Reverse engineering using computational algebra

Matthew Macauley

Department of Mathematical Sciences
Clemson University
http://www.math.clemson.edu/~macaule/

Algebraic Biology

What is reverse engineering?

Sometimes, complex biological systems can seem a bit like this: (click here!).

Systems biology is the study of systems of biological components.

A central problem in systems biology is to use experimental data to infer the structure of a system such as a gene regulatory network.

Modeling approaches

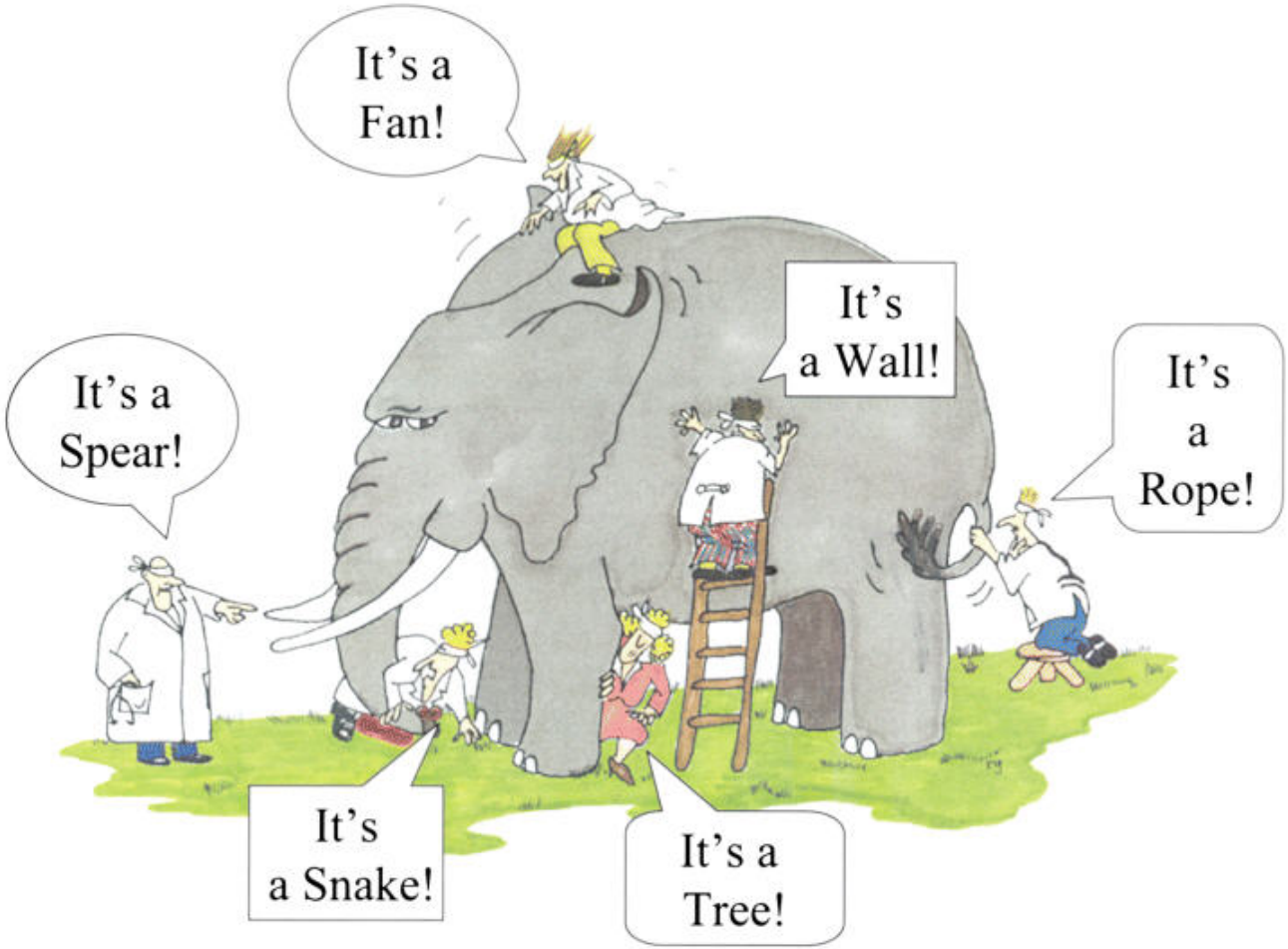
- **Bottom-up**: Build a network from the known local information about every single object.
- **Top-down** ("Reverse-engineering"): View the system as a black box, then use the available data to make a model.

Previously, we've mostly studied the first approach to modeling. In this lecture, we'll focus on the second approach.

Many problems in statistics (e.g., linear regression) deal with the second approach.

The blind men and the elephant

An old parable from India tells of several blind men who try to determine what an elephant looks like just by touch.

