

Genome Rearrangements

Study Chapters 5.3-5.5

Python Tutorial on 2/5 5pm-7pm, Location TBD

From Last Time

 We developed a SimpleReversalSort algorithm that sorts by extending its prefix on every iteration (n-1) steps.

On

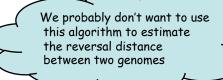
Flip 1: 1 <u>6 2</u> 3 4 5

Flip 2: 1 2 <u>6 3</u> 4 5

Flip 3: 1 2 3 <u>6 4</u> 5

Flip 4: 1 2 3 4 6 5

Flip 5: 1 2 3 4 5 6





• But it could have been sorted in two flips:

$$\pi$$
: 6 1 2 3 4 5



Approximation Algorithms

- Today's algorithms find *approximate* solutions rather than *optimal* solutions
- The approximation ratio of an algorithm \mathcal{A} on input π is:

$$\mathcal{A}(\pi)$$
 / OPT(π)

where

 $\mathcal{A}(\pi)$ - solution produced by algorithm \mathcal{A} OPT(π) - optimal solution of the problem



Approximation Ratio/Performance Guarantee

- Approximation ratio (performance guarantee) of algorithm *A*: max approximation ratio over all inputs of size *n*
 - For a minimizing algorithm \mathcal{A} (like ours):
 - Approx Ratio = $\max_{|\pi| = n} \mathcal{A}(\pi) / \text{OPT}(\pi) \ge 1.0$
 - For maximization algorithms:
 - Approx Ratio = $\min_{|\pi| = n} \mathcal{A}(\pi) / \text{OPT}(\pi) \le 1.0$

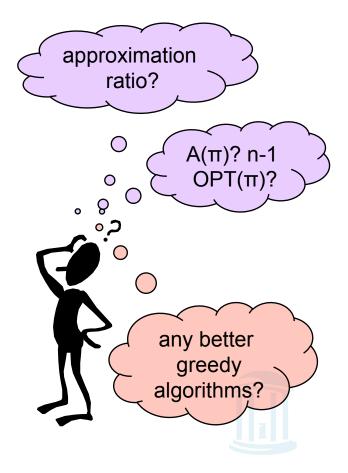


Approximation Ratio

SimpleReversalSort(π) 1 for $i \leftarrow 1$ to n-1 $j \leftarrow \text{position of element } i \text{ in } \pi \text{ (i.e., } \pi_i = i)$ 3 if $j \neq i$ 4 $\pi \leftarrow \pi \ \rho(i,j)$ output π 6 if π is the identity permutation 7 return

```
Step 0: <u>6 1</u> 2 3 4 5
Step 1: 1 <u>6 2</u> 3 4 5 Step 1: <u>5 4 3 2 1</u> 6
Step 2: 1 2 6 3 4 5 Step 2: 1 2 3 4 5 6
Step 3: 1 2 3 <u>6 4</u> 5
Step 4: 1 2 3 4 <u>6 5</u>
Step 5: 1 2 3 4 5 6
```

Step 0: 6 1 2 3 4 5



New Idea: Adjacencies

)

$$\pi = \pi_1 \pi_2 \pi_3 \dots \pi_{n-1} \pi_n$$

• A pair of neighboring elements π_i and π_{i+1} are *adjacent* if

$$\pi_{i+1} = \pi_i \pm 1$$

For example:

$$\pi = 1 \ 9 \ 3 \ 4 \ 7 \ 8 \ 2 \ 6 \ 5$$

• (3, 4) or (7, 8) and (6,5) are adjacent pairs



Breakpoints

Breakpoints occur between neighboring non-adjacent elements:

$$\pi = 1 | 9 | 3 | 4 | 7 | 8 | 2 | 6 | 5$$

- Pairs (1,9), (9,3), (4,7), (8,2) and (2,5) define 5 breakpoints of permutation π
- $b(\pi)$ # breakpoints in permutation π



