Profiling

1 Synopsis

- `{TCA}` is a great package. But it is running unexpectedly slowly. A moderately sized project (400,000 features * 1000 Samples * 6 Cell Types, `vars.mle = FALSE`) couldn't converge after 10 hours and hit out of memory error with 120GB of RAM.
- After learning about how to use `TCA::tca()` correctly and some optimization, we can achieve at least **13.3x** increase in speed and **2x** decrease in memory usage compared to running `TCA::tca()` version 1.2.1 sequentially. On Windows computers, `TCA::tca()` version 1.2.1 with `parallel = TRUE` is likely to be even slower than sequential runs in certain situations (See "Other findings" below).
- In addition to the optimization, added `split_input()` to shuffle the features before splitting them row-wise and `tca_split()` as a wrapper to run `TCA::tca()` in parallel over the independent chunks of X. See (vignettes/tca_split.pdf)

2 Methods

- Use the `TCA::test_data()` function to simulate data under different scenarios
- Profile `TCA::tca()` fits with `profvis::profvis()` and identify bottlenecks
- Create replicates of fit results from `{TCA}` version 1.2.1 as test fixtures before any changes
- Make small changes, fit the model, and test if all the fit results are within machine tolerance of differences from the test fixtures
- Profile the modded version under sequential, `vars.mle = TRUE`, `refit_W = TRUE`, `TCA::tcareg()` fit, and parallel runs
- Add unit tests to any new functions

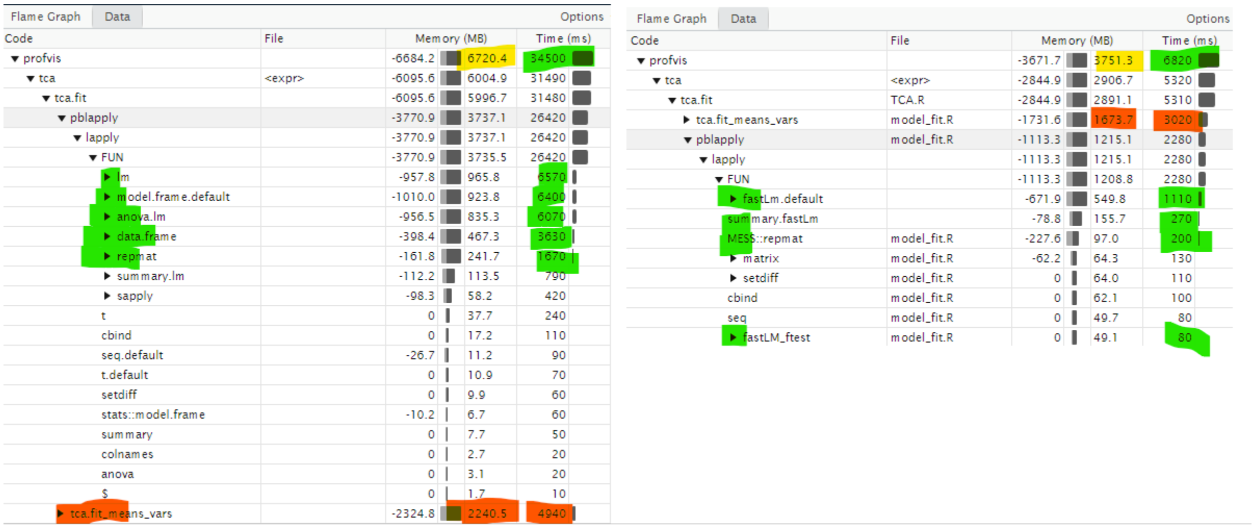
3 Results

- The results of the modifications passed all the included unit tests and generated estimates within machine tolerance of difference from the estimates of the fit produced by version 1.2.1.

3.1 Sequential

- After modifications, running sequentially, we achieved a **6x** speed up in a simulation (Fig 1).

- The major source of speed up achieved is from replacing the `data.frame()`, `lm()`, and `anova()` calls with `RcppEigen::fastLm()` and a minimal implementation of the partial F-test with `./R/Utils.R/fastLM_ftest`. This also helped with memory usage by 2x. This is potentially an unsafe change. But the risk is very small because
  - The constrained optimization step before `fastLm()` has internal checks for matrix positive definiteness. Indeed, testing using rank deficient C1 and C2 matrices tripped the matrix positive definite checks before `fastLm()` is even called.
  - `RcppEigen::fastLm()` returns the correct values for rank deficient matrices, and we can then use `anyNA()` to check for `NA` of p-values for gamma hats if the constrained optimization step didn't throw an error.
  - `NA` is already expected to be taken care of by users.
  - For 5 repetitions, the returned estimates are the same between the `fastLm()` version and `TCA::tca()` version 1.2.1.

