computational details of low-rank matrix completion via adaptive-impute

Alex Hayes

4/26/2019

Motivation

TODO: add references section and save the PDFs in the repository with the code here, etc

TODO: go through and be really really careful with notation. missing some i's in algorithm 2. explain hadamard product. express frobenius inner product of matrices as sum of elements of hadamard products.

Notation: $y->Y$ and treat it as a bitmask matrix

LMAO Adaptative Impute can be abbreviated AI

Notation & Algorithm

Algorithm 1: `AdapativeInitialize`

Input: M, y and r

1 $\hat{p} \leftarrow \frac{1}{nd} \sum_{i=1}^{n} \sum_{j=1}^{d} y_{ij}$

2 $\Sigma_{\hat{p}} \leftarrow M^T M - (1 - \hat{p}) \operatorname{diag}(M^T M)$

3 $\Sigma_{t\hat{p}} \leftarrow MM^T - (1 - \hat{p}) \operatorname{diag}(MM^T)$

4 $\hat{V}_i \leftarrow \mathbf{v}_i(\Sigma_{\hat{p}})$ for $i = 1, ..., r$

5 $\hat{U}_i \leftarrow \mathbf{u}_i(\Sigma_{t\hat{p}})$ for $i = 1, ..., r$

6 $\tilde{\alpha} \leftarrow \frac{1}{d-r} \sum_{i=r+1}^{d} \boldsymbol{\lambda}_i(\Sigma_{\hat{p}})$

7 $\hat{\lambda}_i \leftarrow \frac{1}{\hat{p}} \sqrt{\boldsymbol{\lambda}_i(\Sigma_{\hat{p}}) - \tilde{\alpha}}$ for $i = 1, ..., r$

8 $\hat{s}_i \leftarrow$ sign stuff for $i = 1, ..., r$

9 **return** $\hat{s}_i, \hat{\lambda}_i, \hat{U}_i, \hat{V}_i$ *for* $i = 1, ..., r$

Then we can construct an approximation

$$\hat{M} = \sum_{i=1}^{r} \hat{s}_i \hat{\lambda}_i \hat{U}_i \hat{V}_i^T \tag{1}$$

Algorithm 2: `AdapativeImpute`

Input: M, y, r and $\varepsilon > 0$

1 $Z^{(1)} \leftarrow \texttt{AdaptiveInitialize}(M, y, r)$

2 repeat

3 $\quad \tilde{M}^{(t)} \leftarrow P_\Omega(M) + P_\Omega^\perp(Z_t)$

4 $\quad \hat{V}_i^{(t)} \leftarrow \mathbf{v}_i(\tilde{M}^{(t)})$ for $i = 1, ..., r$

5 $\quad \hat{U}_i^{(t)} \leftarrow \mathbf{u}_i(\tilde{M}^{(t)})$ for $i = 1, ..., r$

6 $\quad \tilde{\alpha}^{(t)} \leftarrow \frac{1}{d-r} \sum_{i=r+1}^{d} \boldsymbol{\lambda}_i^2(\tilde{M}^{(t)})$

7 $\quad \hat{\lambda}_i^{(t)} \leftarrow \sqrt{\boldsymbol{\lambda}_i^2(\tilde{M}^{(t)}) - \tilde{\alpha}^{(t)}}$ for $i = 1, ..., r$

8 $\quad Z^{(t+1)} \leftarrow \sum_{i=1}^{r} \hat{\lambda}_i^{(t)} \hat{U}_i^{(t)} \hat{V}_i^{(t)^T}$

9 $\quad t \leftarrow t + 1$

10 until $\|Z_{t+1} - Z_t\|_F^2 / \|Z_{t+1}\|_F$

11 return $\hat{\lambda}_i^{(t)}, \hat{U}_i^{(t)}, \hat{V}_i^{(t)}$ *for* $i = 1, ..., r$

Pre-requisites

The Matrix package

reference: https://cran.r-project.org/web/packages/Matrix/vignettes/Intro2Matrix.pdf

```r
library(Matrix)

set.seed(17)

M <- rsparsematrix(8, 12, nnz = 30) # small example, not very sparse
summary(M)

# note that Matrix objects are S4 classes so we access their
# slots using the @ symbol
class(M)

M@x  # vector of values in M
M@i  # corresponding row indices

# if you want column indices you need a dgTMatrix
M2 <- as(M, "dgTMatrix")
M2@j  # corresponding column indices // only for dgCMatrix object

M %*% t(M)
```

Summations and norms

```r
M^2    # square each element in M elementwise, return as sparse matrix
M@x^2  # square each element in M elementwise, return as vector of nonzeros

# the second version is much faster
bench::mark(
  sum(M^2),
  sum(M@x^2),
  sum(colSums(M^2)),
  norm(M, type = "F")^2,
  iterations = 20
)

sum(M^2) == sum(M@x^2)  # sums are the same

norm(M, type = "F")^2 == sum(M^2)  # and equal the Frobenius norm squared
```

The projections $P_\Omega(A)$ and $P_\Omega^\perp(A)$ where Ω indicates the observed elements of a matrix M and A is another matrix with the same dimensions as M.

```r
y <- as(M, "lgCMatrix")  # indicator matrix only
all.equal(y * M, M)  # don't lose anything multiplying by indicators

A <- matrix(1:(8*12), 8, 12)

all.equal(dim(A), dim(M))  # appropriate to practice projections with

# Omega indicates whether an entry of M was observed

# P_Omega (A)
A * y

!y

# P_Omega^perp (A): NOTE: this results in a *dense* matrix
A * (1 - y)

all(A * y + A * (1 - y) == A)  # can recover A from both projections together
```

crossproducts

```r
bench::mark(
  crossprod(M),     # dsCMatrix -- most specialized class, want this
  crossprod(M, M),  # dgCMatrix
  t(M) %*% M,       # dgCMatrix
```

