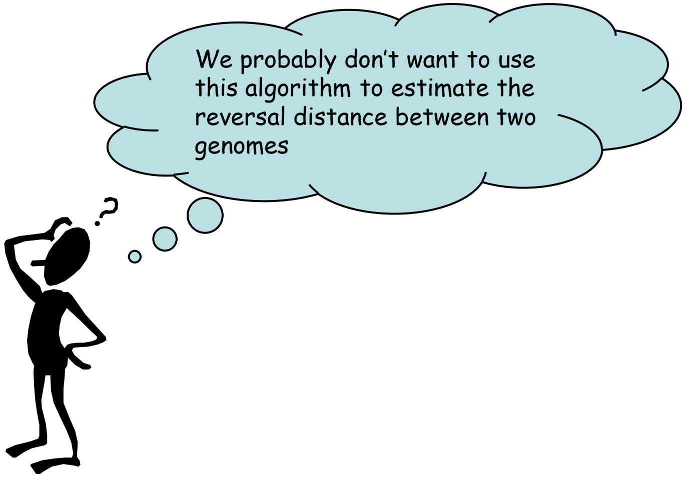
Genome Rearrangements

Study Chapters 5.3-5.5

Recap

- We developed a SimpleReversalSort algorithm that extends the sorted prefix on every iteration.
- On

π: $\underline{6\ 1}\ 2\ 3\ 4\ 5$
Flip 1: $1\ \underline{6\ 2}\ 3\ 4\ 5$
Flip 2: $1\ 2\ \underline{6\ 3}\ 4\ 5$
Flip 3: $1\ 2\ 3\ \underline{6\ 4}\ 5$
Flip 4: $1\ 2\ 3\ 4\ \underline{6\ 5}$
Flip 5: $1\ 2\ 3\ 4\ 5\ 6$



- But it could have been sorted in two flips:

π: $\underline{6\ 1\ 2\ 3\ 4\ 5}$
Flip 1: $\underline{5\ 4\ 3\ 2\ 1}\ 6$
Flip 2: $1\ 2\ 3\ 4\ 5\ 6$

Approximation Algorithms

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

$$\mathcal{A}(\pi) \,/\, \mathrm{OPT}(\pi)$$

where

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

Approximation Ratio/Performance Guarantee

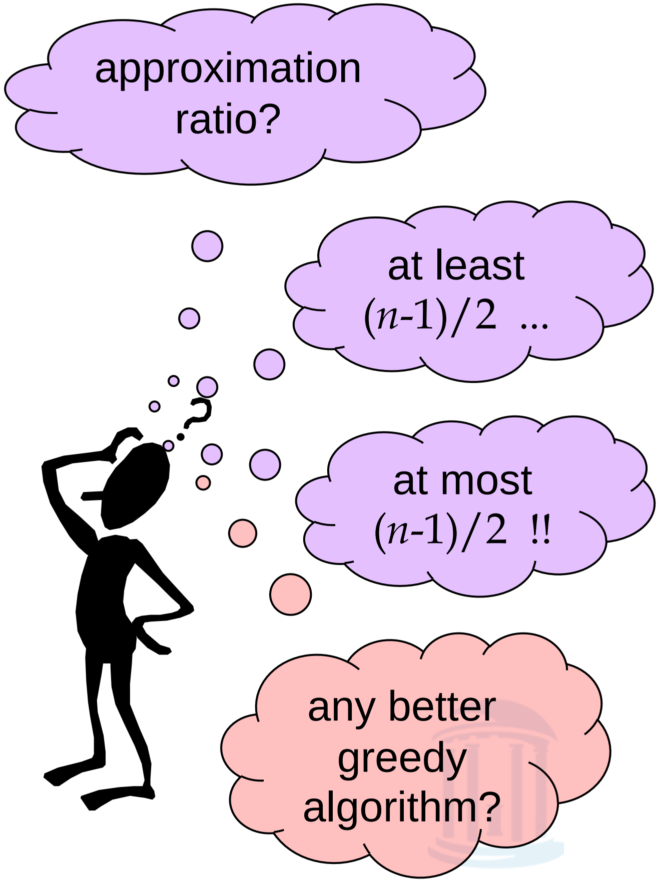
- Approximation ratio (performance guarantee) of algorithm $\mathcal{A}$: max approximation ratio over all inputs of size n
  - For a minimizing algorithm $\mathcal{A}$ (like ours):
    - Approx Ratio = $\max_{|\pi| = n} \mathcal{A}(\pi) / \mathrm{OPT}(\pi) \geq 1.0$
  - For maximization algorithms: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

