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Introduction to Data Mining
05 - Clustering

Benjamin Paaßen

WS 2023/2024, Bielefeld University

Exercise Submission

- Sheet 02 is out today

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$\Rightarrow$ Please use moodle exclusively for your submissions, from now on

1. K-Means algorithm

2. Gaussian Mixture Models

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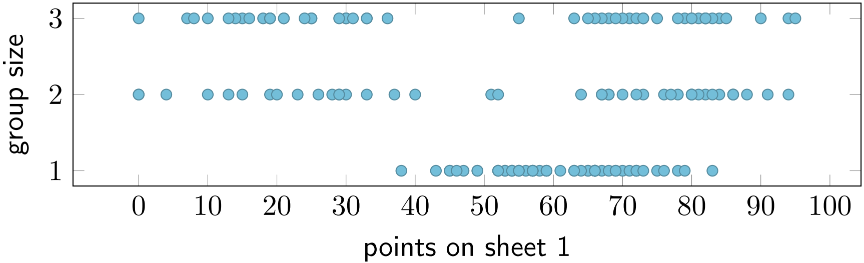

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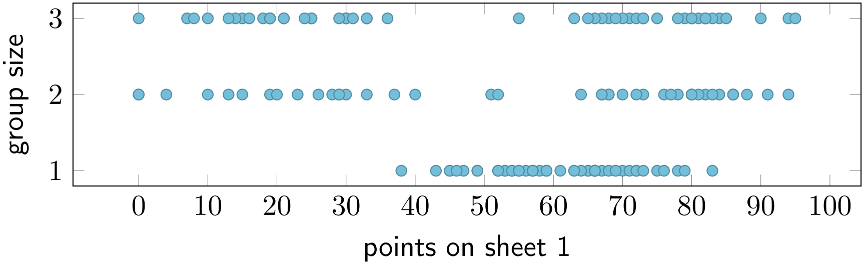

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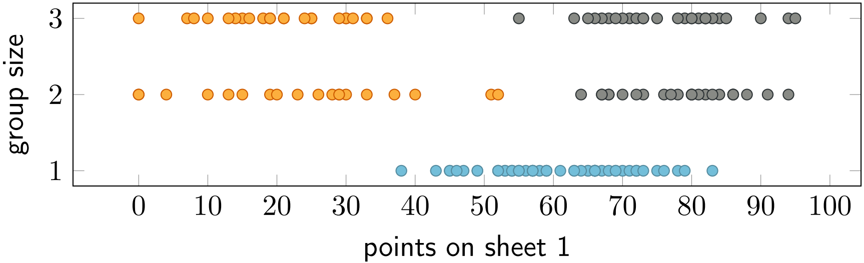

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K-Means algorithm

Autoencoding Setup

observable data

x

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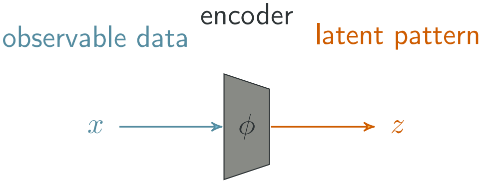

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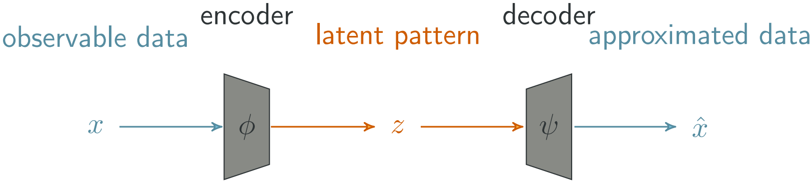

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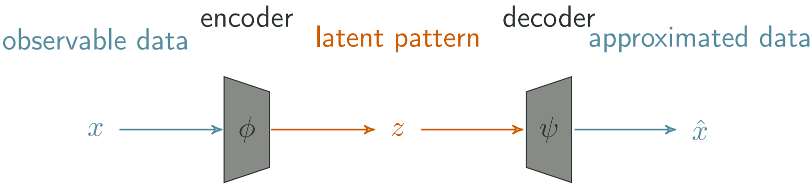

