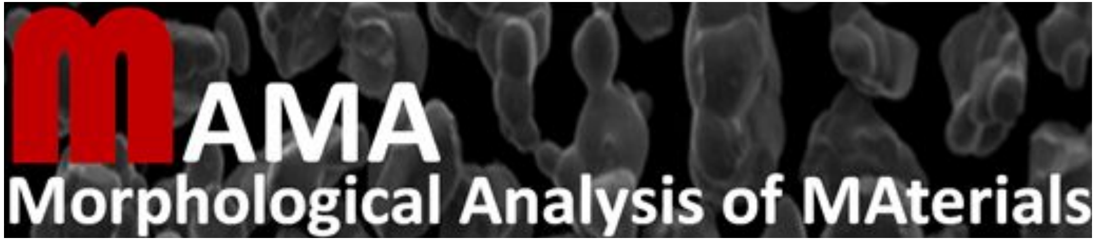
Securing our Technical Leadership in Hierarchical Watersheds

Reid Porter, Kari Sentz (CCS-3)
Brian Patterson (MST-6)

9/13/2021

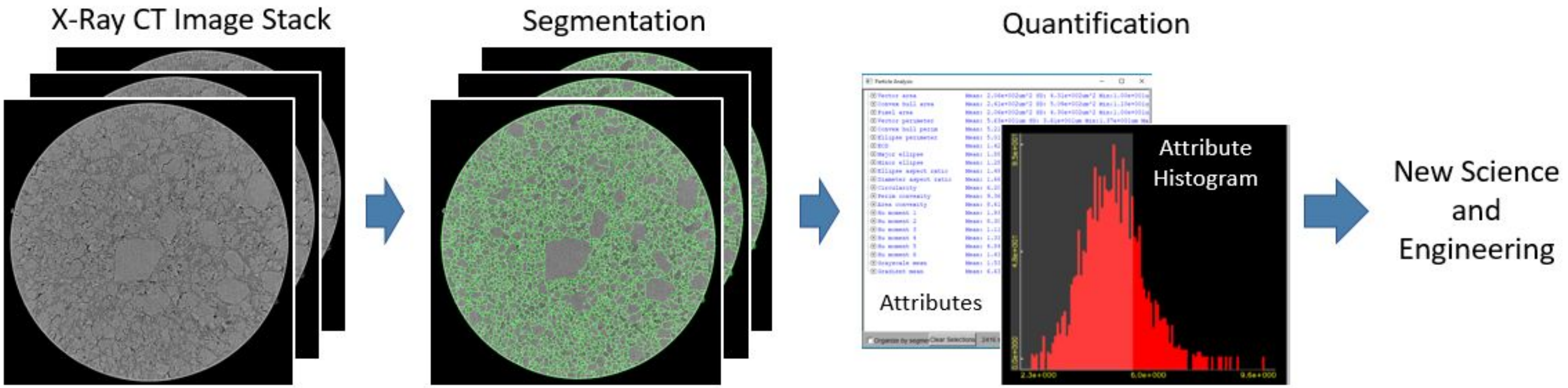
LA-UR-21-29829



- High-throughput, automated image quantification enables basic science and new applications.

