Joint Modeling of the Microscale and Mesoscale in Materials Systems: A Tutorial and Research Update

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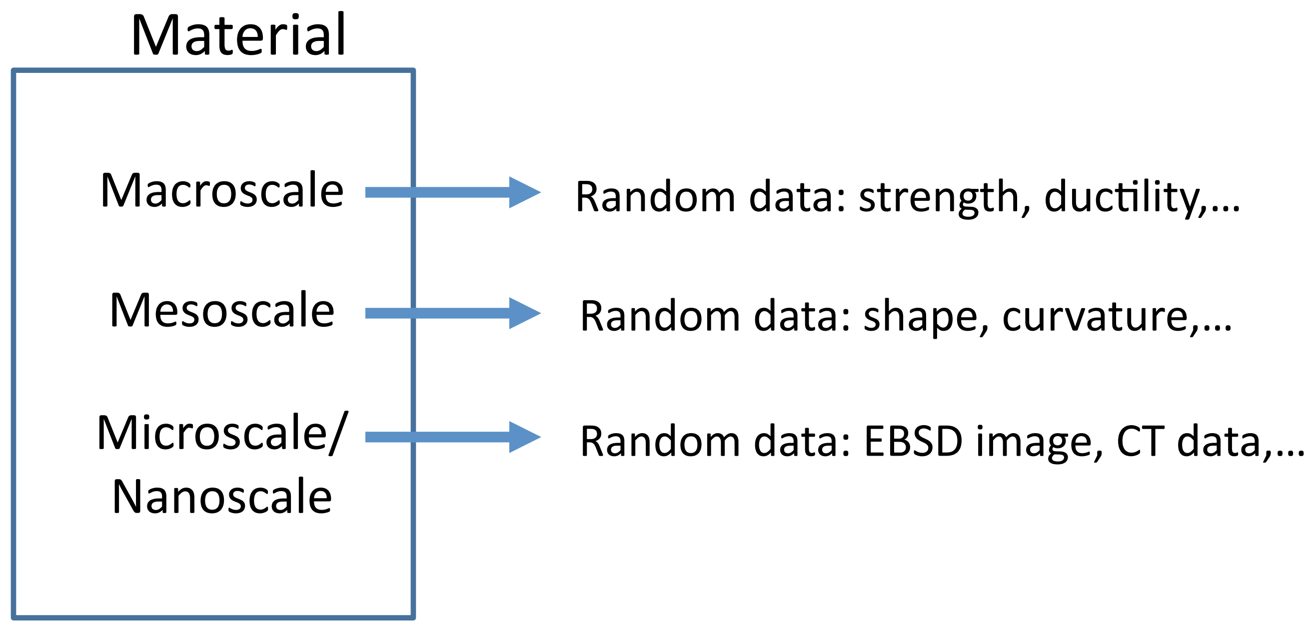
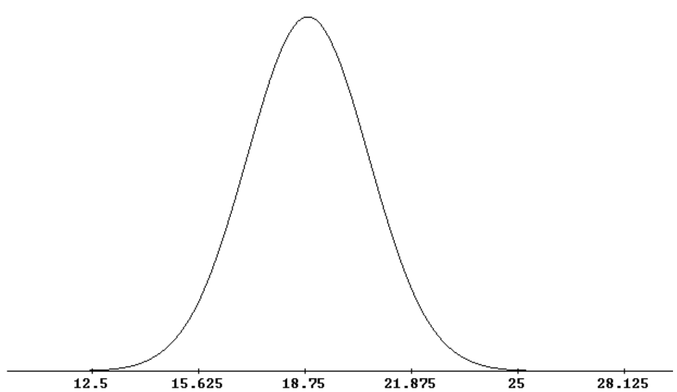
Probability theory is nothing but common sense reduced to calculation. *Pierre Simon Laplace*

