Learning Issues in & Image Segmentation

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The Problem of Data Clustering

Given: Set of n objects $x_1, \ldots, x_n$ (e. g. points in Euclidean space).

Clustering problem: Group $x_1, \ldots, x_n$ into k groups of similar objects. These groups are called *clusters*.

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Note: The number k of clusters is usually predefined, i. e. an input parameter.
The similarity measure depends on the problem.

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Semantics Problem: *How should we infer objects from segments?*

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Result: Segments are connected regions assigned to the same cluster.

Problem Formalization

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- Objects: Data set $(x_1, \ldots, x_n) =: \mathbf{x}$
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Clustering solutions are defined by instances of the assignment vector $\mathbf{c}$.

Cost Function Idea

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Interpretation: Assignment of *dissimilar objects* to the same cluster produces *high costs*.

Cost Function-Based Clustering

Algorithmic solution: Compute assignment $\mathbf{c}^*$ for which costs $H(\mathbf{c})$ are minimal:

$$\mathbf{c}^* = \underset{\mathbf{c} \in \{1,\ldots,k\}^n}{\operatorname{argmin}} \; H(\mathbf{c}|\mathbf{x})$$

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Advantage of cost function approach: Attempts to separate *model design* from *algorithmic issues*.

Cost Function Optimization

Trade-off problem

- *Simple cost functions:* Easy to optimize, but not suitable to capture complex dependencies.
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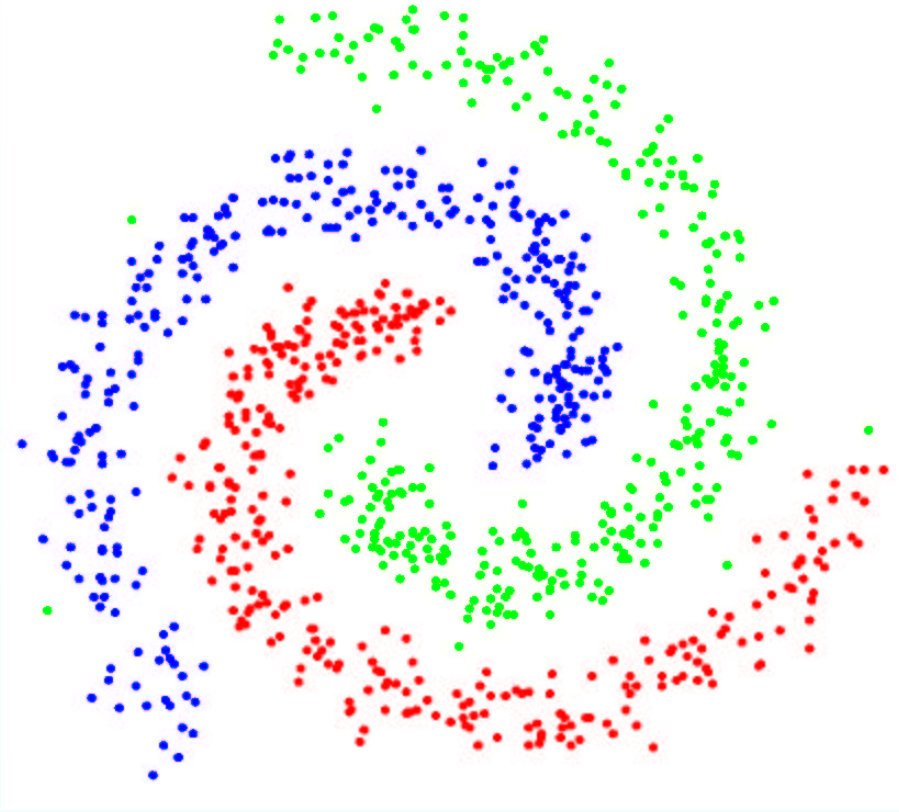
Example: A cost function with simple structure may e. g. be of the form $H\left(\mathbf{c}|\mathbf{x}\right) = \sum_{i=1}^{n} f\left(c_i|x_i\right)$. Costs are evaluated separately for each object.

Extension: incorporate neighborhood information in cluster assignment



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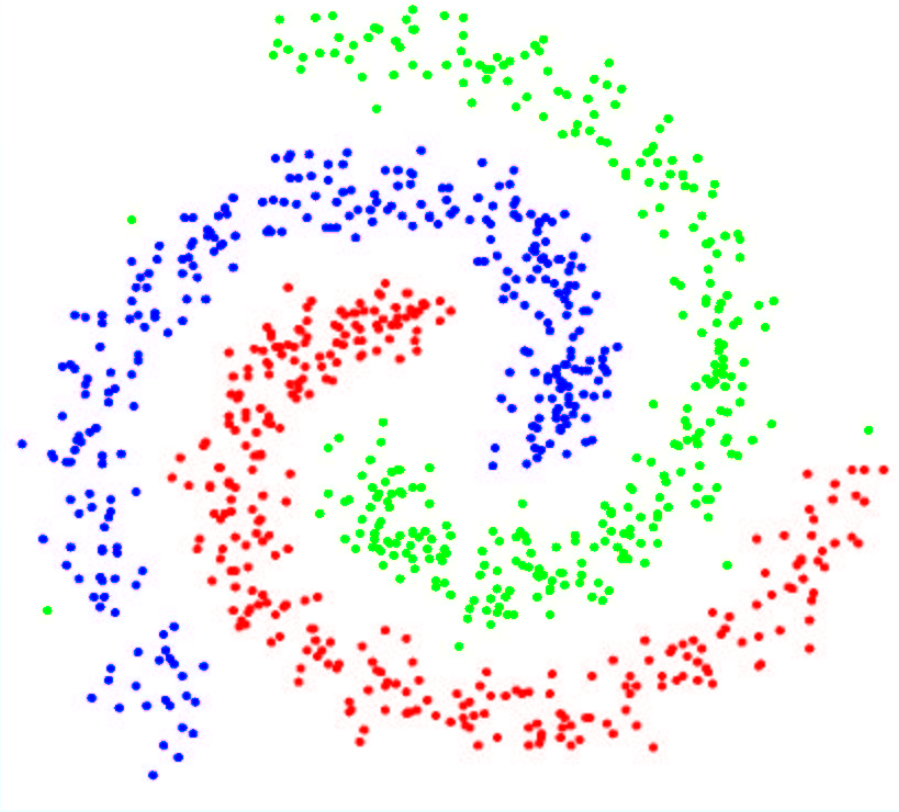

$\Rightarrow$ Object-wise evaluation of costs not sufficient, more complex cost functions required.

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Clustering: Unsupervised methods; no previously labeled data available.

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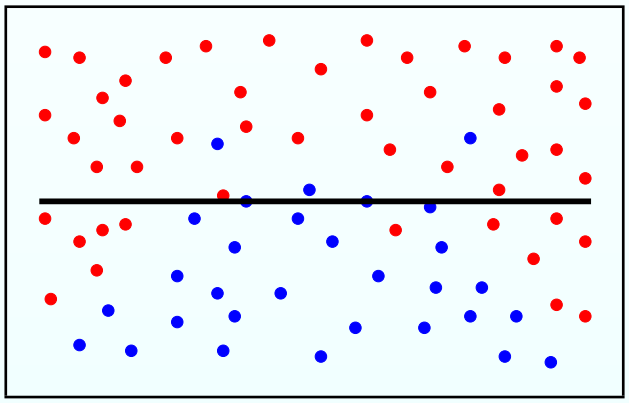
Clustering: Unsupervised partitioning of object space by quality criterion! **How to optimize cluster criterion?**

Generalization Problem in Classification

Underfitting



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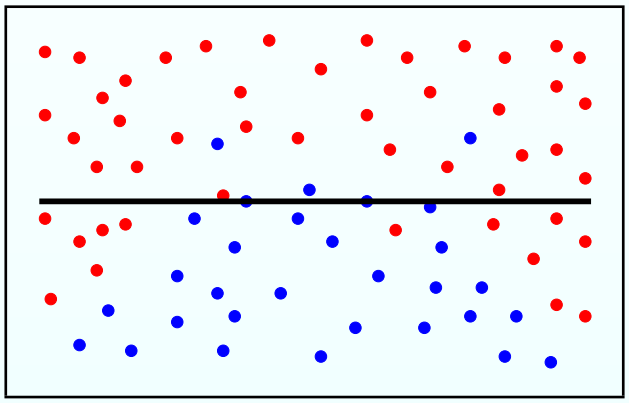
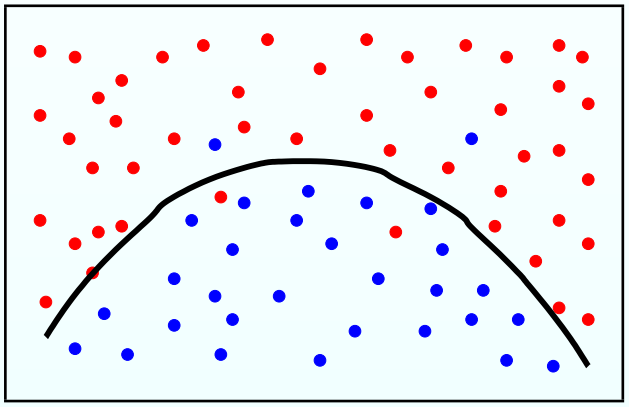
Underfitting $\longleftrightarrow$





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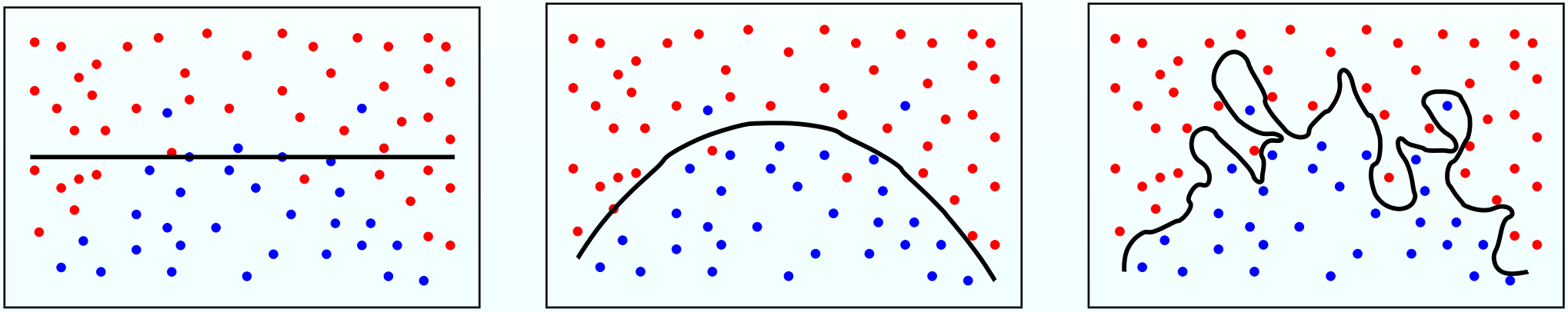

Complexity of Hypothesis Class has to be **controlled**, e.g., restricted to avoid overfitting.

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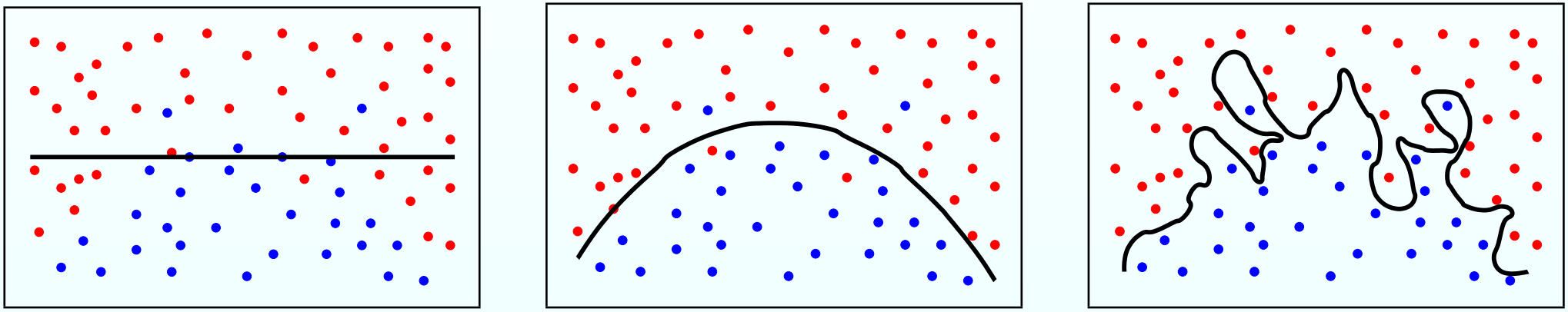

Complexity of Hypothesis Class has to be **controlled**, e.g., restricted to avoid overfitting. **Key Problem in ML,**

Statistical and Computational Learning Theory

Structure of the Tutorial

Part 1: **Basic Concepts** of data clustering

- K-means clustering, histogram/distributional clustering
- graph theoretic approaches: pairwise clustering, NCut
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Part 3: **Validation** of clustering solutions

- agreement measure
- gap statistic
- stability analysis

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Vector data:	n vectors in $\mathbb{R}^d$.
Histogram data:	n histograms in $\mathbb{R}^d$.
Proximity data:	$n \times n$ pairwise proximity matrix.
Much harder problem	structure hidden in n^2 pairwise relations.

Part I: Clustering Principles

- **Compactness**
  - K-Means
  - Histogram Clustering
  - Pairwise Data Clustering (Average Association)
  - Constant Shift Embedding
  - Parametric Distributional Clustering

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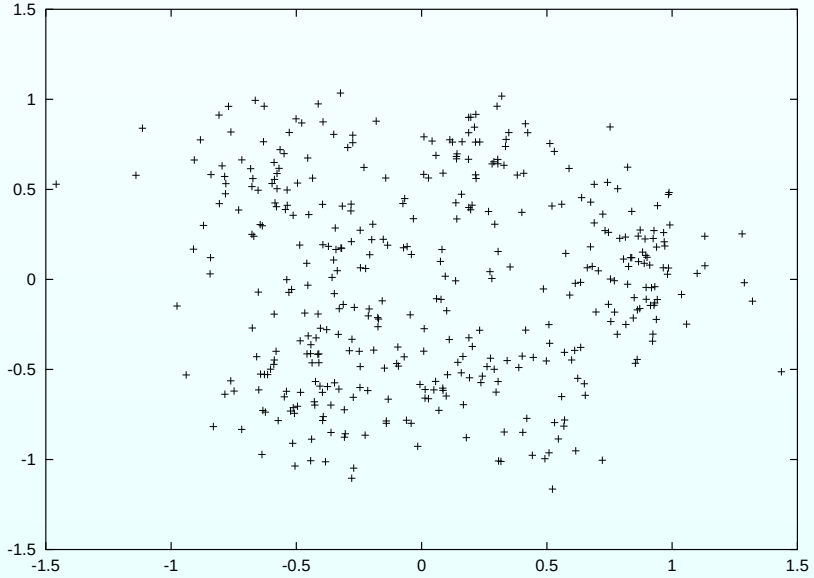

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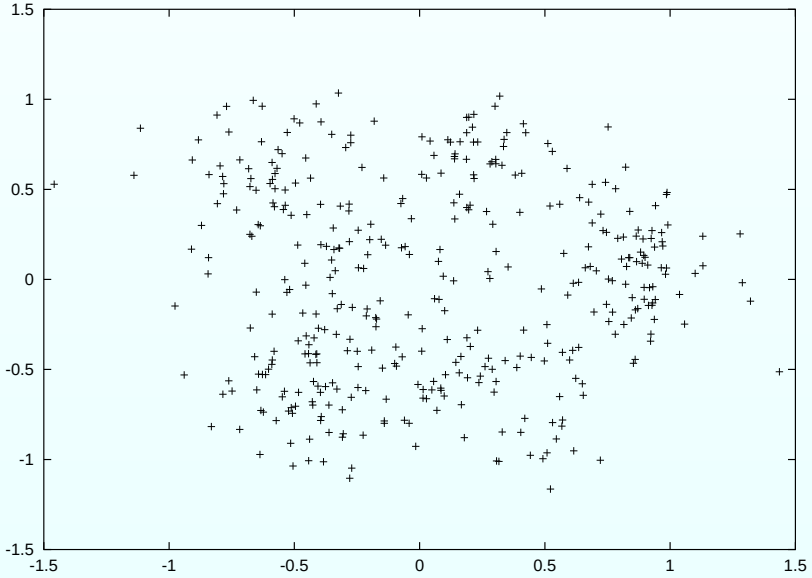
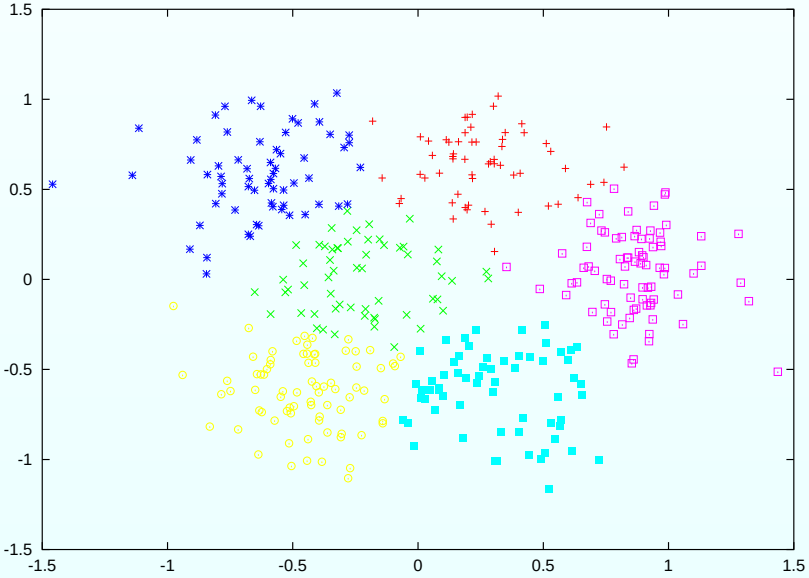


With cluster labels:



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Problem: Find c and y_ν that minimize

$$H^{\text{km}}(c, y) = \sum_{i=1}^{n} ||x_i - y_{c(i)}||^2$$

Mixed combinatorial and continuous optimization problem

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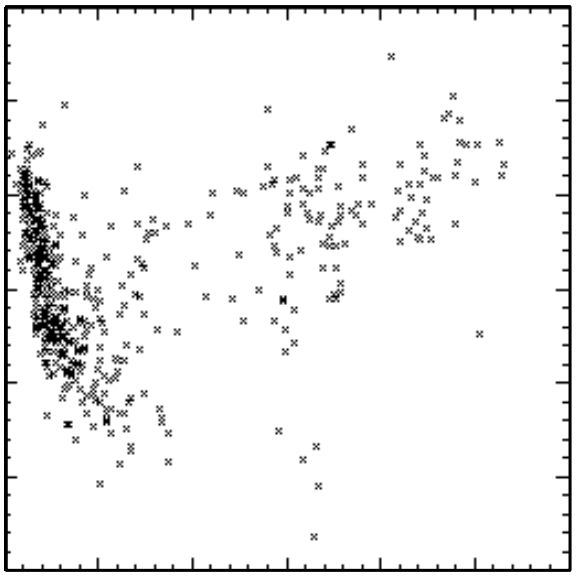
   - Keep assignments $c(i)$ fixed and estimate prototypes

$$y_\nu = \frac{1}{|\mathcal{C}_\nu|} \sum_{i:c(i)=\nu} x_i$$

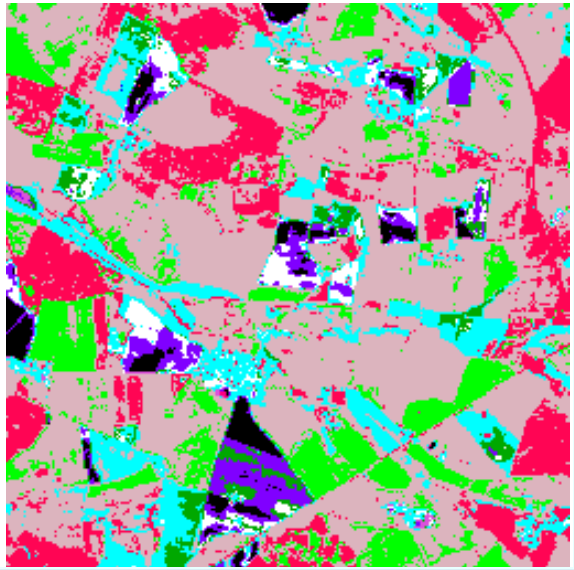
k-Means Segmentation of LANDSAT Images

Vectorial Data : $\mathbf{x}_i \in \mathbb{R}_+^6$

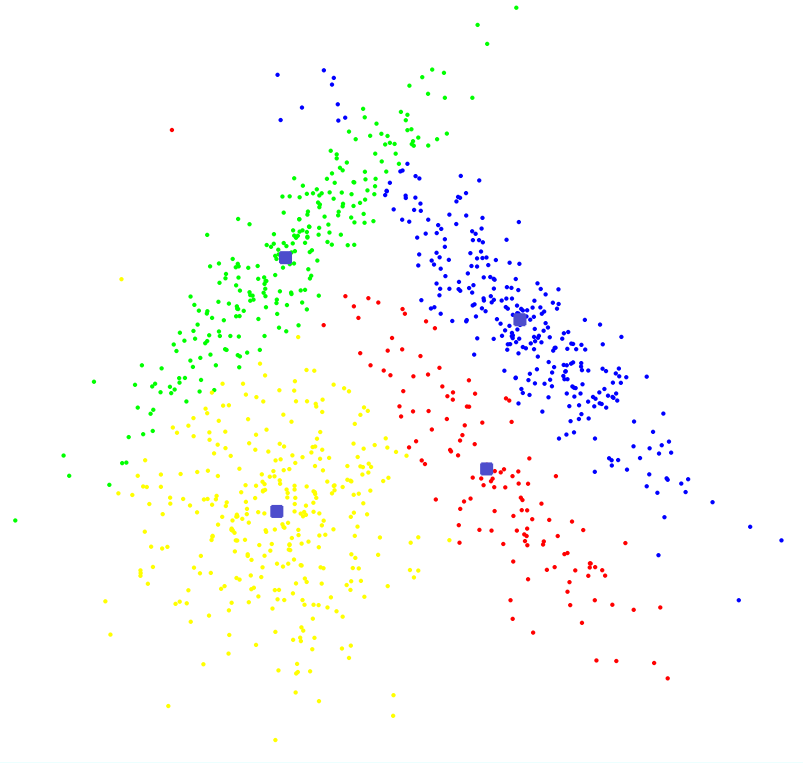


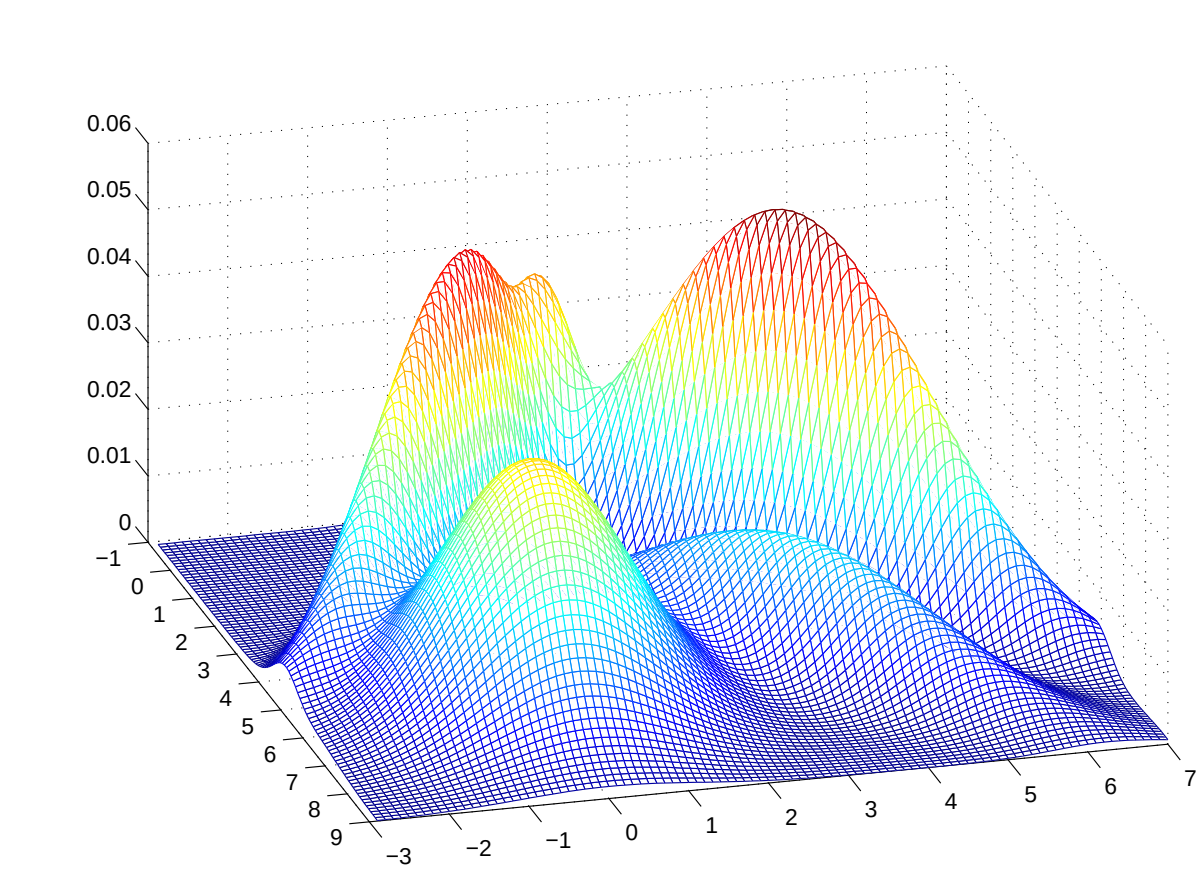
$k = 13$

$c : \mathbb{R}_+^6 \rightarrow \{1, \ldots, k\}$



Example Mixture Model

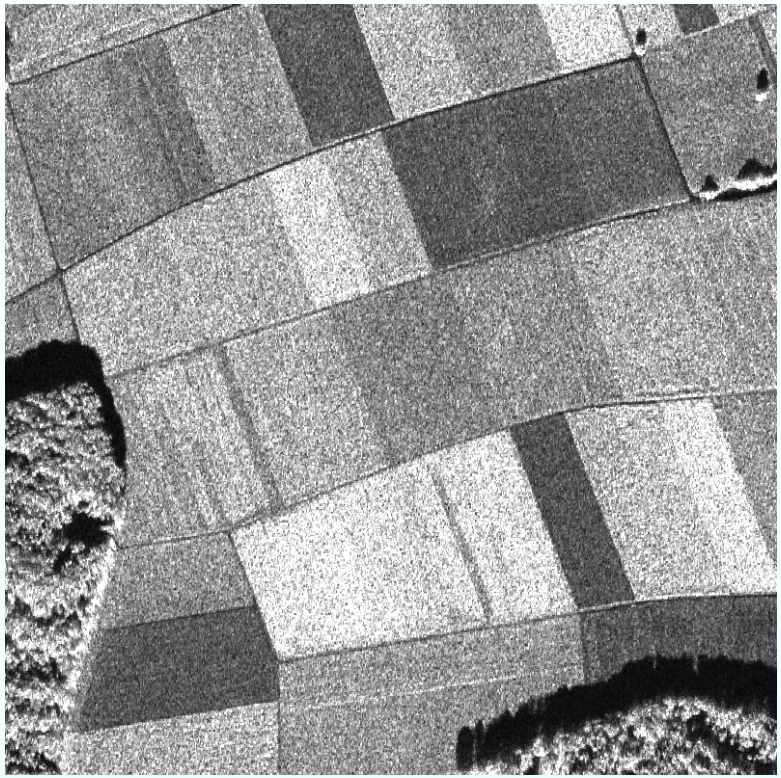




Parametric Distributional Clustering

related to

histogram clustering



- Consider sites on a grid.