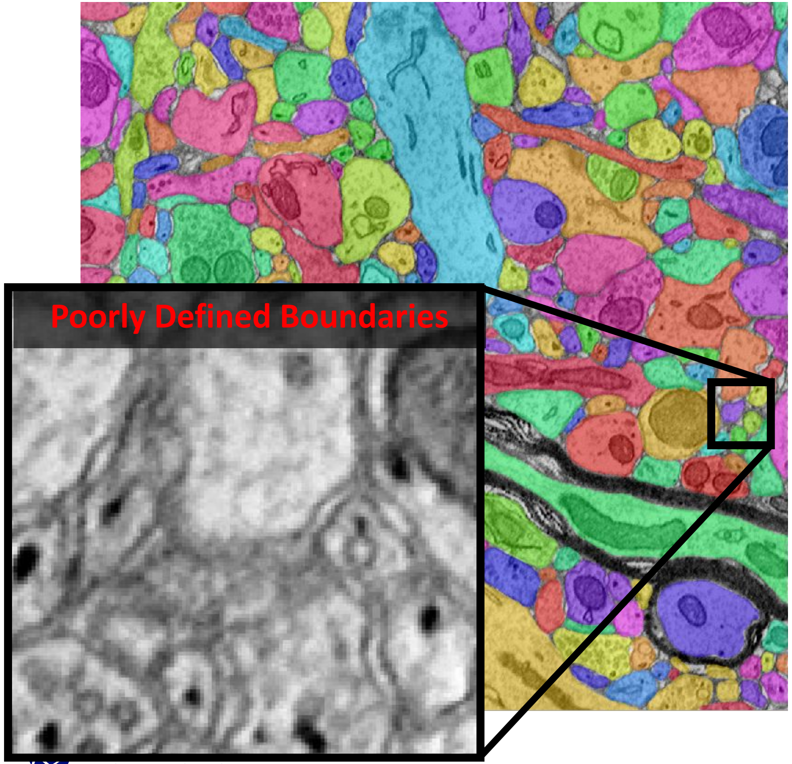
MAMA CURRENT USERS

- DOE NATIONAL LABORATORIES
- GOVERNMENT AGENCIES
- INTERNATIONAL PARTNERS
- UNIVERSITY PARTNERS



Why Segmentation is Hard

3D Segmentation of neurites in EM images



Lack of X-ray contrast between crystals and binder

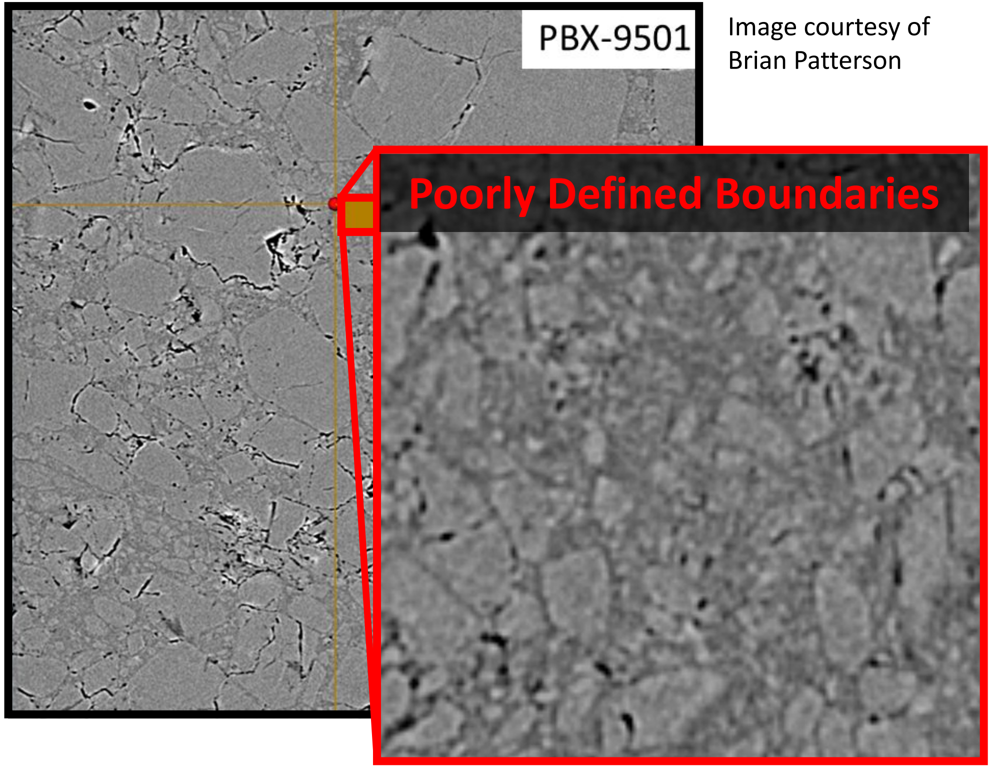
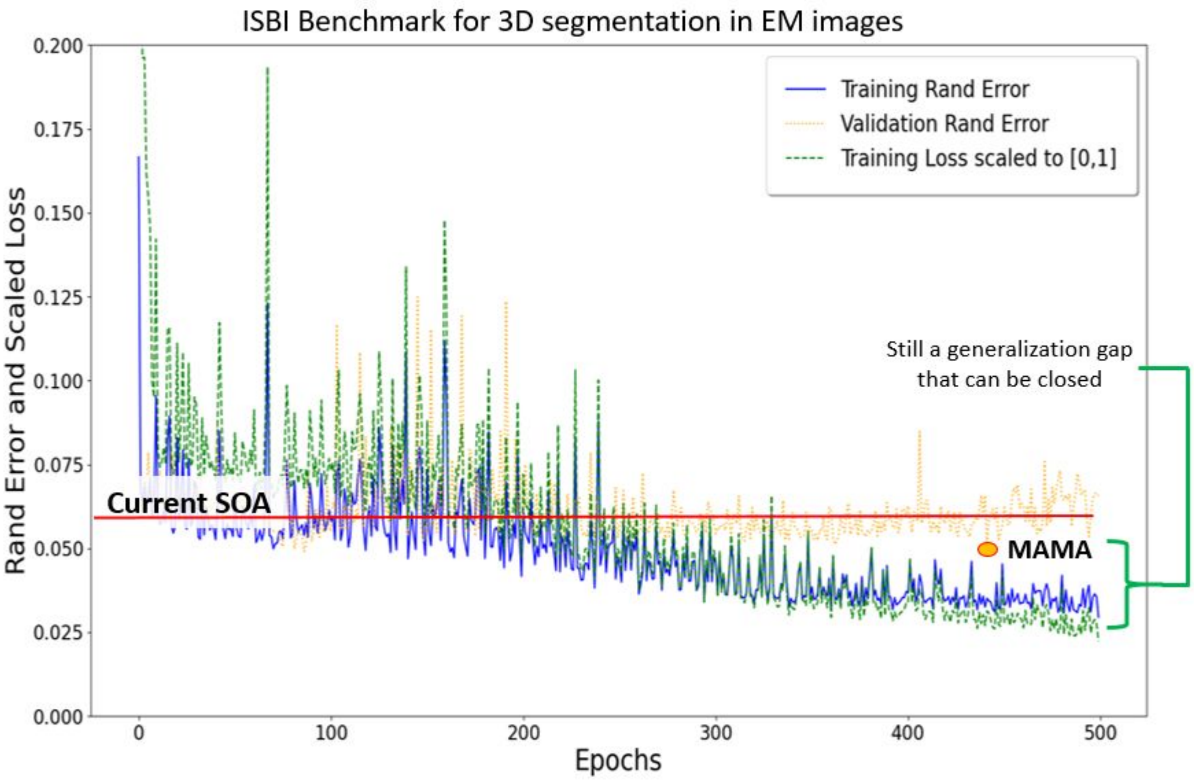
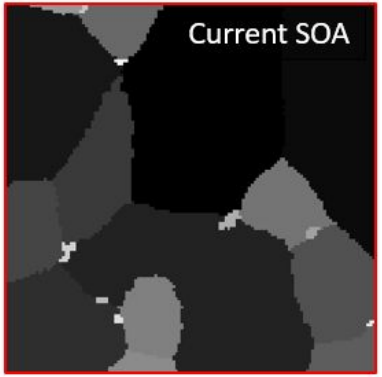
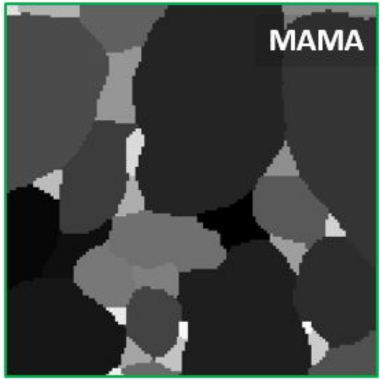