Approximation Ratio

```
SimpleReversalSort($\pi$)
for $i \leftarrow 1$ to $n - 1$
    $j \leftarrow$ position of element $i$ in $\pi$ (i.e., $\pi_j = i$)
    if $j \neq i$
        $\pi \leftarrow \pi \ \rho(i, j)$
        output $\pi$
    if $\pi$ is the identity permutation
        return
```

Step 0: $\underline{6\ 1}$ 2 3 4 5
Step 1: 1 $\underline{6\ 2}$ 3 4 5
Step 2: 1 2 $\underline{6\ 3}$ 4 5
Step 3: 1 2 3 $\underline{6\ 4}$ 5
Step 4: 1 2 3 4 $\underline{6\ 5}$
Step 5: 1 2 3 4 5 6

Step 0: $\underline{6\ 1\ 2\ 3\ 4\ 5}$
Step 1: $\underline{5\ 4\ 3\ 2\ 1}$ 6
Step 2: 1 2 3 4 5 6



New Idea: Adjacencies

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

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

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

- For example:

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

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

Breakpoints

Breakpoints occur between neighboring non-adjacent elements:

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

- 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

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

$$\downarrow \text{ Extending with } \mathit{0} \text{ and } \mathit{10}$$

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

$$\uparrow$$

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(π):

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

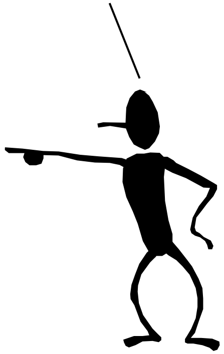
$$0\,|\,\underline{2\ \ 3\,|\,1}\,|\,4\,|\,6\ \ 5\,|\,7 \qquad b(\pi) = 5$$

$$0\ \ 1\,|\,\underline{3\ \ 2}\,|\,4\,|\,6\ \ 5\,|\,7 \qquad b(\pi) = 4$$

$$0\ \ 1\ \ 2\ \ 3\ \ 4\,|\,\underline{6\ \ 5}\,|\,7 \qquad b(\pi) = 2$$

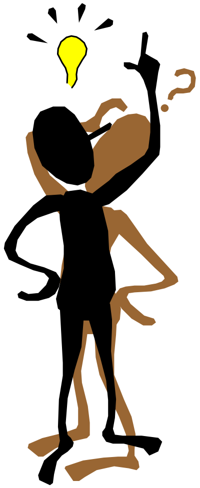
$$0\ \ 1\ \ 2\ \ 3\ \ 4\ \ 5\ \ 6\ \ 7 \qquad b(\pi) = 0$$

$$\textit{required reversals} \geq \frac{b(\pi)}{2}$$



Sorting By Reversals: A Better Greedy Algorithm

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



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

Does it always terminate?

How can we be sure that removing some breakpoints does not introduce others?

New Concept: *Strips*

- Strip: an interval between two consecutive breakpoints in a permutation
  - Decreasing strip: *strip* of elements in decreasing order (e.g. 6 5 and 3 2).
  - Increasing strip: *strip* of elements in increasing order (e.g. 7 8)

