analysis

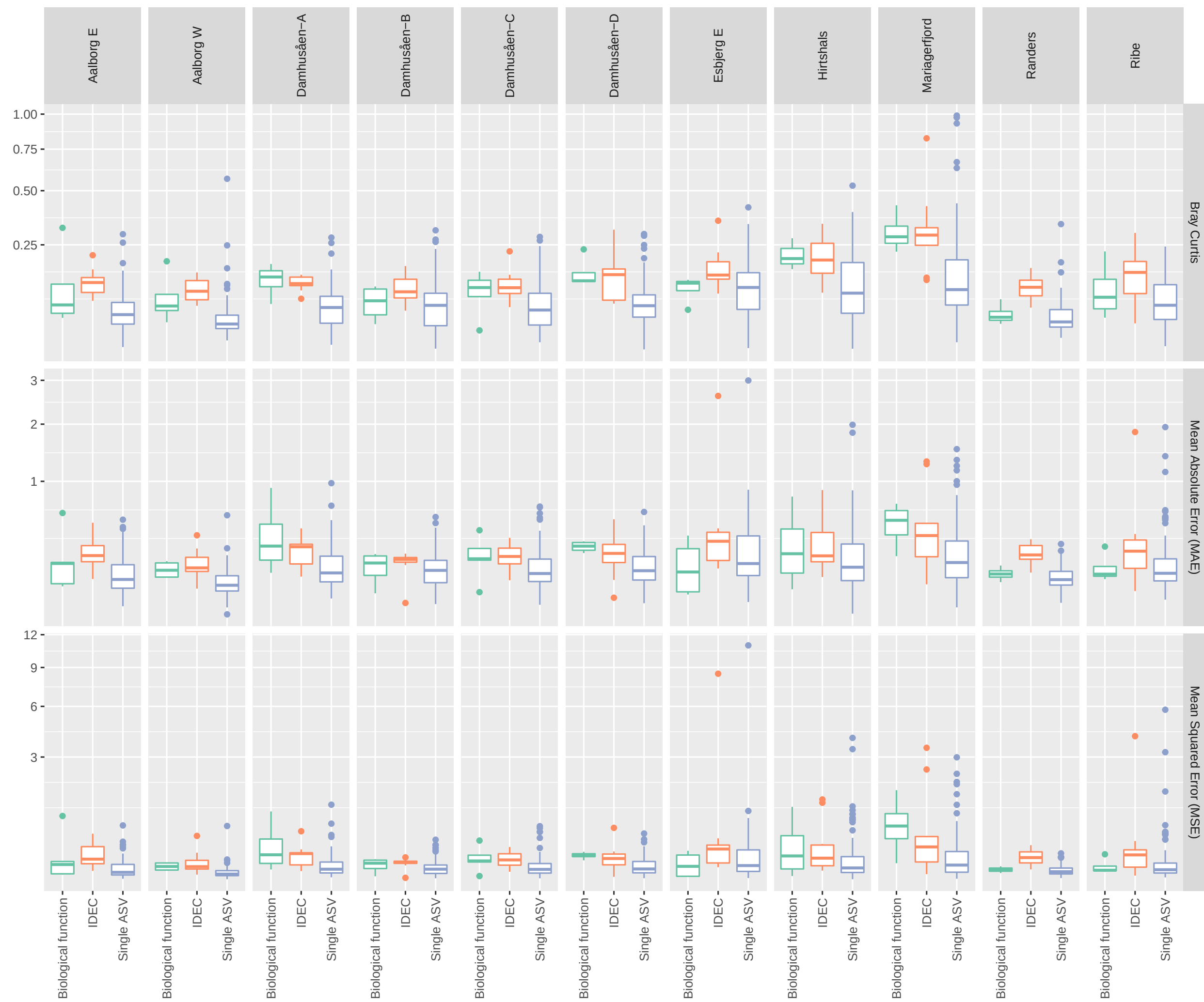
KSA

2022-05-13

Prediction accuracy across WWTPs

top 100 ASVs, 10 iterations, 200 epochs, smoothing factor 8

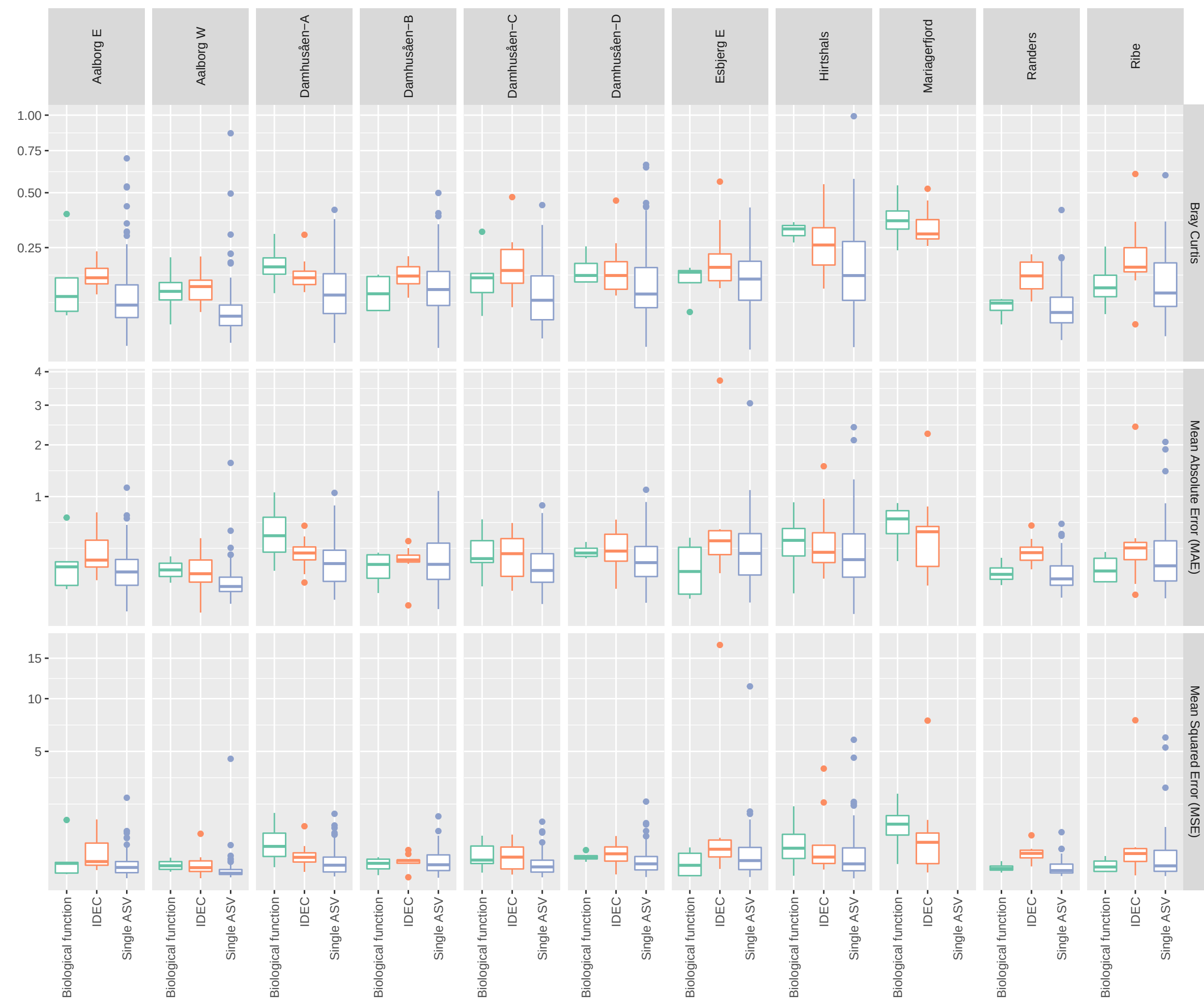
```
plot_all("results/20220420")
```



```
# "only_pos_func": false,
# "pseudo_zero": 0.01,
# "max_zeros_pct": 0.60,
# "top_n_taxa": 100,
# "num_features": 10,
# "iterations": 10,
# "max_epochs_lstm": 200,
# "window_size": 10,
# "num_clusters_idec": 10,
# "tolerance_idec": 0.001,
# "splits": [
#     0.75,
#     0.10,
#     0.15
# ]
```