3

```
    check = FALSE
)
```

the `drop()` function helps us manage dimensions

```
one_col <- matrix(1:4)
one_row <- matrix(5:8, nrow = 1)

drop(one_col)
drop(one_row)

c(one_col)  # same thing, less explicit. use drop to be explicit
```

diagonal of crossproduct

```
v_sign == colSums(svd_M$v * v_hat)
diag(t(svd_M$v) %*% v_hat)
diag(crossprod(svd_M$v, v_hat))

bench::mark(
  colSums(svd_M$v * v_hat),
  crossprod(rep(1, d), svd_M$v * v_hat),
  iterations = 50,
  check = FALSE
)

# write a diag_crossprod helper
```

```
rhos <- matrix(1:12, ncol = 4, byrow = TRUE)

bench::mark(
  diag(crossprod(rhos)),
  diag(t(rhos) %*% rhos),
  colSums(rhos * rhos),
  crossprod(rep(1, nrow(rhos)), rhos^2),
  check = FALSE
)



rhos <- matrix(1:12, ncol = 4, byrow = TRUE)

bench::mark(
  diag(tcrossprod(rhos)),
  diag(crossprod(t(rhos))),
  diag(rhos %*% t(rhos)),
```

```
    rowSums(rhos * rhos),
    check = FALSE
)
```

what we get from `eigen()` and `svd()`: slightly different stuff: `u`, `d` and `v` versus `values` and `vectors`

NOTE: RSpectra *only* does truncated decompositions. if you want the full decomposition, you have to use base R stuff. different algos.

Brief aside in sign ambiguity

yada yada yada the signs of the left and right singular vectors are not identified in SVD

A more elegant solution as proposed in @bro_resolving_2007 and used in Karl's paper is to take inner products

NOTE TO SELF: identifying the signs of a single SVD is a much harder task than comparing two SVDs and seeing if they are the same up to sign differences. we only need to check if they are the same up to sign differences.

```r
set.seed(17)
M <- rsparsematrix(8, 12, nnz = 30) # small example, not very sparse

# number of singular vectors to compute
k <- 4

s <- svd(M, k, k)
s2 <- svds(M, k, k)

# irritating: svd() always gives you all the singular values even if you
# only request the first K singular vectors
s$u %*% diag(s$d[1:k]) %*% t(s$v)

# based on the flip_signs function of
# https://stats.stackexchange.com/questions/134282/relationship-between-svd-and-pca-how-to-use-svd-to-p
equal_svds <- function(s, s2) {

  # svd() always gives you all the singular values, but we only
  # want to compare the first k
  k <- ncol(s$u)

  # the term sign(s$u) * sign(s2$u) performs a sign correction

  # isTRUE because output of all.equal is not a boolean, it's something
  # weird when the inputs aren't equal. lol why
```

```
  u_ok <- isTRUE(
    all.equal(s$u, s2$u * sign(s$u) * sign(s2$u), check.attributes = FALSE)
  )

  v_ok <- isTRUE(
    all.equal(s$v, s2$v * sign(s$v) * sign(s2$v), check.attributes = FALSE)
  )

  d_ok <- isTRUE(all.equal(s$d[1:k], s2$d[1:k], check.attributes = FALSE))

  u_ok && v_ok && d_ok
}
```

Linear algebra facts

Throughout these computations, we will repeatedly use several key facts about eigendecompositions, singular value decompositions (SVD) and the relationship between the two.

https://en.wikipedia.org/wiki/Gramian_matrix X'X – positive semi-def, so the singular values of M'M are the same as the eigenvalues

question: if A, B positive, is sum(svd(A - B)$d) $== sum(svd(A)$d)$ - sum(svd(B)$d)

answer: NO! can't split into two easy computations and then combine them possibly use this to get some sort of bound?

think about what happens as p_hat -> 0

A key observation here is that $M^T M$ and

Fact: sum of squared singular values is `trace(A^T A)` https://math.stackexchange.com/questions/2281721/sum-of-singular-values-of-a-matrix

Fact: for symmetric positive definite matrices the eigendecomp is equal to the singular value decomp

Fact: sum of eigenvalues of M is equal to trace(M)

Consequence: for pos def symmetric M the sum of the singular values is trace(M) as well

Again computing `alpha` deserves some explanation.