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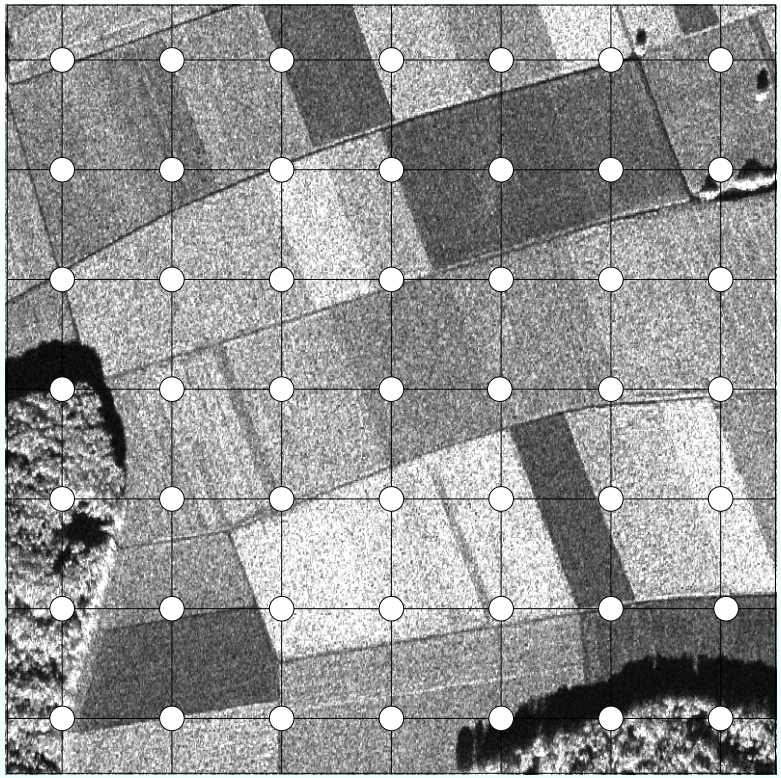

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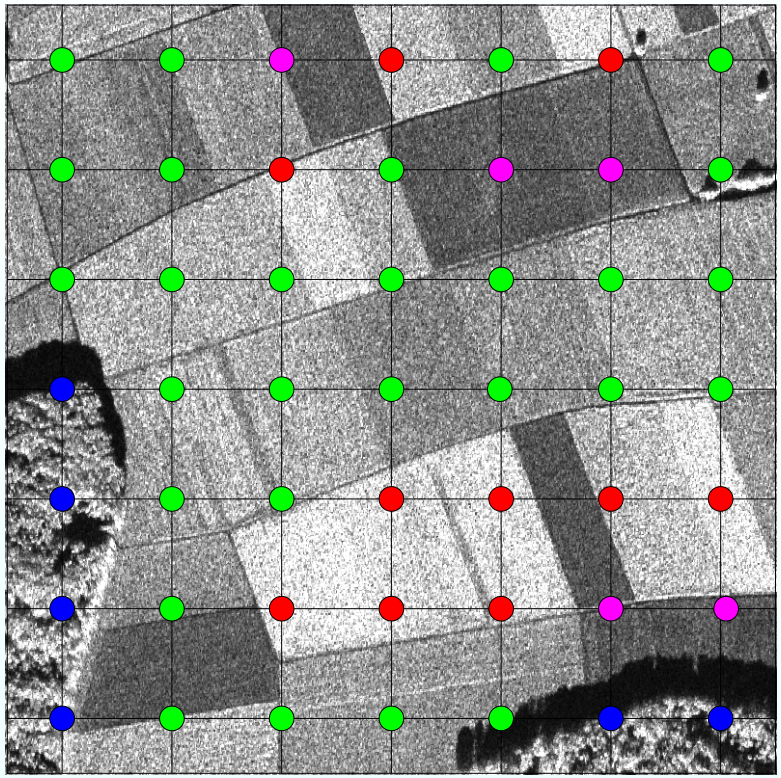

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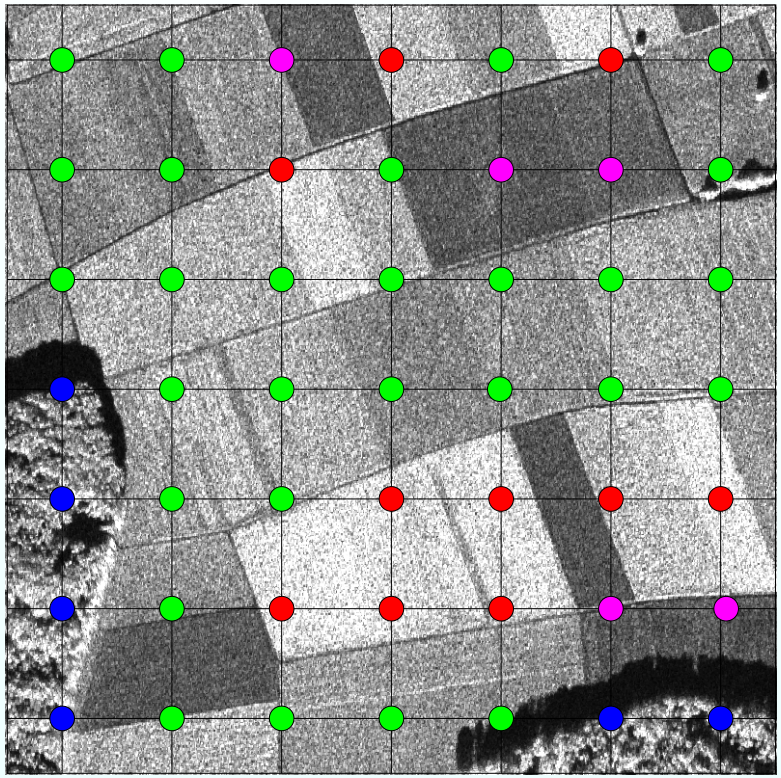

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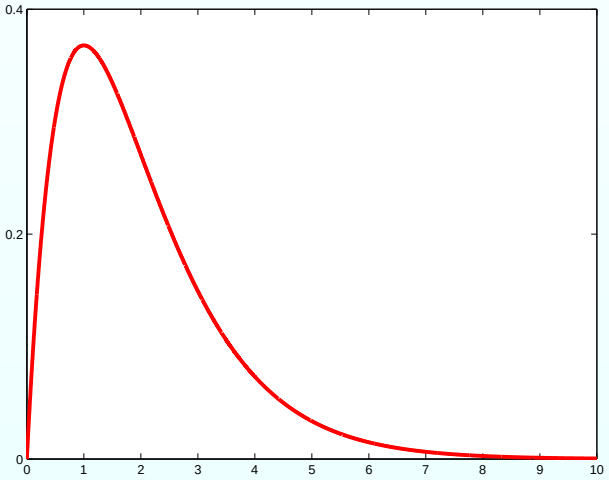
- Cluster memberships encoded by $\mathbf{c} \in \{1, \ldots, k\}^n$

Assumed Sampling Process

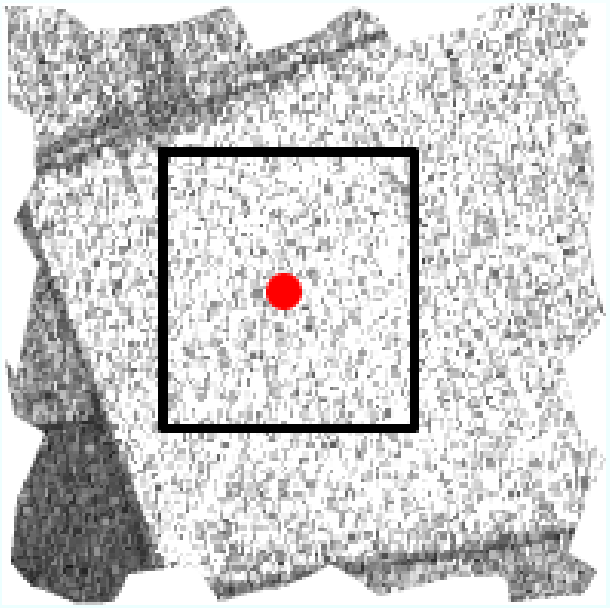
Mixture density

$p(x|\nu)$



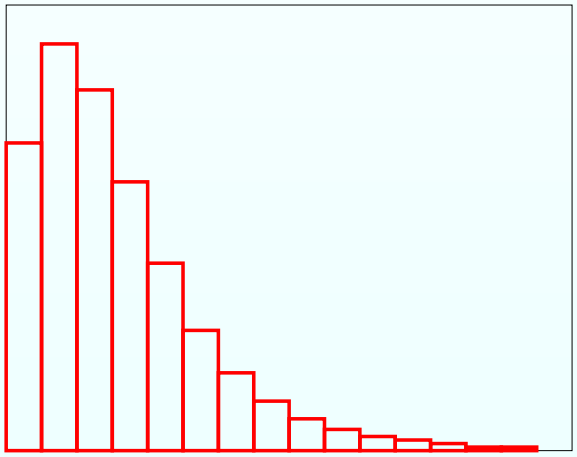
pixel values

$\{x \in \mathcal{N}_i\}$

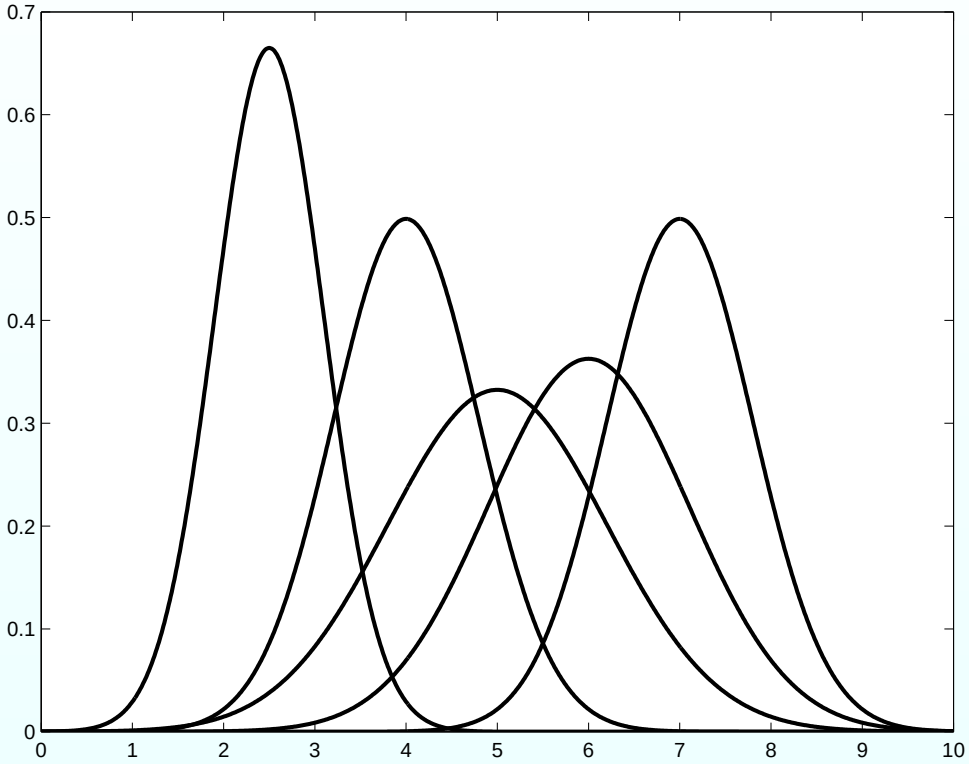


local histogram

$n_{ij}, 1 \leq j \leq m$



Gaussian Mixture Models



A single selection of Gaussian prototypes $g_\alpha(x)$ is used to create mixture densities $p\left(x|\ \nu\right) = \sum_\alpha p_{\alpha|\ \nu} g_\alpha\left(x\right)$.

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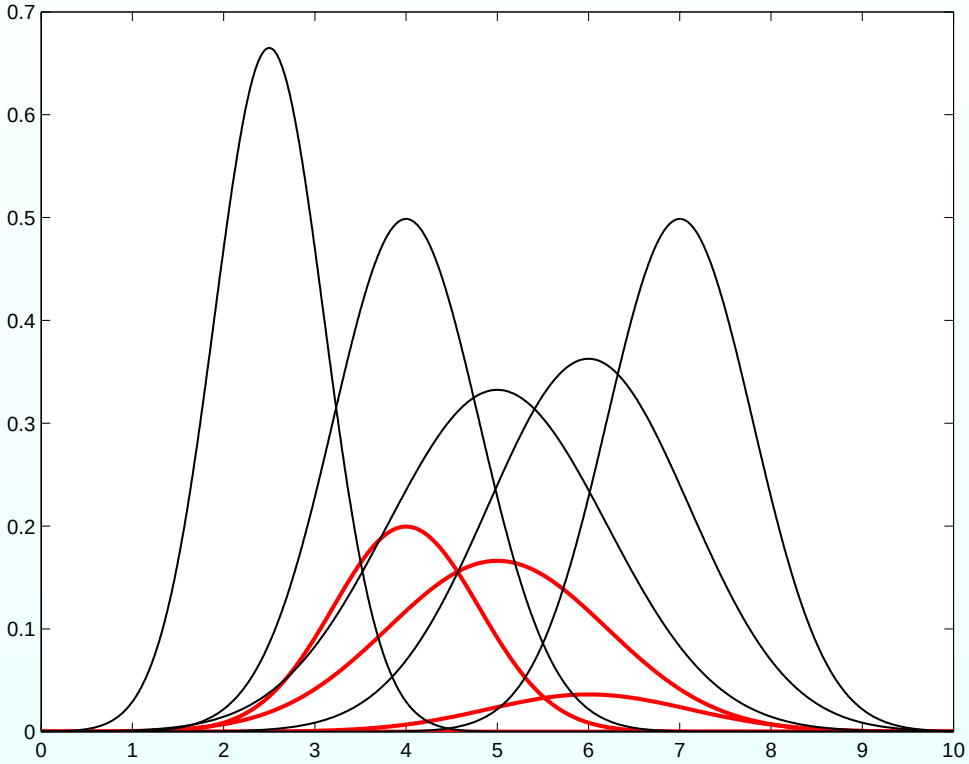

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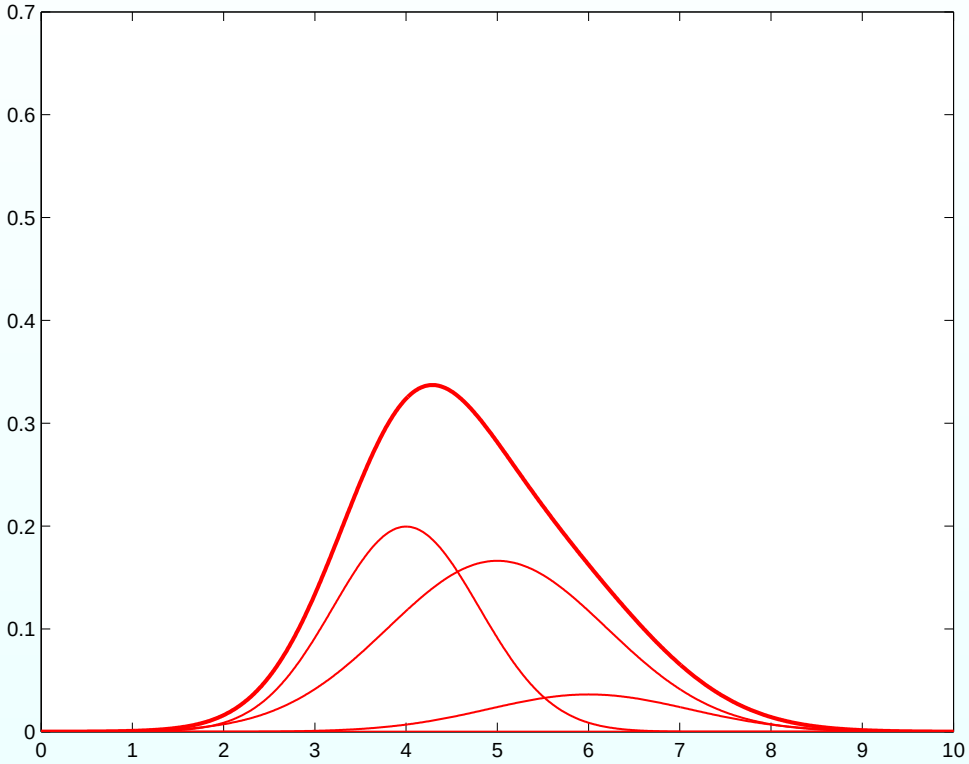

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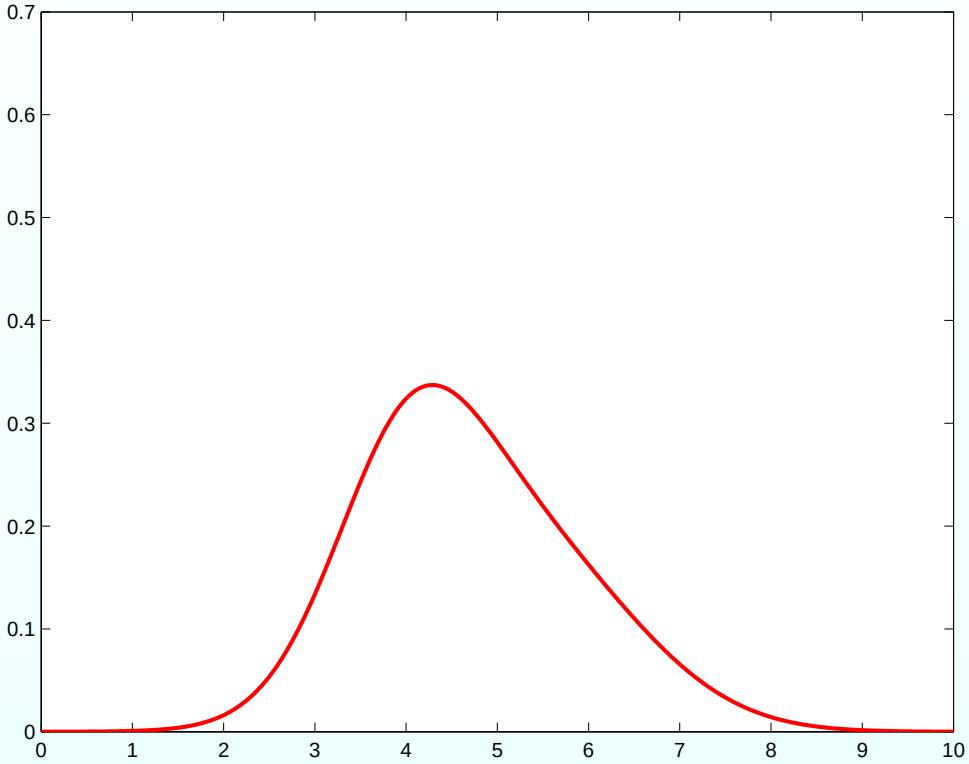

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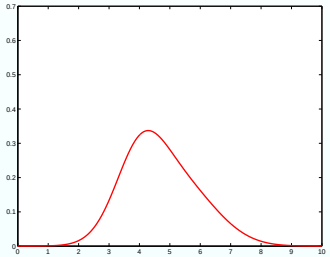

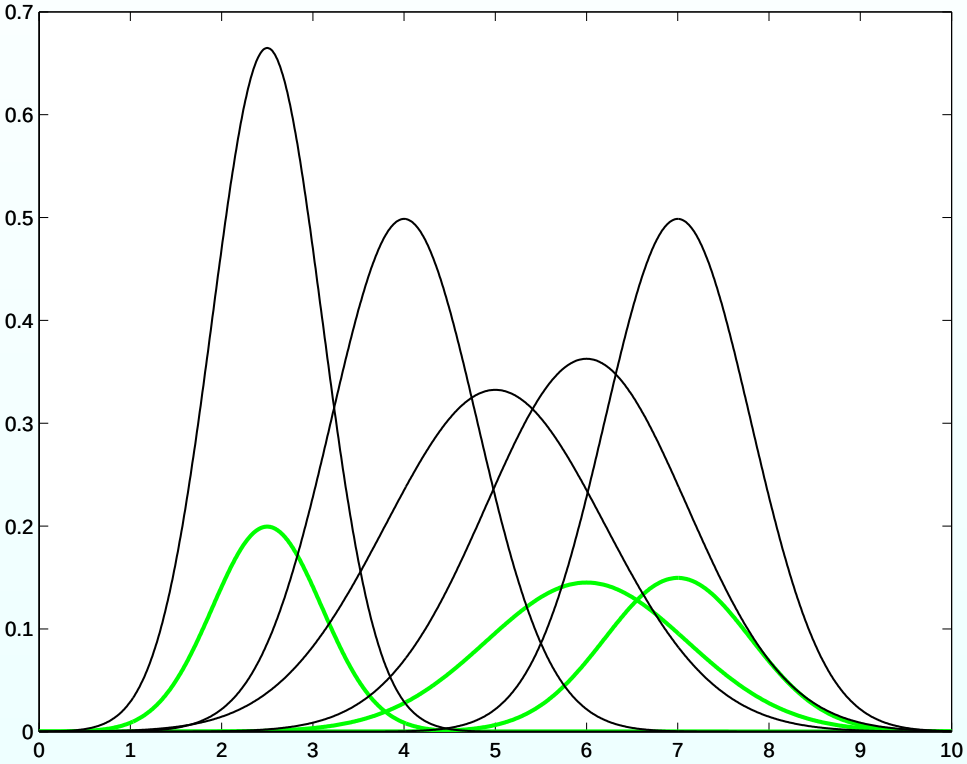

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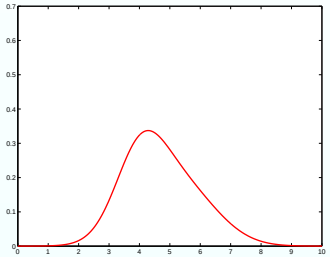

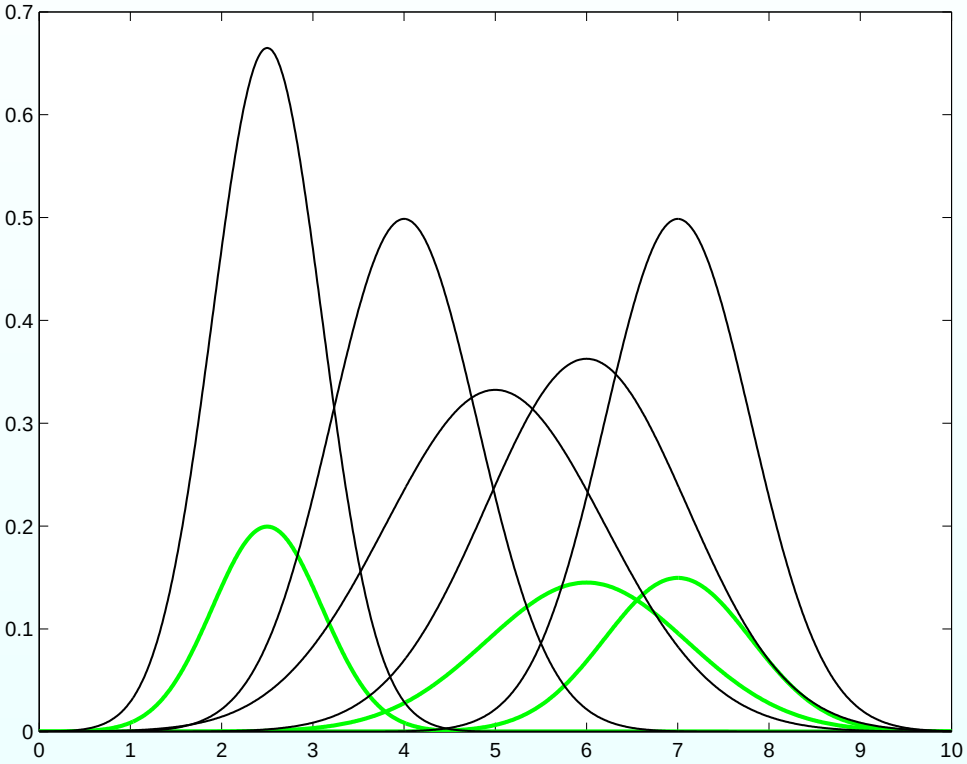

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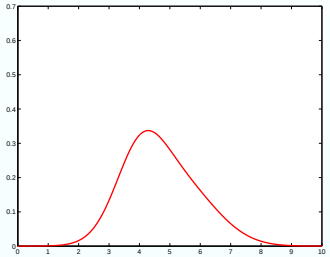

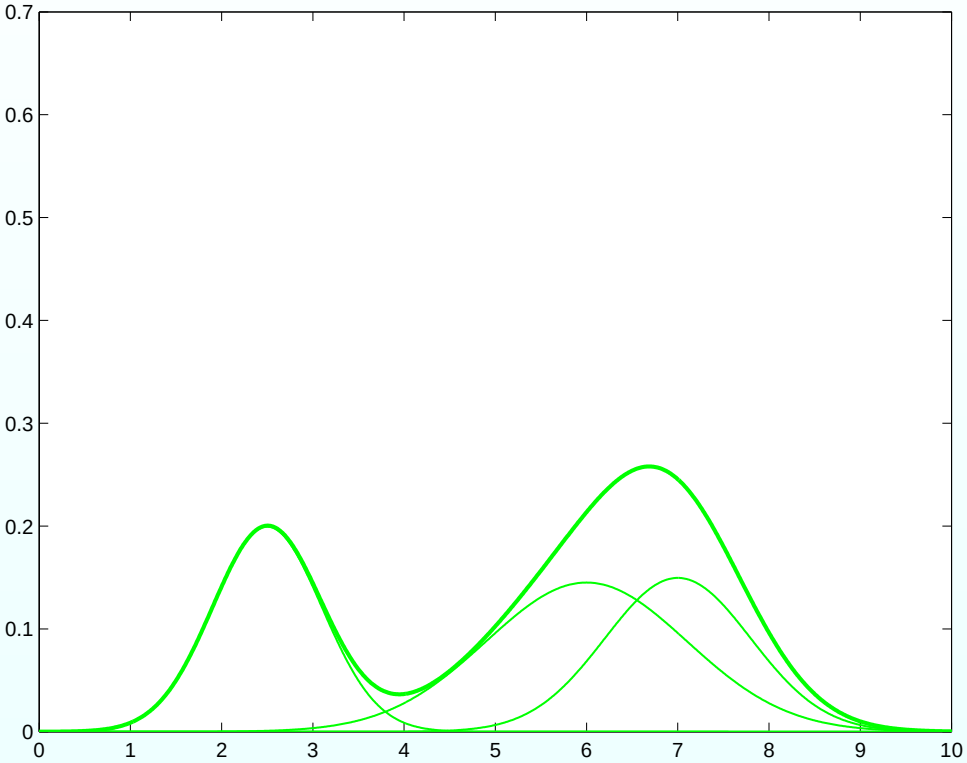

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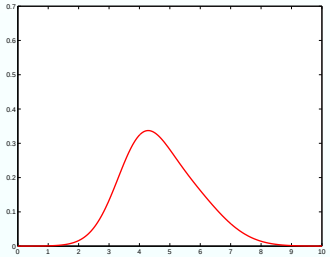

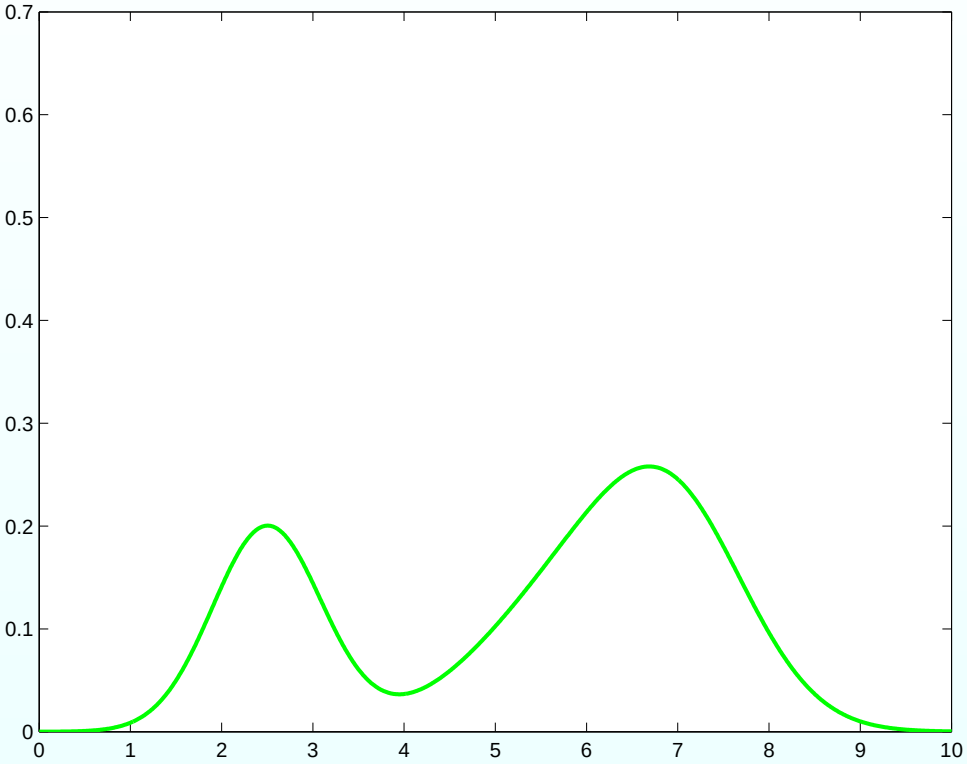

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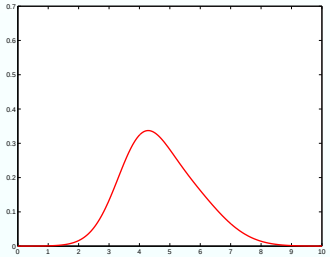