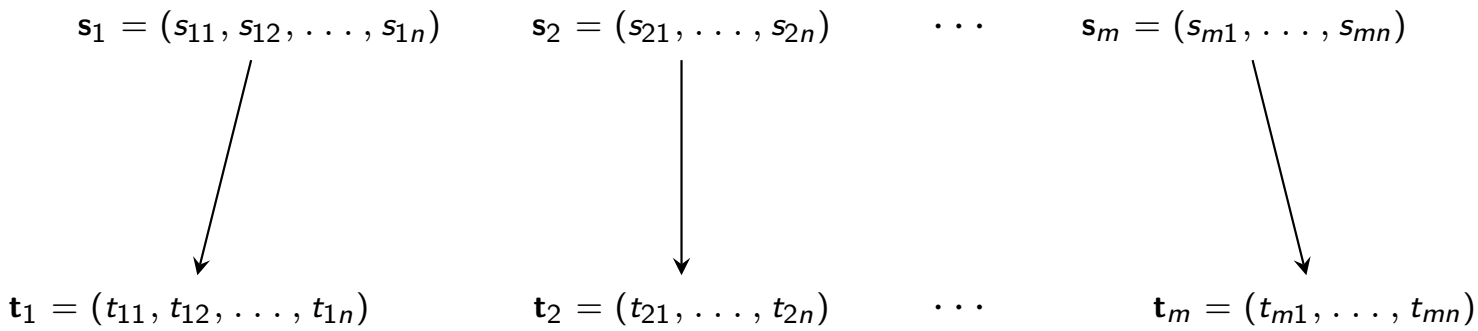


The blind men are trying to reverse engineer an elephant from just a few data points.

Inferring a Boolean model (elephant) from data (observations)

Consider a Boolean network on n nodes, with update function $f : \mathbb{F}_2^n \to \mathbb{F}_2^n$. There are 2^n input states.

Suppose we don't know the actual function f, but through experimental data, we are able to observe several transitions:



Reverse engineering

Start with experimental data (observations) and reconstruct the model (elephant). The two main features are:

(i) the network topology, or wiring diagram,

(ii) the Boolean functions at each node: $f = (f_1, \ldots, f_n)$.

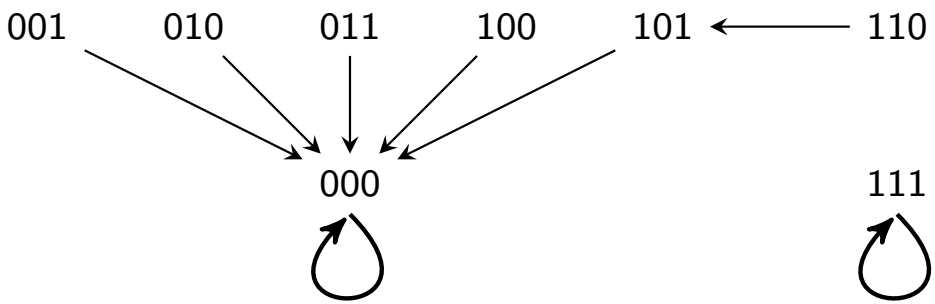
This problem is not just limited to models over $\mathbb{F}_2 = \{0, 1\}$; it works for models over larger finite fields $\mathbb{F}$. We will call such models local models.

Inferring a Boolean network (elephant) from data (observations)

Consider the following Boolean network:

$$f_1(x_1, x_2, x_3) = x_1 \wedge x_2 = x_1 x_2$$
$$f_2(x_1, x_2, x_3) = x_1 \wedge x_2 \wedge x_3 = x_1 x_2 x_3$$
$$f_3(x_1, x_2, x_3) = x_1 \wedge x_2 = x_1 x_2 \,.$$

The state space of $f = (f_1, f_2, f_3)$ is the following graph:



Question

What if we only knew part of this state space, e.g.,

$$(1,1,0) \longrightarrow (1,0,1) \longrightarrow (0,0,0) \longrightarrow (0,0,0)\,.$$

Could we recover the individual functions? How many possible models could yield this "fragment"?

Reverse engineering the model space

Broad goal

Find "the best" local model $f = (f_1, \ldots, f_n)$ that fits the data:

Input states: $\mathbf{s}_1, \ldots, \mathbf{s}_m \in \mathbb{F}^n$

Output states: $\mathbf{t}_1, \ldots, \mathbf{t}_m \in \mathbb{F}^n$

with $f(\mathbf{s}_i) = \mathbf{t}_i$

Note that: $f(\mathbf{s}_i) = (f_1(\mathbf{s}_i), f_2(\mathbf{s}_i), \ldots, f_n(\mathbf{s}_i)) = (t_{i1}, t_{i2}, \ldots, t_{in}) = \mathbf{t}_i$.

Question

What if no models fit the data? (This is actually impossible.)

What if many models fit the data?