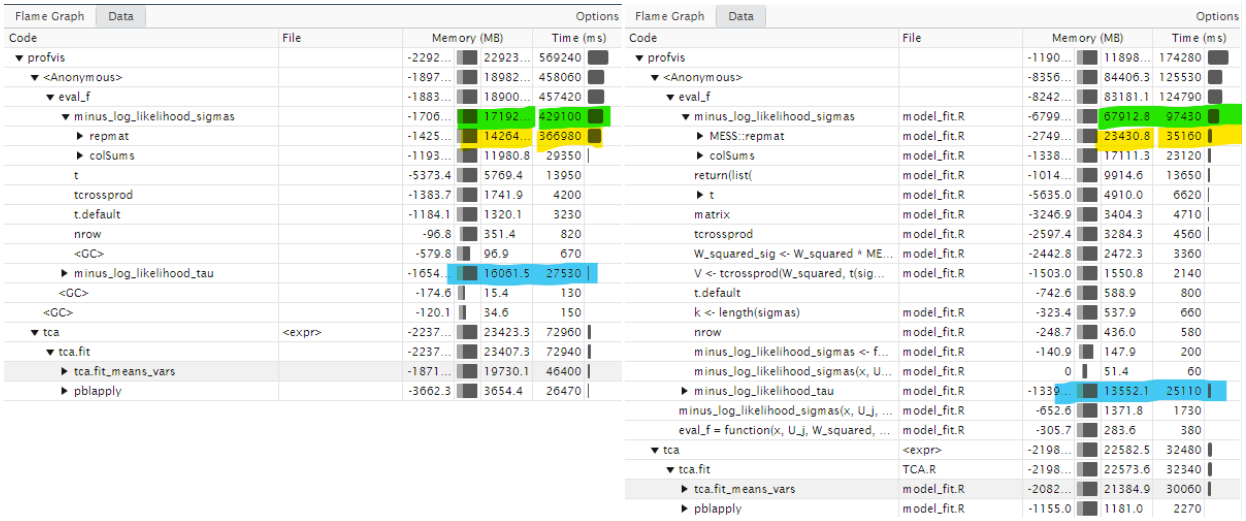


Code	File	Memory (MB)		Time (ms)
▼ profvis		-6684.2	6720.4	34500
▼ tca	<expr>	-6095.6	6004.9	31490
▼ tca.fit		-6095.6	5996.7	31480
▼ pblapply		-3770.9	3737.1	26420
▼ lapply		-3770.9	3737.1	26420
▼ FUN		-3770.9	3735.5	26420
▶ lm		-957.8	965.8	6570
▶ model.frame.default		-1010.0	923.8	6400
▶ anova.lm		-956.5	835.3	6070
▶ data.frame		-398.4	467.3	3630
▶ repmat		-161.8	241.7	1670
▶ summary.lm		-112.2	113.5	790
▶ sapply		-98.3	58.2	420
t		0	37.7	240
cbind		0	17.2	110
seq.default		-26.7	11.2	90
t.default		0	10.9	70
setdiff		0	9.9	60
stats::model.frame		-10.2	6.7	60
summary		0	7.7	50
colnames		0	2.7	20
anova		0	3.1	20
$		0	1.7	10
▶ tca.fit_means_vars		-2324.8	2240.5	4940

Code	File	Memory (MB)		Time (ms)
▼ profvis		-3671.7	3751.3	6820
▼ tca	<expr>	-2844.9	2906.7	5320
▼ tca.fit	TCA.R	-2844.9	2891.1	5310
▶ tca.fit_means_vars	model_fit.R	-1731.6	1673.7	3020
▼ pblapply	model_fit.R	-1113.3	1215.1	2280
▼ lapply		-1113.3	1215.1	2280
▼ FUN		-1113.3	1208.8	2280
▶ fastLm.default		-671.9	549.8	1110
summary.fastLm		-78.8	155.7	270
MESS::repmat	model_fit.R	-227.6	97.0	200
▶ matrix	model_fit.R	-62.2	64.3	130
▶ setdiff	model_fit.R	0	64.0	110
cbind	model_fit.R	0	62.1	100
seq	model_fit.R	0	49.7	80
▶ fastLM_ftest	model_fit.R	0	49.1	80

Figure 1: `tca()` ver 1.2.1 (left) vs modded (right), `tca()` fit time of version 1.2.1 decreased by 6x. Memory usage decreased by 2x

  - Since it looks like `{TCA}` is only running partial F-tests between 2 models, we don't need the extra information of `lm()` objects or the checks and formatting of `stats::anova()` calls. Implementing a minimal version of the partial F-test helped reduced fit time.
  - We can also use `lm.fit()` instead of `RcppEigen::fastLm()`. `lm.fit()` comes with more safety checks and probably is only slightly slower than `fastLm()`.
- The second source of speed up comes from replacing `pracma::repmat()` calls with `MESS::repmat()`, which directly calls C codes. This change helps because the optimization steps repeatedly calls on `pracma::repmat()`. This reduced the `tca.fit_means_vars()` times by **1.6x**.
- The main resource consumer of the `vars.mle = TRUE` fit is from `nloptr()` to estimate sigma. Achieved a **3.3x** improvement through `fastLM` and replacing the replacing the `repmat()` calls (Fig 2).



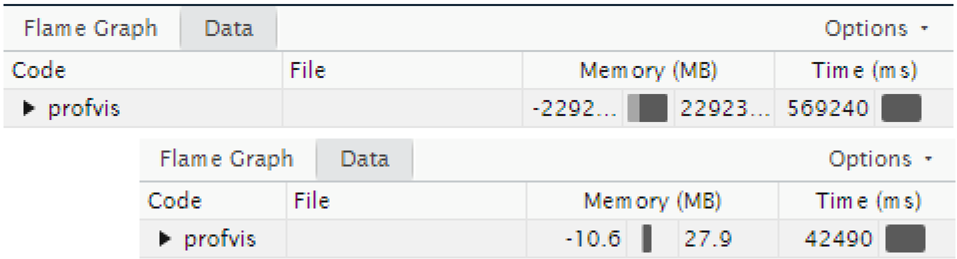
Code	File	Memory (MB)		Time (ms)
▼ profvis		-2292...	22923...	569240
▼ <Anonymous>		-1897...	18982...	458060
▼ eval_f		-1883...	18900...	457420
▼ minus_log_likelihood_sigmas		-1706...	17192...	429100
▶ repmat		-1425...	14264...	366980
▶ colSums		-1193...	11980.8	29350
t		-5373.4	5769.4	13950
tcrossprod		-1383.7	1741.9	4200
t.default		-1184.1	1320.1	3230
nrow		-96.8	351.4	820
<GC>		-579.8	96.9	670
▶ minus_log_likelihood_tau		-1654...	16061.5	27530
<GC>		-174.6	15.4	130
<GC>		-120.1	34.6	150
▼ tca	<expr>	-2237...	23423.3	72960
▼ tca.fit		-2237...	23407.3	72940
▶ tca.fit_means_vars		-1871...	19730.1	46400
▶ pblapply		-3662.3	3654.4	26470

