Machine Learning Department
School of Computer Science
Carnegie Mellon University

Bayesian Nonparametrics
+
Graph Neural Networks

Matt Gormley
Lecture 25
Dec. 7, 2022

Reminders

- 10-618 Mini-Project
  - Team Formation Due: Tue, Nov 29
  - Proposal Due: Thu, Dec 1
  - Summary & Code Due: Fri, Dec 9
- Practice Problems 2
  - Out: Wed, Dec 8
- Exam 2:
  - Thu, Dec 15, 5:30 – 7:30 PM

Chinese Restaurant Process & Stick-breaking Constructions

DIRICHLET PROCESS

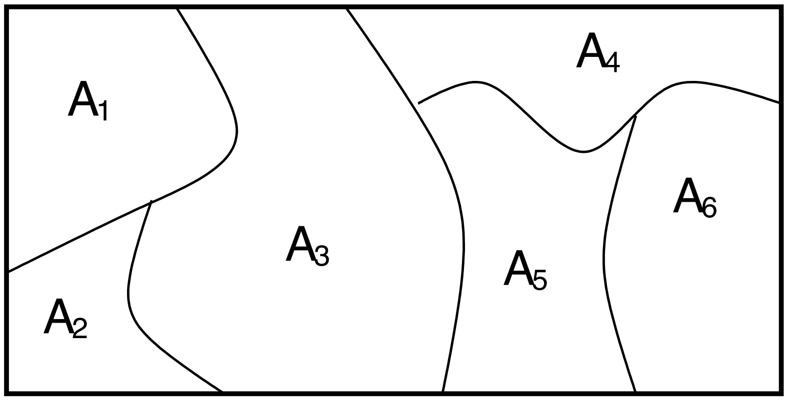
Dirichlet Process

Ferguson Definition

- Parameters of a DP:
  1. Base distribution, H, is a probability distribution over Θ
  2. Strength parameter, $\alpha \in \mathcal{R}$
- We say $G \sim \mathrm{DP}(\alpha, H)$
  if for any partition $A_1 \cup A_2 \cup \ldots \cup A_K = \Theta$
  we have:
  $(G(A_1), \ldots, G(A_K)) \sim \mathrm{Dirichlet}(\alpha H(A_1), \ldots, \alpha H(A_K))$

In English: the DP is a distribution over probability measures s.t. marginals on finite partitions are Dirichlet distributed

A partition of the space Θ

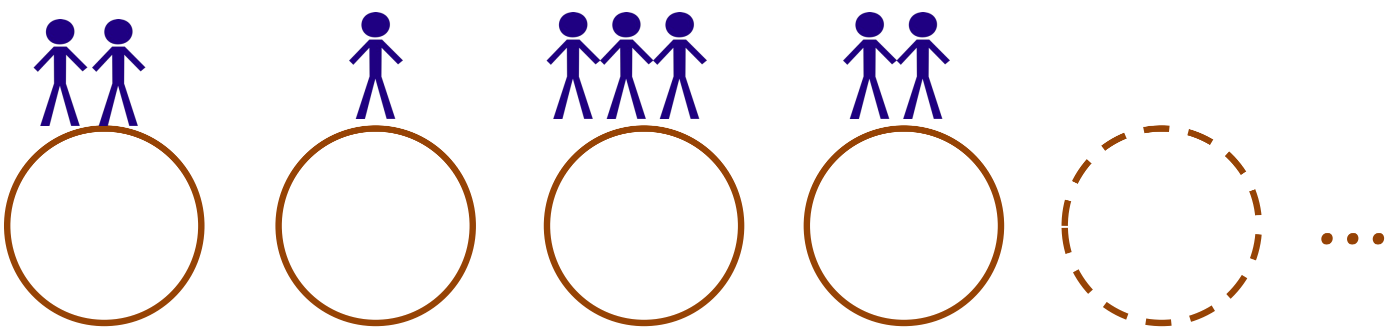


Chinese Restaurant Process

- Imagine a Chinese restaurant with an infinite number of tables
- Each customer enters and sits down at a table
  - The first customer sits at the first unoccupied table
  - Each subsequent customer chooses a table according to the following probability distribution:

    $p(kth\ occupied\ table) \propto n_k$
    $p(next\ unoccupied\ table) \propto \alpha$

    where n_k is the number of people sitting at the table k



$$\frac{2}{8+\alpha} \qquad \frac{1}{8+\alpha} \qquad \frac{3}{8+\alpha} \qquad \frac{2}{8+\alpha} \qquad \frac{\alpha}{8+\alpha}$$

Chinese Restaurant Process & Stick-breaking Constructions

DIRICHLET PROCESS MIXTURE MODEL

CRP Mixture Model

- Draw n cluster indices from a CRP:

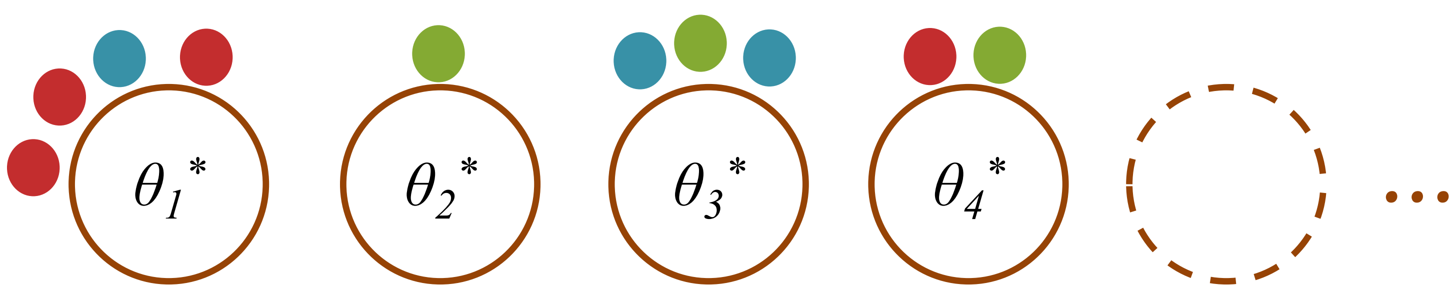
  $z_1, z_2, \ldots, z_n \sim CRP(\alpha)$
- For each of the resulting K clusters:

  $\theta_k^* \sim H$

  where H is a base distribution
- Draw n observations:

  $$x_i \sim p(x_i \mid \theta^*_{z_i})$$

Customer i orders a dish x_i (observation) from a table-specific distribution over dishes θ_k^* (cluster parameters)



(color denotes different values of x_i)

CRP Mixture Model

- Draw n cluster indices from a CRP:
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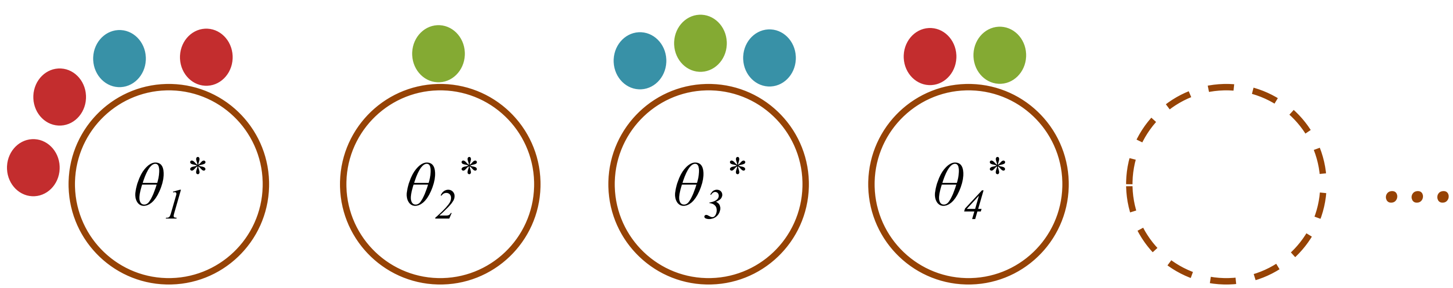
  where H is a base distribution
- Draw n observations:
  $$x_i \sim p(x_i \mid \theta^*_{z_i})$$

- The Gibbs sampler is easy thanks to **exchangeability**
- For each observation, we remove the customer / dish from the restaurant and resample as if they were the **last to enter**
- If we **collapse out the parameters,** the Gibbs sampler draws from the conditionals:

  $z_i \sim p(z_i \mid \mathbf{z}_{-i}, \mathbf{x})$



(color denotes different values of x_i)

CRP Mixture Model

Overview of 3 Gibbs Samplers for Conjugate Priors

- Alg. 1: (uncollapsed)
  - Markov chain state: per-customer parameters $\theta_1, \ldots, \theta_n$
  - For $i = 1, \ldots, n$: Draw $\theta_i \sim p(\theta_i \mid \boldsymbol{\theta}_{-i}, \boldsymbol{x})$

All the thetas except θ_i

- Alg. 2: (uncollapsed)
  - Markov chain state: per-customer cluster indices $z_1, \ldots, z_n$ and per-cluster parameters $\theta_1^*, \ldots, \theta_k^*$
  - For $i = 1, \ldots, n$: Draw $z_i \sim p(z_i \mid \boldsymbol{z}_{-i}, \boldsymbol{x}, \boldsymbol{\theta}^*)$
  - Set K = number of clusters in $\boldsymbol{z}$
  - For $k = 1, \ldots, K$: Draw $\theta_k^* \sim p(\theta_k^* \mid \{x_i : z_i = k\})$
- Alg. 3: (collapsed)
  - Markov chain state: per-customer cluster indices $z_1, \ldots, z_n$
  - For $i = 1, \ldots, n$: Draw $z_i \sim p(z_i \mid \boldsymbol{z}_{-i}, \boldsymbol{x})$

CRP Mixture Model

- Q: How can the Alg. 2 Gibbs samplers permit an infinite set of clusters in finite space?
- A: Easy!
  - We are only representing a finite number of clusters at a time – those to which the data have been assigned
  - We can always bring back the parameters for the "next unoccupied table" if we need them

CRP-MM vs. DP-MM

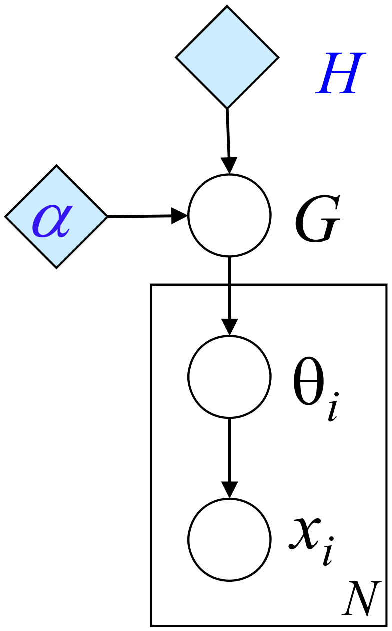
Dirichlet Process: For both the CRP and stick-breaking constructions, if we marginalize out G, we have the following predictive distribution:

$$\theta_{n+1} | \theta_1, \ldots, \theta_n \sim \frac{1}{\alpha + n} \left(\alpha H + \sum_{i=1}^{n} \delta_{\theta_i} \right)$$

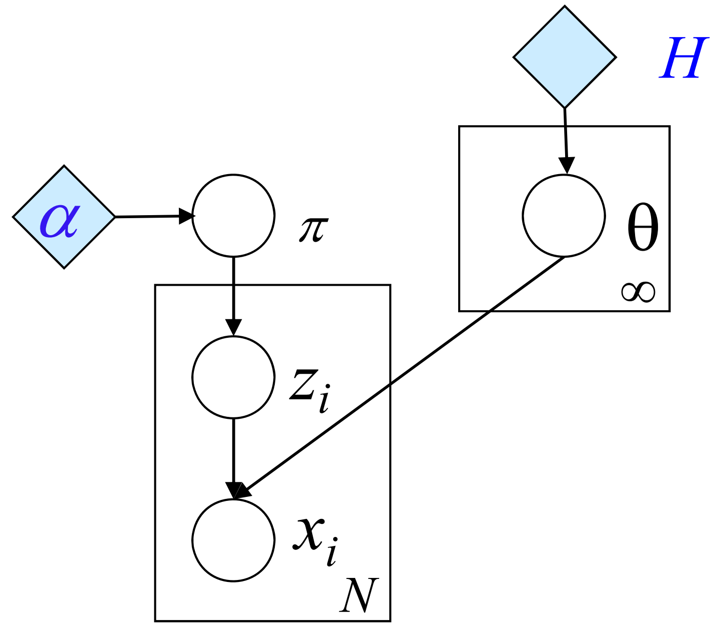
(Blackwell-MacQueen Urn Scheme)

The Chinese Restaurant Process Mixture Model is just a different construction of the Dirichlet Process Mixture Model where we have marginalized out G

Graphical Models for DPMMs



The Pólya urn construction



The Stick-breaking construction

Figure from Blei & Jordan (2006)

Example: DP Gaussian Mixture Model

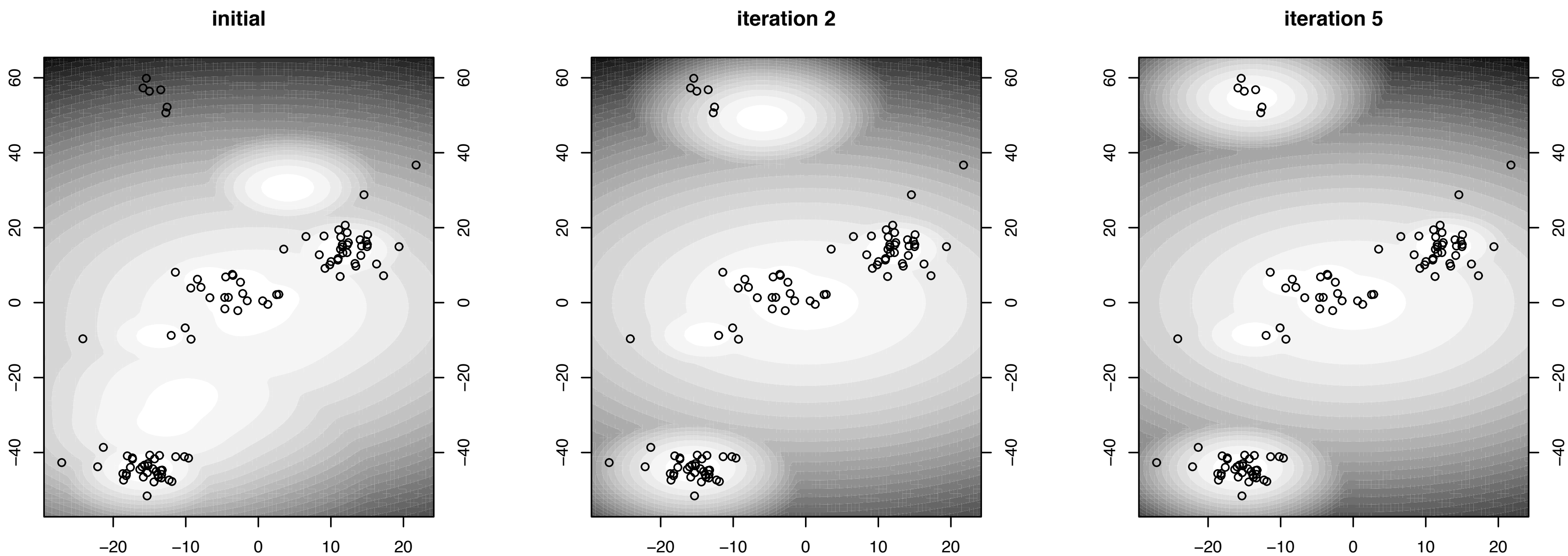


Figure 2: The approximate predictive distribution given by variational inference at different stages of the algorithm. The data are 100 points generated by a Gaussian DP mixture model with fixed diagonal covariance.

Example: DP Gaussian Mixture Model

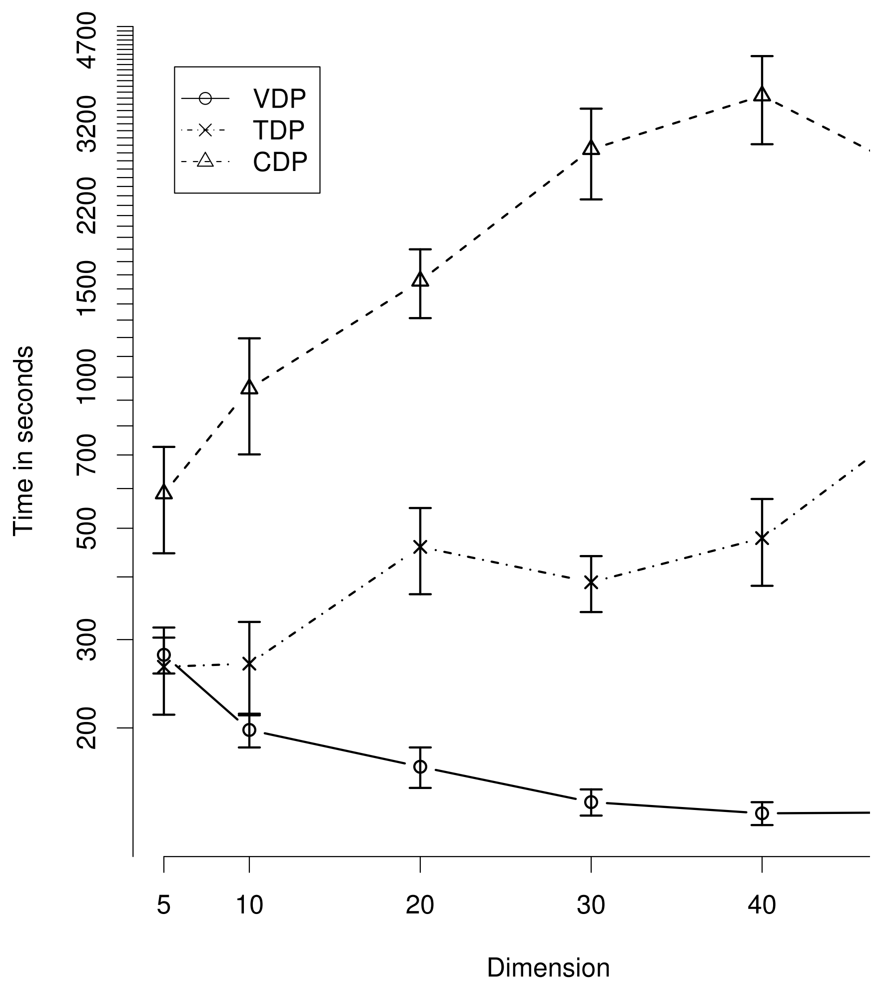
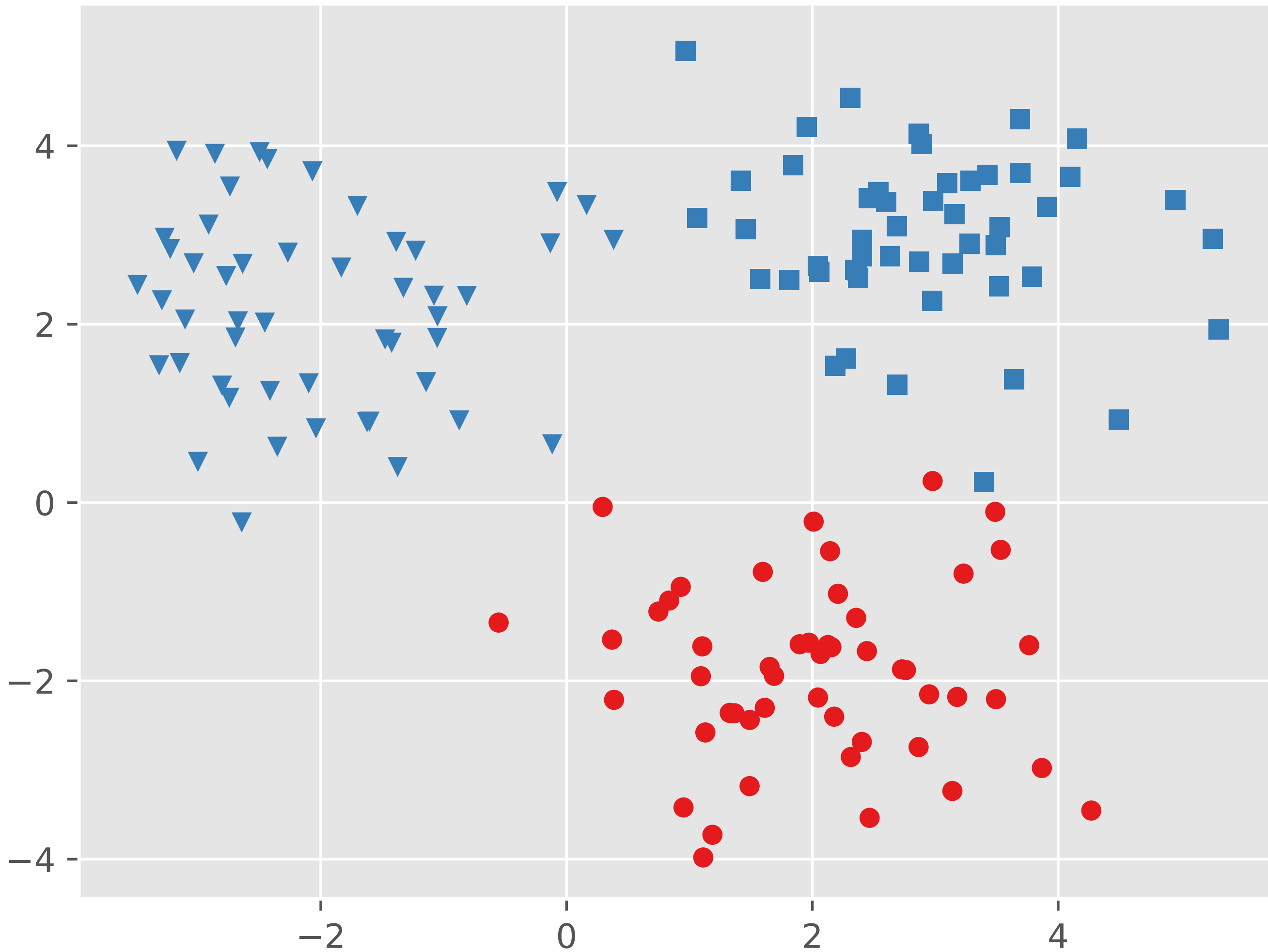


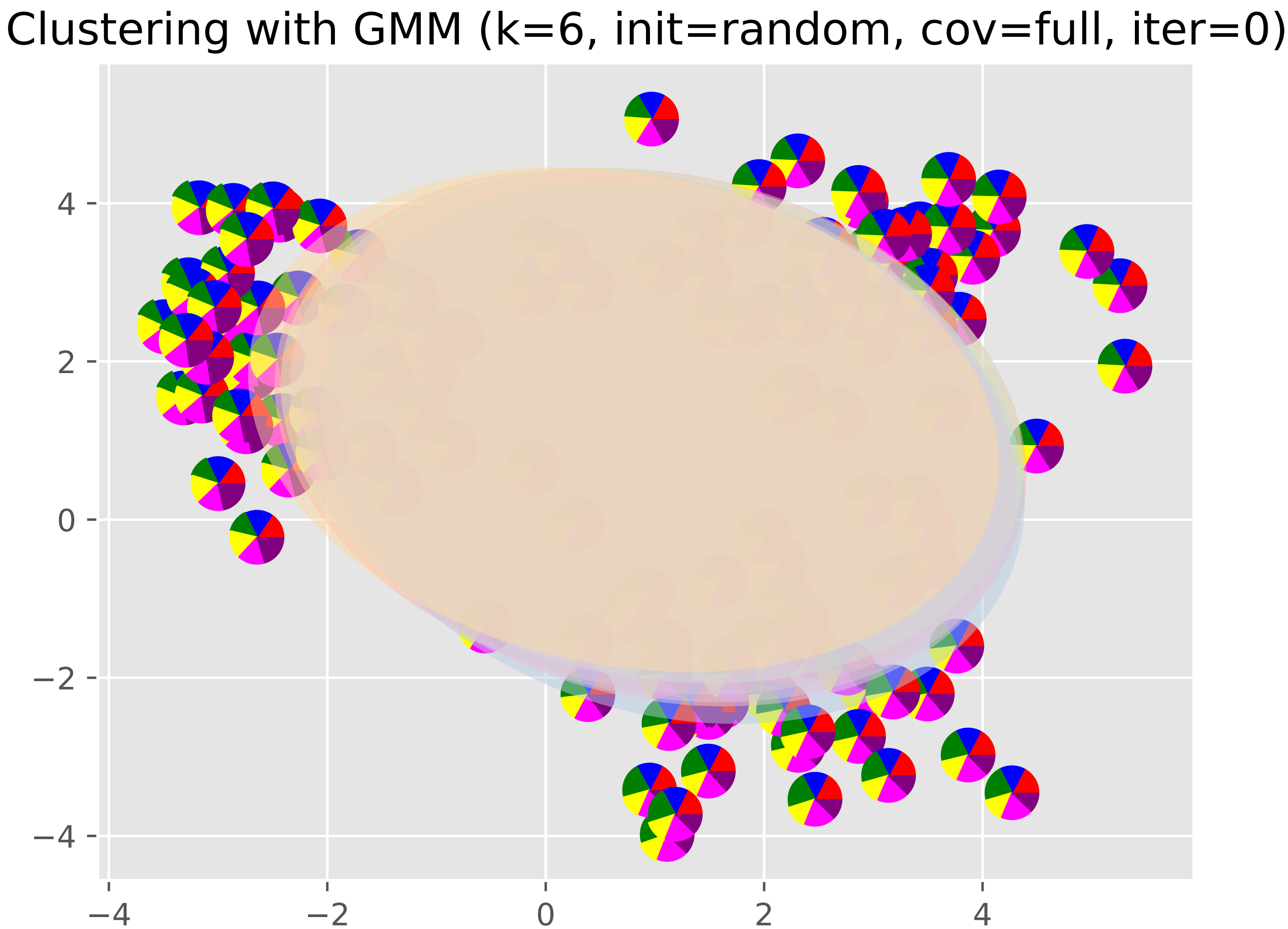
Figure 3: Mean convergence time and standard error across ten data sets per dimension for variational inference, TDP Gibbs sampling, and the collapsed Gibbs sampler.