First, we'll find all local models that fit the data. This is called the model space:

$$F_1 \times \cdots \times F_n = \left\{ (f_1, \ldots, f_n) \mid f_j(\mathbf{s}_i) = t_{ij} \text{ for all } i \text{ and } j \right\}.$$

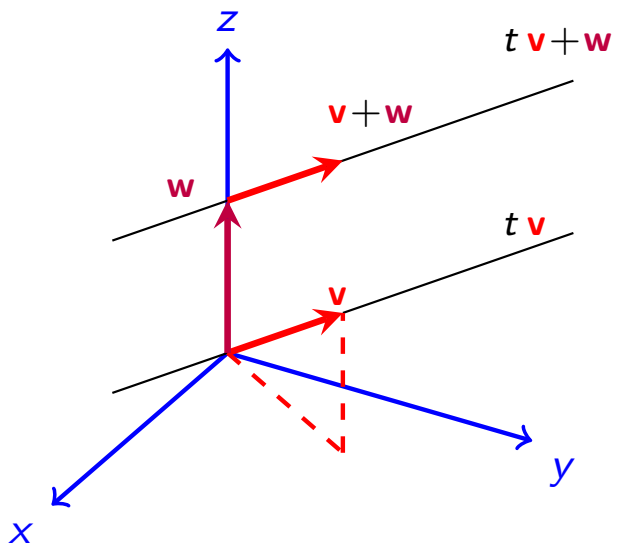
Once we do this, the new problem becomes choosing the "best" one. This is called model selection.

Similar problems in other areas of mathematics

1. Parametrize a line in $\mathbb{R}^n$.
2. Parametrize a plane in $\mathbb{R}^n$.
3. Solve the underdetermined system $\mathbf{Ax} = \mathbf{b}$.
4. Solve the differential equation $x'' + x = 2$.

Parametrize a line in $\mathbb{R}^n$

Suppose we want to write the equation for a line that contains a vector $\mathbf{v} \in \mathbb{R}^n$:



This line, which *contains the zero vector*, is $t\mathbf{v} = \{t\mathbf{v} : t \in \mathbb{R}\}$.

Now, what if we want to write the equation for a line parallel to $\mathbf{v}$?

This line, which *does not contain the zero vector*, is

$$t\mathbf{v} + \mathbf{w} = \{t\mathbf{v} + \mathbf{w} : t \in \mathbb{R}\}.$$

Note that ANY particular $\mathbf{w}$ on the line will work!!!

Solve an underdetermined system $\mathbf{Ax} = \mathbf{b}$

Suppose we have a system of equations that has "too many variables," so there are infinitely many solutions.

For example:

$$\begin{aligned} 2x + y + 3z &= 4 \\ 3x - 5y - 2z &= 6 \end{aligned} \qquad \text{"}\mathbf{Ax} = \mathbf{b} \text{ form"}: \qquad \begin{bmatrix} 2 & 1 & 3 \\ 3 & -5 & -2 \end{bmatrix} \begin{bmatrix} x \\ y \\ z \end{bmatrix} = \begin{bmatrix} 4 \\ 6 \end{bmatrix}.$$

How to solve:

1. Solve the related homogeneous equation $\mathbf{Ax} = \mathbf{0}$ (this is null space, $\mathrm{NS}(A)$);
2. Find any particular solution $\mathbf{x}_p$ to $\mathbf{Ax} = \mathbf{b}$;
3. Add these together to get the general solution: $\mathbf{x} = \mathrm{NS}(A) + \mathbf{x}_p$.

This works because geometrically, the solution space is just a line, plane, etc.

Here are two possible ways to write the solution:

$$C \begin{bmatrix} 1 \\ 1 \\ -1 \end{bmatrix} + \begin{bmatrix} 2 \\ 0 \\ 0 \end{bmatrix}, \qquad C \begin{bmatrix} 1 \\ 1 \\ -1 \end{bmatrix} + \begin{bmatrix} 10 \\ 8 \\ -8 \end{bmatrix}.$$

Linear differential equations

Solve the differential equation $x'' + x = 2$.

How to solve:

1. Solve the related homogeneous equation $x'' + x = 0$. The solutions are $x_h(t) = a\cos t + b\sin t$.
2. Find any particular solution $x_p(t)$ to $x'' + x = 2$. By inspection, we see that $x_p(t) = 2$ works.
3. Add these together to get the general solution:

$$x(t) = x_h(t) + x_p(t) = a\cos t + b\sin t + 2.$$

Note that while the general solution above is unique, its presentation need not be.

For example, we could write it this way:

$$x(t) = x_h(t) + x_p(t) = a(2\cos t - 3\sin t) + b\sin t + (2 - \cos t + 8\sin t).$$

Here, the particular solution has (unnecessary) "extra terms" that vanish on the homogeneous part, $x'' + x = 0$.

Reverse engineering: Problem statement

Recall that a local model over $\mathbb{F}$ is an n-tuple $f = (f_1, \ldots, f_n)$ of functions $f_i : \mathbb{F}^n \to \mathbb{F}$.