Image courtesy of Brian Patterson

MAMA Segmentation is competitive with SOA

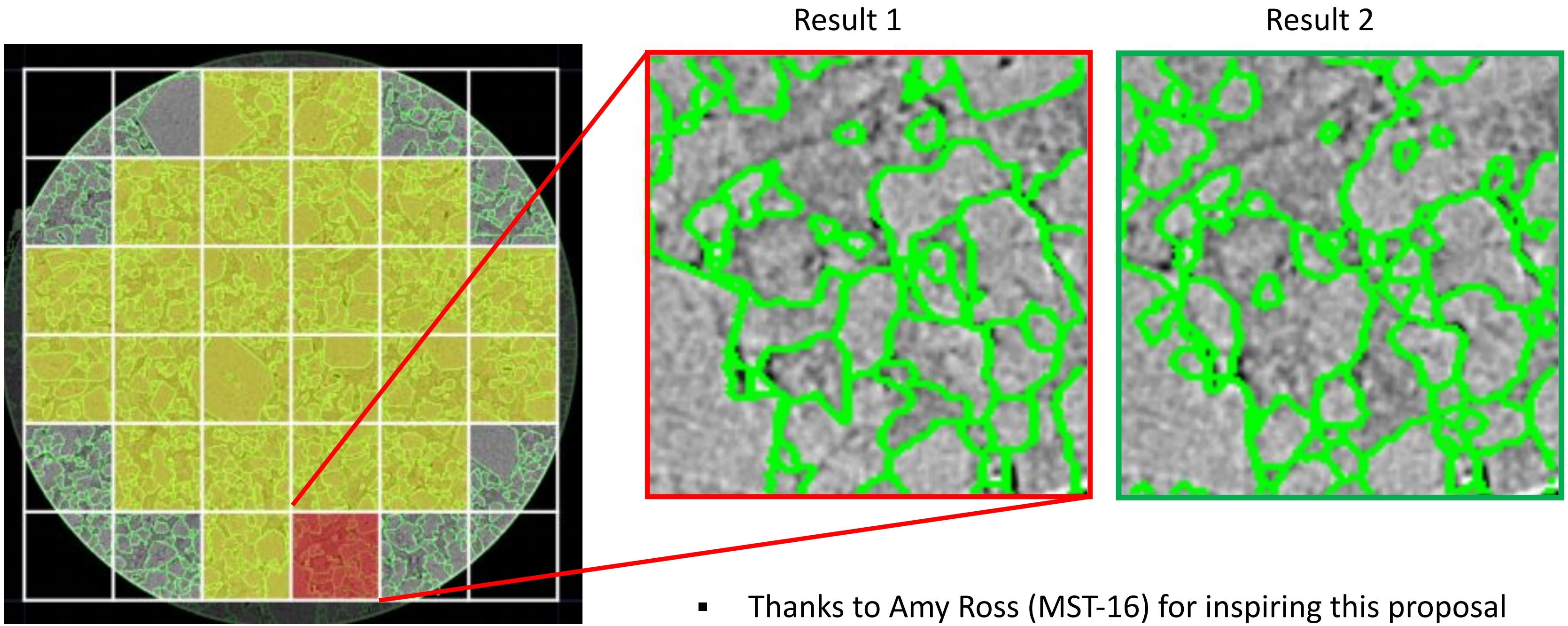






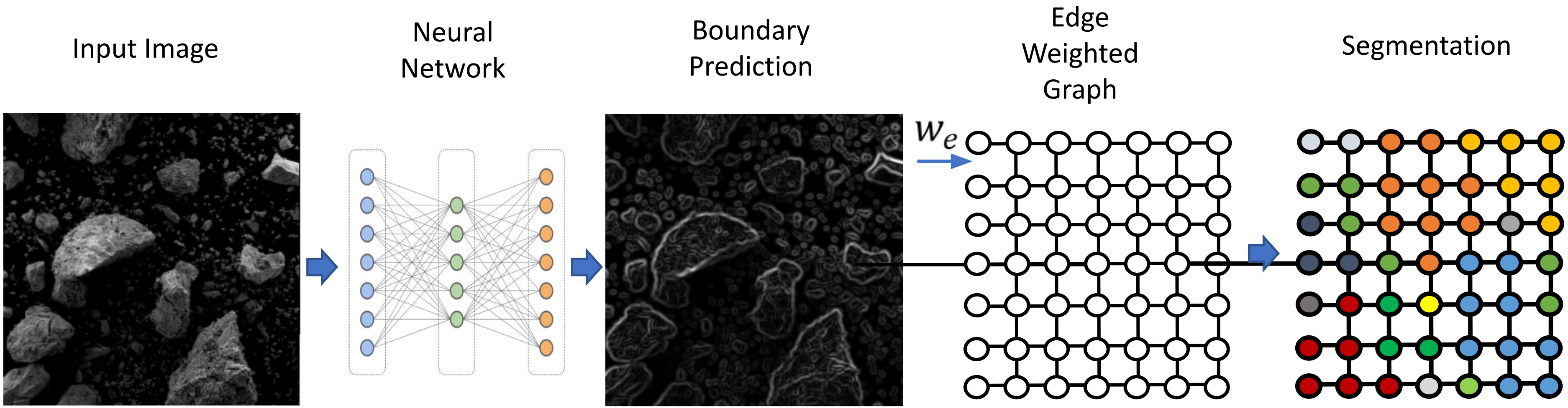
The Need for Segmentation Uncertainty

- PBX-9501 dataset courtesy of Brian Patterson.



- Thanks to Amy Ross (MST-16) for inspiring this proposal and identifying a unique dataset and opportunity.

Segmentation as Graph Coloring/Partitioning



- Neural network with logistic function outputs: $w_e \approx p_e$
- How does the segmentation uncertainty relate to the edge uncertainty?

Probabilistic Graph Coloring/Partitioning

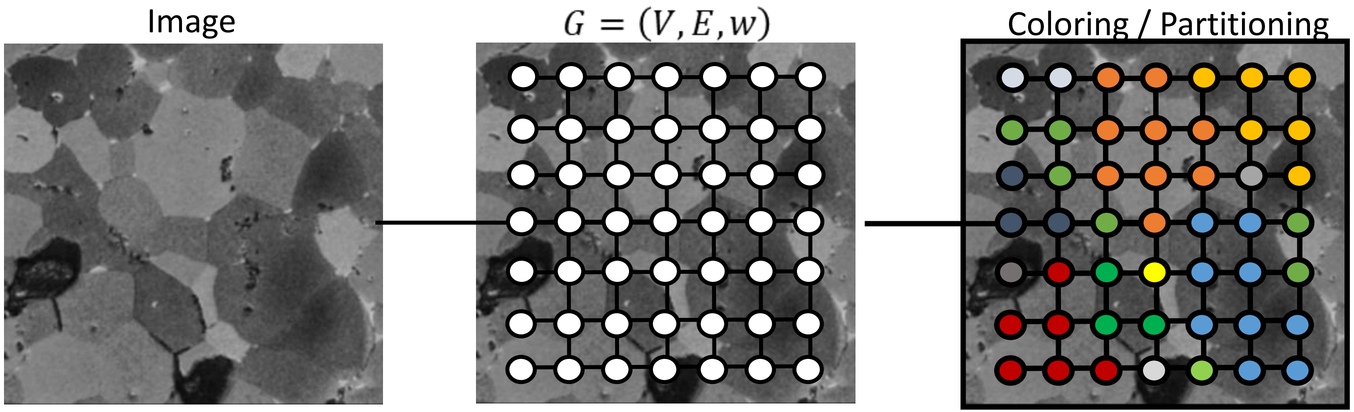


Image with P pixels

Edge weighted graph

Labels $y_i \in \{1, 2, \ldots, |V|\}$

Potts model: $\hat{Y} = argmin_Y \sum_{e_{ij} \in E} I(y_i \neq y_j) w_{ij}$

Gibbs distribution: $p(y|w, \beta) = \exp\left(-\beta \sum_{e_{ij} \in E} I(y_i \neq y_j) w_{ij} \;\; - \log Z_y\right)$

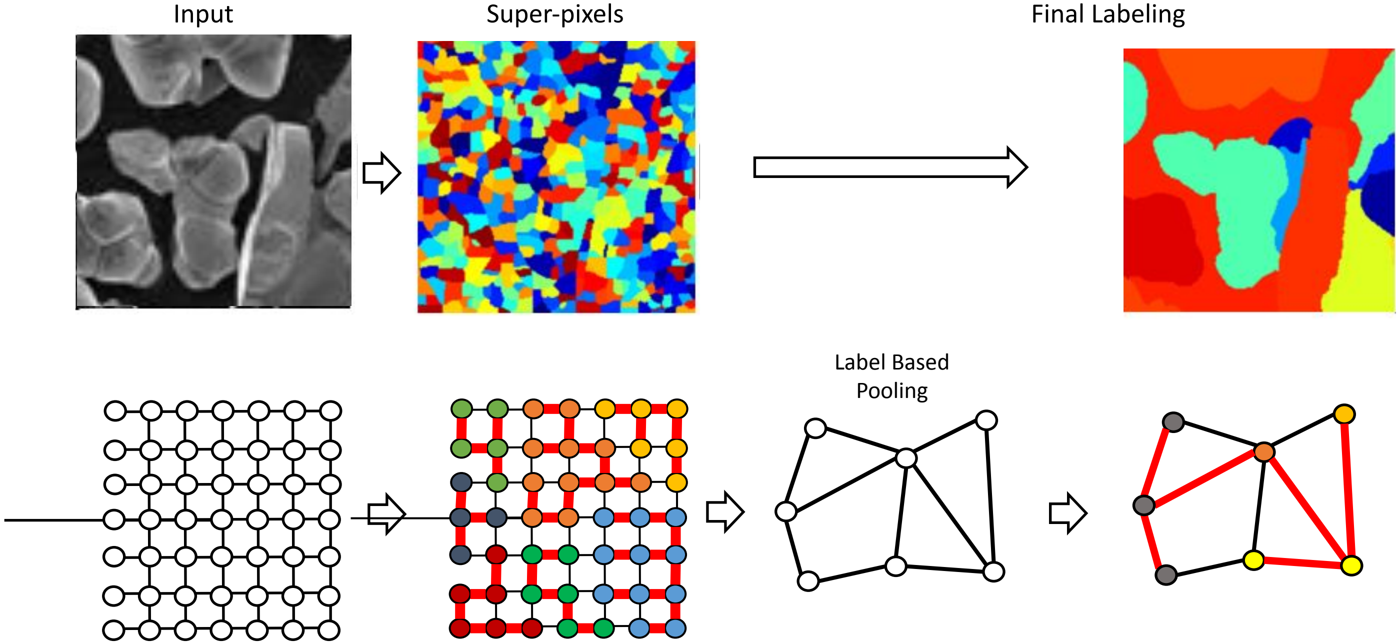
Estimate marginal: $p(y_i, y_j | \theta)$

Size of θ: $|V||V||E|$

Kappes, J. H., et al. (2015). Probabilistic Correlation Clustering and Image Partitioning Using Perturbed Multicuts, Cham, Springer International Publishing.