Extending Permutations

• One can place two elements $\pi_0 = 0$ and $\pi_{n+1} = n+1$ at the beginning and end of π respectively

$$\pi = 1 \mid 9 \mid 3 \mid 4 \mid 7 \mid 8 \mid 2 \mid 6 \mid 5$$

Extending with 0 and 10

 $\pi = 0 \mid 1 \mid 9 \mid 3 \mid 4 \mid 7 \mid 8 \mid 2 \mid 6 \mid 5 \mid 10$

A new breakpoint was created after extending

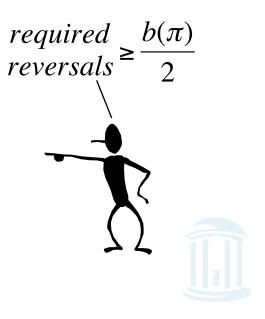
An extended permutation of n can have at most (n+1) breakpoints, (n-1) between elements plus 2)



Reversal Distance and Breakpoints

- Breakpoints are the bottlenecks for sorting by reversals once they are removed, the permutation is sorted.
- Each "useful" reversal eliminates at least 1 and at most 2 breakpoints.
- Consider the following application of SimpleReversalSort(Extend(π)):

$$\pi = 2 \ 3 \ 1 \ 4 \ 6 \ 5$$
 $0 \ 2 \ 3 \ 1 \ 4 \ 6 \ 5 \ 7$
 $b(\pi) = 5$
 $0 \ 1 \ 3 \ 2 \ 4 \ 6 \ 5 \ 7$
 $b(\pi) = 4$
 $0 \ 1 \ 2 \ 3 \ 4 \ 6 \ 5 \ 7$
 $b(\pi) = 2$
 $0 \ 1 \ 2 \ 3 \ 4 \ 5 \ 6 \ 7$
 $b(\pi) = 0$



Sorting By Reversals:

A Better Greedy Algorithm

BreakPointReversalSort(π)

- 1 while $b(\pi) > 0$
- 2 Among all possible reversals, choose reversal ρ minimizing $b(\pi \bullet \rho)$
- 3 $\pi \leftarrow \pi \cdot \rho(i, j)$
- 4 output π
- 5 return



The "greedy" concept here is to reduce as many breakpoints as possible

Does it always terminate?

What if no reversal reduces the number of breakpoints?

0 1 2 5 6 7 3 4 8 9

New Concept: Strips

- Strip: an interval between two consecutive breakpoints in a permutation
 - Decreasing strip: strip of elements in decreasing order (e.g. 65 and 32).
 - Increasing strip: strip of elements in increasing order (e.g. 78)

0 1 9 4 3 7 8 2 5 6 10

- A *single-element strip* can be declared either increasing or decreasing. We will choose to declare them as decreasing with exception of extension strips (with 0 and n+1)



Reducing the Number of Breakpoints

Consider π = 1 4 6 5 7 8 3 2

$$0 \ 1 \ 4 \ 6 \ 5 \ 7 \ 8 \ 3 \ 2 \ 9$$
 $b(\pi) = 5$

If permutation π contains at least one decreasing strip, then there exists a reversal ρ which decreases the number of breakpoints (i.e. $b(\pi \bullet \rho) < b(\pi)$).



How can we be sure that we decrease the number of breakpoints?



Consider $\pi = 14657832$

0 1 4 6 5 7 8 3 2 9
$$b(\pi) = 5$$

- Choose the decreasing strip with the smallest element k in π (it'll always be the rightmost)
- Find k 1 in the permutation (it'll always be flanked by a breakpoint)
- Reverse the segment between k and k-1 the breakpoint flanking k-1



Consider
$$\pi$$
 = 1 4 6 5 7 8 3 2

reduced by 1!

$$0 \ 1 \ 2 \ 3 \ 8 \ 7 \ 5 \ 6 \ 4 \ 9$$
 $b(\pi) = 4$

$$b(\pi) = 4$$

- Choose the decreasing strip with the smallest element k in π (it'll always be the rightmost)
- Find k 1 in the permutation (it'll always be flanked by a breakpoint)
- Reverse the segment between k and k-1
- Repeat until there is no decreasing strip



Consider π = 1 4 6 5 7 8 3 2

0 1 2 3 8 7 5 6 4 9
$$b(\pi) = 4$$

- Choose the decreasing strip with the smallest element k in π (it'll always be the rightmost)
- Find k-1 in the permutation (it'll always be flanked by a breakpoint)
- Reverse the segment between k and k-1
- Repeat until there is no decreasing strip



Consider π = 1 4 6 5 7 8 3 2

0 1 2 3 4 6 5 7 8 9
$$b(\pi) = 2$$

- Choose the decreasing strip with the smallest element k in π (it'll always be the rightmost)
- Find k-1 in the permutation (it'll always be flanked by a breakpoint)
- Reverse the segment between k and k-1
- Repeat until there is no decreasing strip



Consider
$$\pi$$
 = 1 4 6 5 7 8 3 2

0 1 2 3 4 6 5 7 8 9
$$b(\pi) = 2$$

- Choose the decreasing strip with the smallest element k in π (it'll always be the rightmost)
- Find k-1 in the permutation (it'll always be flanked by a breakpoint)
- Reverse the segment between k and k-1
- Repeat until there is no decreasing strip



Consider
$$\pi$$
 = 1 4 6 5 7 8 3 2

No breakpoint left!