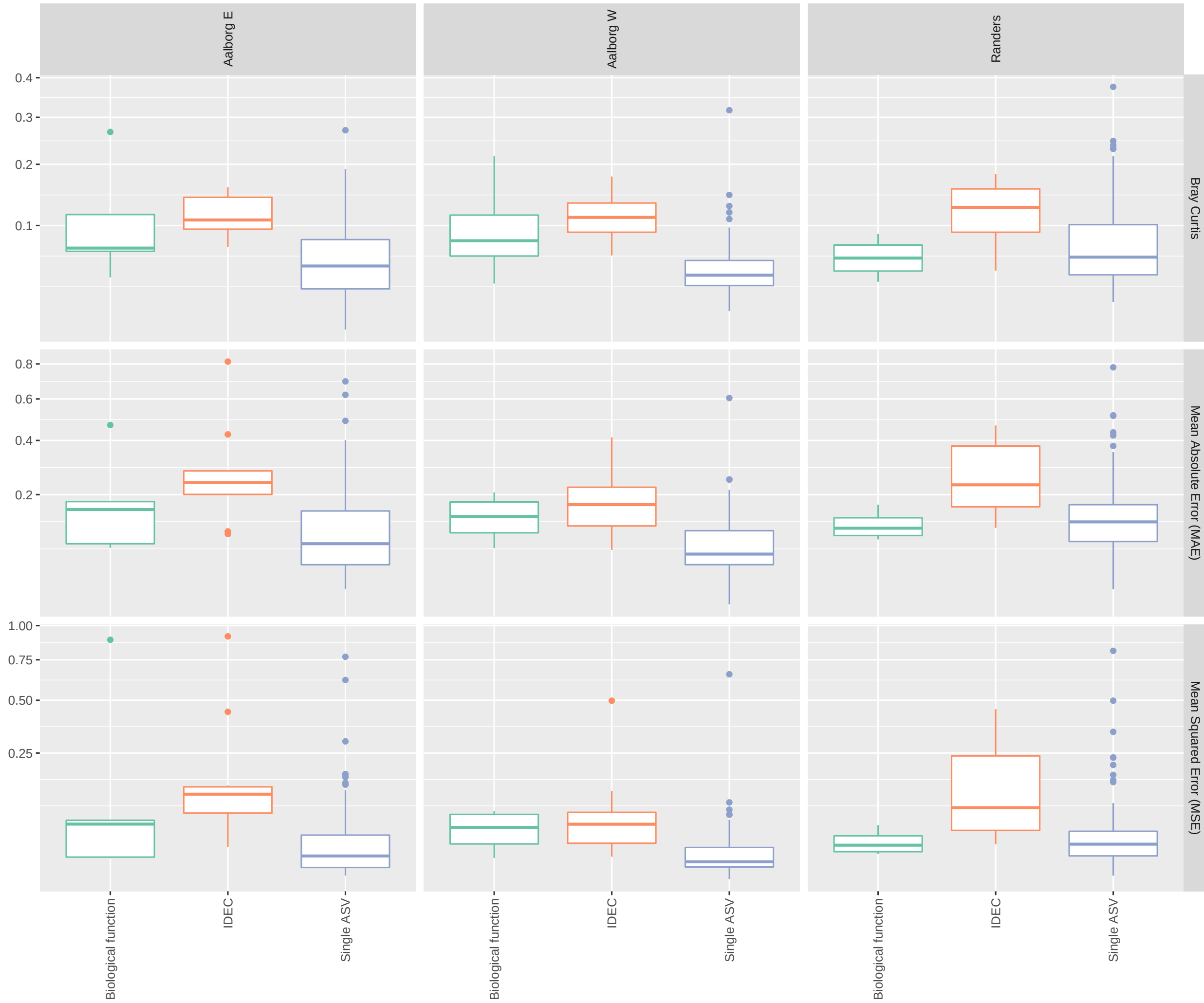
1 iteration, 1000 max epochs

```
# "only_pos_func": false,
# "pseudo_zero": 0.01,
# "max_zeros_pct": 0.60,
# "top_n_taxa": 100,
# "num_features": 10,
# "iterations": 1,
# "max_epochs_lstm": 1000,
# "window_size": 10,
# "num_clusters_idec": 10,
# "tolerance_idec": 0.001,
# "splits": [
#     0.75,
#     0.10,
#     0.15
# ]
plot_all("results/20220421")
```



10 iterations, 2000 max epochs, window size 20

```
# "only_pos_func": false,
# "pseudo_zero": 0.01,
# "max_zeros_pct": 0.60,
# "top_n_taxa": 100,
# "num_features": 10,
# "iterations": 10,
# "max_epochs_lstm": 2000,
# "window_size": 20,
# "num_clusters_idec": 10,
# "tolerance_idec": 0.001,
# "splits": [
#     0.75,
#     0.10,
#     0.15
# ]
plot_all("results/20220422")
```



top 200 ASVs, windows size 10, 20 IDEC clusters

```
# "only_pos_func": false,
# "pseudo_zero": 0.01,
# "max_zeros_pct": 0.60,
# "top_n_taxa": 200,
# "num_features": 10,
# "iterations": 10,
# "max_epochs_lstm": 2000,
# "window_size": 10,
# "num_clusters_idec": 20,
# "tolerance_idec": 0.001,
# "splits": [
#     0.75,
#     0.10,
#     0.15
# ]
plot_all("results/20220427")
```

5 IDEC clusters

```
# "only_pos_func": false,
# "pseudo_zero": 0.01,
# "max_zeros_pct": 0.60,
# "top_n_taxa": 200,
# "num_features": 10,
# "iterations": 10,
# "max_epochs_lstm": 2000,
# "window_size": 10,
# "num_clusters_idec": 5,
# "tolerance_idec": 0.001,
# "splits": [
#     0.75,
#     0.10,
#     0.15
# ]
plot_all("results/20220429")
```