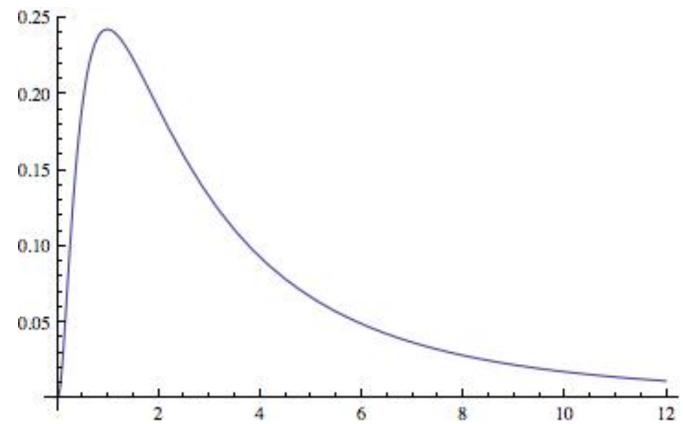


Can we unify all of this random data? Probability theory provides the mathematical framework to do this through *joint modeling*.

Modeling of two random variables: An example

Consider two random variables: air temperature T and atmospheric pressure P. Assume for the sake of argument these have the probability density functions shown:



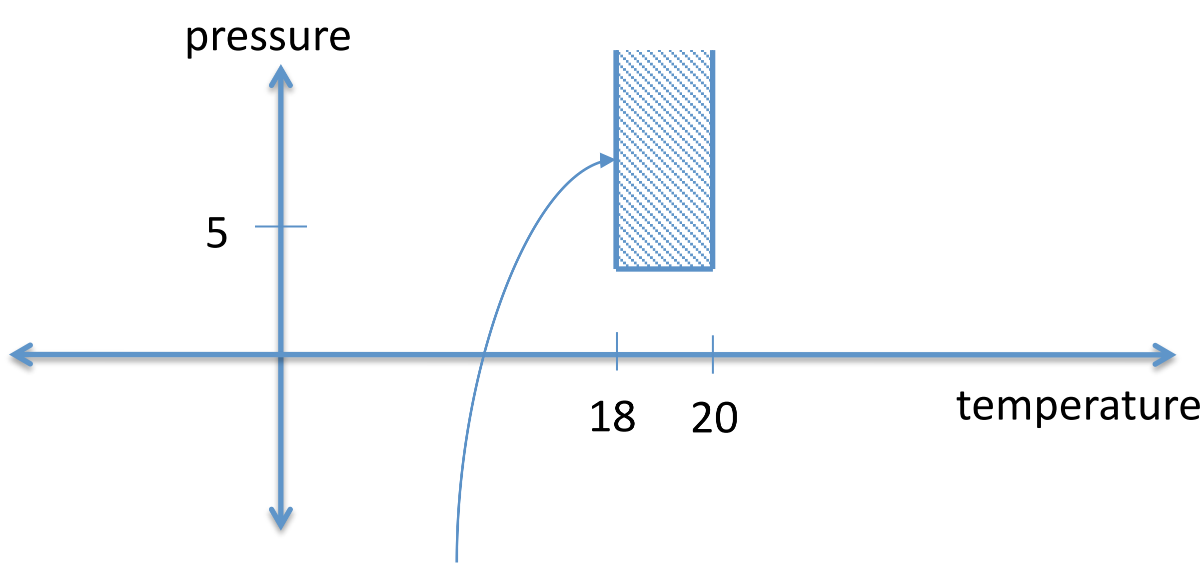


We can compute Prob(18^o<T<20^o) and Prob(P>5 pressure units) from these densities, but we cannot compute P(18^o<T<20^o AND P>5) from them, unless T and P are independent.

We need a *joint distribution* for T and P to do this.

The joint probability density function

The *joint probability density function* of T and P completely characterizes the probabilistic behavior of T and P (at least for the purposes of this discussion). This is a real-valued function defined on the x-y plane.



We integrate the joint density function over this region to get P (18^o<T<20^o AND P>5).