The associated finite dynamical system (FDS) map is

$$f : \mathbb{F}^n \longrightarrow \mathbb{F}^n, \qquad f : \mathbf{x} \longmapsto (f_1(\mathbf{x}), \ldots, f_n(\mathbf{x})).$$

If $\mathbb{F} = \mathbb{F}_p$ then each $f_i : \mathbb{F}_p^n \to \mathbb{F}_p$ is a polynomial in $\mathbb{F}_p[x_1, \ldots, x_n]/\langle x_1^p - x_1, \ldots, x_n^p - x_n \rangle$.

Goal

Given a set of data:

$$\begin{array}{l} \text{Input states: } \mathbf{s}_1, \ldots, \mathbf{s}_m \in \mathbb{F}^n \\ \text{Output states: } \mathbf{t}_1, \ldots, \mathbf{t}_m \in \mathbb{F}^n \end{array} \qquad \text{with } f(\mathbf{s}_i) = \mathbf{t}_i$$

Construct the model space $F_1 \times \cdots \times F_n$ of all local models $f = (f_1, \ldots, f_n)$ that fit the data:

$$f(\mathbf{s}_i) = (f_1(\mathbf{s}_i), \ldots, f_n(\mathbf{s}_i)) = (t_{i1}, \ldots, t_{in}) = \mathbf{t}_i.$$

We'll find each $F_1, \ldots, F_n$ separately.

Reverse engineering: How to find F_j

We wish to find the set F_j of all local functions (polynomials!) f_j that fit the data:

$$F_j = \{f_j : f_j(\mathbf{s}_1) = t_{1j},\ \ldots\ , f_j(\mathbf{s}_m) = t_{mj}\}\,.$$

Define the set I (it is actually an "ideal" of the polynomial ring $\mathbb{F}[x_1, \ldots, x_n]$)

$$\begin{aligned} I &= \{h : h(\mathbf{s}_i) = 0 \text{ for all } i = 1, \ldots, m\} \\ &= \{\text{all polynomials that vanish on the data}\}. \end{aligned}$$

Theorem

The set of polynomials that fit the data at node j is

$$F_j = f_j + I = \{f_j + h : h \in I\}\,,$$

where f_j is any one particular polynomial that fits the data.

Thus, to find F_j, we need to do two things:

1. Find the ideal I; (*all* solutions to $\{f_j(\mathbf{s}_i) = 0,\ \forall i\}$)
2. Find *any* polynomial f_j that fits the data. (*one* solution to $\{f_j(\mathbf{s}_i) = t_{ij},\ \forall i\}$)

Reverse engineering: How to find I and f_j

1. *Finding I*: Define $I(\mathbf{s}_i)$ to be the set of polynomials that vanish on $\mathbf{s}_i$:

$$\begin{aligned} I(\mathbf{s}_i) &= \{\text{all polynomials } h_i \text{ such that } h_i(\mathbf{s}_i) = 0\} \\ &= \{(x_1 - s_{i1})g_1(\mathbf{x}) + (x_2 - s_{i2})g_2(\mathbf{x}) + \cdots + (x_n - s_{in})g_n(\mathbf{x})\} \\ &= \langle x_1 - s_{i1}, x_2 - s_{i2}, \ldots, x_n - s_{in} \rangle \end{aligned}$$

   Clearly, the set I of polynomials that vanish on all $\mathbf{s}_i$ (for $i = 1, \ldots, m$) is

$$I = \bigcap_{i=1}^{m} I(\mathbf{s}_i)\,.$$

2. *Finding f_j*: There are many algorithms. Lagrange interpolation is one of them.

   In this lecture, we will learn another method which has the Chinese remainder theorem lurking behind the scenes.

   We'll get started with this now.

Finding f_j (one method)

For each data point $\mathbf{s}_i$ $(i = 1, \ldots, m)$, we'll construct an *r*-polynomial that has the following property:

$$r_i(\mathbf{x}) = \begin{cases} 1 & \mathbf{x} = \mathbf{s}_i \\ 0 & \mathbf{x} \neq \mathbf{s}_i \end{cases}$$

Once we have these, the polynomial $f_j(\mathbf{x})$ we seek will be

$$f_j(\mathbf{x}) = t_{1j} r_1(\mathbf{x}) + t_{2j} r_2(\mathbf{x}) + \cdots + t_{mj} r_m(\mathbf{x}) \,.$$

One way to construct the *r*-polynomials:

$$r_i(\mathbf{x}) = \prod_{\substack{k=1 \\ k \neq i}}^{m} b_{ik}(\mathbf{x}) \,,$$

where

$$b_{ik}(\mathbf{x}) = (s_{i\ell} - s_{k\ell})^{p-2}(x_\ell - s_{k\ell})$$

and ℓ is any coordinate in which $\mathbf{s}_i$ and $\mathbf{s}_k$ differ. (We'll take the *first* coordinate for simplicity.)

Remark

When our systems are Boolean (over $\mathbb{F}_2$), then this reduces to $b_{ik}(\mathbf{x}) = x_\ell - s_{k\ell}$.