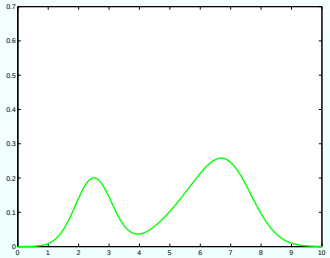

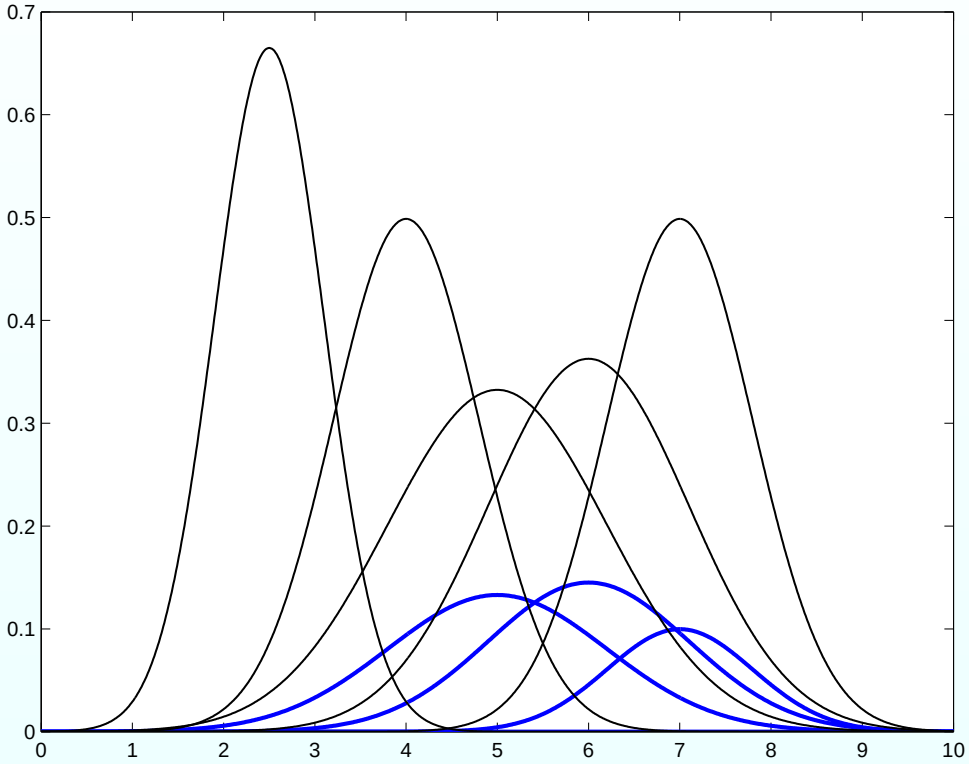

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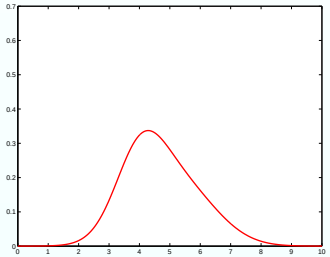

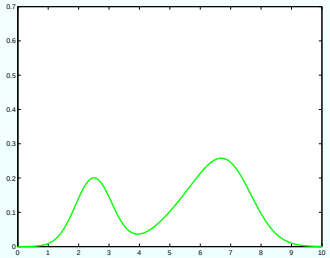

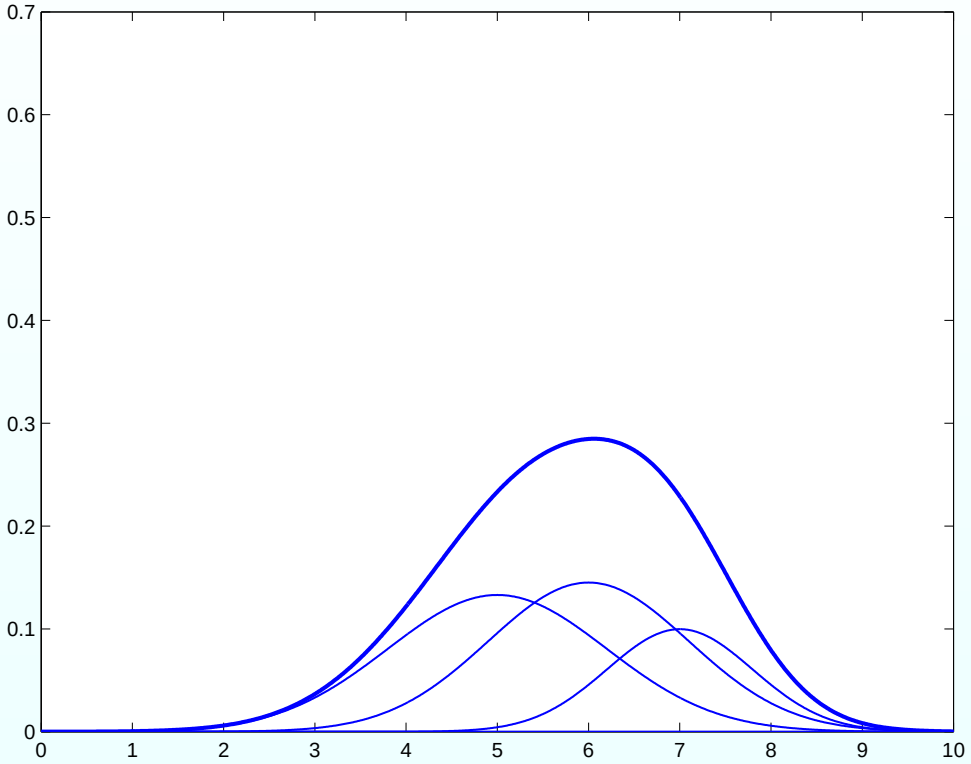

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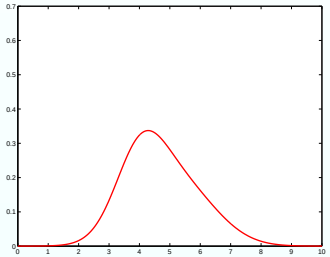

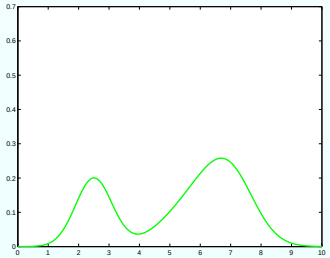

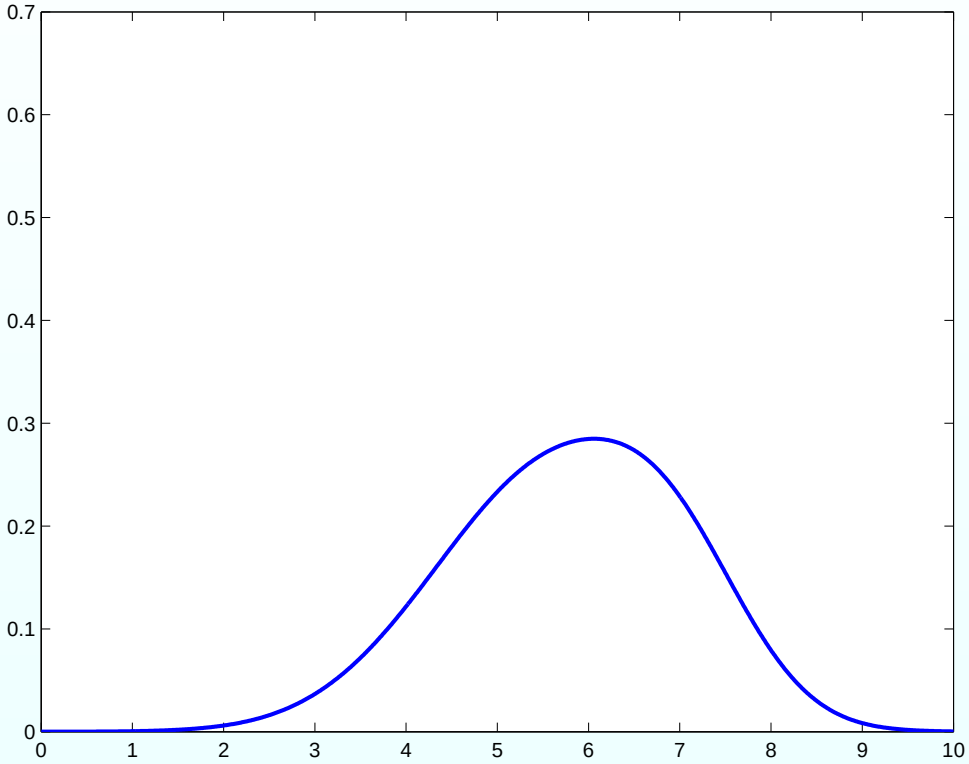

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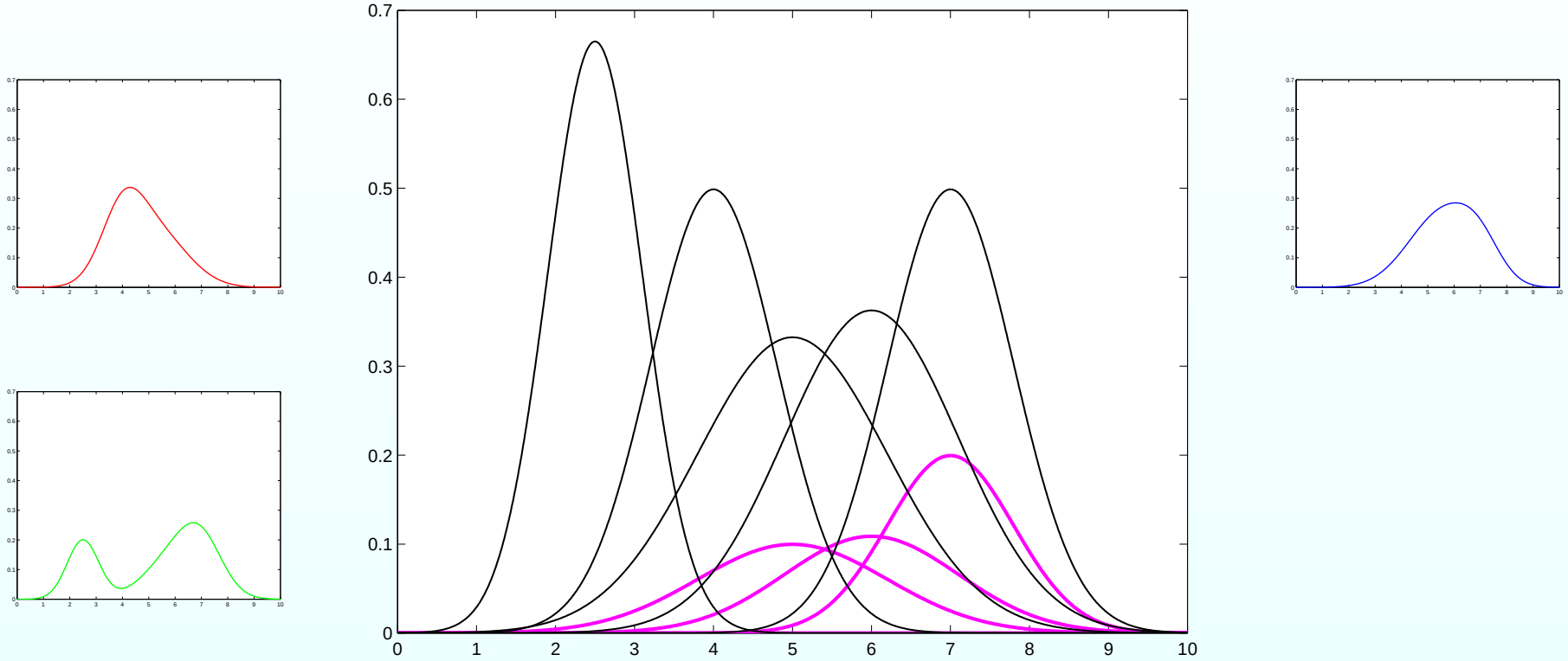

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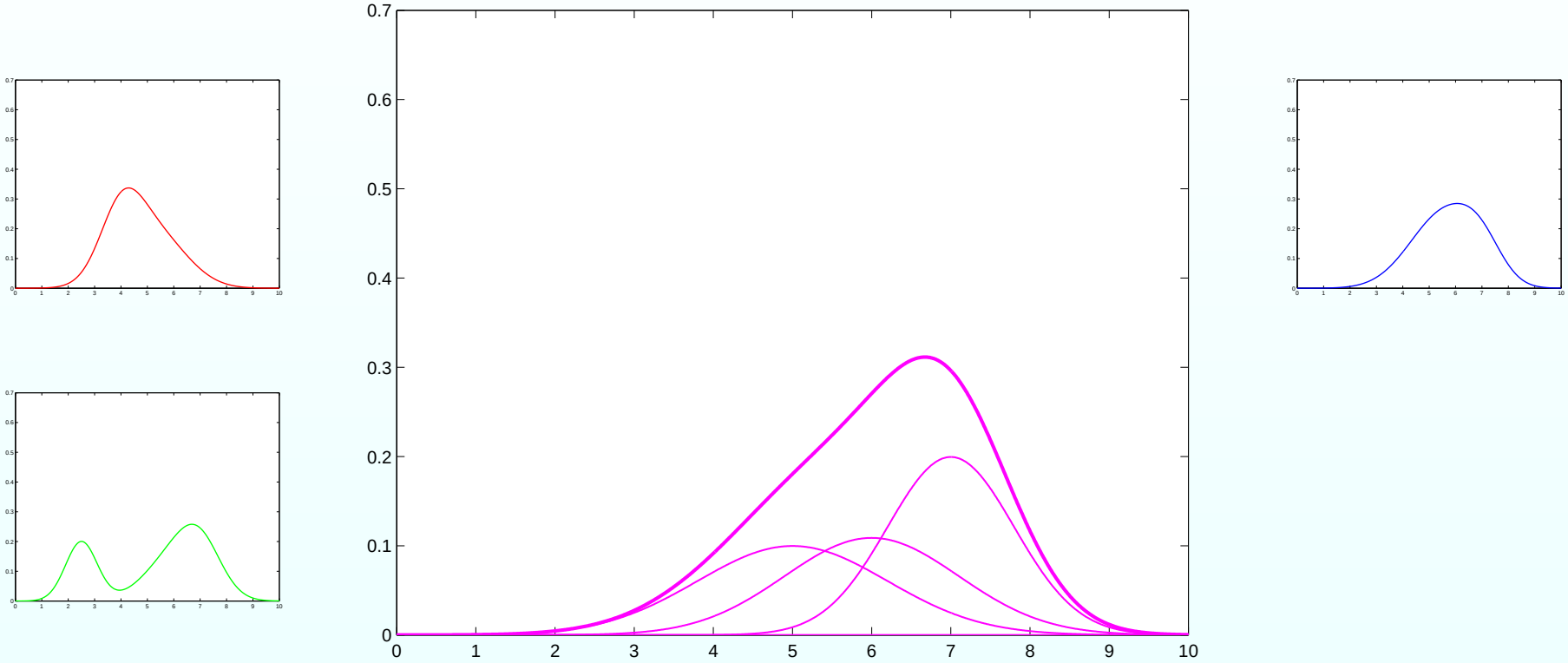

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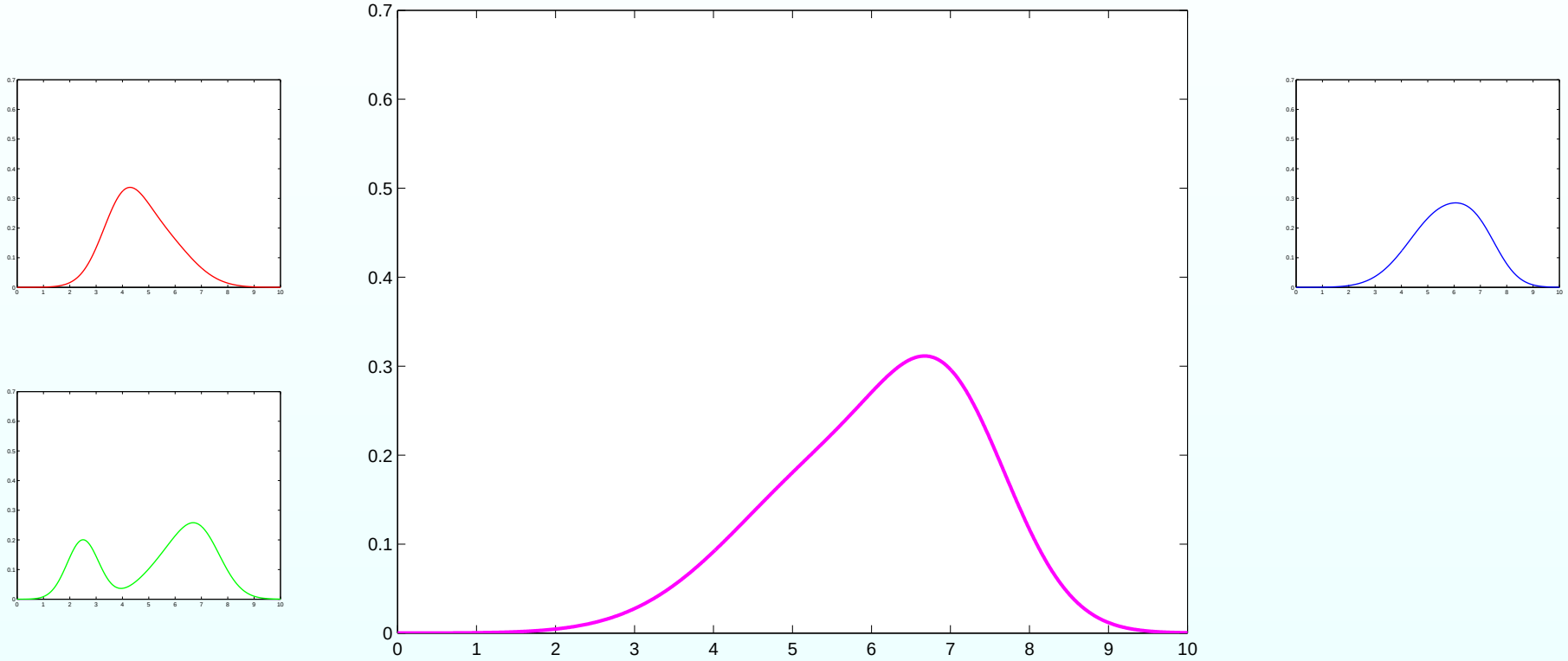

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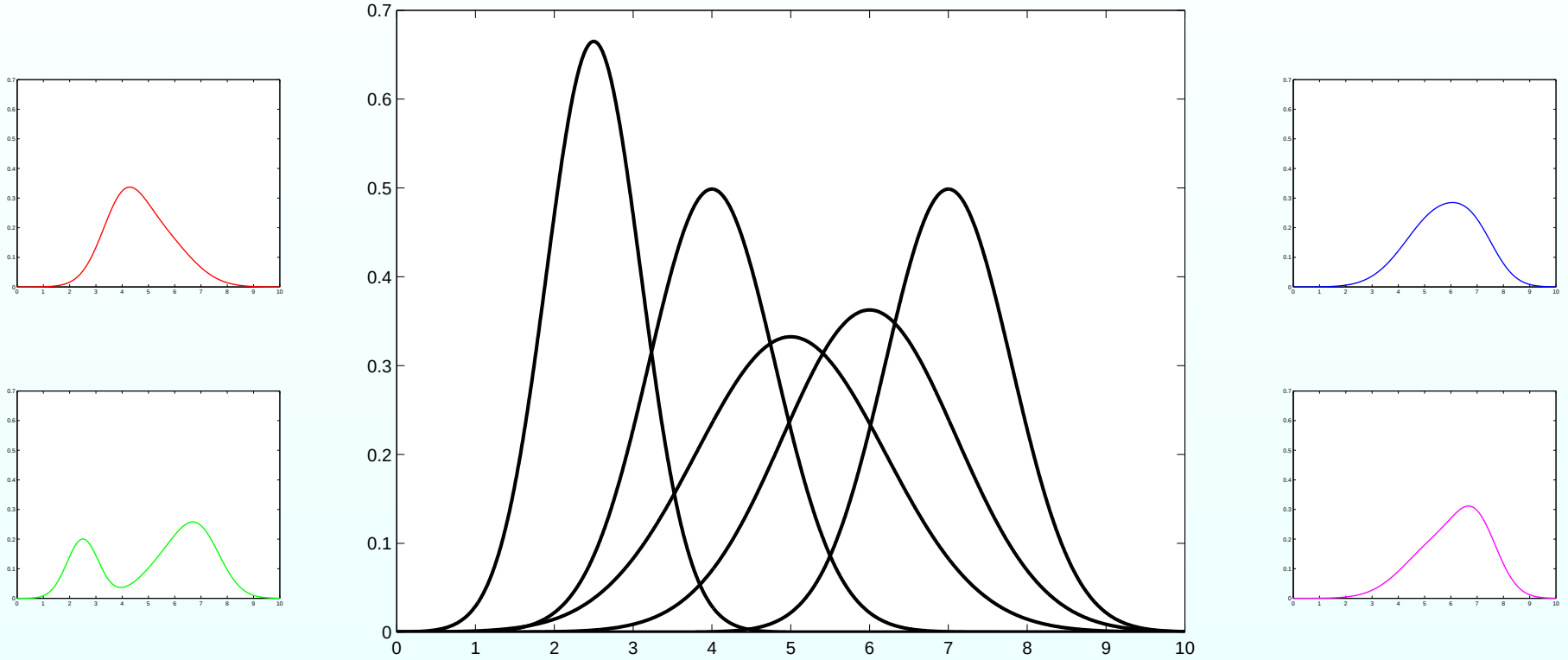

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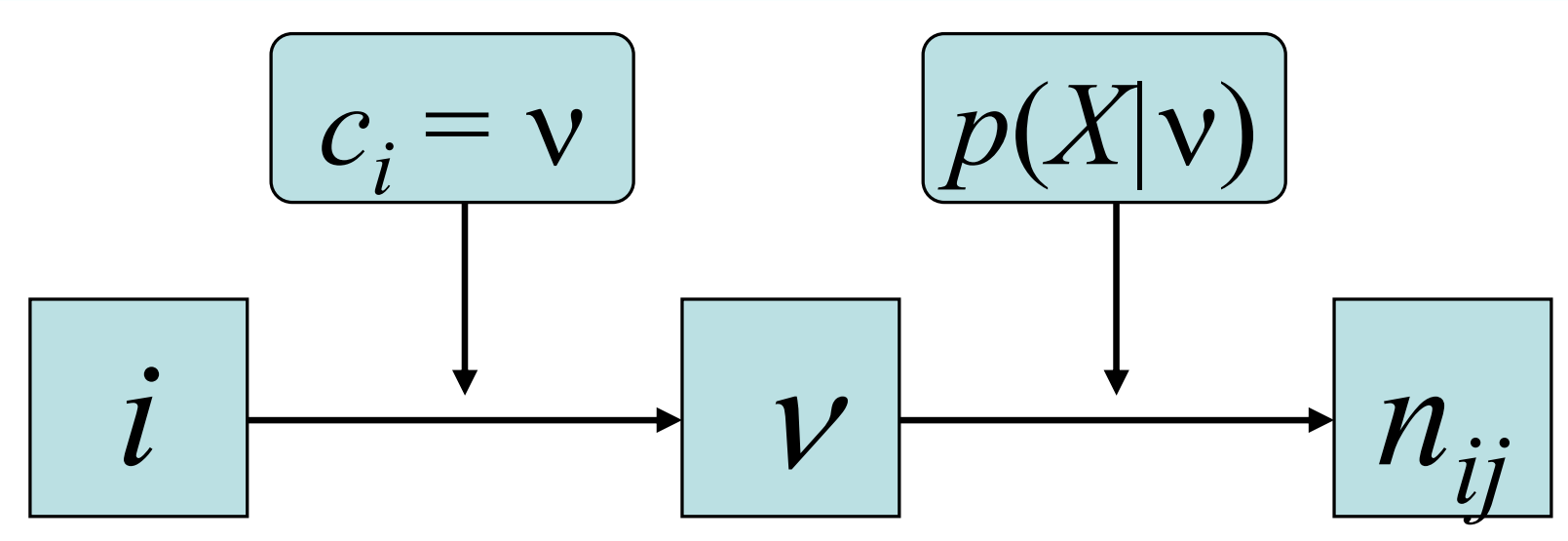
Generative Model



Color values only depend on cluster membership!

Maximum Likelihood Approach

Prior of assignment function $\mathbf{c}$:

$$p\left(\mathbf{c}|\ \theta\right) = \prod_{i=1}^{n} p_{\mathbf{c}(i)}$$

Data likelihood for given $\mathbf{c}$:

$$p\left(\mathcal{X}|\ \mathbf{c}, \theta\right) \ = \ \prod_{i=1}^{n} \left[\prod_{j=1}^{m} \left(\sum_{\alpha=1}^{\ell} p_{\alpha|\ \mathbf{c}(i)} \tilde{G}_{\alpha}(j) \right)^{n_{ij}} \right]$$

Cost Function for PDC

Cost function = negative log-likelihood:

$$H = -\sum_i \left[\log p_{\mathbf{c}(i)} + \sum_j n_{ij} \log \left(\sum_\alpha p_{\alpha|\,\mathbf{c}(i)} \tilde{G}_\alpha(j) \right) \right]$$

Interpretation as **two-part coding scheme**:
Expected codelength when encoding the cluster memberships and, based on that information, encoding the individual color values.

Hermes, Zöller, Buhmann, 2002

Information Bottleneck

Essential idea:

- Find efficient code $X \mapsto \tilde{X}$ ($\tilde{X}$ is a codebook vector)
- Preserve relevant information about context variable Y

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Tradeoff is made explicit by cost functional

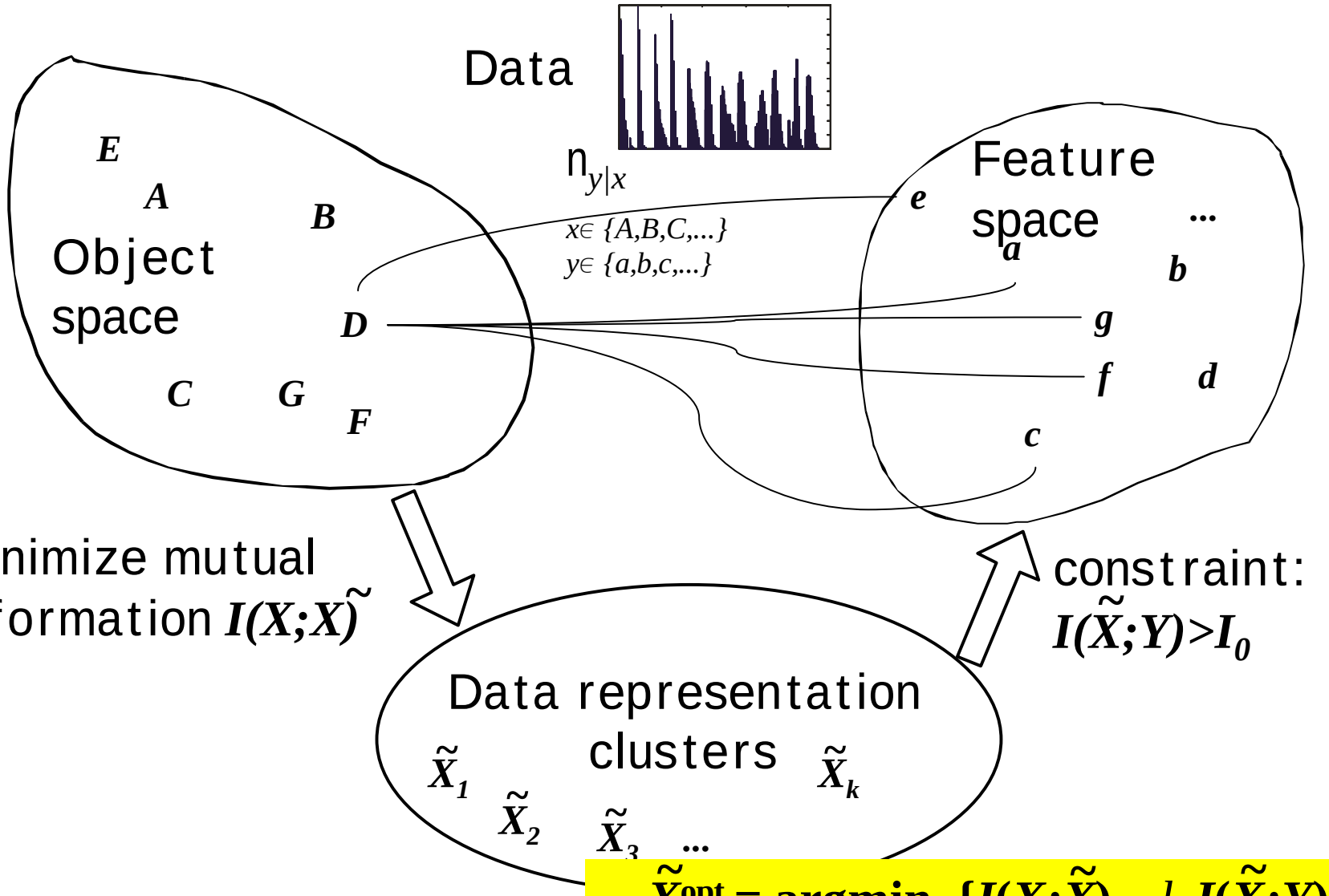
$$H^{IB} = I\left(X;\, \tilde{X}\right) - \lambda I\left(\tilde{X};\, Y\right) \;,$$

where $I(A;\, B)$ is the mutual information between two random variables A and B, $\lambda > 0$.

