Markow Random Fields: A Pervasive Approach for Microstructure Synthesis

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Outline

• Introduction to Markov Random Fields
• Computational approach
• Applications
  – Microstructure sampling
    • Comparison of statistical features with experimental image
    • Comparison of physical properties
  – 3D reconstruction from 2D orthogonal sections
    • A multiscale algorithm for improved efficiency
Probabilistic models

- Probabilistic Models
  - Graphical Models
    - Directed
    - Chordal
    - Undirected

- Bayesian Networks
- Markov Random Fields
1D Markov Chain

Ordered Markov property is the assumption that a node only depends on its immediate parents, not on all predecessors in the ordering.

\[ p(x_n|x_i, i < n) = p(x_n|x_{n-1}) \]

\[ p(x) = p(x_0) \prod_{n=1}^{N} p(x_n|x_{n-1}) \]
1D Markov chain (second order)

\[ p(x_1:T) = p(x_1, x_2) \prod_{t=3}^{T} p(x_t|x_{t-1}, x_{t-2}) \]
Markov Random Fields

- Undirected graph
  - Symmetric and more natural for 2D, 3D image data
- Pairwise, local and global Markov properties

- **Pairwise** $1 \perp 7 | \text{rest}$
- **Local** $1 \perp \text{rest} | 2, 3$
- **Global** $1, 2 \perp 6, 7 | 3, 4, 5$
MRFs for 2D data

Microstructures = Markov random fields: a set of n neighbor pixels completely determine the probability of the next pixel.

Ising model

Higher order interactions
Inference Problems

Find unknown pixel $X_8$ given the rest of the image.
• Need to compute $P(X_8 \mid X_3, X_7, X_9, X_{13})$
• Building explicit probability tables from experimental images intractable, especially for higher order interactions

A harder problem: Sample a new image given an experimental image
• Start from a small seed image and `grow' image based on its neighbors
• $P(p \mid \text{known neighbor pixels}) = ?$
• This is related to the previous problem, but only a part of the neighborhood is known
Sampling approach

- Sample patches in the experimental image that look similar to the neighborhood. All patches within 10% of the closest match are stored in a list. The center pixel values of patches in the list give a histogram for the unknown pixel.
- The similarity measure is based on a least square distance with Gaussian weighting. The distance is normalized by the number of known pixels.
- Tradeoff: PDF may not stay valid as neighbor pixels are filled in; but works well nevertheless.
Example: Sampling polycrystals

- **Experimental sample**
- **Computational estimation of microstructure field**

Diagram showing:
- Synthesized Image
- Seed Image

Graphs and images illustrating the comparison between experimental and computational samples.
Example: Sampling polycrystals

**Experimental sample**

**Computational estimation of microstructure field**
Two-phase microstructure – Effect of window size

Sample | Window Size 3 | Window Size 5
--- | --- | ---

Window Size 7 | Window Size 9 | Window Size 11

Microstructure is a silver-tungsten composite from Umekawa et al (1965)
Two-phase microstructure

- Units of Stress is in GPa
- Average Stress Value for synthesized image = 7.19 GPa
- Average Stress Value for sample image = 7.36 GPa
Microstructure properties

Longer Range Correlation

Shorter Range Correlation

Experimental result Umekawa et al (1965),
Polycrystalline microstructure

Color blot indicating crystal orientations in experimental image (left) and the synthesized image (right).

AA3002 alloy, Wittridge, Knutsen 1999
Microstructure properties

Results from Crystal Plasticity Simulations

Stress-strain response

Young’s modulus

Stress (MPa) vs. Equivalent Strain

Young’s modulus (GPa) vs. Rotation Angle (Degree)
Comparison of experimental and synthesized image

Stress distribution under y-axis tensile test

Sample

Synthesized

Stress histogram (# of pixels with a given stress, stress value is indicated above bars)

Sample

MRF

Stress distribution under y-axis tensile test
Particle Shape Analysis (Collaboration with de Graef group)

- Using our MRF code they generated different synthetic microstructures and generated two density maps
  - Second Order Moment Invariant Maps (SOMIM)
  - Projected Moment Invariant Maps (PMIM)
- These density maps show the distribution of shapes throughout an image.
- Hellinger distance (modified Bhattacharya coefficient) measures the similarity of the two distributions, and a value close to zero indicated good synthesis.
3D reconstruction from 2D samples

- Problem: Generate 3D microstructures from 2D orthogonal image sections
- State-of-the-art methods based on matching statistical features, restricted to simple (e.g. two phase) microstructures
- Direct extension of MRF sampling is computational expensive
- A multiscale optimization approach is proposed: Low resolution 3D images are first constructed (16x16x16) and then progressively refined.
The minimization of the cost function allows reconstruction of 3D images through matching of 3D slices at different voxels to the representative 2D micrographs and while ensuring patches from the 2D micrographs mesh together seamlessly in the 3D image.
EM algorithm

**M-step**: finds the best matching windows in the 2D micrographs along the x-, y- and z- directions for every voxel $v$

**E-step**: $V_v$ is the weighted average of the colors at locations corresponding to voxel $v$ in the best matching windows of various voxels in the solid microstructure.
**EM algorithm**

**Expectation step:** Minimize the cost function with respect to $V_v$

$$V_v = \left( \sum_{i \in \{x,y,z\}} \sum_u \omega_{u,v}^i S_{u,v}^i \right) / \left( \sum_{i \in \{x,y,z\}} \sum_u \omega_{u,v}^i \right)$$

**Maximization step:** Minimize cost function with respect to the set of input neighborhoods $S_v$ keeping $V_v$ fixed at the value estimated in the E-step.

$$S_v^x = \arg \min_{S_{x,w}} \sum_u \omega_{v,u}^x \| V_{v,u}^x - S_{u}^x \|^2$$

Iterate until convergence (i.e. until $S_v$ unchanged between iterations)
Multiresolution Code Demo
Example 1: Disperse Spheres

Experiment

Synthesized

(a)  (b)

(c)
Example 2: Anisotropic case

Experiment

Synthesized

(a)  (b)  (c)
Example 3: Polycrystalline case

Experiment

Synthesized

(a)

(b)

(c)
Conclusions

• Microstructures are mathematically well described as MRFs

• Synthesized microstructures have similar stereological properties (autocorrelation function, grain size histograms, grain shape, orientation distribution function), stress distribution (histograms) under tensile loading and overall stress—strain response.

• Extension to 3D microstructures