MAMA’s “Hierarchical Watershed” Method

- Hierarchical segmentation as a multi-layered graph



- Two-layer energy function:

$$E(Z,Y,X) = \sum_{e_{ij}\in E} g_2(z_i, z_j, X, Y) + \sum_{v_i\in V_Y} \sum_{e_{mn}\in v_i} g_1(y_m, y_n, X)$$

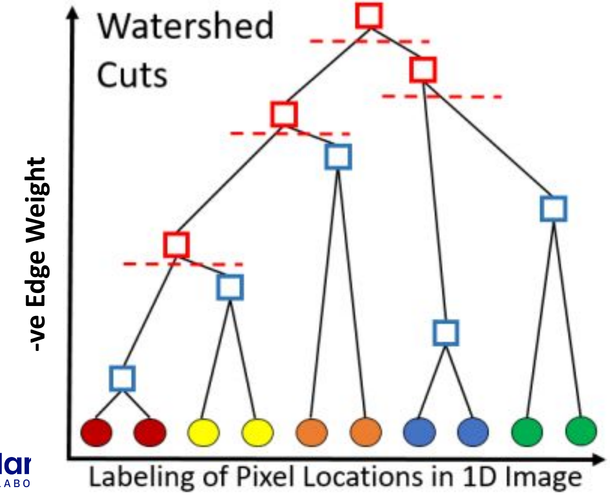
MAMA’s “Hierarchical Watershed” Method

- Two-layer energy function: $$E(Z,Y,X) = \sum_{e_{ij} \in E_Y} g_2(z_i, z_j, X, Y) + \sum_{v_i \in V_Y} \sum_{e_{mn} \in v_i} g_1(y_m, y_n, X)$$
- A tractable subset of energy functions based around dynamic programming

Minimum Spanning Forrest

Local basins of weighted graph

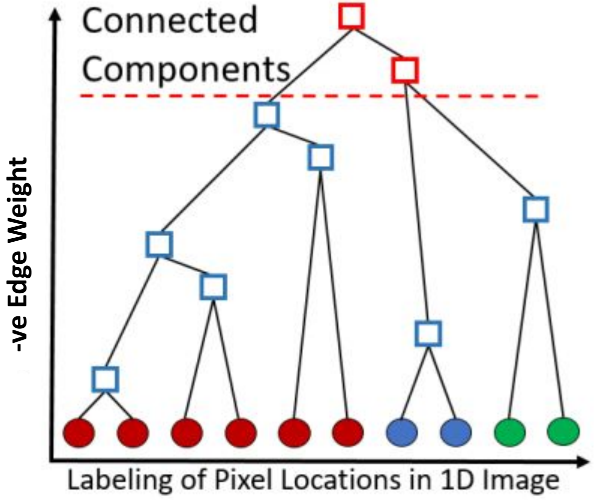
g_1



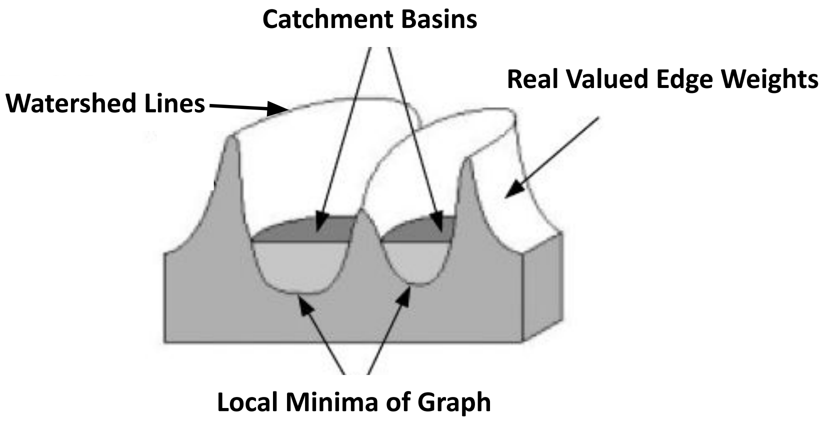
Minimum Spanning Tree

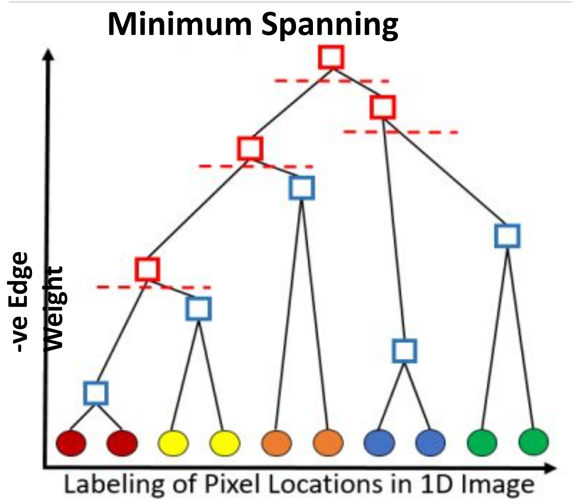
Global threshold on weighted graph

g_2



Watershed Segmentation





Probabilistic Watershed

- Consider all possible spanning forests is actually tractable!

$t \in \mathcal{T}$	Spanning tree
$f \in \mathcal{F}$	Spanning forest
$w(t), w(f)$	Sum of tree/forest weights

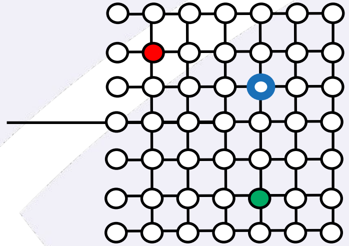
$$P(f) = \frac{w(f)}{\sum_{f' \epsilon \mathcal{F}} w(f')}$$ Gibbs distribution over all possible forests

Matrix tree theorem:

$$w(\mathcal{T}) = \sum_{t \epsilon \mathcal{T}} w(t) = \sum_{t \epsilon \mathcal{T}} \prod_{e \epsilon E_t} w(e) = \frac{1}{|V|} \det\left(L + \frac{1}{|V|} \mathbb{1}\mathbb{1}^T\right)$$

Sanmartin, E. F., et al. (2019). Probabilistic Watershed: Sampling all spanning forests for seeded segmentation and semi-supervised learning: 2776-2787.

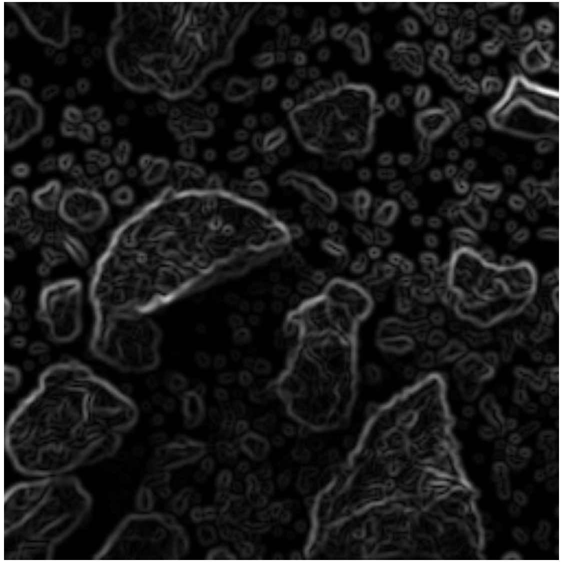
- For each vertex estimate probability that it will appear in a tree associated with a particular minima.



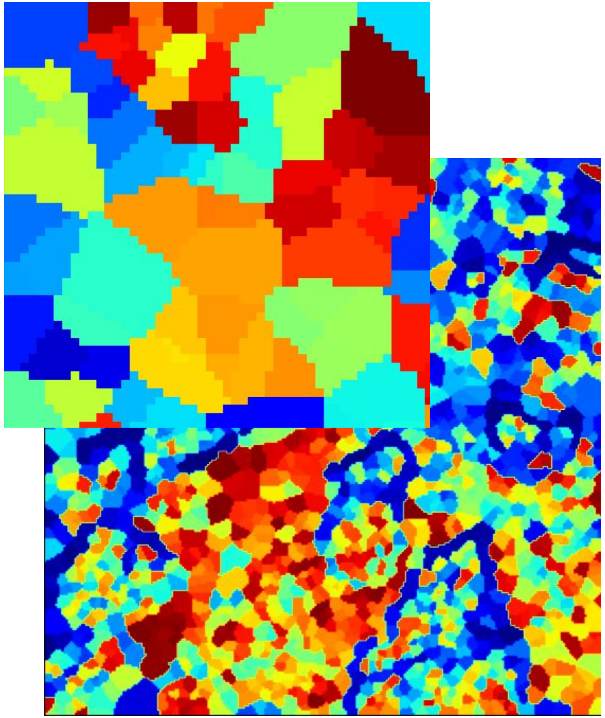
- Equivalent to a diffusion type model where vertex is assigned to a minima it is most likely to visit first on a random walk.