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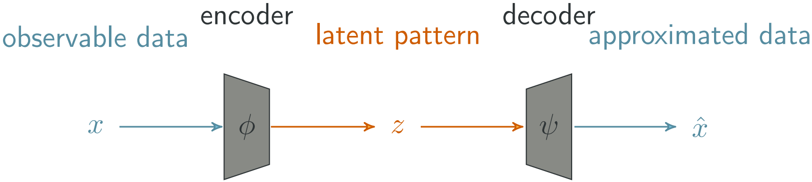

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$\Rightarrow$ decoder: $\psi(z) = \mu_z \in \mathbb{R}^m$ (discrete catalogue of "prototypes")

Optimal encoder

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- For each x, directly optimize reconstruction error

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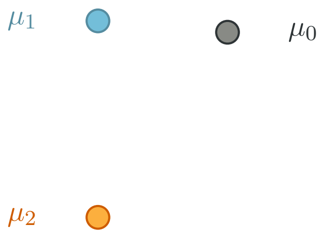

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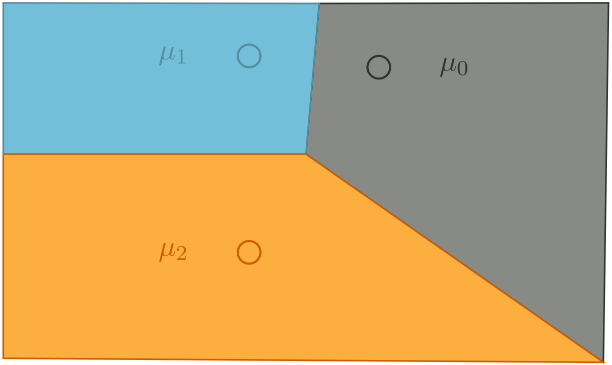

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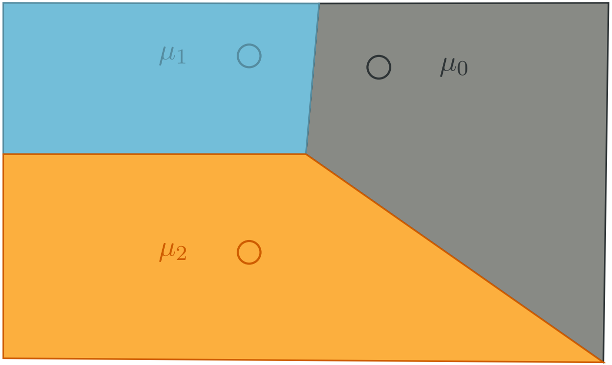

Voronoi tesselation

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- Unfortunately, this is NP-hard :(

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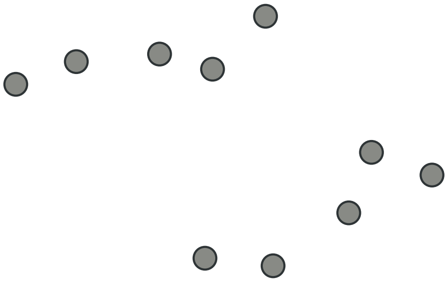
- Setting gradient to zero yields $\mu_k = \frac{1}{|\mathcal{P}_k|} \sum_{i \in \mathcal{P}_k} x_i$.

Visualization



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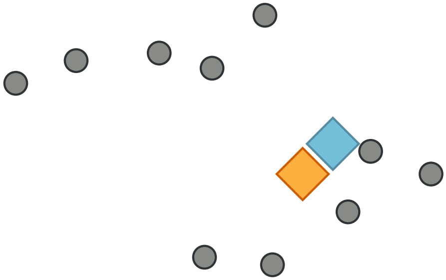

