NOTES ON COMPUTATIONAL HOMOLOGY

???

Abstract. We work out some details of algorithms for computing homology, persistent or otherwise.

1. Persistent homology

First, we study the reduction algorithm for persistent homology described in Edelsbrunner and Harer [**?**, pp. 152 – 156] ("E & H"). Specifically, we analyze the algorithm described by the pseudocode on p. 153 E & H. We prove the claim made on p. 155 ibid that if $i < j$, column i in the reduced matrix R is all 0, and the "lowest 1" in column j is in row i, then the homology class "born" in column i "dies" in column j. Moreover, the space of cycles is spanned by the chains corresponding to the columns in the V matrix corresponding to the 0 columns in the R matrix.

First, of all, what do E & H mean by "lowest 1" in a column? (They don't seem to explain that.) Apparently, they mean the *largest* index in the column that's 1 (i.e, not 0; we're working over $\mathbb{Z}/2$). Such a 1 will be in the lowest position if the matrix is written out in the usual way. If ℓ is a column index, let $low(\ell)$ be the index of the lowest 1 in column ℓ of R. Thus, $low(\ell)$ is the maximal index of the non-zero elements of column ℓ in R.

Let K be the complex under consideration. The simplices in the complex are partially ordered by a function $f : K \to \mathbb{R}$ (p. 150, E & H). This is important in the "Elder Rule" (E & H, p. 151). However, this ordering is not refined enough. For example, suppose two classes are "born" with the addition of simplices σ and τ and $f(\sigma) = f(\tau)$. But suppose with the addition of some other simplex ρ, the two classes later merge. Then one class dies but the other persists. Which one dies? Which one persists? To avoid such difficulties we need a more refined way to measure "time". Suppose the simplices in the complex K are ordered in a fashion that is "compatible" with f (p. 152 E & H). Write $\sigma_1 < \ldots < \sigma_N$. (There might also be a "simplex" in dimension -1 in order to capture reduced homology in dimension 0.) Define a new function $\tilde{f}$ that simply assigns to the j^{th} simplex in the ordering the number j. Then for any pair of simplices in K, one is more "elder" than the other w.r.t. $\tilde{f}$. In particular, we may identify chains with the set of 0-1 vectors of length N.

In a slight extension of the algorithm, we consider homology relative to a complex that belongs to all the subcomplexes corresponding to the values of the function This corresponds to removing some simplices for K. In terms of matrices, this means removing

Date: 7/8/'11.

some rows and columns. *Note: That the i^{th} row is removed if and only if the i^{th} column is removed.* In particular, an identity matrix is transformed to another identity matrix, just of a smaller dimension. (Section VII.3 E & H, "Extended Persistence", discusses relative homology, but apparently deals with different issues to the ones I care about.)

Write

$$R = \partial \cdot V,$$

where ∂ is the matrix of the boundary operator and "$\cdot$" denotes matrix multiplication. Thus, the k^{th} column in R is the image under ∂ of the the k^{th} column in V. Let σ_i denote the simplex whose boundary is given by the i^{th} column of ∂. We will at times refer to the column index as "time".

As observed in E & H, all three matrices, R, ∂, and V are all 0 below the main diagonal. *In fact, the diagonals of ∂ and R are both 0 as well.* This is because the columns of ∂ are "compatibly ordered" (p. 152 E & H). So all faces of a simplex σ strictly precede it in the ordering.

On the other hand, the main diagonal of V is all 1's. To see this imagine running the algorithm initializing V to the identity matrix. Suppose that by the j^{th} passage through the loop in the pseudo code on p. 153 E & H the diagonal of V still consists entirely of 1's. Nothing happens in the algorithm that will cancel a 1 in the diagonal of V. Specifically, if $j_0 < j$ and column j_0 is added to column j, then $j_0 < j$ means that only entries in the j^{th} above the diagonal entry (j, j) can be changed. Hence, by induction, the main diagonal of V consists entirely of 1's. Since all entries of V below the main diagonal are 0, if follows that the column space of V consists of all 0-1 vectors of length N. I.e., any chain can be represented as a sum of columns of V.