- reference: https://math.stackexchange.com/questions/1463269/how-to-obtain-sum-of-square-of-eigenvalues-without-fir
- Frobenius norm (A) = trace(crossprod(A))
- TODO: how we know this thing is strictly positive to prevent sqrt() from exploding

```
## STOPPED HERE: WHY ARE the following not the same?
  isSymmetric(sigma_p)
  eigen(sigma_p)$values
  sum(diag(sigma_p))
```

```r
sum(svd(sigma_p)$d)
sum(eigen(sigma_p)$values)


# let's think just about the first term for a moment
sum(diag(MtM / p_hat^2))
sum(svd(MtM / p_hat^2)$d)


sum(colSums(M^2 / p_hat^2))


# has some negative eigenvalues

# Fact: for a symmetric matrix, the singular values are the *absolute* values
# of the eigenvalues

# https://www.mathworks.com/content/dam/mathworks/mathworks-dot-com/moler/eigs.pdf

eigen(sigma_p)$values
sum(eigen(sigma_p)$values)
sum(abs(eigen(sigma_p)$values))
sum(svd(sigma_p)$d)
sum(abs(diag(sigma_p)))


# those agree so what about the second term

# note to self: alpha should be positive
# issue karl ran into:
# https://math.stackexchange.com/questions/381808/sum-of-eigenvalues-and-singular-values
# how to get the sum of singular values itself (start):
# https://math.stackexchange.com/questions/569989/sum-of-singular-values-of-ab

# options when sigma_p is not positive definite:
# - calculate the full SVD
# - set alpha to zero (don't truncate the singular values)
# - this lower bounds the average of the remaining singular values
# -

# positive semi-definite is enough since symmetric and eigen/singular values
# of zero don't matter

# this is only an issue in the initialization. in the iterative updates
# we use the squared singular values, which we can more easily calculate
# the sum of
```

```
  # ask Karl what he wants to do about this: computing a full SVD is gonna be really expensive.
```

FACT: sum(diag(crossprod(M))) == sum(M^2)

Reference implementation

```
library(RSpectra)
library(Matrix)
```

```
adaptive_initialize <- function(M, r) {

  p_hat <- nnzero(M) / prod(dim(M))  # line 1

  MtM <- crossprod(M)
  MMt <- tcrossprod(M)

  # need to divide by p^2 from Cho et al 2016 to get the "right"
  # singular values / singular values on a comparable scale

  # both of these matrices are symmetric, but not necessarily positive
  # this has important implications for the SVD / eigendecomp relationship

  sigma_p <- MtM / p_hat^2 - (1 - p_hat) * diag(diag(MtM))  # line 2
  sigma_t <- MMt / p_hat^2 - (1 - p_hat) * diag(diag(MMt))  # line 3

  # crossprod() and tcrossprod() return dsCMatrix objects,
  # sparse matrix objects that know they are symmetric

  # unfortunately, RSpectra doesn't support dsCMatrix objects,
  # but does support dgCMatrix objects, a class representing sparse
  # but not symmetric matrices

  # support for dsCMatrix objects in RSpectra is on the way,
  # which will eliminate the need for the following coercions.
  # see: https://github.com/yixuan/RSpectra/issues/15

  sigma_p <- as(sigma_p, "dgCMatrix")
  sigma_t <- as(sigma_t, "dgCMatrix")

  svd_p <- svds(sigma_p, r)  # TODO: is eigs_sym() faster?
  svd_t <- svds(sigma_t, r)

  v_hat <- svd_p$v  # line 4
```

```r
  u_hat <- svd_t$u   # line 5

  n <- nrow(M)
  d <- ncol(M)

  # NOTE: alpha is incorrect due to singular values and eigenvalues
  # being different when sigma_p is not positive

  alpha <- (sum(diag(sigma_p)) - sum(svd_p$d)) / (d - r)   # line 6
  lambda_hat <- sqrt(svd_p$d - alpha) / p_hat              # line 7

  svd_M <- svds(M, r)

  v_sign <- crossprod(rep(1, d), svd_M$v * v_hat)
  u_sign <- crossprod(rep(1, n), svd_M$u * u_hat)
  s_hat <- drop(sign(v_sign * u_sign))

  lambda_hat <- lambda_hat * s_hat   # line 8

  list(u = u_hat, d = lambda_hat, v = v_hat)
}
```

It's worth commenting on computation of `alpha` and `s_hat`.

When we compute `alpha` in line 20 `adaptive_initialize()`, we don't want to do the full eigendecomposition of $\Sigma_{\hat{p}}$ since that could take a long time, so we use trick and recall that the trace of a matrix (the sum of it's diagonal elements) equals the sum of all the eigenvalues. Then we subtract off the first r eigenvalues, which we do compute, and are left with $\sum_{i=r+1}^{d} \lambda_i(\Sigma_{\hat{p}})$.

```r
adaptive_impute <- function(M, r, epsilon = 1e-7) {

  s <- adaptive_initialize(M, r)
  Z <- s$u %*% diag(s$d) %*% t(s$v)   # line 1
  delta <- Inf

  while (delta > epsilon) {

    y <- as(M, "lgCMatrix")   # indicator if entry of M observed
    M_tilde <- M + Z * (1 - y)   # line 3

    svd_M <- svds(M_tilde, r)

    u_hat <- svd_M$u   # line 4
    v_hat <- svd_M$v   # line 5
```

```r
    d <- ncol(M)

    alpha <- (sum(M_tilde^2) - sum(svd_M$d^2)) / (d - r)  # line 6

    lambda_hat <- sqrt(svd_M$d^2 - alpha)  # line 7

    Z_new <- u_hat %*% diag(lambda_hat) %*% t(v_hat)

    delta <- sum((Z_new - Z)^2) / sum(Z^2)
    Z <- Z_new

    print(glue::glue("delta: {round(delta, 8)}, alpha: {round(alpha, 3)}"))
  }


  Z
}
```

Finally we can do a minimal sanity check and see if this code even runs, and see if we are recovering something close-ish to implanted low-rank structure.

```r
n <- 500
d <- 100
r <- 5

A <- matrix(runif(n * r, -5, 5), n, r)
B <- matrix(runif(d * r, -5, 5), d, r)
M0 <- A %*% t(B)

err <- matrix(rnorm(n * d), n, d)
Mf <- M0 + err


p <- 0.3
y <- matrix(rbinom(n * d, 1, p), n, d)
dat <- Mf * y

init <- adaptive_initialize(dat, r)
filled <- adaptive_impute(dat, r)
```

Low-rank implementation

The reference implementation has some problems. As our data matrix M gets larger, we can no longer fit the dense representation of $\hat{M}$ and $Z^{(t)}$ into memory. Instead, we need to work with just the low rank components $\hat{\lambda}, \hat{U}$ and $\hat{V}$.