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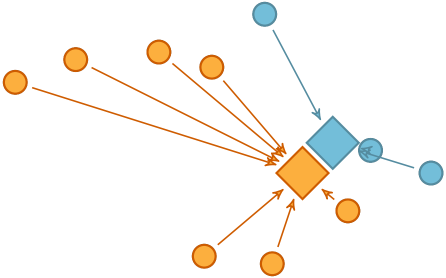

assignment step

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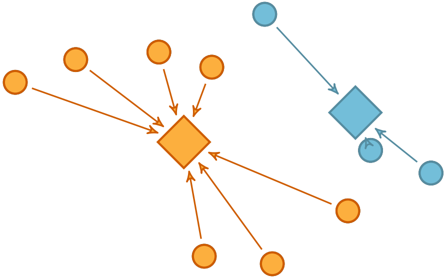

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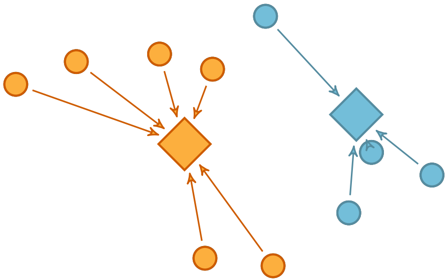

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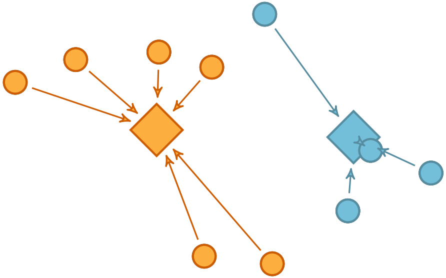

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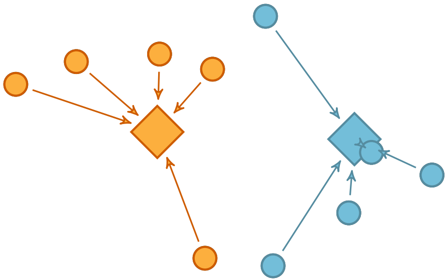

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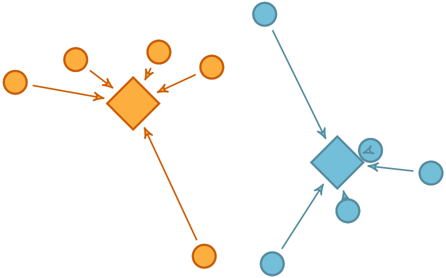

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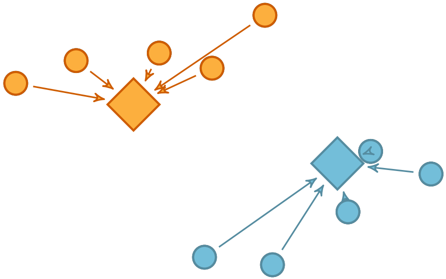

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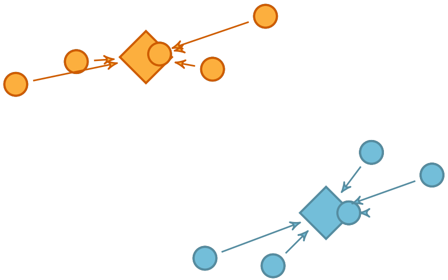

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K-means procedure

function KMeans(data matrix $\boldsymbol{X}$ with N rows and m columns, desired number of clusters K)

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  return $\mu_1, \ldots, \mu_K$.
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- **note!** in practice, K-means mostly stops already after ca. 10-30 iterations

Example: non-normalized data

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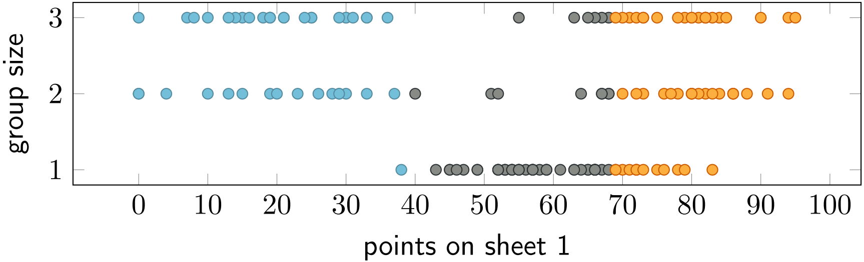