If the i^{th} column in R is all 0's then obviously, the cycle represented by the i^{th} column of V is a cycle, call it z. What does it mean to say that z represents a homology class that is "born" at column i? It means that it's not homologous to a cycle that appears in an earlier column. More precisely, for the cycle represented by the i^{th} column to *not* be born at "time" $\tilde{f}(\sigma_i) := i$, there must be some chain, c, involving only columns up to i, inclusive, s.t. $\partial c + z$ is a cycle composed of columns strictly before the i^{th}. But V has 1's all along its diagonal. In particular, σ_i is a term in z. Thus, σ_i must appear in ∂c. But that means, since the diagonal of ∂ is 0, the chain c involves at least one column strictly *after* i. This proves that z represents a class "born" at i.

We prove that the columns of V corresponding to columns of R consisting only of 0's span the space of cycles. Clearly, every such column is a cycle. Suppose z is a cycle. A observed above, we may think of z as a 0-1 vector of length N and represented as a sum of columns of V. Suppose that z is the sum of columns $j_1 < \cdots < j_k$ of V and suppose that for some $i = 1, \ldots, k$ the j_i^{th} column of R that is not all 0. If the j_i^{th} column of R is not all 0, then that column has a lowest 1. Assume that among all such columns, column j_i has the lowest lowest 1. (Thus, $low(j_\nu)$ with $\nu = i$ is maximal among all the columns, j_ν, in the sum z.) From the specification of the algorithm there there will be exactly one such column. Then in ∂z, there's nothing to cancel the lowest 1 in column j_i of R, so the boundary cannot be 0, contradiction. This proves that the columns of V corresponding to columns of R consisting only of 0's span the space of cycles.

Suppose $z := \sum_{i=1}^{k} \sigma_{j_i}$ is a (reduced) cycle. We show that after reduction, column j_k is all 0's. From what we just proved there are columns $i_1, \ldots, i_m$ of V s.t. if $z_{i_1}, \ldots, z_{i_k}$ are the, say, d-dimensional chains represented by columns $i_1 < \ldots < i_m$ of the matrix V then $z = \sum_{\ell=1}^{m} z_{i_\ell}$ and each column $i_1 < \ldots < i_m$ of the matrix R is 0. Since the main diagonal of V is all 1's and there are only 0's below the main diagonal of V, we must have $i_m = j_k$.

Finally, we show that if the j^{th} column R is non-zero and its lowest 1 is in row i (i.e., $low(j) = i$), then the i^{th} column of R must be all 0 and the homology class born at i must perish at j. Let y be the chain in column j and x be the chain in column i of V. Write

$$\partial y = \sum_{p=1}^{i} \eta_p \sigma_p \text{ and } x = \sum_{\ell=1}^{i} \epsilon_\ell \sigma_\ell,$$

where the η_p's and ϵ_ℓ's are all 0 or 1, of course. Since V has 1's all along its main diagonal, $\epsilon_i = 1$. Since $i = low(j)$ we also have $\eta_i = 1$. Now

$$0 = \partial^2 y = \partial(\partial y).$$

Therefore, from what we just proved, the i^{th} column of R, which is the same as ∂x, is all 0. I.e., x is a cycle. Let $z = x - \partial y$. Then the σ_i's in x and ∂y cancel so

$$z = \sum_{t=1}^{i-1} \zeta_t \sigma_t \text{ and } \partial z = \partial x - \partial^2 y = 0.$$

I.e., $x = \partial y + z$, where z is a cycle that comes from a "time" before i. Thus, y is "dead" at "time" j. This means that at time j the cycle x is homologous to a cycle that was born no later than x was. By the "Elder Rule" (E & H, p. 151) this means that x is "dead" at time j. (This seems a little different from how E & H define the "Elder Rule".)

But couldn't x "die" *before* j? In that case there would be a chain w carried by $\sigma_1, \ldots, \sigma_{j-1}$ s.t. the cycle $x - \partial w$ is carried by $\sigma_1, \ldots, \sigma_{i-1}$. But then we must have $low(w) = i$, contradicting the fact that after the reduction the first column whose lowest 1 is in row i is column j.