Tishby et al., 1999

Information Bottleneck

(**Tishby, Pereira, Bialek** IT Allerton Conf. 1999)

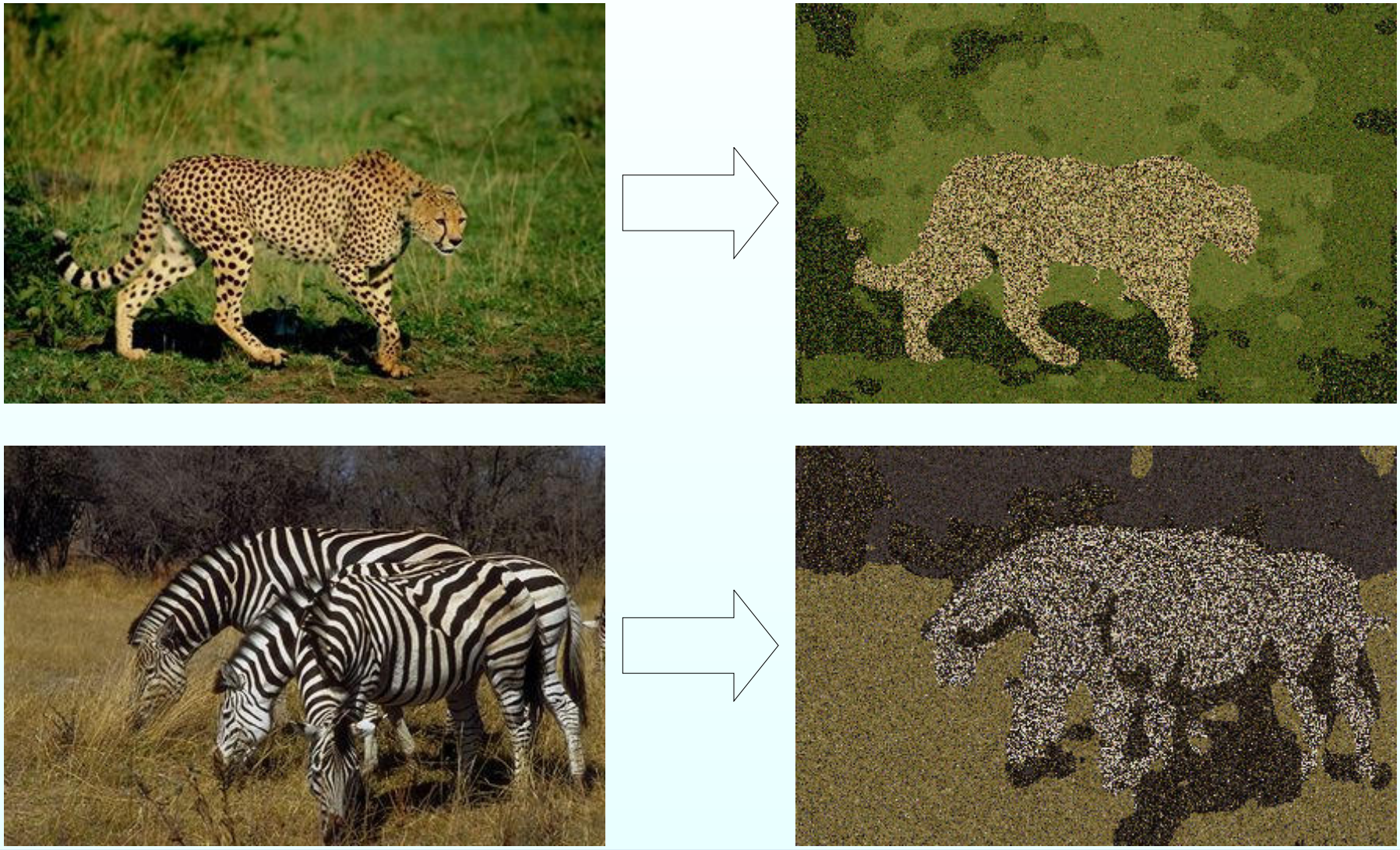


$$\tilde{X}^{opt} = \text{argmin}_{\tilde{X}}\{I(X;\tilde{X}) - \lambda\, I(\tilde{X};Y)\}$$

PDC Segmentation

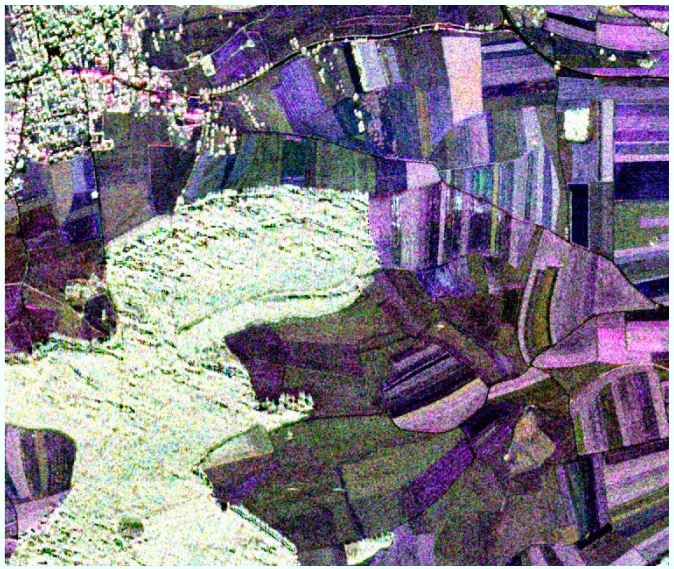
PDC Segmentation

PDC Resampling

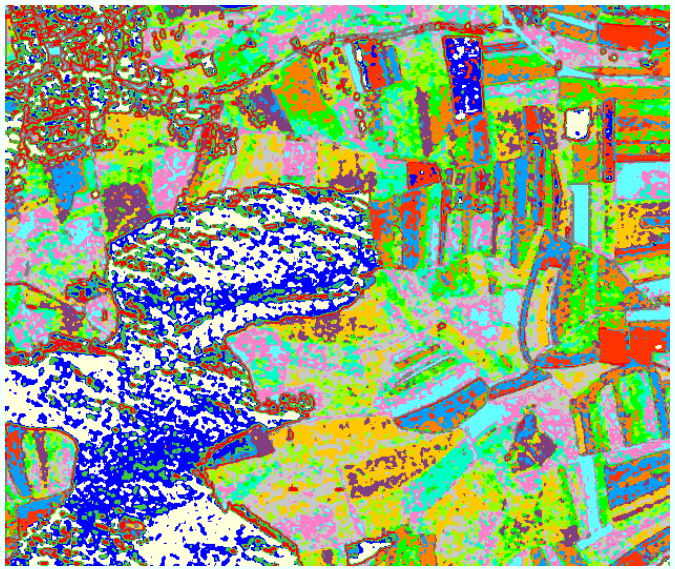


SAR Imagery

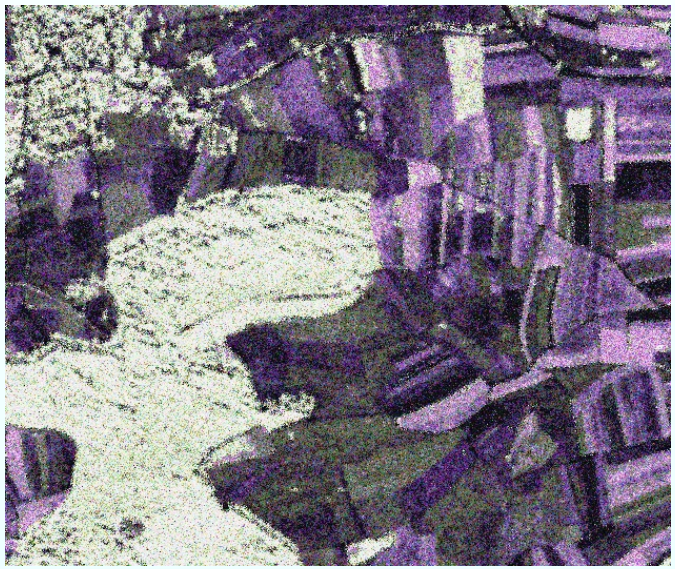
Polarimetric synthetic aperture radar image, L-band



original



segmentation

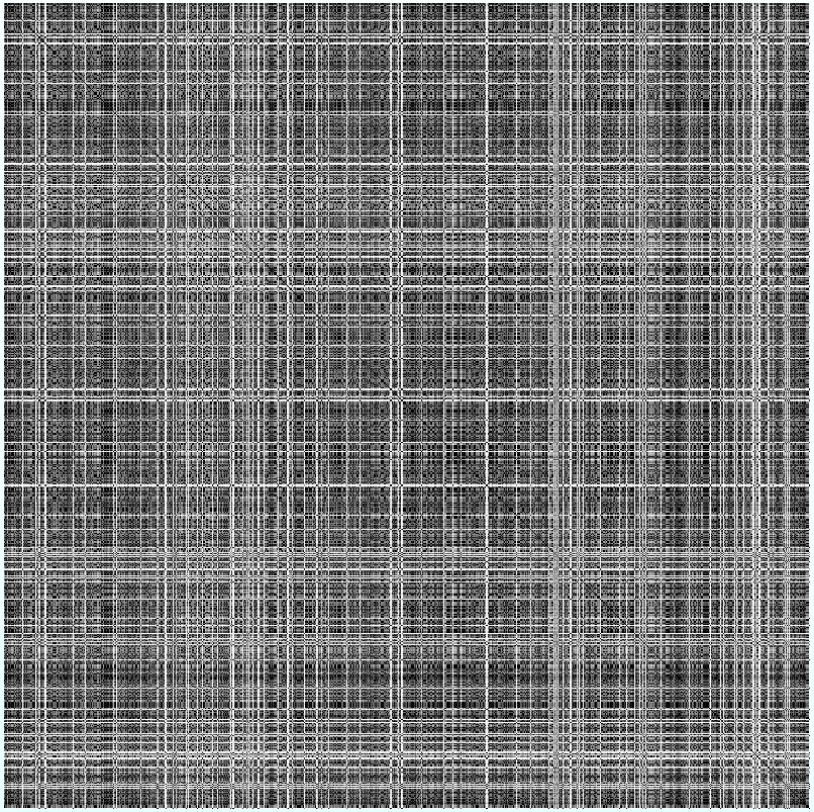


resampled

Proximity Data

Clustering: find **compact subsets** in dissimilarity data

Raw prox. data:



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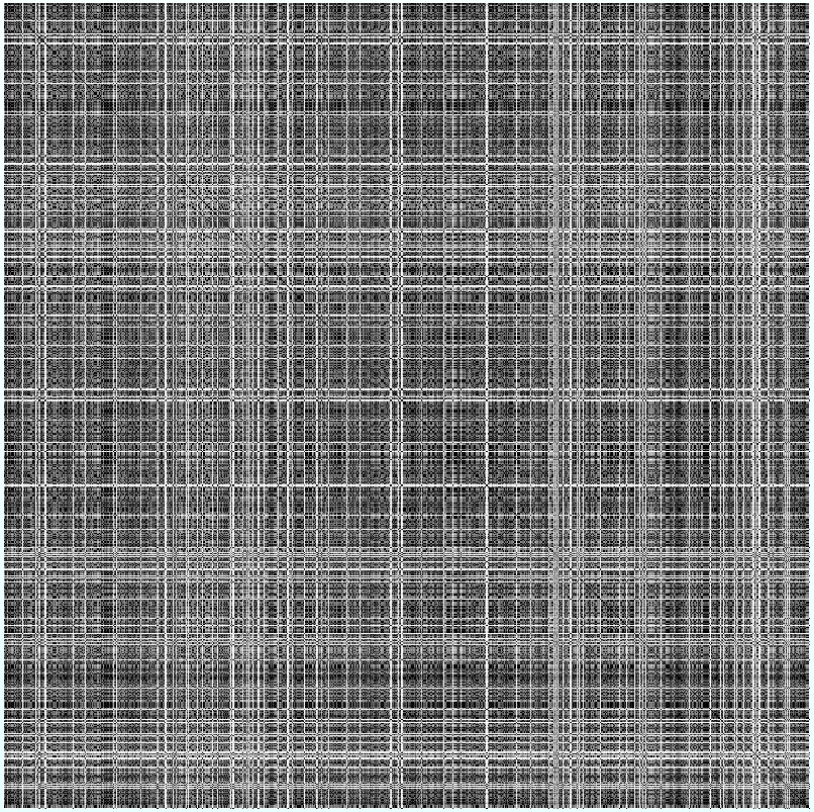
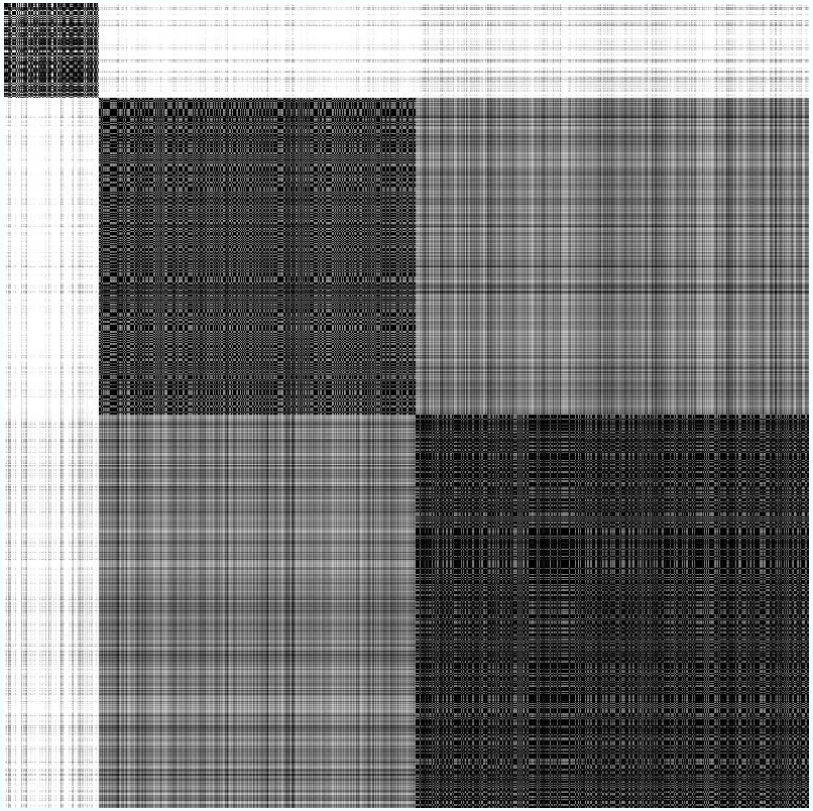


Permuted according to cluster labels:



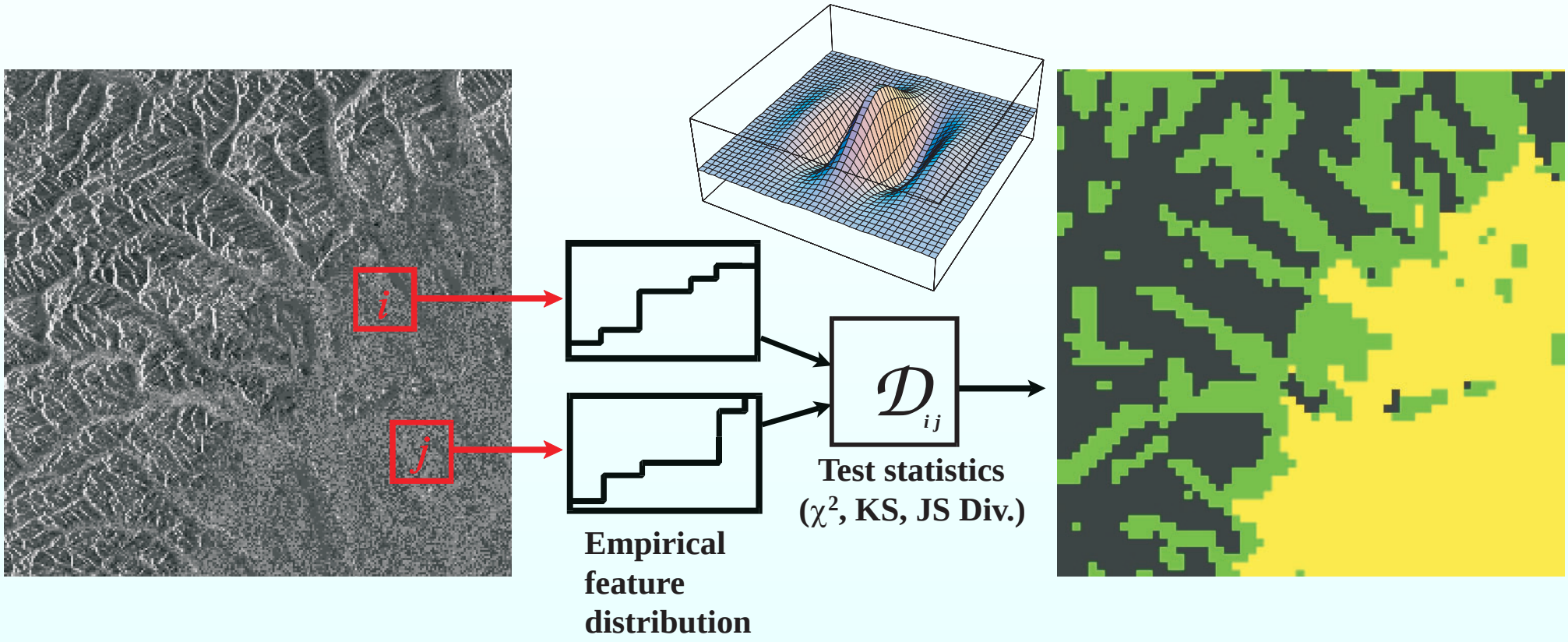
Proximity Data: Example

- Abundant in many applications, e.g. linguistics, psychology, **molecular biology**.
- **Example:** pairwise alignment scores between sequences.

```
       130       140       150       160       170
SDEGSDLAHAVDAEQAFAEGAQAADAVEATPVEPVKVRERKRTFHYPDGLKDYVTAI
 ::       .: :  ..:  ...::    : .: : ::.:. ::::.::.:::  .
LDE-------IDNETELVE--ETTDA----PKKPKK-REKKKIFHYPNGLEDYVHYL
120                 130           140         150       160
```

Proximity Data in Segmentation

SAR imagery analysed by Gabor filters



The Pairwise Clustering Cost Function

Idea: emphasize **compact** clusters by minimizing normalized sum of **intra-cluster dissimilarities**

$$H^{\text{pc}}(c; D) = \sum_{\nu=1}^{k} \frac{1}{|\mathcal{C}_\nu|} \sum_{(i,j):c_i=c_j=\nu} D_{ij},$$

with assignment vector $c \in \{1, \ldots, k\}^n$ and $\mathcal{C}_\nu = \{i : c_i = \nu\}$.

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Euclidean distances: if $D_{ij} = \|x_i - x_j\|^2$ then

$$H^{\text{pc}}(c; \mathcal{X}) = H^{\text{km}} = \sum_{\nu=1}^{k} \sum_{i:c_i=\nu} \|x_i - y_\nu\|^2 \quad \text{for means } y_\nu.$$

Invariance Properties of H^{pc}

H^{pc} **invariant** under...

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symmetrizing transformations:

$$\tilde{D}_{ij} = (1/2)(D_{ij} + D_{ji}) \quad \Rightarrow \quad \tilde{H} = H.$$

$\Rightarrow$ **consider only symmetric matrices**.

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additive shifts of the off-diagonal elements D:

$$\tilde{D}_{ij} = D_{ij} + D_0(1 - \delta_{ij}) \quad \Rightarrow \quad \tilde{H} = H + \text{const.}$$

$\Rightarrow$ **shift does not influence assignments!**

Constant Shift Embedding

Define $\tilde{D} = D + \lambda_0(1 - I)$ with smallest eigenvalue λ_0 of centralized matrix $D^c_{ij} = D_{ij} - \frac{1}{n}\sum_{k=1}^{n} D_{ik} - \frac{1}{n}\sum_{k=1}^{n} D_{kj} - \frac{1}{n^2}\sum_{k,l=1}^{n} D_{kl}$, then

Roth et al., IEEE-TPAMI 2003

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3. $\{x_i\}_{i=1}^{n}$ are explicitly found by eigenvalue decomposition.
4. **optimal approximative vectors** (in least-squares sense): projecting on leading eigenvectors (**kernel PCA**).

Roth et al., IEEE-TPAMI 2003

Clustering of Bacterial *GyrB* Sequences

- **Objects:** 84 amino acid sequences from 5 genera.

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Clustering of Bacterial *GyrB* Sequences

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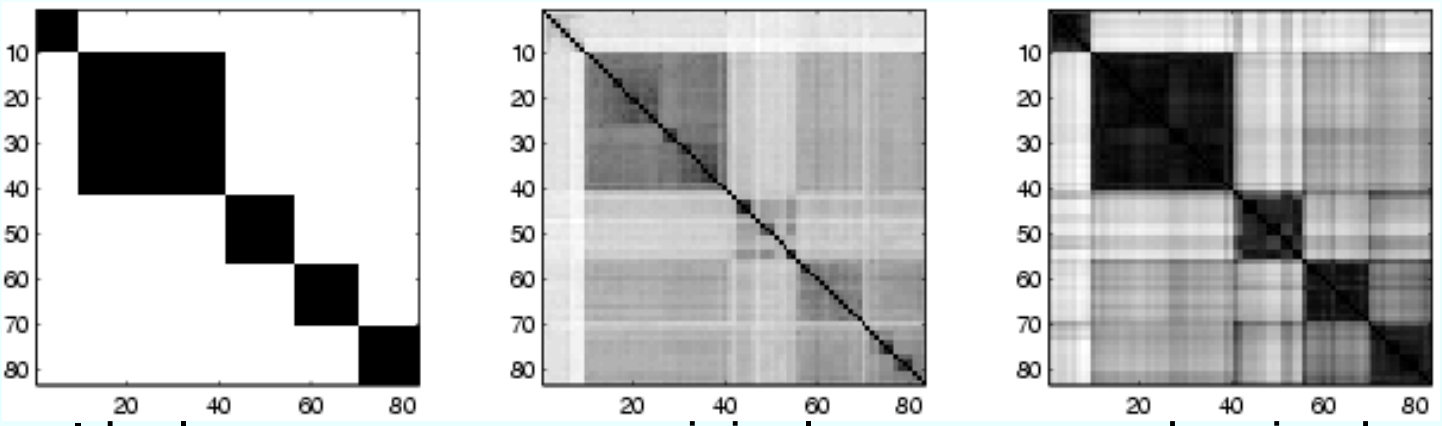
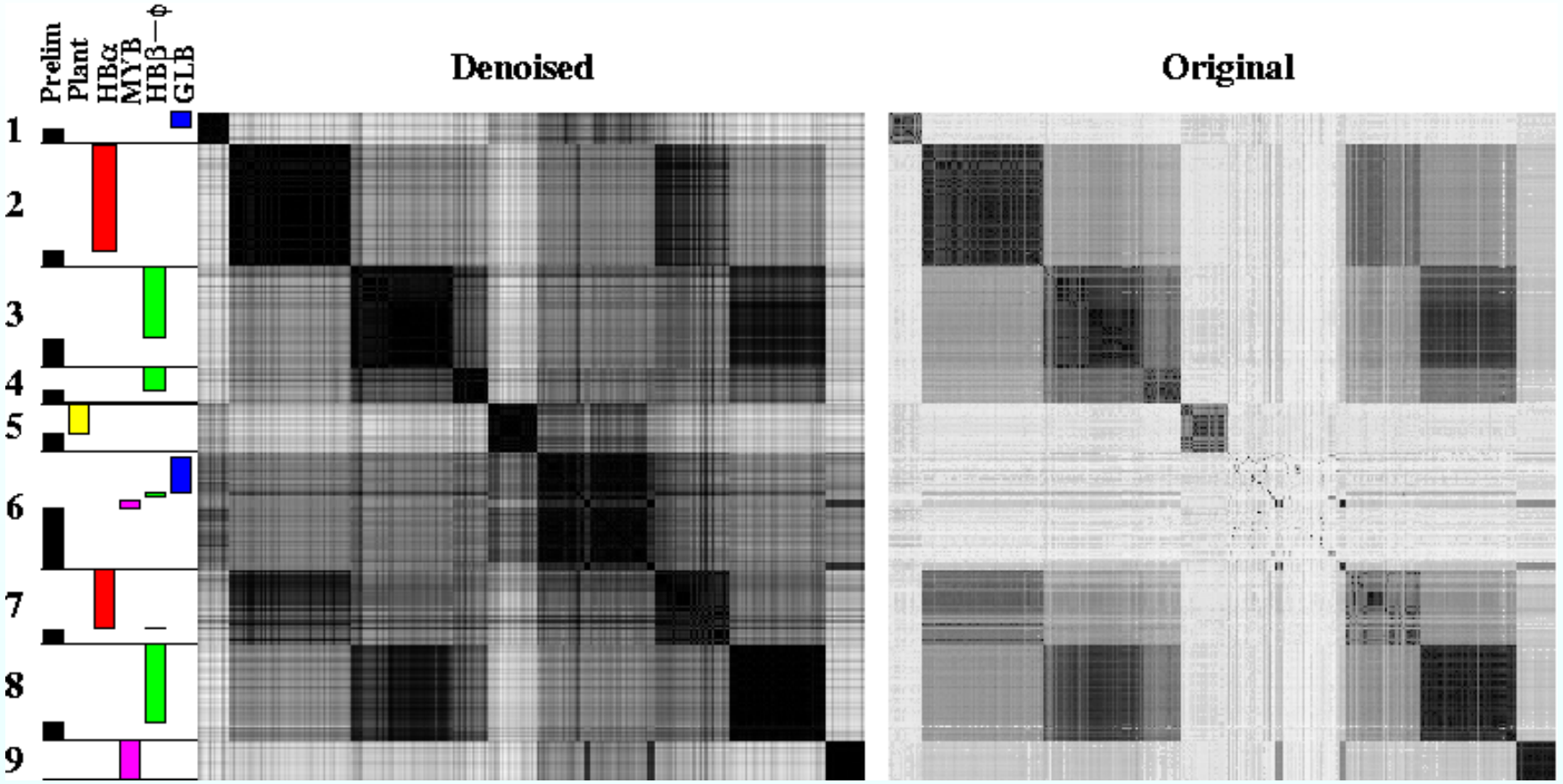
- **Representations:** pairwise alignment scores
- k**-means clustering:** denoised (5 dimensions): 3 misclassifications w.r.t. known ground truth, original (83 dimensions): 17 misclassifications.



Ideal original denoised

Globin Proteins: Cluster Solution



Interpretation: biologically relevant clusters!

Normalized Cut

Minimize the cut, while maximize the association

$$H^{\text{NCut}}(A,B) = \frac{cut(A,B)}{assoc(A,V)} + \frac{cut(B,A)}{assoc(B,V)}$$

Shi & Malik, 2000

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With partition vector $c \in \{-1,1\}^n$ and association matrix $W = (w)_{ij}$:

$$H^{\text{NCut}}(c,W) = \frac{\sum_{c_i>0,c_j<0} -w_{ij}c_ic_j}{\sum_{c_i>0}\sum_{j=1}^{n} w_{ij}} + \frac{\sum_{c_i<0,c_j>0} -w_{ij}c_ic_j}{\sum_{c_i<0}\sum_{j=1}^{n} w_{ij}}$$

Shi & Malik, 2000

Relaxation of NCut

Minimize Rayleigh quotient

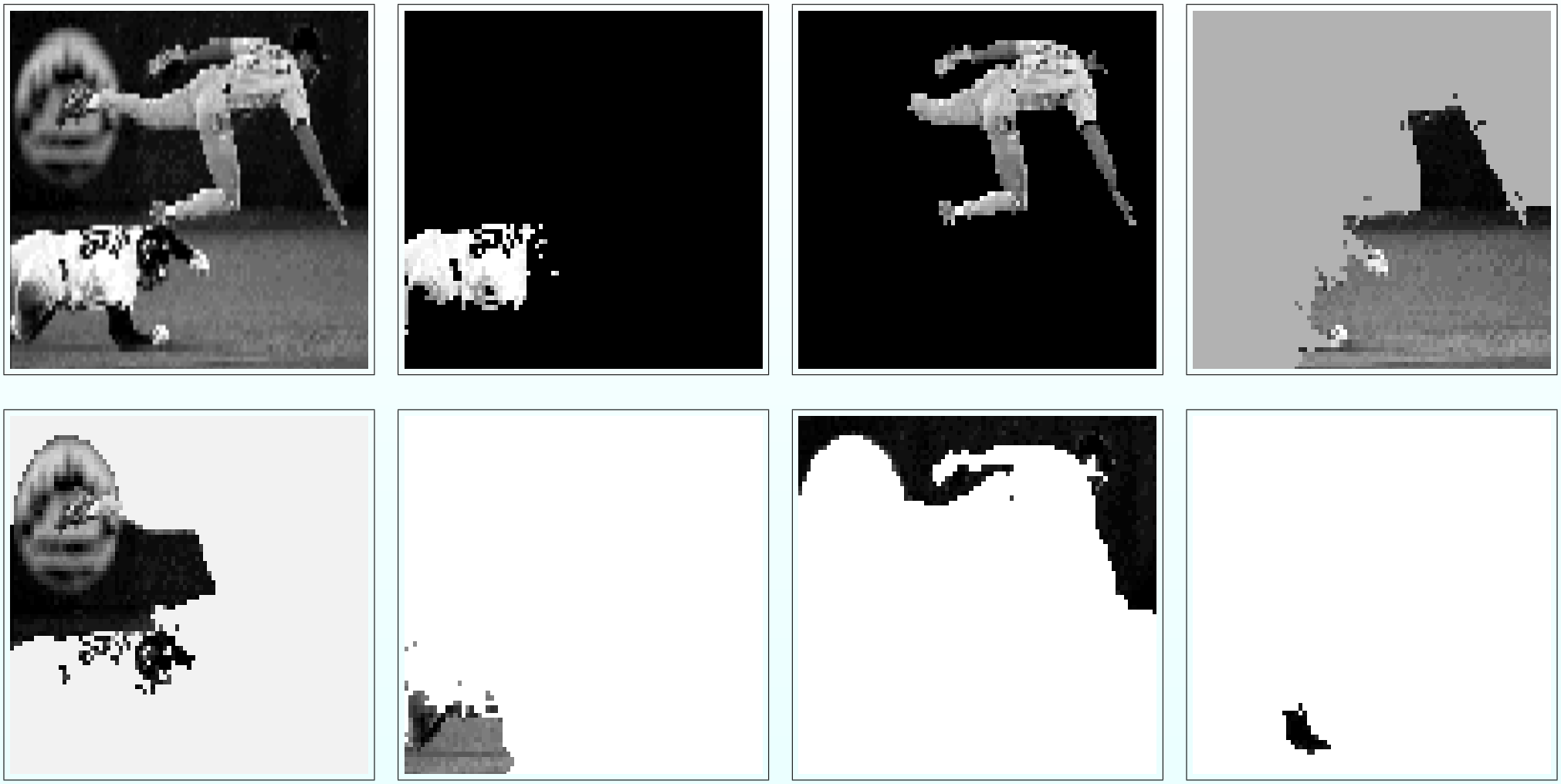
$$\min_c H^{\text{NCut}}(c, W) = \min_y \frac{y^t(D-W)y}{y^t y}$$

$$\text{subject to} \quad y \in \left\{1, \frac{-\sum_{x_i>0} d_i}{\sum_{x_i<0} d_i}\right\}$$

where $D = diag(d_1, \ldots, d_n)$ and $d_i = \sum_{j=1}^{n} w_{ij}$

$x \in [-1, 1]^n$ is the relaxation of the variable vector $c \in \{-1, 1\}^n$.