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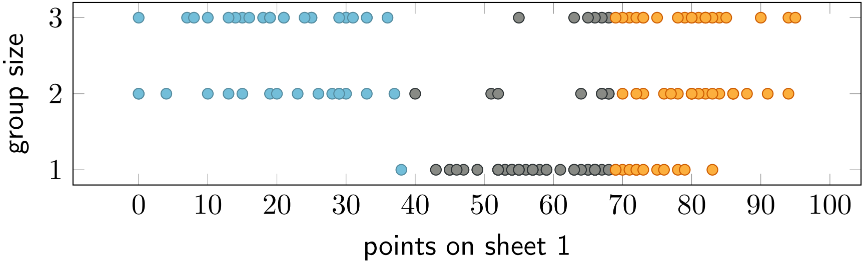

- What is the problem here?

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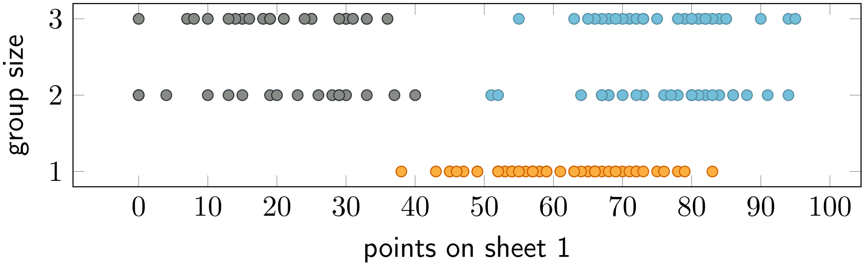

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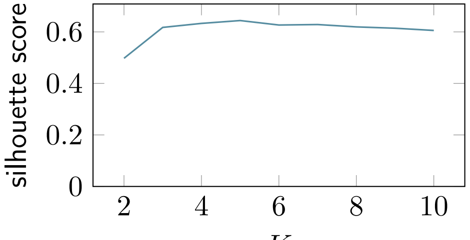

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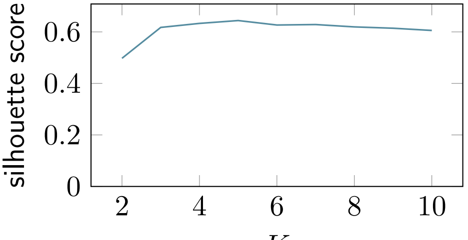

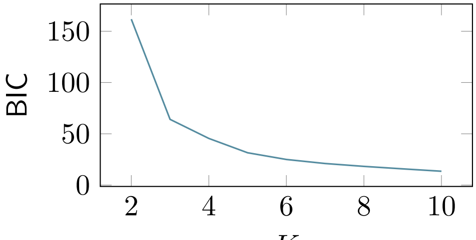

Gaussian Mixture Models

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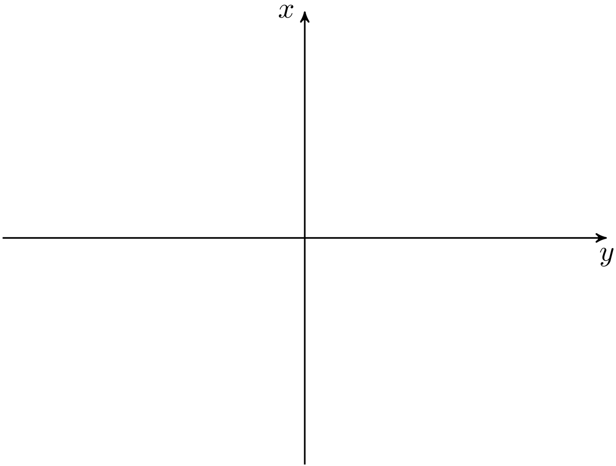
- Step 1: sample latent cluster index k via marginal probability $p_Z(k)$
- Step 2: Sample observable data point x from Gaussian $p_{X|Z}(x|k)$ with mean μ_k and covariance matrix Σ_k