2. "Excision trick"

Let K be a simplicial complex and let L be a subcomplex of K. We apply excision (Munkres [**?**, Theorem 9.1, p. 50]) to the pair (K, L). Define

$$A := \{\sigma \in L : \sigma \text{ is not a face of any } \tau \in K \setminus L\}.$$

Let $U := \bigcup_{\sigma \in A} \operatorname{Int} \sigma$.

Claim: U is the interior, $|L|^\circ$, of the polytope $|L|$ relative to $|K|$. Suppose $x \in |L| \setminus U$. There exists $\zeta \in L$ s.t. $x \in \operatorname{Int} \zeta$. Then ζ is the face of some $\tau \in K \setminus L$. Thus, every neighborhood of x will intersect $\operatorname{Int} \tau$. This means every neighborhood of x will intersect $\tau \setminus |L|$. It follows that $x \notin |L|^\circ$. Therefore, $|L|^\circ \subset U$. Thus, it suffices to show that U is open in $|K|$.

Let $\tau \in K$. First, suppose $\tau \in A$ and let ζ be a face of τ, e.g., $\zeta = \tau$. If $\zeta \in A$, then $\operatorname{Int}\zeta \subset U$. If $\zeta \notin A$, then $\operatorname{Int}\zeta \cap U = \varnothing$, for otherwise $\operatorname{Int}\zeta$ would intersect $\operatorname{Int}\sigma$ for some $\sigma \in A$. But $\zeta \neq \sigma$ so $(\operatorname{Int}\zeta) \cap (\operatorname{Int}\sigma) = \varnothing$. The fact that $\zeta \notin A$ means that ζ is the face of some $\omega \in K \setminus L$. Thus, any face of ζ is the face of $\omega \in K \setminus L$. Hence, no face of ζ is in A. Therefore, if $\zeta \notin A$ then $\zeta \cap U = \varnothing$. Thus, since $\tau = \bigcup_{\zeta \text{ is a face of } \tau} \operatorname{Int}\zeta$,

$$\begin{aligned}
\tau \cap U &= \left(\bigcup_{\zeta \text{ is a face of } \tau \text{ and } \zeta \in A} (\operatorname{Int}\zeta) \cap U \right) \cup \left(\bigcup_{\zeta \text{ is a face of } \tau \text{ and } \zeta \notin A} (\operatorname{Int}\zeta) \cap U \right) \\
&= \bigcup_{\zeta \text{ is a face of } \tau \text{ and } \zeta \in A} \operatorname{Int}\zeta \\
&\subset \tau \setminus \left(\bigcup_{\zeta \text{ is a face of } \tau \text{ and } \zeta \notin A} \operatorname{Int}\zeta \right) \\
&\subset \tau \setminus \left(\bigcup_{\zeta \text{ is a face of } \tau \text{ and } \zeta \notin A} \zeta \right).
\end{aligned}$$

Hence, $\tau \cap U$ is open in τ.

Next, suppose $\tau \in K \setminus A$ and let $\sigma \in A$. Then $\sigma \neq \tau$. Let $\zeta := \tau \cap \sigma$ so ζ is a face of τ and σ. If $\zeta \cap (\operatorname{Int}\sigma) \neq \varnothing$ then $\zeta = \sigma$, so σ is a face of τ, contradicting the definition of A. Therefore, $\zeta \cap (\operatorname{Int}\sigma) = \varnothing$. Hence, $\tau \cap (\operatorname{Int}\sigma) = \varnothing$ and

$$\tau \cap U = \bigcup_{\sigma \in A} \tau \cap (\operatorname{Int}\sigma) = \varnothing.$$

So once again $\tau \cap U$ is open in τ. Thus, by the definition of the topology of $|K|$ (Munkres [**?**, p. 8]), U is open in $|L|$. This completes the proof of the claim that $U = |L|^\circ$.

