Exercise 10, Discrete Mathematics for Bioinformatics

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10.1 Critical Mixed Cycles

To be shown:

$$T \subseteq E \text{ trace} \iff \nexists \text{ critical mixed cycle in } G' = (V, T, H)$$

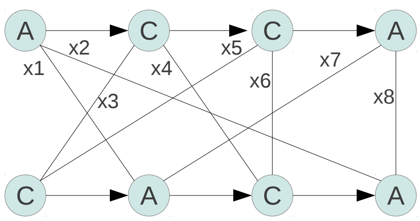
$\Rightarrow$: If T is a trace then it corresponds to an alignment. In this alignment, all edges in T connect vertices in the same column and all arcs in H connect adjacent vertices in the same row in ascending order. Hence, along an edge, the position index of the alignment stays always constant and along an arc the position index of the alignment always increases. The cycle can therefore never be closed.

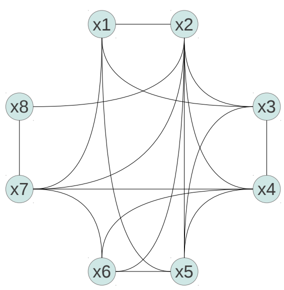
$\Leftarrow$: Let us assume that G' contains a mixed cycle Z which is not critical. Pick the smallest such cycle. By definition, there is one row a^p in the extended alignment graph for which $Z \cap a^p$ is non-consecutive. Call $a^p_{i_0}$ the element in this row with highest position. Now cycle through Z until you return to $Z \cap a^p$. If the return position is $a^p_{i_0}$ then (because there must be other $a^p_i \in Z \cap a^p$) we found a subcycle of Z which contradicts the choice of Z as the smallest subcycle. If the return position is $a^p_{i_1} \neq a^p_{i_0}$ then construct a cycle $Z' = [a^p_{i_0} \dots a^p_{i_1}] \cup [a^p_{i_1} \dots a^p_{i_0}]$ where the second component consists only of directed edges on a^p. Also Z' is smaller than Z, leading to a contradiction. Therefore any mixed cycle in G' must be critical. Inversely, no critical mixed cycle means no cycle at all.

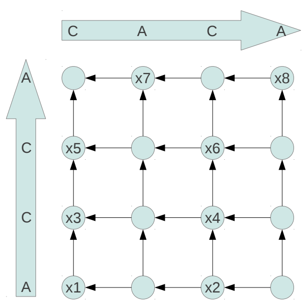
Let us assume this is the case and construct an alignment. We now consider the connected components $\{T_1, \dots, T_n\}$ of (V, T). Let us connect T_i and T_j if any two of their elements are connected in H. The resulting object is acyclic as it inherits the acyclicality from G'. Hence we can topologically order it and thus induce a strict partial order. This, according to the theorem by John Kececioglu, is equvalent to T realizing an alignment.$\square$

10.2 Branch and Cut

a) Here you see the alignment graph $G = (V, E, H)$ (with only the 1-weighted edges drawn), the conflict graph and the pair graph $PG(K_{p,q})$ for the two sequences P and Q.







b) We start solving the LP relaxation of the problem without mixed cycle constraints:

```
MAX x1 + x2 + x3 + x4 + x5  +x6 + x7 + x8

SUBJECT TO
A1:    - x1                                   <= 0
A2:         - x2                              <= 0
A3:              - x3                         <= 0
A4:                   - x4                    <= 0
A5:                        - x5               <= 0
A6:                             - x6          <= 0
A7:                                  - x7     <= 0
A8:                                       - x8 <= 0
B1:    + x1                                   <= 1
B2:         + x2                              <= 1
B3:              + x3                         <= 1
B4:                   + x4                    <= 1
B5:                        + x5               <= 1
B6:                             + x6          <= 1
B7:                                  + x7     <= 1
B8:                                       + x8 <= 1
```

a) optimal value 8, $(1,1,1,1,1,1,1,1)$
   heaviest source-to-sink path: $4 > 1$
   Adding inequality `x2 + x4 + x6 + x7 <= 1`

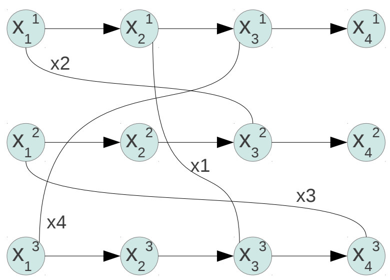
b) optimal value 5, $(1,0,1,0,1,0,1,1)$
   heaviest source-to-sink path: $3 > 1$
   Adding inequality `x1 + x2 + x3 + x5 <= 1`

c) optimal value 3, $(1,0,0,0,0,0,1,1)$
   heaviest source-to-sink path: $2 > 1$
   Adding inequality `x7 + x8 <= 1`

d) optimal value 3, $(1,0,0,0,0,1,0,1)$
   heaviest source-to-sink path: $1 \leq 1$
   integral solution $\Rightarrow$ done

10.3 Branch and Cut

a) Again we start solving the LP relaxation of the problem without mixed cycle constraints:




```
MAX x1 + x2 + x3 + x4

SUBJECT TO
A1:    - x1                 <= 0
```

```
A2:          - x2           <= 0
A3:               - x3      <= 0
A4:                    - x4 <= 0
B1:     + x1                <= 1
B2:          + x2           <= 1
B3:               + x3      <= 1
B4:                    + x4 <= 1
```

a) optimal value 4, $(1, 1, 1, 1)$
shortest path from any node x_i to x_{i-1}: (x_2^3, x_1^3) with length 0
Adding inequality `x1 + x4 <= 1`

b) optimal value 3, $(1, 1, 1, 0)$
shortest path from any node x_i to x_{i-1}: (x_4^3, x_3^3) with length 0
Adding inequality `x1 + x2 + x3 <= 2`

c) optimal value 3, $(0, 1, 1, 1)$
shortest path from any node x_i to x_{i-1}: (x_4^3, x_3^3) with length 0
Adding inequality `x2 + x3 + x4 <= 2`

d) optimal value 2.5, $(0.5, 1, 0.5, 0.5)$
shortest path from any node x_i to x_{i-1}: (x_3^3, x_2^3) with length 1
Could not find a solution!

b) **Branching**
It is not difficult to find a feasible solution with value 2, choosing x_2 and x_3 (*global lower bound*). The current *local upper bound* is 2.5.

First branch: $x1 = 0 \Rightarrow$ optimal value 2, solution $(0, 1, 0, 1) \Rightarrow$ done!

(need no further branch)

c) Adding the constraint `x1 + x2 + x3 + x4 <= 2` to the inequalities from part (a) directly leads to a solution with optimal value 2 and chosen edges x_1 and x_2

d) Proof: