Testing out scaling

cool people

Get a baseline (centered X, centered/scaled Z)

```
# Load in simulation studies
# Not doing the p100 n300 case since a single simulation
# requires over 16 hours on the cluster and many simulations
# need to be done
p = c(5, 15, 25, 50)
n = c(90, 90, 150, 150)
objects_strings = c(
  "simulation_study//p5_n90//res_p5_n90_covdepGE_20220908_215120.Rda",
  "simulation_study//p15_n90//res_p15_n90_covdepGE_20220908_215229.Rda",
  "simulation_study//p25_n150//res_p25_n150_covdepGE_20220825_121750.Rda",
  "simulation_study//p50_n150//res_p50_n150_covdepGE_20220825_090326.Rda"
  # "simulation_study//p100_n300//res_p100_n300_covdepGE_20220824_084919.Rda"
)
results_original = list()
for(sim in 1:length(objects_strings)) {
  load(objects_strings[sim])
  results_original[[sim]] = results
  rm(results)
sim_names_original = paste0("p", p, "_n", n)
results_original = set_names(results_original, sim_names_original)
```

Calculate mean FP/n and FN/n

```
false_positives_baseline = results_original %>%
   map(function(x)
      map_dbl(x, pluck, "FP_n")
)
false_negatives_baseline = results_original %>%
   map(function(x)
      map_dbl(x, pluck, "FN_n")
)

false_positives_baseline %>%
   map_dfr(summary) %>%
   cbind(p, n, .) %>%
   cbind(p, n, .) %>%
   tibble() %>%
   xtable(caption = "False positives per sample - Normalized Z, Centered X")
```

% latex table generated in R 4.2.1 by xtable 1.8-4 package % Mon Nov 14 12:57:01 2022

| - | p | n | Min. | 1st Qu. | Median | Mean | 3rd Qu. | Max. |
|---|-------|--------|------|---------|--------|------|---------|-------|
| 1 | 5.00 | 90.00 | 0.00 | 0.00 | 0.03 | 0.34 | 0.47 | 2.62 |
| 2 | 15.00 | 90.00 | 0.00 | 0.00 | 0.62 | 0.82 | 1.25 | 4.42 |
| 3 | 25.00 | 150.00 | 0.00 | 0.64 | 1.08 | 1.29 | 1.75 | 5.17 |
| 4 | 50.00 | 150.00 | 0.39 | 2.68 | 4.37 | 4.36 | 5.80 | 11.31 |

Table 1: False positives per sample - Normalized Z, Centered X

```
false_negatives_baseline %>%
  map_dfr(summary) %>%
  cbind(p, n, .) %>%
  tibble() %>%
  xtable("False negatives per sample - Normalized Z, Centered X")
```

% latex table generated in R 4.2.1 by xtable 1.8-4 package % Mon Nov 14 12:57:01 2022

| | p | n | Min. | 1st Qu. | Median | Mean | 3rd Qu. | Max. |
|---|-------|--------|------|---------|--------|------|---------|------|
| 1 | 5.00 | 90.00 | 0.00 | 0.78 | 1.03 | 0.99 | 1.29 | 2.16 |
| 2 | 15.00 | 90.00 | 0.00 | 0.89 | 1.32 | 1.41 | 1.99 | 2.98 |
| 3 | 25.00 | 150.00 | 0.00 | 0.77 | 0.92 | 0.91 | 1.10 | 2.00 |
| 4 | 50.00 | 150.00 | 0.08 | 0.92 | 1.13 | 1.19 | 1.40 | 3.28 |

Table 2: False negatives per sample - Normalized Z, Centered X

Goal: reduce mean FP/n (and either reduce or keep constant FN/n)

Data generation

```
set.seed(12345)
n_trials = 100
simulation_list = map2(n, p, function(n,p){
  nj = n \%/\% 3
  replicate(n_trials, generateData(p, nj, nj, nj), F)
})
max_min_scale = function(X) { # Scale each column by max-min
  # Columnwise; subtract min and divide by resulting max
  if(!is.matrix(X)) { # for vectors
    X = as.matrix(X)
  p = ncol(X)
  n = nrow(X)
  # faster with max.col(X) and max.col(-X)
  mins = as.vector(apply(X, 2, min))
  scaled X = t(t(X)-mins)
  maxs = as.vector(apply(scaled_X, 2, max))
  scaled_X = t(t(scaled_X)/maxs)
  return(list(scaled_X = scaled_X, add_invs = mins, mult_invs = maxs))
}
max_min_unscale = function(output) {
  t(t(output$scaled_X)*output$mult_invs + output$add_invs)
}
```

Raw performance (no center/scaling)