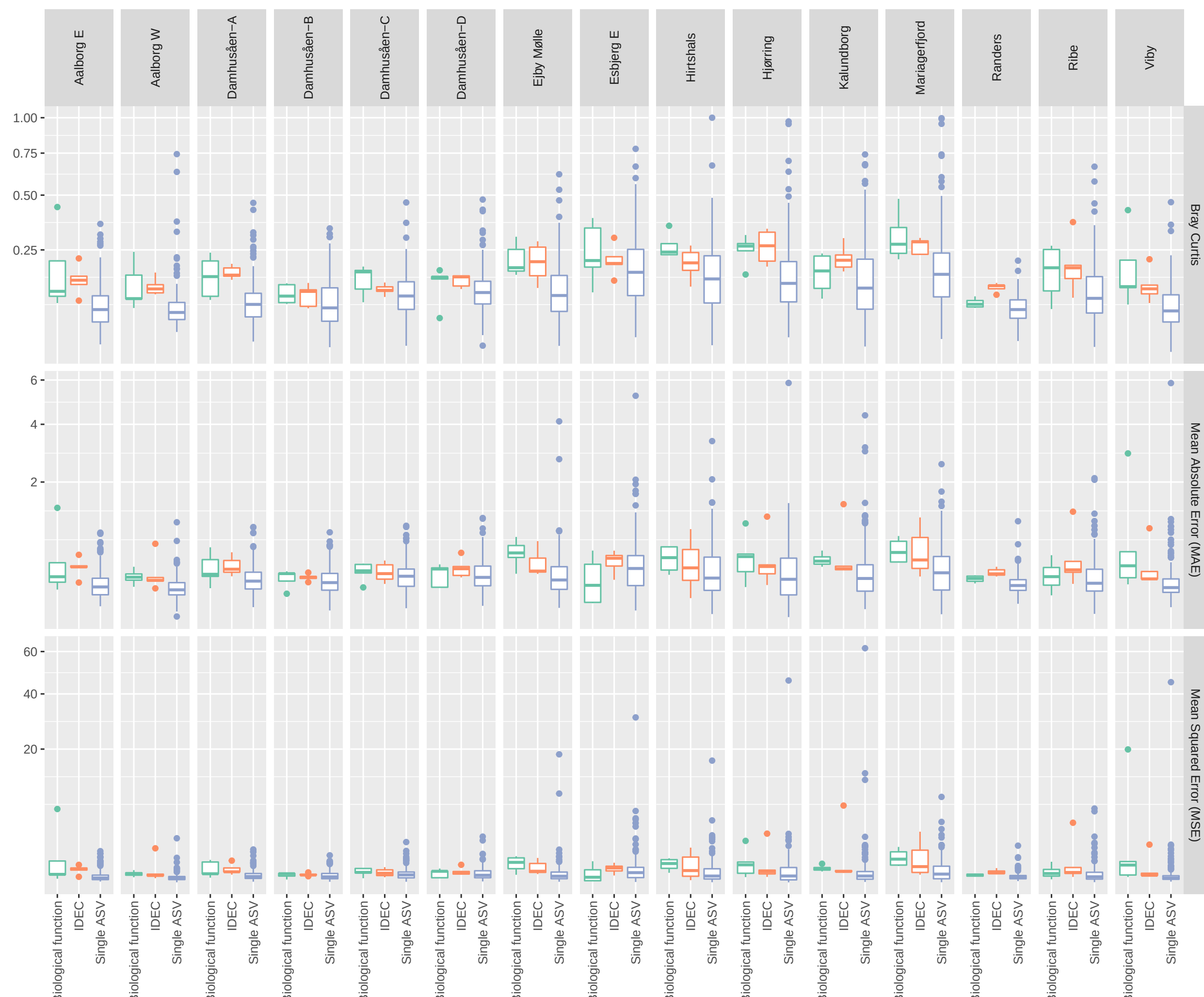
smoothing factor 4

```
# "only_pos_func": false,
# "pseudo_zero": 0.01,
# "max_zeros_pct": 0.60,
# "top_n_taxa": 200,
# "num_features": 10,
# "iterations": 10,
# "max_epochs_lstm": 2000,
# "window_size": 10,
# "num_clusters_idec": 5,
# "tolerance_idec": 0.001,
# "smoothing_factor": 4,
# "splits": [
#     0.75,
#     0.10,
#     0.15
```

```r
# ]
plot_all("results/20220506")
```


```r
# "metadata_date_col": "Date",
# "tax_level": "OTU",
# "tax_add": ["Species", "Genus"],
# "functions": [
#     "AOB",
#     "NOB",
#     "PAO",
#     "GAO",
#     "Filamentous"
# ],
# "only_pos_func": false,
# "pseudo_zero": 0.01,
# "max_zeros_pct": 0.60,
# "top_n_taxa": 200,
# "num_features": 10,
# "iterations": 10,
# "max_epochs_lstm": 2000,
```

```
# "window_size": 10,
# "num_clusters_idec": 5,
# "tolerance_idec": 0.001,
# "smoothing_factor": 4,
# "splits": [
#     0.75,
#     0.10,
#     0.15
# ]
plot_all("results/20220511_updateddata")
```

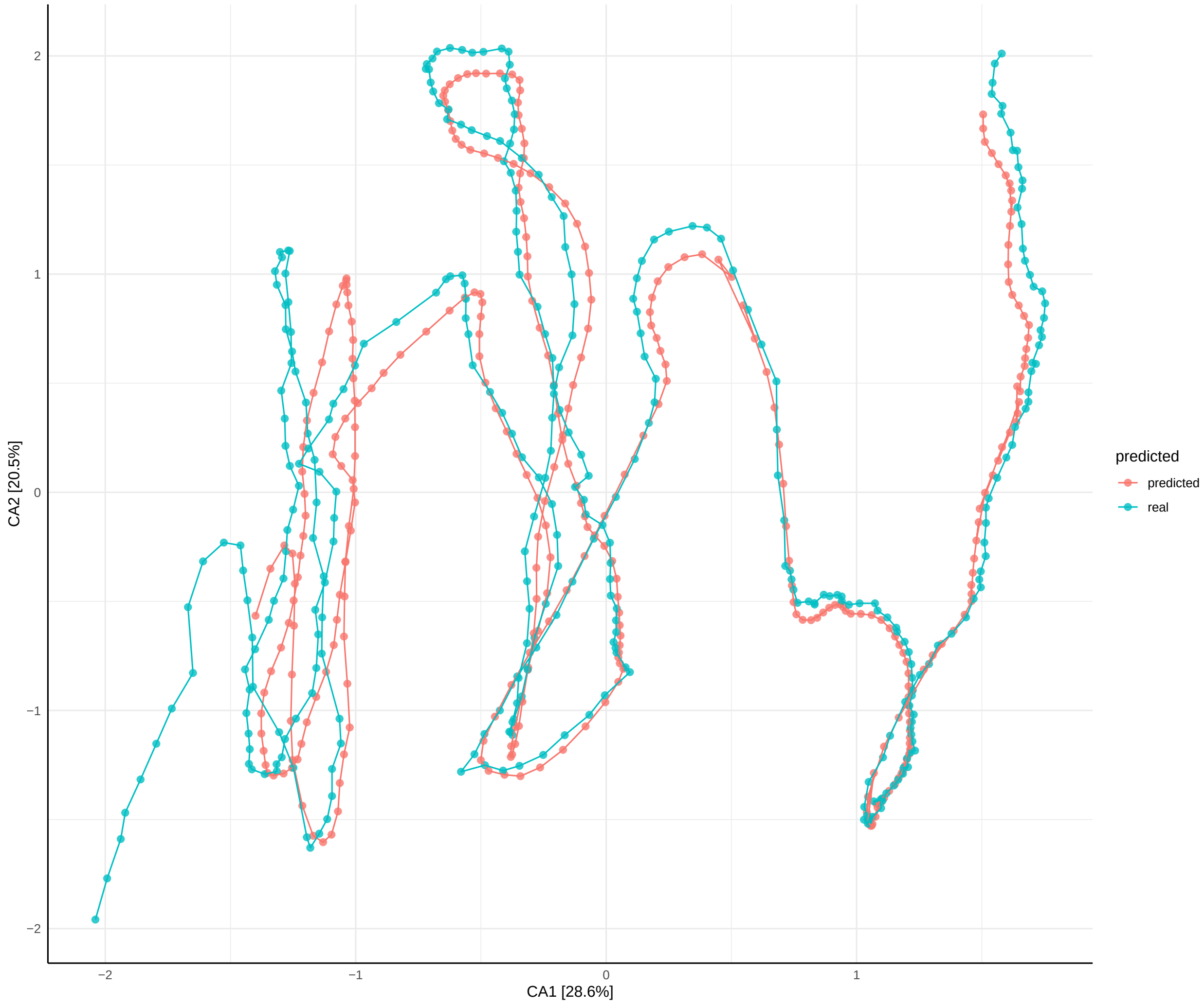


Aalborg West comparison of true vs predicted (smoothing factor 8)