Grady, L. (2006). "Random Walks for Image Segmentation." IEEE transactions on pattern analysis and machine intelligence 28(11): 1768-1783.

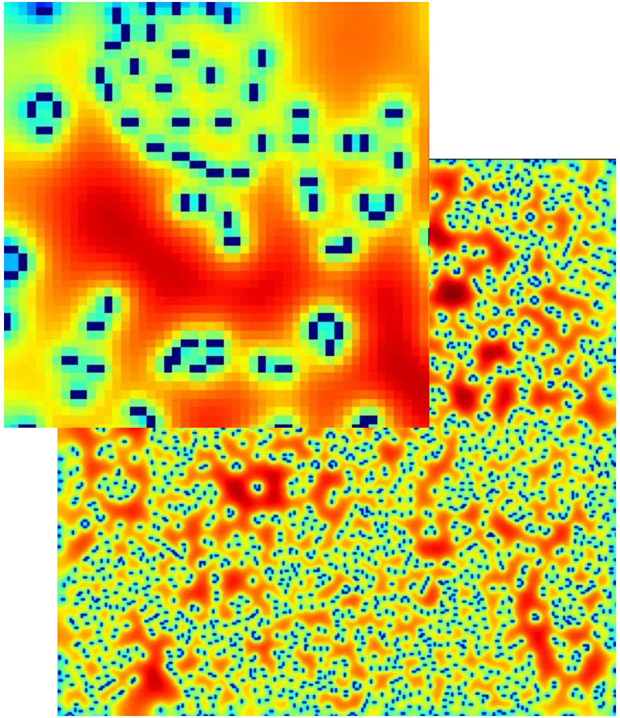
Random Walker



Edge Weights



Segmentation



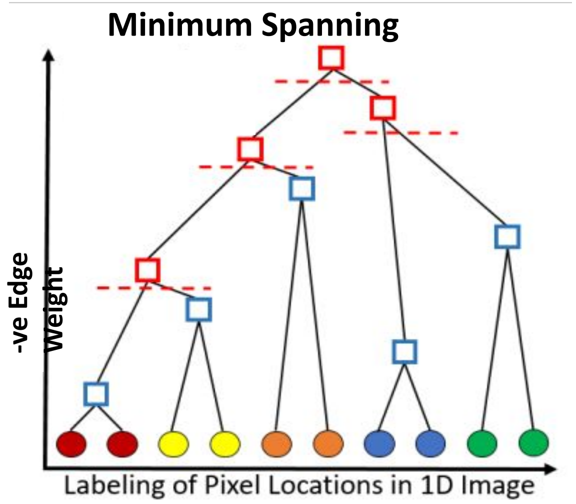
Entropy of Assignment Probabilities

Watershed Segmentation

$$\underset{x}{argmin} \sum_{e_{ij} \in E} w_{ij}^{p} |x_i - x_j|^q \qquad \hat{y} = \begin{cases} 1 & when \quad x_i > 0.5 \\ 0 & otherwise \end{cases}$$

- As $p \to \infty$ we only consider Minimum Spanning Forests.
- This has significant computational advantages.
- The minimum entropy Gibbs distribution.

Couprie, C., et al. (2009). Power watersheds: A new image segmentation framework extending graph cuts, random walker and optimal spanning forest. Computer Vision, 2009 IEEE 12th International Conference on.



- Assign vertex to minima that has the lowest minimax path.

Challa, A. et. al., (2019). Watersheds for semi-supervised classification, IEEE Signal Processing Letters, 26:720-724.

q \ p	0	finite	∞
1	Collapse to seeds	Graph cuts	Power watershed $q = 1$
2	ℓ_2 norm Voronoi	Random walker	Power watershed $q = 2$
∞	ℓ_1 norm Voronoi	ℓ_1 norm Voronoi	Shortest Path Forest

Los Alamos NATIONAL LABORATORY

Connected Component Segmentation

$$\hat{Y} = argmin_Y \sum_{e_{ij} \in E} I(y_i \neq y_j) \min_{P \in \mathcal{P}_{ij}} \left(\max_{ij \in P} (w_{ij}) \right)$$

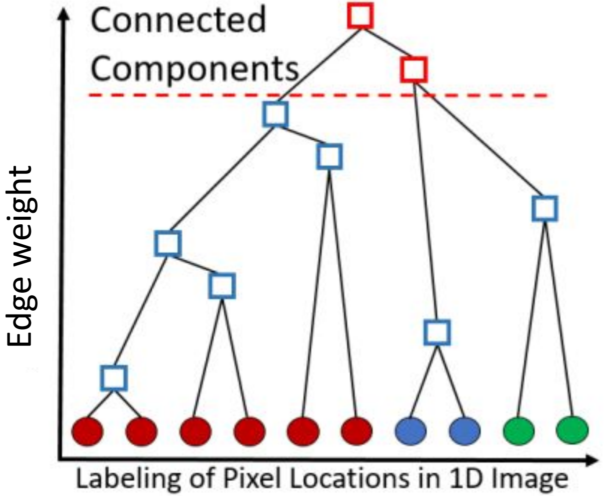
1. Cut negative edges: $w_{ij} < 0$
2. Use Connected Components to label partitions

- Cannot be expressed as MAP solution of an exponential family probabilistic model!

Tarlow, D., et al. (2012). Randomized optimum models for structured prediction. Artificial Intelligence and Statistics, PMLR.