Finding joint distributions

Finding joint distributions of two random variables is generally very difficult. Imagine if we had thousands, or even millions, of random variables…oh wait, we do…

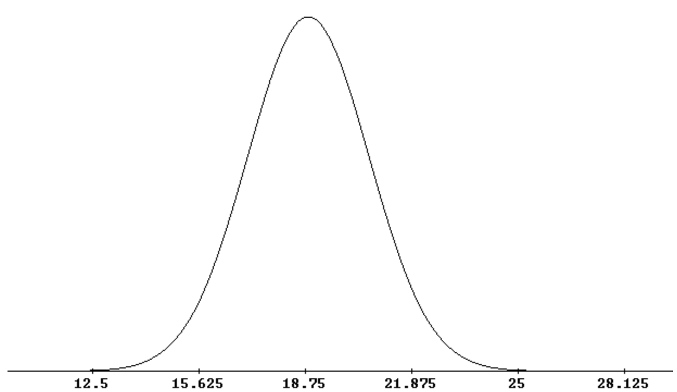
- An MxN image of scalar intensity values has MN random variables.
- The corresponding segmentation has MN random variables (one label per pixel).
- Microstructural features add more random variables to the mix.

All would be hopeless without the concepts of marginal distributions, conditional distributions, and Bayes Theorem.

The marginal density function

The marginal density function is the density function of a random variable (or multiple random variables) resulting from integrating the joint density function over all of the other variables.

For example, for each fixed temperature, we integrate the joint density function of T and P over all values the pressure can take. This gives us the marginal density of T:



The conditional density function

The conditional density function is the density function of a random variable (or multiple random variables) that results from taking cross sections of the joint density function.

For example, for each fixed temperature t, the *conditional density function of P given T=t* is the joint density function of T and P restricted to the plane where temperature equals t.

The conditional density function of P given T=t is the density function of P given that the temperature takes the value t.

Bayes Theorem

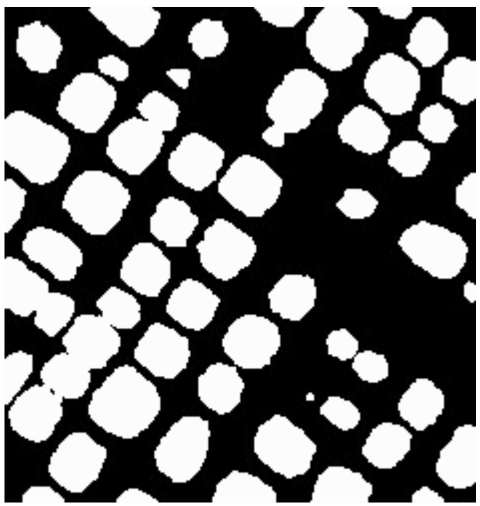
Bayes theorem tells us how we can use conditional and marginal distributions as building blocks to find joint distributions.

- We can also use it to find marginal densities in terms of conditional densities and other marginal densities, and conditional densities in terms of marginal densities and other conditional densities

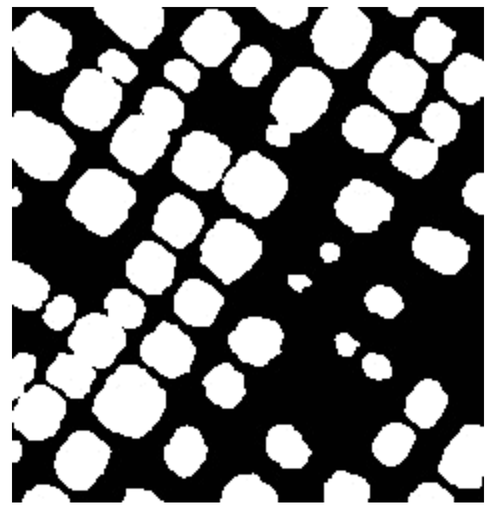
The trick is to write distributions you want to know in terms of distributions you know how to model.