GMM VS. DPMM EXAMPLE

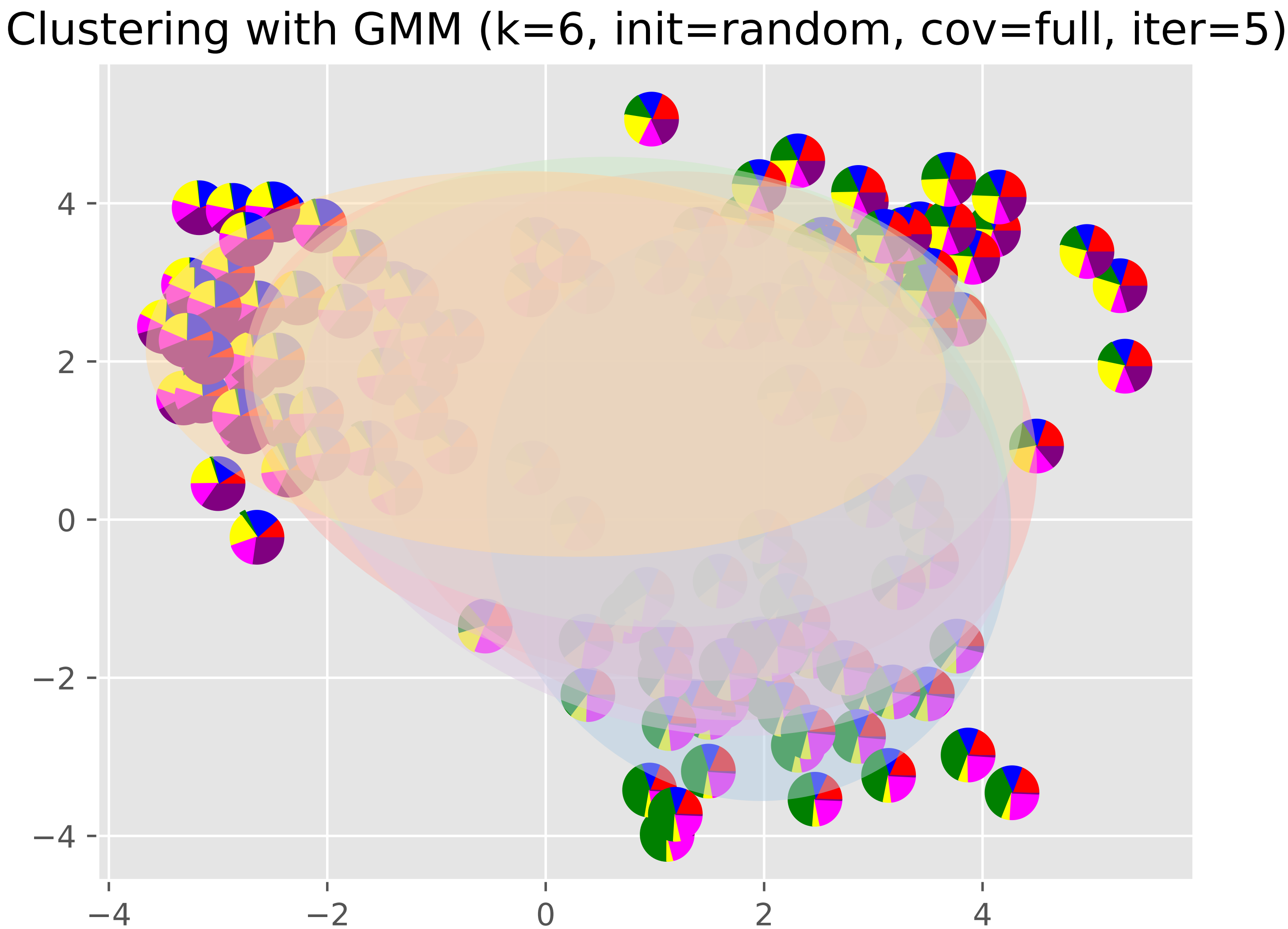
Example: Dataset



Example: GMM

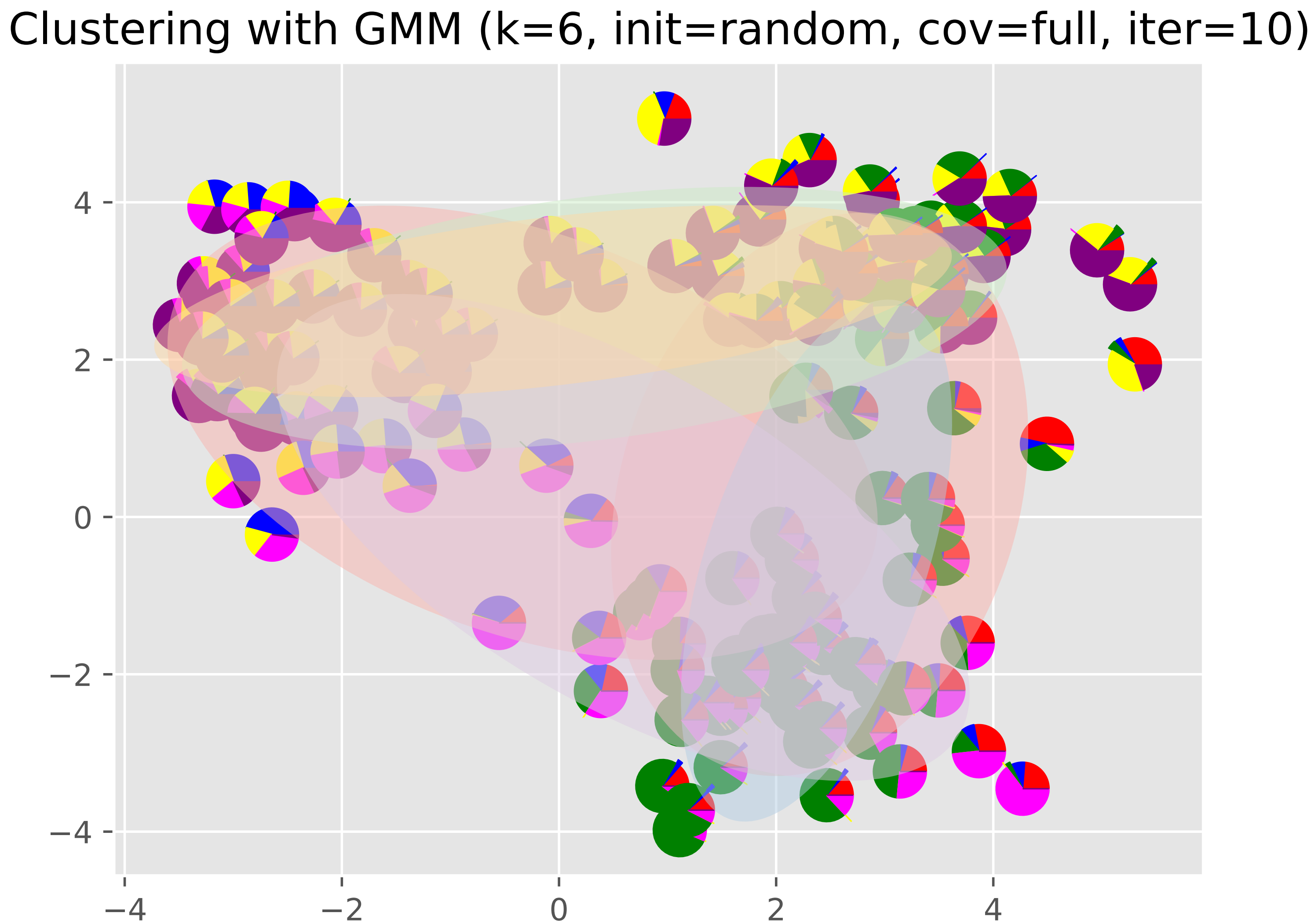

Clustering with GMM (k=6, init=random, cov=full, iter=0)
4
2
0
−2
−4
−4
−2
0
2
4

Example: GMM



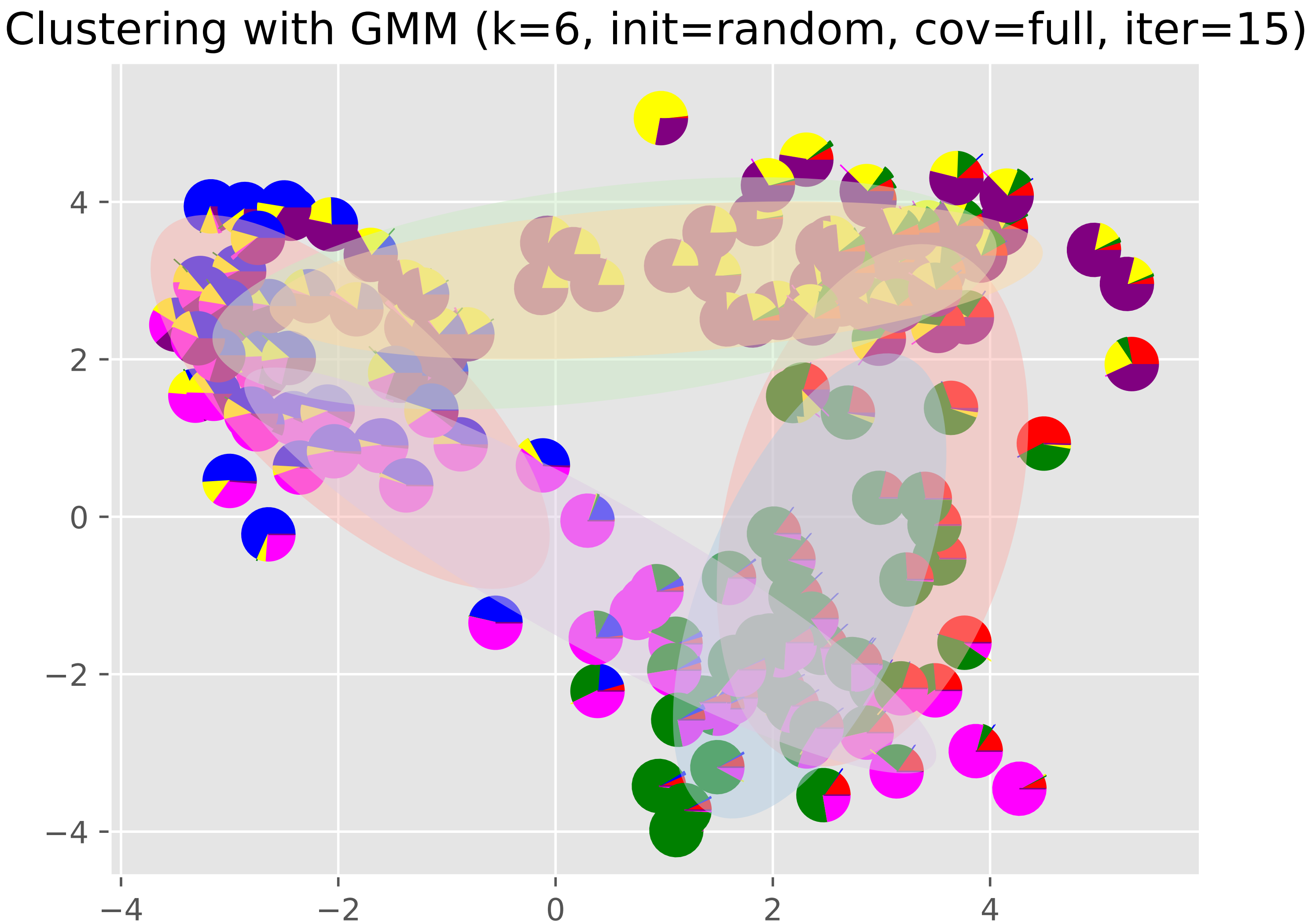
Clustering with GMM (k=6, init=random, cov=full, iter=5)
4
2
0
−2
−4
−4
−2
0
2
4

Example: GMM



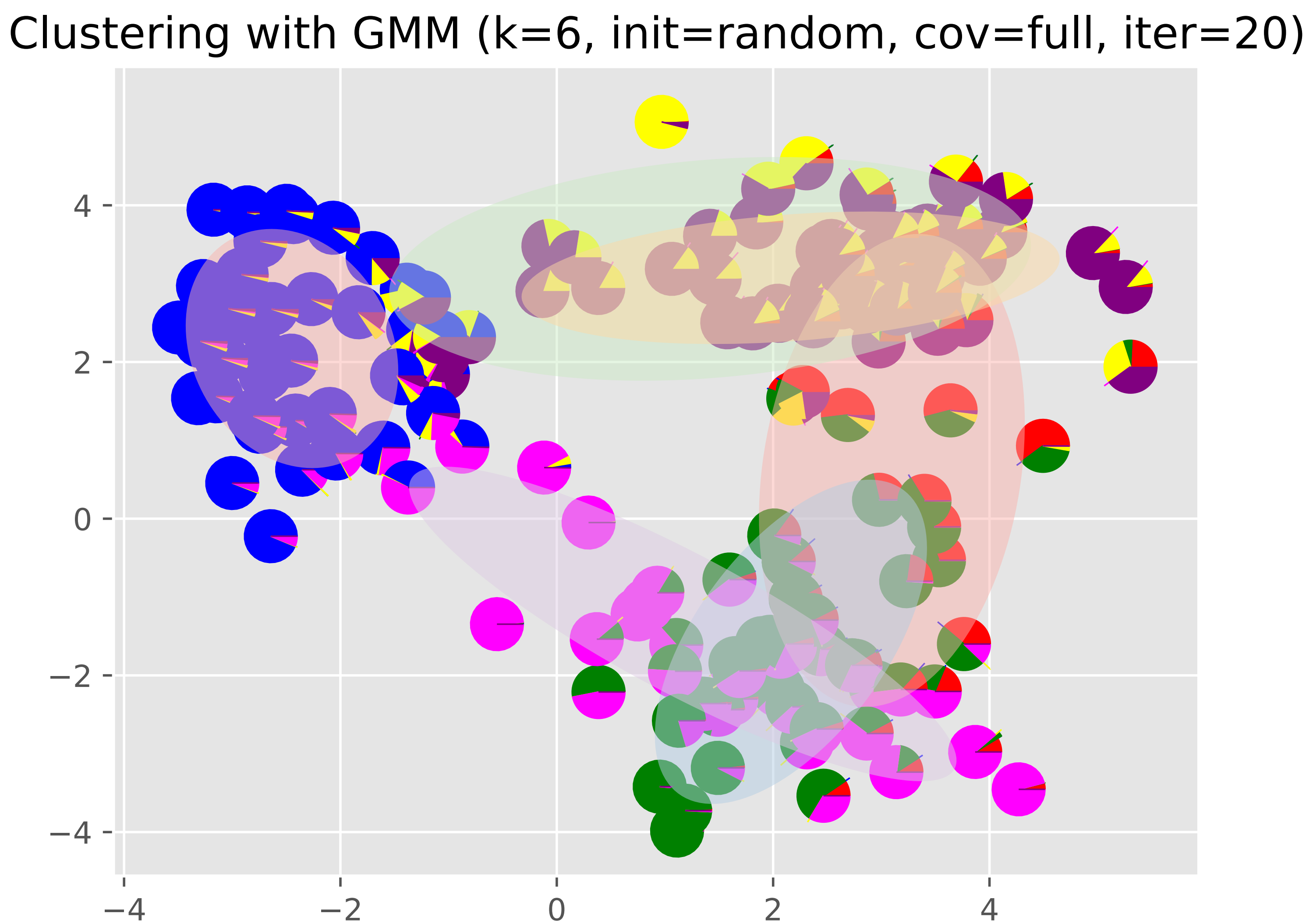
Clustering with GMM (k=6, init=random, cov=full, iter=10)
4
2
0
−2
−4
−4
−2
0
2
4

Example: GMM



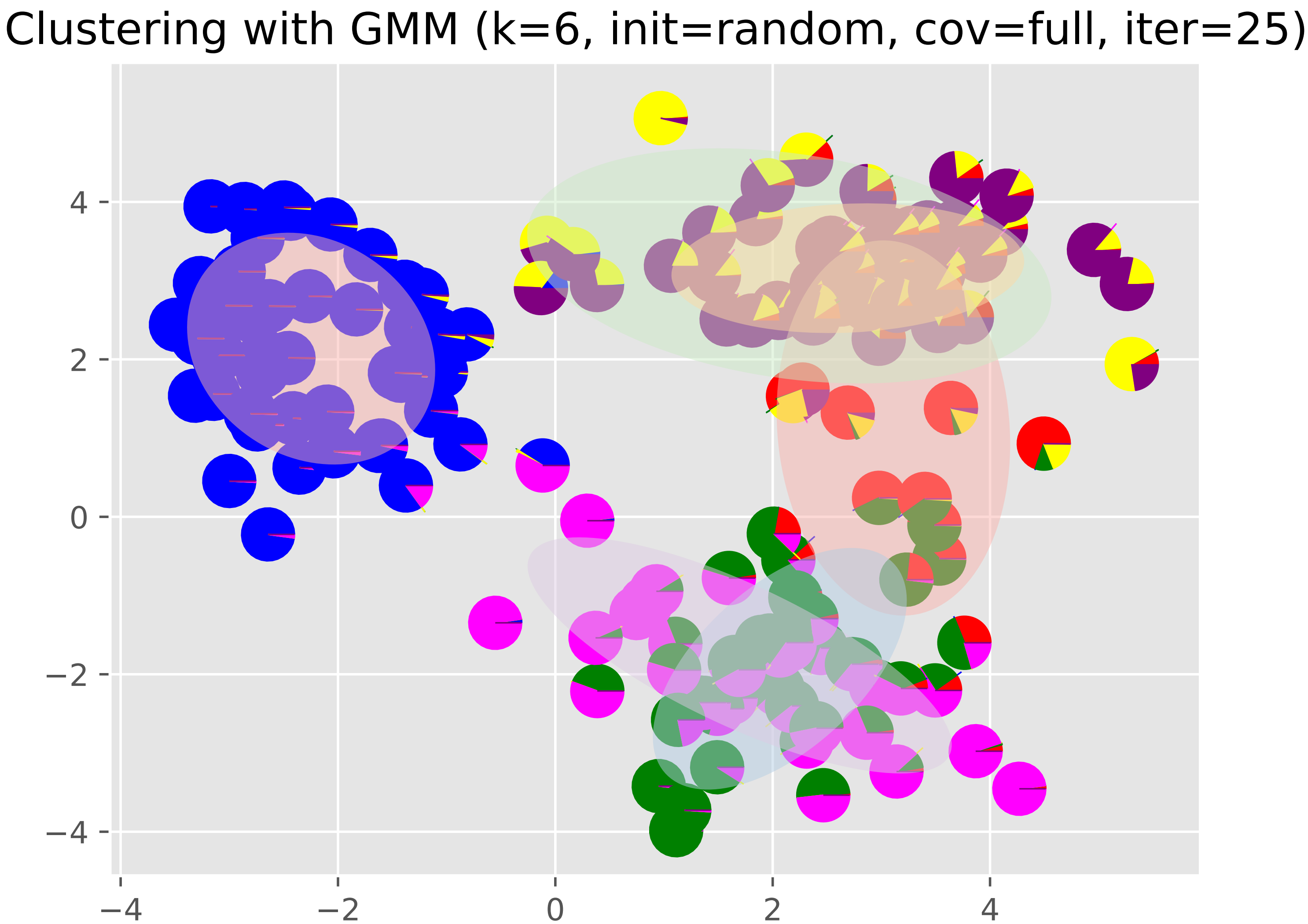
Clustering with GMM (k=6, init=random, cov=full, iter=15)
4
2
0
−2
−4
−4
−2
0
2
4

Example: GMM



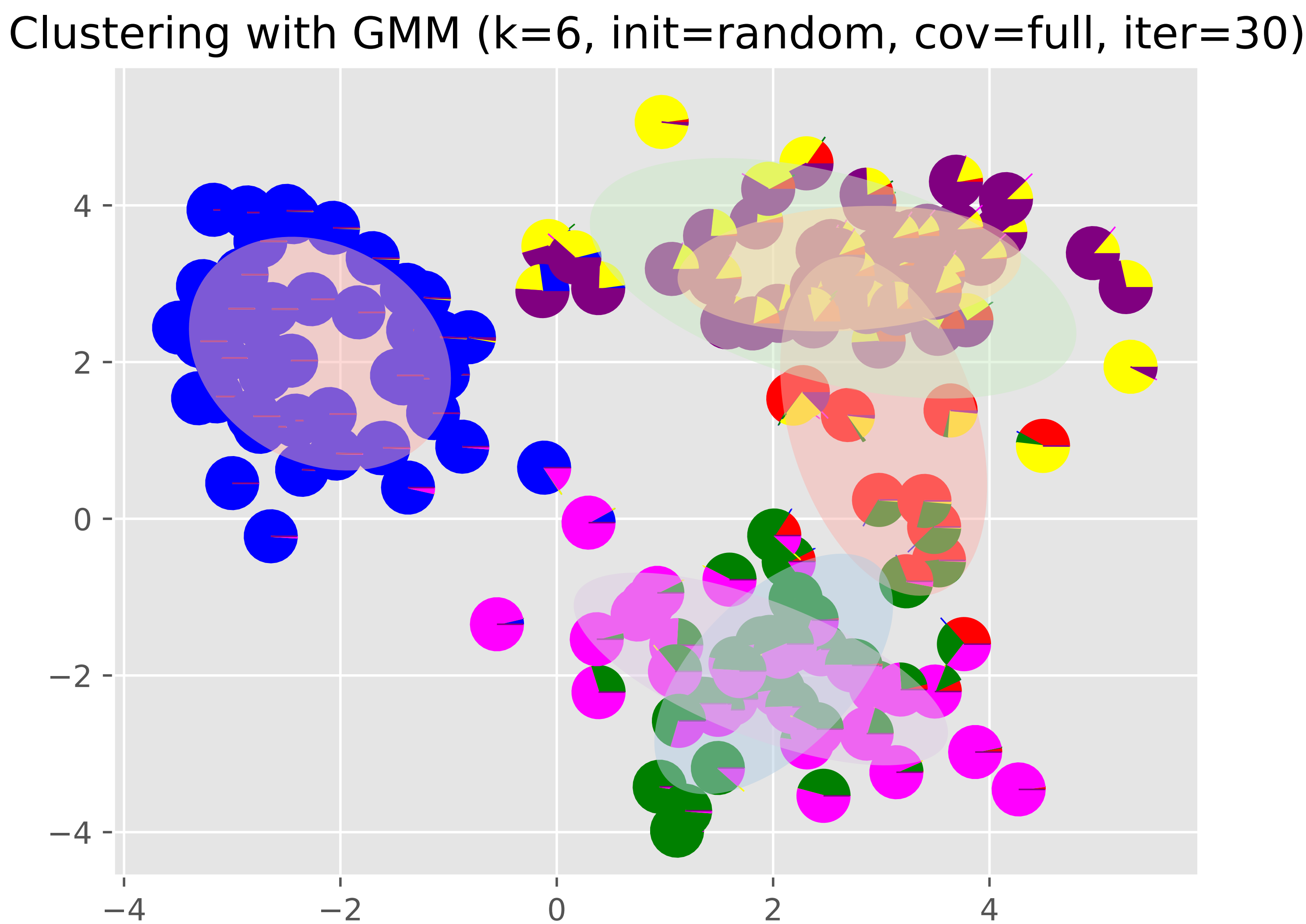
Clustering with GMM (k=6, init=random, cov=full, iter=20)
4
2
0
−2
−4
−4
−2
0
2
4

Example: GMM



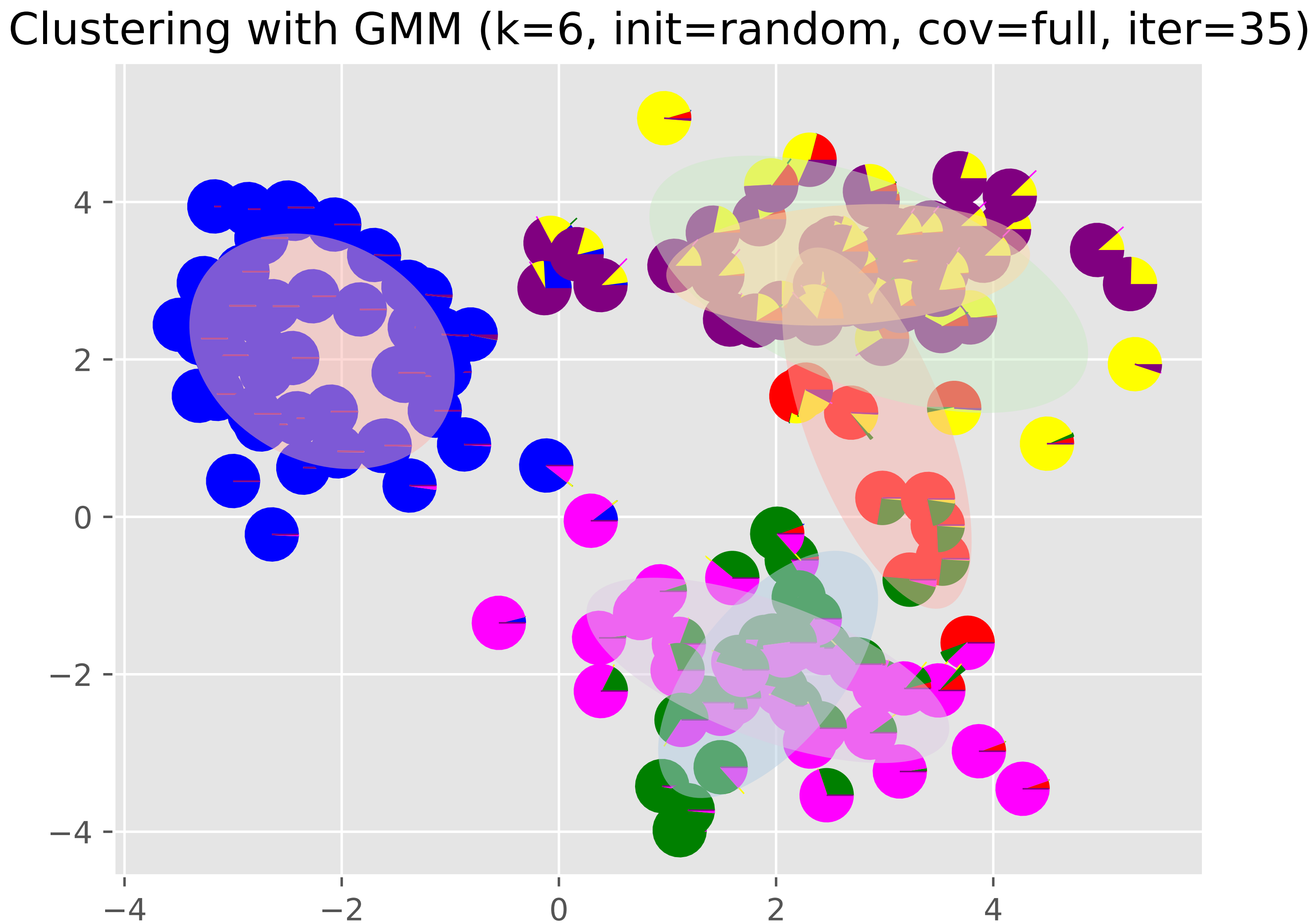
Clustering with GMM (k=6, init=random, cov=full, iter=25)
4
2
0
−2
−4
−4
−2
0
2
4