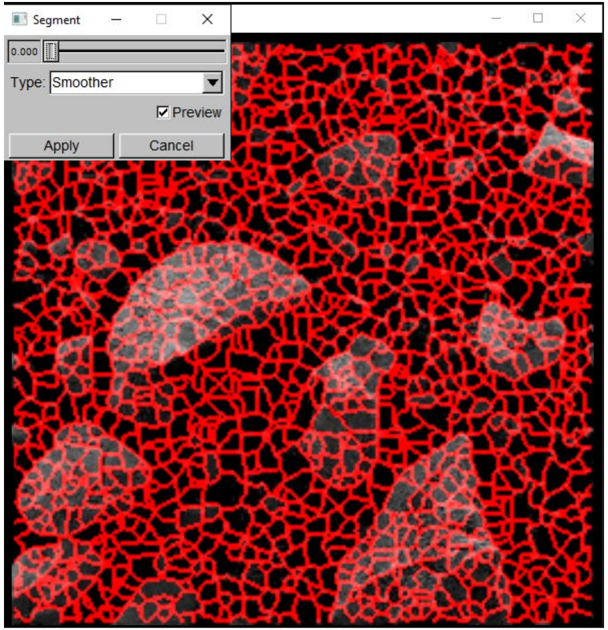
Minimum Spanning Tree

Global threshold on edge weights

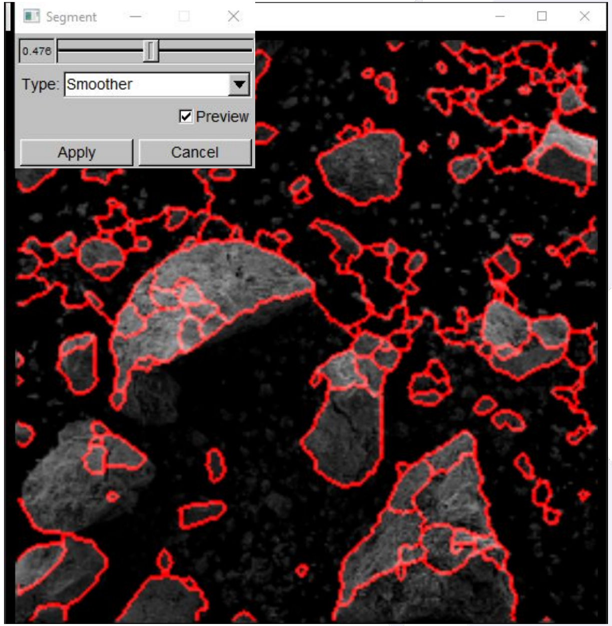


A Hierarchy of Closed Contours

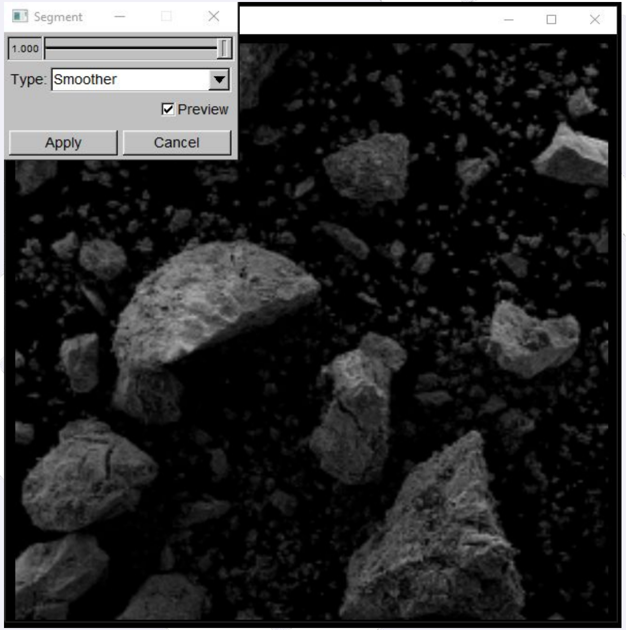
Threshold at leaves



Threshold mid tree

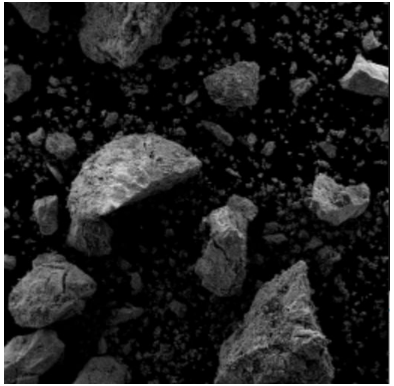


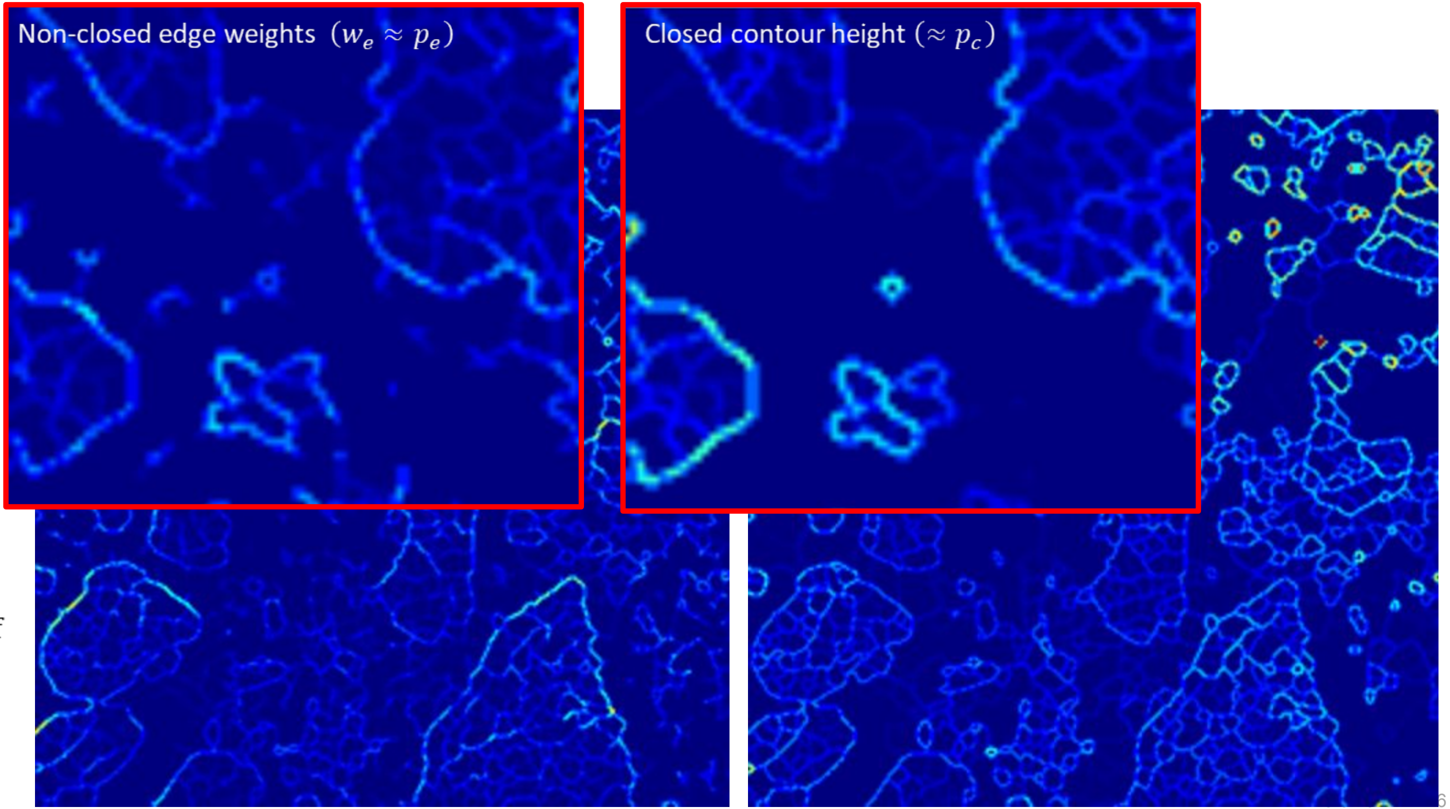
Threshold at root node



Ultra-metric Maps

Height where the Contour Disappears





- Height $\approx$ Confidence
- Captures non-local aspect of segmentation.
- $O(NlogN)$ algorithm

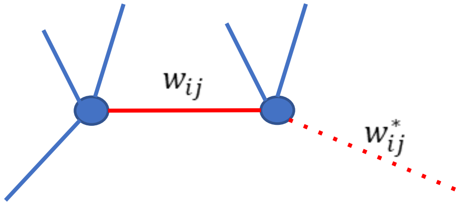
Ultra-metric Maps for Watershed Segmentation

- The Watershed-Cut can be expressed as a MST of a modified graph:

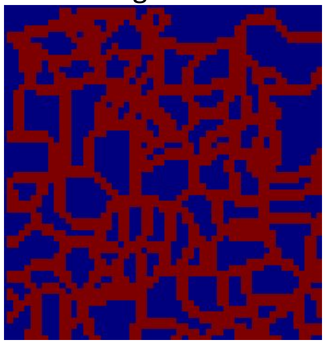
$$\hat{Y} = argmin_Y \sum_{e_{ij} \in E} I(y_i \neq y_j) \min_{P \in \mathcal{P}_{ij}} \left(\max_{ij \in P} \left(w_{ij} - w^*_{ij} \right) \right)$$

$$w^*_{ij} = Max \left(Min_{k \in N_{i \setminus j}} w_{ik},\ Min_{k \in N_{j \setminus i}} w_{kj} \right)$$