0 1 2 3 4 5 6 7 8 9
$$b(\pi) = 0$$

- Choose the decreasing strip with the smallest element k in π (it'll always be the rightmost)
- Find k-1 in the permutation (it'll always be flanked by a breakpoint)
- Reverse the segment between k and k-1
- Repeat until there is no decreasing strip



Consider $\pi = 14657832$

0 1 4 6 5 7 8 3 2 9
$$b(\pi) = 5$$
0 1 2 3 8 7 5 6 4 9 $b(\pi) = 4$
0 1 2 3 4 6 5 7 8 9 $b(\pi) = 2$
0 1 2 3 4 5 6 7 8 9 $b(\pi) = 0$

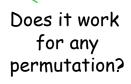
$$b(\pi) = 5$$

$$b(\pi) = 4$$

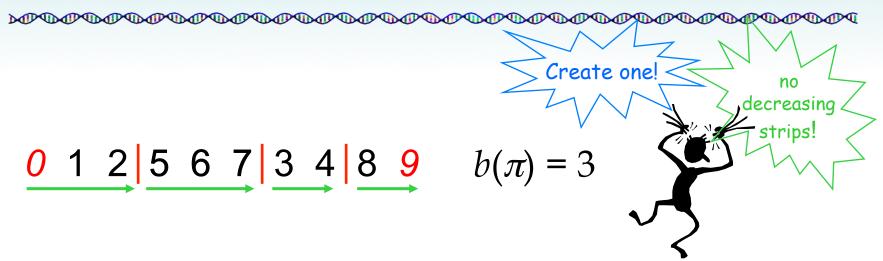
$$b(\pi) = 2$$

$$b(\pi)=0$$

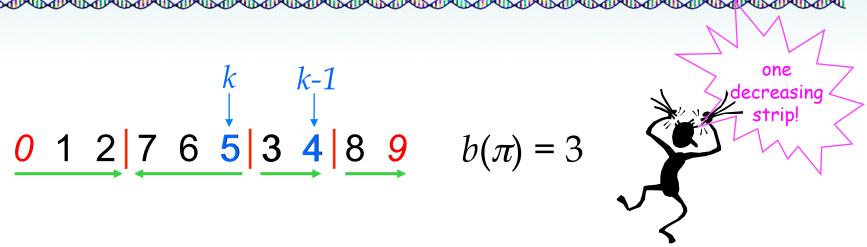
$$d(\pi) = 3$$



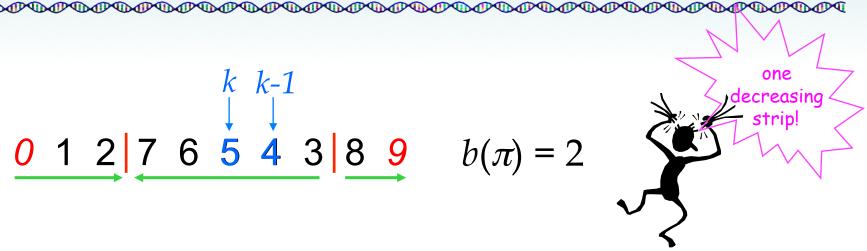




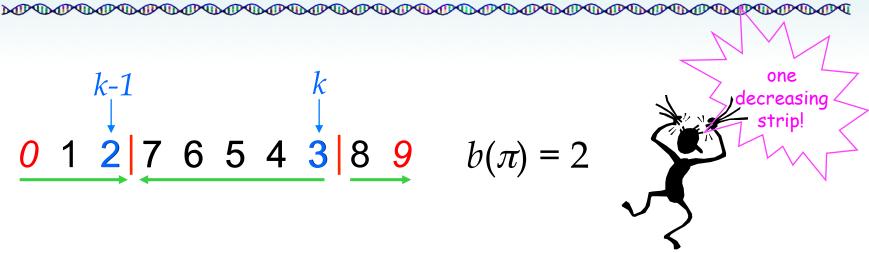
- If there is no decreasing strip, there may be no strip-reversal ρ that reduces the number of breakpoints (i.e. $b(\pi \bullet \rho) \ge b(\pi)$ for any reversal ρ).
- However, reversing an <u>increasing</u> strip creates a decreasing strip, and the number of breakpoints remains unchanged.
- Then the number of breakpoints will be reduced in the following steps.



