L}_\Omega^d, \nu(\mathbf{x};\mathbf{v})) - \frac{1}{2}\sum_{i=1}^n v_i|x_i|^2 + \sum_{i=1}^n v_i x_i \cdot b_i - \frac{1}{2}\int_\Omega |x|^2 \, dx.$$

It can be shown that if $x_i \neq x_j$ for distinct i, j then,

$$\frac{\partial H}{\partial x_i} = v_i(b_i - c_i(\mathbf{x})) \quad \text{for all } i$$

Therefore we can recast our problem as

$$\begin{aligned}
&\text{find } \mathbf{x} \text{ such that,} \\
&x_i \neq x_j \quad if \quad i \neq j, \\
&\mathbf{x} \in \text{argmin } |\nabla H(\mathbf{x})|^2,
\end{aligned}$$

Spatial Distribution

The objective function H has some useful properties:

Theorem (Properties of H)

Let H be defined as above then the following hold:

- *H is concave.*
- *$H \in \mathcal{C}^1(\mathbb{D})$ where*
  $\mathbb{D} = \{\mathbf{x} = (x_1, ..., x_n) \in (\mathbb{R}^d)^n : x_i \neq x_j \text{ for all } i \neq j\}$.
- *The gradient of H is given by,*

$$\nabla H = v_i(b_i - c_i(\mathbf{x}; \mathbf{v}))_{i=1}^n.$$

- *If $\mathbf{x} \in \mathbb{D}$ then,*

$$H(\mathbf{x}) = \sum_{i=1}^{n} v_i(b_i - c_i(\mathbf{x}, \mathbf{v})) \cdot x_i$$

- *If $\mathbf{x} \in \mathbb{D}$ is such that $H(\mathbf{x}) = 0$ then $c_i(\mathbf{x}; \mathbf{v}) = b_i$ for all i.*

Issues

Therefore instead we hope solving:

$$\underset{\mathbf{x}\in\mathbb{R}^{nd}}{\operatorname{argmax}}\, H(\mathbf{x})$$

is equivalent to the NLLS problem.

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Therefore instead we hope solving:

$$\underset{\mathbf{x}\in\mathbb{R}^{nd}}{\operatorname{argmax}}\ H(\mathbf{x})$$

is equivalent to the NLLS problem.

- What if there does not exist a diagram which fits our data exactly, is this approach still sensible? In paticular is the maximum in $\mathbb{D}$
- $H(\mathbf{0}) = 0$.
- If there exists a tessellation which fits our data, is it unique?
- Is the maximum unique?
- What conditions can we impose on the data for there to exist a diagram?

$\nexists$ a diagram case

Lemma (Meyron, 2019)

Given a Laguerre Tesselation with seeds and weights $C = \{x_i, w_i\}$ *if* $x_i^* = \lambda x_i + t$ *for* $\lambda > 0$ *and* $t \in \mathbb{R}^d$ *then there exists* $C^* = (x_i^*, w_i^*)$ *such that,*

$$L_i(C) = L_i(C^*) \quad \text{for all } i.$$

Applying the above to H we find,

$$H(\lambda \mathbf{x}) = \lambda H(\mathbf{x}).$$

We therefore need to restrict $\mathbf{x}$ to a compact set in which H will see every diagram, since if $H(\cdot) > 0$ it is unbounded.

Uniqueness

Theorem (Uniqueness of the Tessellation)

Suppose $\mathbf{x}, \mathbf{y} \in \mathbb{D}$ *are such that,*

$$c_i(\mathbf{x}; \mathbf{v}) = c_i(\mathbf{y}; \mathbf{v}) \quad \text{for all } i,$$

Then

$$L_i(\mathbf{x}; \mathbf{v}) = L_i(\mathbf{y}; \mathbf{v}) \quad \text{for all } i.$$

Proof.

Let T be the optimal transport map between $\mathcal{L}^d_\Omega$ and $\nu(\mathbf{x}; \mathbf{v})$. Define a map S given by,

$$S(x) = x_i \quad \text{if } x \in L_i(\mathbf{y}; \mathbf{v})$$

then since $\mathcal{L}^d_\Omega(S^{-1}(x_i)) = \mathcal{L}^d_\Omega(L_i(Y; \mathbf{v})) = v_i$ S is admissible for the transport problem between $\mathcal{L}^d_\Omega$ and $\nu(X; \mathbf{v})$. Moreover, □

Proof

$$
\begin{aligned}
\mathcal{M}(S) &= \int_\Omega |x - S(x)|^2 \, \mathrm{d}x \\
&= \int_\Omega |x|^2 \, \mathrm{d}x + \sum_{i=1}^{n} \int_{L(Y;\mathbf{v})} |x_i|^2 - 2x \cdot x_i \, \mathrm{d}x \\
&= \int_\Omega |x|^2 \mathrm{d}x + \sum_{i=1}^{n} v_i |x_i|^2 - 2 v_i c_i(\mathbf{y};\mathbf{v}) \\
&= \int_\Omega |x|^2 \mathrm{d}x + \sum_{i=1}^{n} v_i |x_i|^2 - 2 v_i c_i(\mathbf{x};\mathbf{v}) \quad \text{(by assumption)} \\
&= \int_\Omega |x|^2 \mathrm{d}x + \sum_{i=1}^{n} \int_{L(\mathbf{x})} |x_i|^2 - 2x \cdot x_i \, \mathrm{d}x \\
&= \int_\Omega |x - T(x)|^2 \, \mathrm{d}x = \mathcal{M}(T).
\end{aligned}
$$