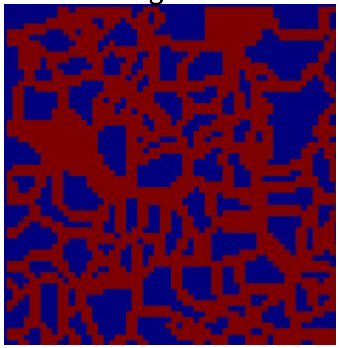
Identify edges on saddles and ridges



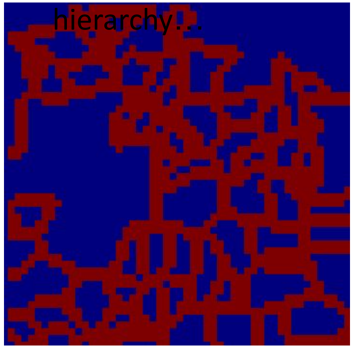
MSF Segmentation



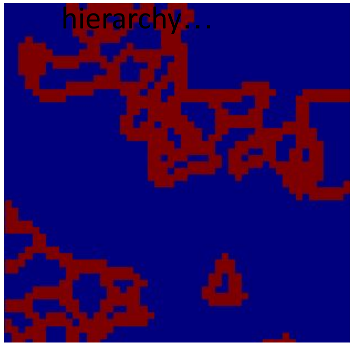
MST Segmentation



Higher in hierarchy…



Higher in hierarchy…

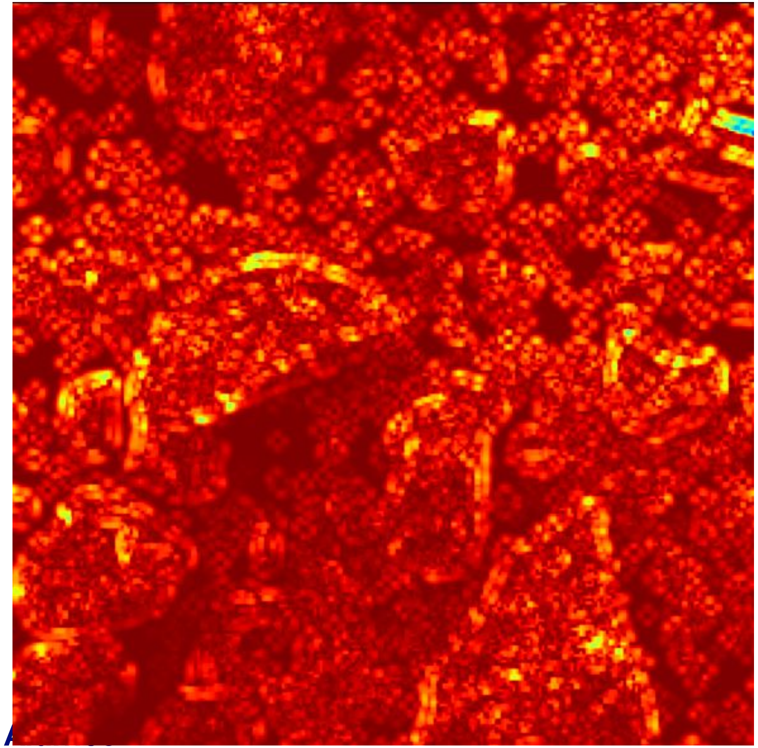


Porter,R., Oyen, D., Zimmer, B.G., "Learning Watershed Cuts Energy Functions", Mathematical Morphology and Its Applications to Signal and Image Processing, 2015.

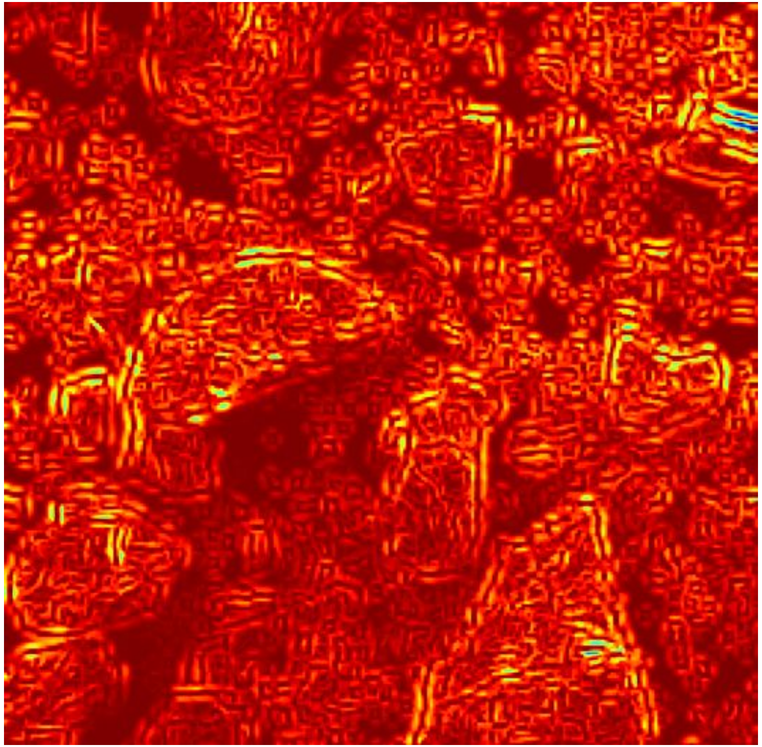
Ultra-metric Maps for Watershed Segmentation

- Likelihood ratio for watershed edge:

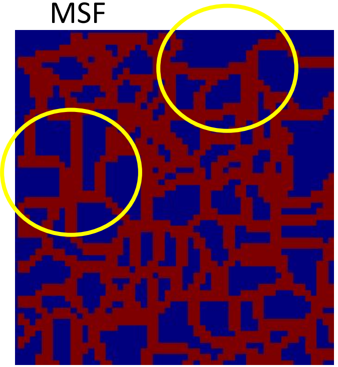
$(w_{ij} - w_{ij}^*) \approx lr_e$

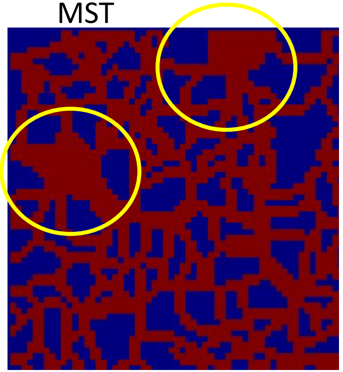


Closed contours (segments) $\approx lr_c$



Flat Zones and the Power Watershed



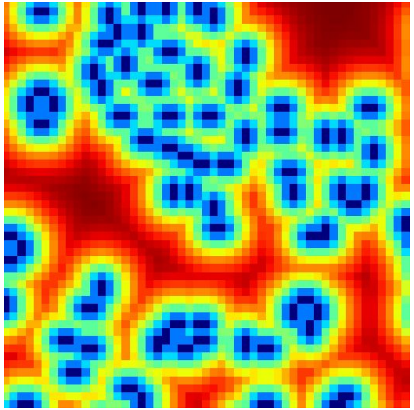


$$\underset{x}{argmin} \sum_{e_{ij} \in E} w_{ij}^{p} |x_i - x_j|^q$$

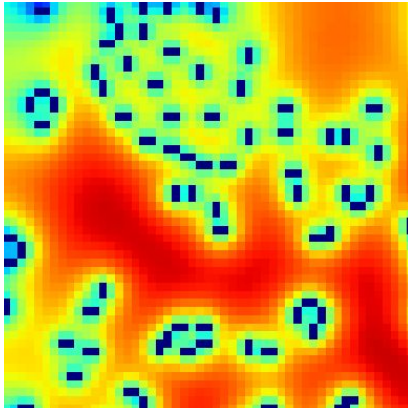
q \ p	0	finite	∞
1	Collapse to seeds	Graph cuts	Power watershed $q = 1$
2	ℓ_2 norm Voronoi	Random walker	Power watershed $q = 2$
∞	ℓ_1 norm Voronoi	ℓ_1 norm Voronoi	Shortest Path Forest

- Watersheds are not well defined when edges are not unique.
- Power Watershed:
  1. Minimum Spanning Forrest for unique edges.
  2. Random Walker solution for flat zones.

- With equal weights, this is equivalent to assigning a vertex to the minima that is closest in terms of geodesic distance.



