

GrafGen Benchmark

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```
# Install packages if needed (uncomment if you haven't installed them)
# install.packages(c("mclust", "aricode", "ggplot2", "ggalluvial"))

library(mclust)      # for adjustedRandIndex
```

```
Package 'mclust' version 6.1.1
Type 'citation("mclust")' for citing this R package in publications.
```

```
library(aricode)      # for NMI
library(ggplot2)      # for plotting bar chart
library(ggalluvial)   # for Sankey plot
```

Read CSV files

```
grafgen    <- read.csv("data/grafgen_clusters.csv", header = TRUE)
fastbaps5 <- read.csv("data/fastBAPS_clusters_c5.csv", header = TRUE)
fastbaps7 <- read.csv("data/fastBAPS_clusters_c7.csv", header = TRUE)
fastbaps8 <- read.csv("data/fastBAPS_clusters_c8.csv", header = TRUE)
fastbaps13 <- read.csv("data/fastBAPS_clusters_c13.csv", header = TRUE)
poppunk   <- read.csv("data/poppunk_clusters.csv", header = TRUE)
#finestructure <- read.csv("finestructure_clusters.csv", header = TRUE)
FS <- read.csv("data/FS_clusters.csv", header = TRUE)
FSsub <- read.csv("data/FSsub_clusters.csv", header = TRUE)
DAPC6 <- read.csv("data/DAPC6_clusters.csv", header = TRUE)
```

Merge by Sample

```
merged <- Reduce(function(x, y) merge(x, y, by = "Sample"),
                 list(grafgen, fastbaps5, fastbaps7,
                      fastbaps8, fastbaps13, FS, FSsub, DAPC6, poppunk))

# Rename cluster columns for clarity
#colnames(merged) <- c("sample_id", "GrafGen", "fastBAPS", "PopPUNK",
#                      "fineSTRUCTURE")
colnames(merged) <- c("sample_id", "GrafGen", "fastBAPS_c5",
                      "fastBAPS_c7", "fastBAPS_c8", "fastBAPS_c13",
                      "FS", "FSsub", "DAPC6", "PopPUNK")
```

Convert clusters to factors (important for ARI/NMI)

```
merged$GrafGen      <- as.factor(merged$GrafGen)
merged$fastBAPS_c5  <- as.factor(merged$fastBAPS_c5)
merged$fastBAPS_c7  <- as.factor(merged$fastBAPS_c7)
merged$fastBAPS_c8  <- as.factor(merged$fastBAPS_c8)
merged$fastBAPS_c13 <- as.factor(merged$fastBAPS_c13)
merged$PopPUNK       <- as.factor(merged$PopPUNK)
merged$FS <- as.factor(merged$FS)
merged$FSsub <- as.factor(merged$FSsub)
merged$DAPC6 <- as.factor(merged$DAPC6)
```

Compute ARI and NMI scores (each method vs GrafGen)

```
ari_vals <- c(
  adjustedRandIndex(merged$GrafGen, merged$fastBAPS_c5),
  adjustedRandIndex(merged$GrafGen, merged$fastBAPS_c7),
  adjustedRandIndex(merged$GrafGen, merged$fastBAPS_c8),
  adjustedRandIndex(merged$GrafGen, merged$fastBAPS_c13),
  adjustedRandIndex(merged$GrafGen, merged$FS),
  adjustedRandIndex(merged$GrafGen, merged$FSsub),
  adjustedRandIndex(merged$GrafGen, merged$DAPC6),
  adjustedRandIndex(merged$GrafGen, merged$PopPUNK))
```

```

)
nmi_vals <- c(
  NMI(merged$GrafGen, merged$fastBAPS_c5),
  NMI(merged$GrafGen, merged$fastBAPS_c7),
  NMI(merged$GrafGen, merged$fastBAPS_c8),
  NMI(merged$GrafGen, merged$fastBAPS_c13),
  NMI(merged$GrafGen, merged$FS),
  NMI(merged$GrafGen, merged$FSsub),
  NMI(merged$GrafGen, merged$DAPC6),
  NMI(merged$GrafGen, merged$PopPUNK)
)
methods <- c("fastBAPS_c5", "fastBAPS_c7", "fastBAPS_c8",
            "fastBAPS_c13", "FS", "FSsub", "DAPC6", "PopPUNK")

```

Prepare data frame for bar plot

