Bioinformatics I

WS 15/16

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Assignment 5

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Theoretical Assignment - Comparison with at most l mismatches

General we are now only looking at the worst case scenario, which means uniform distributed mistmatches in an alignment. Also we only look at k >= 1, as k = 0 is in our application not a useful result. Assume two sequences of length t with l mismatches.

Than both sequences contain l tuples of length $L = \lfloor \frac{t}{l+1} \rfloor$ and one tuple which has a length of maximal $\lfloor \frac{t}{l+1} \rfloor$.

So both sequences share l or l+1 k-tuples, if $k=\lfloor\frac{t}{l+1}\rfloor$, and for each $k\leq\lfloor\frac{t}{l+1}\rfloor$ they share $(l+1)*\lfloor\frac{L}{k}\rfloor$ k-tuples.

Theoretical Assignment - Linear programming by hand

The feasible region of this linear program is shown in figure 1, where the red line is constraint 1, green line is constraint 2, constraint 3 is drawn as a blue line and the yellow line is constraint 4.

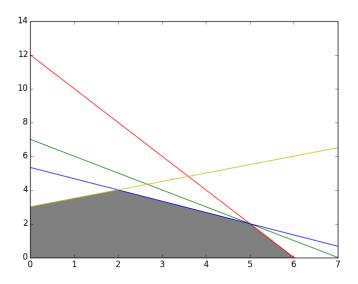


Figure 1: feasible region of linear program (grey area)

solution if t=s=1

Generally we only used integers in this task. The constraint for the algorithm are as following if t and s value is 1 now:

$$max.1 * x_1 + 1 * x_2 \tag{1}$$

$$s.t.2 * x_1 + x_2 \le 12 \tag{2}$$

$$2 * x_1 + 3 * x_2 \le 7 \tag{3}$$

$$-1 * x_1 + 2 * x_2 \le 16 \tag{4}$$

$$x_1, x_2 \ge 0 \tag{5}$$

the next step we started to compute each line of the tuple. Starting with constraint 3 under the aspect of constraint 5. All possible tuples respectively to both constraints from the assignment are:

$$temp1 = \{(0,7); (1,6); (2,5); (3,4); (4,3); (5,2); (6,1); (7,0)\}$$

the constraint 2 was applied to temp1:

$$temp2 = \{(0,7); (1,6); (2,5); (3,4); (4,3); (5,2); \}$$

the next constraint (constraint 4) was applied:

$$temp3 = \{(5,2)\}$$

but not least the last constraint (4) is checked and the remaining tuple from the last step is valid: $r = \{(5,2)\}$

the final result for the Algorithm with s=t=1 is the tuple: (5,2). Solving the formula with this numbers leads us to the following maximal value: $1 * x_1 + 1 * x_2 = 5 + 2 = 7$

How to make unsolvable?

To get a not solvable algorithm for example the following constraint could be added:

$$x_1 + x_2 \ge 7 \tag{6}$$

a new constraint just needs to be a contradiction to another constraint.

How to get infinite solutions with t and s?

The linear program has infinite solutions, if we assign the following values to s and t:

$$s = x_2$$

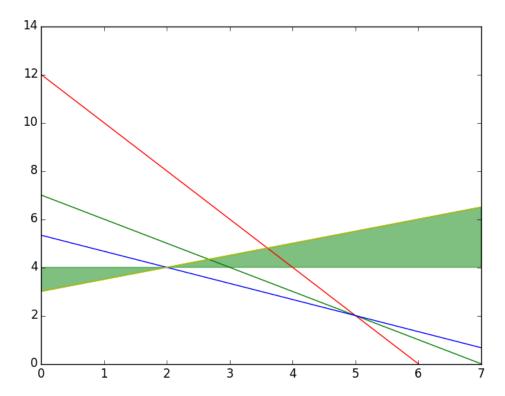
$$t = -x_1$$

These values would lead to the equation $x_2 * x_1 + (-x_1) * x_2$, which is always zero. So the maximal result is zero and you can fill in arbitrary numbers to get this result, i.e. infinite solutions.

how to make the points a optimal solution?

For the first point $P_1 = (0,3)$ we have to set s = -1 and t = 1. That result in a maximal value for (0,3) because we cannot set x_2 arbitrary big due to constraint 4. And if we assign a bigger value to x_1 , would decrease the result. Also we would violate constraint 2, if x_1 is to big.

$$P2 = (2,4)$$



To achive that P(2,4) is the only maximal value, we need to use the borders used in figure. The lower one is described by the maximal constraint (4) (equation 9)and the higher one is described by the horizontal line at $x^2 = 4$. Next we can define relations, for the variables m_2 and c_2 of the searched linear equation. These are shown in equation 12 and .

$$-1x_1 + 2x_2 = 6 (8)$$

$$\Leftrightarrow x_2 = \frac{1}{2}x_1 + 3\tag{9}$$

$$= x_2 = m_1 x_1 + c_1 \tag{10}$$

(11)

$$m_1 > m_2 > 0 \tag{12}$$

$$c_1 < c_2 < 4$$
 (13)

(14)

So any linear equation, which lies in the green area of figure , is a possible solution. We will now just choose one and define $c_2 = 3.5 = \frac{7}{2}$ according to relation . From this now we can deduce $m_2 = \frac{1}{4}$ as shown in Equation 16 so that P(2,4) is the only intersection with the feasible region.

$$4 = m_2 * 2 + 3.5 \tag{15}$$

$$m_2 = \frac{4 - 3.5}{2} = \frac{1}{4} \tag{16}$$

(17)

The last step is now to get s and t, this is achieved by forming the found linear equation back to the desired form (Equation 20). The complete result is for $s = \frac{-1}{14}$ and for $t = \frac{2}{7}$.

$$x_2 = \frac{1}{4} * x_1 + \frac{7}{2} \tag{18}$$

$$\Leftrightarrow -\frac{1}{4}x_1 + x_2 = \frac{7}{2} \tag{19}$$

$$\Leftrightarrow -\frac{1}{14}x_1 + \frac{2}{7}x_2 = 1 \tag{20}$$

$$\Rightarrow s = -\frac{1}{14}; t = \frac{2}{7} \tag{21}$$

(22)

P3 = (1,3)

To make $P_4 = (6,0)$ the maximum we set s = 1 and t = -1. We cannot set x_1 to a bigger value than 6 without violating constraint 1.

Theoretical Assignment - Bonus: Carillo-Lipman bound

The Carrillo-Lipman bound is defined by $B_{pq} := B(A) - (\sum_{i < j} s(\hat{A}_i, \hat{A}_j) - s(\hat{A}_p, \hat{A}_q))$, where B(A) is a score for the alignment computed by a heuristic and $s(\hat{A}_i, \hat{A}_j)$ is the score of a optimal alignment of sequences i and j. If we have just two sequences p and q, this equation would be simplified as

$$B_{pq} = B(A) - (s(\hat{A}_p, \hat{A}_q) - s(\hat{A}_p, \hat{A}_q)) = B(A).$$

So the Carrillo-Lipman bound for two sequences is just the computed score by a heuristic.