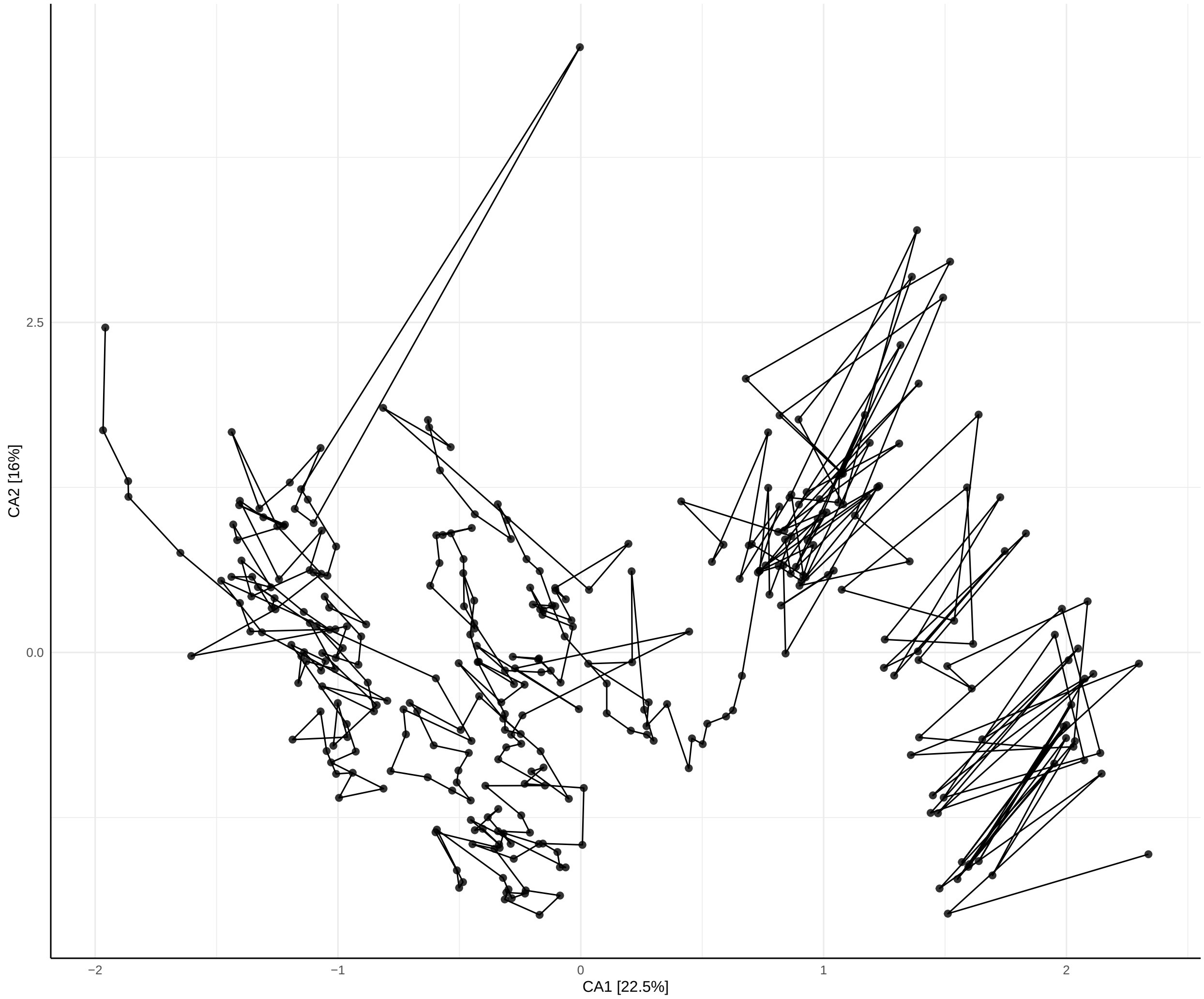
Correspondence Analysis

```
# Configuration:
# {
#     "abund_file": "data/datasets/Aalborg W/ASVtable.csv",
#     "taxonomy_file": "data/datasets/Aalborg W/taxonomy.csv",
#     "metadata_file": "data/metadata.csv",
#     "results_dir": "results",
#     "metadata_date_col": "Date",
#     "tax_level": "OTU",
#     "tax_add": ["Species", "Genus"],
#     "functions": [
#         "AOB",
#         "NOB",
#         "PAO",
#         "GAO",
#         "Filamentous"
#     ],
#     "only_pos_func": false,
#     "pseudo_zero": 0.01,
#     "max_zeros_pct": 0.60,
#     "top_n_taxa": 200,
#     "num_features": 10,
#     "iterations": 10,
#     "max_epochs_lstm": 2000,
#     "window_size": 10,
#     "num_clusters_idec": 5,
#     "tolerance_idec": 0.001,
#     "smoothing_factor": 8,   # <-------------
#     "splits": [
#         0.75,
#         0.10,
#         0.15
#     ]
# }
results_dir <- "results/20220429/results_20220429_182545"
AAW_20220429 <- combine_abund(
  results_dir,
  cluster_type = "abund"
)

AAW_20220429_reformatted <- load_data_reformatted(results_dir)

# run data (here smoothing factor 8)
amp_ordinate(
  AAW_20220429,
  type = "ca",
  sample_color_by = "predicted",
  sample_trajectory = "Date"
```

```
)
```