```

df_plot <- data.frame(
  Method = rep(methods, 2),
  Metric = rep(c("ARI", "NMI"), each = length(methods)),
  Score = c(ari_vals, nmi_vals)
)

```

Bar plot of ARI and NMI scores

```

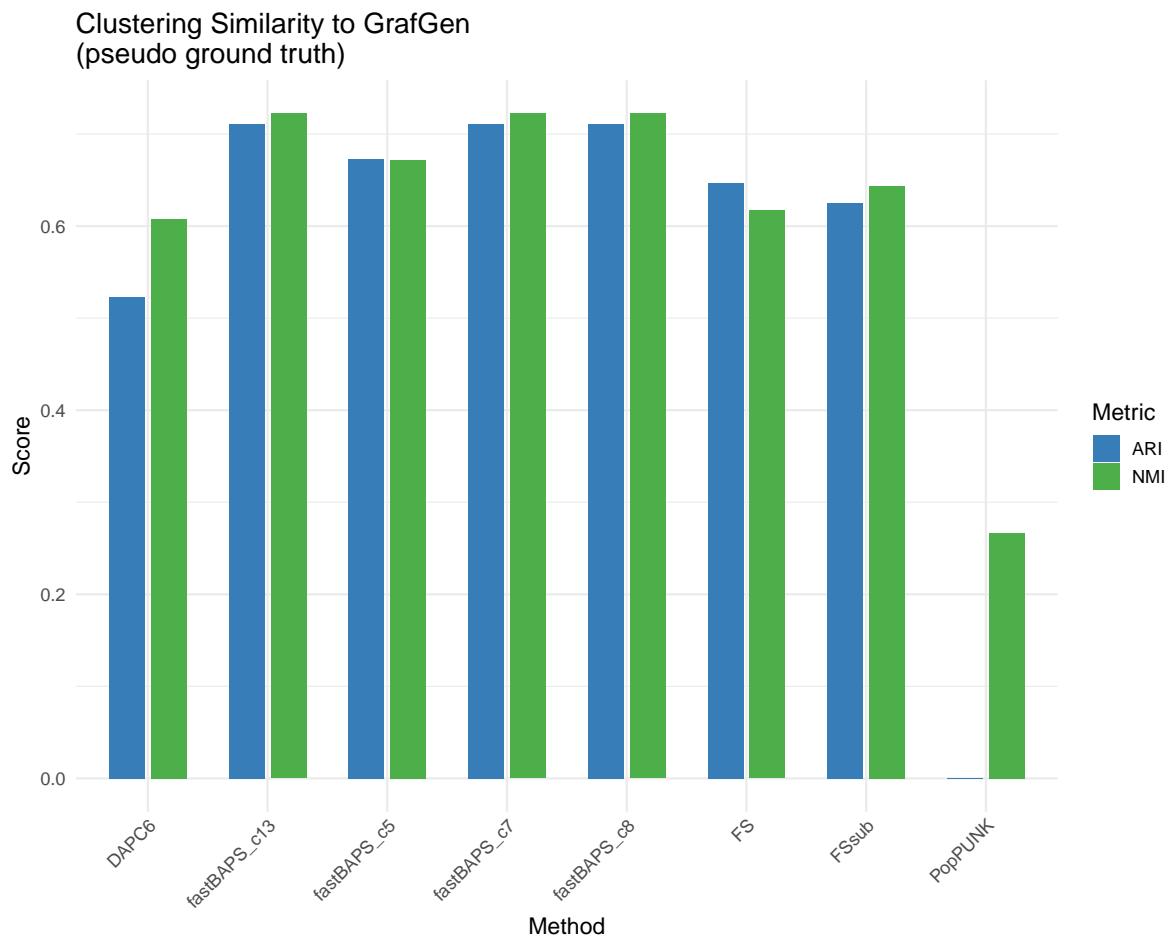
#pdf(file="results/ARI-NMI.barplot.pdf")
ggplot(df_plot, aes(x = Method, y = Score, fill = Metric)) +
  geom_bar(stat = "identity",
            position = position_dodge(width = 0.7),
            width = 0.6) +
  labs(title = "Clustering Similarity to GrafGen\n(pseudo ground truth)",
       y = "Score",
       x = "Method") +
  scale_fill_manual(values = c("ARI" = "#377eb8", "NMI" = "#4daf4a")) +
  theme_minimal(base_size = 14) +
  # smaller `t` value moves it closer

```