Code	File	Memory (MB)		Time (ms)
▼ profvis		-1190...	11898...	174280
▼ <Anonymous>		-8356...	84406.3	125530
▼ eval_f		-8242...	83181.1	124790
▼ minus_log_likelihood_sigmas	model_fit.R	-6799...	67912.8	97430
▶ MESS::repmat	model_fit.R	-2749...	23430.8	35160
▶ colSums	model_fit.R	-1338...	17111.3	23120
return(list(	model_fit.R	-1014...	9914.6	13650
▶ t	model_fit.R	-5635.0	4910.0	6620
matrix	model_fit.R	-3246.9	3404.3	4710
tcrossprod	model_fit.R	-2597.4	3284.3	4560
W_squared_sig <- W_squared * ME...	model_fit.R	-2442.8	2472.3	3360
V <- tcrossprod(W_squared, t(sig...	model_fit.R	-1503.0	1550.8	2140
t.default		-742.6	588.9	800
k <- length(sigmas)	model_fit.R	-323.4	537.9	660
nrow	model_fit.R	-248.7	436.0	580
minus_log_likelihood_sigmas <- f...	model_fit.R	-140.9	147.9	200
minus_log_likelihood_sigmas(x, U...	model_fit.R	0	51.4	60
▶ minus_log_likelihood_tau	model_fit.R	-1339...	13552.1	25110
minus_log_likelihood_sigmas(x, U_j, ...	model_fit.R	-652.6	1371.8	1730
eval_f = function(x, U_j, W_squared, ...	model_fit.R	-305.7	283.6	380
▼ tca	<expr>	-2198...	22582.5	32480
▼ tca.fit	TCA.R	-2198...	22573.6	32340
▶ tca.fit_means_vars	model_fit.R	-2082...	21384.9	30060
▶ pblapply	model_fit.R	-1155.0	1181.0	2270

Figure 2: vars.mle = TRUE, 1.2.1 (left) vs modded (right)

3.2 Parallel

- Combine with the above changes and running in parallel over chunks of X, not using the parallel parameter in `tca()`, we achieved a **13.3x** speed up in a simulation with `vars.mle = TRUE` (Fig 3).



Code	File	Memory (MB)		Time (ms)
▶ profvis		-2292...	22923...	569240

Code	File	Memory (MB)		Time (ms)
▶ profvis		-10.6	27.9	42490

Figure 3: `tca()` 1.2.1 sequential (top) vs modded parallel by chunk X (bottom). The memory usage is inaccurate for the parallel fit

- Summarizing this github question, this parallel implementation is valid because `tca()` *sort of* do not use information between features for the estimations.
  - Technically, `tau_hat` is inducing dependencies among features in X if its estimated from the data. But, it is just one parameter and since we have so many features, the results won't change much between chunks.
- To be even extra cautious about accuracy, which doesn't seem to be necessary, for this very favorable speed up, we can
  - Make sure the chunk size is big enough. This is needed to minimize the overhead of parallel anyway. It is probably optimal to have the number of chunks equal to the number of cores to parallel over.
  - Randomly shuffle features into chunks.
  - Don't estimate tau from the data. Estimating tau from already published data of similar population that we are studying and using that estimate should be more than enough.
- `refit_W`, which uses information across features, is invalid for this. If `refit_W` is needed, run the most informative sites instead of the whole epi-genome and use the resulting estimated W on each chunks as described.
- A good workflow might be to fit with the alternative optimization for model iteration and then fit one final fit with `vars.mle = TRUE`.

4 Changelog

[23/03/27]

- Fixed bugs in `split_input()`. Added unit tests for `split_input()` and `tca_split()`

[23/03/26]

- Added wrappers for running `tca()` by chunks of matrix X in `./R/tca_split.R`.

[23/03/25]

- Moved some function calls outside of `minus_log_likelihood_tau()` and `minus_log_likelihood_sigmas()` to shave off a couple of seconds through possible repeated calls of `nrow()` and `length()` in `nloptr::nloptr()`.

[23/03/24]

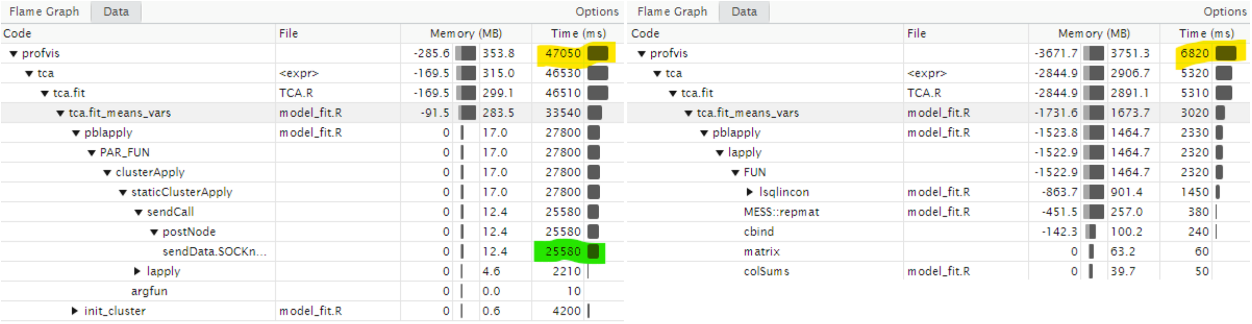
- Replaced all the `pracma::repmat()` calls with `MESS::repmat()` calls, except for the `tcareg()` related functions (because `tcareg()` is fast enough).
- Added test for no result change from ver 1.2.1 for `vars.mle = TRUE`.
- Added test for no result change from ver 1.2.1 for `refit_W()`.