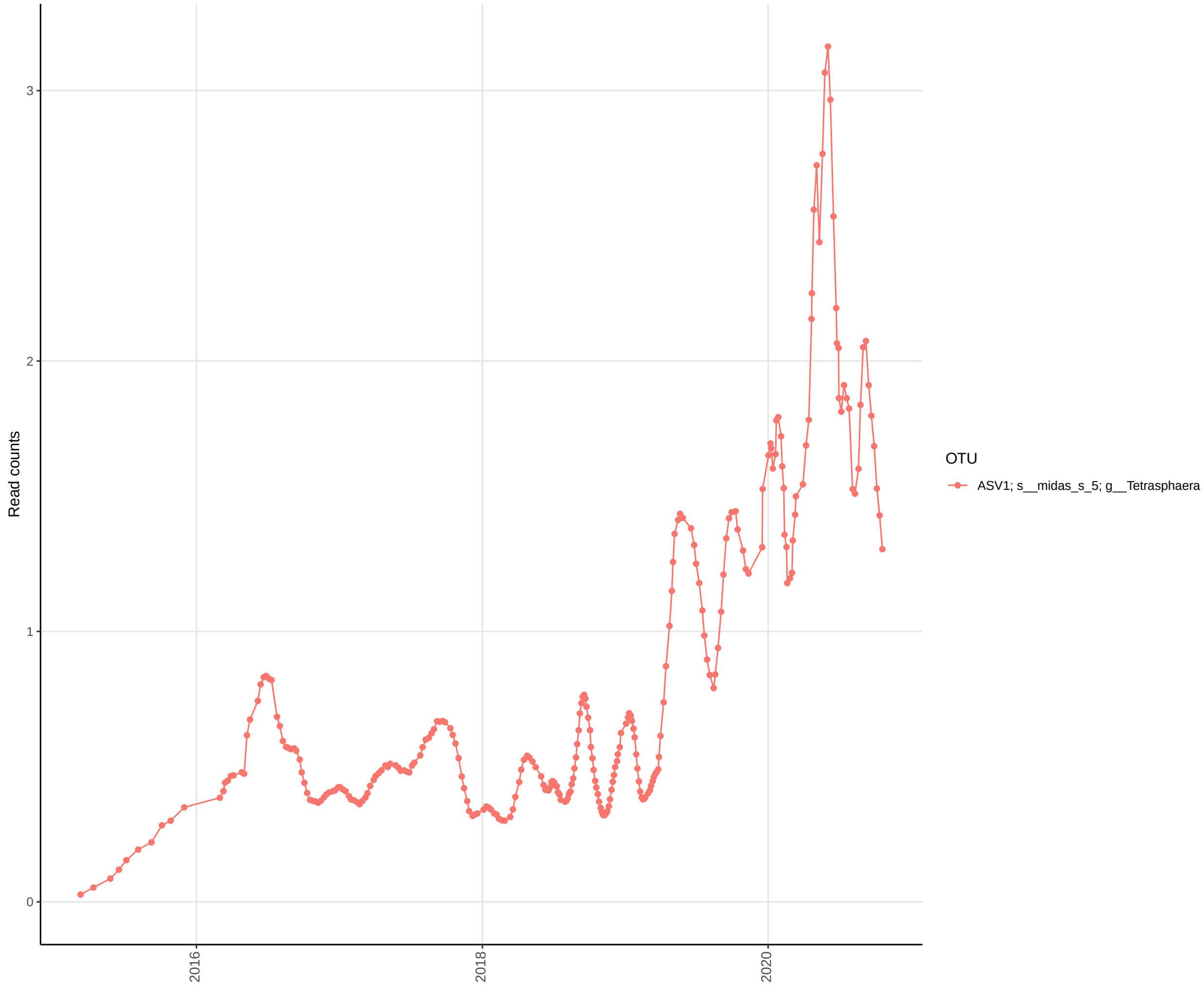



```
# raw reformatted data (here not smoothed)
amp_ordinate(
  AAW_20220429_reformatted,
  type = "ca",
  sample_trajectory = "Date"
)
```

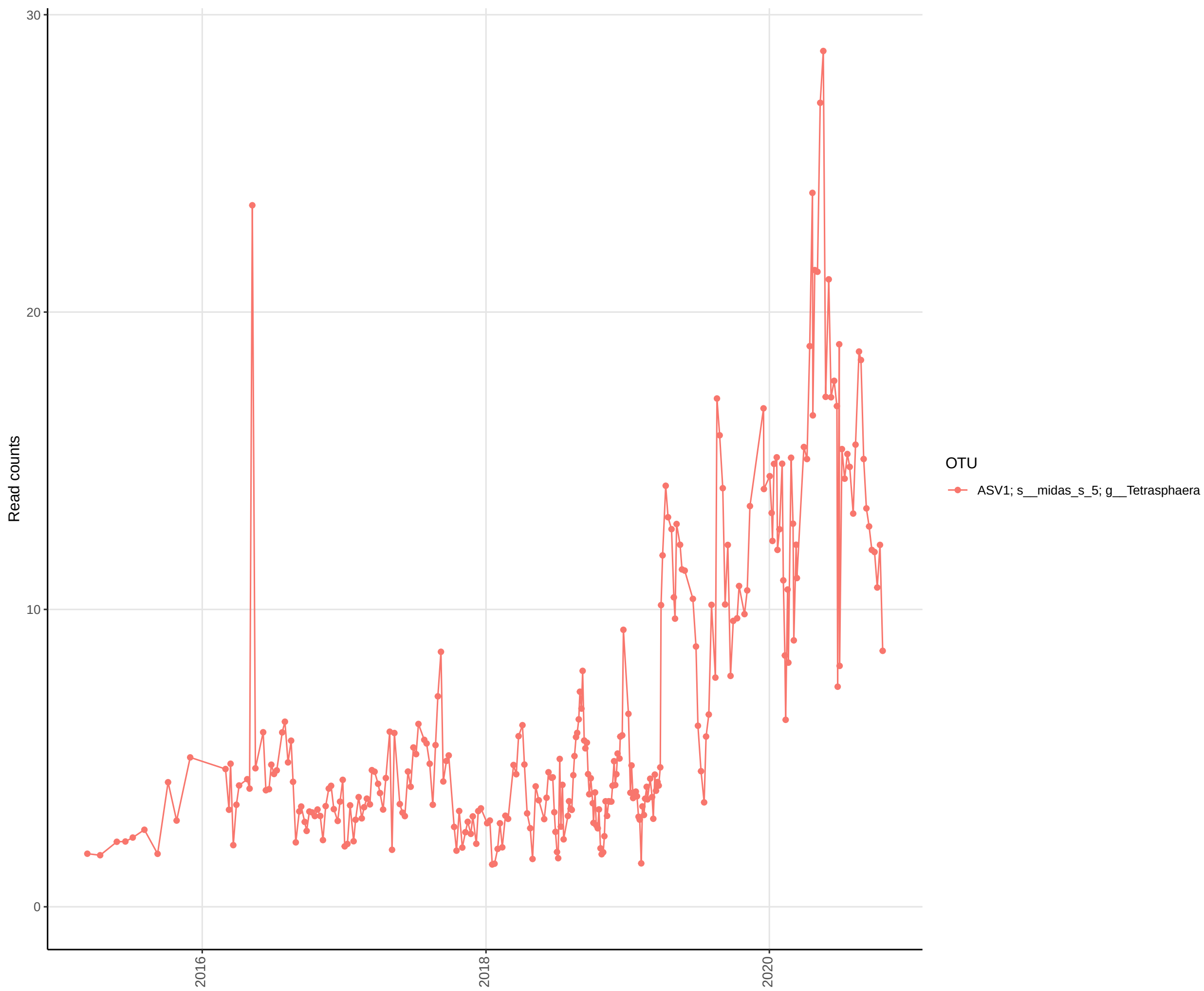


Time Series example ASV1

```
# run data (here smoothing factor 8)
amp_timeseries(
  amp_subset_taxa(
    AAW_20220429,
    "ASV1; s__midas_s_5; g__Tetrasphaera",
    normalise = FALSE
  ),
  time_variable = "Date",
  normalise = FALSE
)
```




```
# raw reformatted data (here not smoothed)
amp_timeseries(
  amp_subset_taxa(
    AAW_20220429_reformatted,
    "ASV1; s__midas_s_5; g__Tetrasphaera",
    normalise = FALSE
  ),
  time_variable = "Date",
  normalise = FALSE
)
```