This leads us to following implementation:

```r
low_rank_adaptive_initialize <- function(M, r) {

  M <- as(M, "dgCMatrix")

  p_hat <- nnzero(M) / prod(dim(M))  # line 1

  # NOTE: skip explicit computation of line 2
  # NOTE: skip explicit computation of line 3

  eig_p <- eigen_helper(M, r)
  eig_t <- eigen_helper(t(M), r)

  lr_v_hat <- eig_p$vectors  # line 4
  lr_u_hat <- eig_t$vectors  # line 5

  d <- ncol(M)
  n <- nrow(M)

  # NOTE: alpha is again incorrect since we work with eigenvalues
  # rather than singular values here
  sum_eigen_values <- sum(M@x^2) / p^2 - (1 - p) * sum(colSums(M^2))
  lr_alpha <- (sum_eigen_values - sum(eig_p$values)) / (d - r)  # line 6

  lr_lambda_hat <- sqrt(eig_p$values - lr_alpha) / p_hat  # line 7

  # TODO: Karl had another sign computation here that he said was faster
  # but it wasn't documented anywhere, so I'm going with what was in the
  # paper

  lr_svd_M <- svds(M, r)

  # v_hat is d by r
  lr_v_sign <- crossprod(rep(1, d), lr_svd_M$v * lr_v_hat)
  lr_u_sign <- crossprod(rep(1, n), lr_svd_M$u * lr_u_hat)
  lr_s_hat <- c(sign(lr_v_sign * lr_u_sign))  # line 8

  lr_lambda_hat <- lr_lambda_hat * lr_s_hat

  list(u = lr_u_hat, d = lr_lambda_hat, v = lr_v_hat)
}
```

What does `eigen_helper()` do? Describe the return object (also do this for svds)

```r
# Take the eigendecomposition of t(M) %*% M - (1 - p) * diag(t(M) %*% M)
# using sparse computations only
eigen_helper <- function(M, r) {
  eigs_sym(
    Mx, r,
    n = ncol(M),
    args = list(
      M = M,
      p = nnzero(M) / prod(dim(M))
    )
  )
}


# compute (t(M) %*% M / p^2 - (1 - p) * diag(diag(t(M) %*% M))) %*% x
# using sparse operations

# TODO: divide the second term by p^2 like in the reference implementatio
Mx <- function(x, args) {
  drop(
    crossprod(args$M, args$M %*% x) / args$p^2 - (1 - args$p) * Diagonal(ncol(args$M), colSums(args$M^2)
  )
}
```

Now we check that `Mx` works

```r
x <- rnorm(12)
p <- 0.3
out <- (t(M) %*% M / p^2 - (1 - p) * diag(diag(t(M) %*% M))) %*% x
out2 <- Mx(x, args = list(M = M, p = p))
all.equal(as.matrix(out), as.matrix(out))
```

TODO: update alg description to divide by p^2 to get the right singular values

Quickly check that the components works before we try the code that integrates them all together

Finally, sanity check this by comparing to the reference implementation. These don't agree, which isn't great:

```r
lr_init <- low_rank_adaptive_initialize(dat, r)

# some weird stuff is happening with the singular values but I'm
# going to not worry about it for the time being

equal_svds(init, lr_init)
```

Space-efficient adaptive impute

TODO: figure out the actual space complexity

Recall the algorithm looks like

$$\hat{M} = \sum_{i=1}^{r} \hat{s}_i \hat{\lambda}_i \hat{U}_i \hat{V}_i^T \tag{2}$$

Algorithm 3: `AdapativeImpute`

Input: M, y, r and $\varepsilon > 0$

1 $Z^{(1)} \leftarrow \texttt{AdaptiveInitialize}(M, y, r)$

2 repeat

3 $\quad \tilde{M}^{(t)} \leftarrow P_\Omega(M) + P_\Omega^\perp(Z_t)$

4 $\quad \hat{V}_i^{(t)} \leftarrow \mathbf{v}_i(\tilde{M}^{(t)})$ for $i = 1, ..., r$

5 $\quad \hat{U}_i^{(t)} \leftarrow \mathbf{u}_i(\tilde{M}^{(t)})$ for $i = 1, ..., r$

6 $\quad \tilde{\alpha}^{(t)} \leftarrow \frac{1}{d-r} \sum_{i=r+1}^{d} \boldsymbol{\lambda}_i^2(\tilde{M}^{(t)})$

7 $\quad \hat{\lambda}_i^{(t)} \leftarrow \sqrt{\boldsymbol{\lambda}_i^2(\tilde{M}^{(t)}) - \tilde{\alpha}^{(t)}}$ for $i = 1, ..., r$

