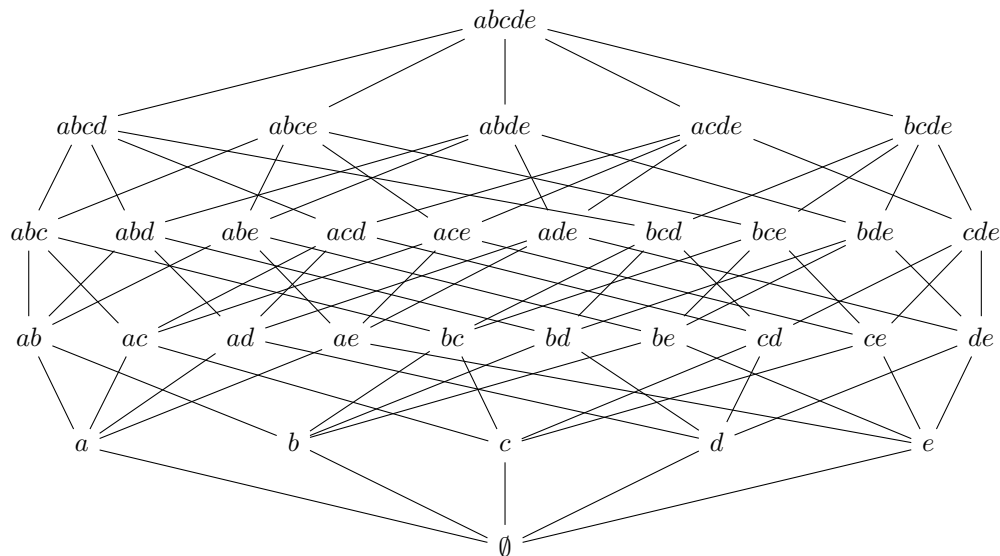


Read: Chapter 6 of *Algebraic and Combinatorial Computational Biology* (Robeva & Macauley, 2018). Inferring interactions in molecular networks via primary decompositions of monomial ideals. By M. Macauley and B. Stigler, pages 175–210.

Chapter 3 of *Mathematical Concepts and Methods in Modern Biology* (Robeva & Hodge, 2013). Inferring the topology of gene regulatory networks: an algebraic approach to reverse engineering. By B. Stigler and E. Dimitrova, pages 75–90.

Exercises.

1. Consider the simplicial complex $\Delta = \{\emptyset, a, b, c, d, e, ab, ac, ad, bc, cd, ce, abc\}$ over the set $X = \{a, b, c, d, e\}$. The 5-dimensional Boolean lattice 2^X is shown below.
 - (i) Sketch the simplicial complex and find the maximal faces.
 - (ii) Draw a dashed or colored line that “cuts” the Boolean lattice into two halves – below the line are the faces and above are the non-faces.
 - (iii) Circle each node in the Boolean lattice 2^X corresponding to a maximal face of Δ .
 - (iv) Box each node that corresponds to a minimal non-face.
 - (v) Find the Stanley-Reisner ideal I_{Δ^c} and compute its primary decomposition.



2. Consider a Boolean network $f = (f_1, f_2, f_3)$ whose (synchronous) phase spaces consists of the following:

$$(0, 0, 1) \xrightarrow{f} (1, 0, 1) \xrightarrow{f} (1, 1, 1) \xrightarrow{f} (1, 1, 0) \xrightarrow{f} (0, 1, 0) \xrightarrow{f} (0, 0, 0).$$

In this problem, you will reverse-engineer the wiring diagram.

- (a) Do the following steps for each $k = 1, 2, 3$.

- i. Write down the corresponding set of *data*

$$\mathcal{D}_k := \{(\mathbf{s}_1, t_{1k}), \dots, (\mathbf{s}_5, t_{5k})\}$$

that arises from the k^{th} coordinate of this time-series.

- ii. Compute the monomials $m(\mathbf{s}_i, \mathbf{s}_j)$ for which $t_{ik} \neq t_{jk}$, and find the ideal $I_{\Delta_k^c}$ of non-disposable sets.
- iii. Find the primary decomposition of $I_{\Delta_k^c}$.
- iv. Find all min-sets of \mathcal{D}_k , and sketch a wiring diagram for each. Only include edges incident to x_k .
- (b) Repeat Steps (ii)–(iv) from Part (a) but to find the signed min-sets. That is, use the pseudomonomials $p(\mathbf{s}_i, \mathbf{s}_j)$ to compute the ideal $J_{\Delta_k^c}$ of signed non-disposable sets.

3. Consider the following *time series* of a 3-node algebra model over \mathbb{F}_3 :

$$(1, 1, 1) \xrightarrow{f} (2, 0, 1) \xrightarrow{f} (2, 0, 0) \xrightarrow{f} (0, 2, 2) \xrightarrow{f} (0, 2, 2).$$

For reference, here are the input vectors \mathbf{s}_i and output vectors \mathbf{t}_i :

$$\begin{aligned} \mathbf{s}_1 &= (s_{11}, s_{12}, s_{13}) = (1, 1, 1), & \mathbf{t}_1 &= (t_{11}, t_{12}, t_{13}) = (2, 0, 1), \\ \mathbf{s}_2 &= (s_{21}, s_{22}, s_{23}) = (2, 0, 1), & \mathbf{t}_2 &= (t_{21}, t_{22}, t_{23}) = (2, 0, 0), \\ \mathbf{s}_3 &= (s_{31}, s_{32}, s_{33}) = (2, 0, 0), & \mathbf{t}_3 &= (t_{31}, t_{32}, t_{33}) = (0, 2, 2), \\ \mathbf{s}_4 &= (s_{41}, s_{42}, s_{43}) = (0, 2, 2), & \mathbf{t}_4 &= (t_{41}, t_{42}, t_{43}) = (0, 2, 2). \end{aligned}$$

- (a) Find polynomials f_1, f_2, f_3 in $\mathbb{F}_3[x_1, x_2, x_3]/\langle x_1^3 - x_1, x_2^3 - x_2, x_3^3 - x_3 \rangle$ that fit the data. That is, $f_j(\mathbf{s}_i) = t_{ij}$ for all $i = 1, 2, 3, 4$.
- (b) For each $i = 1, 2, 3, 4$, write down the ideal $I_i = I(\mathbf{s}_i)$ of polynomials that vanish on the data point \mathbf{s}_i .
- (c) Compute a Gröbner basis for the ideal I of polynomials that vanish on *all* of the input data points. You may use Sage, Singular, or Macaulay2, but use the graded reverse lexicographical monomial order **GRevLex** (this is the default).
- (d) Write the *model space* of the time series using your answer to Part (a) as the particular solution.
- (e) Compute the *normal form* of f_1, f_2, f_3 with respect to \mathcal{G} by reducing them modulo the ideal I . Write the model space using this particular solution.
- (f) Repeat Parts (c)–(e) using lex (**Lex**), and then graded lex (**GLex**).
- (g) How big is the model space? How big is the vanishing ideal?