```

theme(axis.text.x = element_text(angle = 45,
                                  vjust = 1, # moves text downward, closer to axis
                                  hjust = 1,
                                  margin = margin(t = 0) # remove top margin
                                )
)

```



```
#dev.off()
```

Prepare data for Sankey plot (all four methods)

```

df_sankey <- merged[, c("sample_id", "GrafGen",
                        "fastBAPS_c5",
                        "fastBAPS_c7",
                        "fastBAPS_c8",
                        "fastBAPS_c13",
                        "FS",
                        "FSsub",
                        "DAPC6",
                        "PopPUNK")]

head(df_sankey)

```

	sample_id	GrafGen	fastBAPS_c5	fastBAPS_c7	fastBAPS_c8
1	HpGP-ALG-001	hpgpMediterranea	2	2	2
2	HpGP-ALG-002	hpgpEuroamerica	2	2	2
3	HpGP-ALG-003	hpgpEuroamerica	2	2	2
4	HpGP-ALG-004	hpgpMediterranea	2	2	2
5	HpGP-ALG-005	hpgpMediterranea	2	2	2
6	HpGP-ALG-006	hpgpMediterranea	2	2	2
	fastBAPS_c13	FS	FSsub	DAPC6	PopPUNK
1	2	1	hspSEurope	1	2424
2	2	1	hspSEurope	1	2423
3	2	1	hspSEurope	1	2422
4	2	1	hspSEurope	1	2421
5	2	1	hspSEurope	1	2420
6	2	1	hspSEurope	1	2419

```
write.csv(df_sankey, file="results/df_sankey.csv")
```

Create Sankey plot showing flow across clusterings

```
library(dplyr)
```

Attaching package: 'dplyr'

The following objects are masked from 'package:stats':

filter, lag

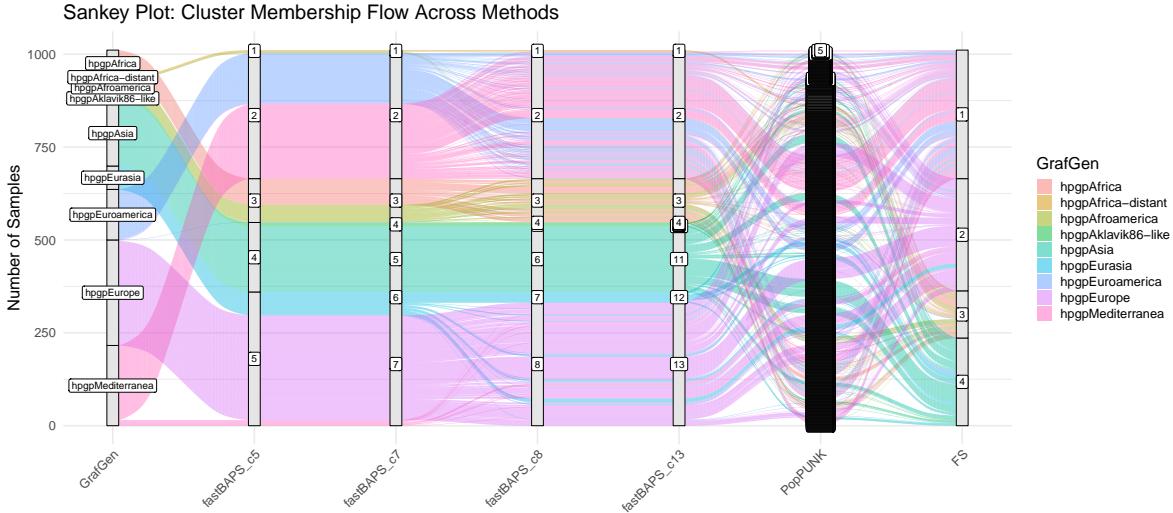
The following objects are masked from 'package:base':

intersect, setdiff, setequal, union