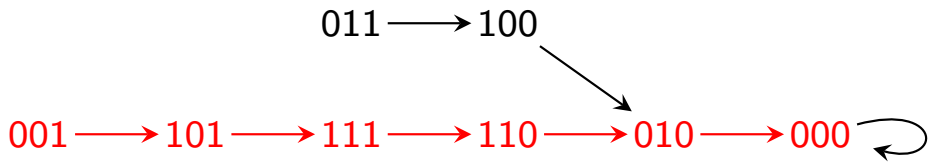
A Boolean example

Consider the following model of the *lac* operon, which implicitly assumes that A degrades slower than M or B.

$$\begin{cases} f_M = x_A \\ f_B = x_M \\ f_A = L \vee (B \wedge L_m) \vee (A \wedge \overline{B}). \end{cases}$$

If lactose levels are low, then $L = L_m = 0$, and this model reduces to the one at left (left) with state space (right):

$$\begin{cases} f_1 = x_3 \\ f_2 = x_1 \\ f_3 = (x_2 + 1)x_3. \end{cases}$$



Exercise

Let's reverse engineer the Boolean network from just knowing the 6 red nodes and 5 transitions.

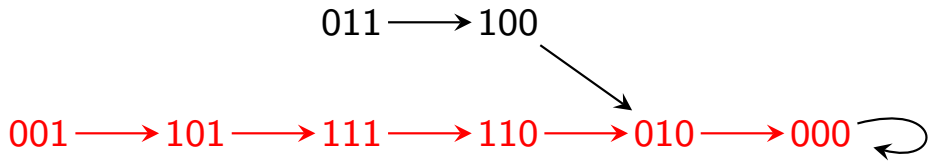
In other words, find all triples of polynomials $f = (h_1, h_2, h_3)$ such that:

- $f(0,0,1) = (h_1(0,0,1),\ h_2(0,0,1),\ h_3(0,0,1)) = (1,0,1)$,
- $f(1,0,1) = (h_1(1,0,1),\ h_2(1,0,1),\ h_3(1,0,1)) = (1,1,1)$,
- $f(1,1,1) = (h_1(1,1,1),\ h_2(1,1,1),\ h_3(1,1,1)) = (1,1,0)$,
- $f(1,1,0) = (h_1(1,1,0),\ h_2(1,1,0),\ h_3(1,1,0)) = (0,1,0)$,
- $f(0,1,0) = (h_1(0,1,0),\ h_2(0,1,0),\ h_3(0,1,0)) = (0,0,0)$,

A Boolean example (cont.)

Since we know the original functions *a priori*, we secretly know the answer to this.

$$(f_1, f_2, f_3) = (x_3,\ x_1,\ (x_2+1)x_3).$$



The ideal of polynomials that vanish on each $\mathbf{s}_k$ is:

```
I1 = ideal(x1, x2, x3-1);
I2 = ideal(x1-1, x2, x3-1);
I3 = ideal(x1-1, x2-1, x3-1);
I4 = ideal(x1-1, x2-1, x3);
I5 = ideal(x1, x2-1, x3);
```

The ideal of polynomials that vanish on *every* $\mathbf{s}_k$ is:

```
I = intersect{I1,I2,I3,I4,I5};
```

Thus, the complete model space is

$$F_1 \times F_2 \times F_3, \qquad F_j = f_j + I\,.$$

If we hadn't known f_1, f_2, f_3 *a priori*, then we'd have to find our own particular solution that fits the data. We'll do that now.

A Boolean example (cont.)

We're looking for a single solution $f = (f_1, f_2, f_3)$ that fits the data.

We know how to do this. For example:

$$\begin{aligned} f_1(\mathbf{x}) &= t_{11} r_1(\mathbf{x}) + t_{21} r_2(\mathbf{x}) + t_{31} r_3(\mathbf{x}) + t_{41} r_4(\mathbf{x}) + t_{51} r_5(\mathbf{x}) \\ &= 1 r_1(\mathbf{x}) + 1 r_2(\mathbf{x}) + 1 r_3(\mathbf{x}) + 0 r_4(\mathbf{x}) + 0 r_5(\mathbf{x}) = r_1(\mathbf{x}) + r_2(\mathbf{x}) + r_3(\mathbf{x}) \,, \end{aligned}$$

where

$$r_1(\mathbf{x}) = \prod_{\substack{k=1 \\ k \neq 1}}^{5} b_{1k}(\mathbf{x}) = b_{12}(\mathbf{x}) b_{13}(\mathbf{x}) b_{14}(\mathbf{x}) b_{15}(\mathbf{x}) \,.$$