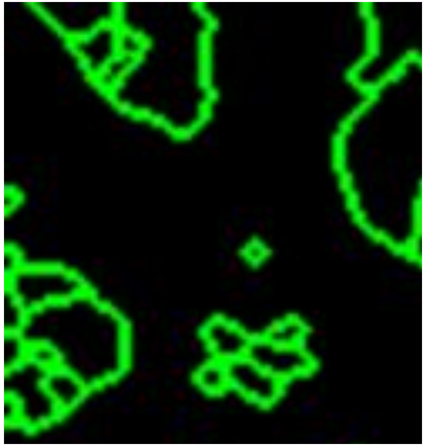
Geodesic distance



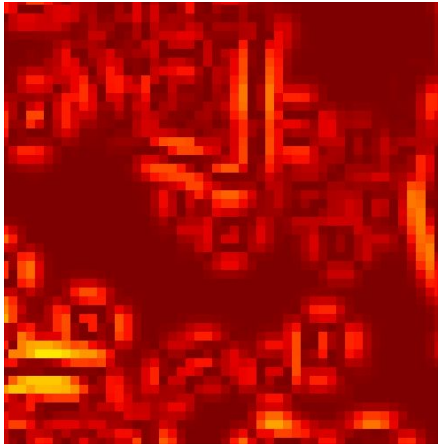
Random Walker

Ultra-metric Likelihood Ratios

Segmentation

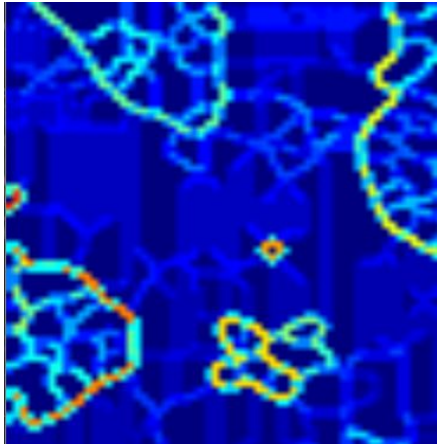


Watershed
Ultra-metric Confidence Map



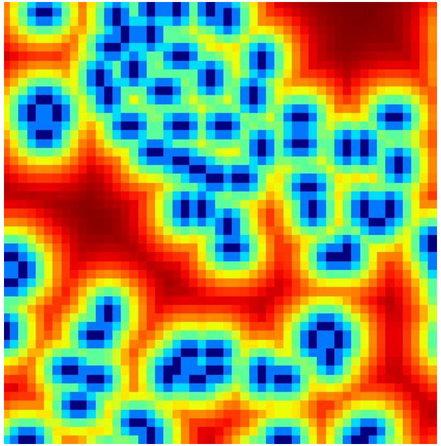
Uncertainty

Connected Component
Ultra-metric Confidence Map



Confidence

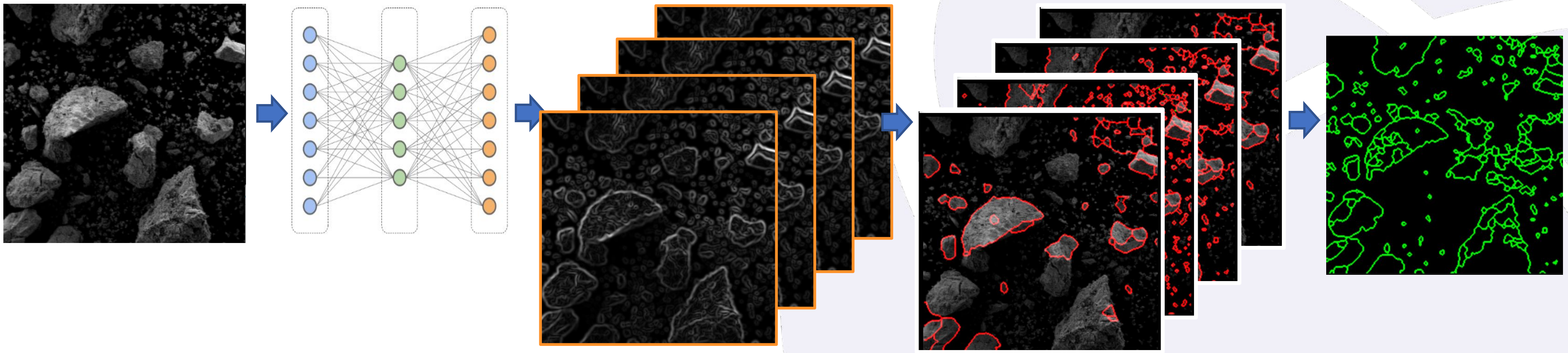
Geodesic Distance
Ultra-metric Confidence Map



Uncertainty

- MAMA's Segmentation method is not a MAP solution to a standard exponential family probabilistic model.
- Ultra-metric Likelihood Ratios provide a segmentation centric worst case estimate for confidence.

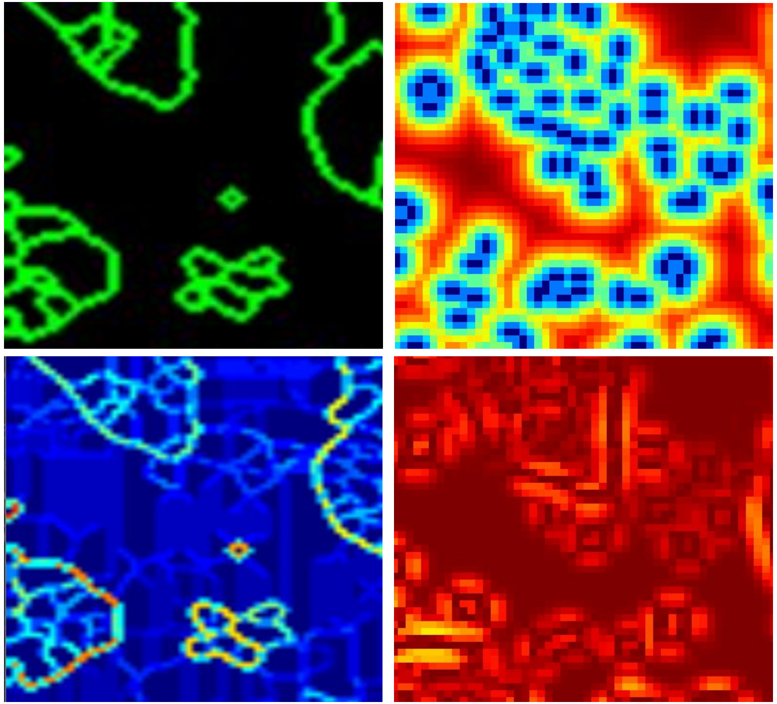
Ensemble and Perturbation Methods



- Ultra-metric distances have been used to weight votes in an ensemble.
- Sampling multiple segmentations can provide probability estimates and also smooth gradient estimates in end-to-end learning.

L. Zheng, T. Li and C. Ding, "Hierarchical Ensemble Clustering," *2010 IEEE International Conference on Data Mining*, 2010, pp. 1199-1204, doi: 10.1109/ICDM.2010.98.

Securing our Technical Leadership in Hierarchical Watersheds



Top Left) Hierarchical watershed segmentation of particles in SEM imagery and the associated ultra-metric likelihood maps that together provide a method specific estimate of confidence. Top Right) uncertainty (red) is highest in plateaus of the input image. Bottom Right) uncertainty (red) in super-pixels. Bottom Left) Confidence (red) of final segmentation boundaries.

Project Description: The objective is to provide uncertainty estimates for hierarchical watersheds (HWS). Success in this project will provide a much needed (and requested) qualification to automated image analysis and strengthen our case for using HWS in production environments.

Project Outcomes

Mentorship:

- Supported full time (but late starting) GRA.
- Provided technical guidance towards a PhD in materials image analysis for a GRA in PT-3 (expected Dec’ 2021).

Publications:

- “Synthetic-to-Real Domain Adaptation for Autonomous Driving”, Har Simrat Singh, Sunil Thulasidasan, Aqueel Jivan and Reid Porter, Accepted for presentation at the SMC Data Challenge 2021.
- “End-to-end learning of Hierarchical Watersheds”, Reid Porter, revisions to be submitted Oct’2021

Proposal: Enabling Manufacturing Proposal: Automated Grain Delineation and Quantification for Production Processes, Kari Sentz (PI), with P-3 and MST-16 (not funded).

PI: Reid Porter
Total Project Budget: $60k
ISTI Focus Area: Verifiable AI & ML

END