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)*

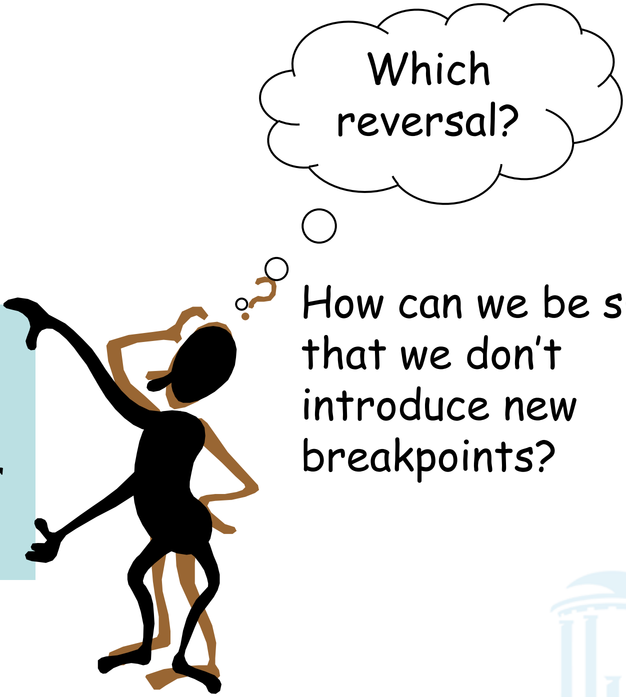
Reducing the Number of Breakpoints

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

$\underrightarrow{0\;\;1} \mid \underleftarrow{4} \mid \underleftarrow{6\;\;5} \mid \underrightarrow{7\;\;8} \mid \underleftarrow{3\;\;2} \mid \underrightarrow{9}$ $\qquad b(\pi) = 5$

Theorem:

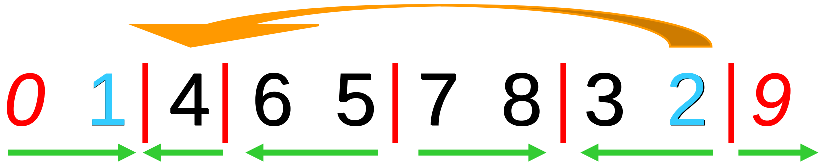
> If permutation π contains at least one decreasing strip, then there exists a reversal ρ which decreases the number of breakpoints (i.e. $b(\pi \bullet \rho) < b(\pi)$).



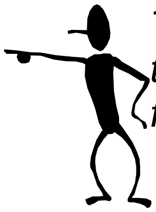
How can we be sure that we don't introduce new breakpoints?

Proof by Example

Consider π = 1 4 6 5 7 8 3 2



$b(\pi) = 5$



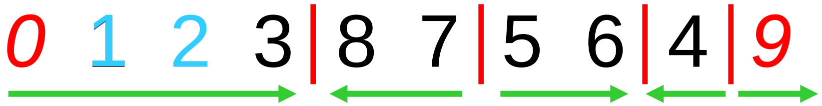
Thus, removing the breakpoint flanking k-1

- Choose the decreasing strip with the smallest element *k* in π
  - *k will be rightmost in the strip*
- Find *k – 1* in the permutation
  - *k-1 will be rightmost in an increasing strip*
- Reverse the segment following *k-1 up through k*
  - *making k-1 and k consecutive*

Continuing the Example

After the first reversal …

reduced by 1!



0 1 2 3 | 8 7 | 5 6 | 4 | 9

$b(\pi) = 4$

- Repeat until there is no decreasing strip

Continuing the Example

Second application of the theorem

0 1 2 3 | 8 7 | 5 6 | 4 | 9

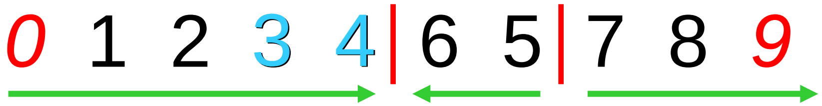
$b(\pi) = 4$

- Choose the decreasing strip with the smallest element *k* in π
  - *k will be rightmost in the strip*
- Find *k – 1* in the permutation
  - *k-1 will be rightmost in an increasing strip*
- Reverse the segment following *k-1 up through k*
  - *making k-1 and k consecutive*

Continuing the Example

After the reversal

reduced by 2!