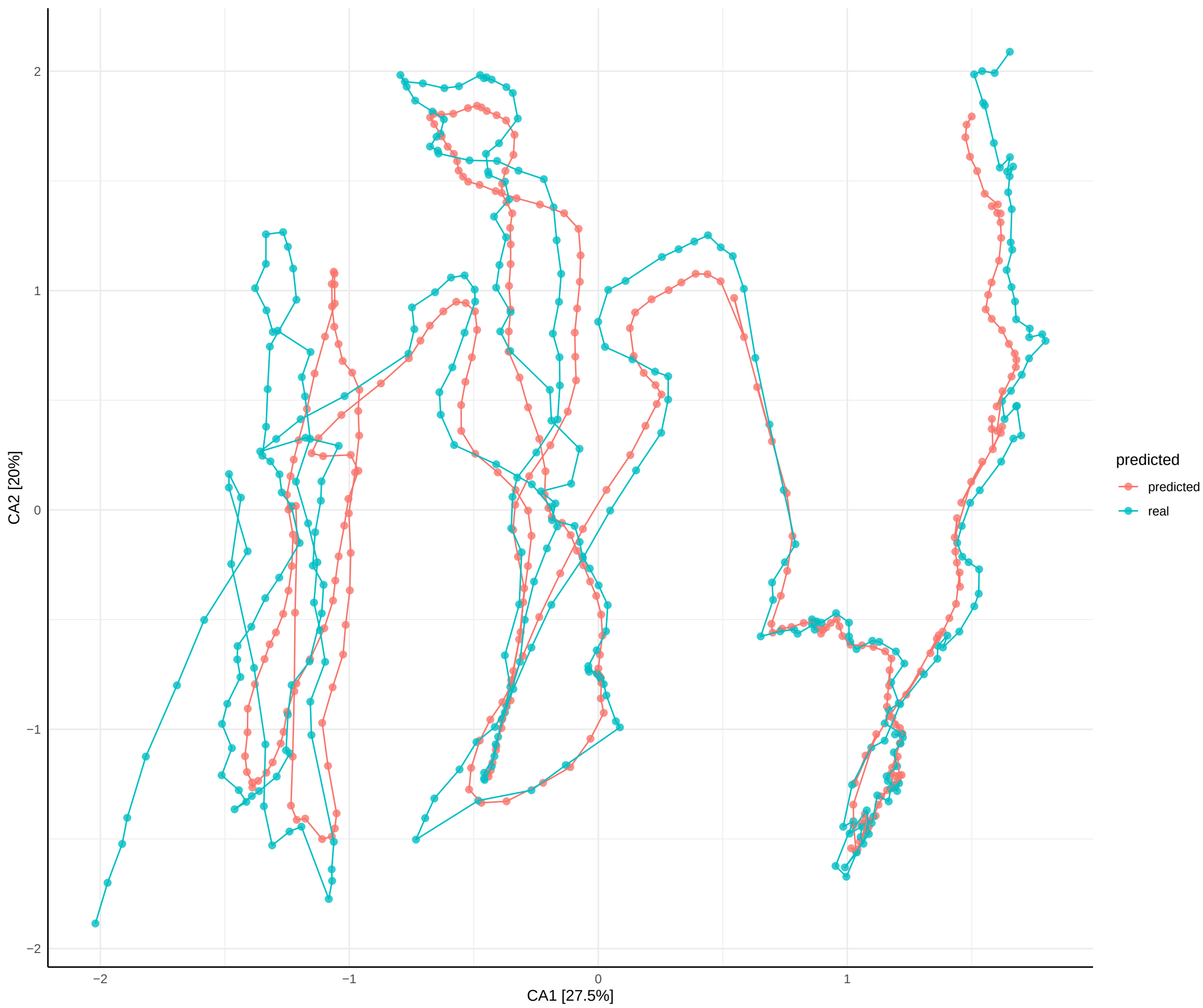


Aalborg West comparison of true vs predicted (smoothing factor 4)

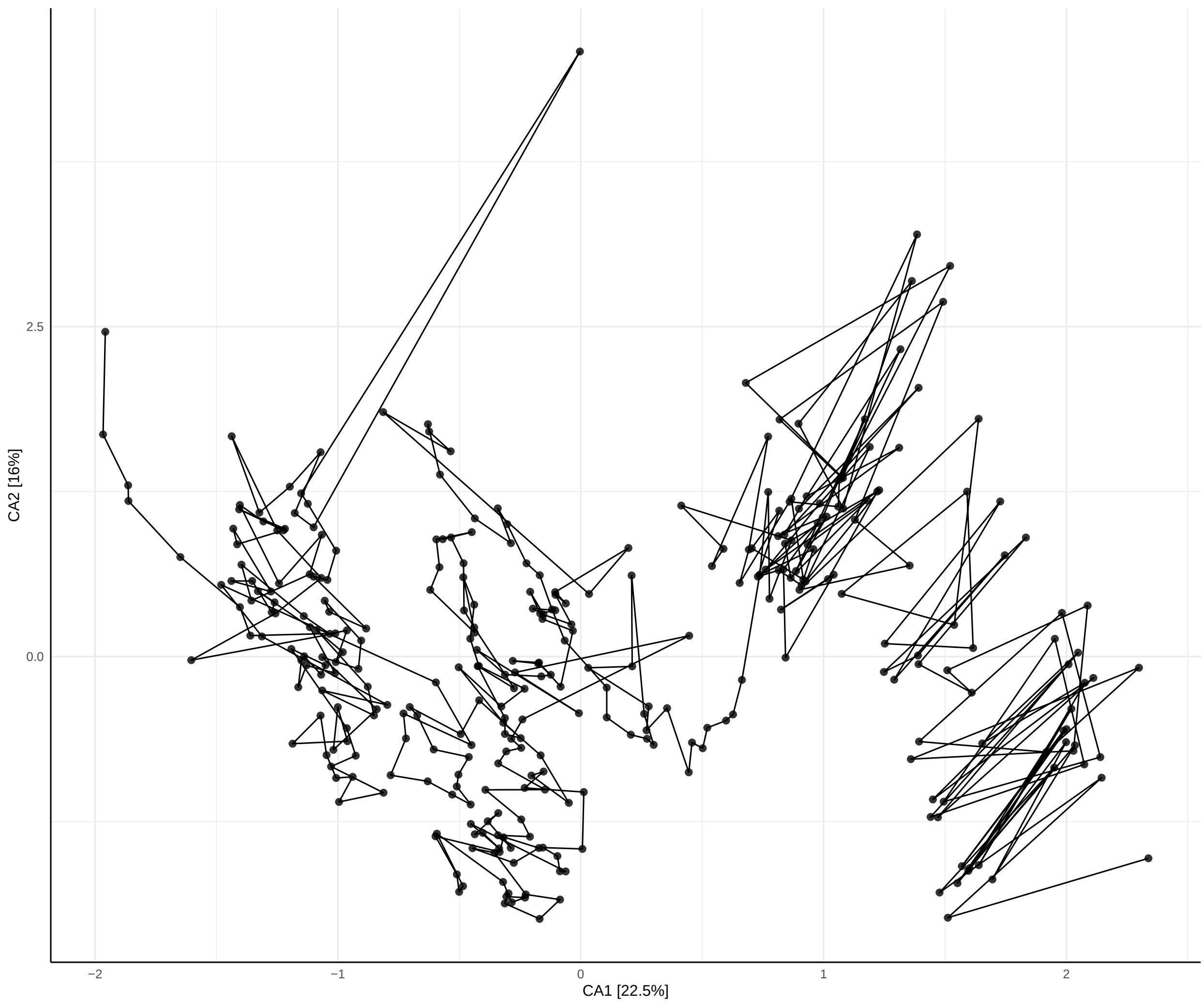
Correspondence Analysis

```
# Configuration:
# {
#     "abund_file": "data/datasets/Aalborg W/ASVtable.csv",
#     "taxonomy_file": "data/datasets/Aalborg W/taxonomy.csv",
#     "metadata_file": "data/metadata.csv",
#     "results_dir": "results",
#     "metadata_date_col": "Date",
#     "tax_level": "OTU",
#     "tax_add": ["Species", "Genus"],
#     "functions": [
#         "AOB",
#         "NOB",
```

```r
#         "PAO",
#         "GAO",
#         "Filamentous"
#     ],
#     "only_pos_func": false,
#     "pseudo_zero": 0.01,
#     "max_zeros_pct": 0.60,
#     "top_n_taxa": 200,
#     "num_features": 10,
#     "iterations": 10,
#     "max_epochs_lstm": 2000,
#     "window_size": 10,
#     "num_clusters_idec": 5,
#     "tolerance_idec": 0.001,
#     "smoothing_factor": 4,   # <-------------
#     "splits": [
#         0.75,
#         0.10,
#         0.15
#     ]
# }
results_dir <- "results/20220506/results_20220506_182133"
AAW_20220506 <- combine_abund(
  results_dir,
  cluster_type = "abund"
)

AAW_20220506_reformatted <- load_data_reformatted(results_dir)

# run data (here smoothing factor 8)
amp_ordinate(
  AAW_20220506,
  type = "ca",
  sample_color_by = "predicted",
  sample_trajectory = "Date"
)
```