Example of the power of conditional probability

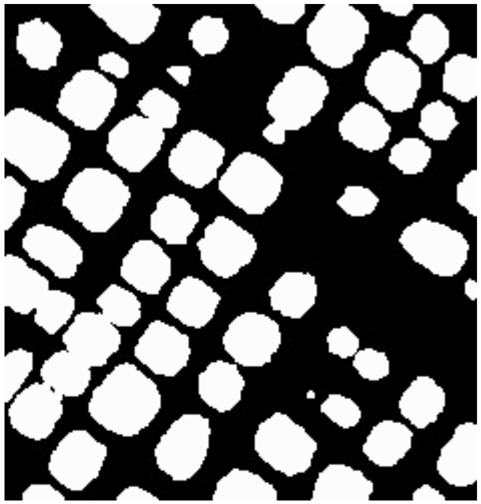
Let's consider a 2D slice of a nickel alloy. Which microstructure is more likely?



OR



Now, which of these microstructures….



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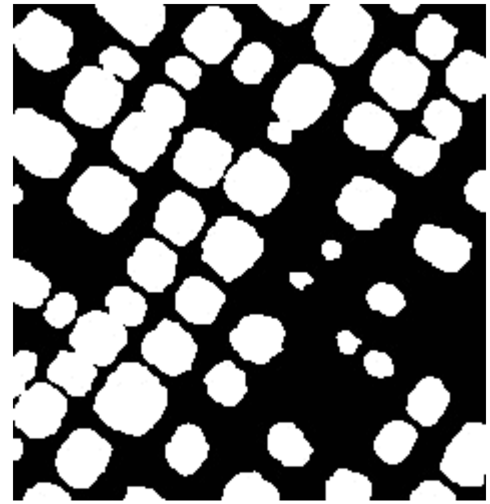
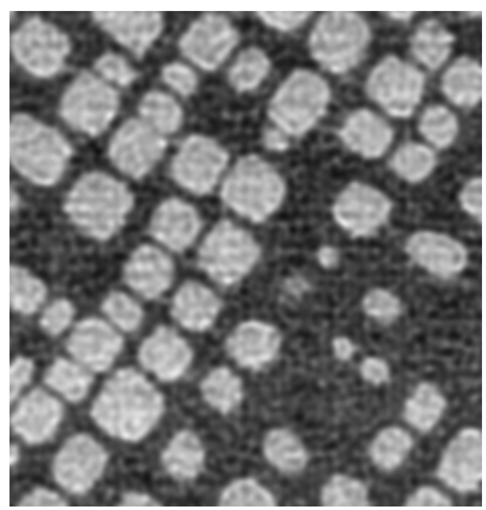


is more likely given that the measured image is:



The Ising/MRF model

The Markov random field (MRF) model, based on the Ising model from physics, provides a very useful joint distribution for an image.

- This gives a joint distribution of MN random variables with a specific spatial structure

Like the Ising model, the MRF model is specified using local interactions. It can model boundaries well, but it is difficult to impose prior information at the mesoscale

The marked point process (MPP) model

Like the MRF, the MPP model gives a joint distribution of random variables with spatial structure.