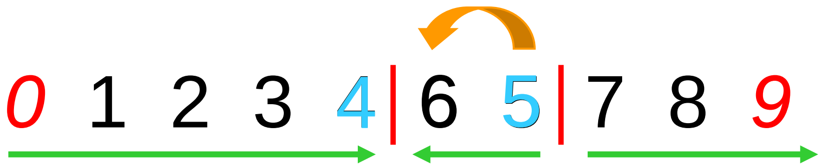
0 1 2 3 4 | 6 5 | 7 8 9

$b(\pi) = 2$

- Repeat until there is no decreasing strip

Continuing the Example

Third and final application of the theorem



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

- Choose the decreasing strip with the smallest element *k* in π
  - *k will be rightmost in the strip*
- Find *k – 1* in the permutation
  - *k-1 will be rightmost in an increasing strip*
- Reverse the segment following *k-1 up through k*
  - *making k-1 and k consecutive*

Continuing the Example

After the reversal

No breakpoint left!

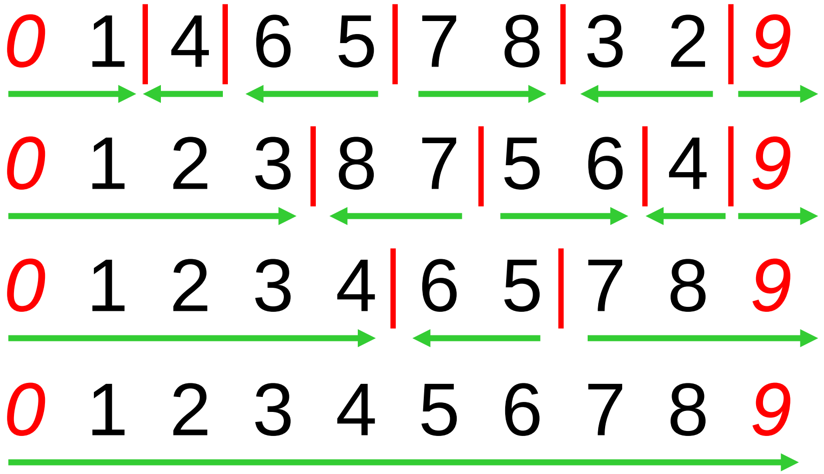
0 1 2 3 4 5 6 7 8 9

$b(\pi) = 0$

- Sequence is sorted

Things to Consider

Consider π = 1 4 6 5 7 8 3 2



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

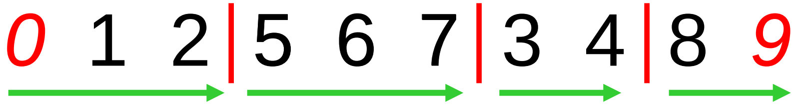
0 1 2 3 | 8 7 | 5 6 | 4 | 9 $b(\pi) = 4$