$\mathbf{s}_1 = (0, 0, 1)$

$\downarrow$

$\mathbf{s}_2 = (\underline{1}, 0, 1) = \mathbf{t}_1$

$\downarrow$

$\mathbf{s}_3 = (\underline{1}, 1, 1) = \mathbf{t}_2$

$\downarrow$

$\mathbf{s}_4 = (\underline{1}, 1, 0) = \mathbf{t}_3$

$\downarrow$

$\mathbf{s}_5 = (0, \underline{1}, 0) = \mathbf{t}_4$

$\downarrow$

$(0, 0, \underline{0}) = \mathbf{t}_5$

Recall that $b_{1k}(\mathbf{x}) = x_\ell - s_{k\ell}$, where ℓ is the first coordinate that $\mathbf{s}_1$ differs from $\mathbf{s}_k$.

skip $k = 1$

$$\begin{aligned} b_{12}(\mathbf{x}) &= (x_1 - s_{21}) = x_1 + 1 \\ b_{13}(\mathbf{x}) &= (x_1 - s_{31}) = x_1 + 1 \\ b_{14}(\mathbf{x}) &= (x_1 - s_{41}) = x_1 + 1 \\ b_{15}(\mathbf{x}) &= (x_2 - s_{52}) = x_2 + 1 \end{aligned}$$

Now, $r_1(\mathbf{x}) = (x_1 + 1)^3 (x_2 + 1) = (x_1 + 1)(x_2 + 1)$.

A Boolean example (cont.)

Recall that $b_{ik}(\mathbf{x}) = x_\ell - s_{k\ell}$, where ℓ is the first coordinate that $\mathbf{s}_i$ differs from $\mathbf{s}_k$.

$\mathbf{s}_1 = (0,0,1)$
$\downarrow$
$\mathbf{s}_2 = (1,0,1) = \mathbf{t}_1$
$\downarrow$
$\mathbf{s}_3 = (1,1,1) = \mathbf{t}_2$
$\downarrow$
$\mathbf{s}_4 = (1,1,0) = \mathbf{t}_3$
$\downarrow$
$\mathbf{s}_5 = (0,1,0) = \mathbf{t}_4$
$\downarrow$
$(0,0,0) = \mathbf{t}_5$

$$b_{21}(\mathbf{x}) = (x_1 - s_{11}) = x_1$$
skip $k = 2$
$$b_{23}(\mathbf{x}) = (x_2 - s_{32}) = x_2 + 1$$
$$b_{24}(\mathbf{x}) = (x_2 - s_{42}) = x_2 + 1$$
$$b_{25}(\mathbf{x}) = (x_1 - s_{51}) = x_1$$

$$b_{31}(\mathbf{x}) = (x_1 - s_{11}) = x_1$$
$$b_{32}(\mathbf{x}) = (x_2 - s_{22}) = x_2$$
skip $k = 3$
$$b_{34}(\mathbf{x}) = (x_3 - s_{43}) = x_3$$
$$b_{35}(\mathbf{x}) = (x_1 - s_{51}) = x_1$$

$$b_{41}(\mathbf{x}) = (x_1 - s_{11}) = x_1$$
$$b_{42}(\mathbf{x}) = (x_2 - s_{22}) = x_2$$
$$b_{43}(\mathbf{x}) = (x_3 - s_{33}) = x_3 + 1$$
skip $k = 4$
$$b_{45}(\mathbf{x}) = (x_1 - s_{51}) = x_1$$

$$b_{51}(\mathbf{x}) = (x_2 - s_{12}) = x_2$$
$$b_{52}(\mathbf{x}) = (x_1 - s_{21}) = x_1 + 1$$
$$b_{53}(\mathbf{x}) = (x_1 - s_{31}) = x_1 + 1$$
$$b_{54}(\mathbf{x}) = (x_1 - s_{42}) = x_1 + 1$$
skip $k = 5$

Recall that $x_i^k = x_i$, and $(x_j + 1)^k = x_j + 1$, so the "r-polynomials" are

$$r_1(\mathbf{x}) = (x_1 + 1)(x_2 + 1)$$
$$r_2(\mathbf{x}) = x_1(x_2 + 1)$$
$$r_3(\mathbf{x}) = x_1 x_2 x_3$$
$$r_4(\mathbf{x}) = x_1 x_2 (x_3 + 1)$$
$$r_5(\mathbf{x}) = (x_1 + 1)x_2$$

A Boolean example (cont.)

We can now compute our particular solution (f_1, f_2, f_3) that fits the data, using:

$$\boxed{f_j(\mathbf{x}) = t_{1j}r_1(\mathbf{x}) + t_{2j}r_2(\mathbf{x}) + \cdots + t_{mj}r_m(\mathbf{x})}.$$