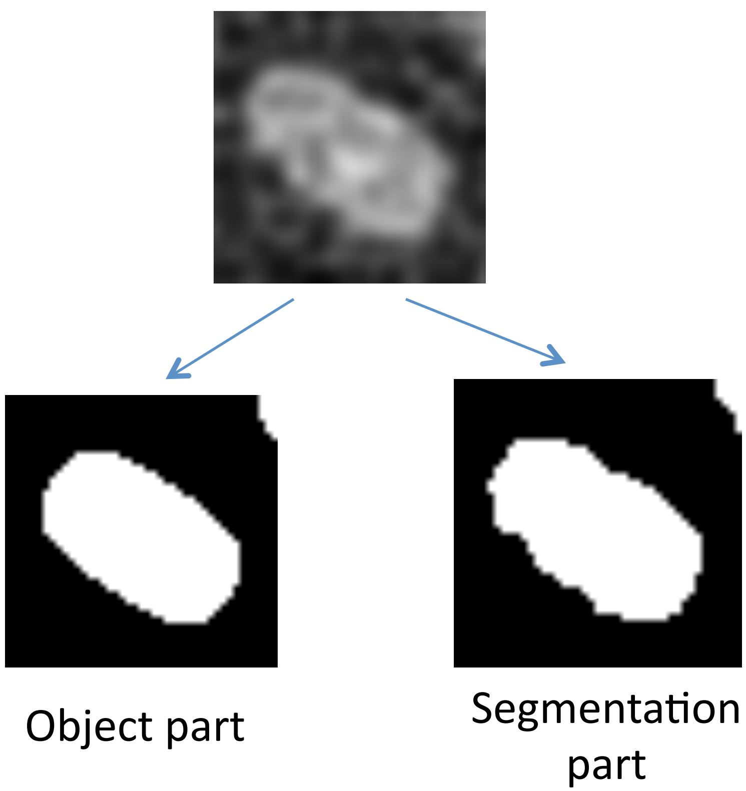
In the MPP model spatial locations of objects are modeled as random variables. This makes it generally better for microstructural features.

We have combined an MPP model for mesoscale prior information and an MRF model for microscale prior information.

COMBINE MARKOV RANDOM FIELD AND MARKED POINT PROCESS

A Segmentation Object Combination (SOC) is advanced to realize image analysis at pixel level and object level simultaneously.

Define the SOC field U, $u_i = \{w_i, x_{w_i}\} \in U$ is a SOC element.



Object part: Object model is used to impose the global constraint. The parameters of the object describe the shape geometrically.

❑Marked Point Process model

Segmentation part: Segmentation of the corresponding object is used to impose the local constraint.

❑Markov Random Field model

COMBINE MARKOV RANDOM FIELD AND MARKED POINT PROCESS

Combining prior information leads to the likelihood function

$$P(u \mid y) = \frac{1}{z}\exp\left[-\Theta(u \mid y)\right]$$

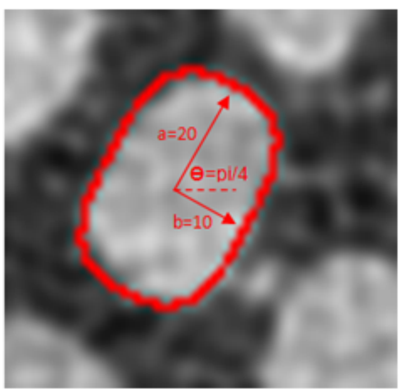
$$= \frac{1}{z}\exp\left\{-\sum_{w_i \in \Omega_w}\left[l(y \mid w_i) + \frac{\min\left\{E(x_{w_i} \mid \hat{y}(w_i))\right\}}{\sum_{s \in D_{w_i}} 1}\right] - \sum_{w_i, w_j \in \Omega_w} t(w_i, w_j)\right\}$$

Measured image model

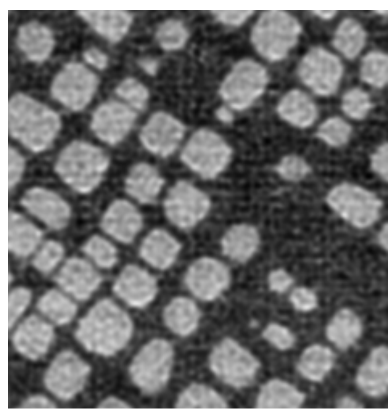
Microscale prior (MRF)

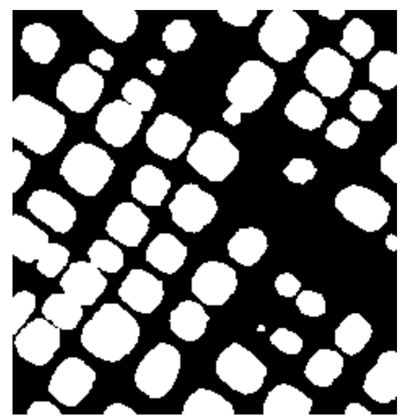
Mesoscale prior (MPP)

Multiple Birth and Death algorithm is adopted to obtain the MAP configuration of *u*.