[23/03/23]

- Replaced `data.frame()` calls and `lm()` calls in `./R/model_fit.R`.
- Added `fastLM_ftest()` to `./R/utils.R` to calculate partial F-tests.
- Added test for no result change from ver 1.2.1.

5 Other findings

- The use of the parallel parameter in `TCA::tca()` might be more situational.
- On a Windows machine, the overhead caused by data being shuffled back and forth by PSOCK increased the fit time by **7x** in a small simulation.



Code	File	Memory (MB)		Time (ms)
▼ profvis		-285.6	353.8	47050
▼ tca	<expr>	-169.5	315.0	46530
▼ tca.fit	TCA.R	-169.5	299.1	46510
▼ tca.fit_means_vars	model_fit.R	-91.5	283.5	33540
▼ pblapply	model_fit.R	0	17.0	27800
▼ PAR_FUN		0	17.0	27800
▼ clusterApply		0	17.0	27800
▼ staticClusterApply		0	17.0	27800
▼ sendCall		0	12.4	25580
▼ postNode		0	12.4	25580
sendData.SOCKn...		0	12.4	25580
▶ lapply		0	4.6	2210
argfun		0	0.0	10
▶ init_cluster	model_fit.R	0	0.6	4200

Code	File	Memory (MB)		Time (ms)
▼ profvis		-3671.7	3751.3	6820
▼ tca	<expr>	-2844.9	2906.7	5320
▼ tca.fit	TCA.R	-2844.9	2891.1	5310
▼ tca.fit_means_vars	model_fit.R	-1731.6	1673.7	3020
▼ pblapply	model_fit.R	-1523.8	1464.7	2330
▼ lapply		-1522.9	1464.7	2320
▼ FUN		-1522.9	1464.7	2320
▶ lsqlincon	model_fit.R	-863.7	901.4	1450
MESS::repmat	model_fit.R	-451.5	257.0	380
cbind		-142.3	100.2	240
matrix		0	63.2	60
colSums	model_fit.R	0	39.7	50

Figure 4: parallel = TRUE, num_cores = 6 in `tca()` (left) vs sequential (right) PSOCK

- On a Linux machine, the performance using 3 clusters is slower than the sequential run by **1.1x** in a simulation. However, on a HPC where small latency can add up or where huge data is passed to `TCA::tca()`, the data has to be replicated for each fork and the performance might worsen and consume much more memory for slower speed.

6 Profiling

- Below are **unorganized** thoughts and notes taken throughout the process.

```
library(profvis) # Profiling tool
library(devtools)
library(tictoc)
near <- dplyr::near
load_all()
```

```
# Simulate the data
set.seed(1234)
library(TCA) # Version 1.2.1
data <- test_data(100, 10000, 6, 1, 1, 0.01)
# tca.mdl <- tca(X = data$X, W = data$W, C1 = data$C1, C2 = data$C2)
lapply(data, dim)
```

6.1 Windows machine

- Cluster type will be set to PSOCK. This would be the worst case scenario for TCA since PSOCK has to shuttle data back and forth between the workers and this massively increases the overhead. In the results below, the fit time was increased by 7x.

```r
set.seed(1234)
# Run the data sequentially first. This is the results for ver 1.2.1.
prof_obj <- profvis({
  tca(X = data$X, W = data$W, C1 = data$C1, C2 = data$C2)
})
saveRDS(prof_obj, "./assets/1_2_1_sequential_n100_m1e5.rds")

# 1.2.1 vars.mle = TRUE
prof_obj <- profvis({
  tca(
    X = data$X, W = data$W, C1 = data$C1, C2 = data$C2,
    vars.mle = TRUE
  )
})
saveRDS(prof_obj, "./assets/1_2_1_sequential_vars.mle_n100_m1e5.rds")

# Then remove.packages("TCA") and load_all() this branch. Also run sequentially
remove.packages("TCA")
load_all()
prof_obj <- profvis({
  tca(X = data$X, W = data$W, C1 = data$C1, C2 = data$C2)
})
saveRDS(prof_obj, "./assets/modded_sequential_n100_m1e5.rds")

# modded vars.mle = TRUE
prof_obj <- profvis({
  tca(
    X = data$X, W = data$W, C1 = data$C1, C2 = data$C2,
    vars.mle = TRUE
  )
})
saveRDS(prof_obj, "./assets/modded_sequential_vars.mle.n100_m1e5.rds")

# Then test the parallel performance
prof_obj <- profvis({
  tca(
    X = data$X, W = data$W, C1 = data$C1, C2 = data$C2, parallel = TRUE,
    num_cores = 6L
  )
})
saveRDS(prof_obj, "./assets/modded_parallel_n100_m1e5.rds")

# Test the parallel performance chunked by X, vars.mle = TRUE
library(furrr)
prof_obj <- profvis({
  split_X <- split_input(X = data$X, n_chunks = 7)

  plan(multisession, workers = 7)

  res_par <- tca_split(
    X = split_X,
    W = data$W,
    C1 = data$C1,
    C2 = data$C2,
    vars.mle = TRUE,
    max_iters = 20
  )

  plan(sequential)
})
saveRDS(prof_obj, "./assets/modded_parallel_chunk_X_vars.mle_n100_m1e5.rds")
```