Example: GMM



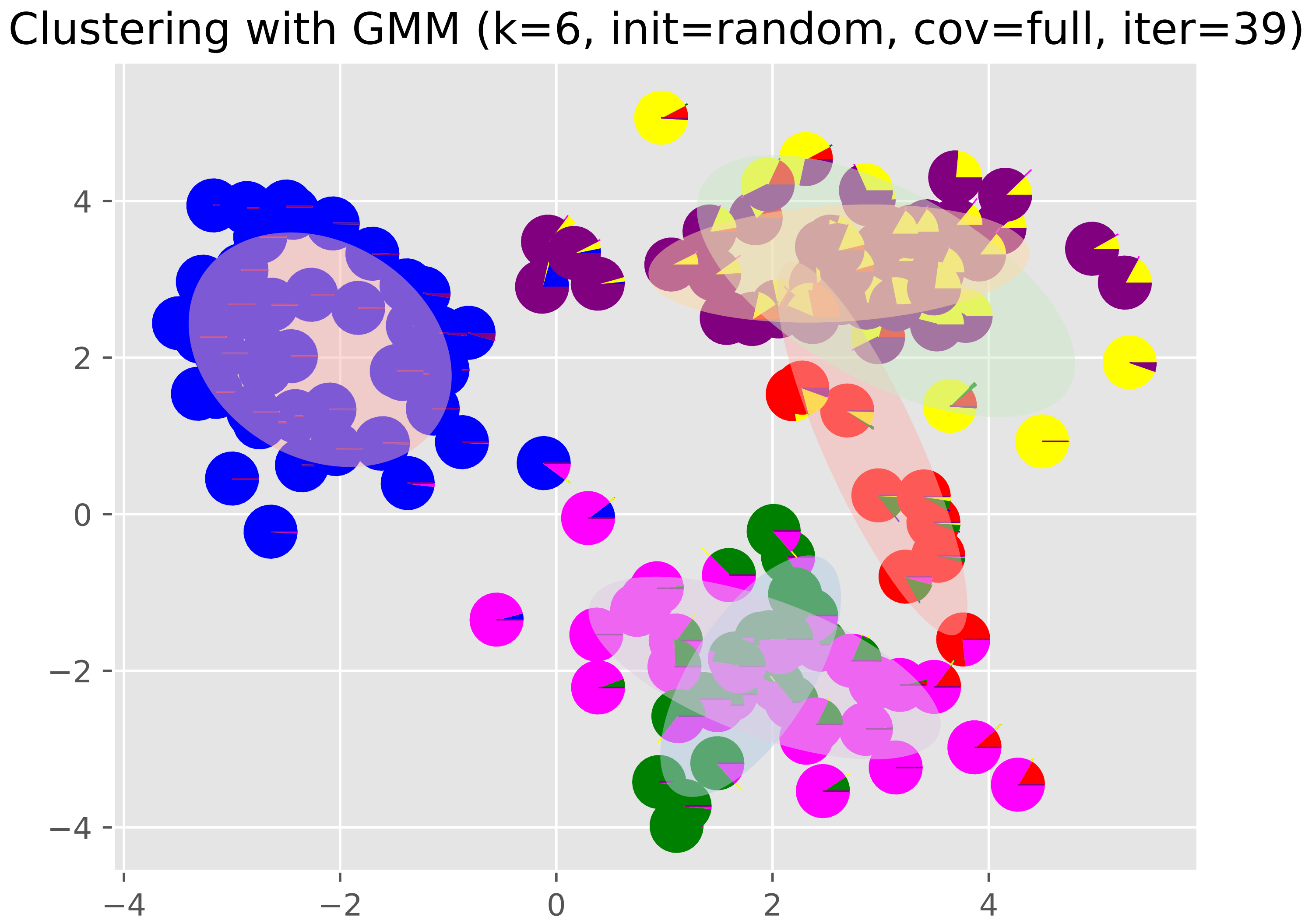
Clustering with GMM (k=6, init=random, cov=full, iter=30)
4
2
0
−2
−4
−4
−2
0
2
4

Example: GMM



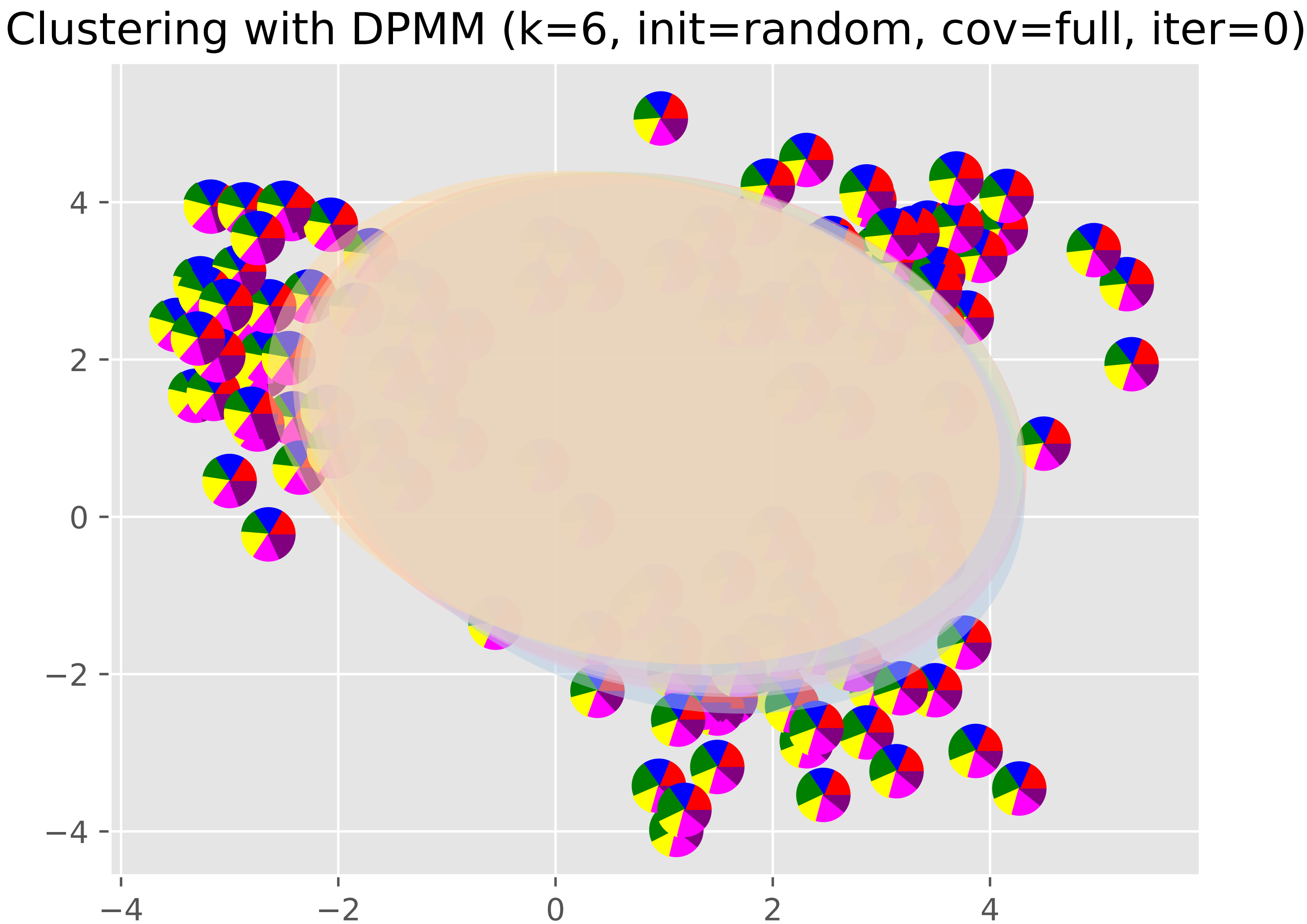
Clustering with GMM (k=6, init=random, cov=full, iter=35)
4
2
0
−2
−4
−4
−2
0
2
4

Example: GMM

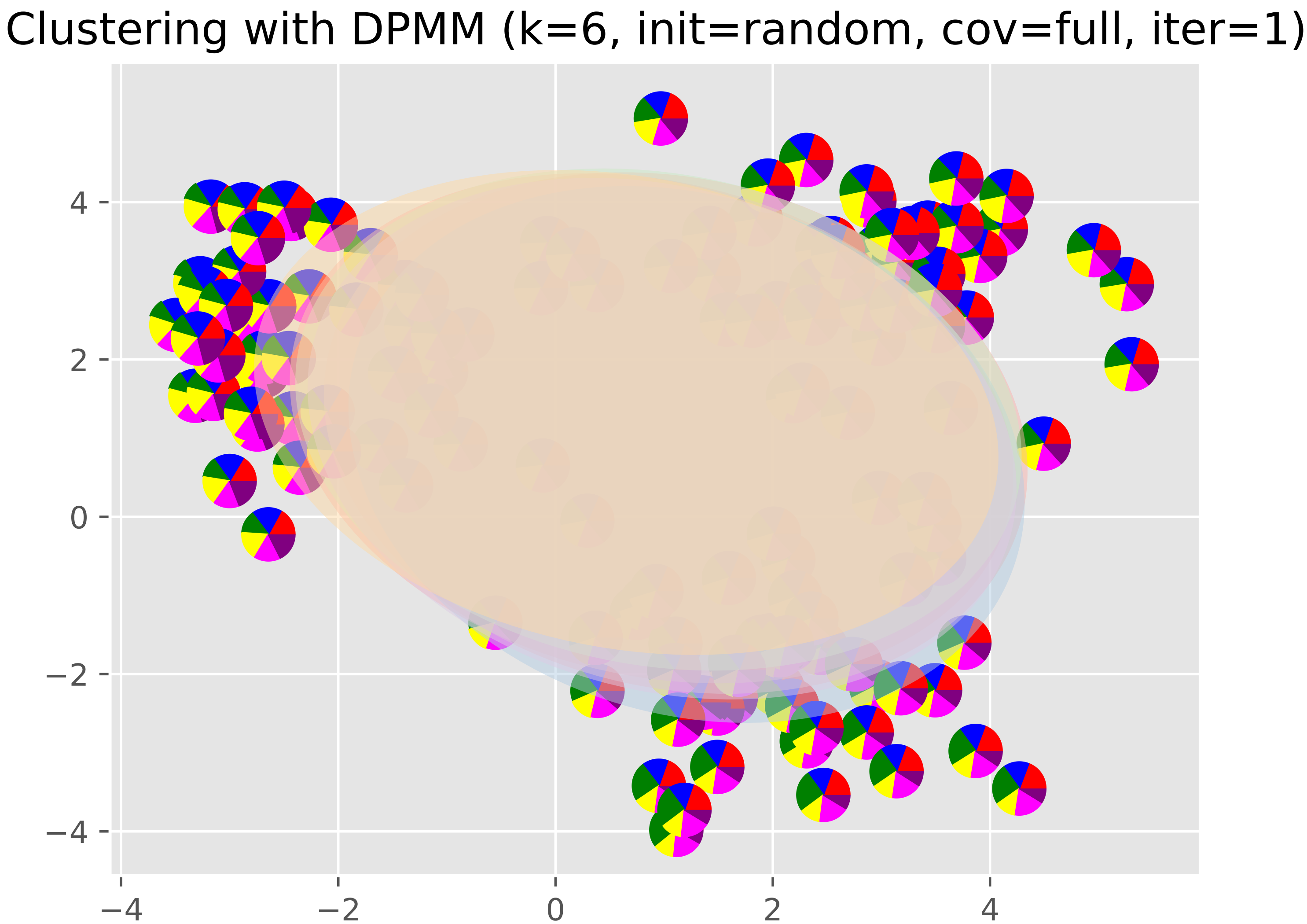


Clustering with GMM (k=6, init=random, cov=full, iter=39)
4
2
0
−2
−4
−4
−2
0
2
4