$\mathbf{s}_1 = (0,0,1)$
$\downarrow$
$\mathbf{s}_2 = (1,0,1) = \mathbf{t}_1$
$\downarrow$
$\mathbf{s}_3 = (1,1,1) = \mathbf{t}_2$
$\downarrow$
$\mathbf{s}_4 = (1,1,0) = \mathbf{t}_3$
$\downarrow$
$\mathbf{s}_5 = (0,1,0) = \mathbf{t}_4$
$\downarrow$
$(0,0,0) = \mathbf{t}_5$

$$\begin{aligned} f_1(\mathbf{x}) &= t_{11}r_1(\mathbf{x}) + t_{21}r_2(\mathbf{x}) + t_{31}r_3(\mathbf{x}) + t_{41}r_4(\mathbf{x}) + t_{51}r_5(\mathbf{x}) \\ &= r_1(\mathbf{x}) + r_2(\mathbf{x}) + r_3(\mathbf{x}) \\ &= 1 + x_2 + x_1x_2x_3 \end{aligned}$$

$$\begin{aligned} f_2(\mathbf{x}) &= t_{12}r_1(\mathbf{x}) + t_{22}r_2(\mathbf{x}) + t_{32}r_3(\mathbf{x}) + t_{42}r_4(\mathbf{x}) + t_{52}r_5(\mathbf{x}) \\ &= r_2(\mathbf{x}) + r_3(\mathbf{x}) + r_4(\mathbf{x}) \\ &= x_1 \end{aligned}$$

$$\begin{aligned} f_3(\mathbf{x}) &= t_{13}r_1(\mathbf{x}) + t_{23}r_2(\mathbf{x}) + t_{33}r_3(\mathbf{x}) + t_{43}r_4(\mathbf{x}) + t_{53}r_5(\mathbf{x}) \\ &= r_1(\mathbf{x}) + r_2(\mathbf{x}) \\ &= 1 + x_2. \end{aligned}$$

Our original FDS was $(f_1, f_2, f_3) = (x_3,\ x_1,\ x_3 + x_2x_3)$, but our algorithm yielded

$$\begin{aligned} (f_1, f_2, f_3) &= (1 + x_2 + x_1x_2x_3,\ x_1,\ 1 + x_2) \\ &= (x_3,\ x_1,\ x_3 + x_2x_3) + (1 + x_2 + x_3 + x_1x_2x_3,\ 0,\ 1 + x_2 + x_3 + x_2x_3) \end{aligned}$$

Remark

Each polynomial in the 2nd term above is in the *vanishing ideal* I. (Why?)

A Boolean example (cont.)