- The data graph shows 2x memory saving and 6x performance increase.

```
seq_1_2_1 <- readRDS("./assets/1_2_1_sequential_n100_m1e5.rds")
seq_1_2_1.mle <- readRDS("./assets/1_2_1_sequential_vars.mle_n100_m1e5.rds")
seq_modded <- readRDS("./assets/modded_sequential_n100_m1e5.rds")
seq_modded.mle <- readRDS("./assets/modded_sequential_vars.mle.n100_m1e5.rds")
seq_parallel_modded <- readRDS("./assets/modded_parallel_n100_m1e5.rds")
chunk_X_modded.mle <- readRDS("./assets/modded_parallel_chunk_X_vars.mle_n100_m1e5.rds")

# 1.2.1 vs modded
seq_1_2_1
seq_modded

# 1.2.1 vs modded mle
seq_1_2_1.mle
seq_modded.mle

# modded sequential vs parallel
seq_modded
seq_parallel_modded

#  1.2.1 vars mle vs chunk by X modded
seq_1_2_1.mle
chunk_X_modded.mle
```

6.2 Linux machine

- The forked cluster is available on linux machines.

```
set.seed(1234)
prof_obj <- profvis({
  tca(X = data$X, W = data$W, C1 = data$C1, C2 = data$C2)
})
saveRDS(prof_obj, "./assets/linux_modded_sequential_n100_m1e5.rds")

prof_obj <- profvis({
  tca(
    X = data$X, W = data$W, C1 = data$C1, C2 = data$C2, parallel = TRUE,
    num_cores = 3L
  )
})
saveRDS(prof_obj, "./assets/linux_modded_parallel_n100_m1e5.rds")
```

- Slower by 1.08x.

```r
seq_fork_modded <- readRDS("./assets/linux_modded_sequential_n100_m1e5.rds")
seq_fork_modded_par <- readRDS("./assets/linux_modded_parallel_n100_m1e5.rds")
seq_fork_modded
seq_fork_modded_par
```

7 Notes

- We see that in `model_fit.R/tca_fit.R`, R is spending
  - High peak memory and decent amount of time to call `tca.fit_means_vars()`.
    This is the internal loop optimization of `tca()`. This is probably where the bottle neck for the loop in parallel mode because the high memory overhead.

  - High peak memory and a lot of time to call `lm()` and subsequently `model.frame.default()`.

  - The `anova.lm()` call to perform partial F tests is also taking a significant amount time.

- Let's try to replace the `data.frame()` call with a straight `cbind()` call to create a X matrix. Then we can use `RcppEigen::fastLm()` to directly call the X data matrix and the vector y.
  - This is potentially a dangerous trade-off between speed and safety. But `NA` is already expected to be taken care of by user. `{quadprog}` has internal check for positive definite matrix. Furthermore, `RcppEigen::fastLm()` returns the correct results for rank deficient matrix. We should be safe to make this trade off. We can create a test case for this.

  - Have to implement an `anova()` method for `RcppEigen::fastLm()`. This is straightforward.

- The `pracma::repmat()` calls are also taking a good amount of time. Looks like the implementation in `{MESS}` accomplish the same thing but calls C code directly so it should be faster. This change would add up since `pracma::repmat()` is called a lot.

8 Replacing codes

- Warning, this might be unsafe

8.1 fastLm

- Replace the `data.frame()` and `lm()` call with `RcppEigen::fastLm`

- Two code chunks to be replaced.

```r
# Before
df <-
  data.frame(y = X_tilde[, j], cbind(
    W / t(repmat(W_norms[, j], k, 1)),
    if (p2 > 0) {
      C2 / t(repmat(W_norms[, j], p2, 1))
    } else {
      C2
    },
    if (p1 > 0) {
      C1_ / t(repmat(W_norms[, j], k * p1, 1))
    } else {
      C1_
    }
  ))
mdl1.fit <- lm(y ~ ., data = df)
mdl1.coef <- summary(mdl1.fit)$coefficients
mdl1.cov.names <- colnames(df)[colnames(df) != "y"]
deltas_gammas_hat_pvals <-
  sapply(mdl1.cov.names, function(x) {
    if (x %in% rownames(mdl1.coef)) {
      return(mdl1.coef[x, "Pr(>|t|)"])
    } else {
      return(NA)
    }
  })
```

```r
# After
mdl1.fit <- RcppEigen::fastLm(
  X = cbind(
    "(Intercept)" = 1.0, # <----------- Remember the intercept
    W / t(repmat(W_norms[, j], k, 1)),
    if (p2 > 0) {
      C2 / t(repmat(W_norms[, j], p2, 1))
    } else {
      C2
    },
    if (p1 > 0) {
      C1_ / t(repmat(W_norms[, j], k * p1, 1))
    } else {
      C1_
    }
  ),
  y = X_tilde[, j]
)
mdl1.coef <- summary(mdl1.fit)$coefficients
# First row is always intercept. Sacrifice some code readability here
# Sacrifice some code readability here by using -1 instead of
## `which(rownames(mdl1.coef) != "(Intercept)")`
deltas_gammas_hat_pvals <- mdl1.coef[-1, "Pr(>|t|)"]
```

Second chunk

```r
# Before
C1_alt <- C1_ / t(repmat(W_norms[, j], k * p1, 1))
for (d in 1:p1) {
  C1_null <- C1_alt[, setdiff(1:(p1 * k), seq(d, k * p1, p1))]
  df <-
    data.frame(y = X_tilde[, j], cbind(W / t(repmat(W_norms[, j], k, 1)), if (p2 > 0) {
      C2 / t(repmat(W_norms[, j], p2, 1))
    } else {
      C2
    }, C1_null))
  mdl0.fit <- lm(y ~ ., data = df)
  anova.fit <- anova(mdl0.fit, mdl1.fit)
  gammas_hat_pvals.joint[d] <- anova.fit$`Pr(>F)`[2]
}
```

```r
# After
for (d in 1:p1) {
  mdl0.fit <- RcppEigen::fastLm(
    X = cbind(
      "(Intercept)" = 1.0, # <----------- Remember the intercept
      W / t(repmat(W_norms[, j], k, 1)),
      if (p2 > 0) {
        C2 / t(repmat(W_norms[, j], p2, 1))
      } else {
        C2
      },
      #### Used to be `C1_null` and `C1_alt`. Removed assignment calls.
      (C1_ / t(repmat(W_norms[, j], k * p1, 1)))[, setdiff(1:(p1 * k), seq(d, k * p1, p1))]
    ),
    y = X_tilde[, j]
  )
  gammas_hat_pvals.joint[d] <- fastLM_ftest(mdl0.fit, mdl1.fit)$`Pr(>F)`
}
```

8.2 repmat

- pracma::repmat() is taking a decent chunk out of the time. MESS::repmat is about 50% faster at the current dimensions.

```r
use_package("MESS")
```

- Replace a bunch of t(repmat ...) with MESS::repmat to remove a t() call and use the more efficient MESS::repmat() call.
- For vars.mle = TRUE, carefully reproduce the gradient calculation and replace with MESS::repmat() as well as removing some repeated calculations.