Example Normalized Cut



Shi & Malik, 2000

Part II: Optimization Methods

Given: cost function to rank different object partitions

Robustness: cost function depends on noisy data

$\Rightarrow$ partition with minimal costs is a r.v. of noisy data

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Candidate Solutions: typical or averages of partitions

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Principle: (Jaynes 1957) **Estimate expectation values of optimization variables which are maximally non-committal with respect to missing data.**

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Algorithm: Markov Chain Monte Carlo or Mean Field Approximation

Metropolis Sampler for Clustering

Input: n objects, cost function $H(c)$
Output: partition $c:$ objects $\rightarrow$ clusters

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Output: partition $c:$ objects $\rightarrow$ clusters

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Variants: Gibbs sampling, importance sampling, (competitive!?)

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$\Rightarrow$ Gibbs distribution $\mathbf{P}(\tilde{\theta}) = \exp\left(-\big(H(c) - F(\tilde{\theta}) \big) / T \right)$

Algorithm Design for Maximum Entropy Estimation

Calculate the Gibbs distribution of object partitions.

$\Rightarrow$ expectation values of optimization variables

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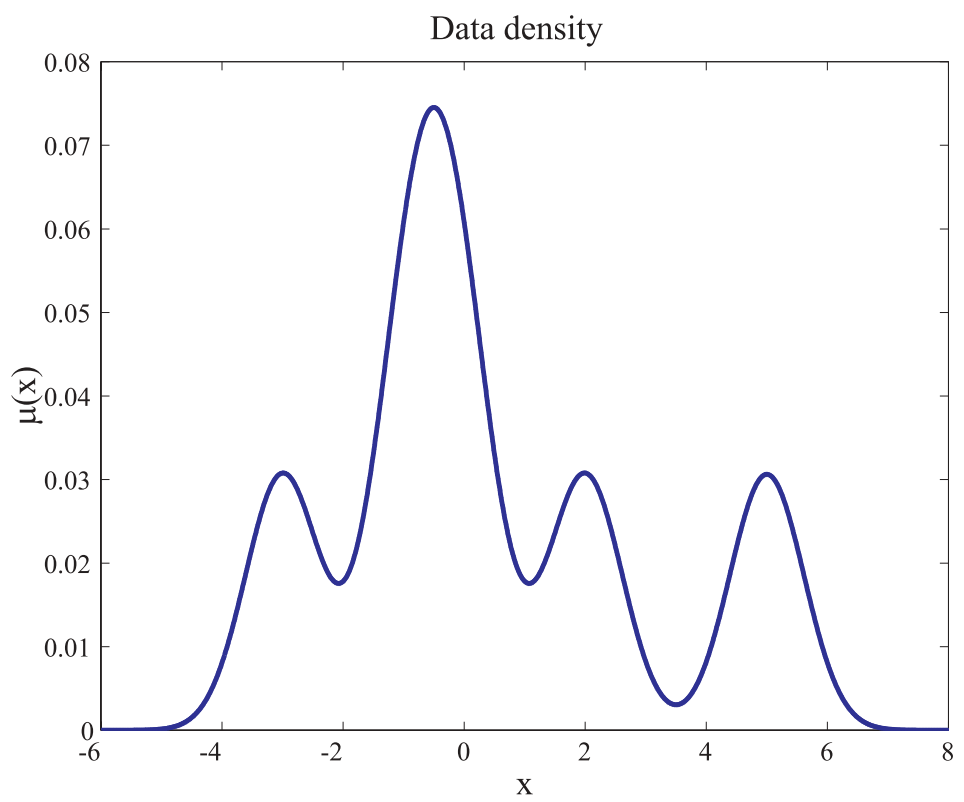
EM-like Iteration: Both steps are iterated until convergence to a local maximum of the entropy is achieved.

Phase Transitions in K-means Clustering

1-dim. mixture model; track centroids as a function of temperature.



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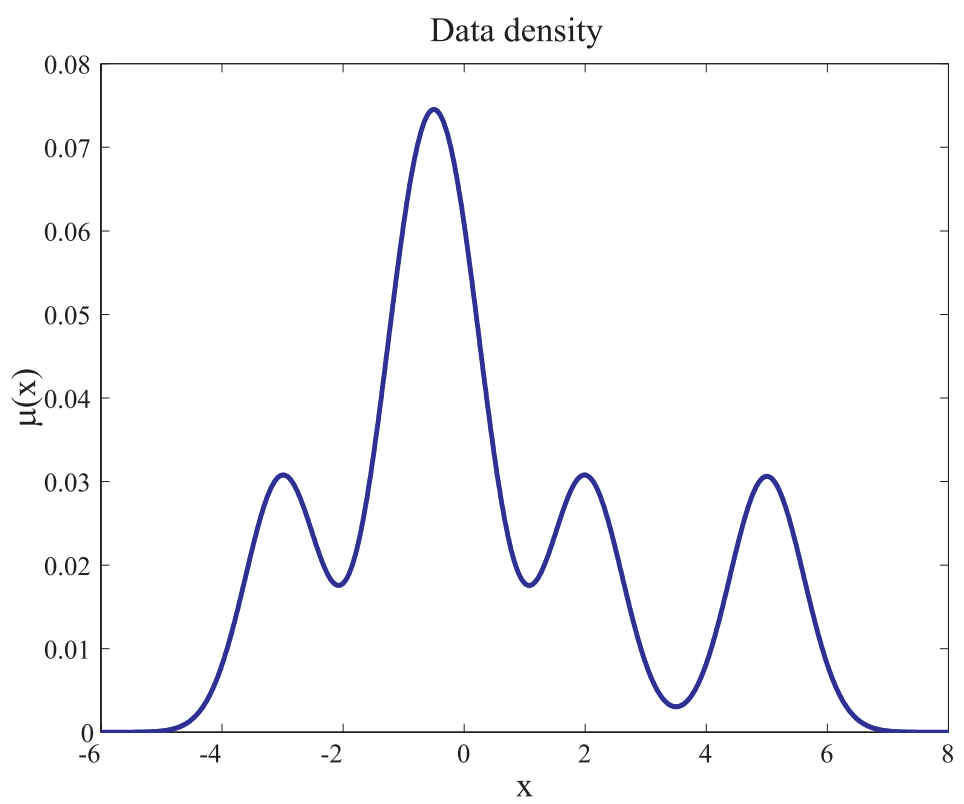

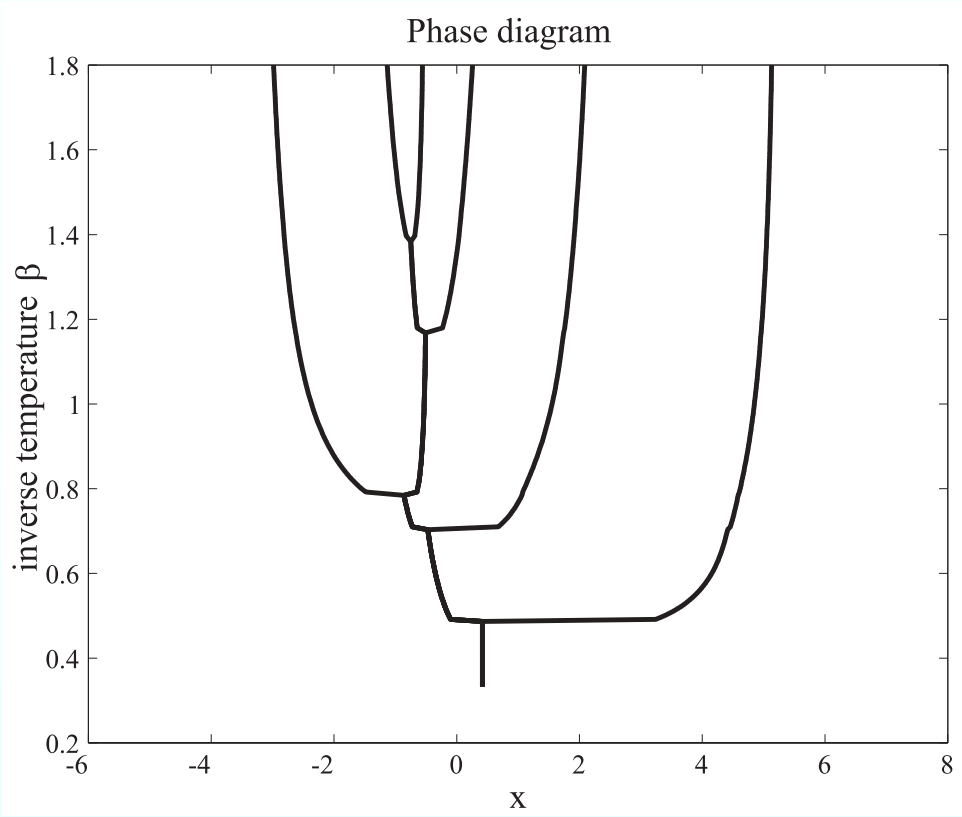

EM Update Scheme for PDC

E-step

$$h_{i\nu} = -\log p_\nu - \sum_j n_{ij} \log \left(\sum_\alpha p_{\alpha|\,\nu} \tilde{G}_\alpha (j) \right)$$

$$q_{i\nu} = E\left[M_{i\nu}\right] \propto \exp\left(-\frac{h_{i\nu}}{T}\right)$$

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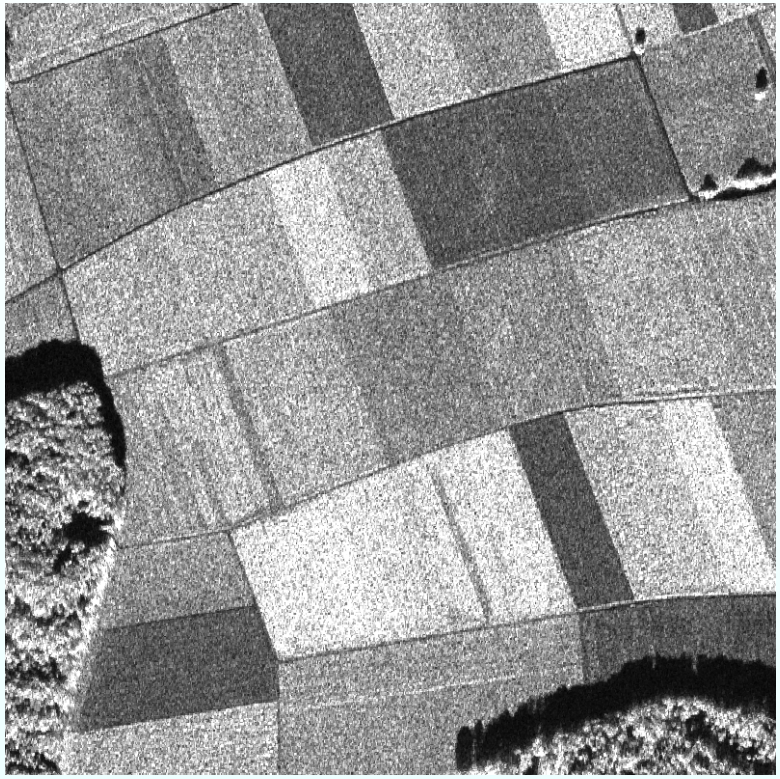
M-step

$$p_\nu = \frac{1}{n} \sum_i q_{i\nu}$$

No closed formula for $p_{\alpha|\,\nu}$, nor for μ_α! We iteratively optimize pairs $p_{\alpha_1|\,\nu}$, $p_{\alpha_2|\,\nu}$ until convergence. Interval bisection is used to optimize Gaussian means μ_α.

Cooling Dynamics of PDC



Level of randomness decreases while lowering the computational temperature.

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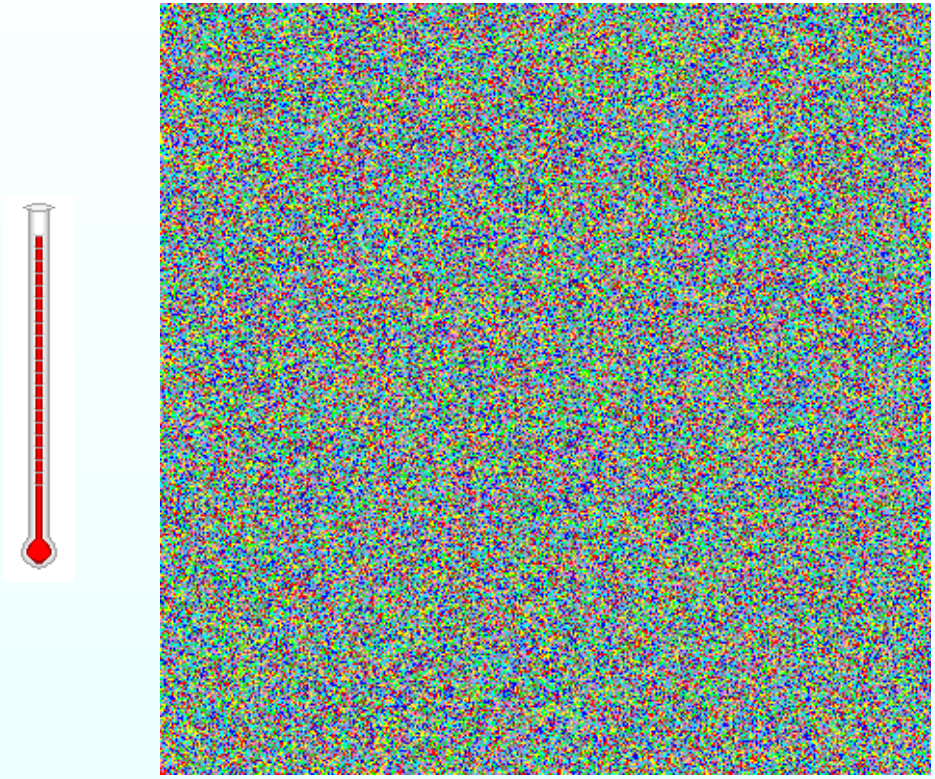

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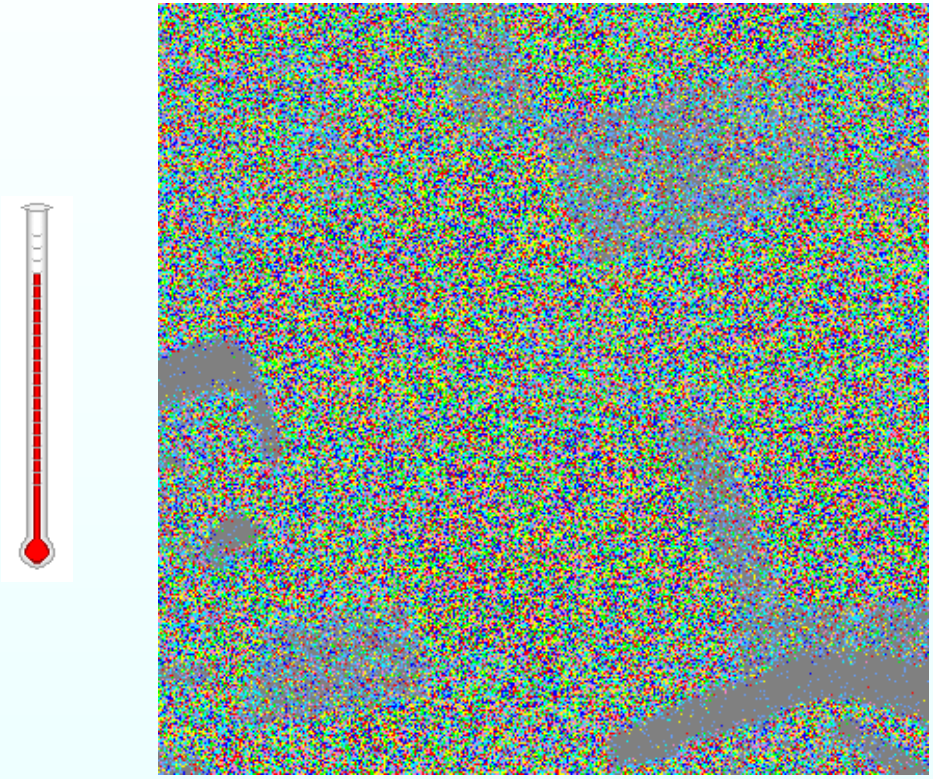

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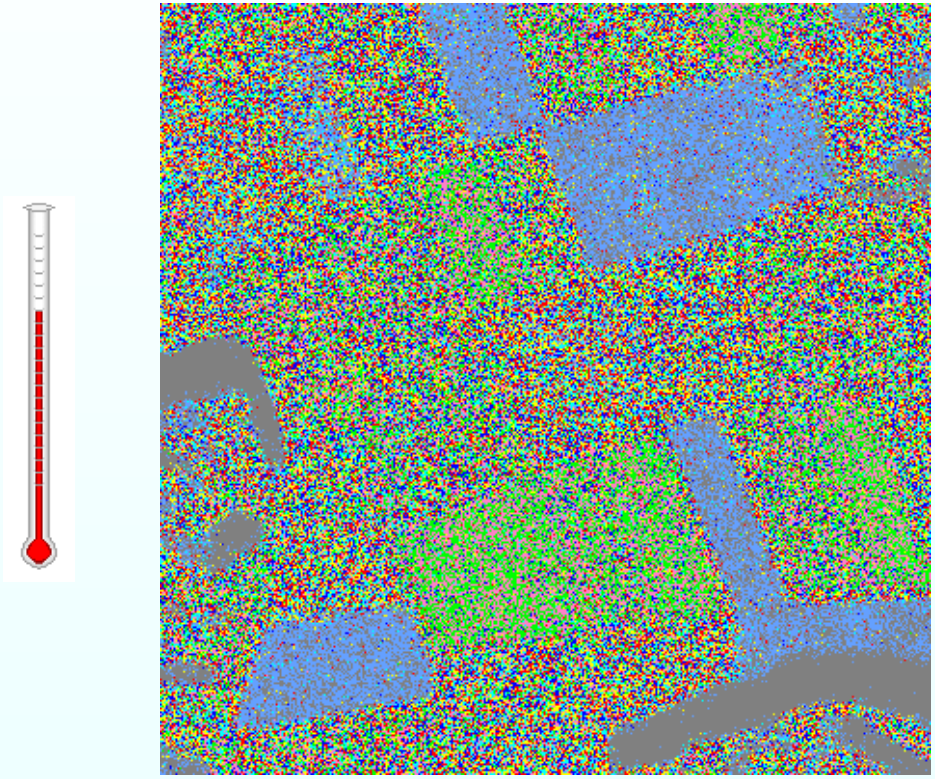

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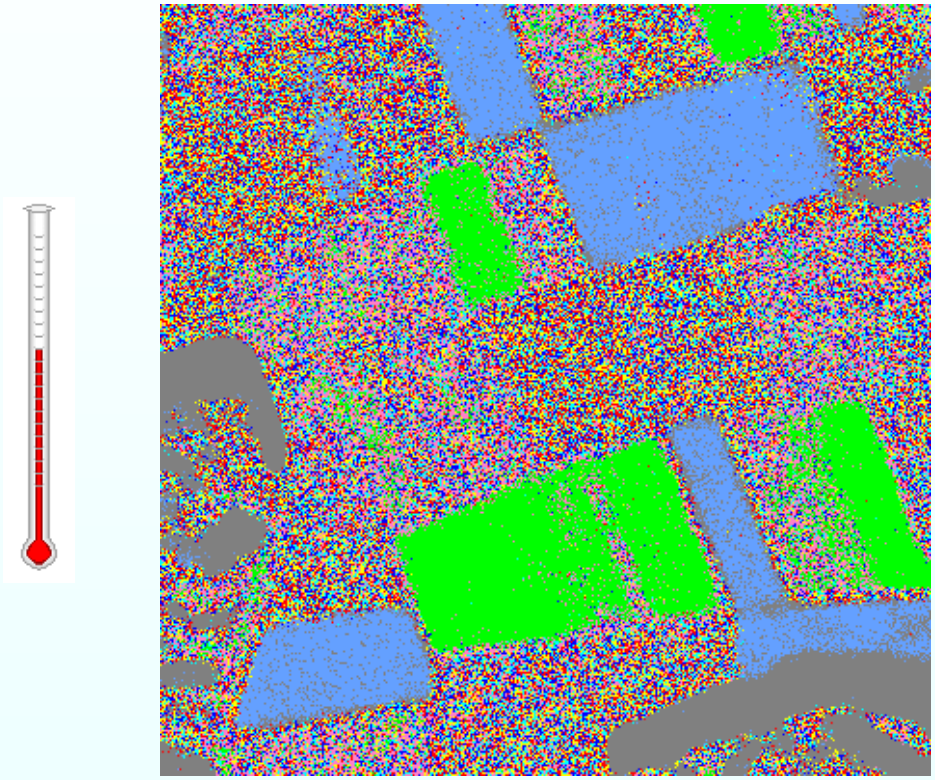

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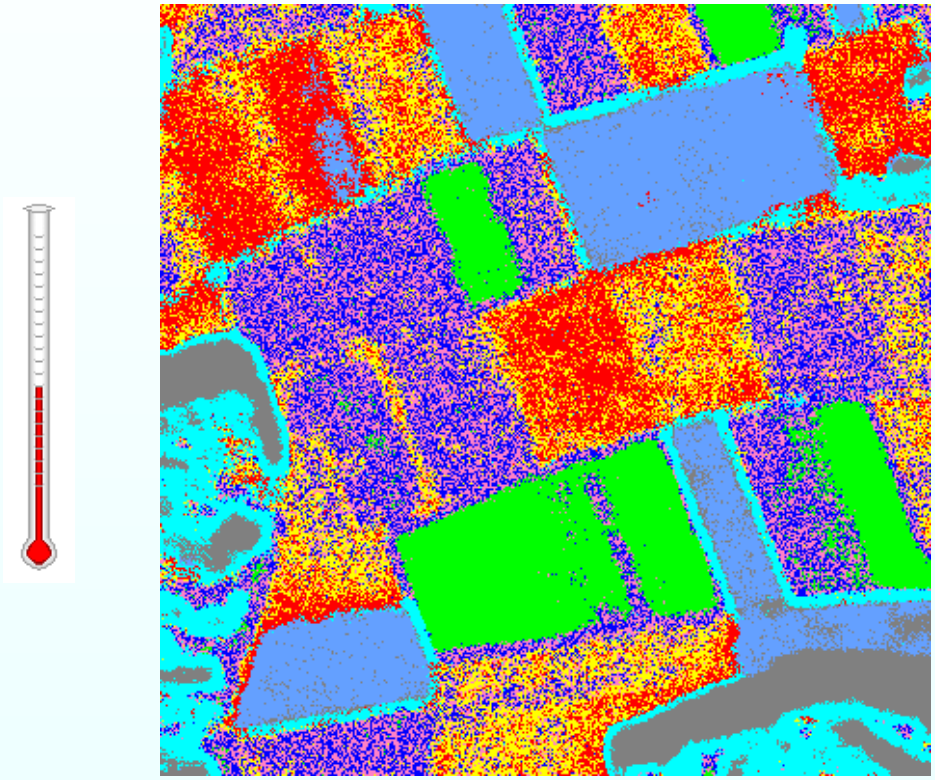

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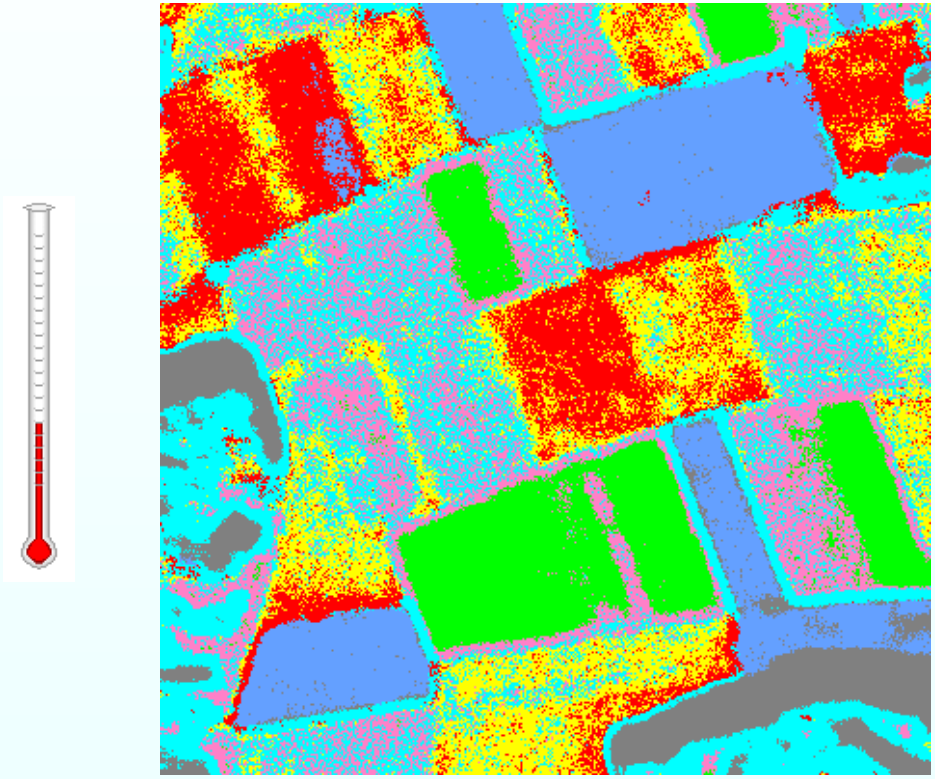

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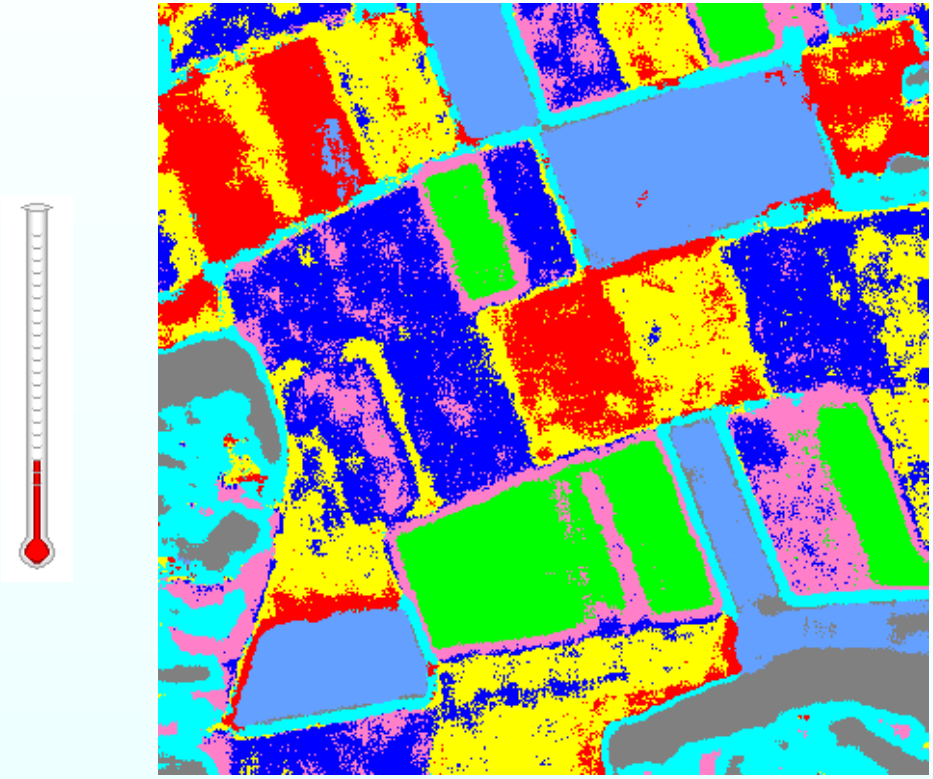

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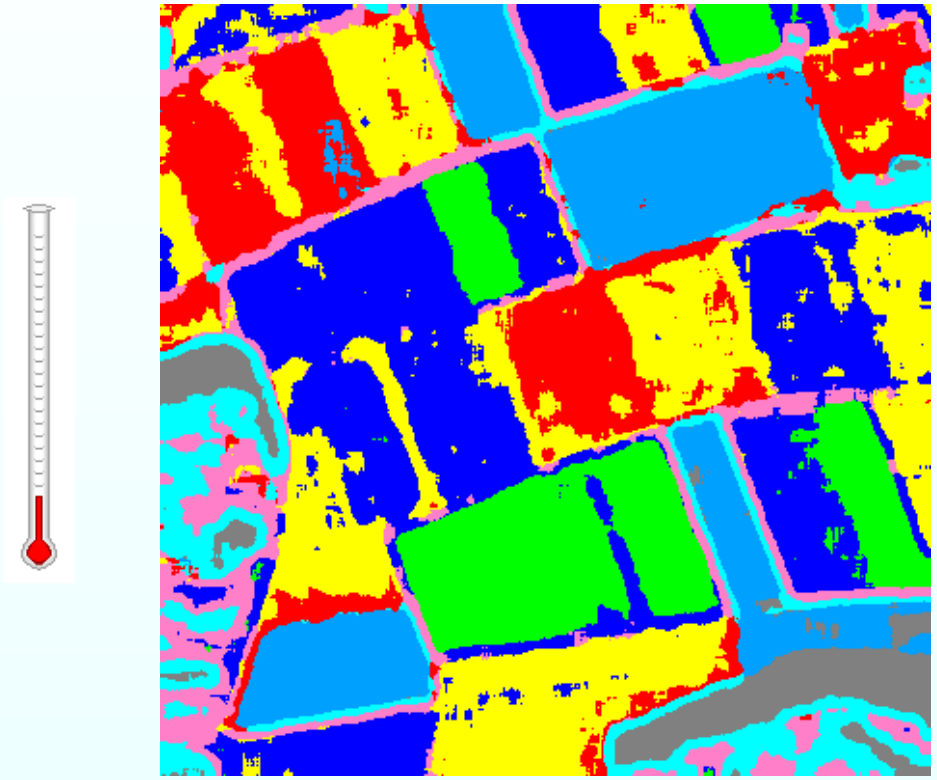