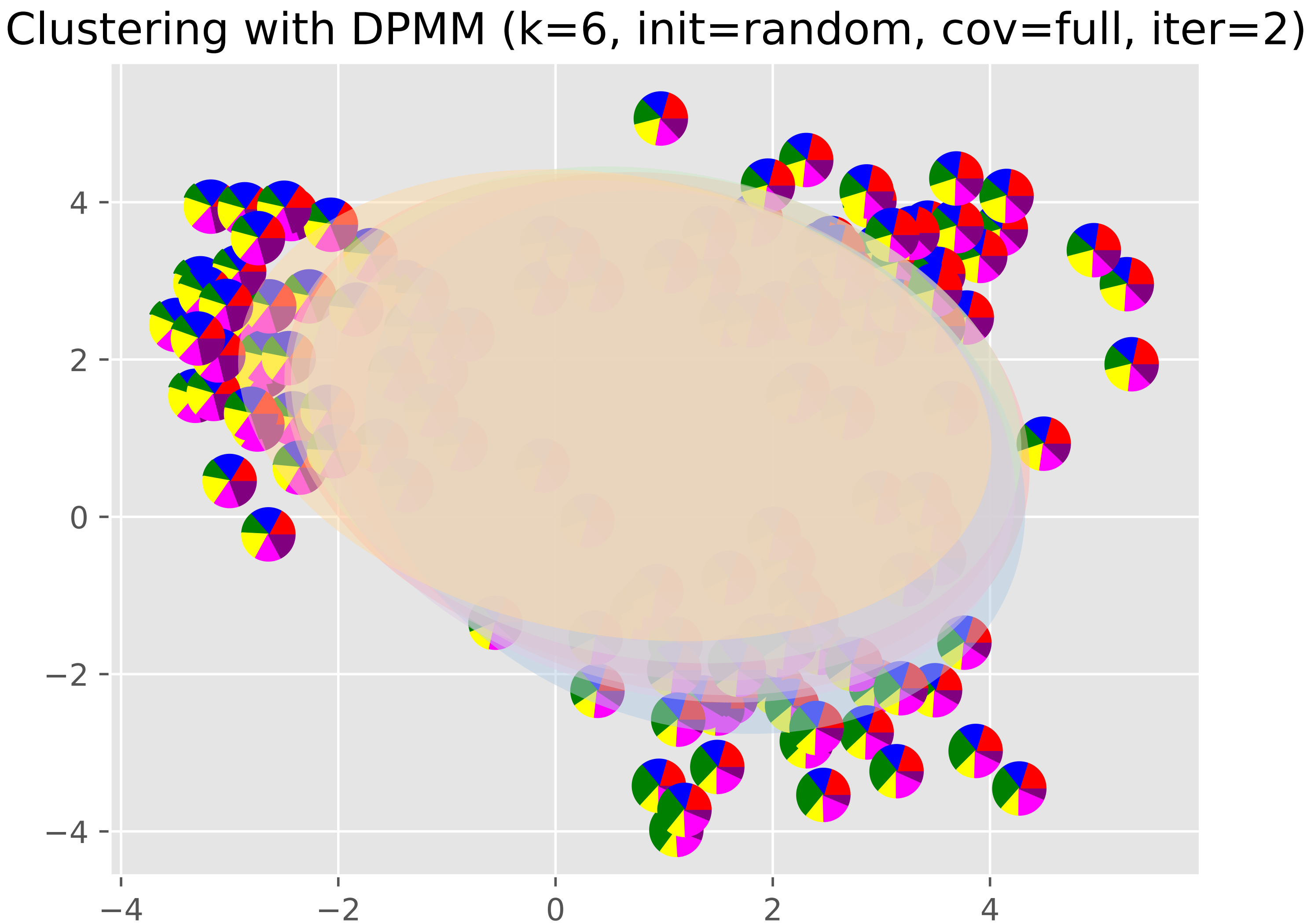
Example: DPMM



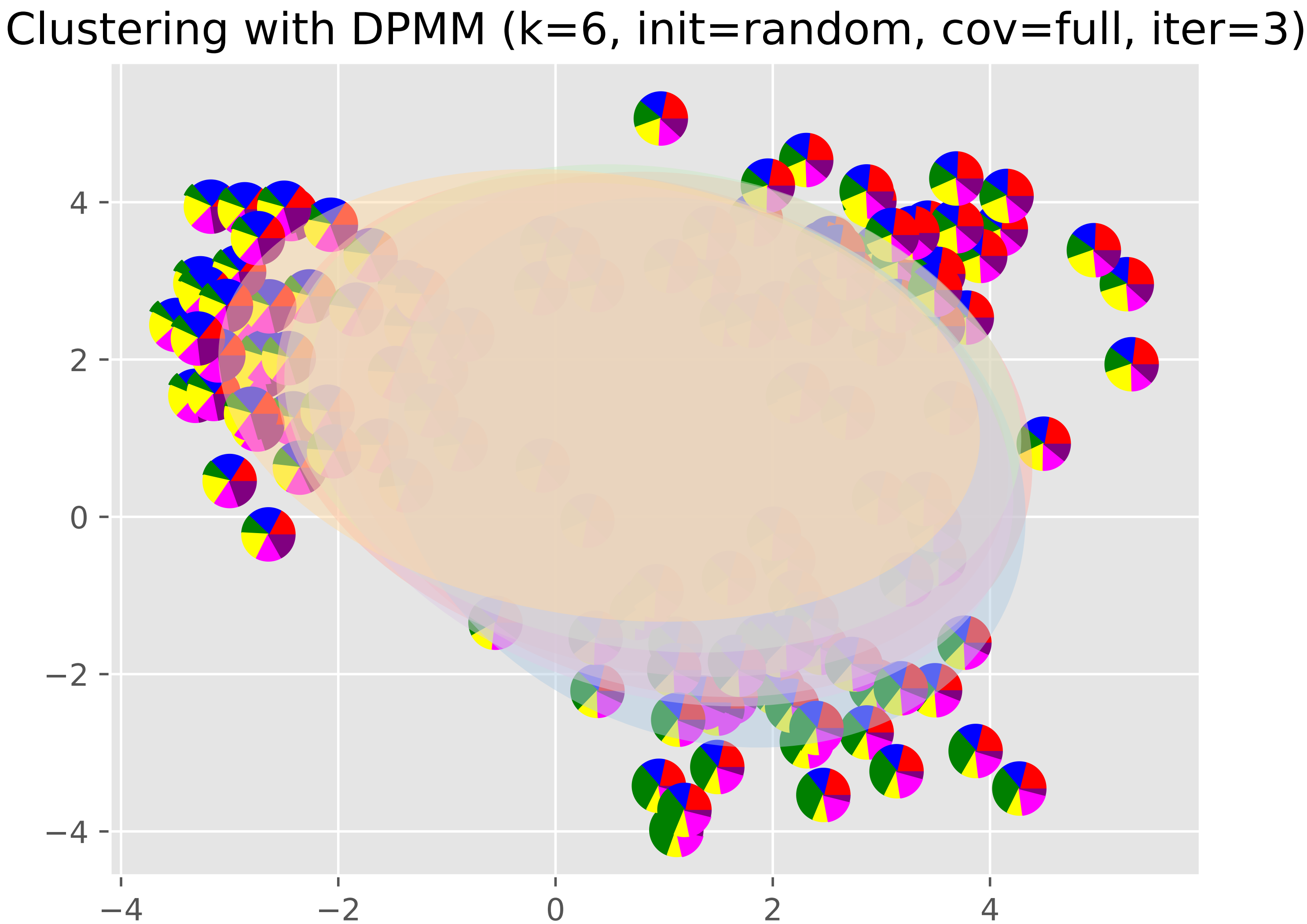
Example: DPMM



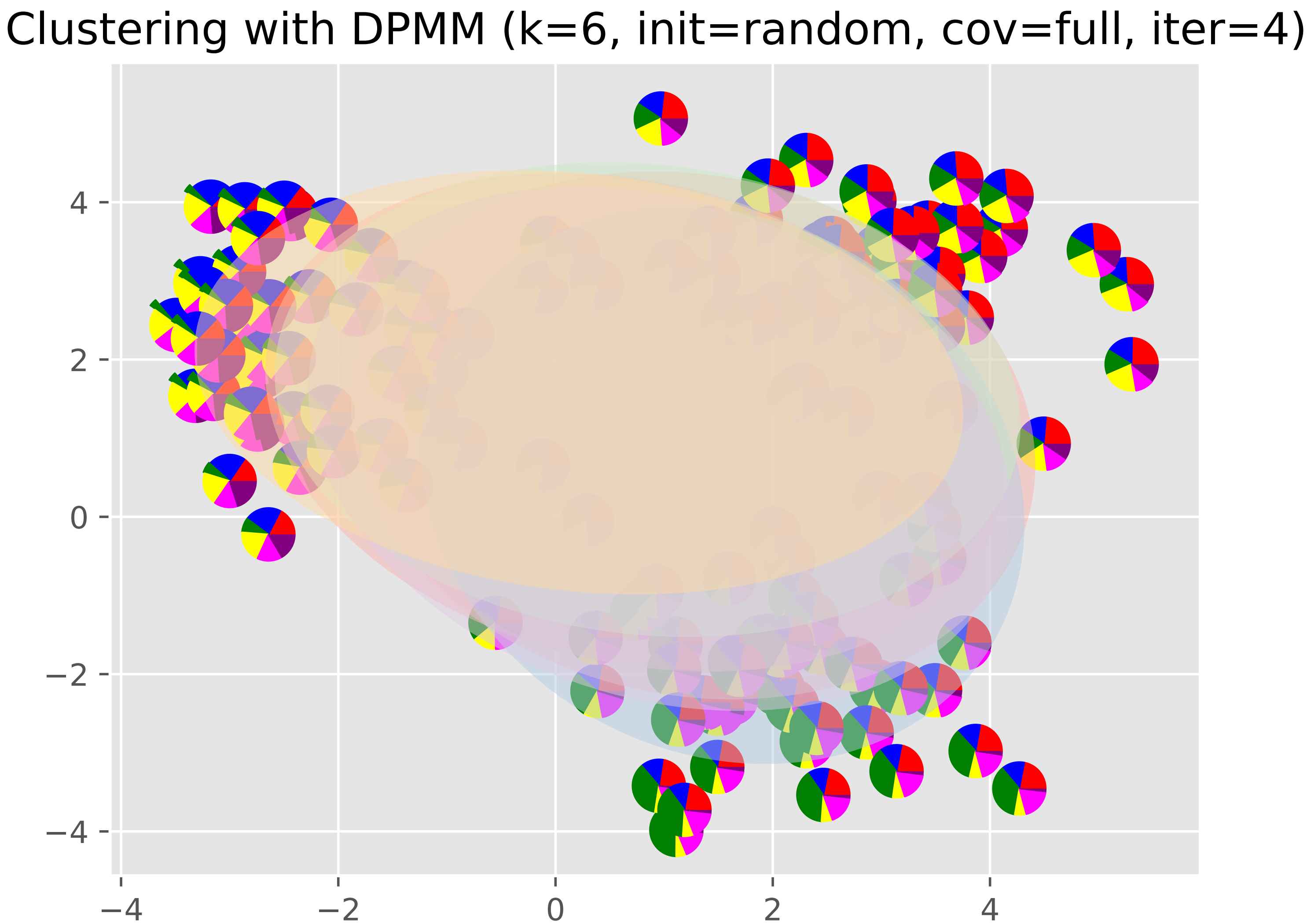
Example: DPMM



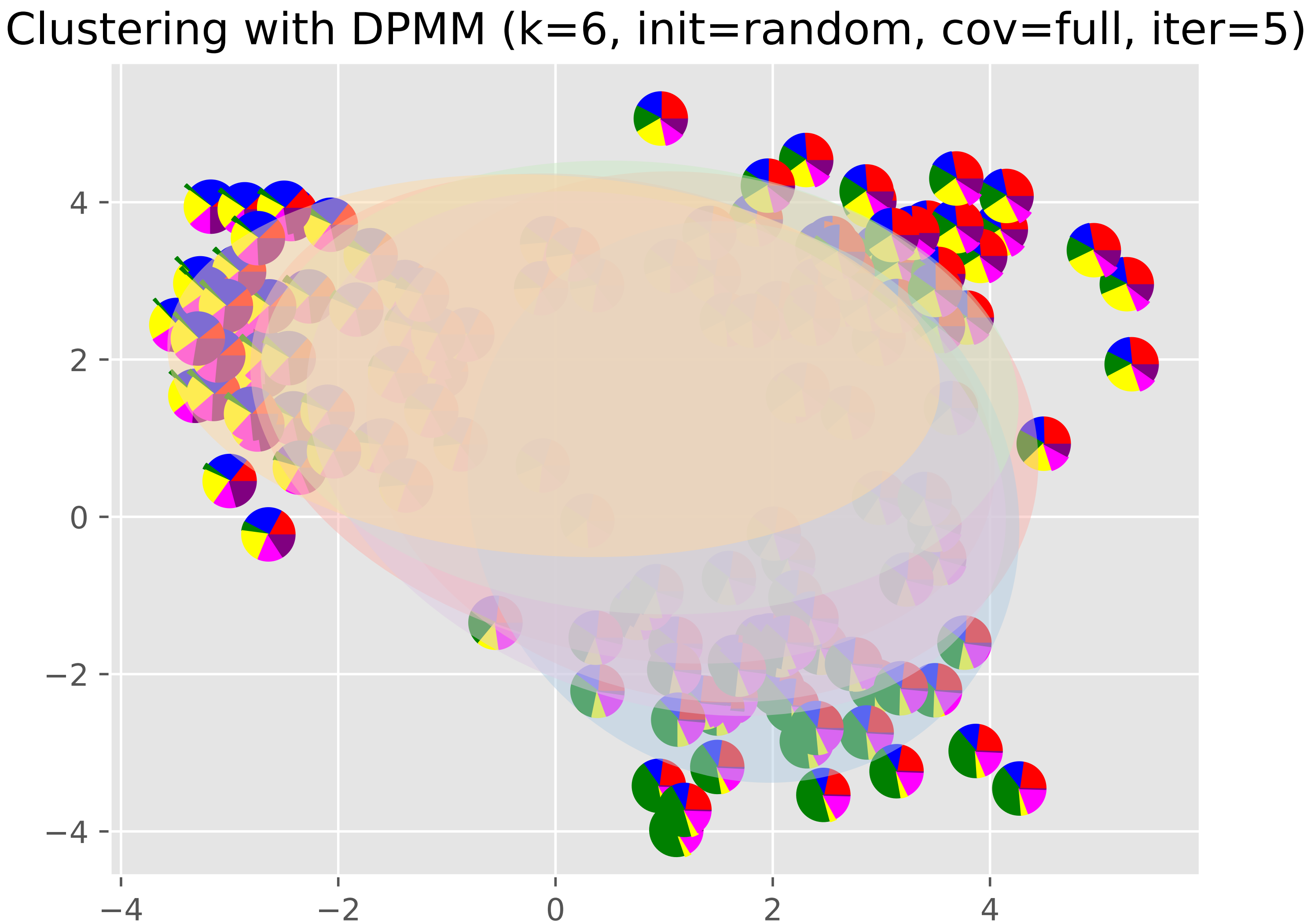
Example: DPMM



Example: DPMM



Example: DPMM



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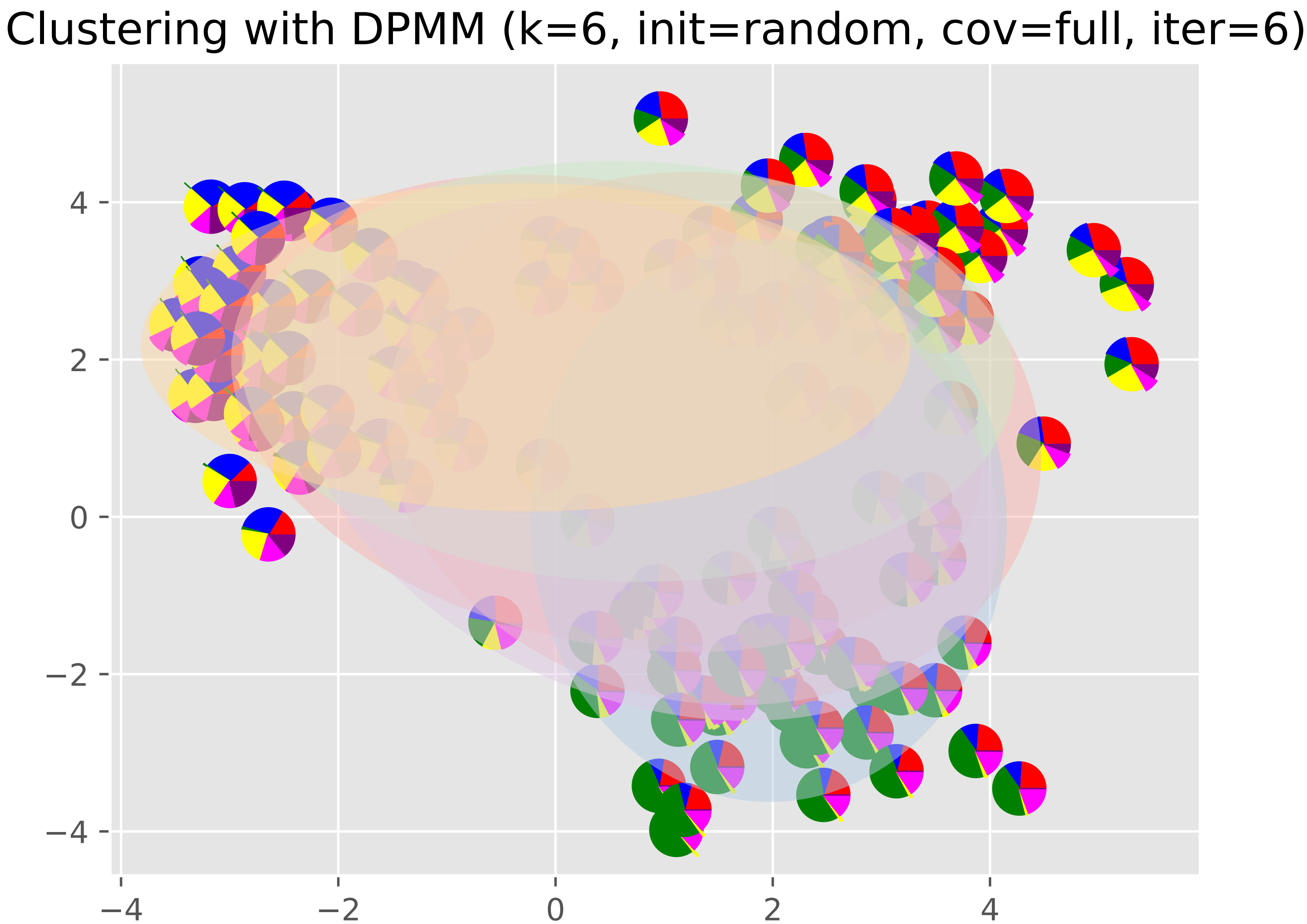

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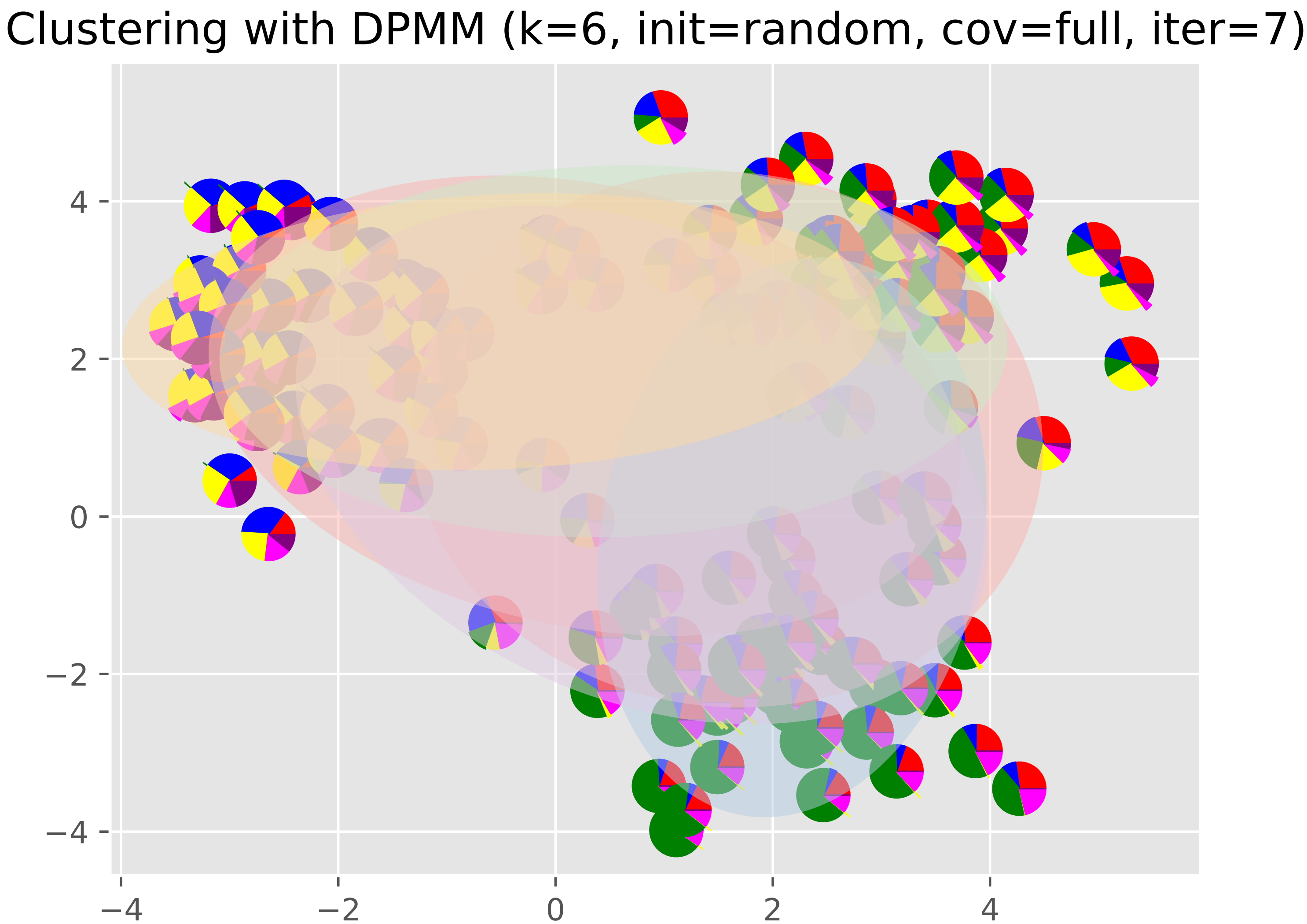

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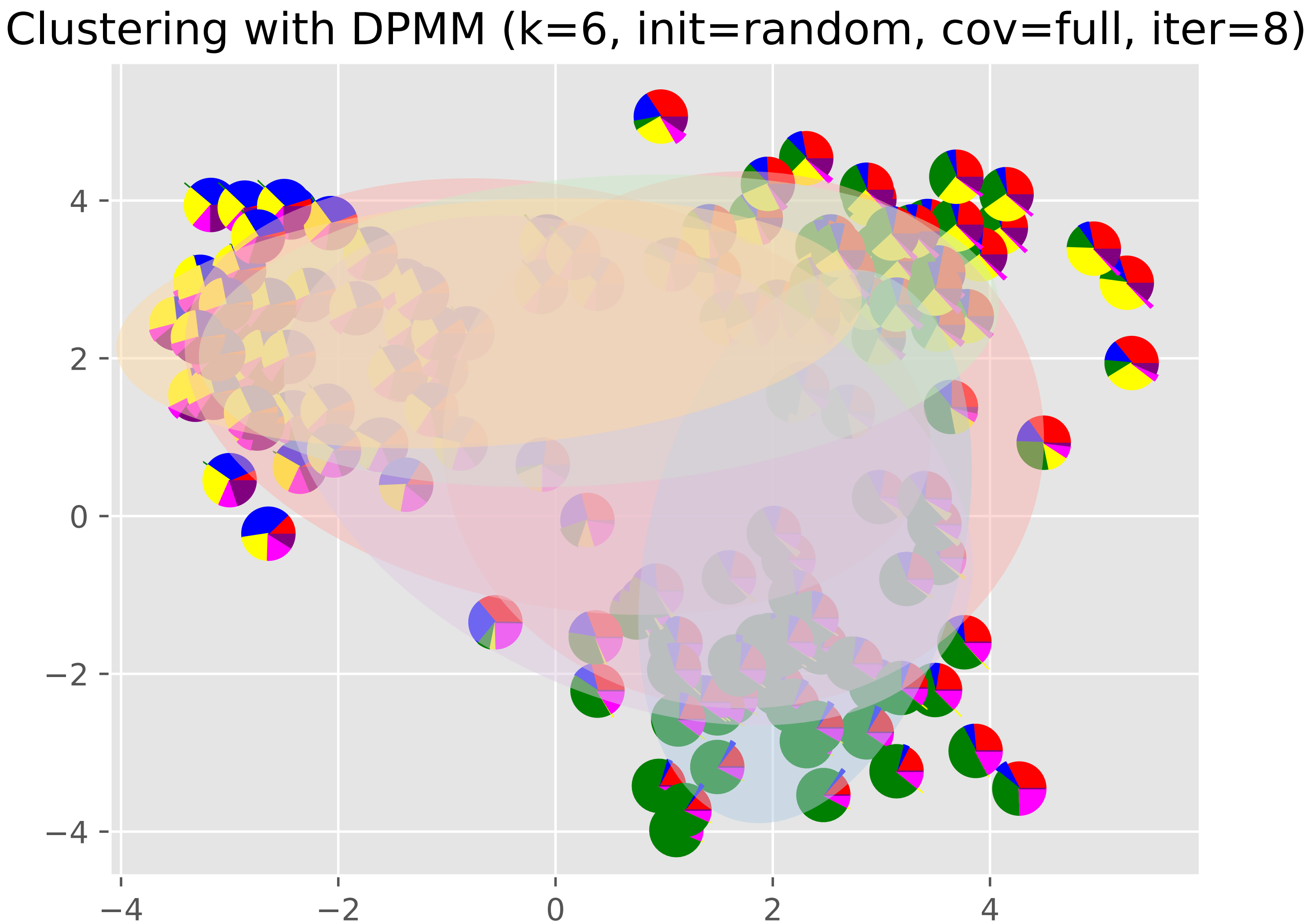
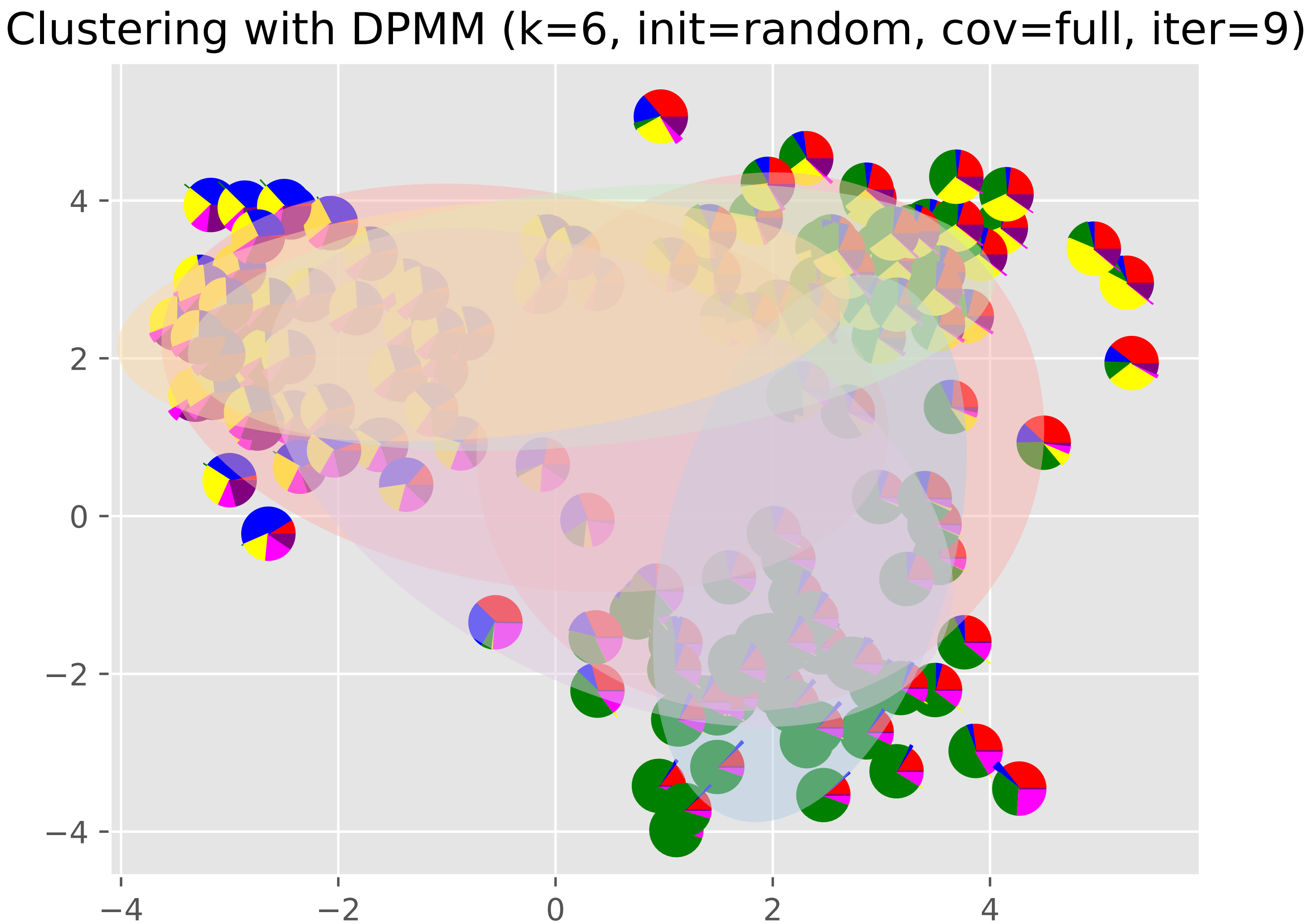
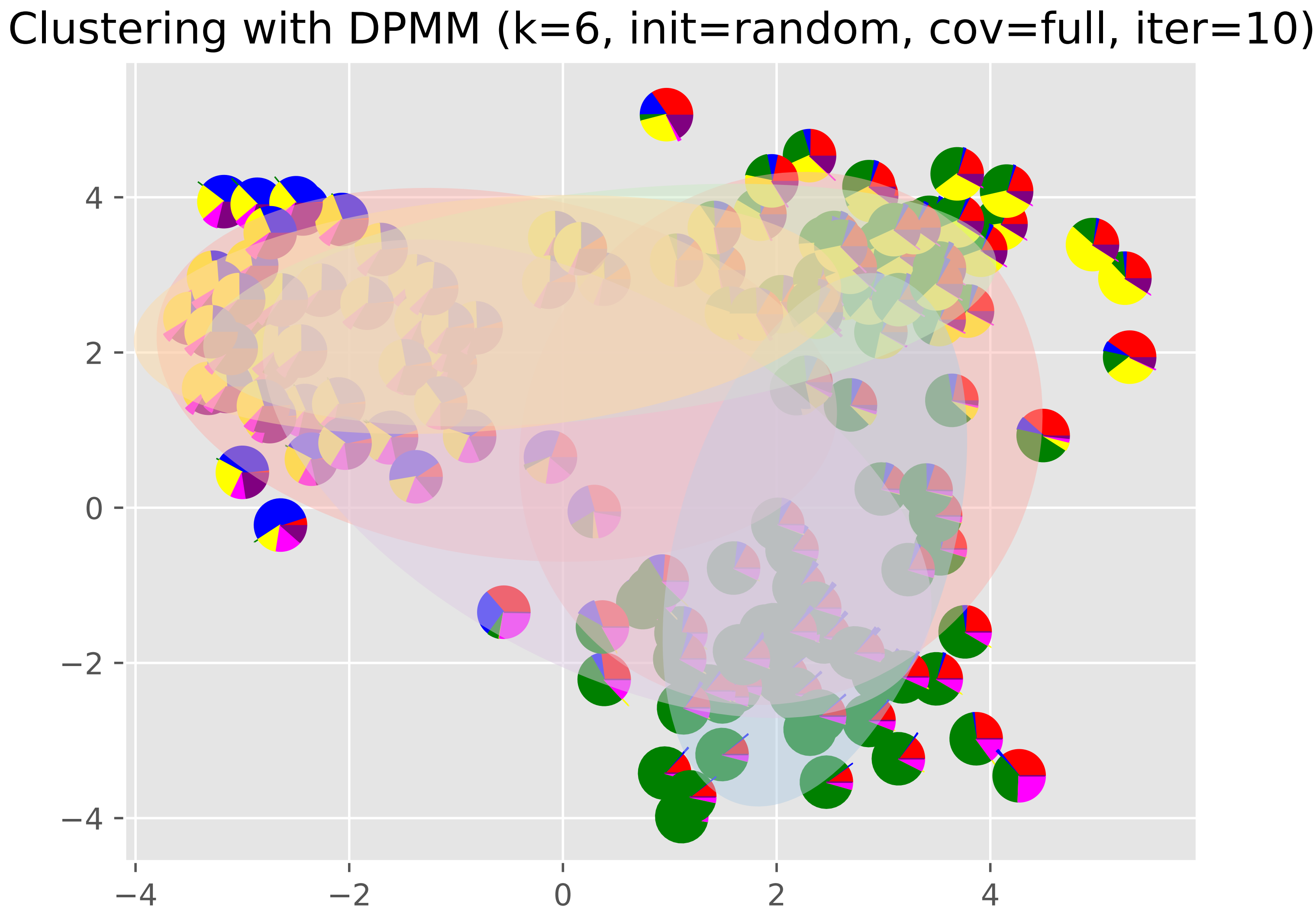