```
# Summarize counts for flows between GrafGen and fastBAPS (as example)
#flow_counts <- df_sankey %>%
#  group_by(GrafGen, fastBAPS) %>%
#  summarise(Freq = n()) %>%
#  ungroup()

#pdf(file="results/Sankey.pdf", height=16, width=24)
# 8. Create Sankey plot showing flow across clusterings
ggplot(df_sankey,
       aes(axis1 = GrafGen, axis2 = fastBAPS_c5, axis3 = fastBAPS_c7,
           axis4 = fastBAPS_c8, axis5 = fastBAPS_c13, axis6 = PopPUNK,
           axis7 = FS)) +
  geom_alluvium(aes(fill = GrafGen), width = 1/12) +
  geom_stratum(width = 1/12, fill = "gray90", color = "black") +
  geom_label(stat = "stratum", aes(label = after_stat(stratum))) +
  scale_x_discrete(limits = c("GrafGen", "fastBAPS_c5", "fastBAPS_c7",
                               "fastBAPS_c8", "fastBAPS_c13", "PopPUNK", "FS"),
                    expand = c(.05, .05)) +
  theme_minimal(base_size = 18) +
  theme(axis.text.x = element_text(angle = 45,
                                    vjust = 1,
                                    hjust = 1,
                                    margin = margin(t = 0) # remove top margin
                                    )) +
  labs(title = "Sankey Plot: Cluster Membership Flow Across Methods",
       y = "Number of Samples")
```

```
Warning in to_lodes_form(data = data, axes = axis_ind, discern =
params$discern): Some strata appear at multiple axes.
Warning in to_lodes_form(data = data, axes = axis_ind, discern =
params$discern): Some strata appear at multiple axes.
Warning in to_lodes_form(data = data, axes = axis_ind, discern =
params$discern): Some strata appear at multiple axes.
```



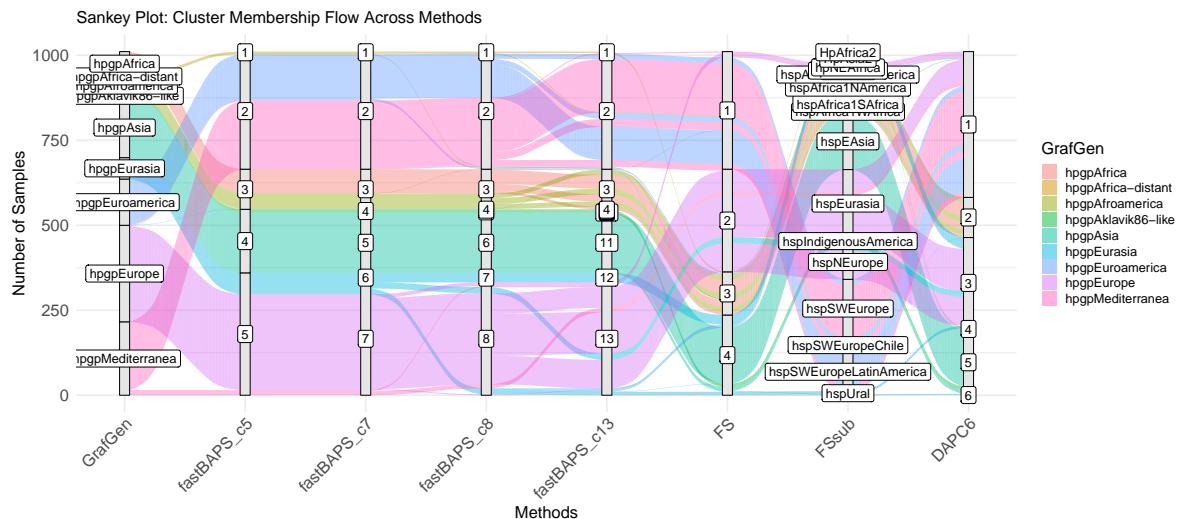
```
# 8.1 Create Sankey plot showing flow across clusterings
ggplot(df_sankey,
       aes(axis1 = GrafGen,
            axis2 = fastBAPS_c5,
            axis3 = fastBAPS_c7,
            axis4 = fastBAPS_c8,
            axis5 = fastBAPS_c13,
            axis6 = FS,
            axis7 = FSsub,
            axis8 = DAPC6)) +
  geom_alluvium(aes(fill = GrafGen), width = 1/12) +
  geom_stratum(width = 1/12, fill = "gray90", color = "black") +
  geom_label(stat = "stratum", aes(label = after_stat(stratum)),
             size = 5, fontface = "plain") +
#  geom_text(data = flow_counts,
#            aes(x = 1.5, y = Freq / 2 + cumsum(Freq) - Freq/2, label = Freq),
#            inherit.aes = FALSE,
#            size = 4) +
  scale_x_discrete(limits = c("GrafGen",
                               "fastBAPS_c5",
                               "fastBAPS_c7",
                               "fastBAPS_c8",
                               "fastBAPS_c13",
                               "FS",
                               "FSsub",
                               "DAPC6"),
                   expand = c(.05, .05)) +
```