Visualization



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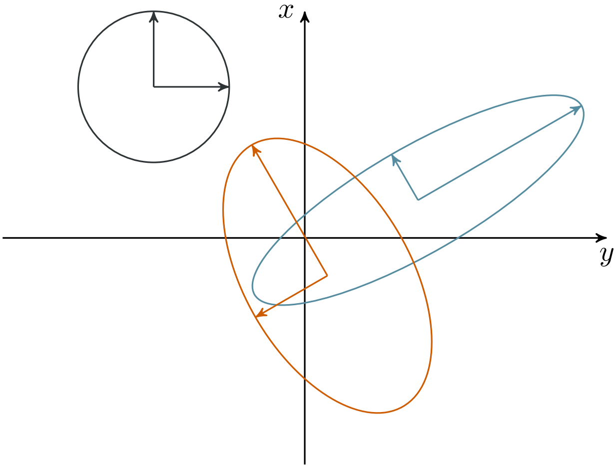

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- Trick: Compute $\gamma_{k,i} = p_{Z|X}(k|x_i)$, then optimize the **expected** negative log likelihood instead:

$$Q = \sum_{i=1}^{N} \sum_{k=1}^{K} -\gamma_{k,i} \cdot \log\left[p_{X|Z}(x_i|k) \cdot p_Z(k)\right]$$

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- Trick: Compute $\gamma_{k,i} = p_{Z|X}(k|x_i)$, then optimize the **expected** negative log likelihood instead:

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Optimization procedure

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⇒ Convex and closed-form solution (see exercises) :)

Visualization

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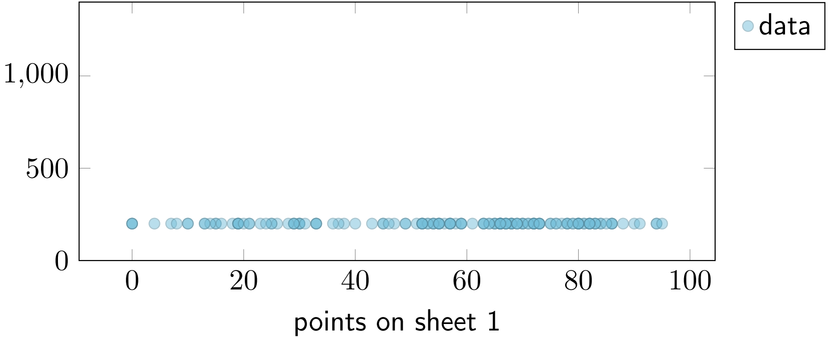

Visualization

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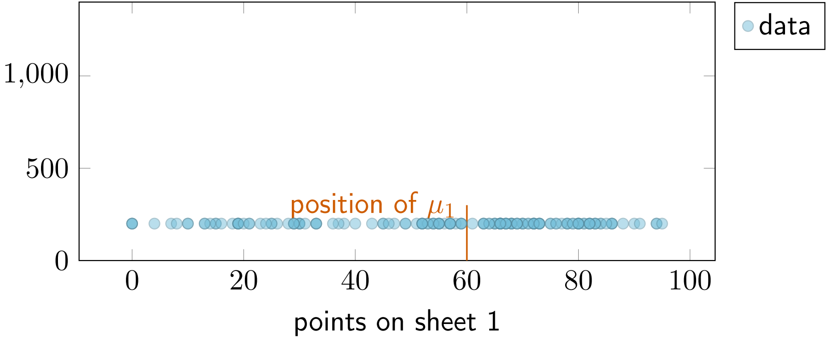

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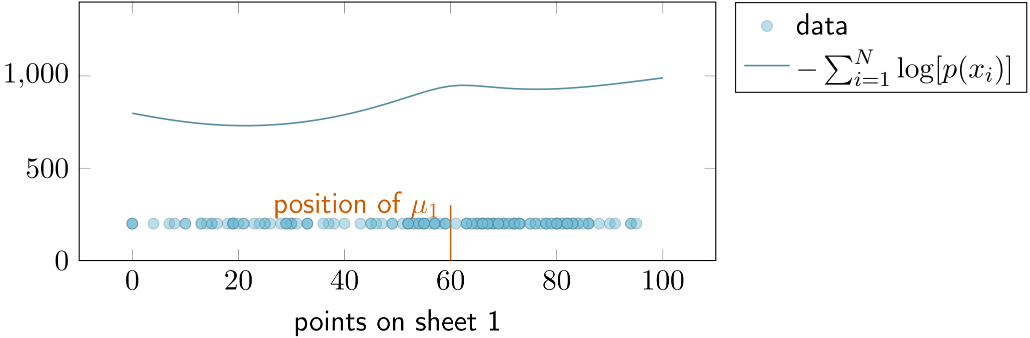