Claim: $|K| \setminus U$ is the polytope of the complex, K', consisting of all simplices in $K \setminus L$ plus all faces of same. I.e., $K' = K \setminus A \supset K \setminus L$. Clearly, K' is a subcomplex of K. Suppose $\sigma \in K'$, i.e., σ is the face of a simplex in $K \setminus L$. Suppose $x \in \sigma \cap U$. Then there exists $\tau \in A$ s.t. $x \in \operatorname{Int}\tau$. This means that τ is a face of σ, which means that τ is a face of a simplex in $K \setminus L$. But $\tau \in A$, a contradiction. Thus, $|K'| \subset |K| \setminus U$. Conversely, let $x \in |K| \setminus U$. Then for every $\sigma \in A$, we have $x \notin \operatorname{Int}\sigma$. But there exists $\tau \in K$ s.t. $x \in \operatorname{Int}\tau$. Hence, $\tau \notin A$, which means that τ is a face of some simplex in $K \setminus L$. I.e., $\tau \in K'$. Therefore $|K| \setminus U \subset |K'|$, as claimed.

Let $L' := L \cap K'$, so L' is a subcomplex of L and $|L'| = |L| \setminus U$. Therefore, by excision (Munkres [**?**, Theorem 9.1, p. 50]), the inclusion map $j' : (K', L') \hookrightarrow (K, L)$ induces an isomorphism in homology. Let $p = 0, 1, \ldots$ and define $f' : C_p(K, L) \to C_p(K', L')$ as follows. Let $c + C_p(L) \in C_p(K, L)$. We may write *uniquely,*

$$c = \sum_{i=1}^{m} \sigma_i,$$

where $\sigma_1, \ldots, \sigma_m \in K \setminus L$. Then $\sigma_1, \ldots, \sigma_m \notin A$. I.e., $\sigma_1, \ldots, \sigma_m \in K'$. Hence the following defines a homomorphism $f' : C_p(K, L) \to C_p(K', L')$,

$$f'\big[c + C_p(L)\big] = c + C_p(L') \in C_p(K')/C_p(L').$$

Next, we show that f' is a chain map. Let $\sigma \in K$ be a p-simplex. Let ζ be a $(p-1)$-face of σ. If $\sigma \in K \setminus L$, then $\zeta \notin A$, so $\zeta \in K'$ and

$$f'\big[\partial(\sigma + C_p(L))\big] = \partial\sigma + C_p(L') = \partial f'(\sigma).$$

Observe $f' = (j'_\#)^{-1}$, where $j'_\# : C_p(K', L') \to C_p(K, L)$ is the induced homomorphism. Therefore, f' induces isomorphisms in homology.

Now suppose that L is acyclic. Let $h : K \to (K, L)$ and $h' : K' \to (K', L')$. Then the following commutes.

$$\begin{tikzcd}
 & \tilde{H}_p(L') \arrow[r] \arrow[d] & \tilde{H}_p(K') \arrow[r, "h'_*"] \arrow[d] & H_p(K', L') \arrow[r] \arrow[d, "\cong"] & \tilde{H}_{p-1}(L') \arrow[d] & \\
0 \arrow[r, equal] & \tilde{H}_p(L) \arrow[r] & \tilde{H}_p(K) \arrow[r, "h_*", "\cong"'] & H_p(K, L) \arrow[r] & \tilde{H}_{p-1}(L) \arrow[r, equal] & 0.
\end{tikzcd} \tag{1}$$

Thus, we can calculate $\tilde{H}_*(K)$ by calculating $H_*(K', L')$ and $C_*(K')/C_*(L')$ will be of lower dimension, sometimes much lower dimension, than $C_*(K)$.

3. "Wave" algorithm for computing persistent relative homology

Suppose we have pairs $(K_1, L_1) \subset \cdots \subset (K_n, L_n)$. In this section we assume that *the complexes L_ℓ are acyclic.* Persistence makes sense for the relative homology groups $H_*(K_r, L_r)$. In this section, we develop an algorithm for computing persistent relative homology (Section VII.3, E & H, "Extended Persistence", discusses relative homology, but apparently deals with different issues to the ones I care about.)

To begin with take $n = 2$ and let $j : (K_1, L_1) \hookrightarrow (K_2, L_2)$ be inclusion. Let (K'_ν, L'_ν) be the "excised" version of (K_ν, L_ν) as described in section **??** ($\nu = 1, 2$). Let $j'_1 : (K'_1, L'_1) \hookrightarrow (K_1, L_1)$ be inclusion and let $f'_{2*} : H_*(K_2, L_2) \to H_*(K'_2, L'_2)$ be an isomorphism as in section **??**.