```

theme_minimal(base_size = 18) +
theme(
  axis.title = element_text(face = "plain", size = 18), # bold axis titles
  axis.text = element_text(face = "plain", size = 18), # bold axis text (ticks)
  plot.title = element_text(face = "plain", size = 18), # bold and bigger title
  axis.text.x = element_text(angle = 45,
                             vjust = 1, # moves text downward, closer to axis
                             hjust = 1,
                             margin = margin(t = 0) # remove top margin
  )
) +
labs(title = "Sankey Plot: Cluster Membership Flow Across Methods",
  x = "Methods",
  y = "Number of Samples")

```

Warning in to_lodes_form(data = data, axes = axis_ind, discern = params\$discern): Some strata appear at multiple axes.
 Warning in to_lodes_form(data = data, axes = axis_ind, discern = params\$discern): Some strata appear at multiple axes.
 Warning in to_lodes_form(data = data, axes = axis_ind, discern = params\$discern): Some strata appear at multiple axes.



```

## all methods
# 8.2 Create Sankey plot showing flow across clusterings
ggplot(df_sankey,

```

```

aes(axis1 = GrafGen,
    axis2 = fastBAPS_c5,
    axis3 = fastBAPS_c7,
    axis4 = fastBAPS_c8,
    axis5 = fastBAPS_c13,
    axis6 = FS,
    axis7 = FSsub,
    axis8 = DAPC6,
    axis9 = PopPUNK)) +
geom_alluvium(aes(fill = GrafGen), width = 1/12) +
geom_stratum(width = 1/12, fill = "gray90", color = "black") +
geom_label(stat = "stratum", aes(label = after_stat(stratum)),
           size = 5, fontface = "plain") +
# geom_text(data = flow_counts,
#           aes(x = 1.5, y = Freq / 2 + cumsum(Freq) - Freq/2, label = Freq),
#           inherit.aes = FALSE,
#           size = 4) +
scale_x_discrete(limits = c("GrafGen",
                             "fastBAPS_c5",
                             "fastBAPS_c7",
                             "fastBAPS_c8",
                             "fastBAPS_c13",
                             "FS",
                             "FSsub",
                             "DAPC6",
                             "PopPUNK"),
                  expand = c(.05, .05)) +
theme_minimal(base_size = 18) +
theme(
  axis.title = element_text(face = "plain", size = 18), # bold axis titles
  axis.text = element_text(face = "plain", size = 18), # bold axis text (ticks)
  plot.title = element_text(face = "plain", size = 18), # bold and bigger title
  axis.text.x = element_text(angle = 45,
                             vjust = 1,
                             hjust = 1,
                             margin = margin(t = 0) # remove top margin
                           )) +
labs(title = "Sankey Plot: Cluster Membership Flow Across Methods",
      x = "Methods",
      y = "Number of Samples")