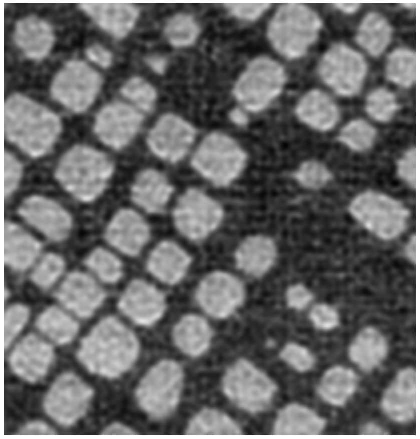


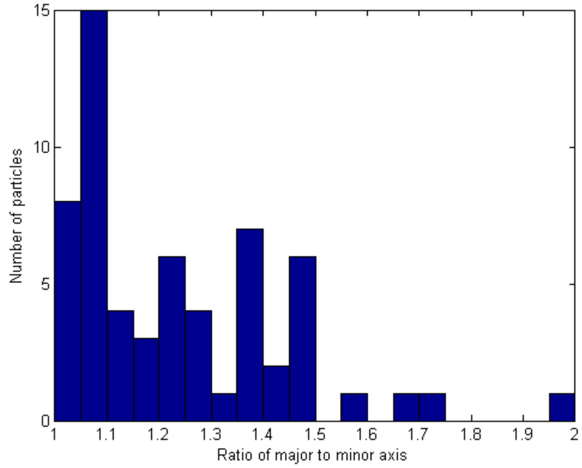
Superellipse model is used for NiCrAl particle (2D)



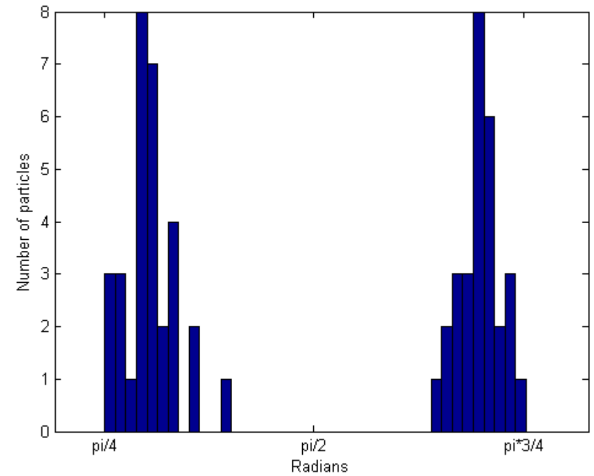


Result (Segmentation part)