8.2.1 minus_log_likelihood_sigmas

```r
# Before
return(list(
  "objective" = -0.5 * (const - sum(log(V)) - sum(U_j / V)),
  "gradient" = -(colSums(W_squared * repmat(sigmas, n, 1) * t(repmat(U_j, k, 1)) /
    repmat(V_squared, 1, k)) - colSums(W_squared * repmat(sigmas, n, 1) / repmat(V, 1, k)))
))
```

```r
# After
W_squared_sig <- W_squared * MESS::repmat(matrix(sigmas, nrow = 1), nrow = n, 1)
return(list(
  "objective" = -0.5 * (const - sum(log(V)) - sum(U_j / V)),
  "gradient" = -(
    colSums(W_squared_sig * MESS::repmat(matrix(U_j), ncol = k) /
      MESS::repmat(V_squared, 1, ncol = k)) -
      colSums(W_squared_sig / MESS::repmat(V, 1, ncol = k))
  )
))
```

8.2.2 minus_log_likelihood_w

```r
# Before
V_rep <- repmat(V, 1, k)
U_i <- tcrossprod(mus, w_i) + crossprod_deltas_c2_i + tcrossprod(gammas, c1_i_) - t(x_i)
U_i_squared <- U_i**2
w_i_rep <- repmat(w_i, m, 1)
fval <- -0.5 * (const - sum(log(V)) - sum(U_i_squared / V))
gval <- colSums(w_i_rep * sigmas_squared / V_rep) + colSums(((mus + C_tilde) * repmat(U_i, 1, k) * V_rep
return(list("objective" = fval, "gradient" = gval))
```

```r
# After
V_rep <- MESS::repmat(V, 1, k)
U_i <- tcrossprod(mus, w_i) + crossprod_deltas_c2_i + tcrossprod(gammas, c1_i_) - t(x_i)
U_i_squared <- U_i**2
w_i_rep <- MESS::repmat(matrix(w_i, nrow = 1), m, 1)
fval <- -0.5 * (const - sum(log(V)) - sum(U_i_squared / V))
w_i_rep_sig <- w_i_rep * sigmas_squared
gval <-
  colSums(w_i_rep_sig / V_rep) +
  colSums((
    (mus + C_tilde) * MESS::repmat(U_i, 1, k) * V_rep -
      w_i_rep_sig * MESS::repmat(U_i_squared, 1, k)
  ) /
    MESS::repmat(V**2, 1, k))
return(list("objective" = fval, "gradient" = gval))
```

8.3 vars.mle = TRUE

- Not really a way to get around the `nloptr()` call that takes the majority of the time to optimize sigma.
- The only "improvement" that's low hanging is remove assignment calls for objects that is used only once in the function to minimize overhead for `nloptr()`

8.4 parallel

- Let's think about the parallel.
- Looks like R is stopping and starting clusters multiple times.
  - Cluster is started twice. Once for the `tca.fit_mean_vars()` and once for p-values of deltas and gammas.
  - RUNNING CLUSTER IS IN GENERALL MUCH SLOWER THAN SEQUENTIAL! This is probably because of overhead.
  - Make sure to only run in sequential mode. But parallel over chunks of X matrix instead.
- Add a stop for if parallel and refit_W is FALSE. We can probably remove all the parallel to be honest and just run the codes over chunks of X.

9 Test

9.1 fastLm

The two code chunks that were replaced has to be tested concurrently

```
data <- test_data(30, 1000, 6, 1, 1, 0.01)
C1_1 <- cbind(data$C1, data$C1)
C2_1 <- cbind(data$C2, data$C2)
tca(X = data$X, W = data$W, C1 = data$C1, C2 = data$C2)
df <- readRDS("./assets/change_1.rds")
X <- cbind("(Intercept)" = 1, df[, which(names(df) != "y")])
y <- df$y

mdl1.fit <- lm(y ~ ., data = df)
mdl1.coef <- summary(mdl1.fit)$coefficients
mdl1.cov.names <- colnames(df)[colnames(df) != "y"]
deltas_gammas_hat_pvals <-
  sapply(mdl1.cov.names, function(x) {
    if (x %in% rownames(mdl1.coef)) {
      return(mdl1.coef[x, "Pr(>|t|)"])
    } else {
      return(NA)
    }
  })

deltas_gammas_hat_pvals

mdl1.fit.1 <- RcppEigen::fastLm(
  X = X,
  y = y
)

mdl1.coef.1 <- summary(mdl1.fit.1)$coefficients
deltas_gammas_hat_pvals.1 <- mdl1.coef.1[-1, "Pr(>|t|)"]
stopifnot(all(dplyr::near(deltas_gammas_hat_pvals, deltas_gammas_hat_pvals.1)))
```

10 Scrap

```
library(profvis)
set.seed(1234)
data <- test_data(1000, 2000, 12, 3, 10, 0.01)

# Sequential
sim_1 <- profvis({
  tca(X = data$X, W = data$W, C1 = data$C1, C2 = data$C2)
})

# Parallel
sim_2 <- profvis({
  tca(X = data$X, W = data$W, C1 = data$C1, C2 = data$C2, parallel = TRUE, num_cores = 4L)
})
```