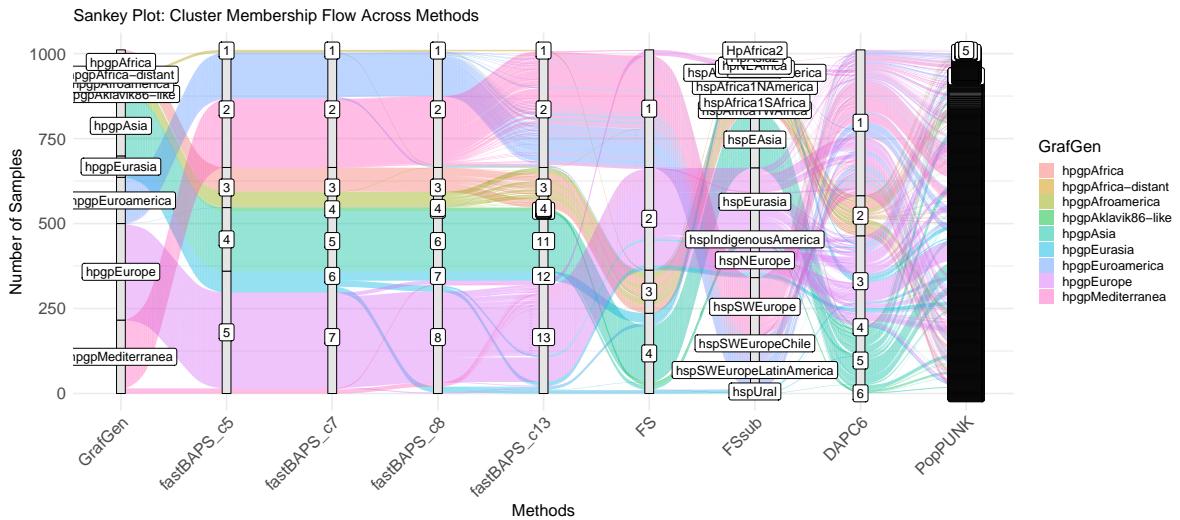
```

Warning in to_lodes_form(data = data, axes = axis_ind, discern =

```

params$discern): Some strata appear at multiple axes.
Warning in to_lodes_form(data = data, axes = axis_ind, discern =
params$discern): Some strata appear at multiple axes.
Warning in to_lodes_form(data = data, axes = axis_ind, discern =
params$discern): Some strata appear at multiple axes.

```



```

# 8.3 Create Sankey plot showing flow across clusterings, no PopPUNK and DAPC6
pdf(file="results/Sankey.pdf", height=16, width=30)
p <- ggplot(df_sankey,
             aes(axis1 = GrafGen,
                  axis2 = fastBAPS_c5,
                  axis3 = fastBAPS_c7,
                  axis4 = fastBAPS_c8,
                  axis5 = fastBAPS_c13,
                  axis6 = FS,
                  axis7 = FSsub)) +
  geom_alluvium(aes(fill = GrafGen), width = 1/12) +
  geom_stratum(width = 1/12, fill = "gray90", color = "black") +
  geom_label(stat = "stratum", aes(label = after_stat(stratum)),
             size = 5, fontface = "bold") +
  # geom_text(data = flow_counts,
  #           aes(x = 1.5, y = Freq / 2 + cumsum(Freq) - Freq/2, label = Freq),
  #           inherit.aes = FALSE,
  #           size = 4) +
  scale_x_discrete(limits = c("GrafGen",
                               "fastBAPS_c5",

```