8 $\quad Z^{(t+1)} \leftarrow \sum_{i=1}^{r} \hat{\lambda}_i^{(t)} \hat{U}_i^{(t)} \hat{V}_i^{(t)^T}$

9 $\quad t \leftarrow t + 1$

10 until $\|Z_{t+1} - Z_t\|_F^2 / \|Z_{t+1}\|_F$

11 return $\hat{\lambda}_i^{(t)}, \hat{U}_i^{(t)}, \hat{V}_i^{(t)}$ for $i = 1, ..., r$

Now we need two things:

1. The SVD of $\tilde{M}^{(t)}$
2. (Certain sums of) the squared singular values.

Sums of squared singular values

For a matrix A, the sum of squared singular values (denoted by λ_i) equals the squared frobenius norm:

$$\sum_{i=1}^{\min(n,d)} \lambda_i^2 = \|A\|_F^2 = \text{trace}(A^T A) \tag{3}$$

Also note that

$$\|A + B\|_F^2 = \|A\|_F^2 + \|B\|_F^2 + 2 \cdot \langle A, B \rangle_F \tag{4}$$

Now we consider $\tilde{M}^{(t)}$. Suppose that unobserved values of M are set to zero, as is the case for M stored in a sparse matrix representation

$$\tilde{M}^{(t)} = P_\Omega(M) + P_\Omega^\perp(Z_t) \tag{5}$$

$$= P_\Omega(M) + P_\Omega^\perp \left(\sum_{i=1}^r \hat{\lambda}_i^{(t)} \hat{U}_i^{(t)} \hat{V}_i^{(t)^T} \right) \tag{6}$$

Now we need

$$||\tilde{M}^{(t)}||_F^2 = \left\| P_\Omega(M) + P_\Omega^\perp \left(\sum_{i=1}^r \hat{\lambda}_i^{(t)} \hat{U}_i^{(t)} \hat{V}_i^{(t)^T} \right) \right\|_F^2 \tag{7}$$

$$= \|P_\Omega(M)\|_F^2 + \left\| P_\Omega^\perp \left(\sum_{i=1}^r \hat{\lambda}_i^{(t)} \hat{U}_i^{(t)} \hat{V}_i^{(t)^T} \right) \right\|_F^2 + 2 \cdot \left\langle P_\Omega(M), P_\Omega^\perp \left(\sum_{i=1}^r \hat{\lambda}_i^{(t)} \hat{U}_i^{(t)} \hat{V}_i^{(t)^T} \right) \right\rangle_F \tag{8}$$

$$= \|P_\Omega(M)\|_F^2 + \left\| P_\Omega^\perp \left(\sum_{i=1}^r \hat{\lambda}_i^{(t)} \hat{U}_i^{(t)} \hat{V}_i^{(t)^T} \right) \right\|_F^2 \tag{9}$$

Where the cancellation in the final line follows because

$$\left\langle P_\Omega(M), P_\Omega^\perp \left(\sum_{i=1}^r \hat{\lambda}_i^{(t)} \hat{U}_i^{(t)} \hat{V}_i^{(t)^T} \right) \right\rangle_F = \sum_{i,j} P_\Omega(M)_{ij} \cdot P_\Omega^\perp(Z_t)_{ij} = \sum_{i,j} 0 = 0 \tag{10}$$

Now we need one more trick, which is that

$$\|Z_t\|_F^2 = \left\| P_\Omega(Z_t) + P_\Omega^\perp(Z_t) \right\|_F^2 = \|P_\Omega(Z_t)\|_F^2 + \left\| P_\Omega^\perp(Z_t) \right\|_F^2 \tag{11}$$

and then

$$\left\| P_\Omega^\perp(Z_t) \right\|_F^2 = \|Z_t\|_F^2 - \|P_\Omega(Z_t)\|_F^2 \tag{12}$$

$$= \sum_{i=1}^r \lambda_i^2 - \|Z_t \odot y\|_F^2 \tag{13}$$

Putting it all together we see

$$||\tilde{M}^{(t)}||_F^2 = \|P_\Omega(M)\|_F^2 + \left\| P_\Omega^\perp \left(\sum_{i=1}^r \hat{\lambda}_i^{(t)} \hat{U}_i^{(t)} \hat{V}_i^{(t)^T} \right) \right\|_F^2 \tag{14}$$

$$= \|M\|_F^2 + \sum_{i=1}^r \lambda_i^2 - \|Z_t \odot y\|_F^2 \tag{15}$$

In code we will have a sparse matrix `M` and a list `s` with elements of the SVD. The first Frobenious norm is quick to calculate, but I am not sure how to calculate the other two frobenius norms.

```r
# s is a matrix defined in terms of it's svd
# G is a sparse matrix
# compute only elements of U %*% diag(d) %*% t(V) only on non-zero elements of G
# G and U %*% t(V) must have same dimensions

# maybe call this svd_perp?
svd_perp <- function(s, mask) {

  # note: must be dgTMatrix to get column indexes j larger
  # what if we used dlTMatrix here?
  m <- as(mask, "dgTMatrix")

  # the indices for which we want to compute the matrix multiplication
  # turn zero based indices into one based indices
  i <- m@i + 1
  j <- m@j + 1

  # gets rows and columns of U and V to multiply, then multiply
  ud <- s$u %*% diag(s$d)
  left <- ud[i, ]
  right <- s$v[j, ]

  # compute inner products to get elements of U %*% t(V)
  uv <- rowSums(left * right)

  # NOTE: specify dimensions just in case
  sparseMatrix(i = i, j = j, x = uv, dims = dim(mask))
}
```