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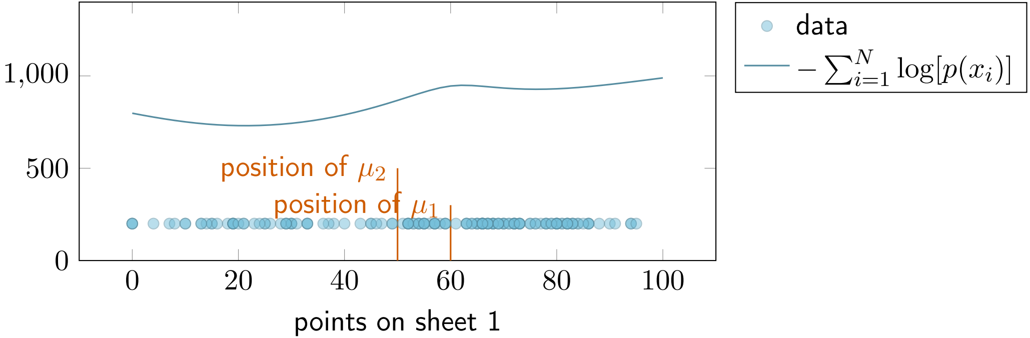

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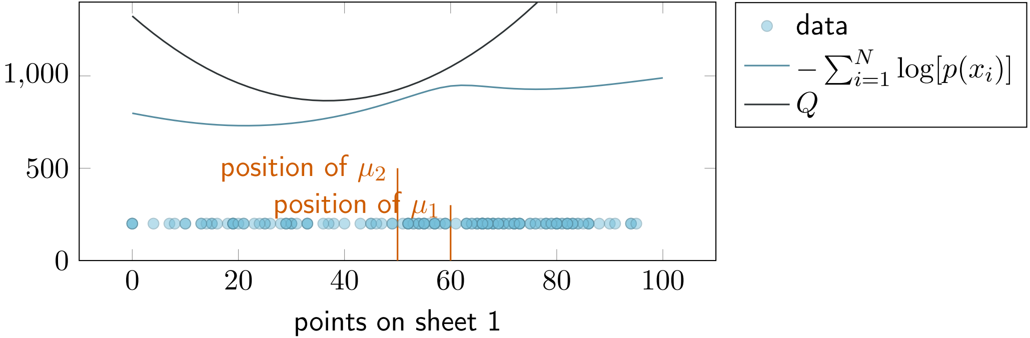

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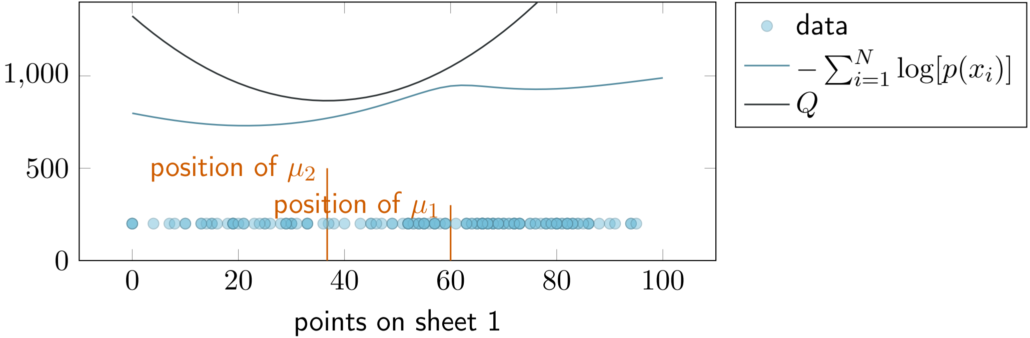