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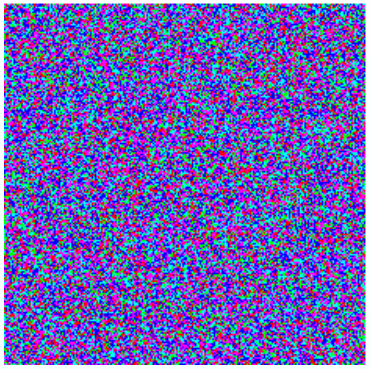

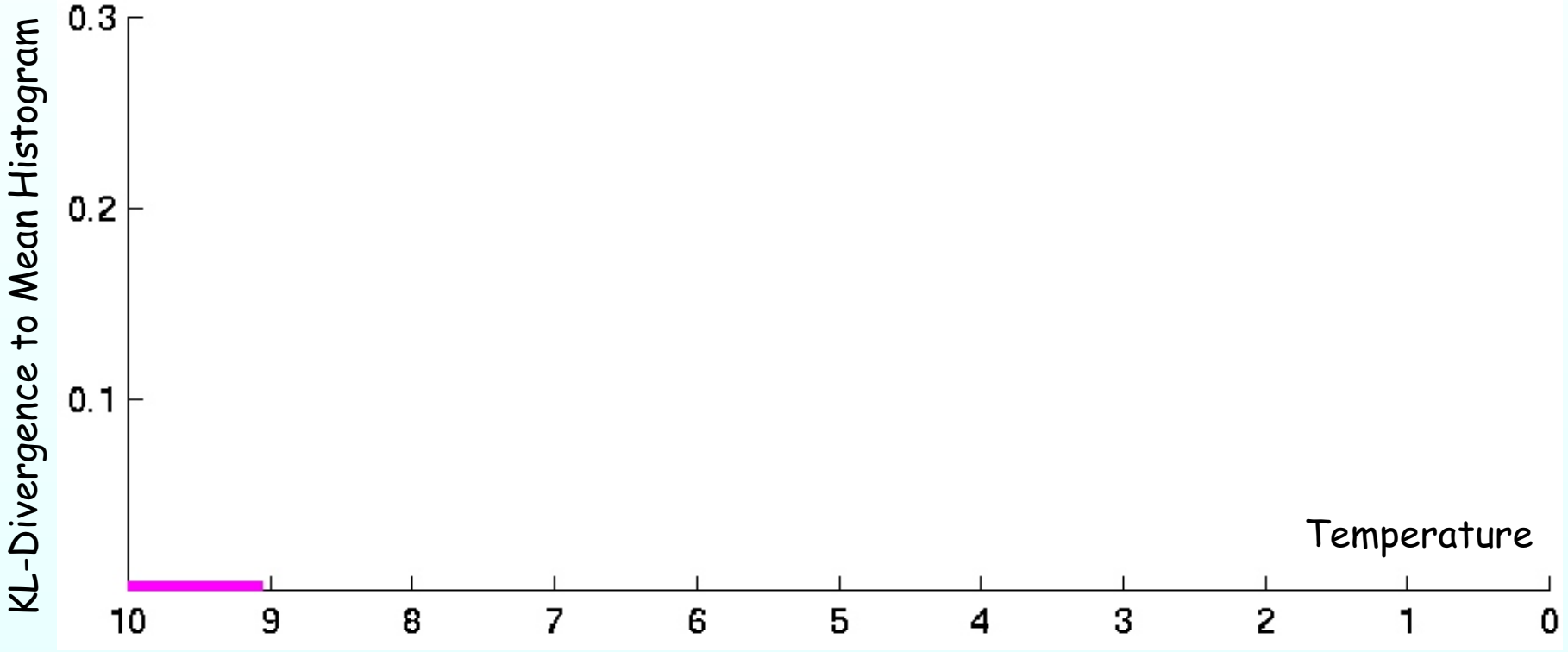

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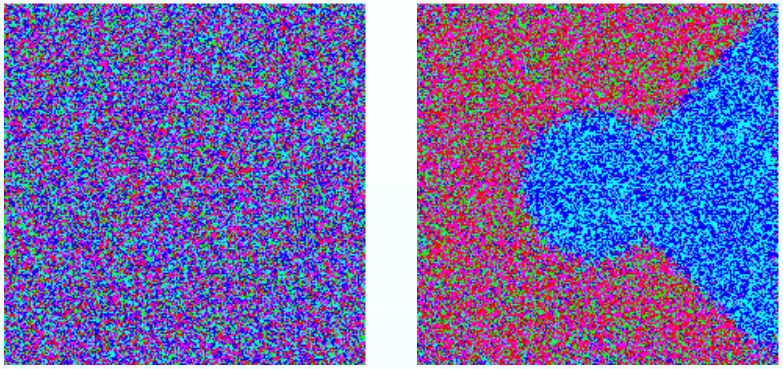

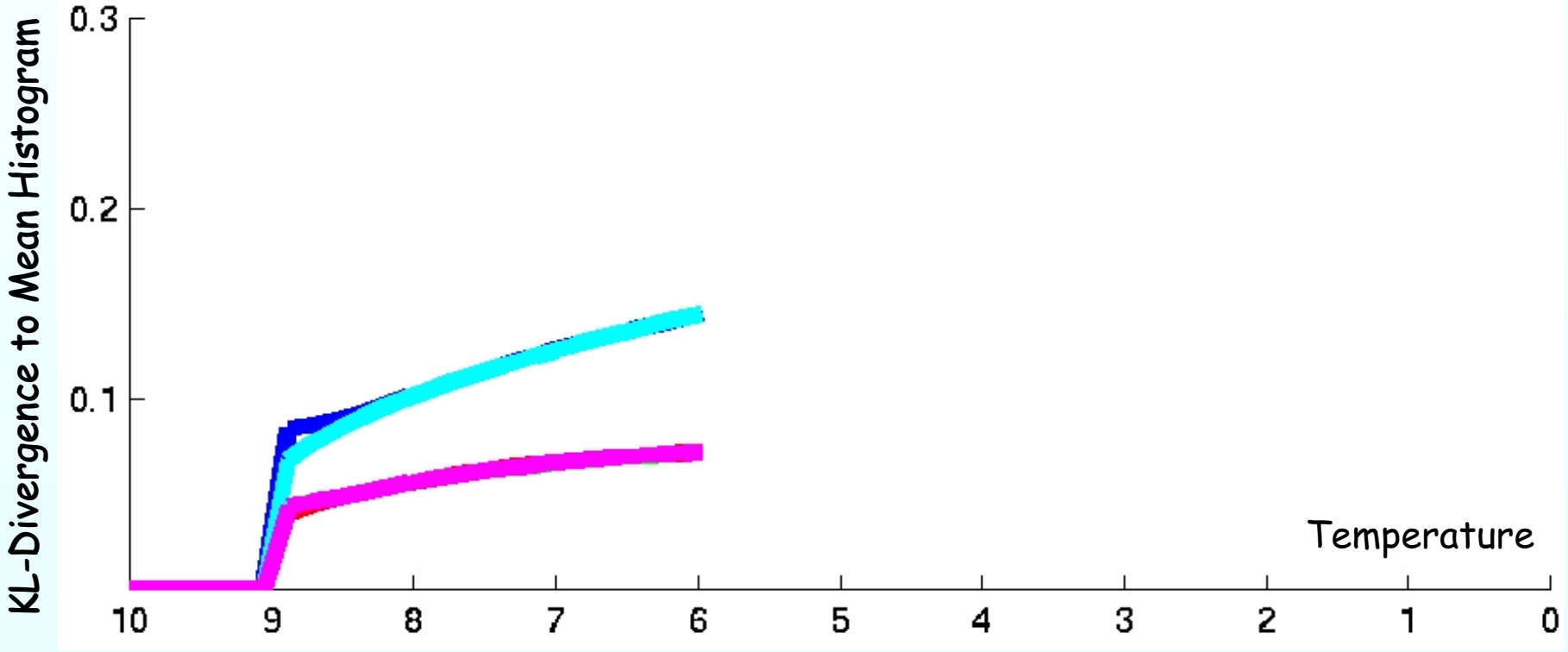

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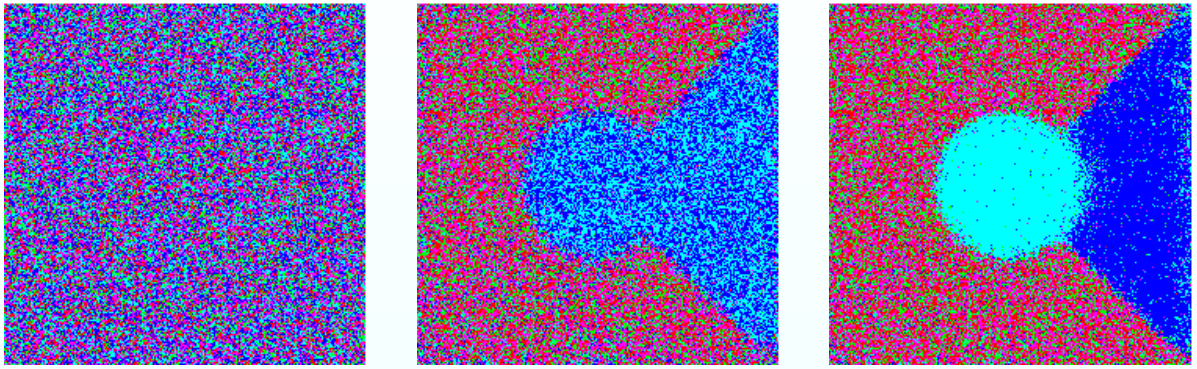

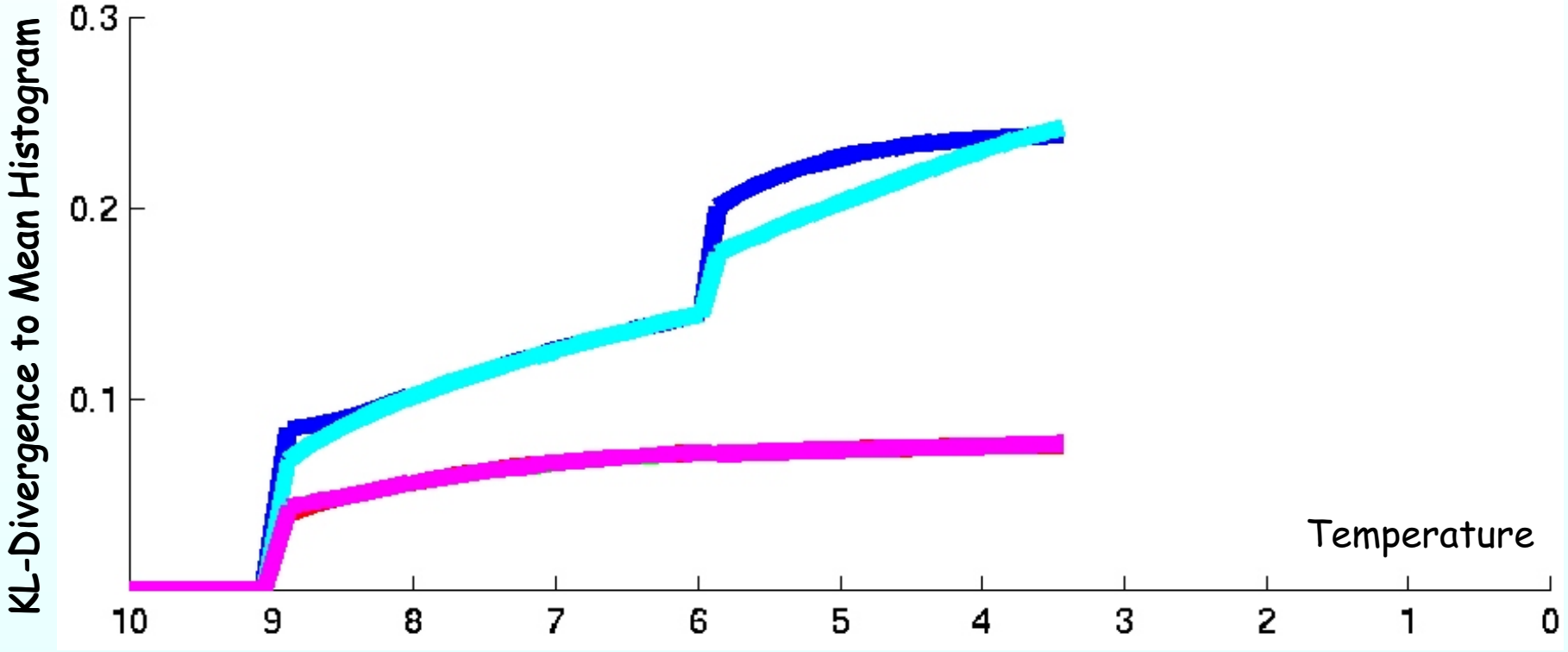

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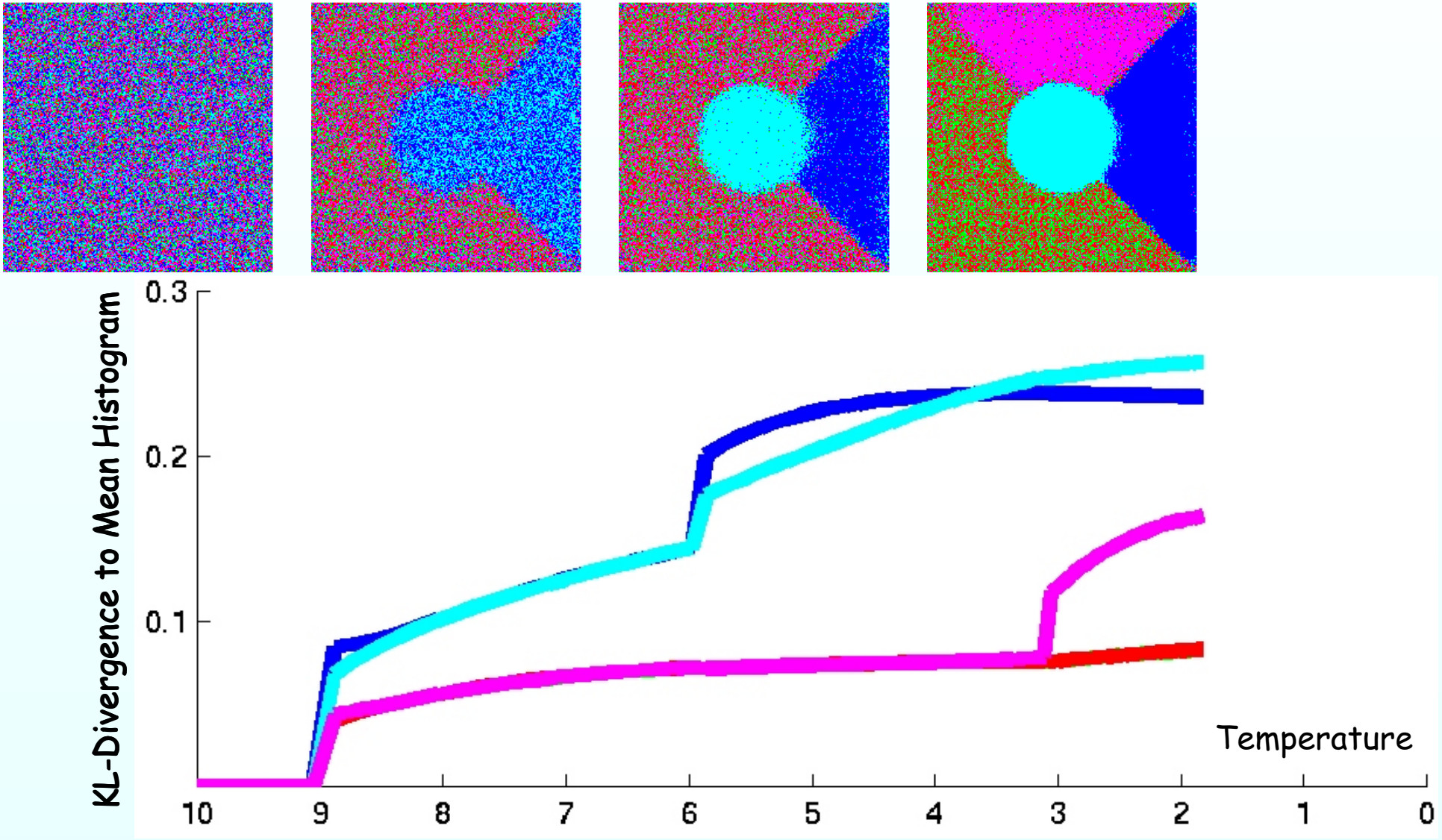

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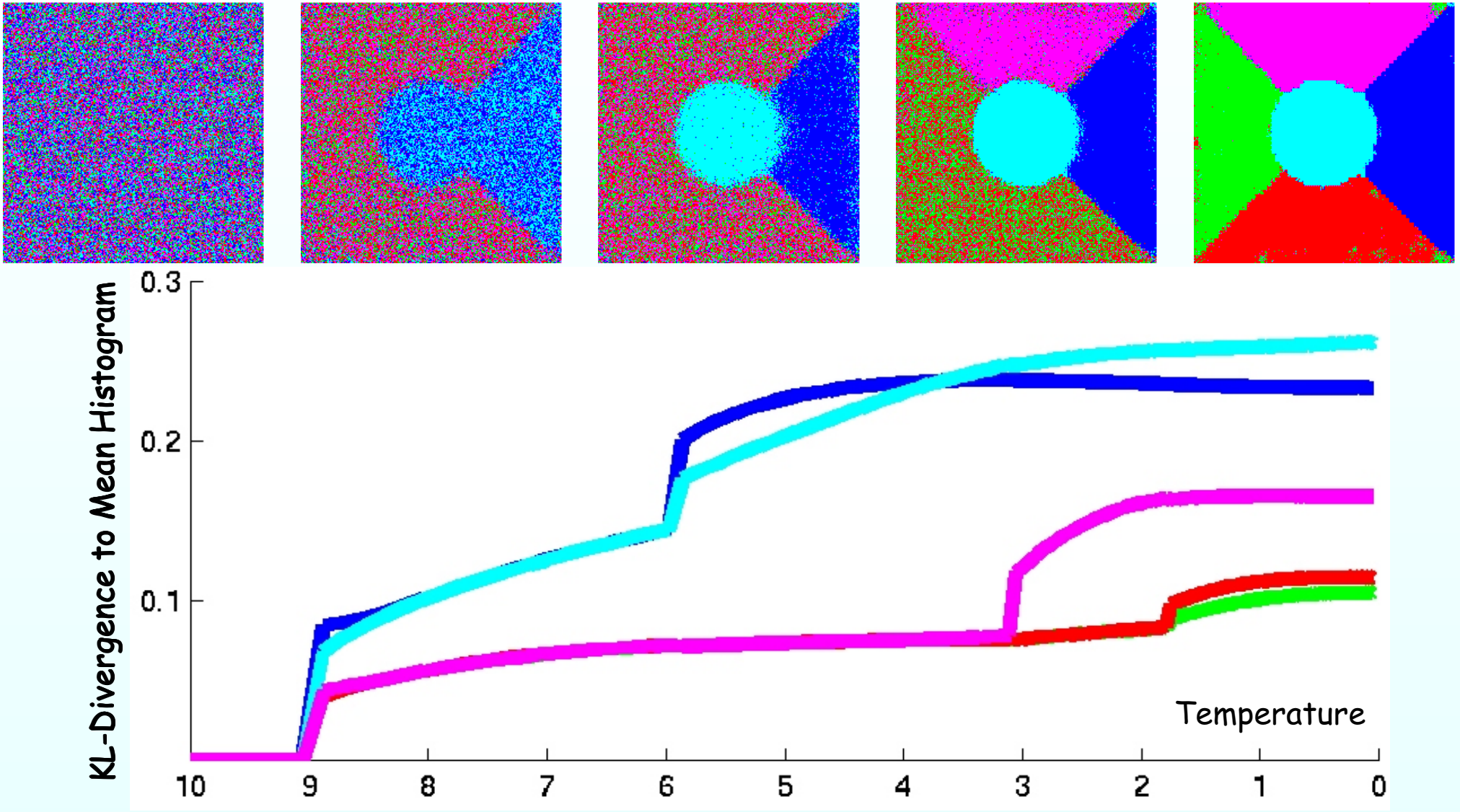
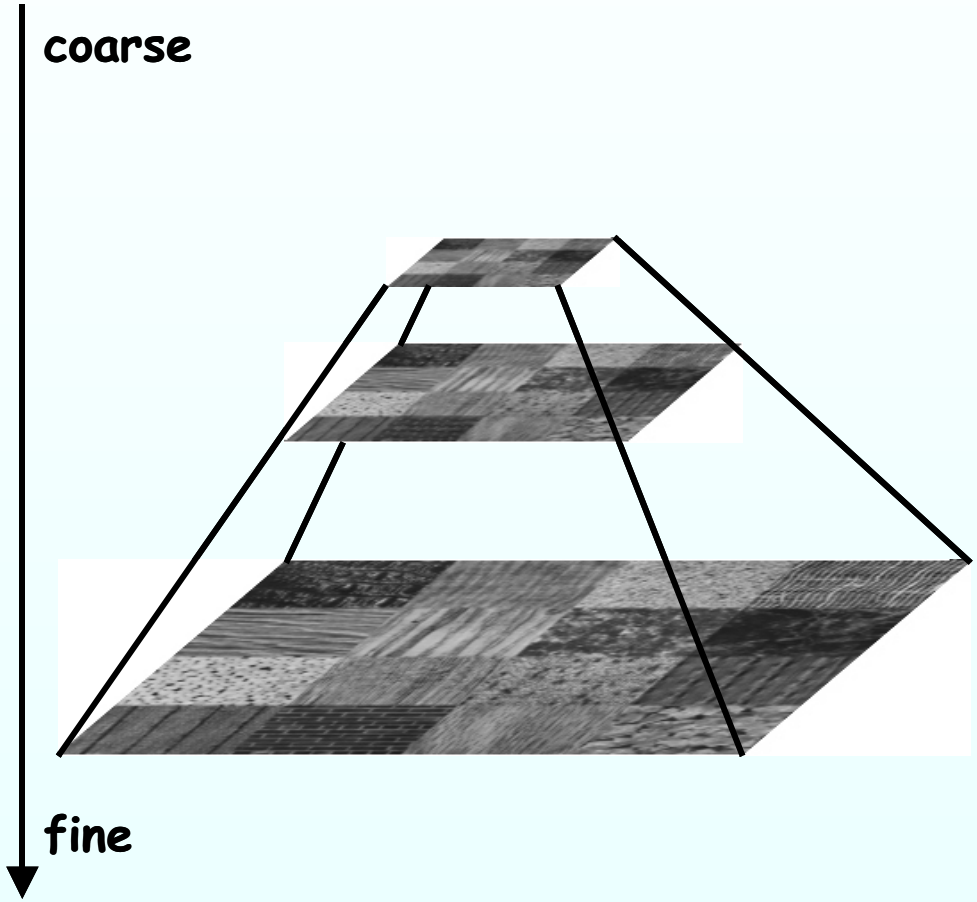


Scales in Vision and their Coupling

Coarsening
Variable Space



Resolution Pyramid

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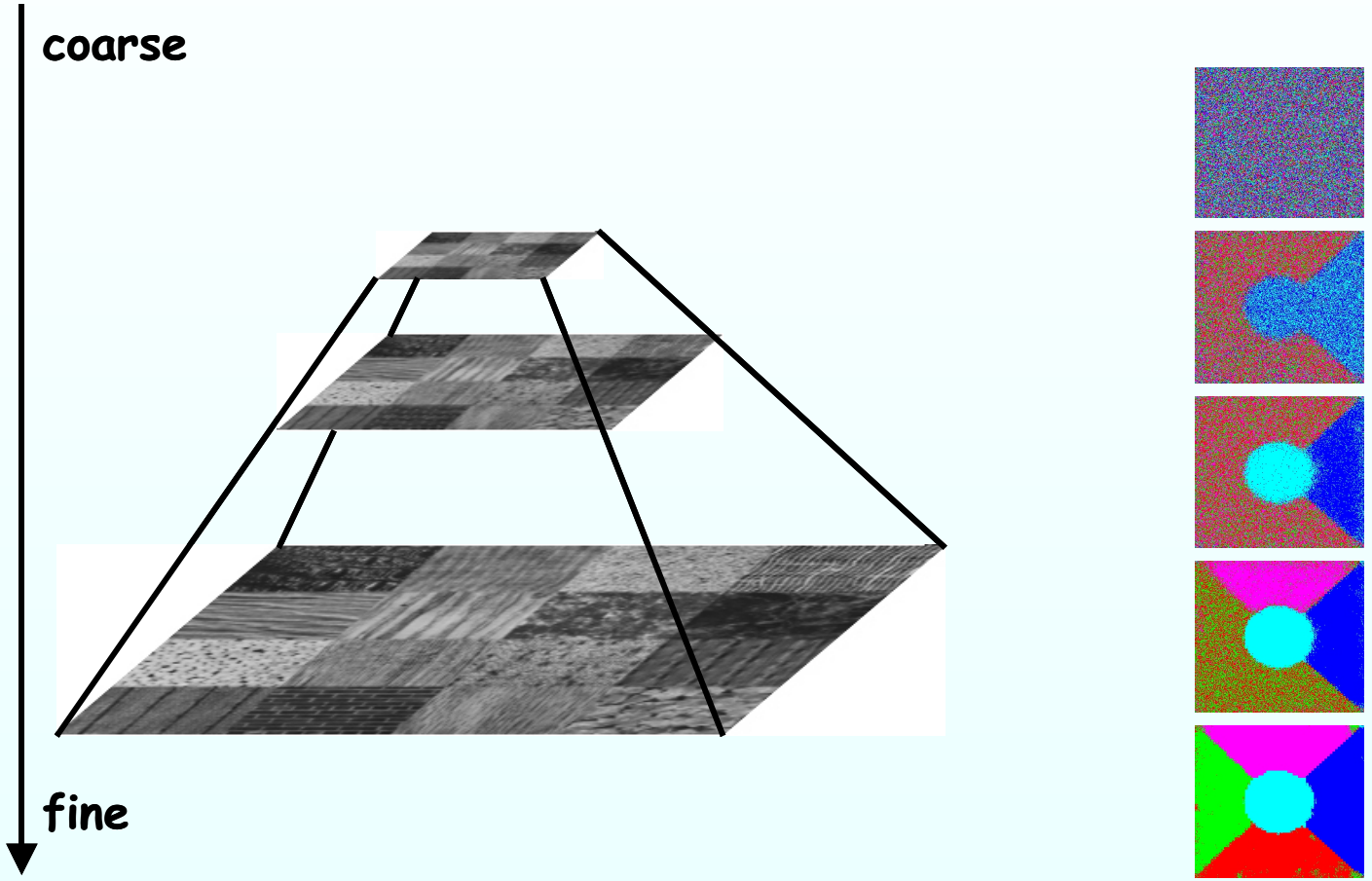
Coarsening
Optimization Criterion