10.1 fastLm

```
rand_y <- rnorm(nrow(mtcars))
df <- cbind(y = rand_y, mtcars)
```

```r
## lm
lm.mdl0.fit <- lm(y ~ mpg + cyl + disp, data = df)
lm.mdl1.fit <- lm(y ~ ., data = df)

## alternatives
X <- cbind("(Intercept)" = 1, as.matrix(mtcars))
X_null <- cbind("(Intercept)" = 1, as.matrix(mtcars)[, c("mpg", "cyl", "disp")])

fastLm.mdl0.fit <- RcppEigen::fastLm(
  X = X_null,
  y = rand_y
)

fastLm.mdl1.fit <- RcppEigen::fastLm(
  X = X,
  y = rand_y
)
```

```r
anova_obj <- anova(lm.mdl0.fit, lm.mdl1.fit)
anova_obj$F
anova_obj$`Pr(>F)`

microbenchmark::microbenchmark(
  anova(lm.mdl0.fit, lm.mdl1.fit),
  fastLM_ftest(lm.mdl0.fit, lm.mdl1.fit),
  times = 1000
)

fastLM_ftest(fastLm.mdl0.fit, fastLm.mdl1.fit)
summary(fastLm.mdl0.fit)
mdl1.fit <- fastLm.mdl0.fit
```

10.1.1 Bug

```r
set.seed(1234)
data <- test_data(500, 5000, 6, 1, 1, 0.01)
tca.mdl <-
  tca(
    X = data$X,
    W = data$W,
    C1 = data$C1,
    C2 = data$C2
  )
```

10.1.2 Positive Definite

```r
X <- matrix(rnorm(100), ncol = 4)
X <- cbind(X, X[, 1], X[, 2])
X
y <- rnorm(nrow(X))

df <- as.data.frame(cbind(X, y))
lm(y ~ ., data = df) |>
```

```r
  summary()

library(RcppEigen)
mdl1.fit <- fastLm(X = X, y = y)

mdl1.coef <- summary(mdl1.fit)$coefficients
# First row is always intercept. Sacrifice some code readability here
# Sacrifice some code readability here by using -1 instead of
## mdl1.coef[`which(rownames(mdl1.coef) != "(Intercept)")`, "Pr(>|t|)"]
deltas_gammas_hat_pvals <- mdl1.coef[-1, "Pr(>|t|)"]
stopifnot("C1 is rank deficient" = !anyNA(deltas_gammas_hat_pvals))
```

10.2 repmat

10.2.1 tca.fit

```r
# tca.fit
# saveRDS(list(a = W_norms[, j], n = k, m = 1), "assets/repmat_optimize.rds")
# stop()
repmat_1 <- readRDS("assets/repmat_optimize.rds")
waldo::compare(
  t(repmat(repmat_1$a, repmat_1$n, repmat_1$m)),
  MESS::repmat(matrix(repmat_1$a), repmat_1$m, repmat_1$n)
)

t(repmat(repmat_1$a, repmat_1$n, repmat_1$m))
MESS::repmat(matrix(repmat_1$a), ncol = repmat_1$n)
waldo::compare(
  pracma::repmat(repmat_1$a, 1000, 1),
  MESS::repmat(matrix(repmat_1$a, nrow = 1), 1000, 1)
)
```

10.2.2 tca.fit_means_vars

```r
# tca.fit_means_vars
# saveRDS(
#   list(
#     W_norms = W_norms,
#     X_tilde = W_tilde,
#     C1_tilde = C1_tilde,
#     C2_tilde = C2_tilde
#   ),
#   "assets/repmat_optimize2.rds"
# )
# stop()
repmat_2 <- readRDS("assets/repmat_optimize2.rds")
waldo::compare(
  apply(repmat_2$X_tilde, 2, function(v) {
    repmat(v, 1, 3)
  }),
  apply(repmat_2$X_tilde, 2, function(v) {
    MESS::repmat(matrix(v), ncol = 3)
  })
)
```

10.2.3 minus_log_likelihood_sigmas

```
# minus_log_likelihood_sigmas
# stop()

repmat_3 <- readRDS("assets/repmat_optimize3.rds")

for (i in names(repmat_3)) {
  assign(i, repmat_3[[i]])
}

gradient <- -(
  colSums(
    W_squared * pracma::repmat(sigmas, n, 1) * t(pracma::repmat(U_j, k, 1)) / pracma::repmat(V_squared,
  ) - colSums(
    W_squared * pracma::repmat(sigmas, n, 1) / pracma::repmat(V, 1, k)
  )
)

gradient2 <- -(
  colSums(
    (
      W_squared *
        MESS::repmat(matrix(sigmas, nrow = 1), nrow = n, 1) *
        MESS::repmat(matrix(U_j), ncol = k)
    ) /
      MESS::repmat(V_squared, 1, ncol = k)
  ) -
    colSums(
      (
        W_squared *
          MESS::repmat(matrix(sigmas, nrow = 1), nrow = n, 1)
      ) /
        MESS::repmat(V, 1, ncol = k)
    )
)

W_squared_sig <- W_squared * MESS::repmat(matrix(sigmas, nrow = 1), nrow = n, 1)

gradient3 <- -(
  colSums(
    (
      W_squared_sig *
        MESS::repmat(matrix(U_j), ncol = k)
    ) /
      MESS::repmat(V_squared, 1, ncol = k)
  ) -
    colSums(
      (
        W_squared_sig
      ) /
```

```
        MESS::repmat(V, 1, ncol = k)
    )
)

waldo::compare(gradient, gradient2)
waldo::compare(gradient, gradient3)
```

