Lecture 8

Wednesday, September 26, 2018 1:57 PM

$|A| = m$
$|B| = n$

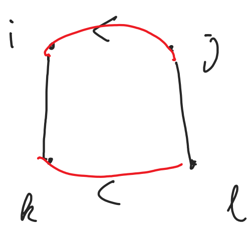
<u>Problem</u> Contact Map Overlap (CMO)

Given two contact maps $C^A = [c^A_{i,j}]$ and $C^B = [c^B_{k,l}]$, Find an alignment that maximizes the number of preserved contacts.

An alignment S is a subset of pairs of $[m] \times [n]$ such that for all distinct pairs $(i,k), (j,l) \in S$ it holds that:

1. $i \neq j$ [unique counterpart in B]
2. $k \neq l$ [unique counterpart in A]
3. $(i < j$ and $k < l)$ or $(j < i$ and $l < k)$ [non-crossing]

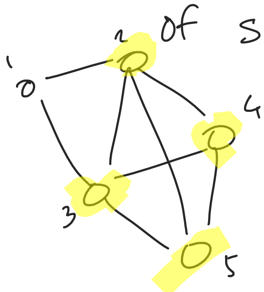
<u>preserved contact</u>



$(i,k) \in S$
$(j,l) \in S$

$c^A_{i,j} = 1$ and $c^B_{k,l} = 1$

<u>Clique</u> Given $G = (V, E)$ and $k \in \mathbb{N}$, is there a clique in G



of size k?

$k = 4$?

$$C^A = \begin{array}{c|ccccc} & 1 & 2 & 3 & 4 & 5 \\ \hline 1 & 0 & 1 & 1 & 0 & 0 \\ 2 & 1 & 0 & 1 & 1 & 1 \\ 3 & 1 & 1 & 0 & 1 & 1 \\ 4 & 0 & 1 & 1 & 0 & 1 \\ 5 & 0 & 1 & 1 & 1 & 0 \end{array}$$

NP-complete

$\hookrightarrow$ very unlikely to solve this problem in $O(\mathrm{poly}(n))$ where $n = |V|$

CLIQUE $\leq_p$ CMO

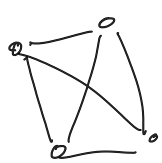
Given $G = (V, E)$ and $k \in \mathbb{N}$

Task: Define C^A and C^B

Idea: – represent G as C^A

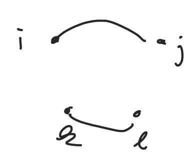
– C^B

K_k is the complete graph on k vertizes.



$K_4 \Longrightarrow C^B$

Integer Linear Programming



$$c_{i,k,j,l} = \begin{cases} 1, & \text{if } C^A_{i,j} = 1 \text{ and } C^B_{k,l} = 1 \\ 0, & \text{otherwise} \end{cases}$$

$i<j$, $k<l$

optimal alignment

$x_{i,k} = 1 \iff (i,k) \in S^{*}$

$x_{i,k} = 1 \quad x_{j,l} = 1$

$$\max \sum_{i=1}^{m} \sum_{k=1}^{n} \sum_{j=i+1}^{m} \sum_{l=k+1}^{n} c_{i,k,j,l} \cdot \cancel{x_{i,k} \cdot x_{j,l}} \; y_{i,k,j,l}$$

s.t.

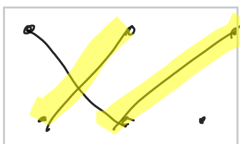
$$\sum_{(i,k) \in I} x_{i,k} \leq 1 \qquad \forall I \in \mathcal{I}$$

$$x_{i,k} \in \{0,1\} \qquad \forall i \in [m], k \in [n]$$

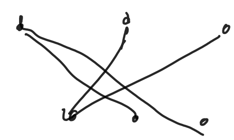
$$y_{ikjl} \leq x_{ik}$$

$$y_{ikjl} \leq x_{jl}$$

$I \in \mathcal{I}$ $\quad$ I is a pairwise incompatible set



this is not pairwise incompatible



maximal pairwise incompatible

$$y_{i,k,j,l} := x_{i,k} \cdot x_{j,l}$$

$y_{i,k,j,l}$	$x_{i,k}$	$x_{j,l}$
0	0	0
0	0	1
0	1	0
1	1	1

$$y_{ikjl} \leq x_{ik}$$

$$y_{ikjl} \leq x_{jl}$$

$$y_{ikjl} \geq x_{ik} + x_{jl} - 1$$