Let $p = 1, 2, \ldots$. On the homology level, we have the composition,

$$f'_{2*} \circ j_* \circ j'_{1*} : H_p(K'_1, L'_1) \to H_p(K'_2, L'_2).$$

What does this look like on the chain level? Let $\sigma \in K'_1 \setminus L'_1$. Then $j'_{1\#}(\sigma + C_p(L'_1)) = \sigma + C_p(L_1)$ and $j_\#(\sigma + C_p(L_1)) = \sigma + C_p(L_2)$. If $\sigma \in L_2$ then $\sigma + C_p(L_2) = 0 \in C_p(K_2)/C_p(L_2)$ so $f'_2\big(\sigma + C_p(L_2)\big) = 0$. If $\sigma \in K_2 \setminus L_2$, then $f'_2(\sigma + C_p(L_2)) = \sigma + C_p(L'_2)$. If $\sigma \notin K'_2$, then $\sigma \in L_2$, so $f'_2\big(\sigma + C_p(L_2)\big) = 0$. Thus,

$$f'_2 \circ j_\# \circ j'_{1\#}\big(\sigma + C_p(L'_1))\big) = \begin{cases} 0, & \text{if } \sigma \notin K'_2, \\ \sigma + C_p(L'_2), & \text{otherwise.} \end{cases}$$

We conclude that $f'_{2*} \circ j_* \circ j'_{1*}$ can be computed without having to consider the bigger complexes K_1, L_1, K_2, L_2.

Let $h_\nu : K_\nu \to (K_\nu, L_\nu)$ be inclusion. Then, as noted in section **??**, since L_ν is acyclic, h_ν induces isomorphisms of homology. Let $k : K_1 \to K_2$ also be inclusion. Note that the following commutes

$$
\begin{array}{ccc}
H_p(K'_1, L'_1) & \xrightarrow{f'_{2*} \circ j_* \circ j_{1*}'} & H_p(K'_2, L'_2) \\
{\scriptstyle j'_{1*}} \big\downarrow \cong & & \cong \big\downarrow {\scriptstyle j'_{2*} = (f'_{2*})^{-1}} \\
H_p(K_1, L_1) & \xrightarrow{j_*'} & H_p(K_2, L_2) \\
{\scriptstyle h_{1*}} \big\uparrow \cong & & \cong \big\uparrow {\scriptstyle h_{2*}} \\
\tilde{H}_p(K_1) & \xrightarrow{k_*} & \tilde{H}_p(K_2).
\end{array}
\tag{2}
$$

It follows that $\alpha \in \tilde{H}_p(K_1)$ persists, i.e., $k_*(\alpha) \neq 0$, if and only if $(j'_{1*})^{-1} \circ h_{1*}(\alpha)$ persists. I.e, one can check persistence working in the smaller complexes (K'_ν, L'_ν).

As another wrinkle, suppose $\bar{K}_i$ is a subcomplex of K_i s.t. inclusion, $\bar{j}_i$, induces an isomorphism in homology. Suppose further that $\bar{K}_1 \subset \bar{K}_2$ and let $\bar{k} : \bar{K}_1 \hookrightarrow \bar{K}_2$ be inclusion. Then the following commutes.

$$
\begin{array}{ccc}
\tilde{H}_p(\bar{K}_1) & \xrightarrow{\bar{k}_*} & \tilde{H}_p(\bar{K}_2) \\
{\scriptstyle \bar{j}_{1*}} \big\uparrow \cong & & \cong \big\uparrow {\scriptstyle \bar{j}_{2*}} \\
\tilde{H}_p(K_1) & \xrightarrow{k_*} & \tilde{H}_p(K_2).
\end{array}
$$

Then a class $x \in \tilde{H}_p(K_1)$ "persists" to $\tilde{H}_p(K_2)$ (i.e., $k_*(x) \neq 0$) if and only if $\bar{j}_{1*}(x) \in \tilde{H}_p(\bar{K}_1)$ "persists" to $\tilde{H}_p(\bar{K}_2)$. Therefore, we can study persistence in K_1, K_2 by studying it in $\bar{K}_1, \bar{K}_2$.