Test max-min scaling

We'll try 3 situations; scaling both X and Z, scaling only Z, and scaling only X

```
min_max_simulation_list = map(simulation_list, function(setup){
    mm_X_data_list = map(setup, function(sim) {
        output = max_min_scale(sim$X)
```

```
sim$X = output$scaled_X
    sim$scaleoutX = output
    sim
  })
  mm_Z_data_list = map(setup, function(sim) {
    output = max_min_scale(sim$Z)
    sim$Z = output$scaled X
    sim$scaleoutZ = output
    sim
  })
  mm_XZ_data_list = map(setup, function(sim) {
    output = max_min_scale(sim$X)
    sim$X = output$scaled_X
    sim$scaleout = output
    output2 = max_min_scale(sim$Z)
    sim$Z = output2$scaled_X
    sim$scaleoutZ = output2
    sim
  })
  list(mm_X_data_list, mm_Z_data_list, mm_XZ_data_list)
})
num_workers <- parallel::detectCores() - 8</pre>
doParallel::registerDoParallel(cores = num_workers)
min_max_X_simulation_results = min_max_simulation_list %>% map(~pluck(.x, 1)) %>%
  map(function(setup){
    simulation_func(n_trials, setup, num_workers, normalize = FALSE)
  })
save(min_max_X_simulation_results, file = "minmax_X_sim.Rda")
min max Z simulation results = min max simulation list %>% map(~pluck(.x, 2)) %>%
  map(function(setup){
    simulation_func(n_trials, setup, num_workers, normalize = FALSE)
  })
save(min_max_Z_simulation_results, file = "minmax_Z_sim.Rda")
min_max_XZ_simulation_results = min_max_simulation_list %>% map(~pluck(.x, 3)) %>%
  map(function(setup){
```

```
simulation_func(n_trials, setup, num_workers, normalize = FALSE)
})
save(min_max_XZ_simulation_results, file = "minmax_XZ_sim.Rda")
```

% latex table generated in R 4.2.1 by xtable 1.8-4 package % Mon Nov 14 12:57:02 2022

| | p | n | Min. | 1st Qu. | Median | Mean | 3rd Qu. | Max. |
|---|-------|--------|-------|---------|--------|-------|---------|-------|
| 1 | 5.00 | 90.00 | 0.00 | 0.37 | 0.64 | 0.81 | 1.19 | 2.53 |
| 2 | 15.00 | 90.00 | 0.78 | 3.03 | 4.13 | 4.08 | 4.78 | 8.49 |
| 3 | 25.00 | 150.00 | 7.57 | 10.16 | 11.87 | 11.89 | 13.53 | 19.25 |
| 4 | 50.00 | 150.00 | 11.09 | 17.41 | 20.21 | 19.86 | 22.22 | 28.53 |

Table 3: False positives per sample - Max/Min Scaled Z

% latex table generated in R 4.2.1 by xtable 1.8-4 package % Mon Nov 14 12:57:02 2022

| | p | n | Min. | 1st Qu. | Median | Mean | 3rd Qu. | Max. |
|---|-------|--------|------|---------|--------|------|---------|------|
| 1 | 5.00 | 90.00 | 0.11 | 0.80 | 1.16 | 1.14 | 1.42 | 2.42 |
| 2 | 15.00 | 90.00 | 0.71 | 1.73 | 2.36 | 2.35 | 2.83 | 4.07 |
| 3 | 25.00 | 150.00 | 0.32 | 1.20 | 1.66 | 1.71 | 2.13 | 4.19 |
| 4 | 50.00 | 150.00 | 1.07 | 1.92 | 2.27 | 2.42 | 2.84 | 4.08 |

Table 4: False negatives per sample - Max/Min Scaled Z

Test Max-min + Normalization

First do a max-min transform to scale, then do the z-transform (or mean 0 center transform in the case of X)

```
num_workers <- parallel::detectCores() - 8
doParallel::registerDoParallel(cores = num_workers)

min_max_norm_X_simulation_results = min_max_simulation_list %>% map(~pluck(.x, 1)) %>%
    map(function(setup){
        simulation_func(n_trials, setup, num_workers, normalize = TRUE)
    })

save(min_max_norm_X_simulation_results, file = "minmax_norm_X_sim.Rda")

min_max_norm_Z_simulation_results = min_max_simulation_list %>% map(~pluck(.x, 2)) %>%
    map(function(setup){
```

```
simulation_func(n_trials, setup, num_workers, normalize = TRUE)
})

save(min_max_norm_Z_simulation_results, file = "minmax_norm_Z_sim.Rda")

min_max_norm_XZ_simulation_results = min_max_simulation_list %>% map(~pluck(.x, 3)) %>%
    map(function(setup){
        simulation_func(n_trials, setup, num_workers, normalize = TRUE)
    })

save(min_max_norm_XZ_simulation_results, file = "minmax_norm_XZ_sim.Rda")
```