Test it

```r
set.seed(17)

M <- rsparsematrix(8, 12, nnz = 30)
s <- svds(M, 5)

y <- as(M, "lgCMatrix")

Z <- s$u %*% diag(s$d) %*% t(s$v)

all.equal(
  svd_perp(s, M),
```

```
  Z * y
)
```

So, to take an eigendecomp you just need to be able to do Mx. To take an SVD, what do you need? matrix vector and matrix transpose vector multiplication

```r
set.seed(17)
r <- 5

M <- rsparsematrix(8, 12, nnz = 30)
y <- as(M, "lgCMatrix")

s <- svds(M, r)
Z <- s$u %*% diag(s$d) %*% t(s$v)

M_tilde <- M + Z * (1 - y)   # dense!

Z_perp <- svd_perp(s, M)
sum_singular_squared <- sum(M@x^2) + sum(s$d^2) - sum(Z_perp@x^2)

all.equal(
  sum(svd(M_tilde)$d^2),
  sum_singular_squared
)
```

SVD of M tilde

```r
set.seed(17)
r <- 5

M <- rsparsematrix(8, 12, nnz = 30)
y <- as(M, "lgCMatrix")

s <- svds(M, r)
Z <- s$u %*% diag(s$d) %*% t(s$v)

M_tilde <- M + Z * (1 - y)   # dense!

svd_M_tilde <- svds(M_tilde, r)
svd_M_tilde

Ax <- function(x, args) {
  drop(M_tilde %*% x)
```

```
}

Atx <- function(x, args) {
  drop(t(M_tilde) %*% x)
}


# is eigs_sym() with a two-sided multiply faster?
args <- list(u = s$u, d = s$d, v = s$v, m = M)
test1 <- svds(Ax, k = r, Atrans = Atx, dim = dim(M), args = args)


test1
svd_M_tilde

all.equal(
  svd_M_tilde,
  test1
)
```

So we're done our first sanity check of the function interface. Let x be a vector. Now we want to calculate

$$\tilde{M}^{(t)}x = \left[P_\Omega(M) + P_\Omega^\perp(Z_t)\right]x \tag{16}$$
$$= \left[P_\Omega(M) - P_\Omega(Z_t) + P_\Omega(Z_t) + P_\Omega^\perp(Z_t)\right]x \tag{17}$$
$$= P_\Omega(M - Z_t)x + Z_t x \tag{18}$$

where we can think of $R_t \equiv P_\Omega(M - Z_t)$ as "residuals" of sorts. Crucially, R_t is sparse, and

$$Z_t x = (\hat{U}\operatorname{diag}(\hat{\lambda}_1, ..., \hat{\lambda}_r)\hat{V}^t)x \tag{19}$$
$$= (\hat{U}(\operatorname{diag}(\hat{\lambda}_1, ..., \hat{\lambda}_r)(\hat{V}^t x))) \tag{20}$$

So now the memory requirement of the computation has been reduced to that of two sparse matrix vector multiplications, rather than that of fitting the dense matrix $P_\Omega^\perp(Z_t)$ into memory.

Similarly, for the transpose, we have

$$\tilde{M}^{(t)^T}x = \left[P_\Omega(M) + P_\Omega^\perp(Z_t)\right]^T x \tag{21}$$
$$= \left[P_\Omega(M) - P_\Omega(Z_t) + P_\Omega(Z_t) + P_\Omega^\perp(Z_t)\right]^T x \tag{22}$$
$$= P_\Omega(M - Z_t)^T x + Z_t^T x \tag{23}$$

This leads us to a second, less memory intensive implementation of `Ax()` and `Atx()`:

17

```r
# input: M, Z_t as a low-rank SVD list s

R <- M - svd_perp(s, M)   # residual matrix
args <- list(u = s$u, d = s$d, v = s$v, r = R)

Ax <- function(x, args) {
  drop(args$r %*% x + args$u %*% diag(args$d) %*% crossprod(args$v, x))
}

Atx <- function(x, args) {
  # TODO: can we use a crossprod() for the first multiplication here?
  drop(t(args$r) %*% x + args$v %*% diag(args$d) %*% crossprod(args$u, x))
}

# is eigs_sym() with a two-sided multiply faster?
test2 <- svds(Ax, k = r, Atrans = Atx, dim = dim(M), args = args)

all.equal(
  svd_M_tilde,
  test2
)
```

```r
low_rank_adaptive_impute <- function(M, r, epsilon = 1e-03) {

  # coerce M to sparse matrix such that we use sparse operations
  M <- as(M, "dgCMatrix")

  # low rank svd-like object, s ~ Z_1
  s <- low_rank_adaptive_initialization(M, r)  # line 1
  delta <- Inf

  norm_M <- sum(M^2)

  while (delta > epsilon) {
    s_new <- low_rank_threshold(s, M, norm_M, r)
    delta <- low_rank_relative_change(s, s_new, M)
    s <- s_new
  }

  s
}
```

$$\mathtt{MtM} = \tilde{M}^{(t)^T} \tilde{M}^{(t)} \tag{24}$$

Extension to a mixture of observed and unobserved missingness

originally solving an optimization vaguely of the form

$$\left\| M - \hat{M} \right\|_F^2 \tag{25}$$

where M is a partially observed matrix. now, we let $M' = YM$ where Y is an indicator of whether or not M was observed. Typically we have some setup like

$$M = \begin{bmatrix} \cdot & \cdot & 3 & 1 & \cdot \\ 3 & \cdot & \cdot & 8 & \cdot \\ \cdot & -1 & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & 2 & \cdot & \cdot & \cdot \\ 5 & \cdot & 7 & \cdot & 4 \end{bmatrix}, \qquad Y = \begin{bmatrix} \cdot & \cdot & 1 & 1 & \cdot \\ 1 & \cdot & \cdot & 1 & \cdot \\ \cdot & 1 & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & 1 & \cdot & \cdot & \cdot \\ 1 & \cdot & 1 & \cdot & 1 \end{bmatrix} \tag{26}$$