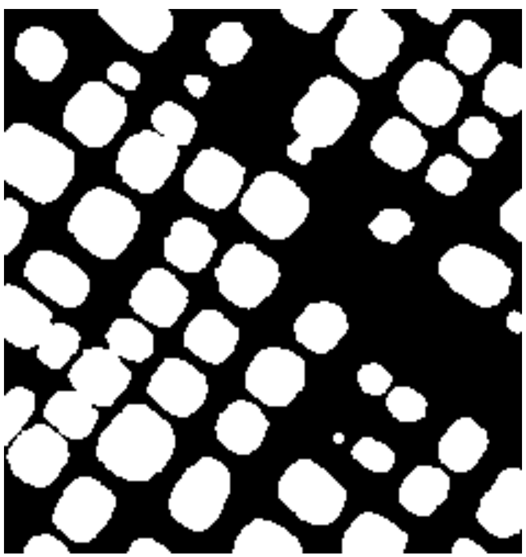


Histogram of major to minor axis ratios

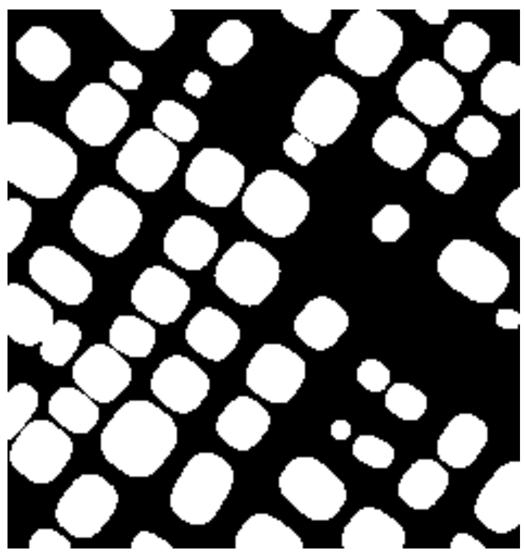


Orientation histogram

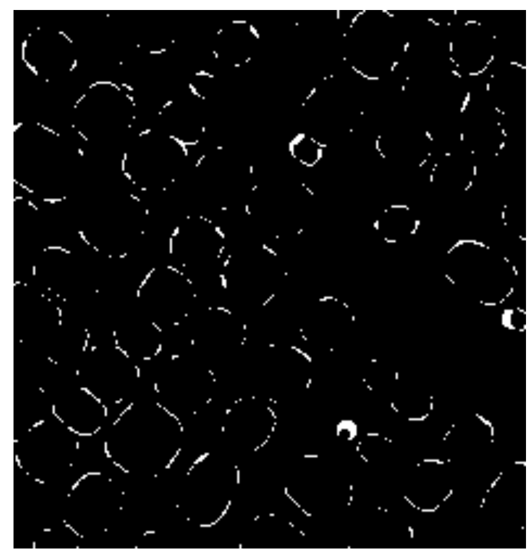
Key point: One unified model, one joint optimization give all of these results



Seg. Part (lambda = 1.5)



