Prof. Dr. Alexander Bockmayr,
Prof. Dr. Knut Reinert,
Sandro Andreotti

January 7, 2011

Discrete Mathematics for Bioinformatics (P1)

WS 2010/11

Exercises 9

1. **Group Work Presentation**

   - Form groups of up to 3 students
   - Read the overview paper by Lancia (available in the lecture wiki) and choose a problem discussed there which is solved by branch-and-cut or Lagrangian relaxation. Prepare to explain a) the problem b) the ILP formulation c) the main point of the solution (e.g. A separation algorithm, or a class of inequalities dropped in Lagrangian relaxation).
   - In the lecture at January 18th each group has to present the problem in a 10 minutes presentation.

   We will organize the groups and selected topics on Monday. You should already communicate between groups since we do not want every group to present the same problem.

   Your presentation should be structured like (example: Sequence alignment):

   - Problem: You can formulate the multiple sequence alignment as a graph problem (show extended alignment graph), formulate trace problem as choosing the maximum weight graph without mixed cycles (demonstrate some examples) (total of 2-3 slides)
   - Translate this into an ILP. (Show ILP and explain inequalities (1-2 slides).
   - The authors solve it by branch-and-cut. The contribution is a polynomial time algorithm for clique inequality separation. (no detailed explanation) (1-2 slides)

2. **Critical Mixed Cycles (NIVEAU II)**
   Prove the following lemma (see lecture script):

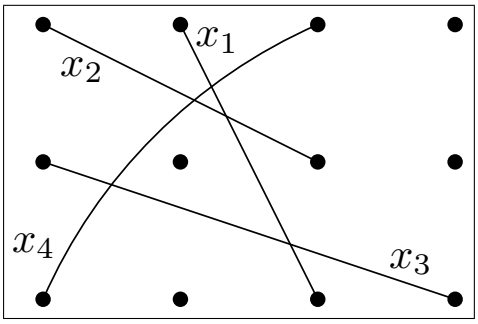
   A subset $T \subseteq E$ is a trace, if and only if $G' = (V, T, H)$ does not contain a critical mixed cycle.

3. **Branch and Cut (NIVEAU I)**
   Apply the cutting plane method to compute an optimal alignment of two sequences "'$ACCA$"' and "'$CACA$"' where a match scores 1 and a mismatch or gap scores 0:

   (a) Draw the alignment graph, the conflict graph, and the pair graph.

   (b) Now start with the trivial (relaxed) LP and add successively clique inequalities which you can find on the longest paths in the pair graph that is labeled with the solution of the last step. Repeat this until you get the optimal alignment.

4. **Branch and Cut (NIVEAU I)**
   Given the following alignment graph:



   All edges have weight 1.

   (a) Try to solve the alignment problem by using branch-and-cut: Add mixed cycle inequalities (see the 'shortest path' method in the script, page 18) to the corresponding (relaxed) LP. Can you reach an optimal solution for the ILP without branching?

   (b) Now use branching to solve the problem.

   (c) Instead of branching, just add the inequality

$$x_1 + x_2 + x_3 + x_4 \leq 2$$

   Can you solve the ILP now?

   (d) Prove that the inequality in (c) is facet-defining.