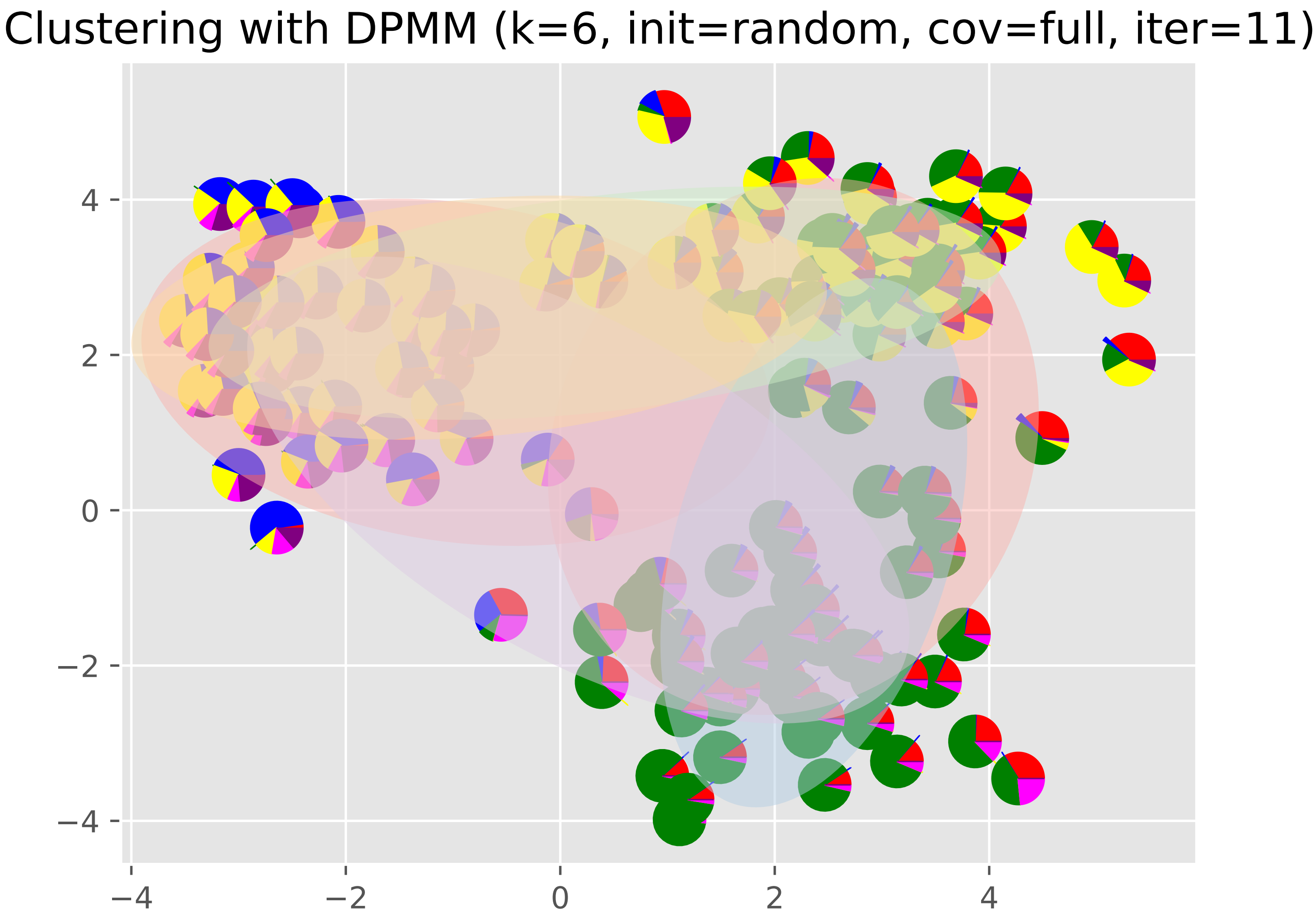
Example: DPMM



Example: DPMM



Example: DPMM



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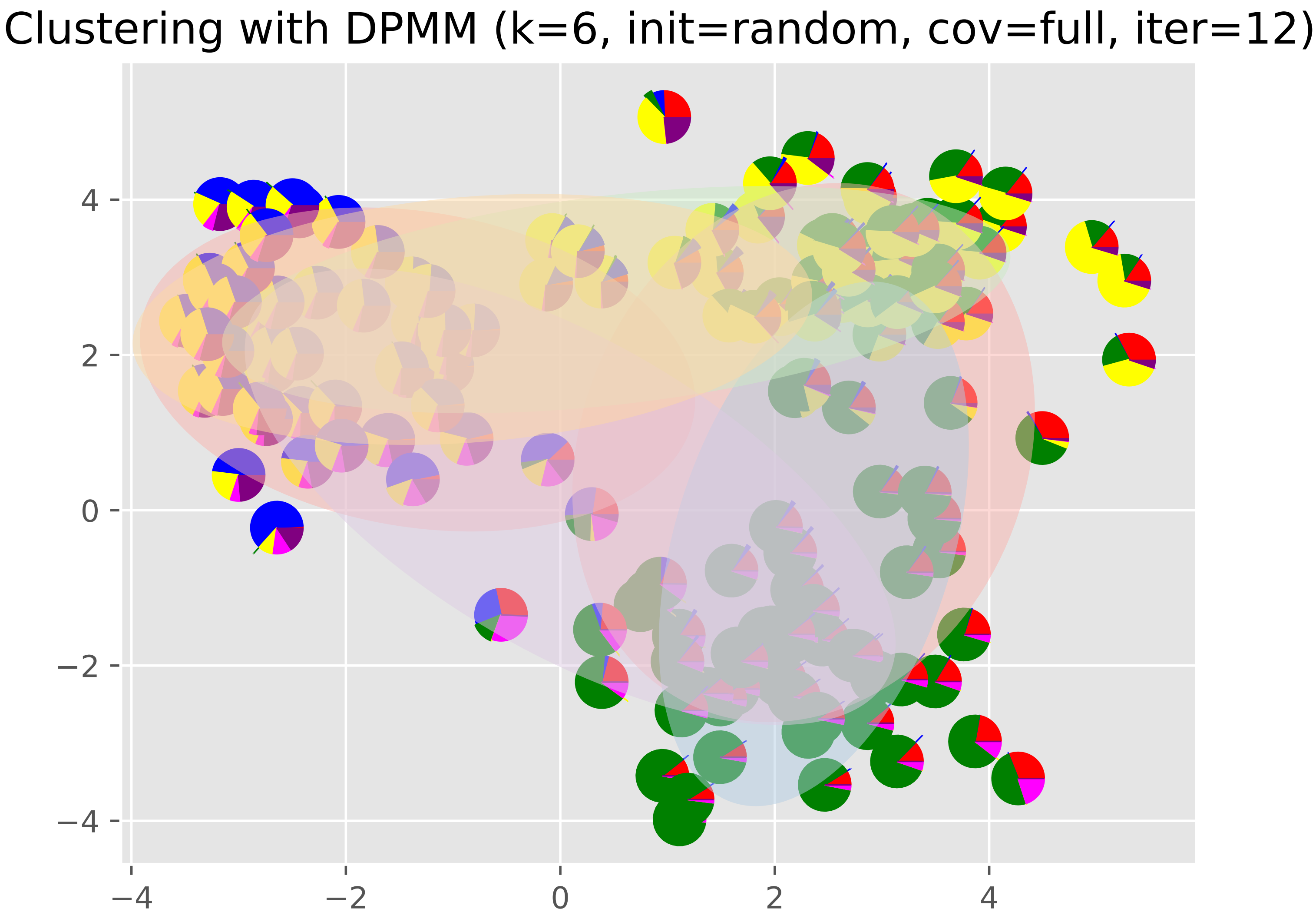
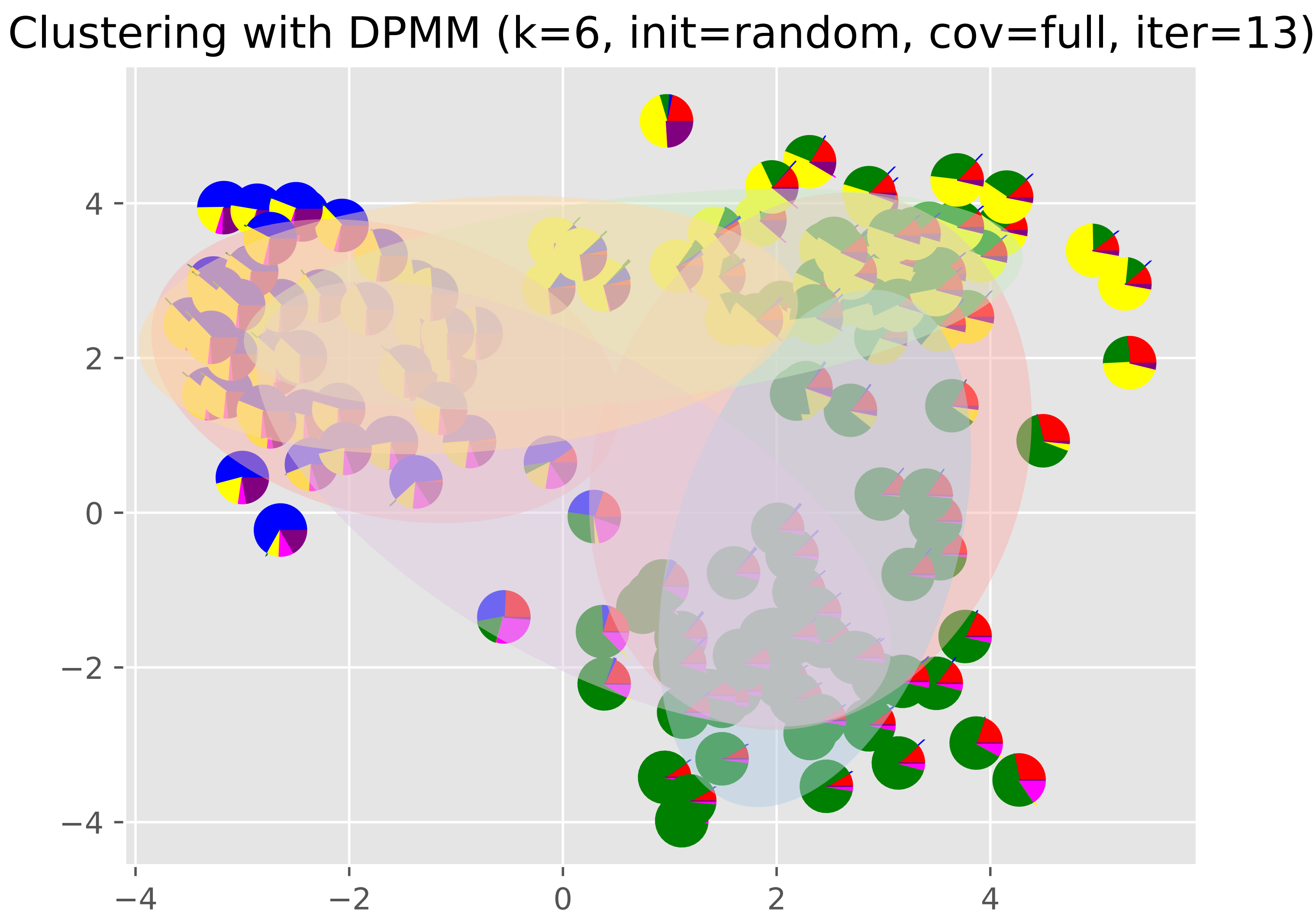


Example: DPMM



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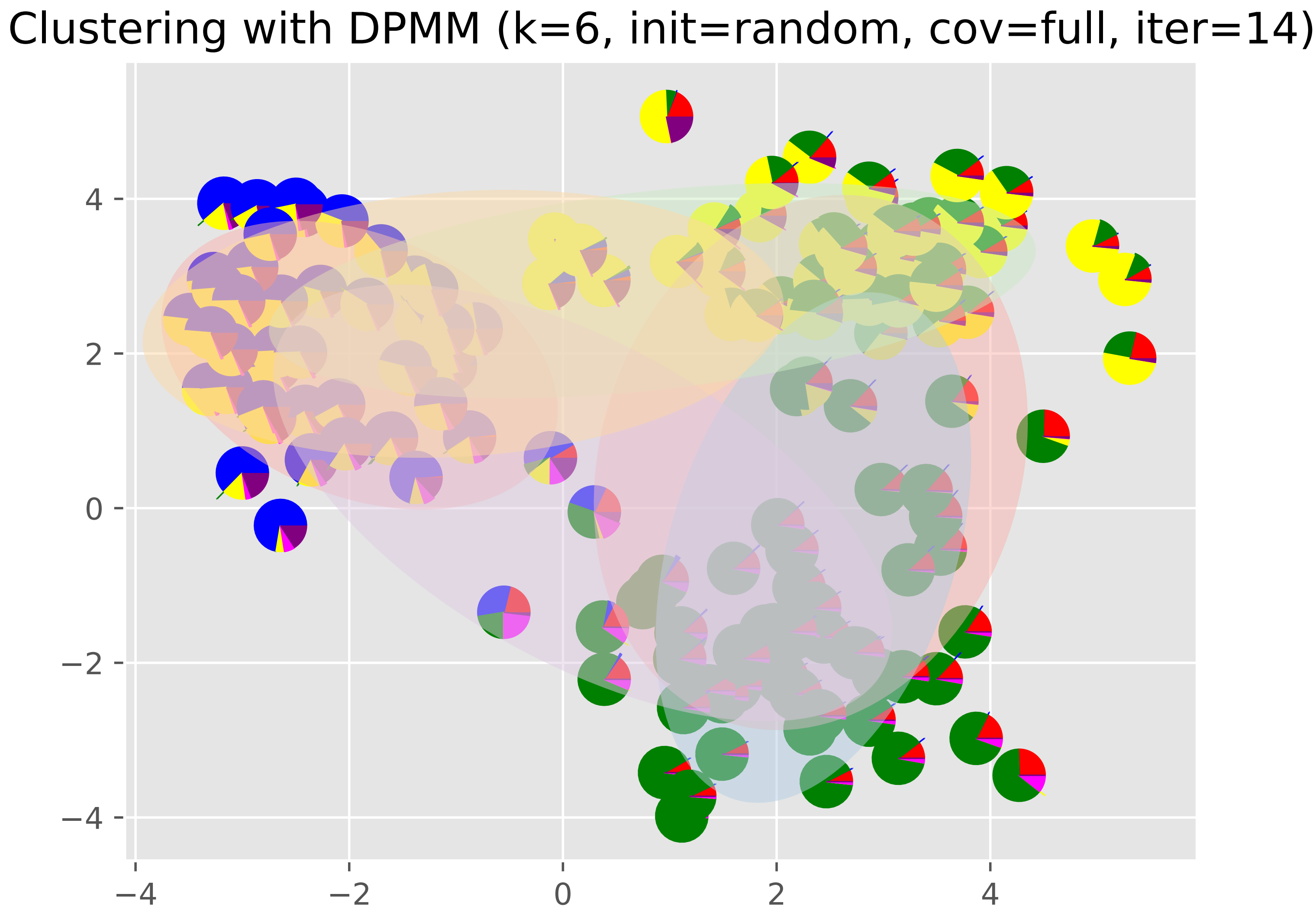

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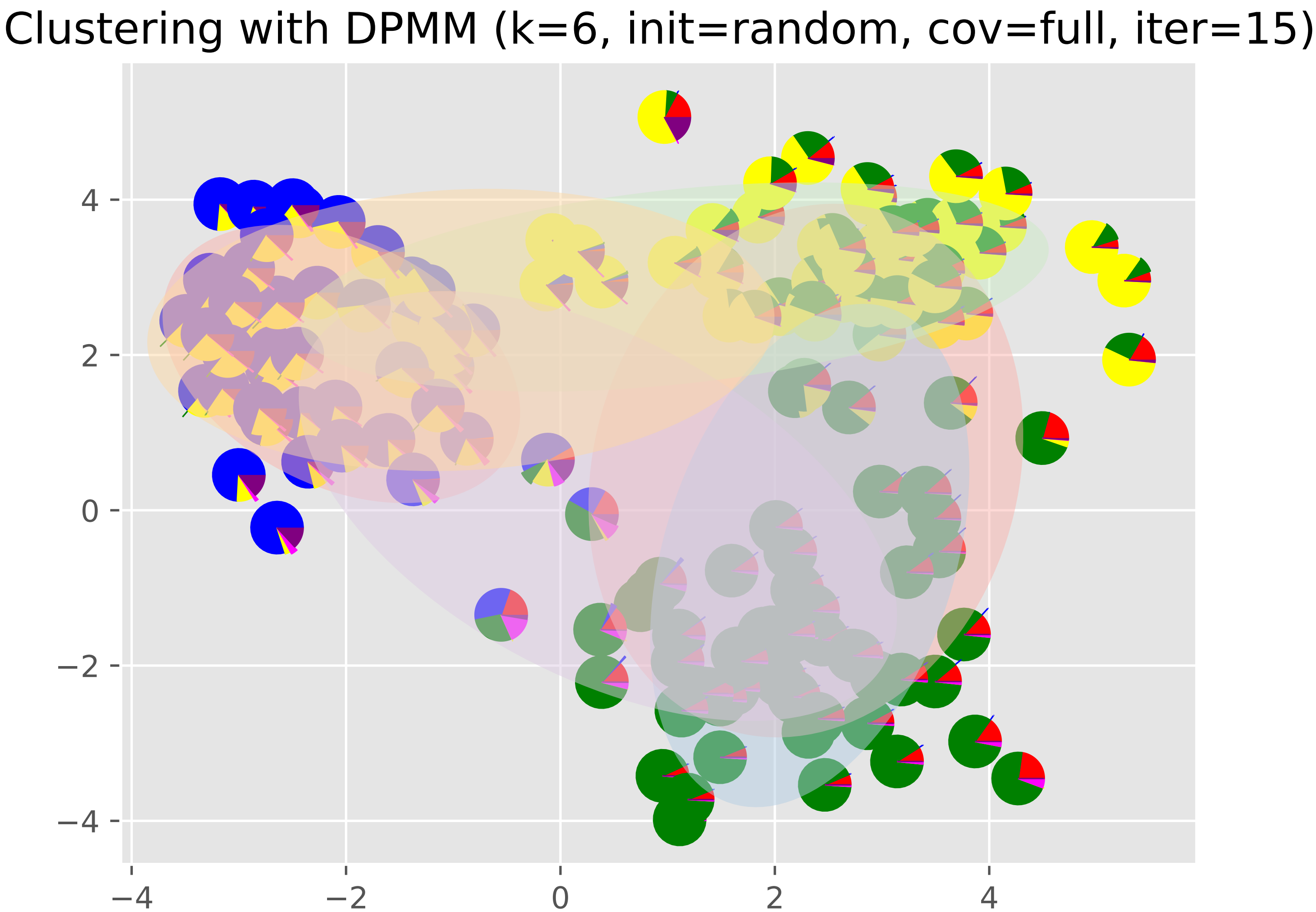

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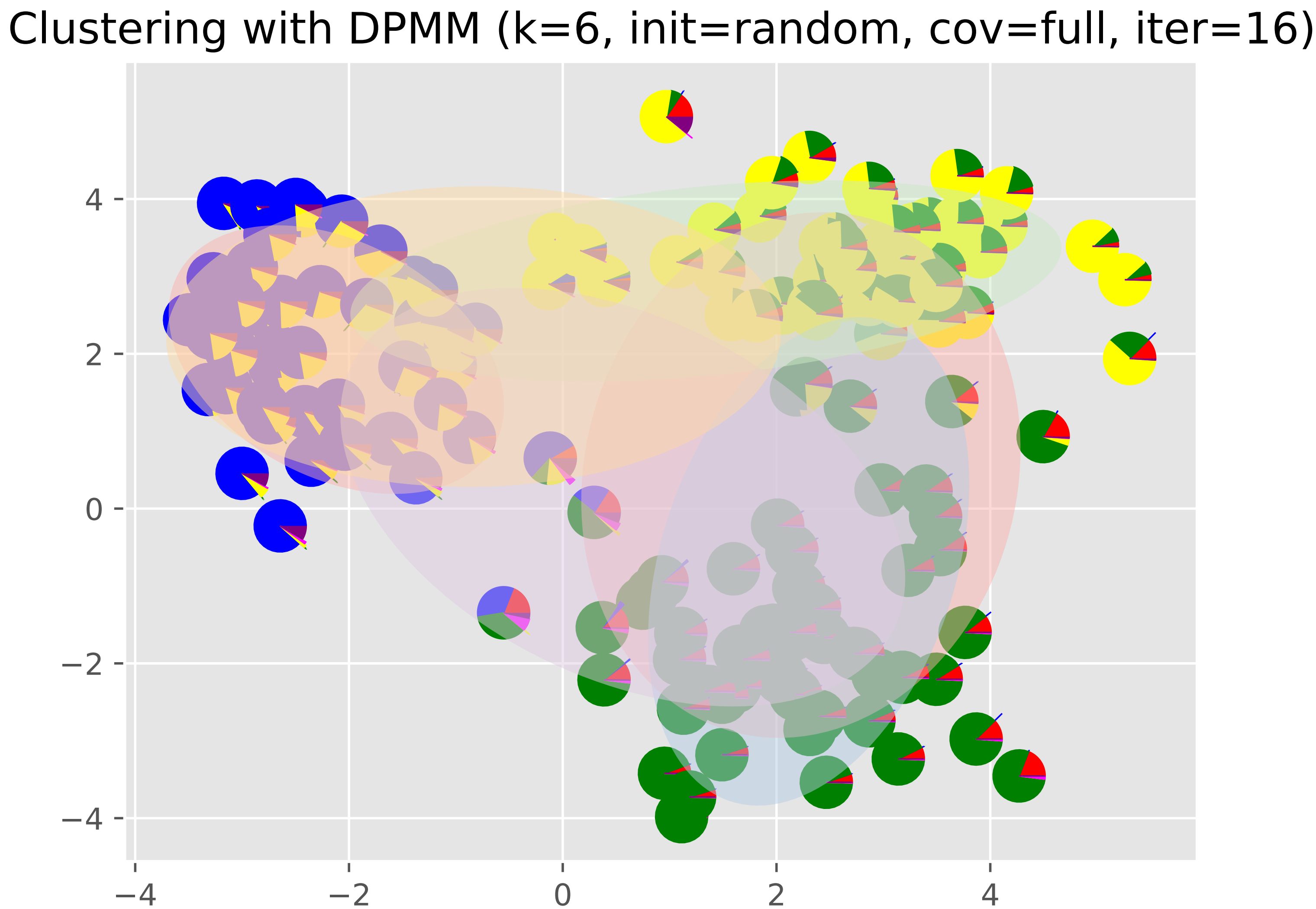
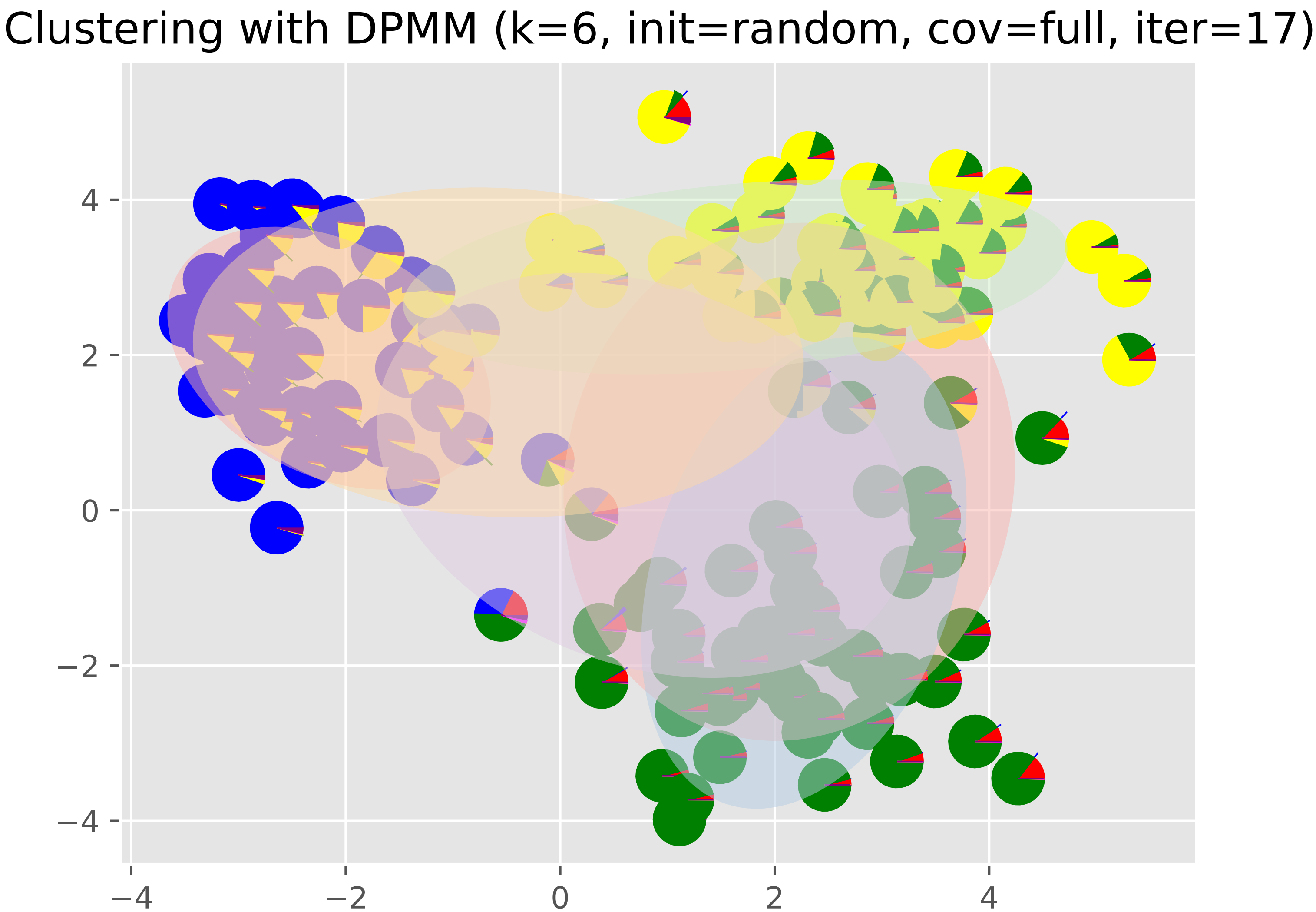


Example: DPMM



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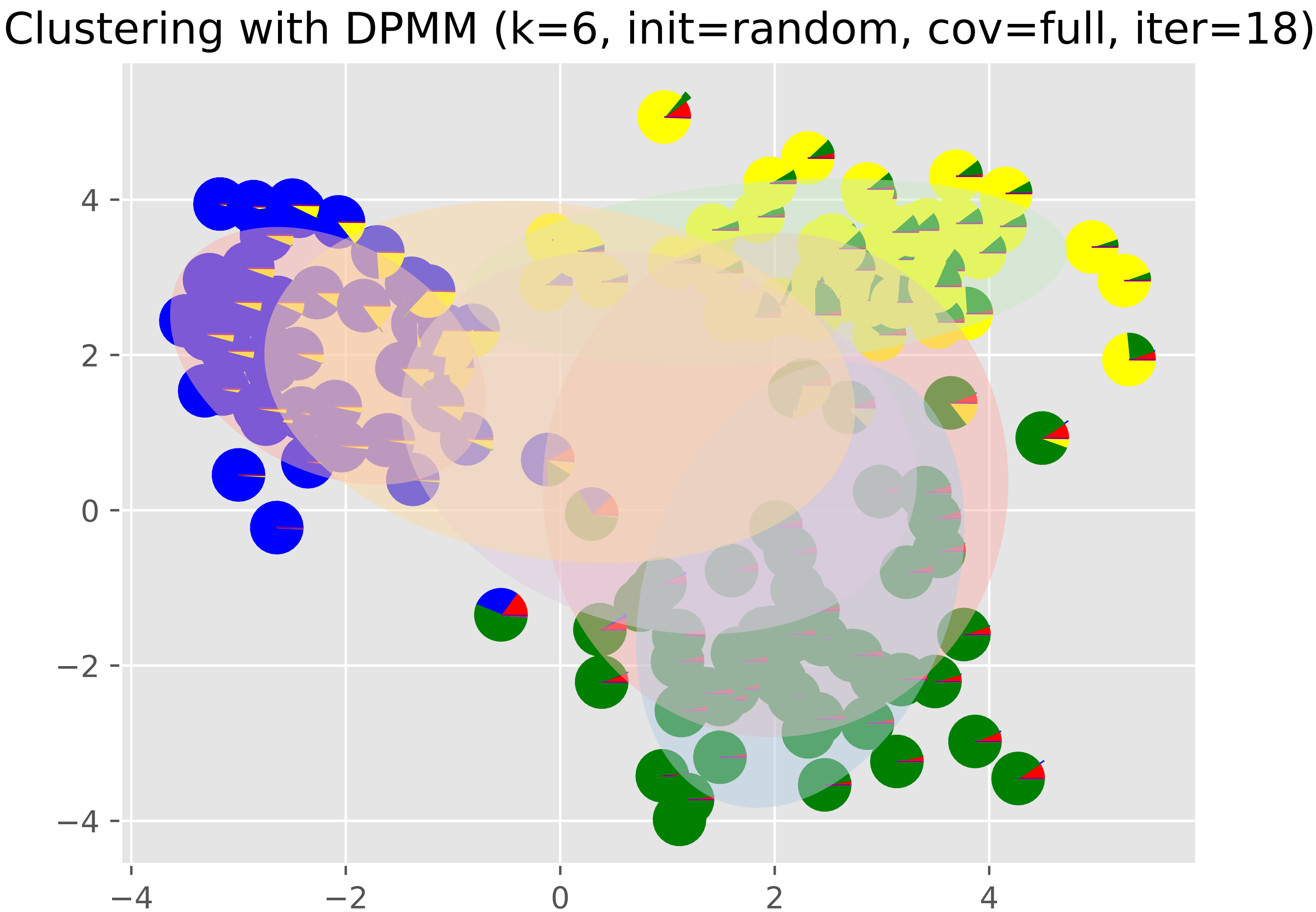