Here the symbol $\cdot$ means that an entry of the matrix was unobserved.

but what we do now is, continuing to represent M as a sparse matrix with no zero entries, is *observe* a bunch of zeros. So we might know that the upper triangle of M has structurally missing zeros that we have observed are missing. These zeros are primarily important because they affect the residuals in our calculations. In this particular case, the take multiplication by M, a sparse operation, and make it into a dense operation.

At this point it becomes useful to introduce some additional notation. Let $\tilde{\Omega}$ be the set of indicies (i, j) such that $M_{i,j}$ is non-zero. Observe that $\tilde{\Omega} \subset \Omega$. Then we have $P_{\tilde{\Omega}}(A) = P_{\Omega}(A)$.

$$M = \begin{bmatrix} 0 & 0 & 3 & 1 & 0 \\ 3 & 0 & 0 & 8 & 0 \\ \cdot & -1 & 0 & 0 & 0 \\ \cdot & \cdot & \cdot & 0 & 0 \\ \cdot & 2 & \cdot & \cdot & 0 \\ 5 & \cdot & 7 & \cdot & 4 \end{bmatrix}, \qquad Y = \begin{bmatrix} 1 & 1 & 1 & 1 & 1 \\ 1 & 1 & 1 & 1 & 1 \\ \cdot & 1 & 1 & 1 & 1 \\ \cdot & \cdot & \cdot & 1 & 1 \\ \cdot & 1 & \cdot & \cdot & 1 \\ 1 & \cdot & 1 & \cdot & 1 \end{bmatrix}, \qquad M' = \begin{bmatrix} \cdot & \cdot & 3 & 1 & \cdot \\ 3 & \cdot & \cdot & 8 & \cdot \\ \cdot & -1 & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & 2 & \cdot & \cdot & \cdot \\ 5 & \cdot & 7 & \cdot & 4 \end{bmatrix} \tag{27}$$

And now we need to figure out how to calculate

$$\tilde{M}^{(t)}x = \left[P_\Omega(M) + P_{\tilde{\Omega}}^\perp(Z_t)\right]x \tag{28}$$

$$= \left[P_\Omega(M) - P_\Omega(Z_t) + P_\Omega(Z_t) + P_{\tilde{\Omega}}^\perp(Z_t)\right]x \tag{29}$$

$$= P_\Omega(M) - P_\Omega(Z_t)x + Z_t x \tag{30}$$

$$= P_{\tilde{\Omega}}(M) - P_\Omega(Z_t)x + Z_t x \tag{31}$$

We already know how to calculate $P_{\tilde{\Omega}}(M)$ and $Z_t x$ using sparse operations, so we're left with $P_\Omega(Z_t)x$. Note that $P_\Omega(Z_t)x \neq P_{\tilde{\Omega}}(Z_t)x$ since Z_t is not necessarily zero on $\tilde{\Omega}^\perp$. In other words $P_{\tilde{\Omega}}^\perp(Z_t) \neq Z_t$.

When Y is dense, there is no way to avoid paying the computational cost of the dense or near dense computation. Our primary concern is fitting Y into memory for large datasets. This is an issue when Y is dense but with no discernible structure that permits a more compact representation.

If we can fit Y into memory, we can do a low-rank computation, only calculating elements $Z_{ij}^{(t)}$ when $Y_{ij} = 1$. When Y is stored as a vector of row indices together with a vector of column indices (plus some information about the dimension), we can write the computation out:

```r
M <- Matrix(
  rbind(
    c(0, 0, 3, 1, 0),
    c(3, 0, 0, 8, 0),
    c(0, -1, 0, 0, 0),
    c(0, 0, 0, 0, 0),
    c(0, 2, 0, 0, 0),
    c(5, 0, 7, 0, 4)
  )
)

Y <- rbind(
  c(1, 1, 1, 1, 1),
  c(1, 1, 1, 1, 1),
  c(0, 1, 1, 1, 1),
  c(0, 0, 1, 1, 1),
  c(0, 1, 0, 1, 1),
  c(1, 0, 1, 0, 1)
)

s <- svds(M, 2)

Y <- as(Y, "CsparseMatrix")

# triplet form
# compressed column matrix form even better but don't
# understand the format
```

```r
Y <- as(Y, "lgCMatrix")
Y <- as(Y, "lgTMatrix")

# ugh: RcppArmadillo only supports dgTMatrix rather than
# lgTMatrix which is somewhat unfortunate

# link: https://cran.r-project.org/web/packages/RcppArmadillo/vignettes/RcppArmadillo-sparseMatrix.pdf

Y

x <- rnorm(5)

# want to calculate
Z <- s$u %*% diag(s$d) %*% t(s$v)
out <- drop((Z * Y) %*% x)
out
```