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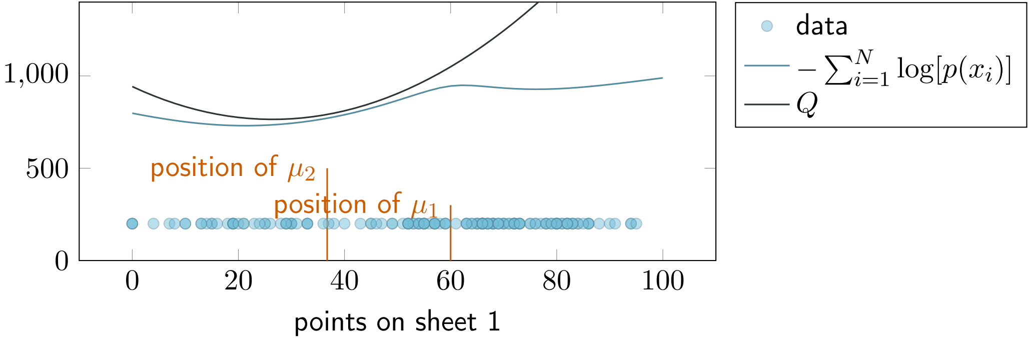

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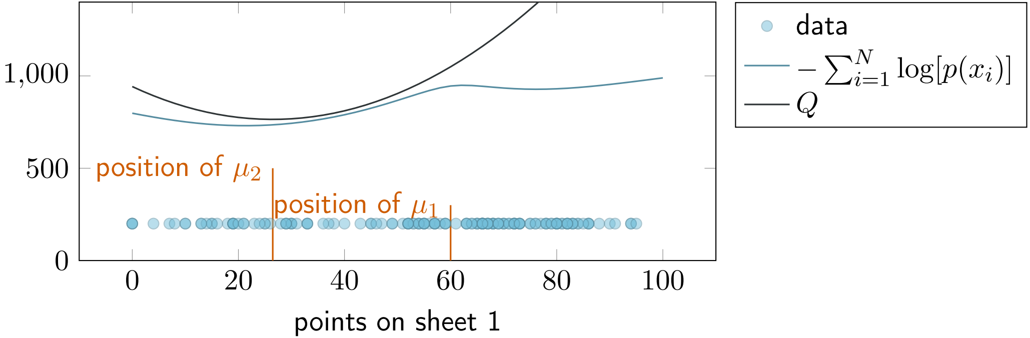

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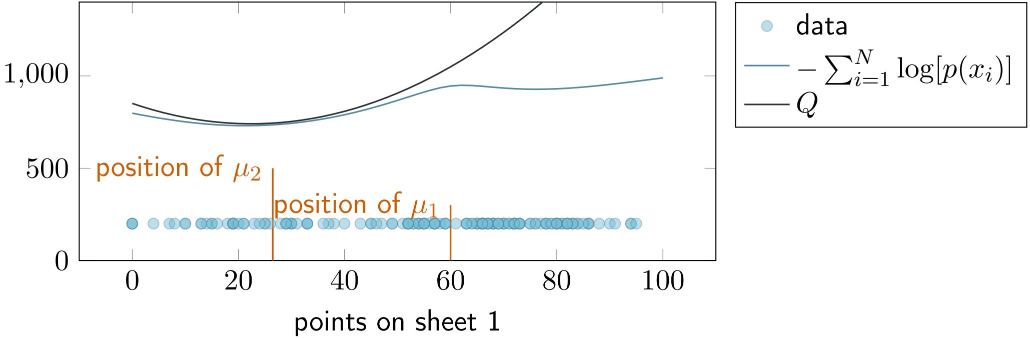

Theory of EM (part 1)

Let $\gamma_{i,k}$ be arbitrary real number s.t. $\sum_{k=1}^{K} \gamma_{i,k} = 1$ and $\gamma_{i,k} \geq 0$ for all i and all k.
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Theory of EM (part 2)

