Segmentation of Polycrystalline Images Using Voronoi Diagrams

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Material development is essential to solving problems our world faces.

- Superalloys: Industrial engineering applications such as aerospace and marine engineering
- Graphene: Applications in medicine and electronics
- Aerogels: Environmental applications
Polycrystalline materials are composed of many crystalline parts that are randomly oriented with respect to each other.

The material’s properties are largely dependent on its microstructure.

Material properties
- conductivity
- strength
- hardness
- corrosion resistance ...

Material microstructure properties
- Grain size
- Grain boundary distribution
- Grain deformations
- Chemical composition ...
Determining a materials properties through analysis of grain boundary structure is crucial to the development of new materials and subsequent advancement of engineering.

Obtaining accurate measurements through imaging can be expensive and tedious.

- Electron Backscatter Diffraction: Equipment and technician costs
- Light optical microscopy: Requires preprocessing of the material and may affect measurement accuracy
Problem Statement

- Given an image of a polycrystalline material, can we implement an algorithm that will produce an accurate segmentation?
- i.e. Can we produce a binary image that accurately represents the grain boundary structure?
Voronoi Diagrams

- We can model grain boundary structure by using Voronoi Diagrams.
- Given a set of generating points $P = \{p_1, p_2, ..., p_n\}$, a plane is partitioned into $n$ regions, $\{R_1, R_2, ..., R_n\}$, such that:
  - Each point $p_i$ lies in exactly one region $R_i$.
  - For any point $q \notin P$ that lies in region $R_i$, the Euclidean distance from $p_i$ to $q$ will be shorter than the Euclidean distance from $p_j$ to $q \forall j \neq i$. 

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Voronoi Diagrams

[Image of Voronoi Diagram]
Voronoi Diagrams
Mean-Curvature Flow of Voronoi Diagrams - Matt Elsey & Dejan Slepčev, 2014

They were interested in gradient flow of Voronoi diagrams and proving universal bounds on coarsening rates.

We followed a similar method while relaxing some constraints such as periodic boundary conditions. (more later)
Given a Voronoi Diagram with:
- Generating points \( P = \{p_1, p_2, ..., p_n\} \)
- Edges \( S = \{s_1, s_2, ..., s_k\} \)
- Vertices \( V = \{v_1, v_2, ..., v_m\} \).

We define the energy of the Voronoi Diagram as:

\[
E = \sum_{s_k \in S} \text{Length}(s_k) = \sum_{i, j \text{ s.t. } \overline{v_i v_j} = s_k \in S} |v_i - v_j|
\]

Using this definition of energy, we can apply gradient descent on the generating points \( P = \{p_1, p_2, ..., p_n\} \) and start to view some dynamics of the Voronoi diagrams.
Piece-wise Constant Mumford-Shah model

$$\sum_i \int_{R_i} (f(x, y) - c_i)^2 dx dy$$

- $f(x, y)$: the target image’s grayscale value at the pixel $(x, y)$
- $c_i$: the average pixel value in region $R_i$ computed from $f$
Model

Using the energy we defined earlier and the piece-wise constant Mumford-Shah we get:

\[ E = \sum_{i, j \text{ s.t. } \vec{v}_i \vec{v}_j = s_k \in S} |\vec{v}_i - \vec{v}_j| + \sum_{i} \int_{R_i} (f(x, y) - c_i)^2 \, dx \, dy \]
Calculating Gradients: First Term

- Edges: \( S = \{ s_1, s_2, \ldots, s_k \} \)
- Vertices: \( V = \{ v_1, v_2, \ldots, v_m \} \)

\[
\frac{\partial E}{\partial p_i} = \sum_{s_i \in S} \sum_{v_i \in \text{vertex}(s_i)} \frac{\partial \text{Length}(s_i)}{\partial v_i} \frac{\partial v_i}{\partial p_i}
\]

\[
\frac{\partial \text{length}(s_i)}{\partial v_i} = \left[ \frac{v_i(x) - v_j(x)}{\text{Length}(s_i)}, \frac{v_i(y) - v_j(y)}{\text{Length}(s_i)} \right]
\]

How to calculate \( \frac{\partial v_i}{\partial p_i} \)?
Calculating Gradients: First Term
Calculating Gradients: First Term
Calculating Gradients: First Term
We now have a way to calculate changes in $v_i$ for perturbations of $p_i$ along two specific directions.

Using a change of basis, we can get the gradient in terms of the standard basis

$$\frac{\partial v}{\partial p_1} = [w_1 \ w_2][s_1 \ s_2]^{-1}$$
Calculating Gradients: Second Term

- \( g(x, y) = (f(x, y) - c_i)^2 \)
- \( \frac{\partial}{\partial p_i} \sum_i \int_{R_i} g(x, y) \, dx \, dy \)
- note that after perturbing a center, the change in the integral comes from the part of the region that is changed.
Calculating Gradients: Second Term
Calculating Gradients: Second Term
Calculating Gradients: Second Term
Calculating Gradients: Second Term

- \( g(x, y) = (f(x, y) - c_i)^2 \)
- \[ \frac{\partial}{\partial p_i} \sum_i \int_{R_i} g(x, y) dxdy = \sum_i \int_{\partial R_i} g(s)v(s)^\perp ds \]
- \[ \approx \sum_i \sum_{s_i \in \text{edges}(R_i)} \sum_{k=1}^{N} g(s)v_k(s)^\perp \Delta s \]
- \[ v(s)^\perp = \frac{L-r}{L} \frac{\partial v_i}{\partial p_1} \hat{n} + \frac{r}{L} \frac{\partial v_j}{\partial p_1} \hat{n} \]
Gradient Descent Video

- play GD_Collision.mp4
Handling Topological Events

- Vertex collisions (handled well by the algorithm)
- Center collisions
- Vertices escape the boundary
- Center regions collapsed
Handling Topological Events - Center Collisions

- Repulsion:

\[ R(p_i, p_j) = R(d_{ij}) = e^{-\frac{1}{\theta^2(r-d_{ij})^2}} \]
Handling Topological Events - Boundary Event

![Graph showing topological events with boundary events labeled as \( p \) and \( p + g \).]
Handling Topological Events - Boundary Event

![Graph showing topological events]

- **p**
- **p**
- **p + g**

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Handling Topological Events - Collapsed Regions

- \( \text{Area}(R_i) \leq \tau \implies \text{Removal of } p_i \)
Gradient Descent Video

play GD_RP.mp4
Image Segmentation Result
Image Segmentation Result

- play Sample_Segment.mp4
Conclusion and Future Work

- Our Model / Algorithm was able to properly handle a preliminary test case segmentation.
- Future Challenges include:
  - Non-Uniform Grain Colors
  - Non-Distinct Grain Colors
  - Generating Point Initialization - Location and Number of points
References


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