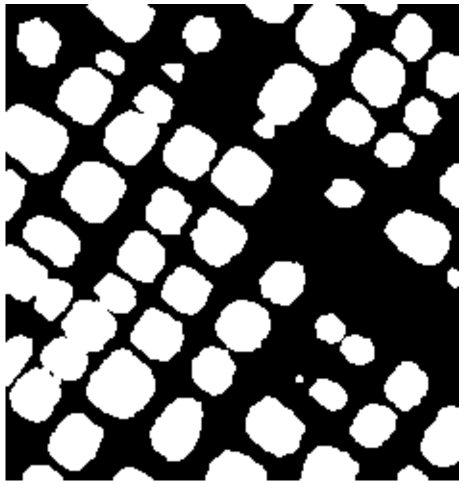
Object part



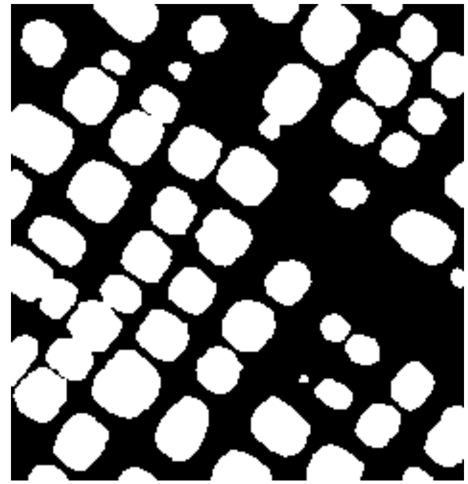
Difference image

There is a regularization parameter λ that balances the MRF and MPP constraints

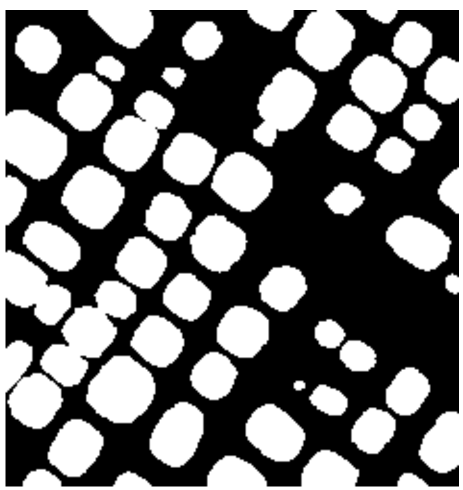
Segmentation part



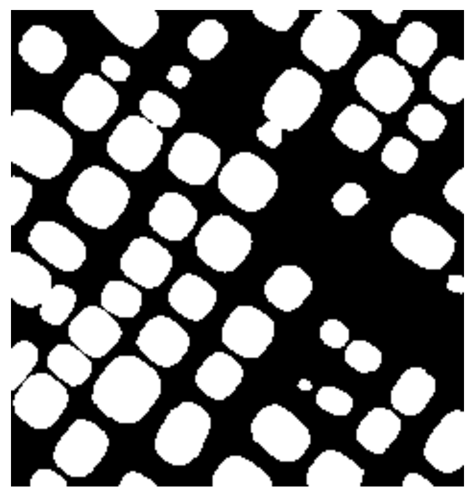
$\lambda = 0$



$\lambda = 1$



$\lambda = 2$



$\lambda = 4$

Extension to 3D segmentation

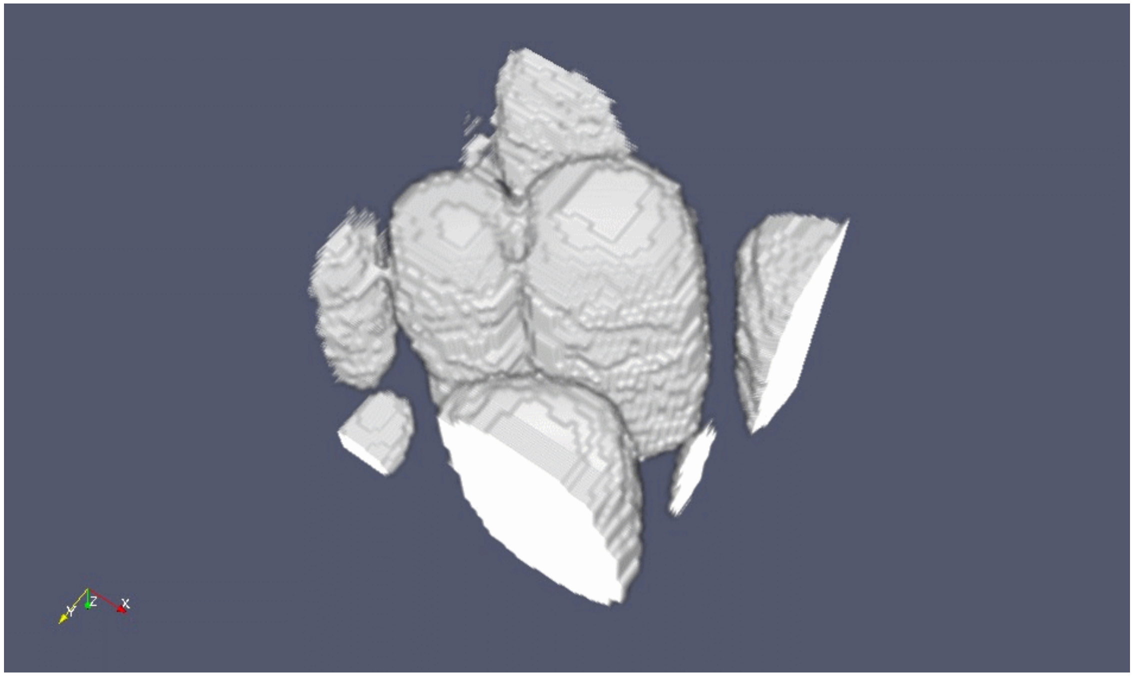


Illustration of geometric constraints' impact on segmentation

Future: Superellipsoid model

$$\left|\frac{x}{a}\right|^n + \left|\frac{y}{b}\right|^n + \left|\frac{z}{c}\right|^n = 1$$