Theorem

Let $g : \mathbb{R}^n \to \mathbb{R}$ *be convex. Suppose that there exists* $x_0 \in \mathbb{R}^n$ *such that, for all* $\lambda > 0$, $x \in \mathbb{R}^n$,

$$g(\lambda(x - x_0) + x_0) = \lambda g(x).$$

(If $x_0 = 0$*, then* g *is 1-positively homogeneous.) Assume that* g *is continuously differentiable on* $\mathbb{R}^n \setminus \{x_0\}$*. Let* $R > 0$ *and* $B_R = \{x \in \mathbb{R}^n : \|x - x_0\| \leq R\}$*. Assume that the global minimum of* g *on* B_R *is achieved at a point* $x^* \in \partial B_R$*. Moreover, assume that* g *is 3-times continuously differentiable in a neighbourhood of* x^* *and* $\ker(D^2 g(x^*)) = \mathrm{span}_{\mathbb{R}}\{x^* - x_0\}$*. Then* x^* *is a local minimiser of* $|\nabla g|$ *on*

Numerical Results

Real Data:

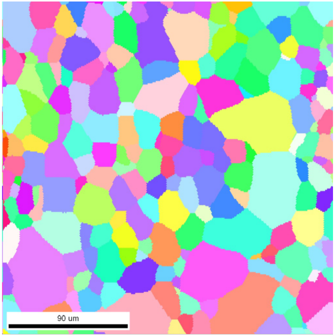


Figure: Data (EBSD)

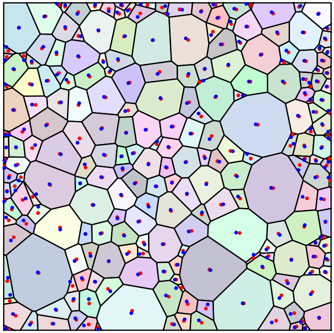


Figure: Model

Figure: Data vs Model, Blue: Target Centroids, Red: Realised Centroids

Numerical Results

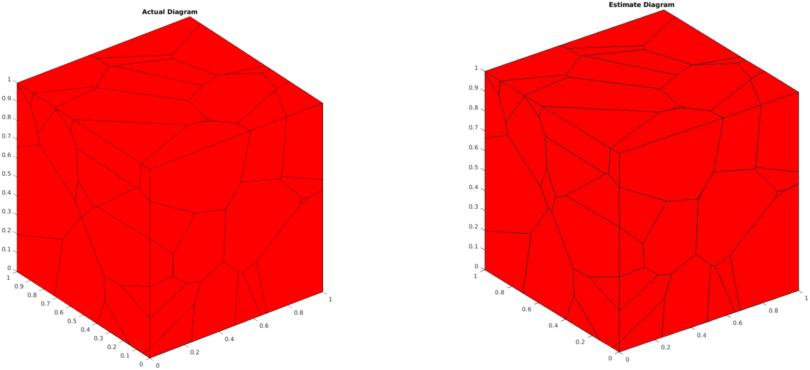
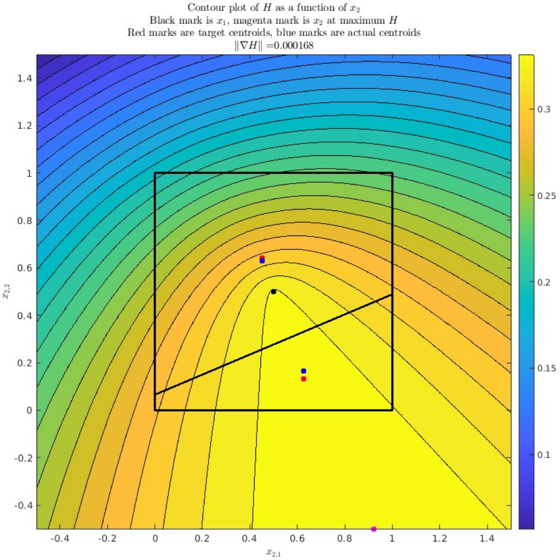


Figure: Simulated Data vs Model

∄ a diagram case



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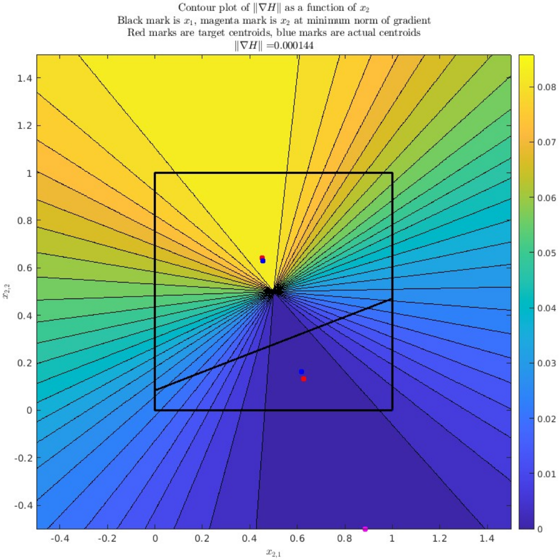

Thanks for listening!