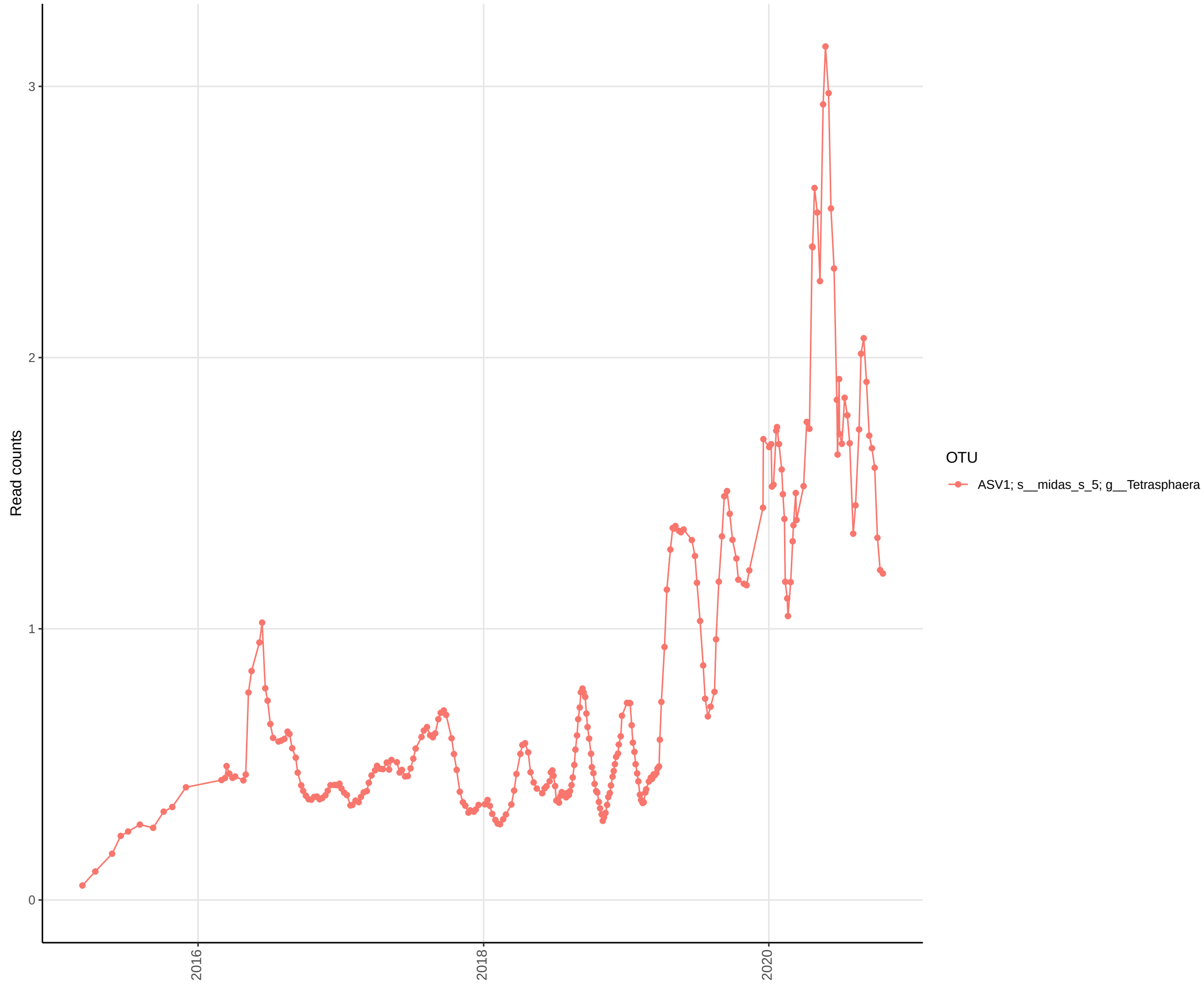



```r
# raw reformatted data (here not smoothed)
amp_ordinate(
  AAW_20220506_reformatted,
  type = "ca",
  sample_trajectory = "Date"
)
```