10.2.4 minus_log_likelihood_w

```
set.seed(1234)
data <- test_data(20, 10000, 6, 1, 1, 0.01)
tca.mdl <- tca(X = data$X, W = data$W, C1 = data$C1, C2 = data$C2, refit_W = TRUE)
```

```
# saveRDS(
#   list(
#     w_i = w_i,
#     w_i_rep = w_i_rep,
#     sigmas_squared = sigmas_squared,
#     V_rep = V_rep,
#     mus = mus,
#     C_tilde = C_tilde,
#     U_i = U_i,
#     k = k,
#     V_rep = V_rep,
#     U_i_squared = U_i_squared,
#     V = V
#   ),
#   "assets/repmat_optimize4.rds"
# )
# stop()

repmat_4 <- readRDS("assets/repmat_optimize4.rds")

for (i in names(repmat_4)) {
  assign(i, repmat_4[[i]])
}

V_rep2 <- MESS::repmat(V, 1, k)
V_rep <- repmat(V, 1, k)
waldo::compare(V_rep2, V_rep)

w_i_rep2 <- MESS::repmat(matrix(w_i, nrow = 1), m, 1)
w_i_rep <- repmat(w_i, m, 1)
waldo::compare(w_i_rep2, w_i_rep)

gval <-
  colSums(w_i_rep * sigmas_squared / V_rep) +
  colSums(
    (
      (mus + C_tilde) * repmat(U_i, 1, k) * V_rep -
        w_i_rep * sigmas_squared * repmat(U_i_squared, 1, k)
    ) /
      repmat(V**2, 1, k)
  )

w_i_rep_sig <- w_i_rep * sigmas_squared
gval2 <-
  colSums(w_i_rep_sig / V_rep) +
  colSums((
    (mus + C_tilde) * MESS::repmat(U_i, 1, k) * V_rep -
      w_i_rep_sig * MESS::repmat(U_i_squared, 1, k)
  ) /
    MESS::repmat(V**2, 1, k))

waldo::compare(gval, gval2)
```

10.3 vars.mle = TRUE

- Not really a way to get around the `nloptr()` call that takes the majority of the time to optimize sigma.
- The only "improvement" that's low hanging is remove extra assignment calls in the function to minimize overhead for `nloptr()`

```
set.seed(1234)
data <- test_data(200, 5000, 6, 1, 1, 0.01)
tca.mdl <-
  tca(
    X = data$X,
    W = data$W,
    C1 = data$C1,
    C2 = data$C2
  )

sequential_vars.alt <- profvis({
  tca.mdl <-
    tca(
      X = data$X,
      W = data$W,
      C1 = data$C1,
      C2 = data$C2
    )
})

sequential_vars.mle <- profvis({
  tca.mdl <-
    tca(
      X = data$X,
      W = data$W,
      C1 = data$C1,
      C2 = data$C2,
      vars.mle = TRUE
    )
})

sequential_vars.mle2 <- profvis({
  tca.mdl <-
    tca(
      X = data$X,
      W = data$W,
      C1 = data$C1,
      C2 = data$C2,
      vars.mle = TRUE
    )
})

saveRDS(sequential_vars.mle, "./assets/sequential_n200_m1e3_vars.mle.rds")
```

```
sequential_vars.mle <- readRDS("./assets/sequential_n200_m1e3_vars.mle.rds")
sequential_vars.mle
```

10.3.1 Rfast::colsums

- Rfast::colsums can be faster than colSums. Use with caution. We can try to benchmark the fit of the results before and after the use of colsums for a close to realistic set of data.

- Rfast is faster, but it doesn't reproduce the result of fit 1.2.1.

```
tm <- matrix(rnorm(25e6), nrow = 5000)

waldo::compare(
  colSums(tm),
  Rfast::colsums(tm),
  tolerance = .Machine$double.eps^0.5
)

microbenchmark::microbenchmark(
  colSums(tm),
  # Rfast::colsums(tm),
  matrixStats::colSums2(tm)
)
```

10.4 split_input

```
data <- test_data(30, 200000, 6, 1, 1, 0.01)
split_X <- split_input(X = data$X, n_chunks = 21)
```

```
fit1 <- tca(X = split_X[[1]], W = data$W, C1 = data$C1, C2 = data$C2, W_C1_C2 = FALSE)
fit2 <- tca(X = split_X[[2]], W = data$W, C1 = data$C1, C2 = data$C2, W_C1_C2 = FALSE)

fit_final <- purrr::map2(fit1, fit2, \(x, y) {
  rbind(x, y)
})
fit_final$mus_hat
```

10.5 tca_split

- Split the work into small chunks and test vs running sequentially and see if the estimates are similar.

- Looks like the smaller the chunks, the more the correlation between the sequential run and the chunked run decreases. This is probably because the sigmas_hat and tau_hat are estimated using information from X. More work to be determined to see if its a trade off between time and accuracy if we just chunk into "small enough" chunks instead.

- If vars.mle = TRUE, the correlation stays high (>0.95) even when chunked into single features/chunk.

```r
library(TCA)
library(furrr)
# devtools::install_github("hhp94/TCA@profiling")

set.seed(1234)
data <- test_data(30, 10000, 6, 1, 1, 0.01)
split_X <- split_input(X = data$X, n_chunks = 10000)
split_X
dim(split_X)

plan(multisession, workers = 7)
res_par <- tca_split(
  X = split_X, W = data$W, C1 = data$C1, C2 = data$C2, vars.mle = TRUE,
  max_iters = 20
)
plan(sequential)

res_seq <- tca(X = data$X, W = data$W, C1 = data$C1, C2 = data$C2)

res_seq |> lapply(dim)
res_seq$tau_hat
res_seq_2$tau_hat

setdiff(names(res_seq), "tau_hat")
sapply(compare_fit(res_seq, res_seq_2), \(x) {
  all(x > 0.96)
})
```