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

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

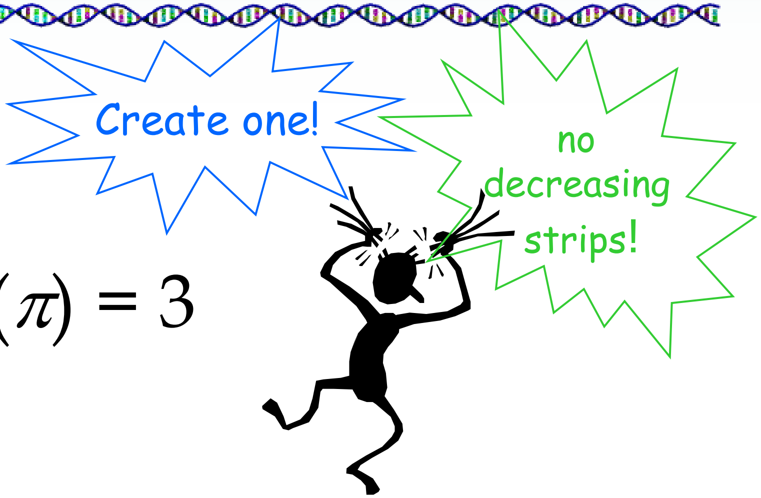
$d(\pi) = 3$

Potential Gotcha



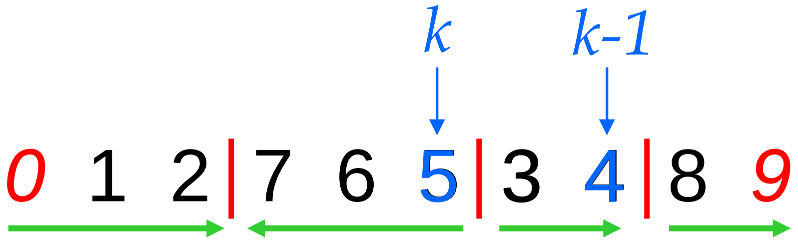
0 1 2 | 5 6 7 | 3 4 | 8 9

$b(\pi) = 3$



- If there is no decreasing strip, there may be no strip-reversal ρ that reduces the number of breakpoints (i.e. $b(\pi \bullet \rho) \geq b(\pi)$ for any reversal ρ).
- 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 step.

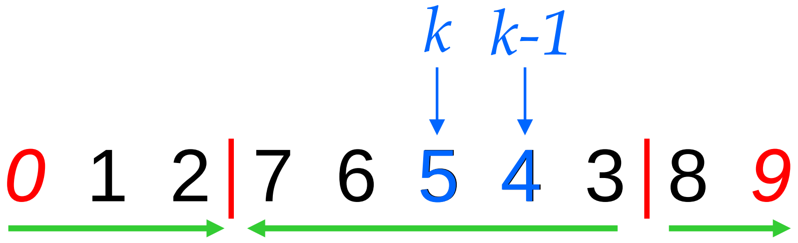
Potential Gotcha



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

- If there is no decreasing strip, there may be no strip-reversal ρ that reduces the number of breakpoints (i.e. $b(\pi \bullet \rho) \geq b(\pi)$ for any reversal ρ).
- 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.

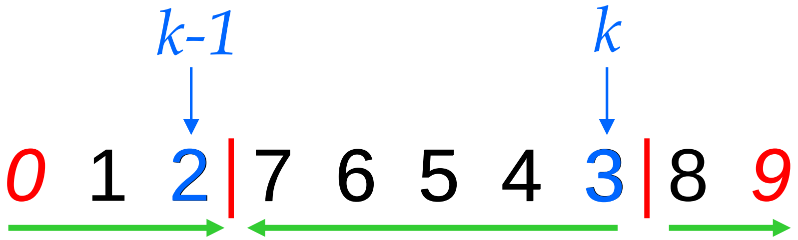
Potential Gotcha



$b(\pi) = 2$

- If there is no decreasing strip, there may be no strip-reversal ρ that reduces the number of breakpoints (i.e. $b(\pi \bullet \rho) \geq b(\pi)$ 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.

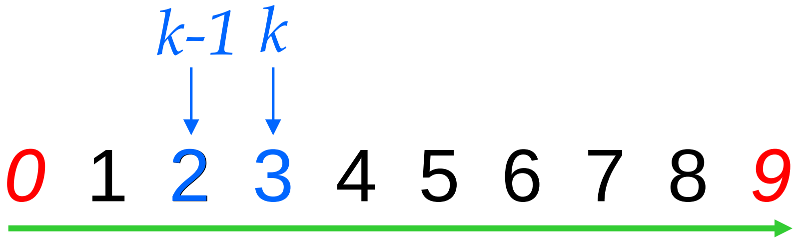
Potential Gotcha



$b(\pi) = 2$

- If there is no decreasing strip, there may be no strip-reversal ρ that reduces the number of breakpoints (i.e. $b(\pi \bullet \rho) \geq b(\pi)$ for any reversal ρ).
- 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.