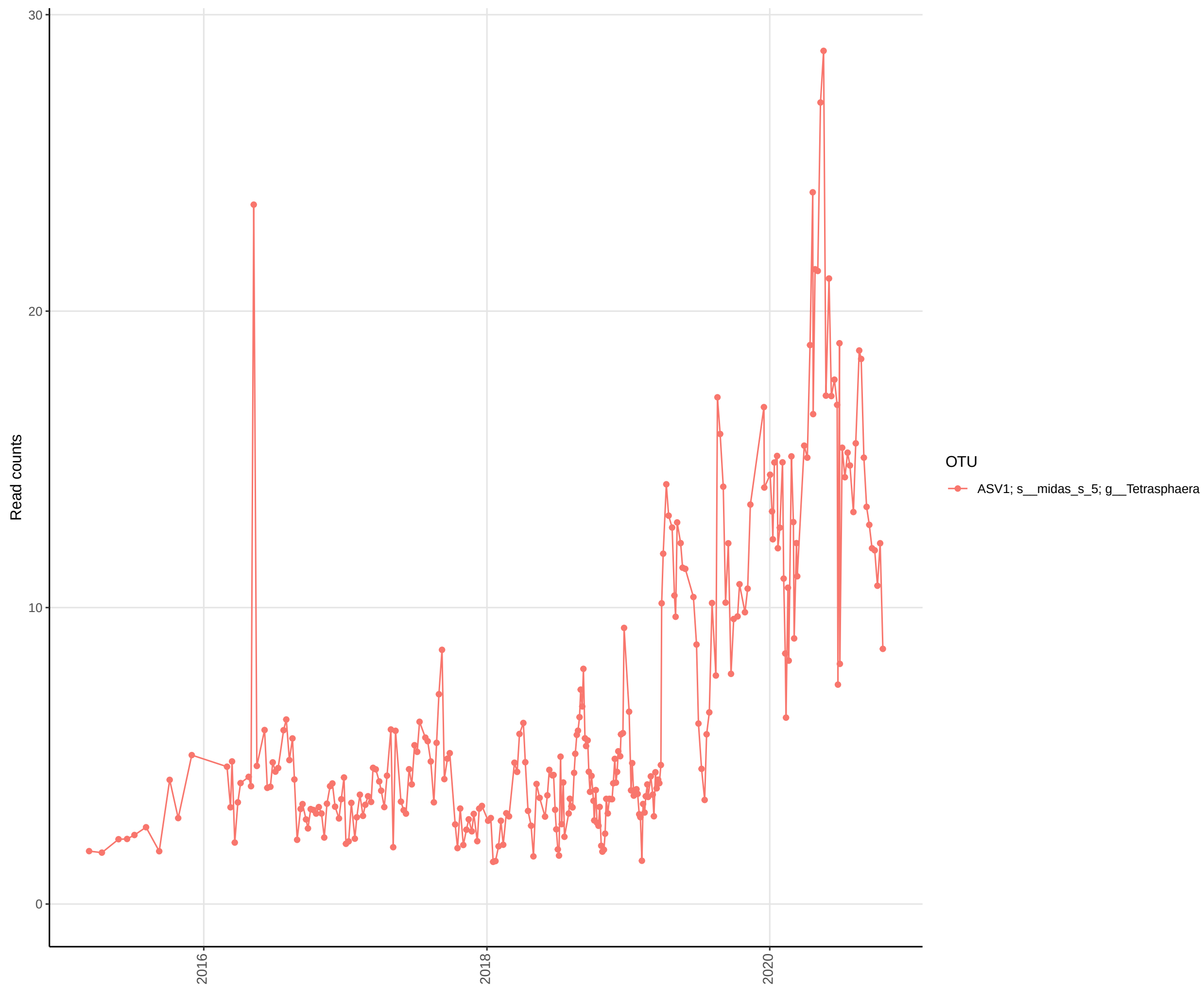


Time Series example ASV1

```
# run data (here smoothing factor 8)
amp_timeseries(
  amp_subset_taxa(
    AAW_20220506,
    "ASV1; s__midas_s_5; g__Tetrasphaera",
    normalise = FALSE
  ),
  time_variable = "Date",
  normalise = FALSE
)
```



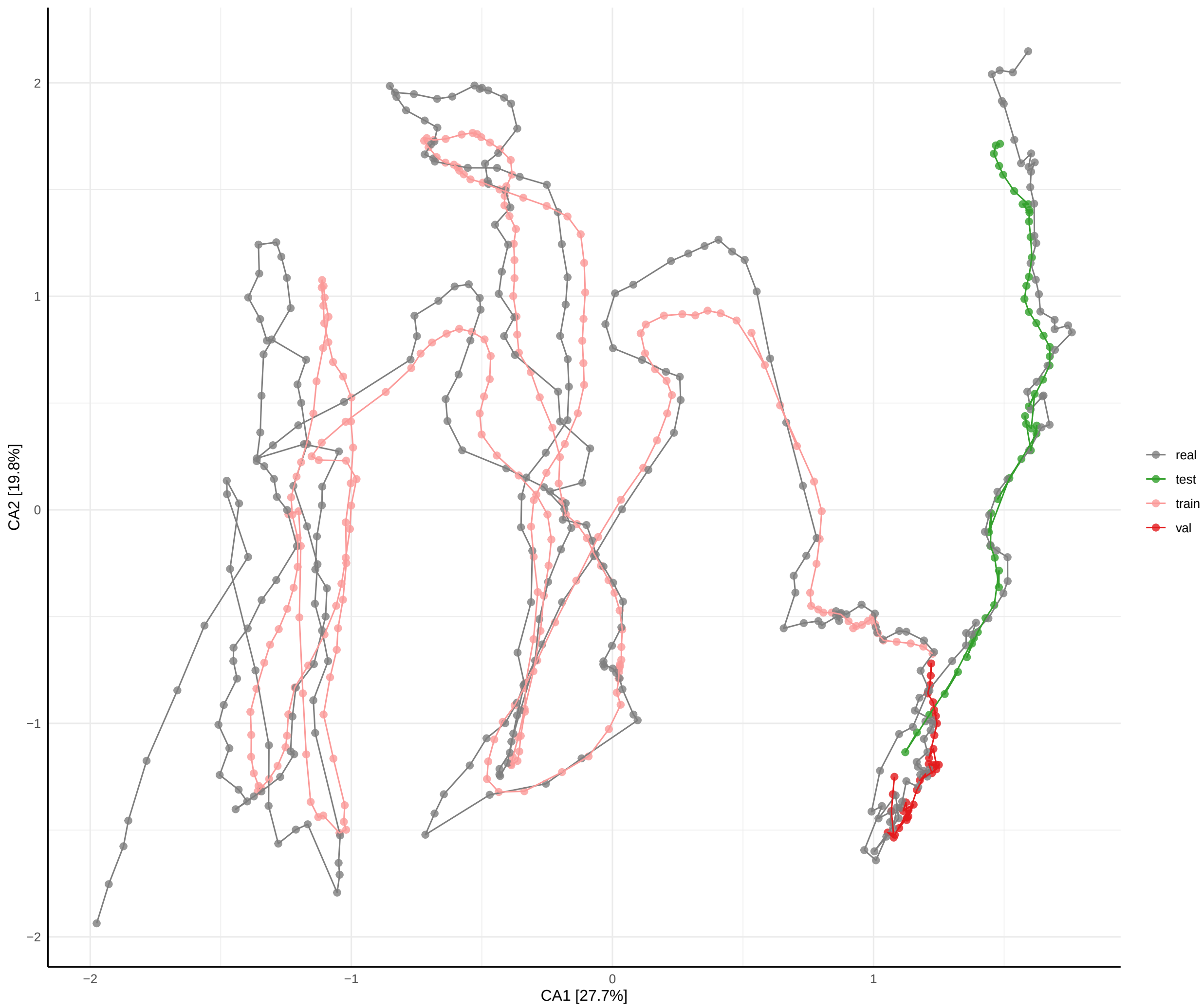

```r
# raw reformatted data (here not smoothed)
amp_timeseries(
  amp_subset_taxa(
    AAW_20220506_reformatted,
    "ASV1; s__midas_s_5; g__Tetrasphaera",
    normalise = FALSE
  ),
  time_variable = "Date",
  normalise = FALSE
)
```



colored

```r
#data set exactly same settings as 20220506, just with additional data output
results_dir <- "results/20220510/results_20220510_190511"
AAW_20220510 <- combine_abund(
  results_dir,
  cluster_type = "abund"
)

AAW_20220510_reformatted <- load_data_reformatted(results_dir)

# run data (here smoothing factor 8)
amp_ordinate(
  AAW_20220510,
  type = "ca",
  sample_color_by = "split_dataset",
  sample_trajectory = "Date"
) +
```

```
  scale_color_manual(
    values = c("grey50", RColorBrewer::brewer.pal(6, "Paired")[c(4:6)])
  ) +
  theme(legend.title = element_blank())
```




```
#five number statistics of sum of reads per data set
list.dirs(
  "results/20220506",
  full.names = TRUE,
  recursive = FALSE
) %>%
  lapply(function(dataset) {
    abund <- fread(
      file.path(dataset, "data_reformatted", "abundances.csv"),
      drop = 1
    )
    fivenum(rowSums(abund))
  })
```