```

    "fastBAPS_c7",
    "fastBAPS_c8",
    "fastBAPS_c13",
    "FS",
    "FSsub"),
  expand = c(.05, .05)) +
theme_minimal(base_size = 20) +
theme(
  axis.title = element_text(face = "bold", size = 20), # bold axis titles
  axis.text = element_text(face = "bold", size = 20), # bold axis text (ticks)
  plot.title = element_text(face = "bold", size = 28), # bold and bigger title
  axis.text.x = element_text(angle = 45,
                             vjust = 1, # moves text downward, closer to axis
                             hjust = 1,
                             margin = margin(t = 0) # remove top margin
                           )
)
+
labs(title = "Sankey Plot: Cluster Membership Flow Across Methods",
      x = "Methods",
      y = "Number of Samples")
print(p)

```

Warning in to_lodes_form(data = data, axes = axis_ind, discern =
params\$discern): Some strata appear at multiple axes.
Warning in to_lodes_form(data = data, axes = axis_ind, discern =
params\$discern): Some strata appear at multiple axes.
Warning in to_lodes_form(data = data, axes = axis_ind, discern =
params\$discern): Some strata appear at multiple axes.

```
dev.off()
```

```

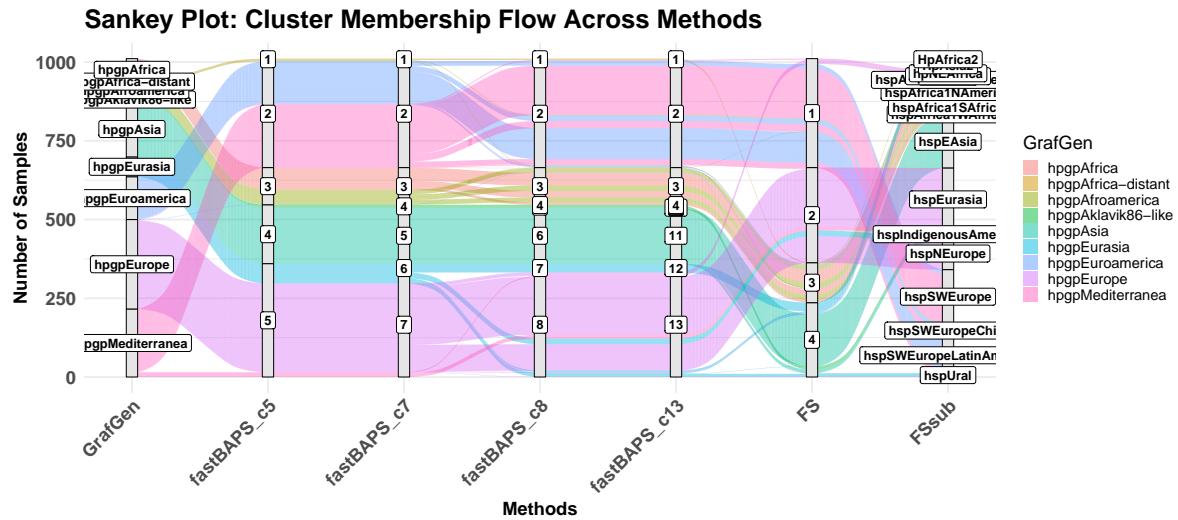
pdf
2

```

```
print(p)
```

Warning in to_lodes_form(data = data, axes = axis_ind, discern =
params\$discern): Some strata appear at multiple axes.
Warning in to_lodes_form(data = data, axes = axis_ind, discern =
params\$discern): Some strata appear at multiple axes.

```
Warning in to_lodes_form(data = data, axes = axis_ind, discern =
params$discern): Some strata appear at multiple axes.
```



Output ARI and NMI in a table and save to CSV

```
results_table <- data.frame(
  Method = methods,
  ARI = round(ari_vals, 3),
  NMI = round(nmi_vals, 3)
)

print(results_table)
```

	Method	ARI	NMI
1	fastBAPS_c5	0.673	0.672
2	fastBAPS_c7	0.711	0.722
3	fastBAPS_c8	0.711	0.722
4	fastBAPS_c13	0.711	0.722
5	FS	0.647	0.617
6	FSub	0.625	0.643
7	DAPC6	0.523	0.607
8	PopPUNK	0.001	0.267

```
write.csv(results_table, "results/clustering_comparison_results.csv",
          row.names = FALSE)
```