Resolution Pyramid

Raising Temperature

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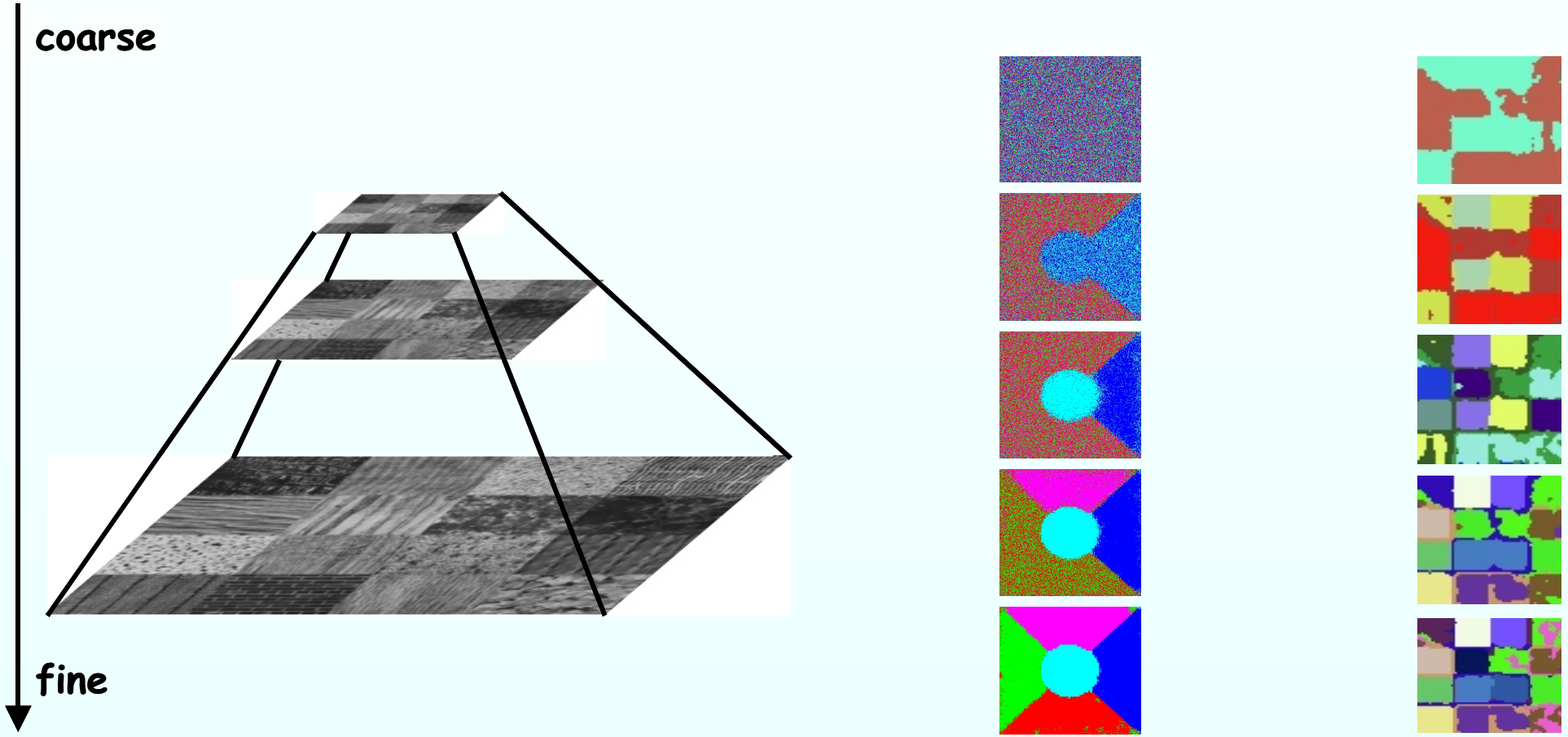
Model Order



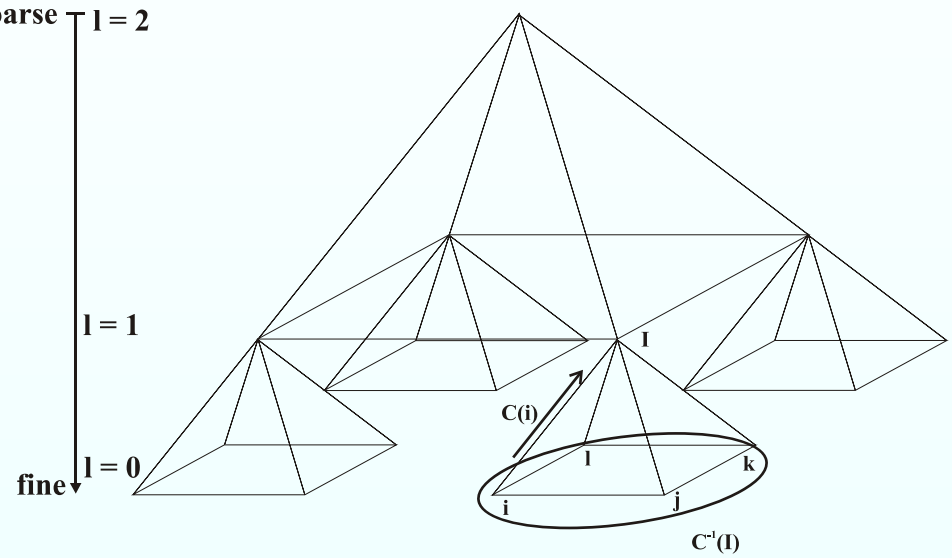
Resolution Pyramid

Raising Temperature

Decr. Number of Segments

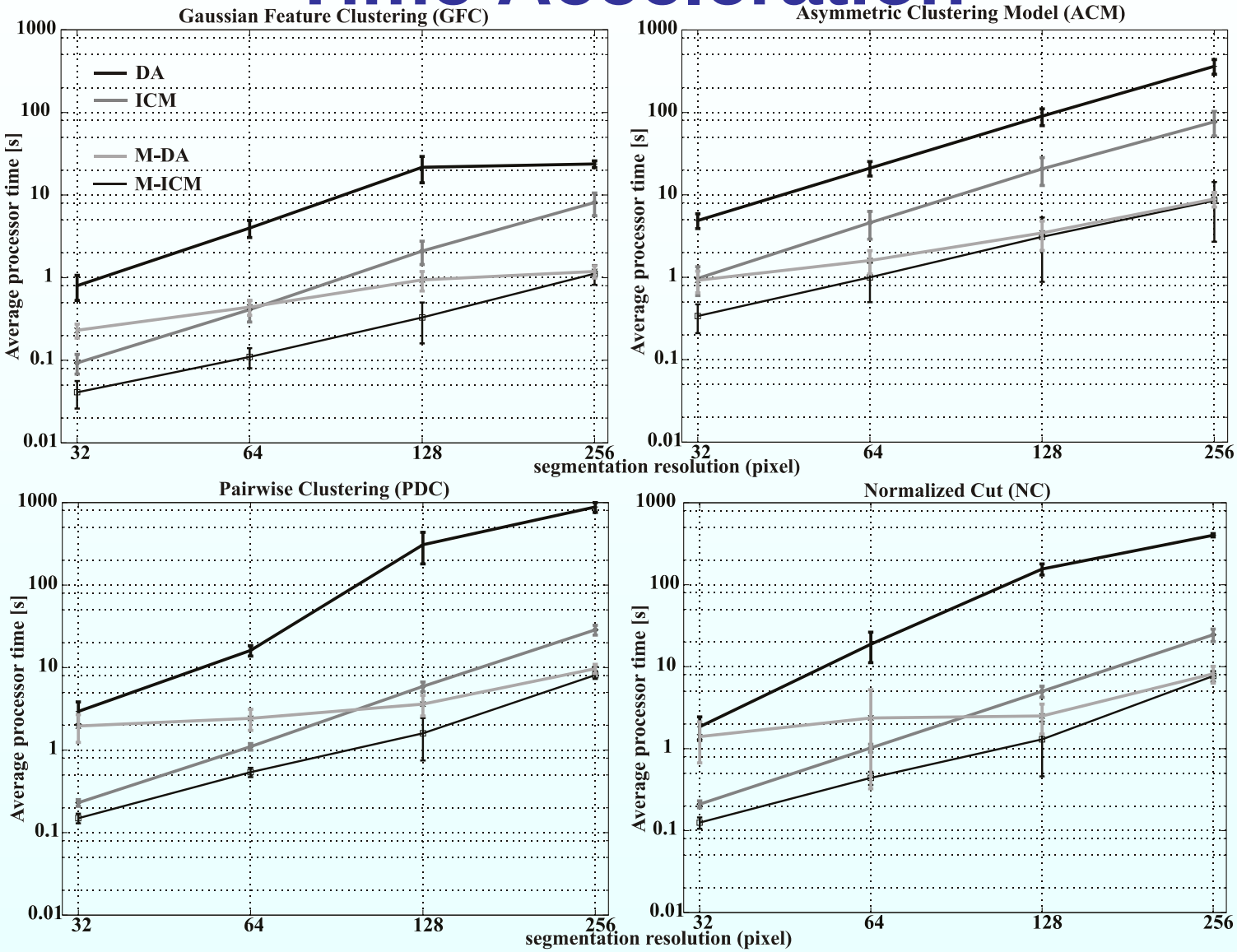
Multi-Scale Optimization

- Coarser set of image sites $S^\ell = \{s_1^\ell, \ldots, s_{n_\ell}^\ell\}$
- Prolongation operator P_ℓ : $S^{\ell+1} \rightarrow S^\ell$ defines map between two resolution levels

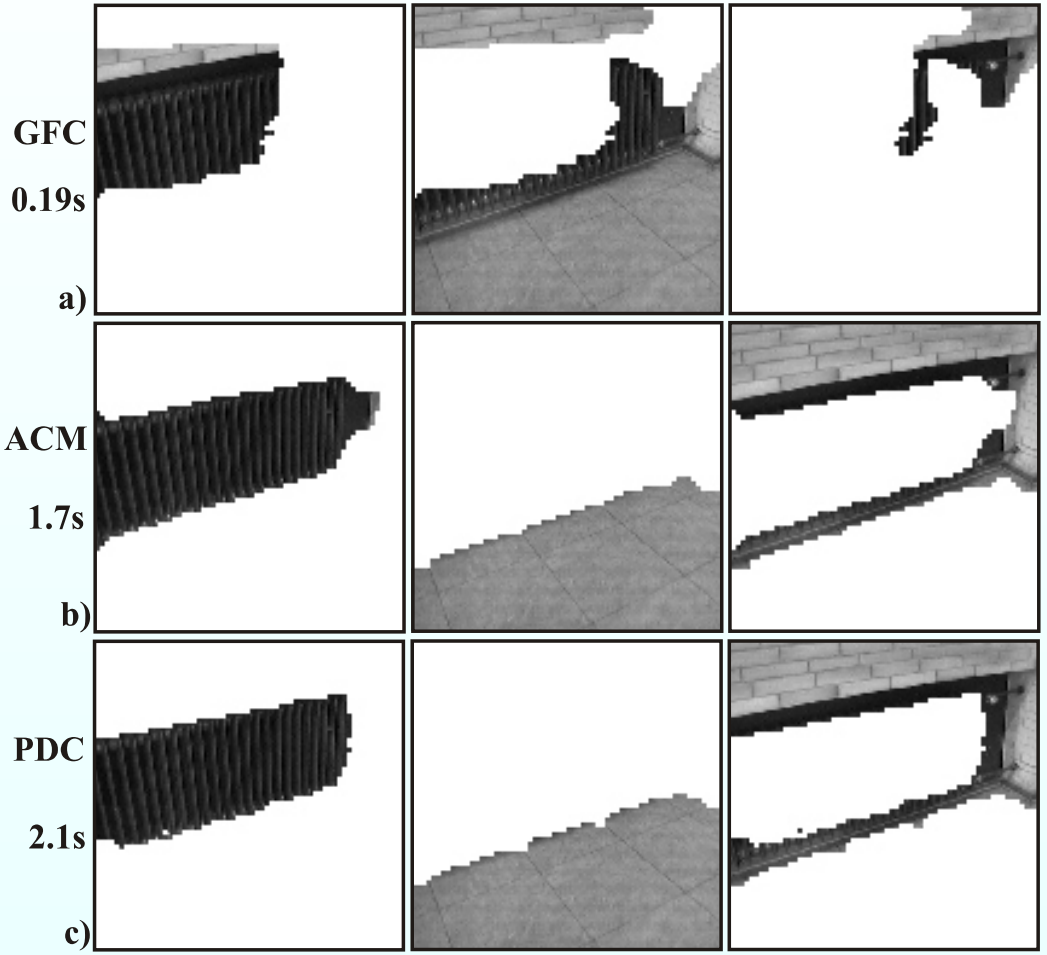


- Multiscale Operator $H^{\ell+1}(S^{l+1}) = \Gamma(H^\ell) = H^\ell(P(S^{\ell+1}))$ maps the value of the objective function

Time Acceleration



Example Multiscale optimization



Part III: Cluster Validation

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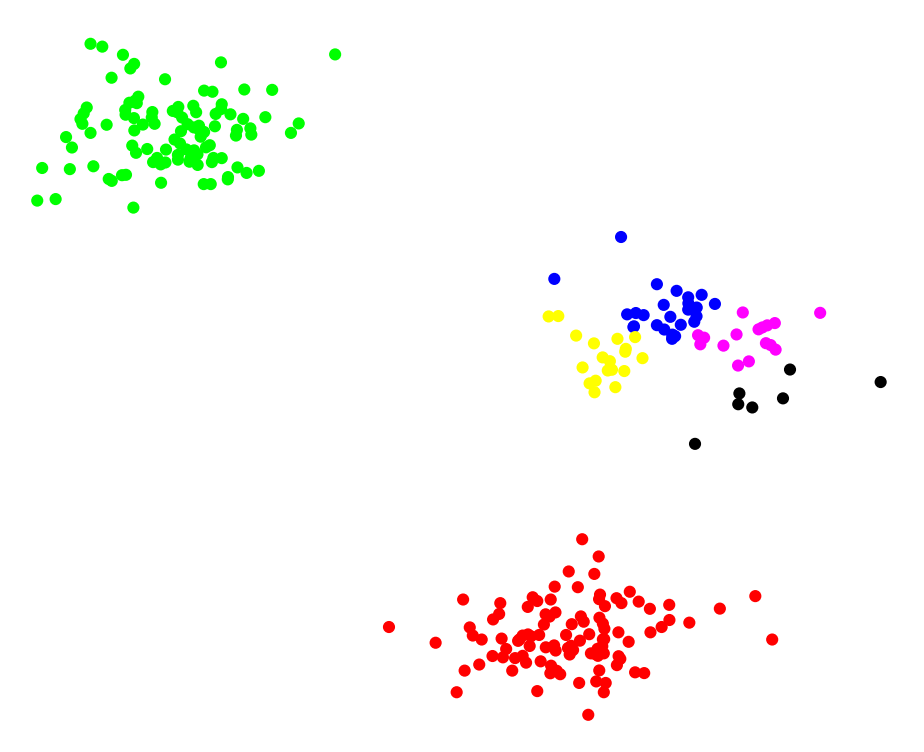

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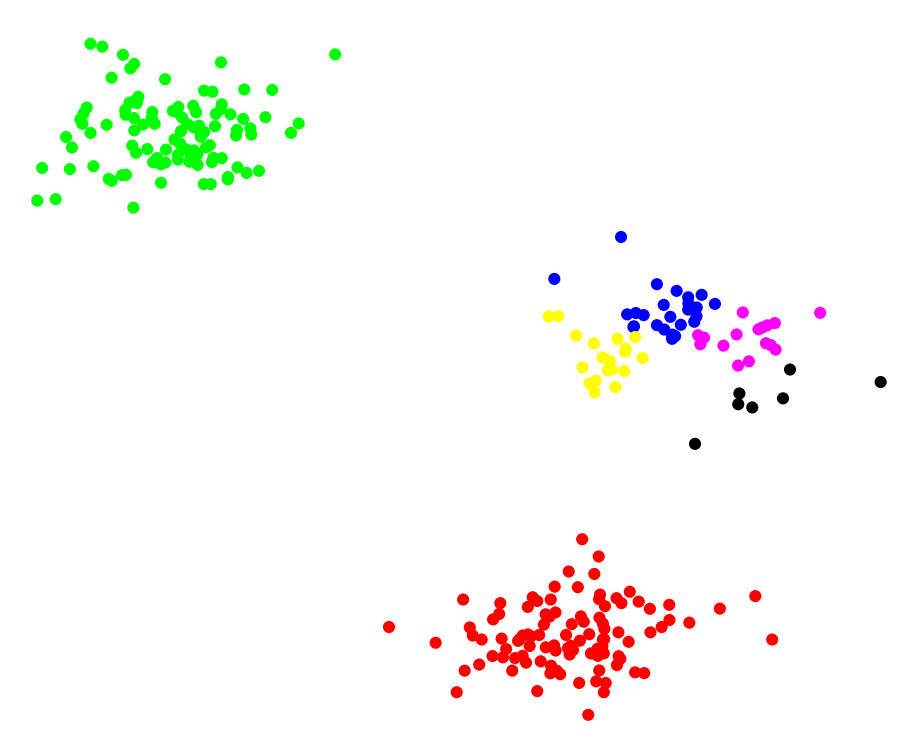

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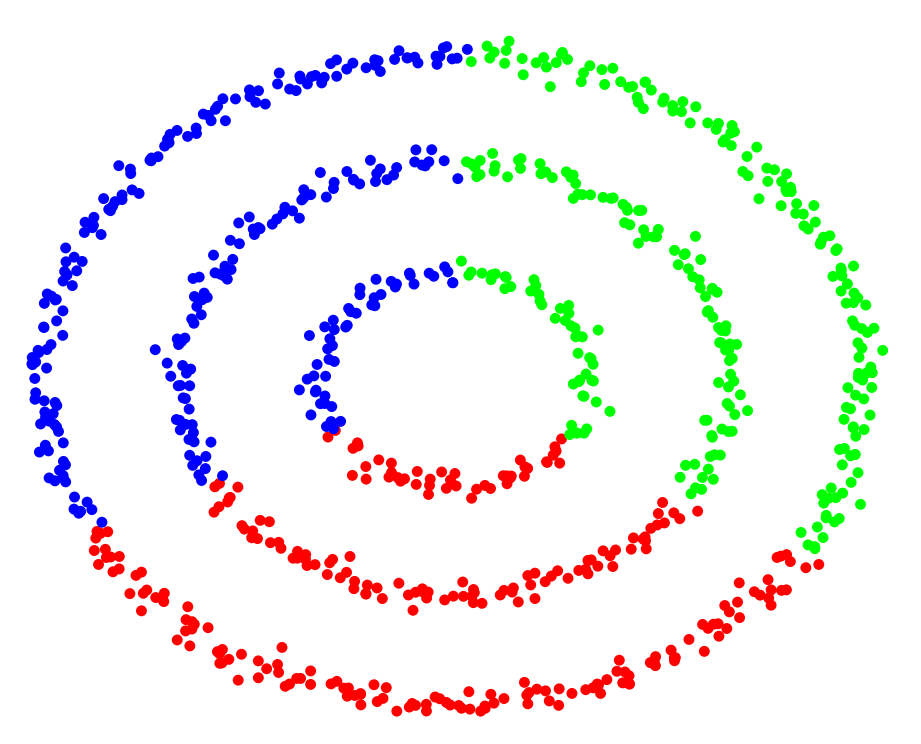

(b) Inappropriate model type.

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Important Question:
What is the appropriate number of clusters k for my data?

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Important Question:
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General approach: Measure quality for different k!

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Add a complexity term to the neg. log-likelihood in model-based clustering!

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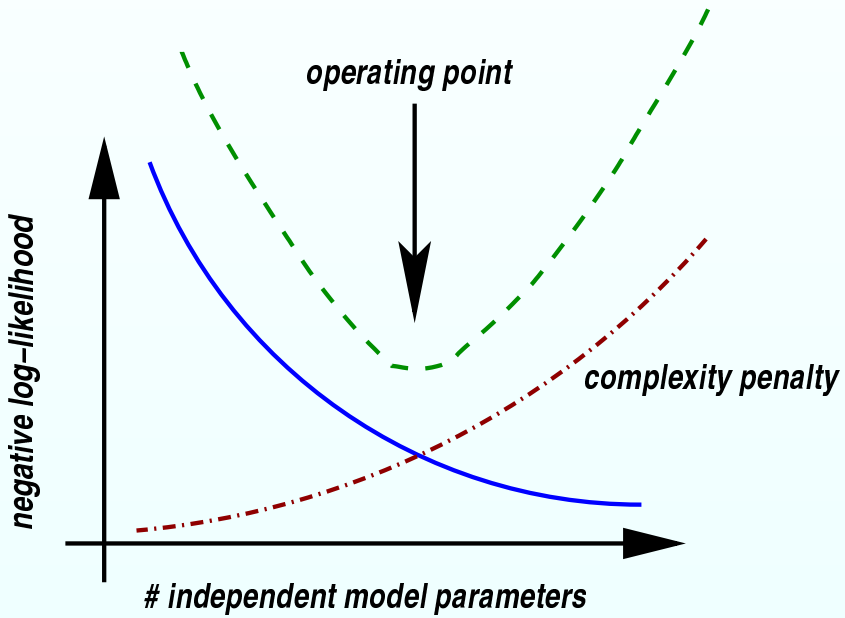
Idea formalized e.g. by

- Rissanen's **Minimum Description Length**.
- Schwartz's **Bayesian Information Criterion**.

Underlying Principle



The (neg.) log-likelihood decreases with increasing model complexity. Correct this with a complexity penalty.

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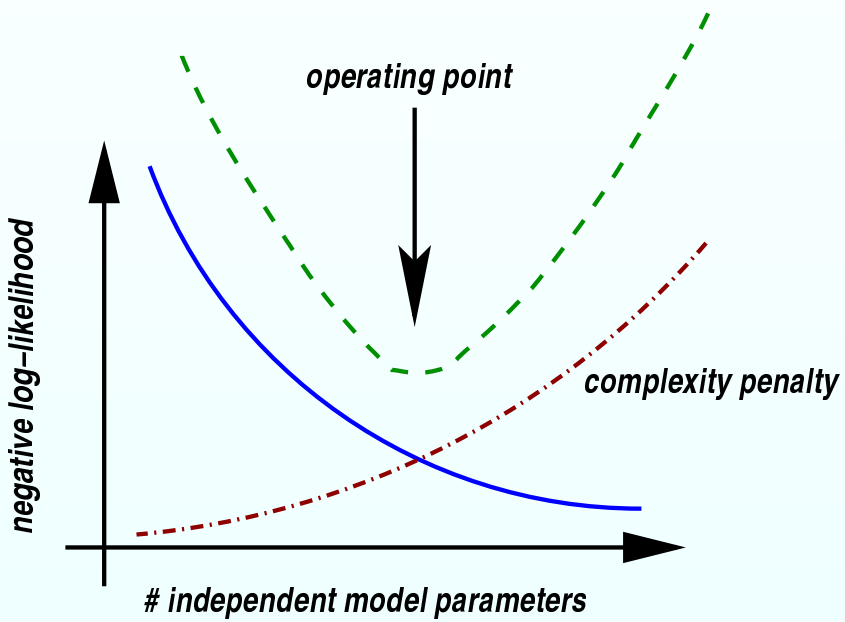

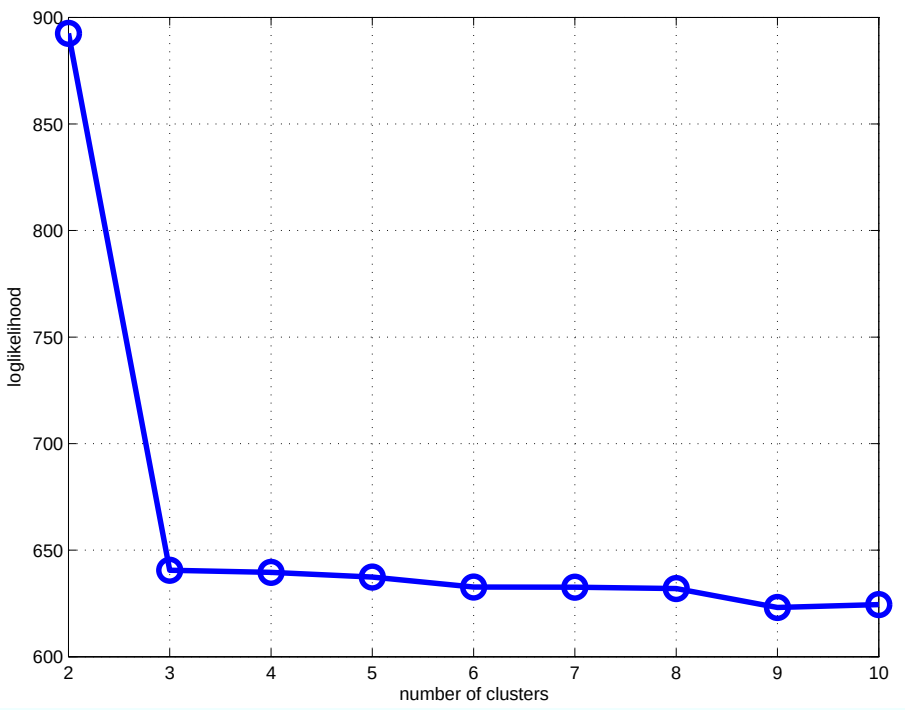

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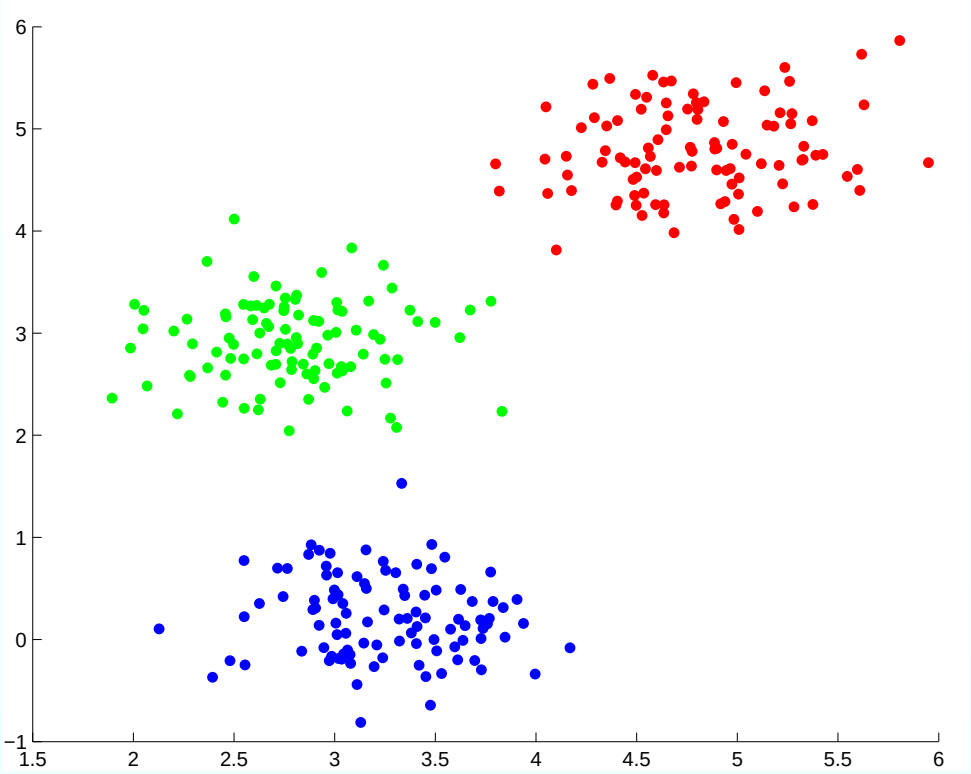
Minimum Description Length *(Rissanen,1978)*

MDL minimizes the overall description length of the data where the description consists of the data and the model parameters.

$$\hat{k} := \underset{1 \le k \le K_{\max}}{\operatorname{argmin}} \left(\underbrace{-\log(\hat{\mathrm{p}}(\mathbf{X} \mid \hat{\Phi}_k))}_{\text{negative loglikelihood}} + \underbrace{\frac{1}{2} k' \log n}_{\text{complexity penalty}} \right)$$

where k' is the number of independent parameters in the model Φ_k.

BIC Validation of a Mixture



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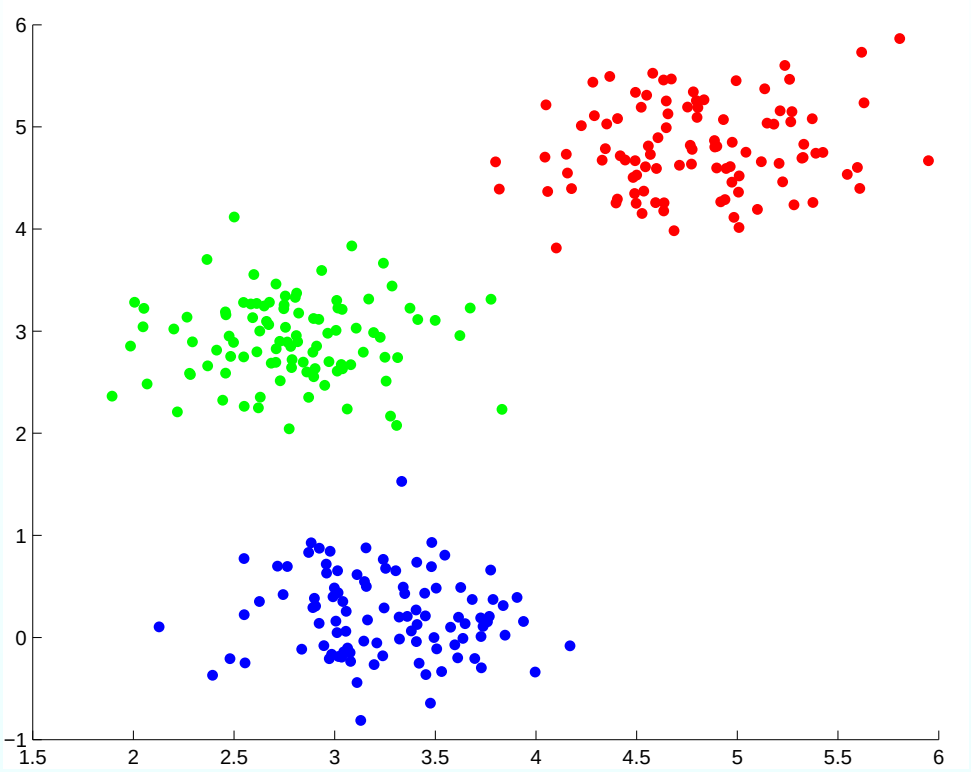

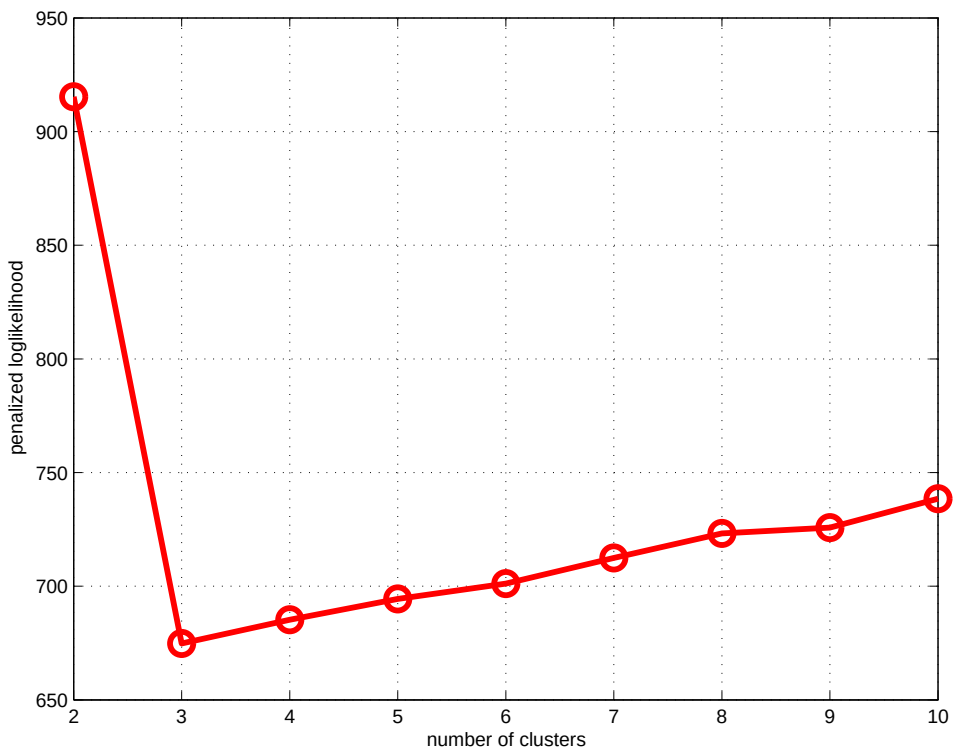

Stability-based Validation *(Lange, Braun, Roth, JB,2002)*

- Many validation methods incorporate a structural bias!