At this point it's worth writing out explicitly how calculate $Z_{ij}^{(t)}$.

$$Z_{ij}^{(t)} = \left(\sum_{\ell=1}^{r} \hat{U}_\ell \hat{d}_\ell \hat{V}_\ell^T \right)_{ij} \tag{32}$$

For a visual reminder, this looks like (using $\mathrm{diag}(\hat{d})$ and $\hat{\Sigma}$ somewhat interchangeably here)

$$Z^{(t)} = \hat{U} \, \mathrm{diag}(\hat{d}) \, \hat{V}^T = \begin{bmatrix} U_1 & U_2 & \dots & U_r \end{bmatrix} \begin{bmatrix} d_1 & 0 & \dots & 0 \\ 0 & d_2 & \dots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \dots & d_r \end{bmatrix} \begin{bmatrix} V_1^T \\ V_2^T \\ \vdots \\ V_r^T \end{bmatrix} \tag{33}$$

$$\begin{bmatrix} U_{11} & U_{12} & \dots & U_{1r} \\ U_{21} & U_{22} & \dots & U_{2r} \\ \vdots & \vdots & \ddots & \vdots \\ U_{n1} & U_{n2} & \dots & U_{nr} \end{bmatrix} \begin{bmatrix} d_1 & 0 & \dots & 0 \\ 0 & d_2 & \dots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \dots & d_r \end{bmatrix} \begin{bmatrix} V_{11} & V_{21} & \dots & V_{d1} \\ V_{12} & V_{22} & \dots & V_{d2} \\ \vdots & \vdots & \ddots & \vdots \\ V_{1r} & V_{2r} & \dots & V_{dr} \end{bmatrix} \tag{34}$$

n x d = (n x r) x (r x r) x (r x d)

(r x d) is after the transpose

$$\begin{bmatrix} U_{11} & U_{12} & \dots & U_{1r} \\ U_{21} & U_{22} & \dots & U_{2r} \\ \vdots & \vdots & \ddots & \vdots \\ U_{n1} & U_{n2} & \dots & U_{nr} \end{bmatrix} \begin{bmatrix} d_1 & 0 & \dots & 0 \\ 0 & d_2 & \dots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \dots & d_r \end{bmatrix} \begin{bmatrix} V_{11} & V_{21} & \dots & V_{d1} \\ V_{12} & V_{22} & \dots & V_{d2} \\ \vdots & \vdots & \ddots & \vdots \\ V_{1r} & V_{2r} & \dots & V_{dr} \end{bmatrix} \tag{35}$$

Also because I never remember anything, recall that Z is $n \times d$, x is $d \times 1$ and Zx is $n \times 1$:

$$(Zx)_i = \sum_{j=1}^{d} Z_{ij} \cdot x_j \tag{36}$$

(recall that X_i always refers to the ith column of X in this document)

```r
# mask as a pair list
# L and Z / svd are both n x d matrices
# x is a d x 1 matrix / vector
masked_svd_times_x <- function(s, mask, x) {

  stopifnot(inherits(mask, "lgTMatrix"))

  u <- s$u
  d <- s$d
  v <- s$v

  zx <- numeric(nrow(u))

  # lgTMatrix uses zero based indexing, add one
  row <- mask@i + 1
  col <- mask@j + 1

  # need to loop over index of indexes
  # double looping over i and j here feels intuitive
  # but is incorrect
  for (idx in seq_along(row)) {
    i <- row[idx]
    j <- col[idx]

    z_ij <- sum(u[i, ] * d * v[j, ])
    zx[i] <- zx[i] + x[j] * z_ij
  }

  zx
}


# how to calculate just one element of the reconstructed
# data using the SVD

i <- 6
j <- 4
```

```
sum(s$u[i, ] * s$d * s$v[j, ])
Z[i, j]

# the whole masked matrix multiply

Z <- s$u %*% diag(s$d) %*% t(s$v)
out <- drop((Z * Y) %*% x)

# check that we did this right
all.equal(
  masked_svd_times_x(s, Y, x),
  out
)
```

This is gonna be painfully slow in R so we rewrite in C++

```
library(Rcpp)

cppFunction(
  depends = "RcppArmadillo",
  "arma::vec masked_svd_times_x_impl(
      const arma::mat& U,
      const arma::rowvec& d,
      const arma::mat& V,
      const arma::vec& row,
      const arma::vec& col,
      const arma::vec& x) {

    int i, j;
    double z_ij;

    arma::vec zx = arma::zeros<arma::vec>(U.n_rows);

    for (int idx = 0; idx < row.n_elem; idx++) {

      i = row(idx);
      j = col(idx);

      // % does elementwise multiplication in Armadillo
      // accu() gives the sum of elements of resulting vector
      z_ij = accu(U.row(i) % d % V.row(j));

      zx(i) += x(j) * z_ij;
```

```
    }

    return zx;
  }")

# wrap with slightly nicer interface
masked_svd_times_x_cpp <- function(s, mask, x) {
  drop(masked_svd_times_x_impl(s$u, s$d, s$v, mask@i, mask@j, x))
}
```

```
bench::mark(
  masked_svd_times_x_cpp(s, Y, x),
  masked_svd_times_x(s, Y, x)
)
```

A naive solution: the epsilon trick

issue: we've moved back into dense computation land

The memory efficient version

asdf

TODO: don't coerce to explicit Matrix class as that is not recommended apparently. alternatives?