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$$\log[p_X(x_i)] = \sum_{k=1}^{K} \gamma_{i,k} \cdot \log[p_{X,Z}(x_i, k)] - \sum_{k=1}^{K} \gamma_{i,k} \cdot \log\left[\frac{p_{Z|X}(k|x_i)}{\gamma_{i,k}}\right] - \sum_{k=1}^{K} \gamma_{i,k} \cdot \log[\gamma_{i,k}]$$

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- We summarize:

$$Q = -\sum_{i=1}^{N} \sum_{k=1}^{K} \gamma_{i,k} \cdot \log[p_{X,Z}(x_i, k)] \qquad \text{(exp. neg. log likelihood)}$$

$$\mathcal{D}_{\mathsf{KL}}(\boldsymbol{\gamma_i} || p_{Z_i|X_i}) = -\sum_{k=1}^{K} \gamma_{i,k} \cdot \log\left[\frac{p_{Z|X}(k|x_i)}{\gamma_{i,k}}\right] \qquad \text{(Kullback-Leibler-Divergence)}$$

$$\mathcal{H}(\boldsymbol{\gamma_i}) = -\sum_{k=1}^{K} \gamma_{i,k} \cdot \log[\gamma_{i,k}] \qquad \text{(entropy)}$$

Theory of EM (part 3)

$$-\sum_{i=1}^{N} \log[p_X(x_i)] = Q - \sum_{i=1}^{N} \mathcal{D}_{\mathsf{KL}}(\boldsymbol{\gamma_i} || p_{Z_i|X_i}) + \mathcal{H}(\boldsymbol{\gamma_i})$$

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$\Rightarrow$ The more clearly defined our clusters get over time, the better Q approximates $\mathcal{L}$

EM algorithm for GMMs

function GMM(data matrix $\boldsymbol{X}$ with N rows and m columns, desired number of Gaussians K)

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end for

return p_Z, $\mu_1, \ldots, \mu_K$, $\Sigma_1, \ldots, \Sigma_K$.

end function

GMM on example data

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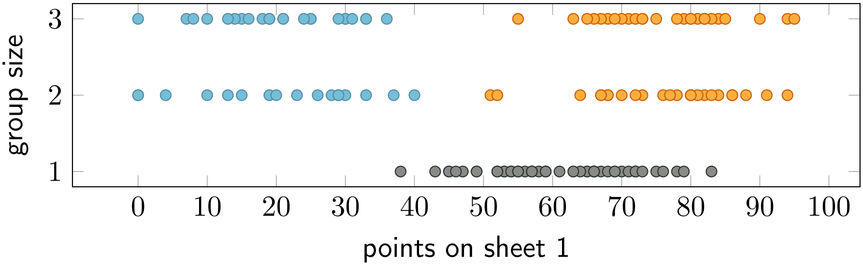

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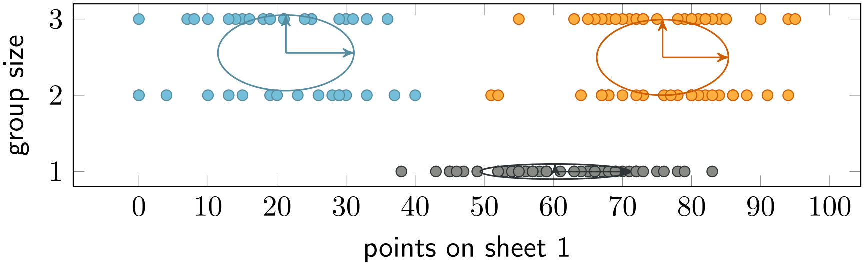

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- K-Means discovers clusters by assigning data to closest prototype and prototypes to cluster means
- Sensitive to data scaling and "unlucky" initializations
- Selection of K: Silhouette score and/or BIC
- Gaussian mixture models can handle scaling and elliptical cluster shapes – but need much more computation

Literature I

Barber, David (2012). **Bayesian Reasoning and Machine Learning**. Cambridge, UK: Cambridge University Press. url: http://www.cs.ucl.ac.uk/staff/d.barber/brml/.

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