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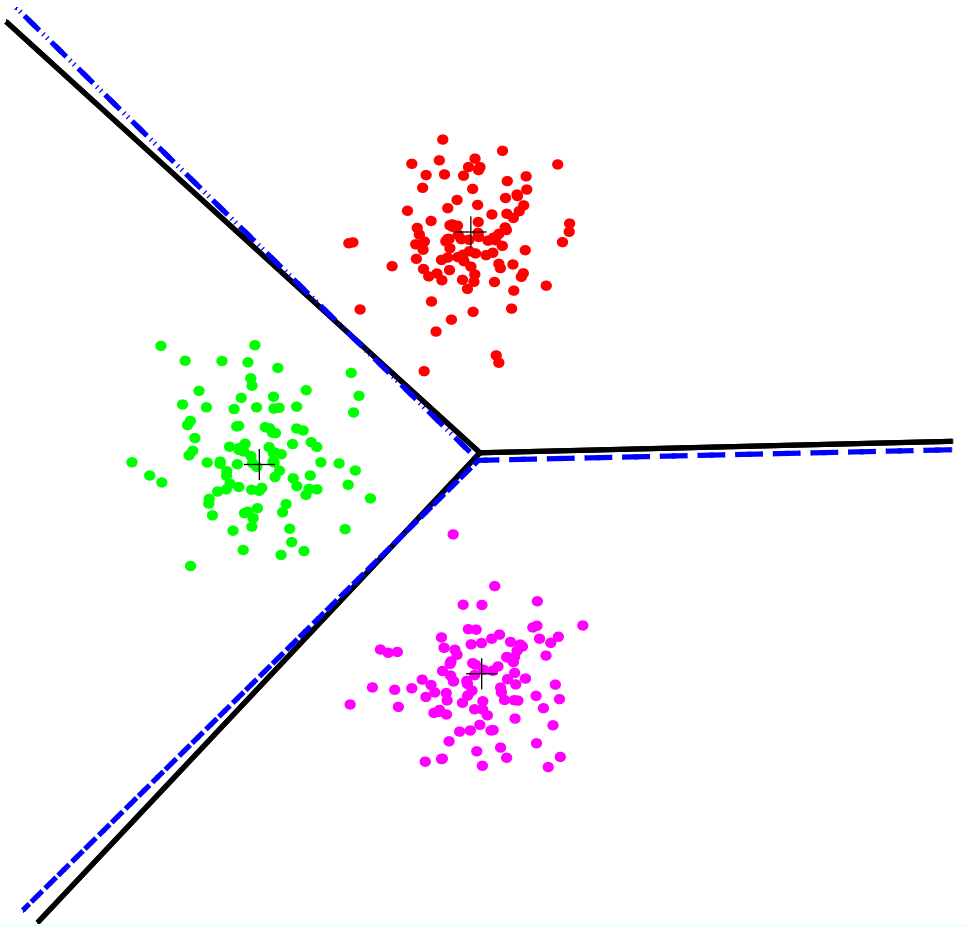
Stability-based Validation *(Lange, Braun, Roth, JB,2002)*

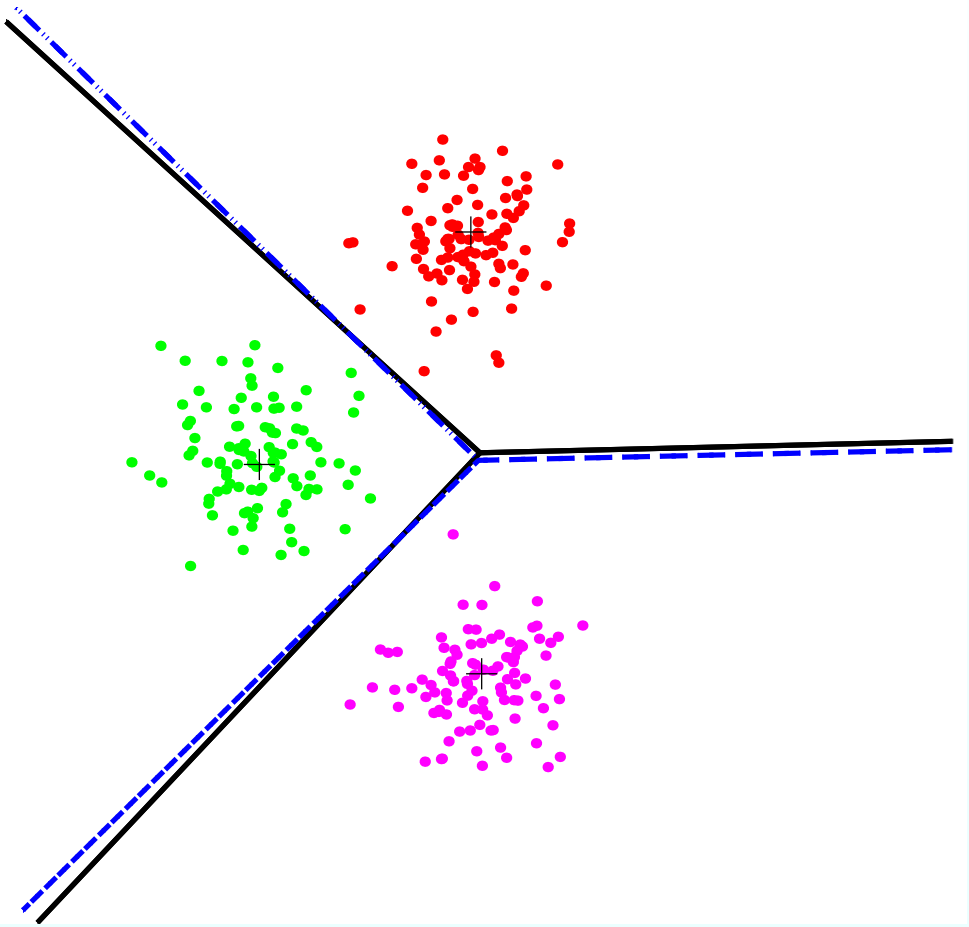
- Many validation methods incorporate a structural bias!
- What to do if no additional a priori knowledge available?
- **Main idea:**

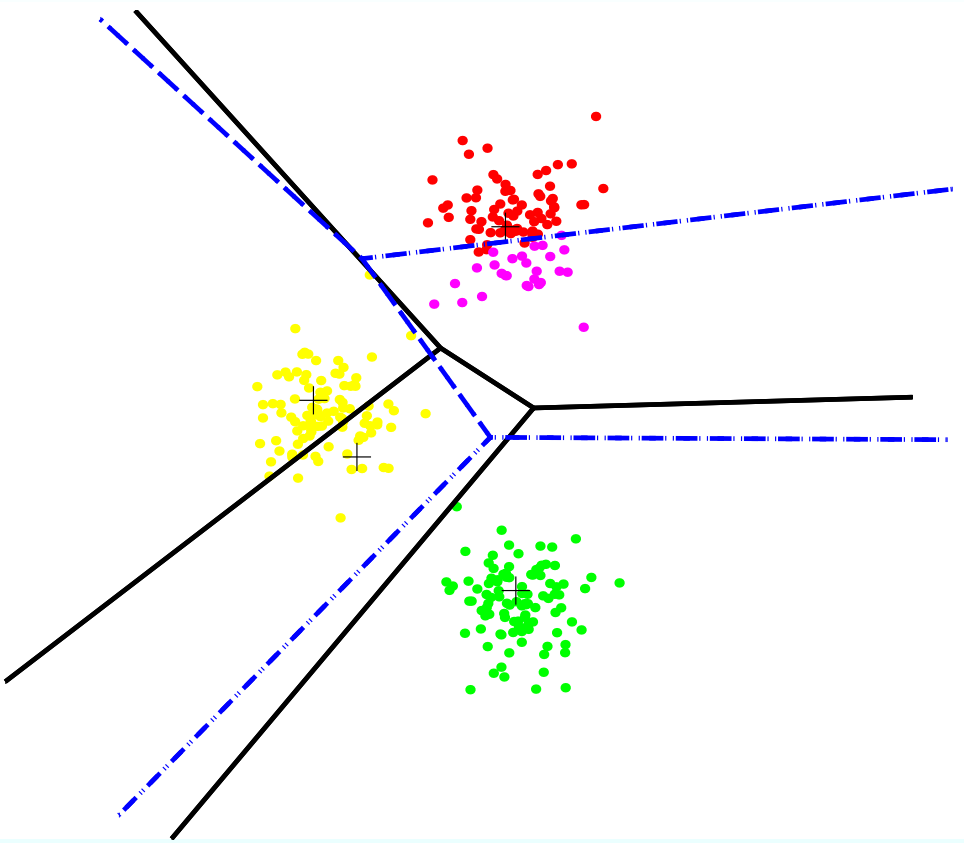
Stability:
Solutions on two data sets from the same source should be similar.

Stability



Stability





Two Sample Scenario

- **General procedure:**

  (i) Draw two data sets from the same source.

  (ii) Cluster both data sets.

  (iii) Compute agreement

Stability := expected agreement of the solutions.

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Stability $:=$ expected agreement of the solutions.

- **In practical applications:** only one data set available.
  - (i) Estimate expected agreement by resampling.
  - (ii) Cluster entire data set with optimal k.

Measuring disagreement

Two labelings on one data set:

disagreement $:=$ Fraction of differently labeled objects.

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3 problems:

1. Clustering solutions are labelings of disjoint sets.
2. Labeling is unique only up to permutation $\pi \in \mathfrak{S}_k$.
3. Fraction of differently labeled points is sensitive to model complexity:

   50% @ $k = 2 \rightarrow$ totally random,

   50% @ $k = 10 \rightarrow$ often acceptable.

Stability Measure: Labelings on disjoint sets

Extend solution from set A to B

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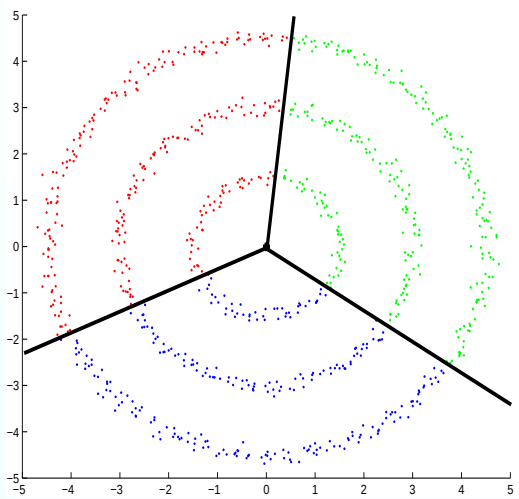
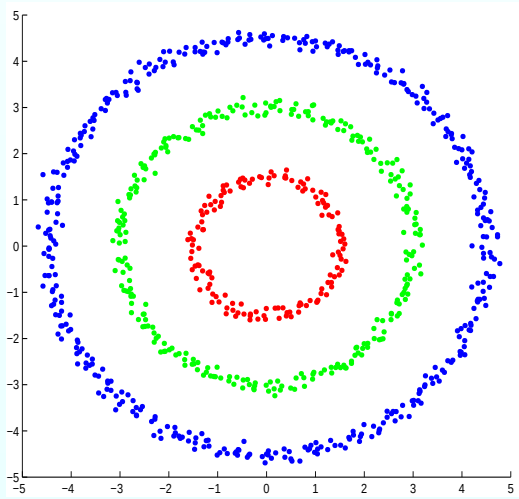
Choose predictor according to meta-principle.





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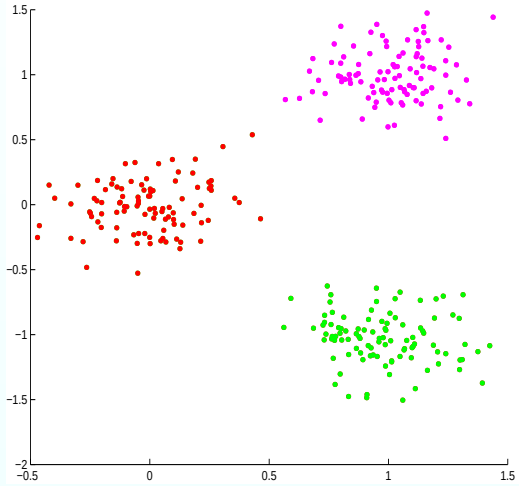

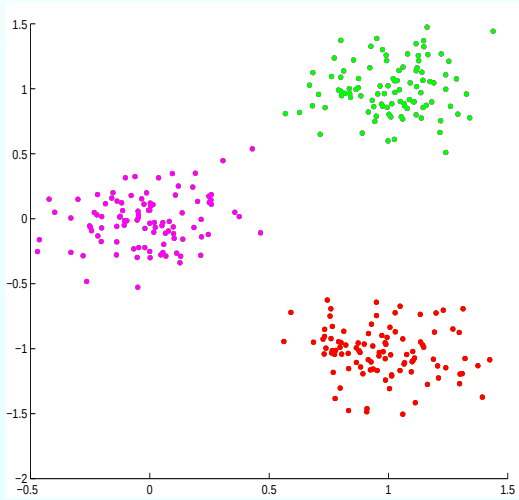

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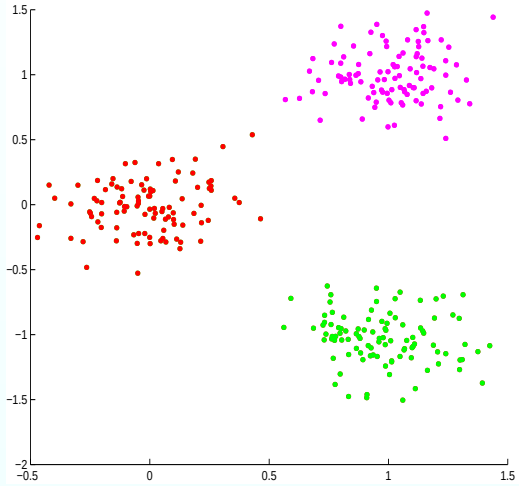
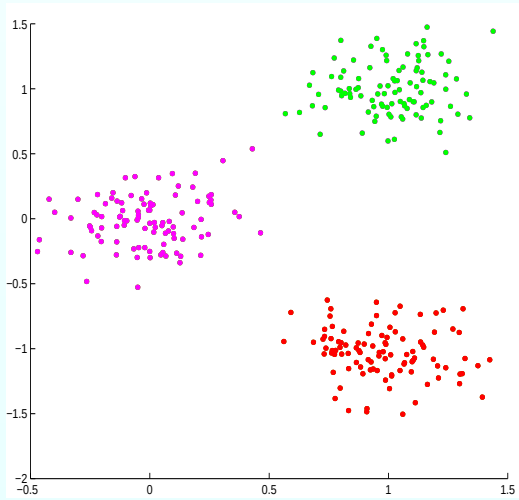


- Labeling unique only up to $\pi \in \mathfrak{S}_k$.
- **Solution:** Stability index $S :=$ expected minimal disagreement over all $\pi \in \mathfrak{S}_k$.
- **Hungarian method** $O(k^3)$.



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$$\rightsquigarrow \boxed{\text{Normalize } S \mapsto \frac{S_k(\alpha)}{S_k(\varrho)}.}$$

The Final Stability Measure

$$\frac{1}{n}\sum_{i=1}^{n} \mathbf{1}\{\alpha(\mathbf{X})_i \neq \qquad g(X_i; \mathbf{X}', \alpha(\mathbf{X}'))\}$$

- Disagreement rate

The Final Stability Measure

$$\min_{\pi \in \mathfrak{S}_k} \frac{1}{n} \sum_{i=1}^{n} \mathbf{1}\{\alpha(\mathbf{X})_i \neq \pi \circ g(X_i; \mathbf{X}', \alpha(\mathbf{X}'))\}$$

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- Permutation symmetry breaking

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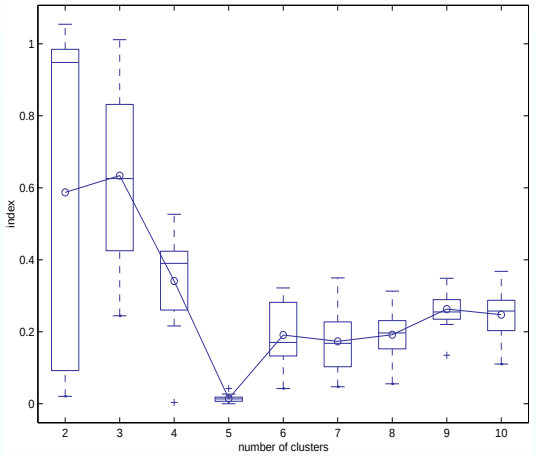
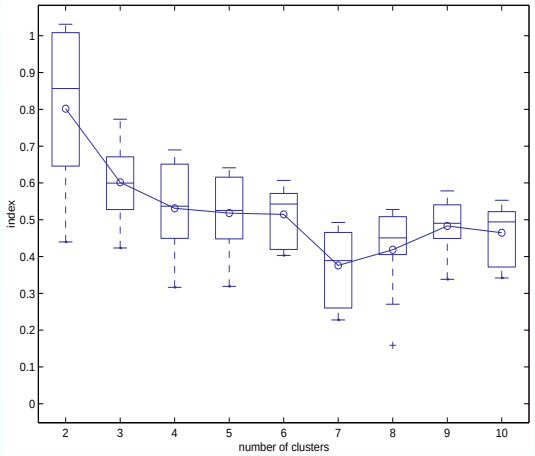
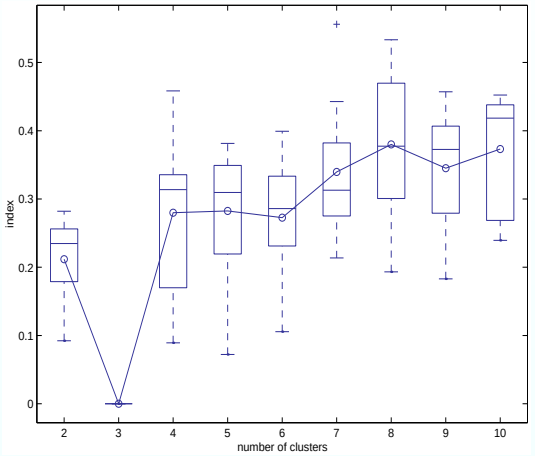
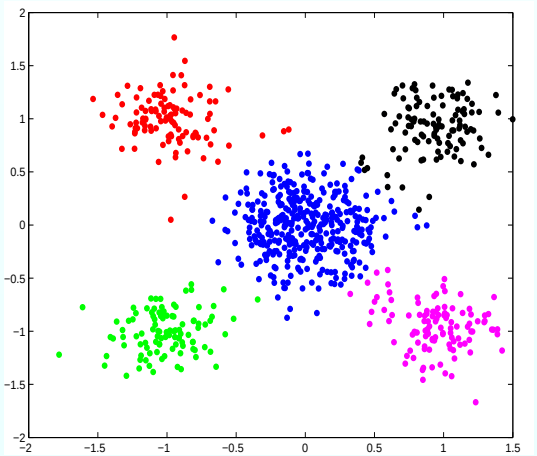
- Disagreement rate
- Permutation symmetry breaking
- Expectation w.r.t. two samples from same source
- Normalize by $S(\varrho)$.
- Estimate $\mathbb{E}_{\mathbf{X},\mathbf{X}'}$ by resampling

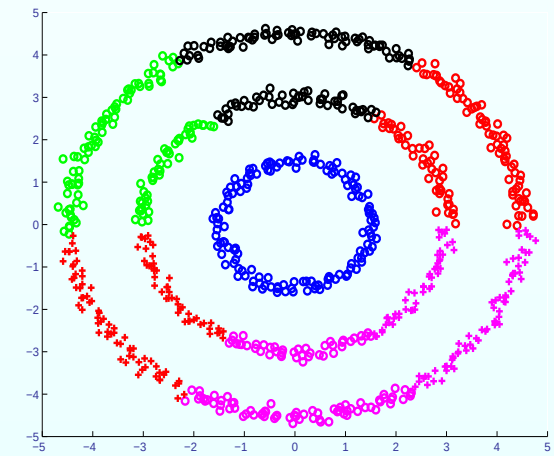
Results on Toy Data

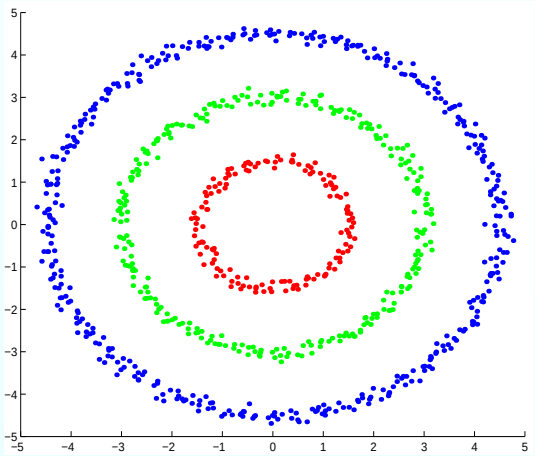












Biological Applications

- Tumor Class Discovery from gene expression data:
  Identify different types of Leukemia
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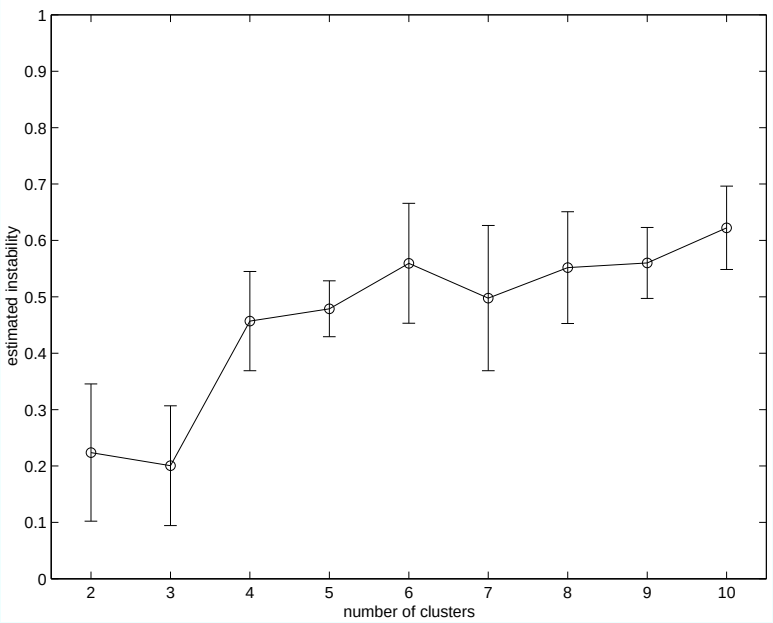
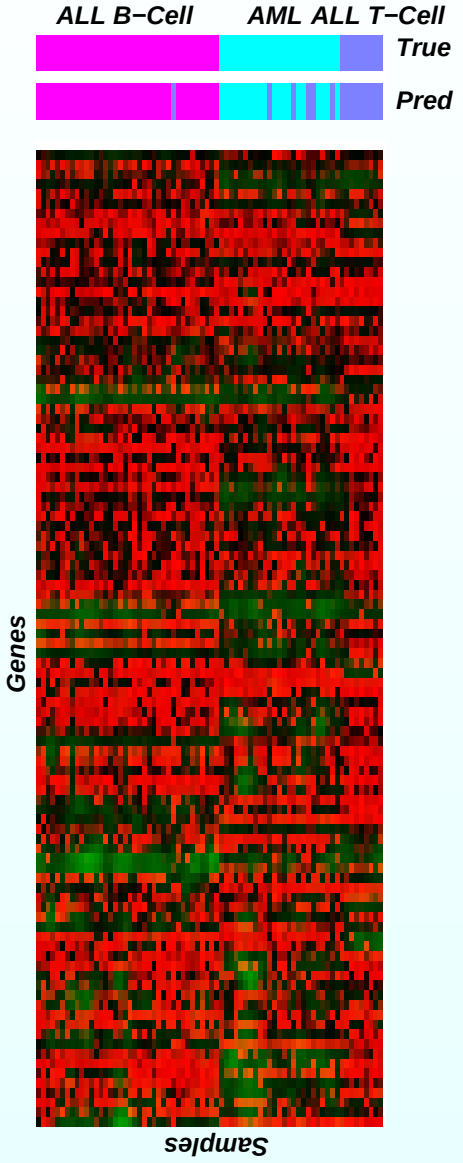
- Clustering of Proteins:
  Find groups of similar proteins
  Pairwise Data
  1200 Globins or Globin-like proteins
  “ground truth”: 5 classes

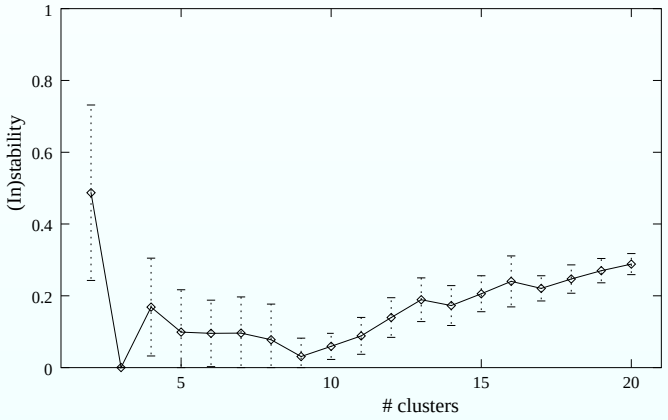
Class Discovery

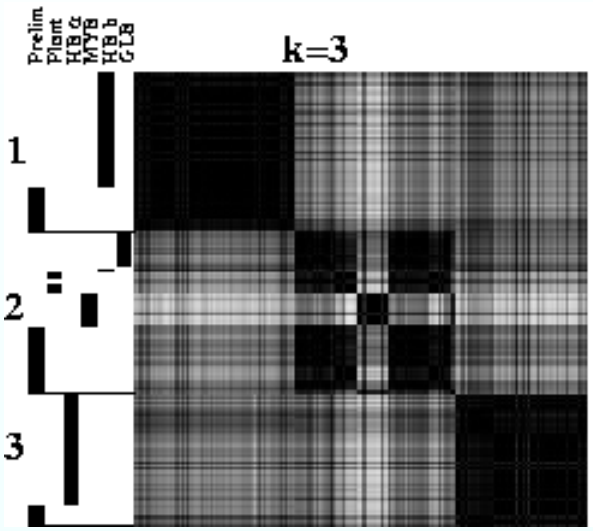


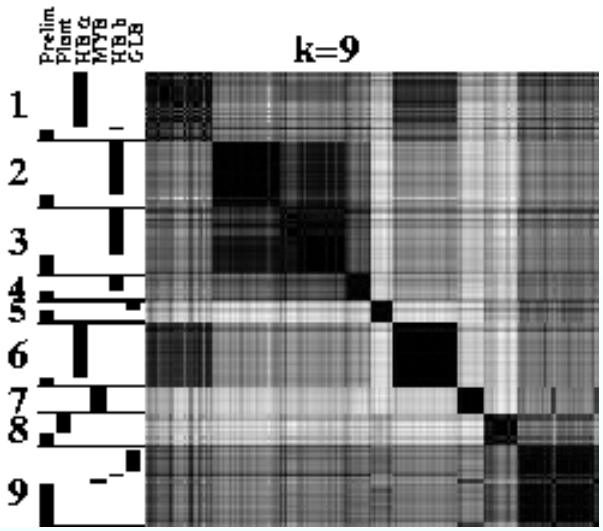


- Two candidates: $k = 3$ and $k = 2$
- Approx. 91 % of the known classes found.

Clustering of Globins







- Two candidates: $k = 3$ und $k = 9$
- Separation of hemoglobin-α and hemoglobin-β from the remaining globins.

Biologically plausible clustering!

Stability: Summary

- **Stability Principle:** Solutions for two data sets from the same source should be similar.
- **No additional assumptions** about the structure of solutions.
- **Good performance** on experimental data sets.

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