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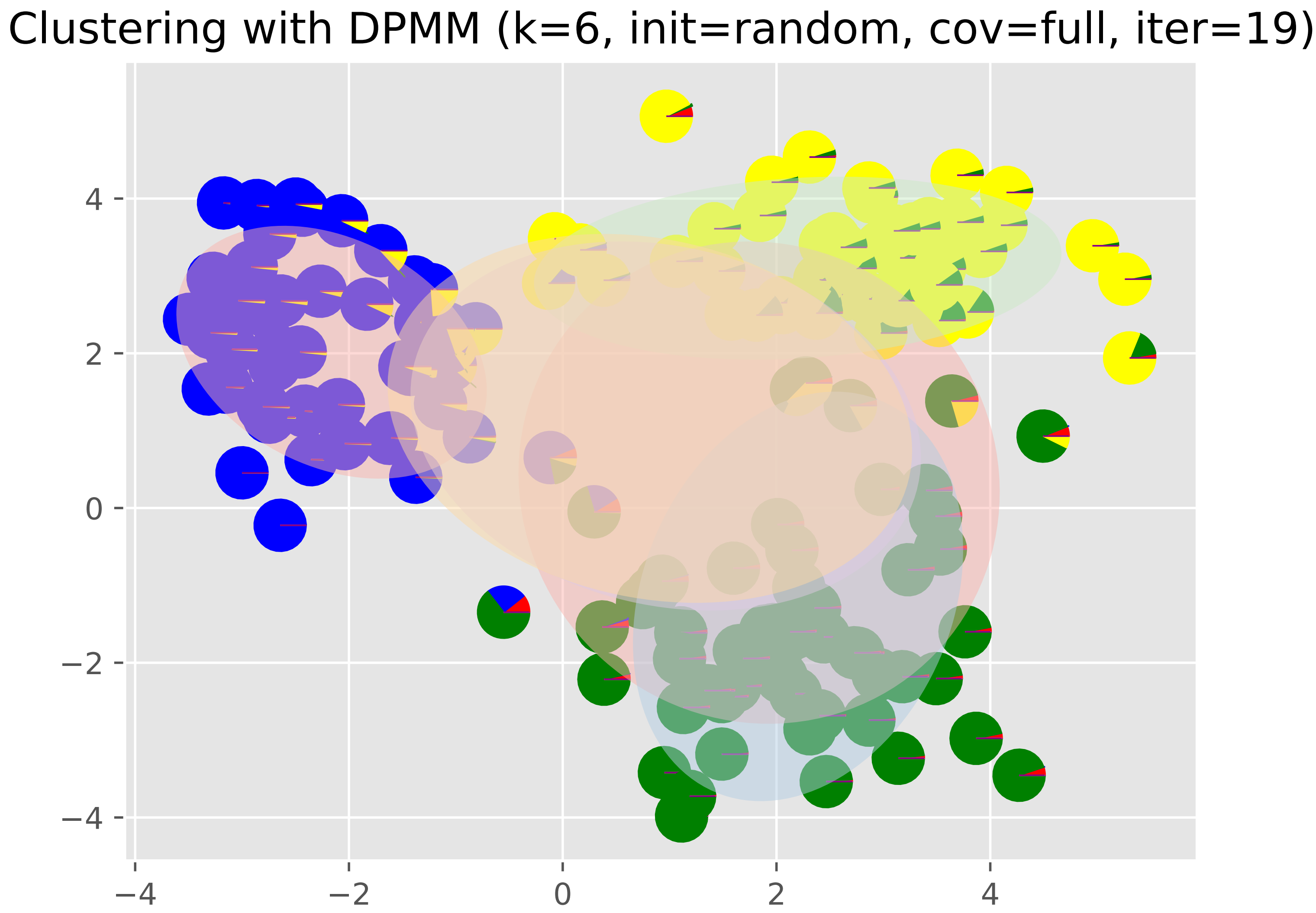

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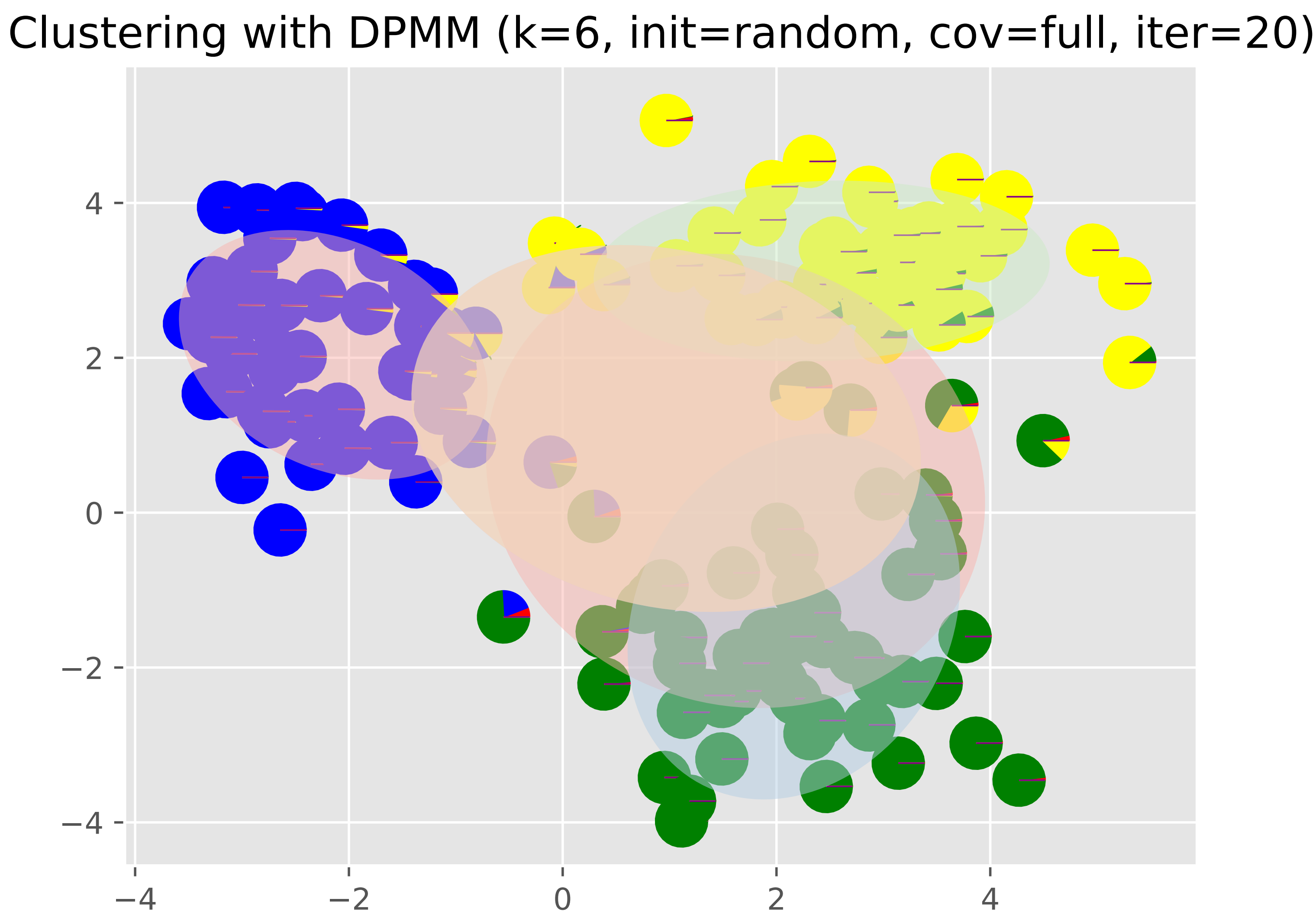

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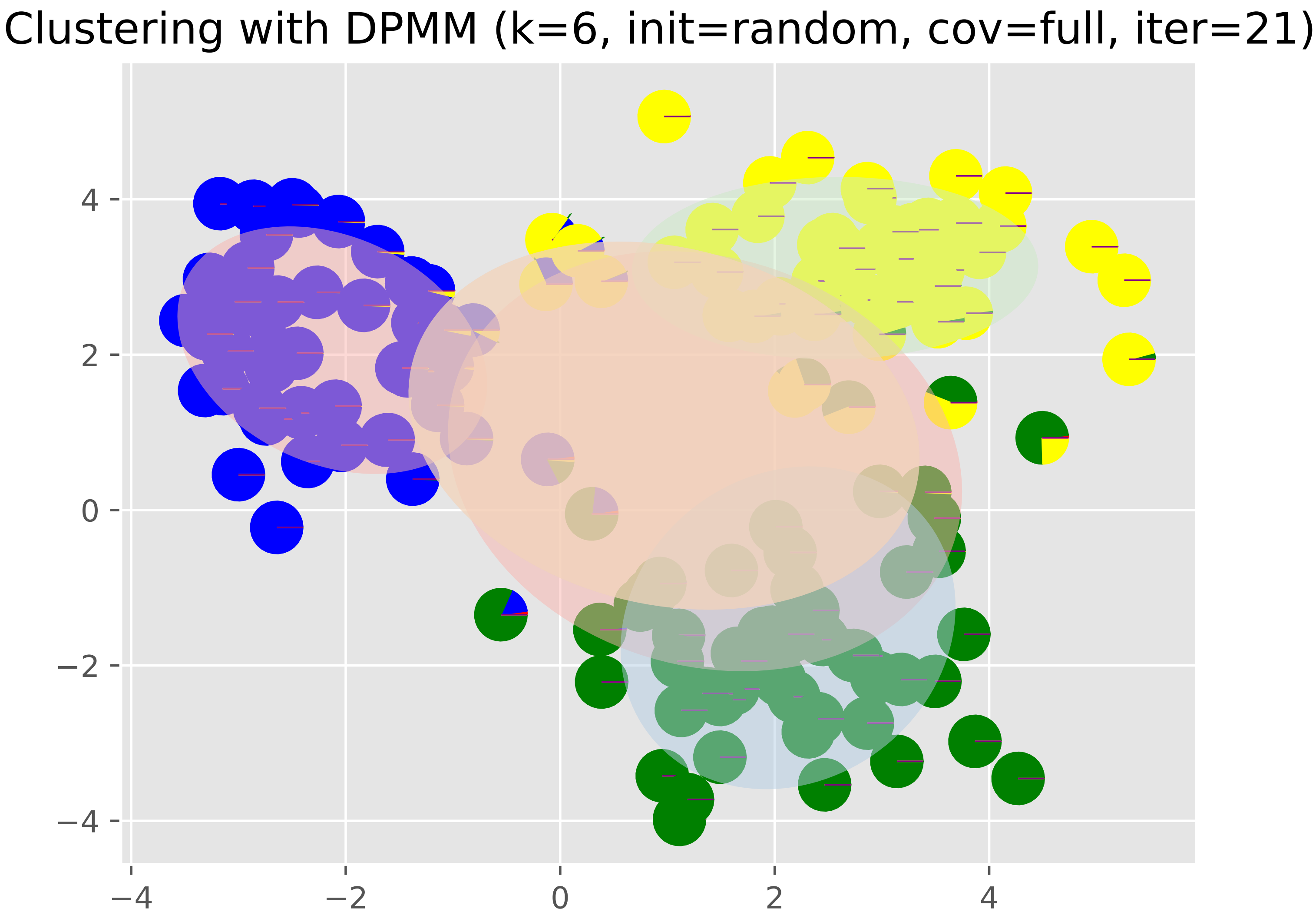

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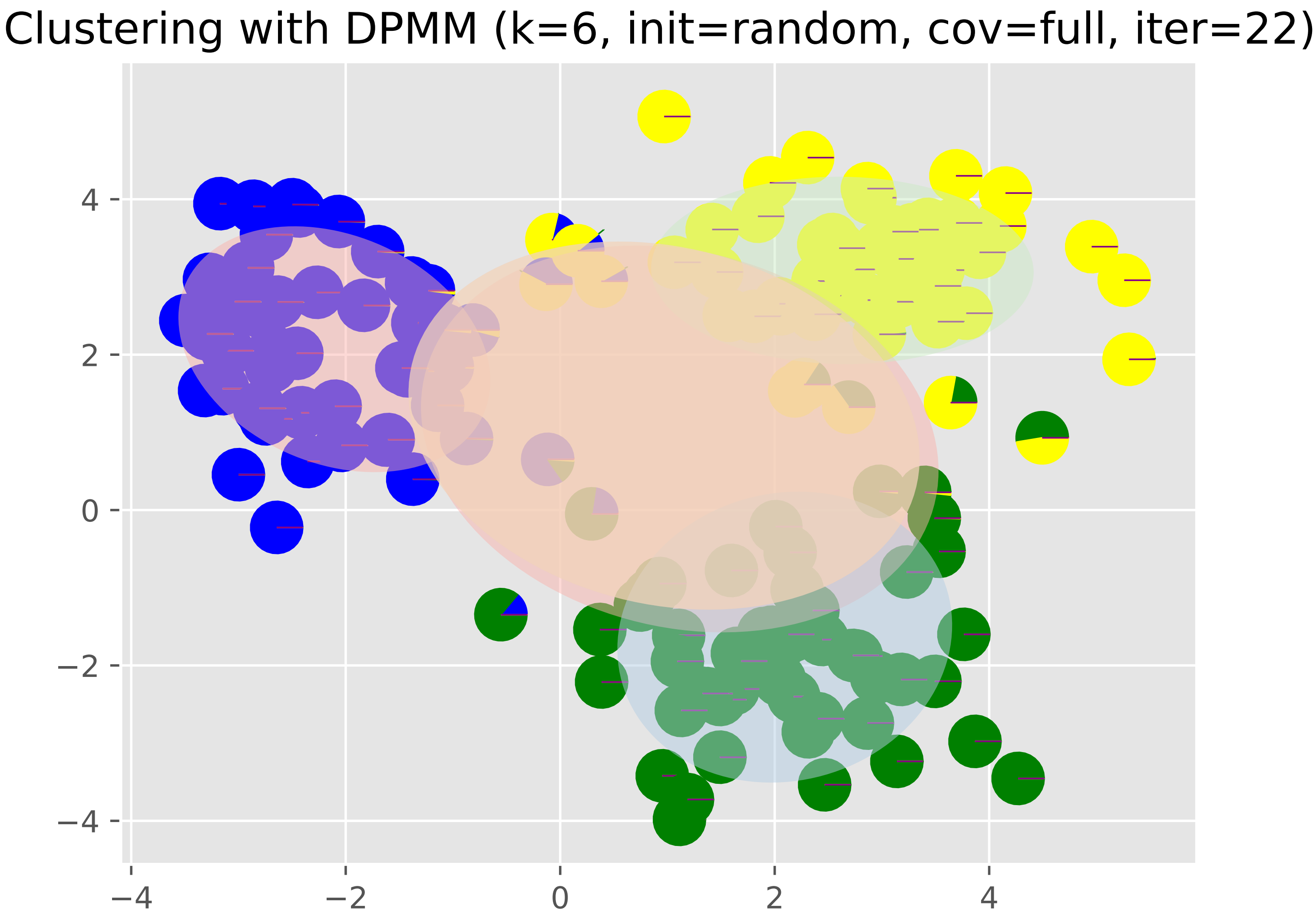

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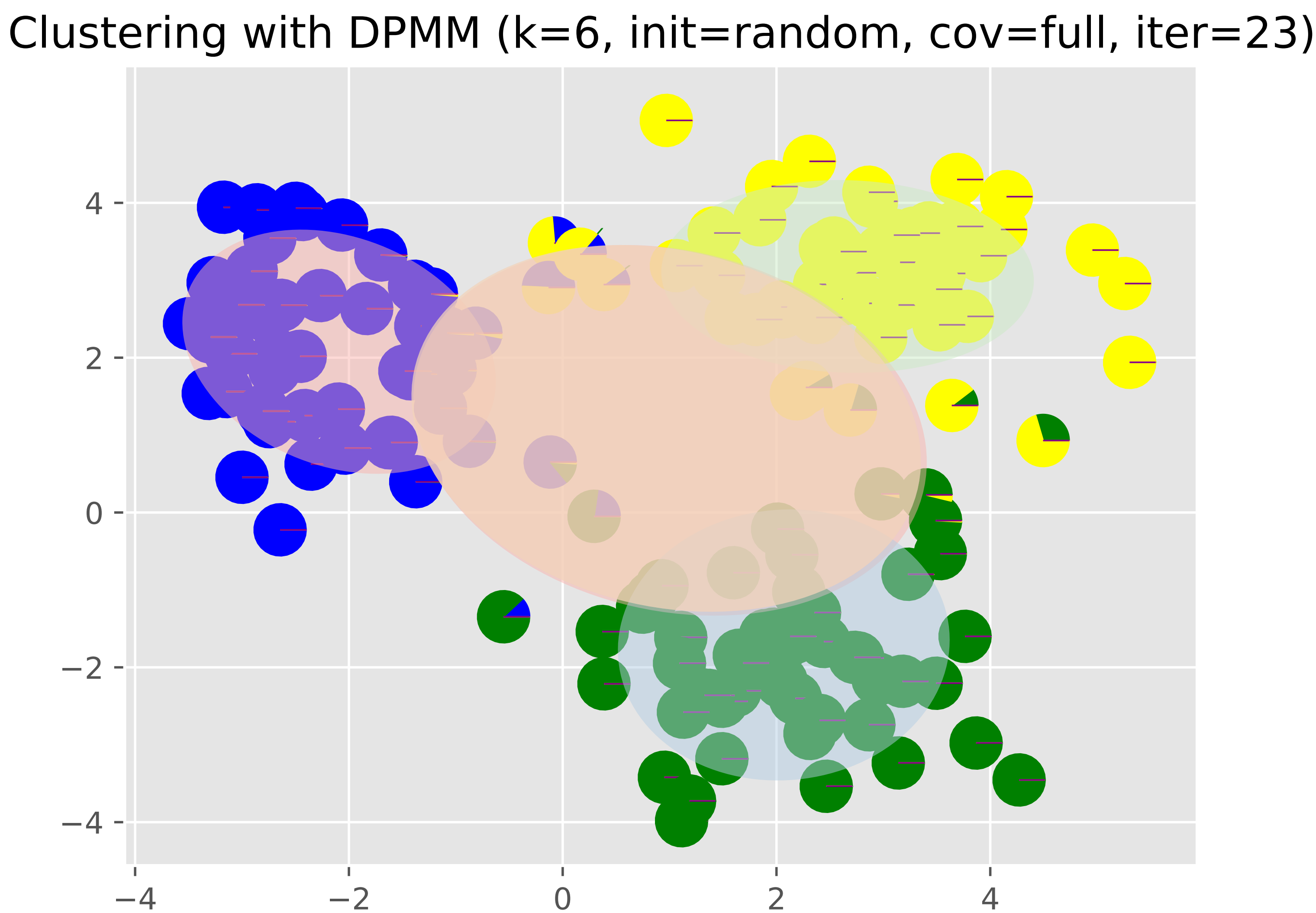

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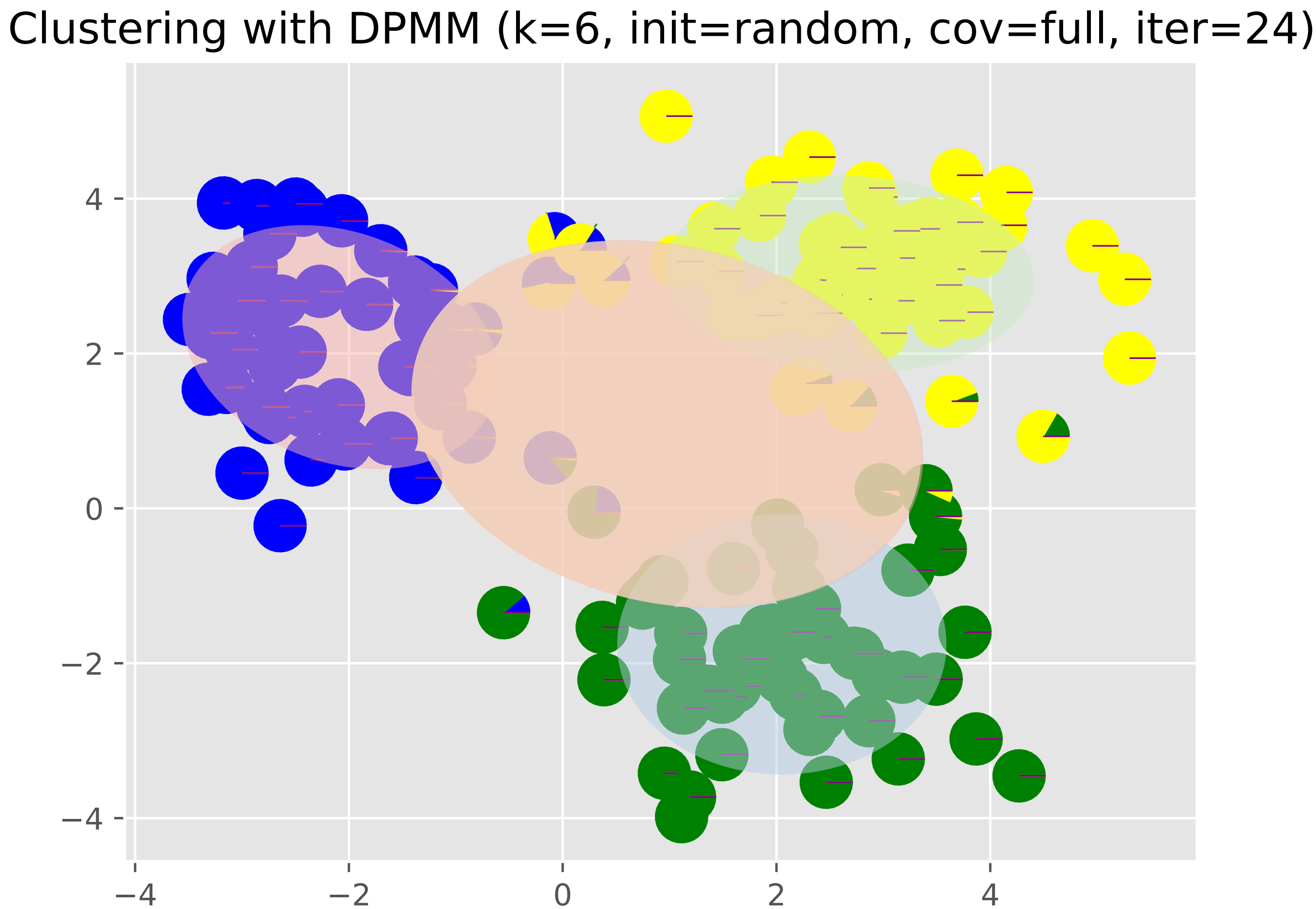

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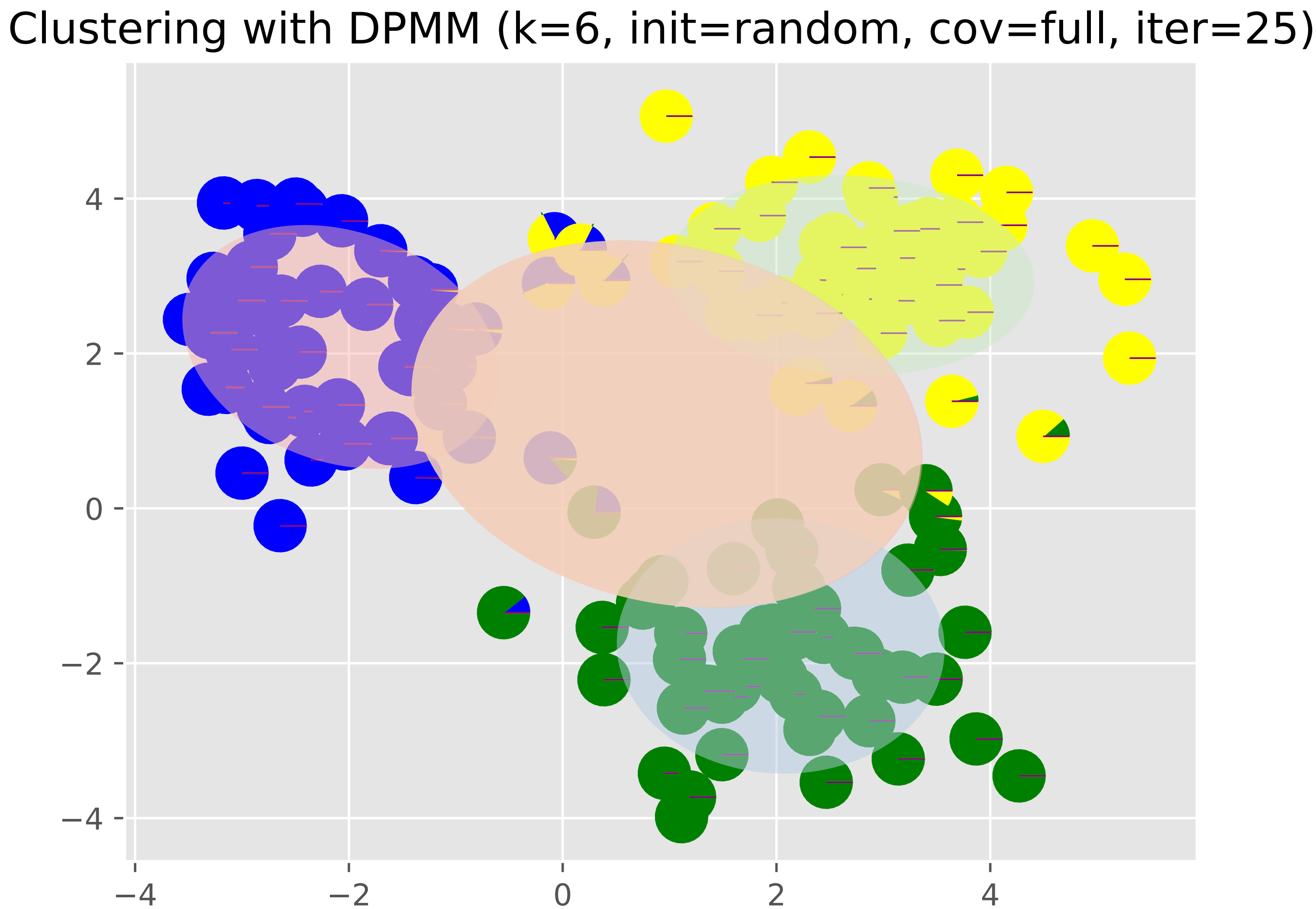


Summary of DP and DP-MM

- **DP** has many **different representations:**
  - Chinese Restaurant Process
  - Stick-breaking construction
  - Blackwell-MacQueen Urn Scheme
  - Limit of finite mixtures
  - etc.
- These representations give rise to a variety of **inference techniques** for the **DP-MM** and related models
  - Gibbs sampler (CRP)
  - Gibbs sampler (stick-breaking)
  - Variational inference (stick-breaking)
  - etc.

HIERARCHICAL DIRICHLET PROCESS (HDP)

Related Models

- Hierarchical Dirichlet Process Mixture Model (HDP-MM)
- Infinite HMM
- Infinite PCFG

HDP-MM

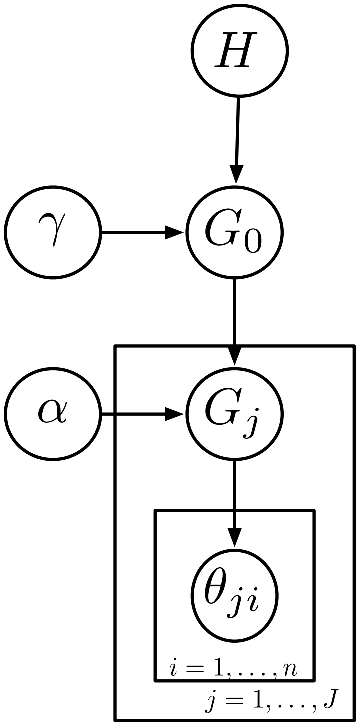
- In LDA, we have *M* independent samples from a Dirichlet distribution.
- The weights are different, but the topics are fixed to be the same.
- If we replace the Dirichlet distributions with Dirichlet processes, each atom of each Dirichlet process will pick a topic *independently* of the other topics.