% latex table generated in R 4.2.1 by xtable 1.8-4 package % Mon Nov 14 12:57:05 2022

| | p | n | Min. | 1st Qu. | Median | Mean | 3rd Qu. | Max. |
|---|-------|--------|------|---------|--------|------|---------|-------|
| 1 | 5.00 | 90.00 | 0.00 | 0.00 | 0.00 | 0.26 | 0.34 | 2.51 |
| 2 | 15.00 | 90.00 | 0.00 | 0.00 | 0.33 | 0.61 | 0.96 | 3.89 |
| 3 | 25.00 | 150.00 | 0.00 | 0.64 | 1.09 | 1.34 | 1.97 | 3.73 |
| 4 | 50.00 | 150.00 | 0.55 | 2.81 | 4.04 | 4.07 | 5.11 | 10.25 |

Table 5: False positives per sample - Max/Min Scaled X and Normalization

% latex table generated in R 4.2.1 by xtable 1.8-4 package % Mon Nov 14 12:57:05 2022

| | p | n | | • | | Mean | 3rd Qu. | Max. |
|---|-------|--------|------|------|------|------|---------|------|
| 1 | 5.00 | 90.00 | 0.00 | 0.78 | | 1.00 | 1.33 | 1.98 |
| 2 | 15.00 | 90.00 | 0.00 | 1.11 | 1.42 | 1.48 | 2.00 | 2.87 |
| 3 | 25.00 | 150.00 | 0.00 | 0.72 | 0.97 | 0.92 | 1.15 | 1.96 |
| 4 | 50.00 | 150.00 | 0.16 | 0.87 | 1.06 | 1.12 | 1.32 | 2.67 |

Table 6: False negatives per sample - Max/Min Scaled X and Normalization

% latex table generated in R 4.2.1 by xtable 1.8-4 package % Mon Nov 14 12:57:05 2022

| | p | n | Min. | 1st Qu. | Median | Mean | 3rd Qu. | Max. |
|---|-------|--------|------|---------|--------|------|---------|-------|
| 1 | 5.00 | 90.00 | 0.00 | 0.00 | 0.00 | 0.24 | 0.27 | 2.60 |
| 2 | 15.00 | 90.00 | 0.00 | 0.00 | 0.36 | 0.63 | 0.94 | 5.04 |
| 3 | 25.00 | 150.00 | 0.00 | 0.60 | 1.10 | 1.34 | 1.99 | 3.80 |
| 4 | 50.00 | 150.00 | 0.32 | 2.74 | 3.88 | 4.08 | 5.23 | 10.27 |

Table 7: False positives per sample - Max/Min Scaled Z and Normalization

% latex table generated in R 4.2.1 by x table 1.8-4 package % Mon Nov 14 12:57:05 2022

| | p | n | Min. | 1st Qu. | Median | Mean | 3rd Qu. | Max. |
|---|-------|--------|------|---------|--------|------|---------|------|
| 1 | 5.00 | 90.00 | 0.00 | 0.80 | 0.94 | 1.03 | 1.41 | 1.93 |
| 2 | 15.00 | 90.00 | 0.04 | 1.11 | 1.49 | 1.53 | 2.02 | 3.09 |
| 3 | 25.00 | 150.00 | 0.00 | 0.72 | 0.97 | 0.95 | 1.24 | 1.97 |
| 4 | 50.00 | 150.00 | 0.19 | 0.88 | 1.08 | 1.15 | 1.36 | 2.67 |

Table 8: False negatives per sample - Max/Min Scaled Z and Normalization

| | p | n | Min. | 1st Qu. | Median | Mean | 3rd Qu. | Max. |
|---|-------|--------|------|---------|--------|------|---------|-------|
| 1 | 5.00 | 90.00 | 0.00 | 0.00 | 0.00 | 0.24 | 0.34 | 1.89 |
| 2 | 15.00 | 90.00 | 0.00 | 0.00 | 0.33 | 0.61 | 0.98 | 3.89 |
| 3 | 25.00 | 150.00 | 0.00 | 0.65 | 1.09 | 1.35 | 1.97 | 3.73 |
| 4 | 50.00 | 150.00 | 0.55 | 2.86 | 3.92 | 4.07 | 5.13 | 10.52 |

Table 9: False positives per sample - Max/Min Scaled X and Z and Normalization

% latex table generated in R 4.2.1 by xtable 1.8-4 package % Mon Nov 14 12:57:05 2022 % latex table generated in R 4.2.1 by xtable 1.8-4 package % Mon Nov 14 12:57:05 2022

| | | p | n | Min. | 1st Qu. | Median | Mean | 3rd Qu. | Max. |
|---|---|-------|--------|------|---------|--------|------|---------|------|
| - | 1 | 5.00 | 90.00 | 0.00 | 0.78 | 0.94 | 1.02 | 1.33 | 1.93 |
| | 2 | 15.00 | 90.00 | 0.02 | 1.08 | 1.41 | 1.47 | 2.00 | 2.87 |
| | 3 | 25.00 | 150.00 | 0.00 | 0.72 | 0.95 | 0.92 | 1.18 | 1.96 |
| | 4 | 50.00 | 150.00 | 0.17 | 0.85 | 1.05 | 1.11 | 1.31 | 2.67 |

Table 10: False negatives per sample - Max/Min Scaled X and Z and Normalization