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$$b(\pi)=0$$



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- However, reversing an increasing strip creates a decreasing strip, and the number of breakpoints remains unchanged.
- Then the number of breakpoints will be reduced in the following steps.

ImprovedBreakpointReversalSort

```
ImprovedBreakpointReversalSort(\pi)
```

```
1 while b(\pi) > 0

2 if \pi has a decreasing strip

3 Among all possible reversals, choose reversal \rho

that minimizes b(\pi \bullet \rho)

4 else

5 Choose a reversal \rho that flips an increasing strip in \pi

6 \pi \leftarrow \pi \bullet \rho

7 output \pi

8 return
```



In Python

```
def improvedBreakpointReversalSort(seq):
  while hasBreakpoints(seq):
       increasing, decreasing = getStrips(seq)
       if len(decreasing) > 0:
           reversal = pickReversal(seq, decreasing)
       else:
        reversal = increasing[0]
       print seq, "reversal", reversal
       seq = doReversal(seq,reversal)
  print seq, "Sorted"
  return
```



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Performance

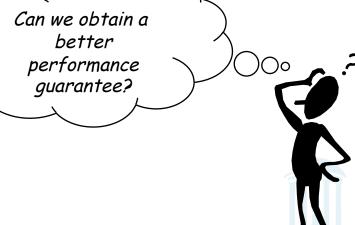
- ImprovedBreakPointReversalSort is an approximation algorithm with a performance guarantee of no worse than 4
 - It eliminates at least one breakpoint in every two steps; at most $2b(\pi)$ steps

- Optimal algorithm eliminates *at most 2 breakpoints* in every step: $d(\pi) \ge b(\pi) / 2$

Approximation ratio:

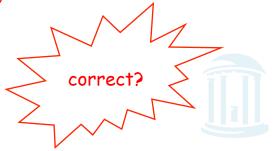
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$$\frac{2b(\pi)}{d(\pi)} \le \frac{2b(\pi)}{\frac{b(\pi)}{2}} = 4$$



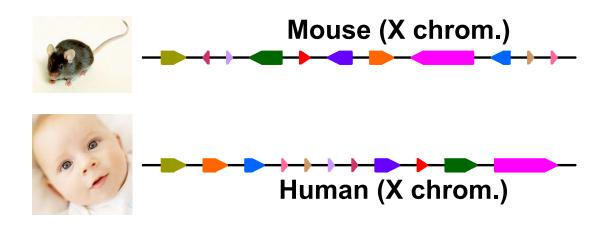
A Better Approximation Ratio

- If there is a decreasing strip, the next reversal reduces $b(\pi)$ by at least one.
- The only bad case is when there is no decreasing strip, as then we need a reversal that does not reduce $b(\pi)$.
 - If we could always choose a reversal reducing $b(\pi)$ and, at the same time, yielding a permutation that again has at least one decreasing strip, the bad case would never occur.
 - If all reversals that reduce $b(\pi)$ create a permutation without decreasing strips, then there exists a reversal that reduces $b(\pi)$ by two?!
 - When the algorithm creates a permutation without decreasing strip, the previous reversal must have reduced $b(\pi)$ by two.
- At most $b(\pi)$ reversals are needed.
- Approximation ratio: $\frac{b(\pi)}{d(\pi)} \le \frac{b(\pi)}{\frac{b(\pi)}{2}} = 2$



Both are Greedy Algorithms

- SimpleReversalSort
 - Attempts to maximize $prefix(\pi)$ at each step
- ImprovedBreakPointReversalSort
 - Attempts to reduce the number of breakpoints at each step
 - Performance guarantee: 2
- Performance guarantee: $\frac{n-1}{2}$





Try it yourself

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Next Time

• Dynamic Programming Algorithms





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