To handle more than two spaces $\cdots \hookrightarrow K_\nu \hookrightarrow K_{\nu+1} \hookrightarrow \cdots$ just concatenate the preceding.

4. Left to right reduction

We describe an algorithm that might be useful for actually computing homology generators. Let M be an $m \times n$ matrix with field entries. (Call the field F.) For $j = 1, \ldots, n$, let M_j denote the j^{th} column of M. For $i = 1, \ldots, m$, let $M[i, j]$ be the entry in the i^{th} row and j^{th} column. Let $M^0 := M$. Do the following for $x = 1, \ldots, n-1$. If $M_x^{x-1} = 0$ (M_x^{x-1} is the x^{th} column of M^{x-1}), then return M^{x-1}. Suppose $M_x^{x-1} \neq 0$. Initialize $M^x := M^{x-1}$. Let $k = i = 1, \ldots, m$ be the smallest index s.t. $M^{x-1}[k, x] \neq 0$. Do the following for $j = x+1, \ldots, n$. If $M^{x-1}[i, j] = 0$, then $M_j^x = M_j^{x-1}$ is unchanged. If $M^{x-1}[i, j] \neq 0$, Let

$$
M_j^x := M_j^{x-1} - \big(M^{x-1}[i, j] / M^{x-1}[i, x]\big) M_x^{x-1}. \tag{3}
$$

In this case $M^x[i,j] = 0$. The final output is a matrix M^{n-1}.

Observe the following. Suppose $j = 1, \ldots, n$ and let $k = i = 1, \ldots, m$ be the smallest index s.t. $M^x[k,j] \neq 0$. Then if $i' = 1, \ldots, i-1$, we will also have $M^{x+1}[i',j] = 0$.

Let $N = M^{n-1}$ be the matrix that results from going through this algorithm (so x goes from 1 to $n-1$). Let $j = 2, \ldots, n$. We prove that $N_j = 0$ if and only if M_j lies in the span of $M_1, \ldots, M_{j-1}$. Clearly, if $N_j = 0$ (e.g., $M_j = 0$), then M_j lies in the span of $M_1, \ldots, M_{j-1}$.

So suppose M_j lies in the span of $M_1, \ldots, M_{j-1}$. We show that $N_j = 0$. We proceed by induction on n. If $j = n = 1$, then $N_j = M_j$ and $M_1, \ldots, M_{j-1}$ spans 0, so the statement is obvious. Don't like that? Okay, try $j = n = 2$. If M_2 lies in the span of M_1, then $M_2 = \alpha M_1$ for some $\alpha \in F$. Whether $\alpha = 0$ or not, M_2 will be zeroed out after the first pass of the algorithm.

Let $\nu = 2, 3, \ldots$ and suppose the statement is true for any $j = 2, \ldots, n$ providing $n \leq \nu$. Let $n = \nu + 1$ and let $k = i_1$ be the smallest k s.t. $M[k,t] \neq 0$ for some $t = 1, \ldots, j-1$. (So if $t = 1, \ldots, j-1$ and $k = 1, \ldots, i_1 - 1$, then $M[k,t] = 0$.) Let $k = x = 1, \ldots, j-1$ be the smallest k s.t $M[i_1,k] \neq 0$. Thus, (i_1, x) is the lexicographically smallest pair of indices to the left of the j^{th} column s.t. the corresponding element of M is non-zero. Then $M^x[i_1,x] \neq 0$. The remainder of the i^{th} row of M^x is 0. In particular, $M^x[i_1,j] = 0$. Remember that we are assuming that M_j lies in the span of $M_1, \ldots, M_{j-1}$. Hence, M^x_j is spanned by M^x_t for $t = 1, \ldots, x-1, x+1, \ldots, j-1$. Consider the matrix obtained from M^x but with column x removed. Apply the induction hypothesis. Then $N_j = 0$ as desired.

Conversely, suppose $N_j = 0$. Then from the way the algorithm works we see that some linear combination of $M_1, \ldots, M_j$ is 0. From (**??**), we see that the coefficient of M_j in that linear combination is 1. Therefore, M_j lies in the span of $M_1, \ldots, M_{j-1}$.