- Because the base measure is *continuous*, we have zero probability of picking the same topic twice.
- If we want to pick the same topic twice, we need to use a *discrete* base measure.
- For example, if we chose the base measure to be $H = \sum_{k=1}^{K} \alpha_k \delta_{\beta_k}$ then we would have LDA again.
- We want there to be an infinite number of topics, so we want an *infinite, discrete* base measure.
- We want the location of the topics to be random, so we want an *infinite, discrete, random* base measure.

HDP-MM

Hierarchical Dirichlet process:

$$G_0 | \gamma, H \sim \mathrm{DP}(\gamma, H)$$
$$G_j | \alpha, G_0 \sim \mathrm{DP}(\alpha, G_0)$$
$$\theta_{ji} | G_j \sim G_j$$



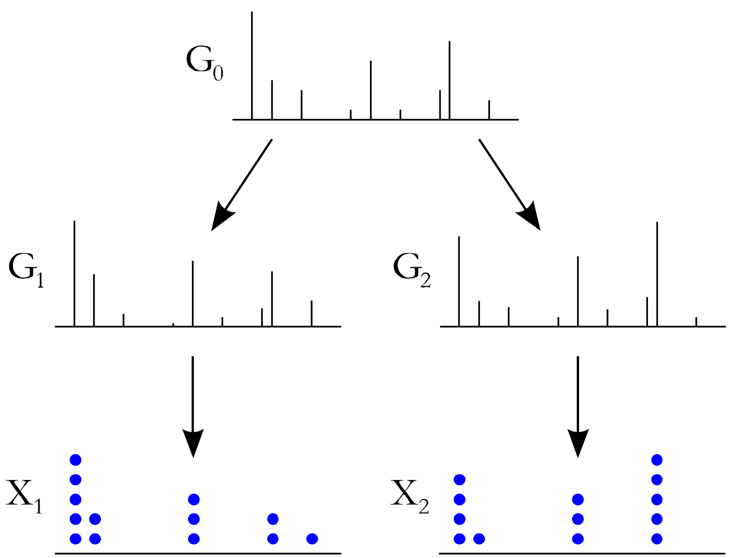


Figure from Teh 2004

HDP-MM

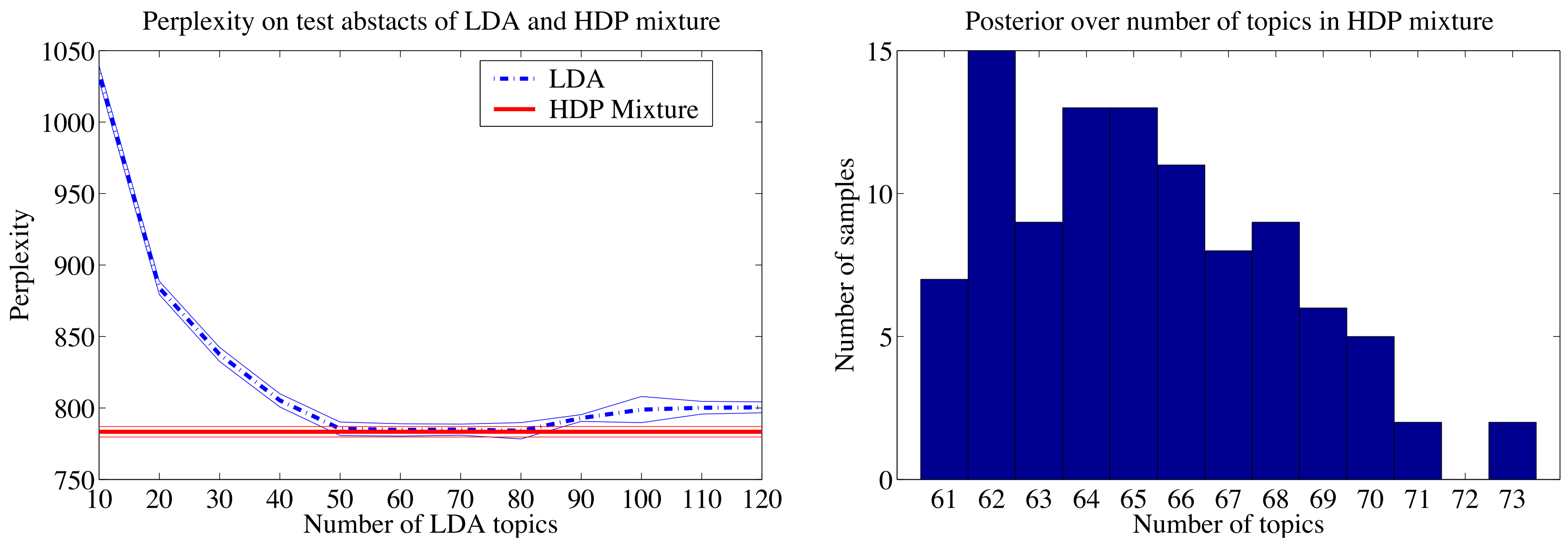


Figure 6: (Left) Comparison of latent Dirichlet allocation and the hierarchical Dirichlet process mixture. Results are averaged over 10 runs; the error bars are one standard error. (Right) Histogram of the number of topics for the hierarchical Dirichlet process mixture over 100 posterior samples.

HDP-HMM (Infinite HMM)

Number of hidden states in Infinite HMM is **countably infinite**

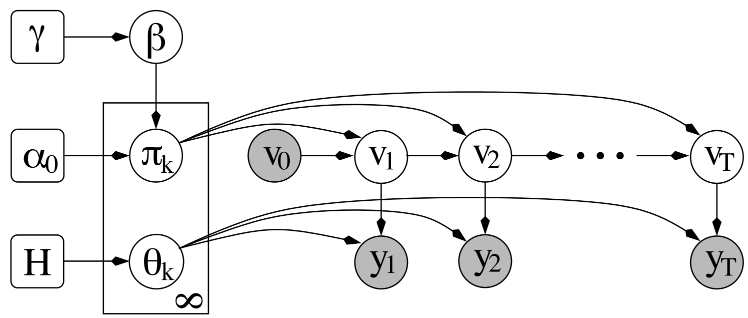


Figure 9: A hierarchical Bayesian model for the infinite hidden Markov model.

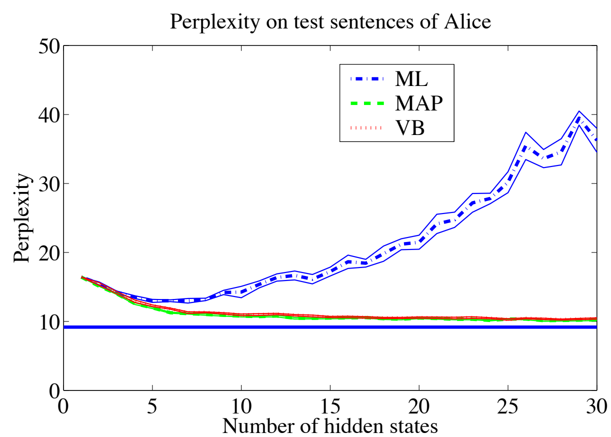


Figure 10: Comparing the infinite hidden Markov model (solid horizontal line) with ML, MAP and VB trained hidden Markov models. The error bars represent one standard error (those for the HDP-HMM are too small to see).

HDP-PCFG (Infinite PCFG)

HDP-PCFG

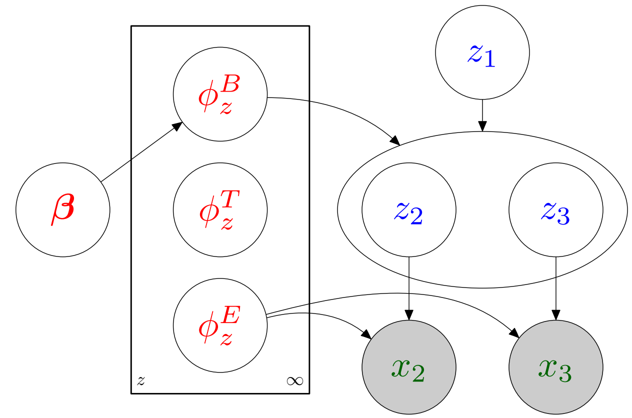
$\boldsymbol{\beta} \sim \mathrm{GEM}(\alpha)$ [draw top-level symbol weights]

For each grammar symbol $z \in \{1, 2, \dots\}$:

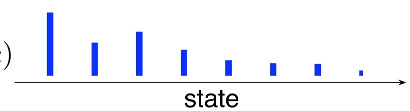
- $\phi_z^T \sim \mathrm{Dirichlet}(\alpha^T)$ [draw rule type parameters]
- $\phi_z^E \sim \mathrm{Dirichlet}(\alpha^E)$ [draw emission parameters]
- $\phi_z^B \sim \mathrm{DP}(\alpha^B, \boldsymbol{\beta}\boldsymbol{\beta}^T)$ [draw binary production parameters]

For each node i in the parse tree:

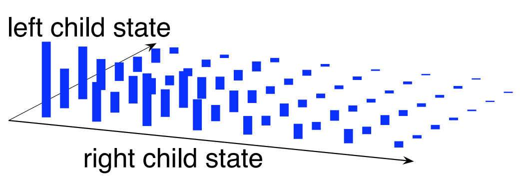
- $t_i \sim \mathrm{Multinomial}(\phi_{z_i}^T)$ [choose rule type]
- If $t_i = \textsc{Emission}$:
  - $x_i \sim \mathrm{Multinomial}(\phi_{z_i}^E)$ [emit terminal symbol]
- If $t_i = \textsc{Binary-Production}$:
  - $(z_{L(i)}, z_{R(i)}) \sim \mathrm{Multinomial}(\phi_{z_i}^B)$ [generate children symbols]



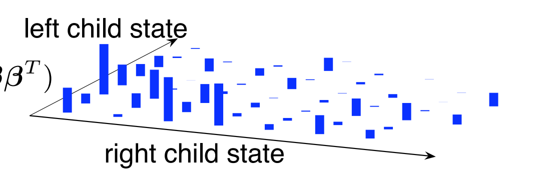
$\boldsymbol{\beta} \sim \mathrm{GEM}(\alpha)$



$\boldsymbol{\beta}\boldsymbol{\beta}^T$



$\phi_z^B \sim \mathrm{DP}(\boldsymbol{\beta}\boldsymbol{\beta}^T)$



Parametric vs. Nonparametric

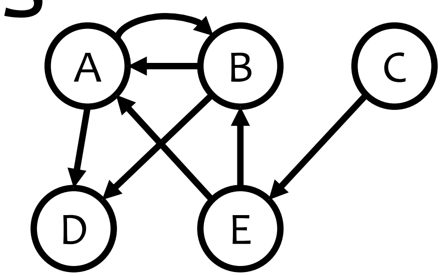
Type of Model	Parametric Example	Nonparametric Example: Construction #1	Nonparametric Example: Construction #2
distribution over counts	Dirichlet-Multinomial Model	Dirichlet Process (DP)	
		Chinese Restaurant Process (CRP)	Stick-breaking construction
mixture	Gaussian Mixture Model (GMM)	Dirichlet Process Mixture Model (DPMM)	
		CRP Mixture Model	Stick-breaking construction
admixture	Latent Dirichlet Allocation (LDA)	Hierarchical Dirichlet Process Mixture Model (HDPMM)	
		Chinese Restaurant Franchise	Stick-breaking construction

Summary of DP and DP-MM

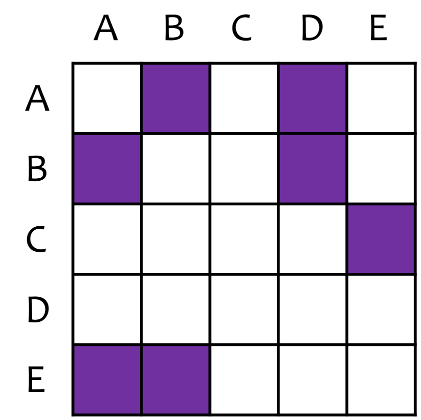
- **DP** has many **different representations:**
  - Chinese Restaurant Process
  - Stick-breaking construction
  - Blackwell-MacQueen Urn Scheme
  - Limit of finite mixtures
  - etc.
- These representations give rise to a variety of **inference techniques** for the **DP-MM** and related models
  - Gibbs sampler (CRP)
  - Gibbs sampler (stick-breaking)
  - Variational inference (stick-breaking)
  - etc.

GRAPH NEURAL NETWORKS

Background: Graphs



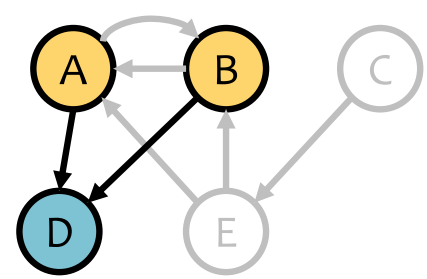
- *Def*: a **graph** $G = (V,E)$ consists of vertices V and edges E
  - vertices are also called nodes
  - Let **node** $v_i \in V$ and $|V| = N$
  - Let **edge** $(v_i, v_j) \in E$ and $|E| = M$
- *Def*: an **adjacency matrix A** for graph G is a binary matrix such that:
  - $A_{i,j} = 1$ if $(v_i, v_j) \in E$
  - $A_{i,j} = 0$ if $(v_i, v_j) \notin E$



- *Def*: an **adjacency list** is simply an ordered version of the set of edges, e.g. list(E)

[(A,B), (A,D), (B,A), (B,D), (C,E), (E,A), (E,B)]

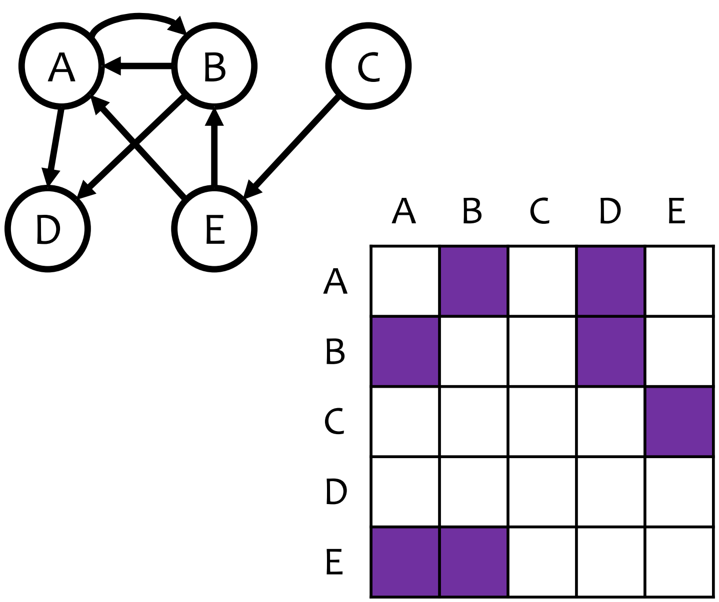
- *Def*: the **neighbors** $N(v_j)$ of a node v_j are all nodes v_i such that $(v_i, v_j) \in E$

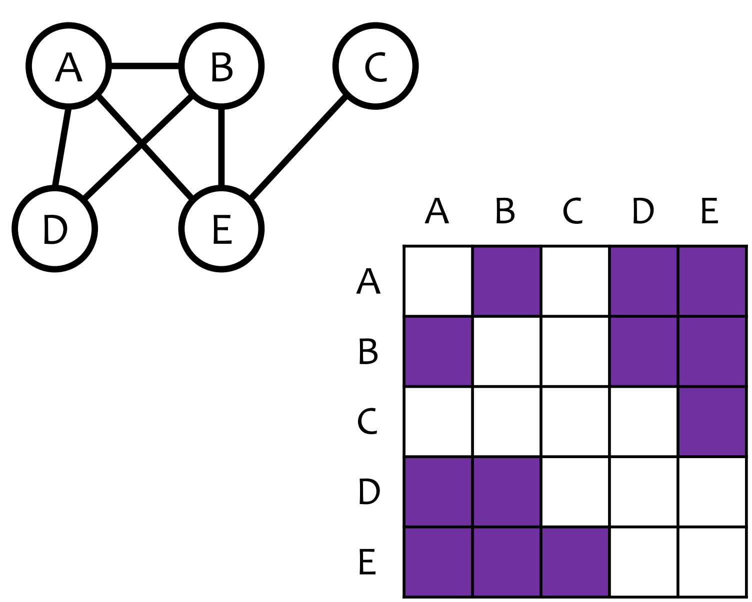


Background: Graphs

- The graph we just defined is a **directed graph** because each **edge** $(v_i, v_j) \in E$ is an **ordered pair**

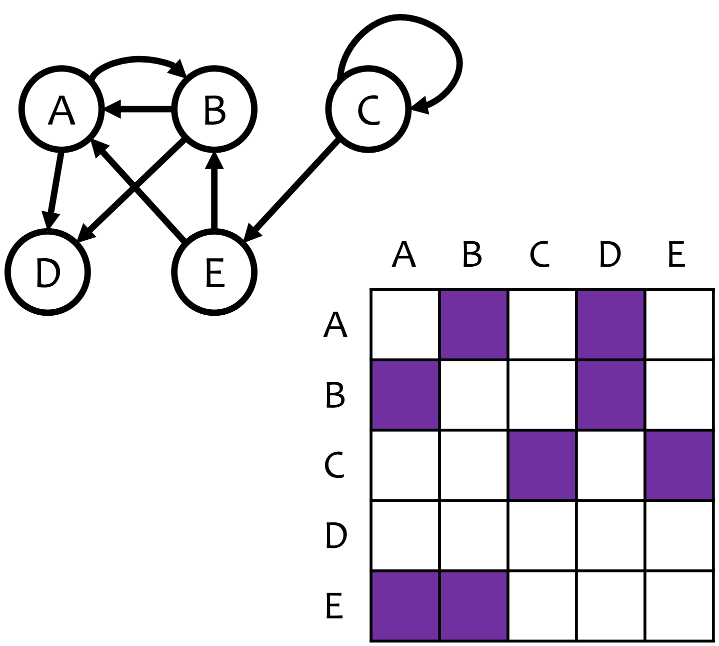
- For an undirected graph:
  $(v_i, v_j) \in E \Rightarrow (v_j, v_i) \in E$
  each undirected edge is just two directed edges
- An **undirected graph** is a special case in which the adjacency matrix is **symmetric**



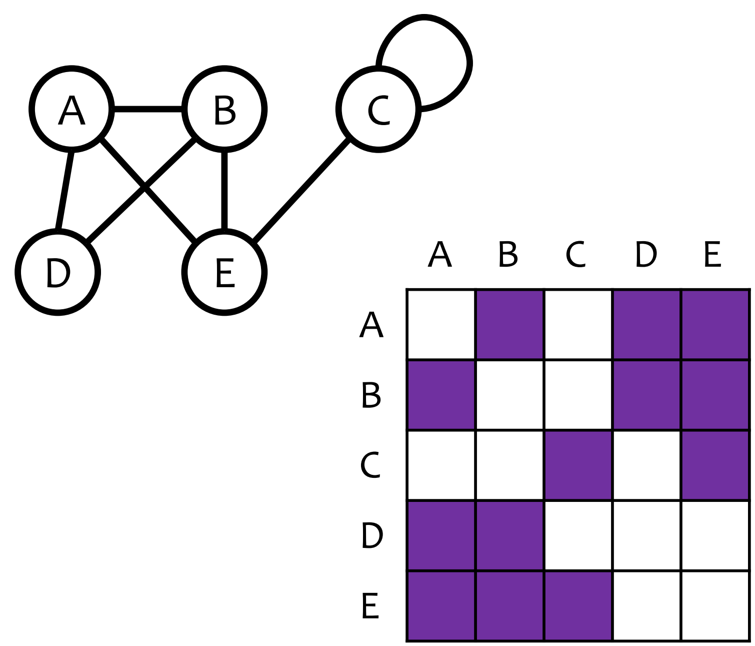


Background: Graphs

- The graph we just defined is a **directed graph** because each **edge** $(v_i, v_j) \in E$ is an **ordered pair**
- *Def*: a **self-loop** $(v_i, v_i) \in E$ is an edge from a node to itself
- A self-loop corresponds to a diagonal entry in the adjacency matrix

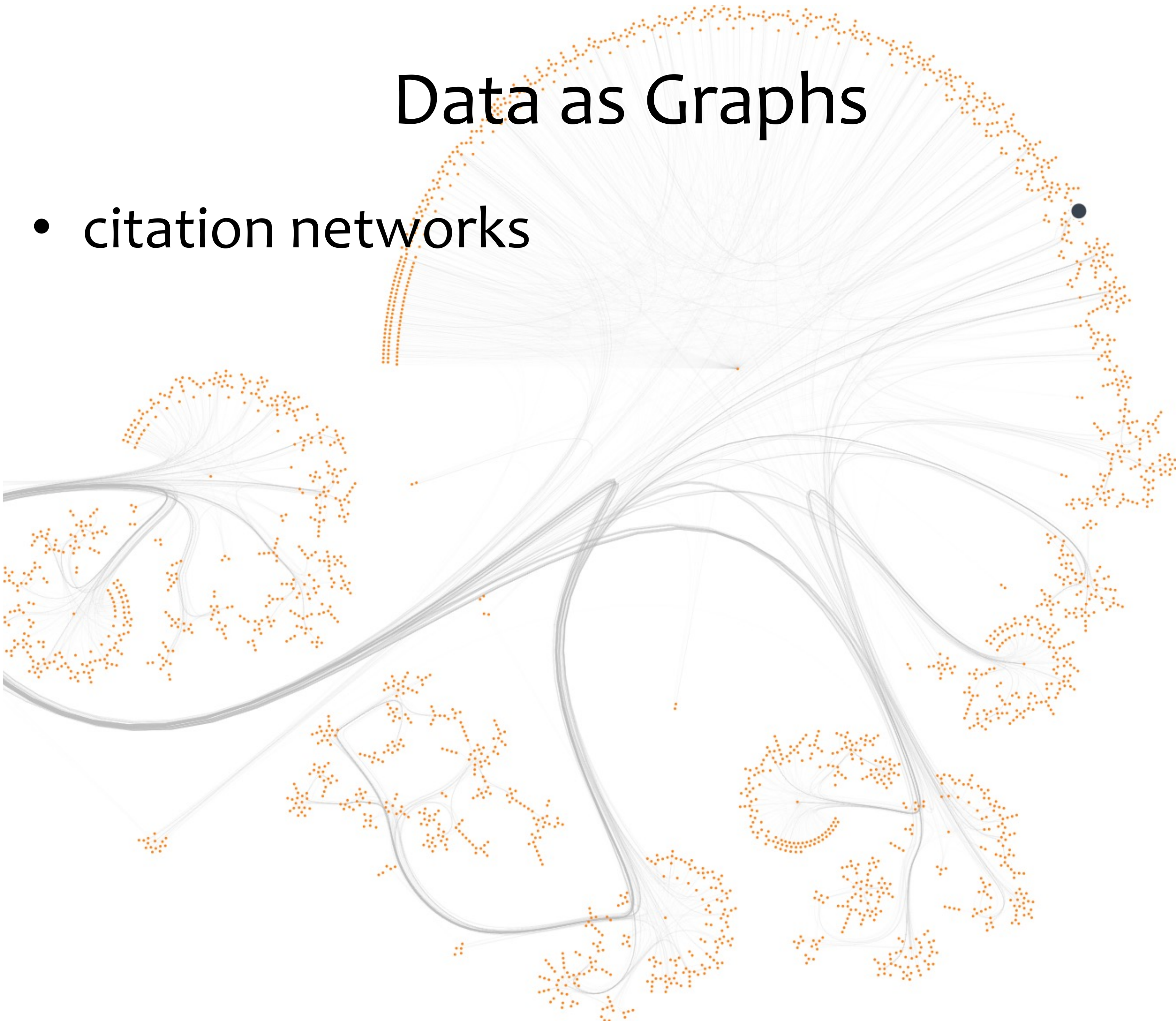


- For an undirected graph: $(v_i, v_j) \in E \Rightarrow (v_j, v_i) \in E$ each undirected edge is just two directed edges
- An **undirected graph** is a special case in which the adjacency matrix is **symmetric**
- (An undirected self-loop is only one directed edge)



Data as Graphs

- citation networks



Data as Graphs

- molecules

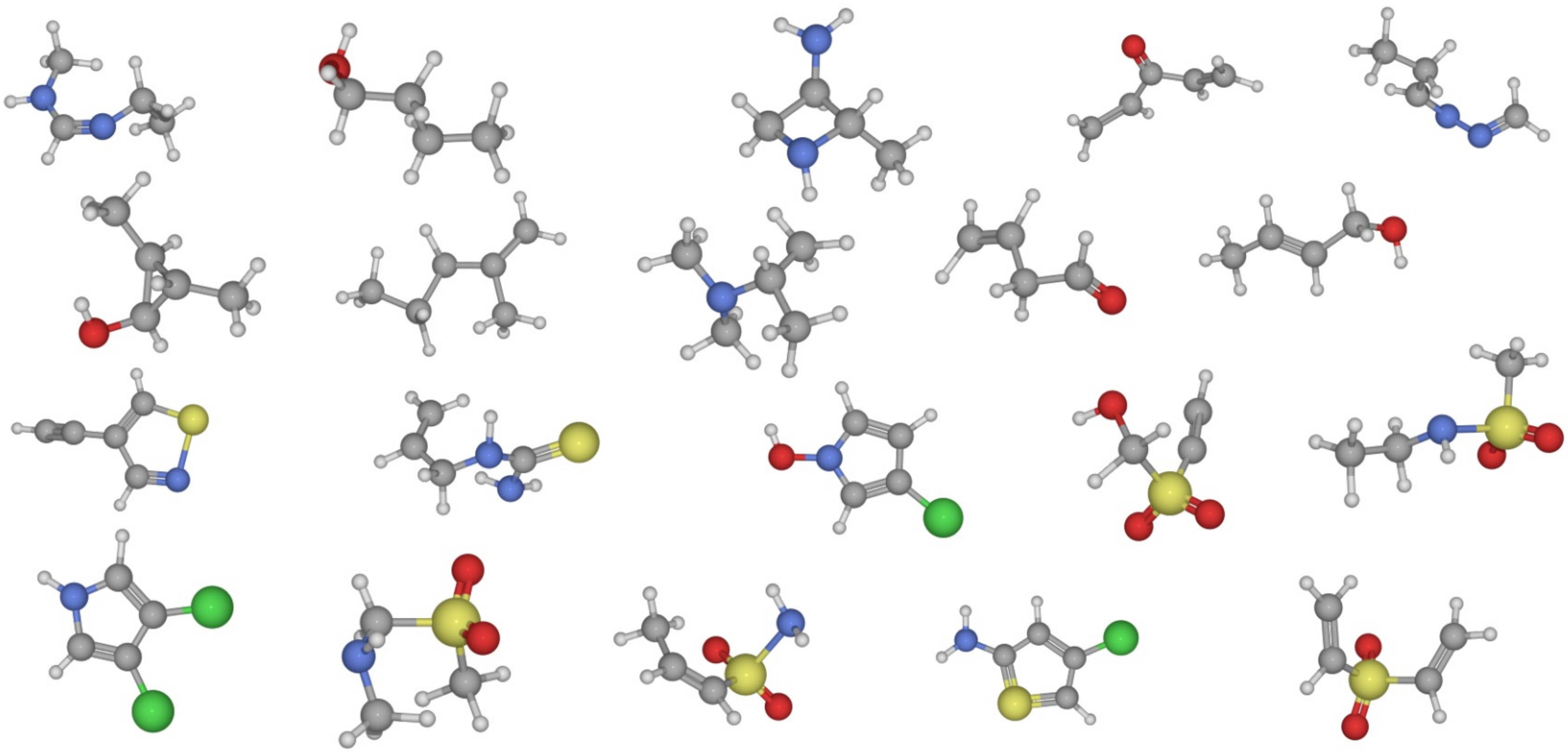


Figure from https://chemrxiv.org/engage/chemrxiv/article-details/6246035d3affe4aa143c3848