Potential Gotcha



$b(\pi) = 0$

- If there is no decreasing strip, there may be no strip-reversal ρ that reduces the number of breakpoints (i.e. $b(\pi \bullet \rho) \geq b(\pi)$ for any reversal ρ).
- 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($\pi$)
while $b(\pi) > 0$
    if $\pi$ has a decreasing strip
        Among all possible reversals, choose reversal $\rho$
                        that minimizes $b(\pi \bullet \rho)$
    else
        Choose a reversal $\rho$ that flips an increasing strip in $\pi$
    $\pi \leftarrow \pi \bullet \rho$
    output $\pi$
return
```

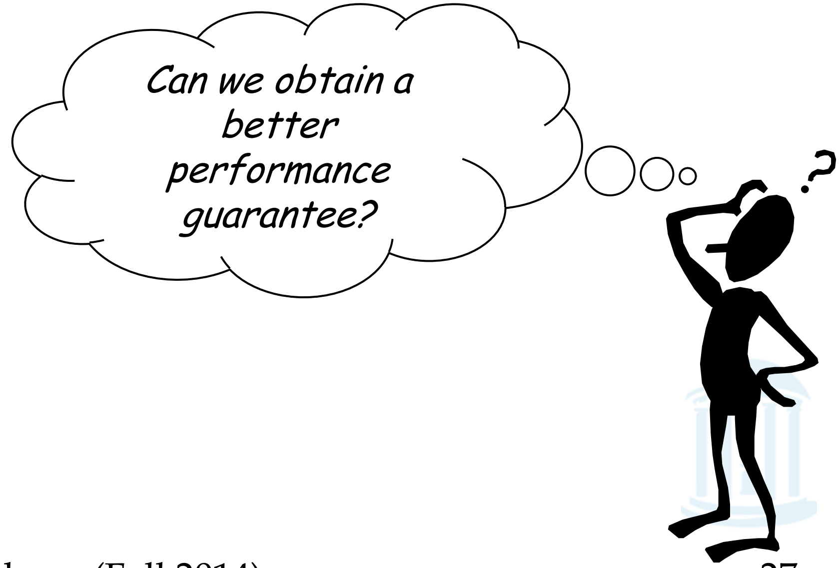
In Python

```
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
```

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: $d(\pi) \geq b(\pi) / 2$
  - Approximation ratio:

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

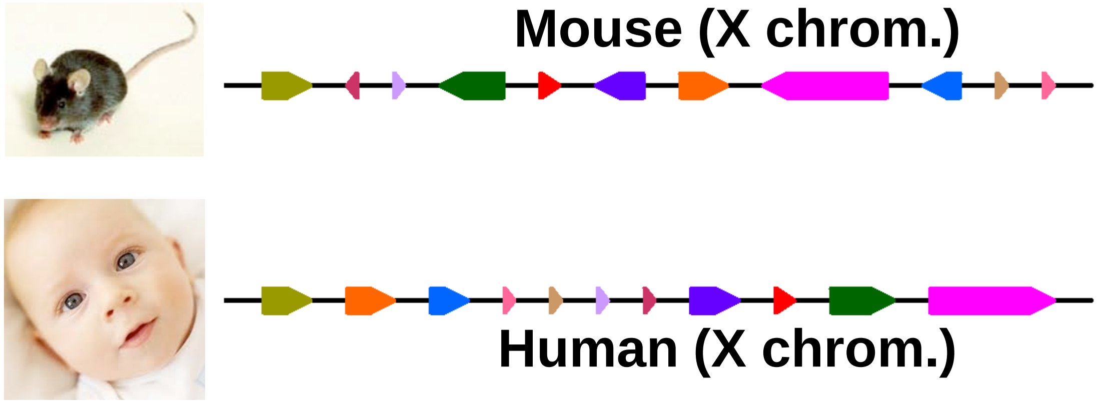


Both are Greedy Algorithms

- SimpleReversalSort
  - Attempts to maximize *prefix*(π) at each step
  - Performance guarantee:

$$\frac{n-1}{2}$$

- ImprovedBreakPointReversalSort
  - Attempts to reduce the number of breakpoints at each step
  - Performance guarantee: 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 a decreasing strip, the previous reversal must have reduced $b(\pi)$ by two.*
- At most $b(\pi)$ reversals are needed.
- Approximation ratio: $$\frac{b(\pi)}{d(\pi)} \le \frac{b(\pi)}{\frac{b(\pi)}{2}} = 2$$

correct?

Try it yourself

0 1 | 3 | 8 7 6 | 2 | 4 5 | 9 *10*

Next Time

- Dynamic Programming Algorithms