Data as Graphs

- semantic parsing

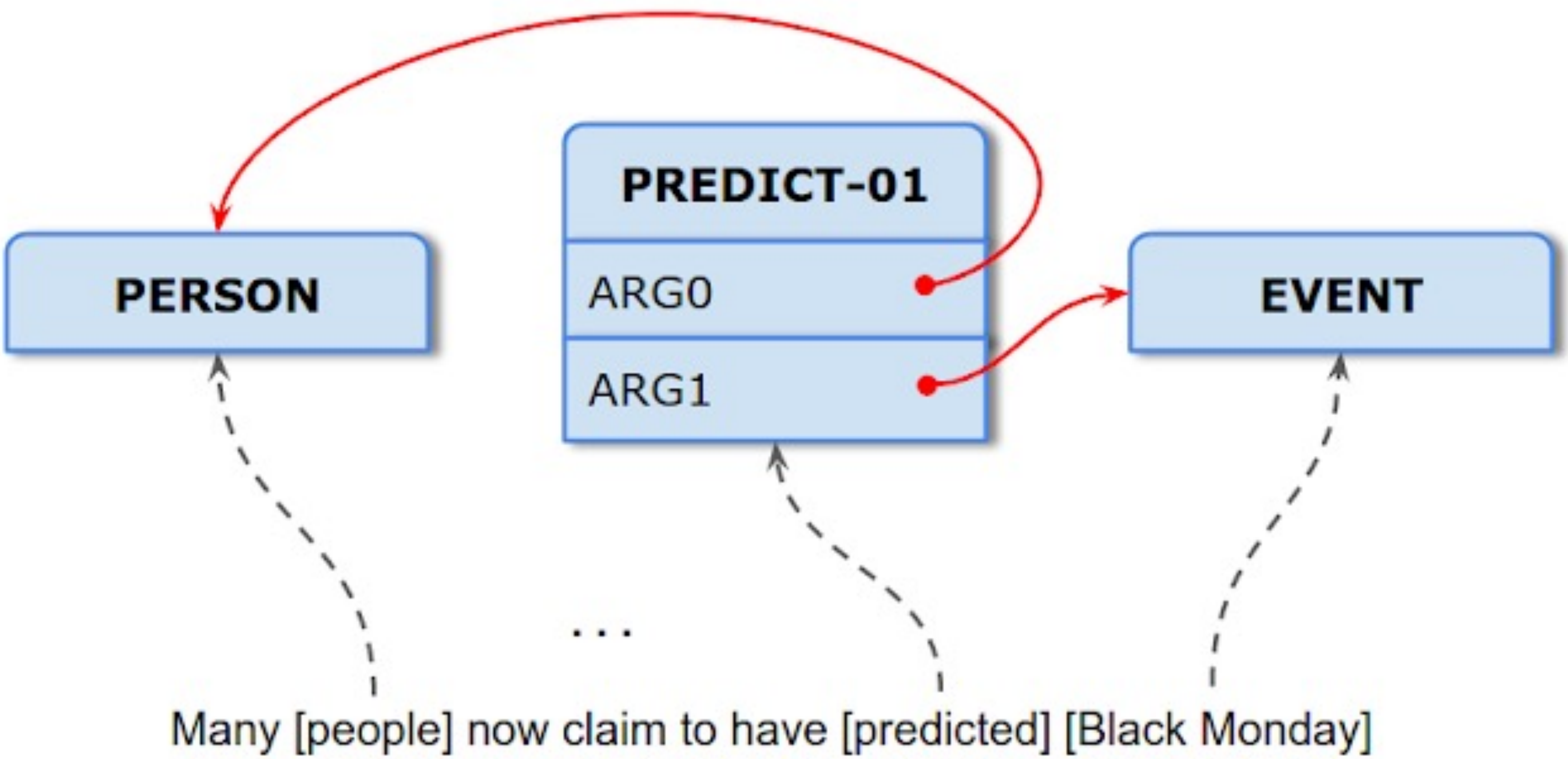
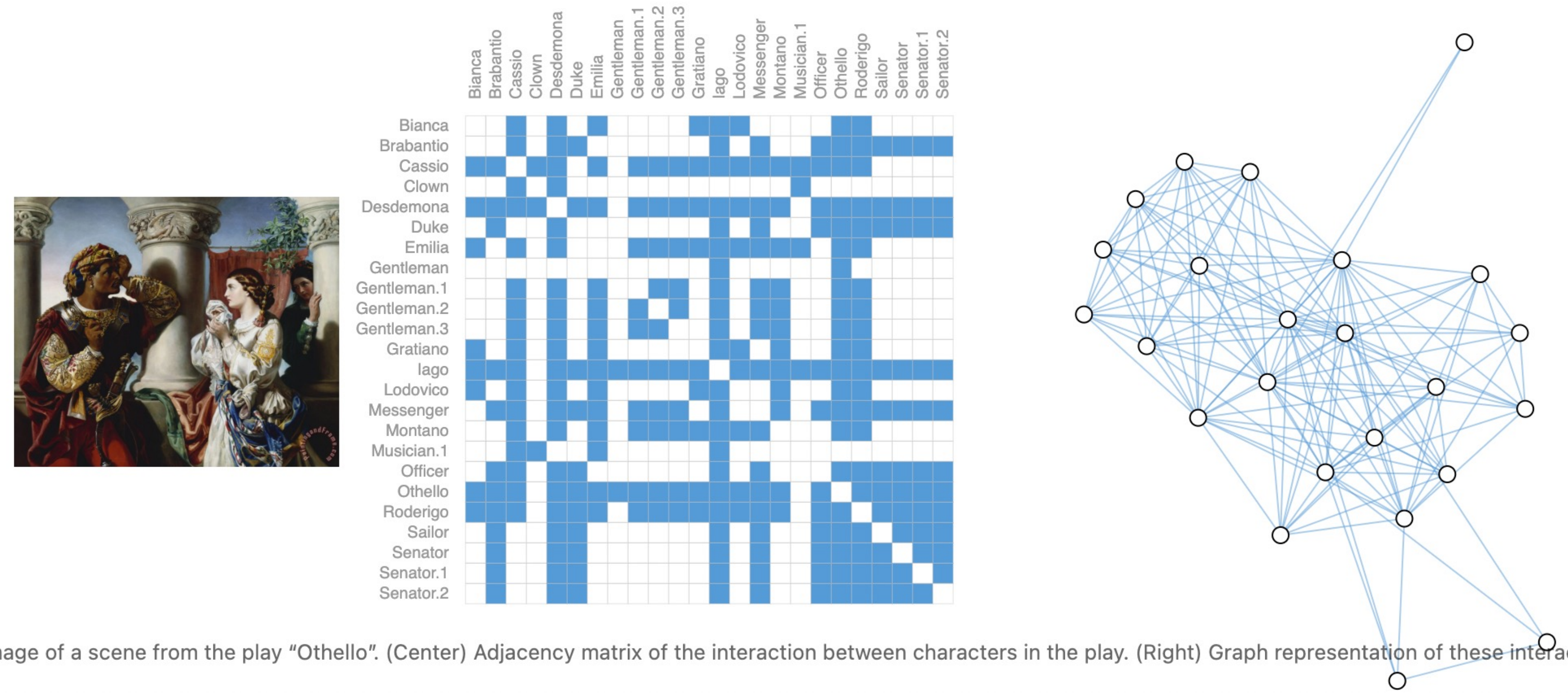


Figure from https://ai.googleblog.com/2017/11/sling-natural-language-frame-semantic.html

Data as Graphs

- social networks

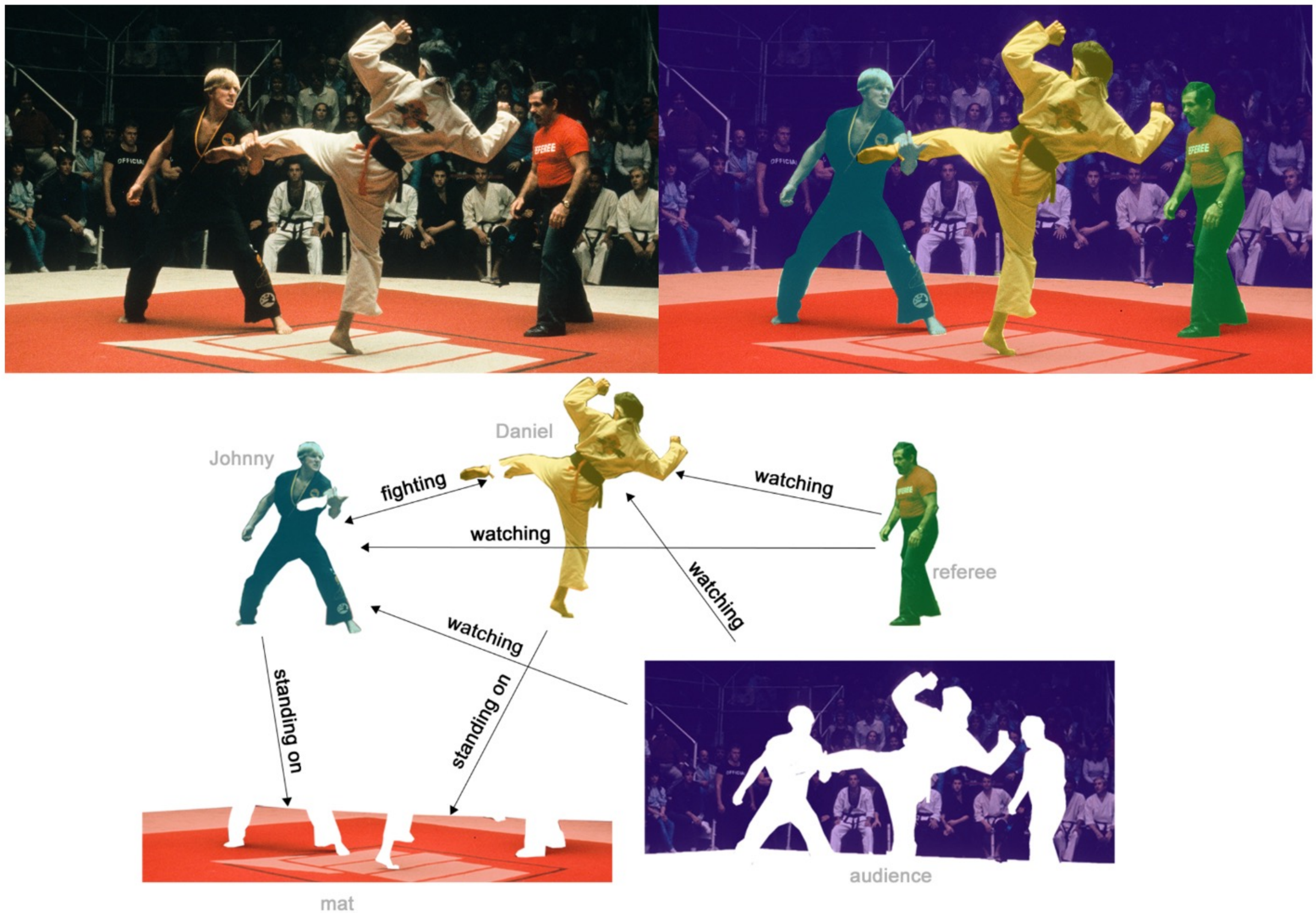


(Left) Image of a scene from the play "Othello". (Center) Adjacency matrix of the interaction between characters in the play. (Right) Graph representation of these interactions.

Figure from https://distill.pub/2021/gnn-intro/

Data as Graphs

- images



In (b), above, the original image (a) has been segmented into five entities: each of the fighters, the referee, the audience and the mat. (C) shows the relationships between these entities.

Figure from https://distill.pub/2021/gnn-intro/

Graph Neural Networks

Decomposition of tasks for GNNs

- *Node-level*
  - **node classification:** predict a label for each node
  - **node regression**: predict a value for each node
- *Edge-level*
  - **edge classification:** predict a label for each edge
  - **link prediction:** predict presence/absence/strength of an edge
- *Graph-level*
  - **graph classification**: predict a label for the entire graph
  - **graph regression**: predict a value for the entire graph

Types of GNNs

A **Taxonomy** of Graph Neural Networks (GNNs) from Wu et al. (2020):

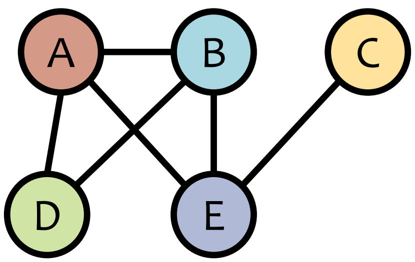
1. Recurrent GNNs
2. Convolutional GNNs
   a. Spectral-based
   b. Spatial-based
3. Graph autoencoders
   a. for network embedding
   b. for graph generation
4. Spatial-temporal GNNs

Taxonomy from https://arxiv.org/pdf/1901.00596.pdf

Node and Edge Representations

- *Def*: each node v has a **node feature vector $\mathbf{x}_v \in \mathbb{R}^M$**
- *Def*: each edge e has an **edge feature vector $\mathbf{x}_e \in \mathbb{R}^{M'}$**
- For undirected graphs, we (usually) assume there is only **one vector per undirected edge** (i.e. not one for each of the two corresponding directed edges)

$\mathbf{x}_A$	.1	-7	…	2
$\mathbf{x}_B$	4	-2	…	3
$\mathbf{x}_C$	-5	1	…	1
$\mathbf{x}_D$	0	3	…	.5
$\mathbf{x}_E$	.6	-.3	…	.1



$\mathbf{x}_{A,B}$	2	.4	…	-2
$\mathbf{x}_{A,D}$	.3	.1	…	-.5
$\mathbf{x}_{A,E}$	-5	1	…	4
$\mathbf{x}_{B,D}$	.9	9	…	-9
$\mathbf{x}_{B,E}$	1	-4	…	7
$\mathbf{x}_{C,E}$	6	-.2	…	0

RECURRENT GRAPH NEURAL NETWORKS

Recurrent GNNs

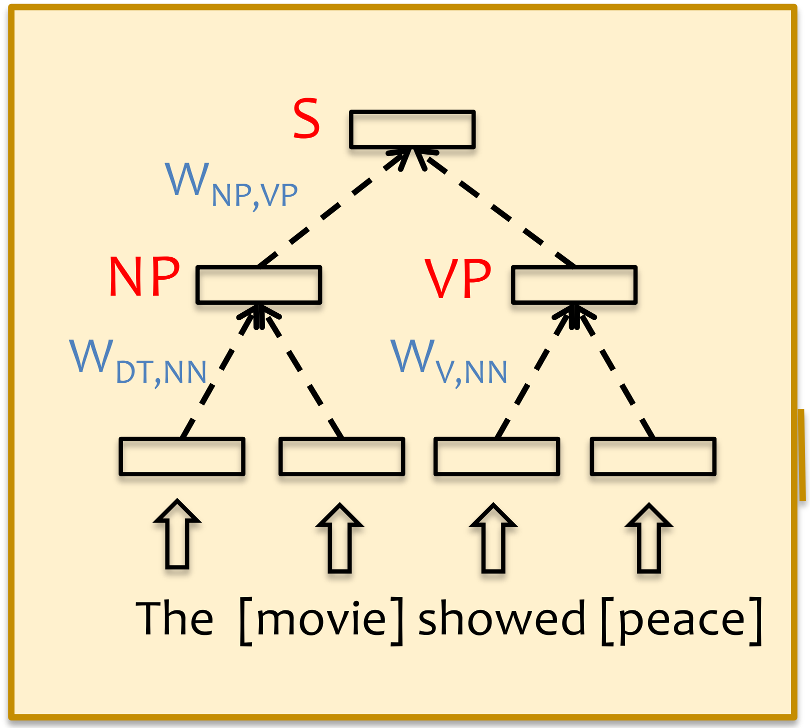
- Some of the early GNNs **capitalized on acyclic graphs** (or acyclic substructure of graphs)

- This is akin to how Loopy Belief Propagation and Tree Reweighted Belief Propagation (two variational message passing techniques that came long before) are implemented

- The **backbone** of these Recurrent GNNs was a **variant of the LSTM**

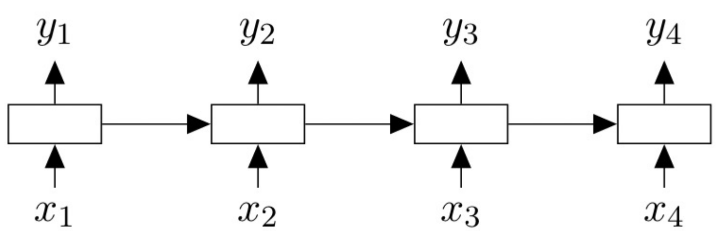
Tree LSTMs

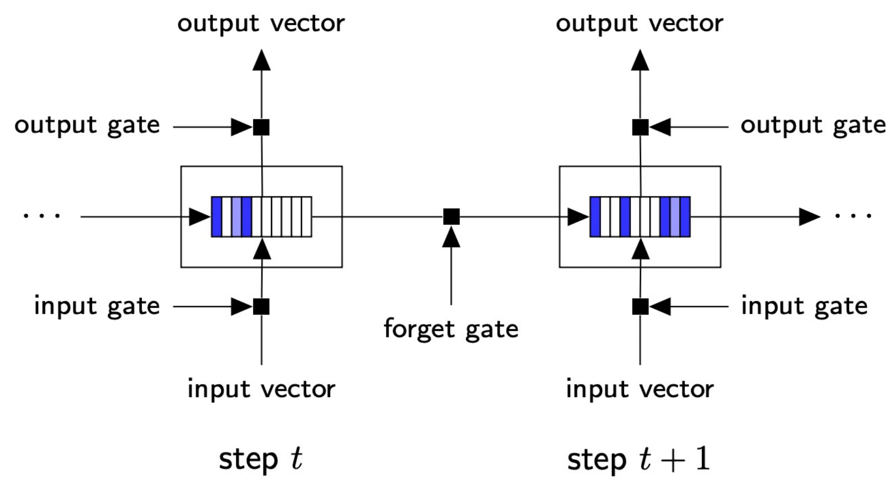
- *Two types*:
  - Child-Sum TreeLSTM (handles binary trees)
  - N-ary TreeLSTM (handles arbitrary trees)
- *Key insight:*
  - generalize the LSTM from chains to trees
  - the **hidden unit** for a non-terminal node is a **parameterized function of its children**



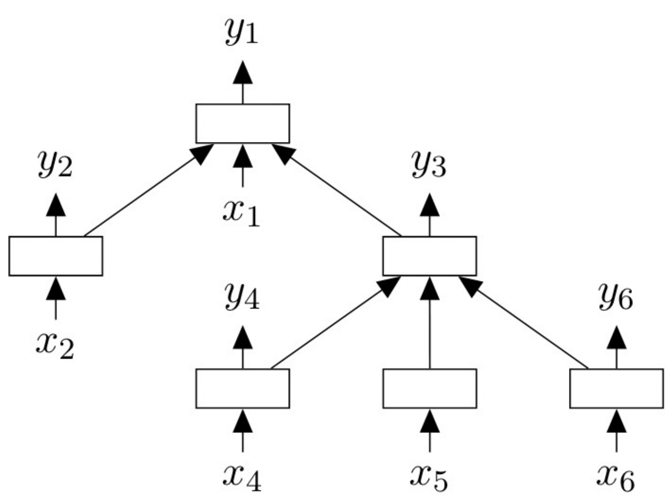
Tree LSTMs

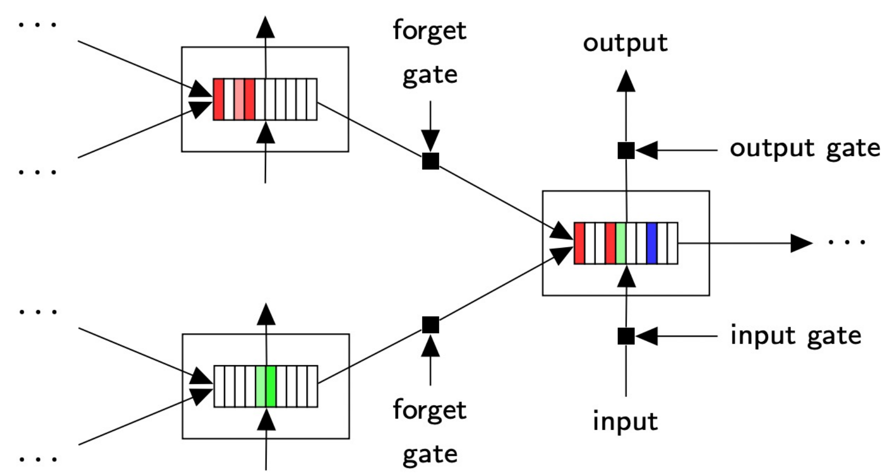
Standard LSTM on a chain





Tree LSTM on an n-ary tree



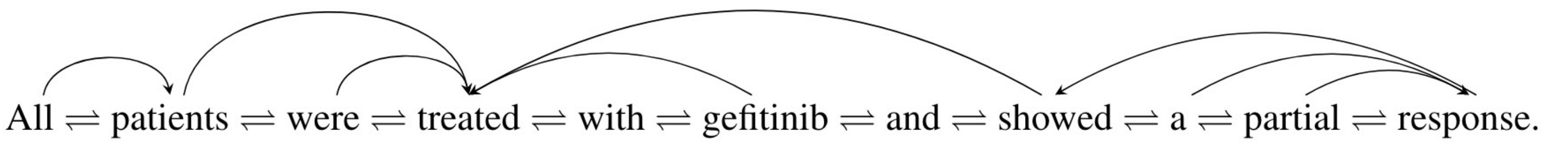


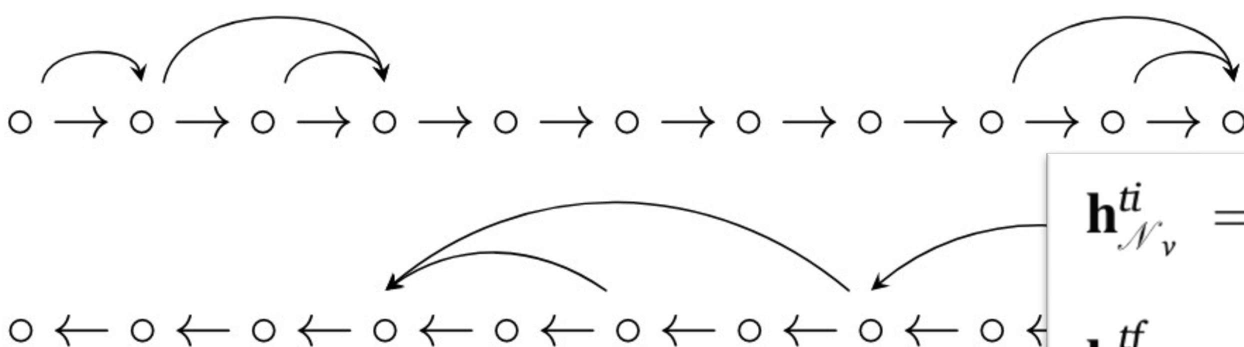
Figures from Tai et al. (2015) https://aclanthology.org/P15-1150

Figures from Tai et al. (2015) ACL slides: https://kaishengtai.github.io/static/slides/treelstm-acl2015.pdf

Graph LSTMs

- The Graph LSTM (Peng et al., 2017) decomposes a directed **cyclic** graph into two directed **acyclic** graphs
- The computation graph first runs a TreeLSTM left-to-right along the first acyclic graph, then right-to-left through the second acyclic graph





$$
\begin{aligned}
\mathbf{h}^{ti}_{\mathcal{N}_v} &= \sum_{k \in \mathcal{N}_v} \mathbf{U}^{i}_{m(v,k)} \mathbf{h}^{t-1}_{k} \\
\mathbf{h}^{tf}_{\mathcal{N}_v k} &= \mathbf{U}^{f}_{m(v,k)} \mathbf{h}^{t-1}_{k} \\
\mathbf{h}^{to}_{\mathcal{N}_v} &= \sum_{k \in \mathcal{N}_v} \mathbf{U}^{o}_{m(v,k)} \mathbf{h}^{t-1}_{k} \\
\mathbf{h}^{tu}_{\mathcal{N}_v} &= \sum_{k \in \mathcal{N}_v} \mathbf{U}^{u}_{m(v,k)} \mathbf{h}^{t-1}_{k}
\end{aligned}
$$

Equations from https://arxiv.org/abs/1812.08434

Figures from https://aclanthology.org/Q17-1008

SPATIAL GRAPH NEURAL NETWORKS

Spatial Graph Neural Networks

Whiteboard:

- Basic node-only GNN
- Basic neighbor-only GNN
- Visualizing the k-hop neighborhood computation graph
- Incorporating self-loops
- Normalization techniques
- Adding edge features