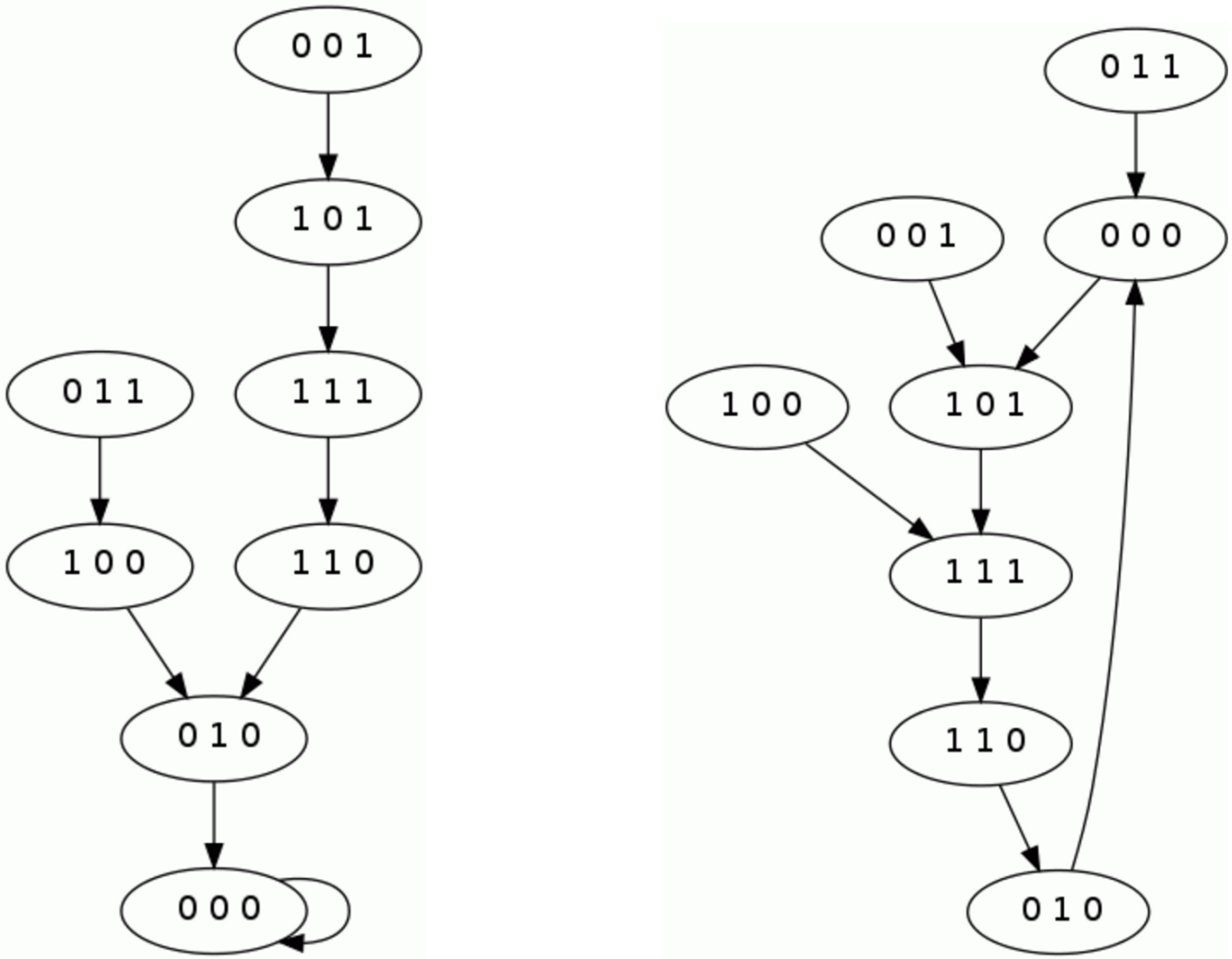


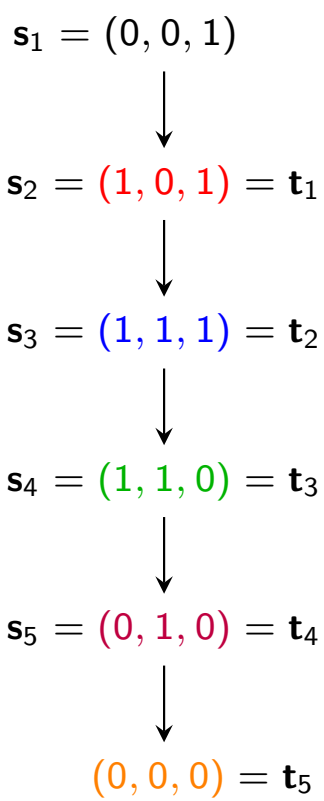
Figure : The original phase space (left), and the reverse-engineered phase space (right).

A Boolean example (cont.)

Now that we found a particular solution $f = (f_1, f_2, f_3)$ that fits the data, we need to (re)compute the ideal I of polynomials that vanish on the data.

We'll use Macaulay2 in Sage:

```
%default_mode macaulay2
R=ZZ/2[x1,x2,x3] / ideal(x1^2-x1, x2^2-x2, x3^2-x3);
```



The ideal of polynomials that vanish on each $\mathbf{s}_k$ is:

```
I1 = ideal(x1, x2, x3-1);
I2 = ideal(x1-1, x2, x3-1);
I3 = ideal(x1-1, x2-1, x3-1);
I4 = ideal(x1-1, x2-1, x3);
I5 = ideal(x1, x2-1, x3);
```

The ideal of polynomials that vanish on *every* $\mathbf{s}_k$ is:

```
I = intersect{I1,I2,I3,I4,I5}
```

To compute a Gröbner basis:

```
G = gens gb I
```

The output is: `| x2x3+x2+x3+1 x1x2+x1x3+x1+x2+x3+1 |`

A Boolean example (cont.)

In conclusion, the set of all Boolean models that fit the data

$$001 \longrightarrow 101 \longrightarrow 111 \longrightarrow 110 \longrightarrow 010 \longrightarrow 000$$

i.e., the model space, is the set

$$F_1 \times F_2 \times F_3, \qquad F_j = f_j + I$$

where I is the vanishing ideal

$$I = \langle g_1, g_2 \rangle = \langle 1 + x_2 + x_3 + x_2x_3,\ 1 + x_1 + x_2 + x_3 + x_1x_2 + x_1x_3 \rangle .$$

Our reverse-engineered BN is slighly different than the "true model":

$$\begin{aligned}(f_1, f_2, f_3) &= (1 + x_2 + x_1x_2x_3,\ x_1,\ 1 + x_2) \\ &= (x_3 + x_1g_1 + g_2,\ \ x_1,\ \ (x_2 + 1)x_3 + g_1)\end{aligned}$$

Note that x_1g_1, 0, and g_1 *must* be in the vanishing ideal I.

Next goal ("model selection")

We would like to be able to recover functions in $F_j = f_j + I$ that have no "extra terms" in I.

A Boolean example (cont.)

Goal ("model selection")

We would like to be able to be able to recover functions in $F_j = f_j + I$ that have no "extra terms" in I.

$$001 \longrightarrow 101 \longrightarrow 111 \longrightarrow 110 \longrightarrow 010 \longrightarrow 000$$

We can do this with Macaulay2. It's called finding the remainder of f_j modulo I, and we use the % symbol.

```
f1 = 1+x2+x1*x2*x3;
f2 = x1;
f3 = 1+x2;
f1%I;
f2%I;
f3%I;
```

The output is: `x3`, `x1`, `x2+1`. Almost the original Boolean model!

Question

What would happen if we:

- added the (original) self-loop at 000 to the data?
- removed the data point $010 \longrightarrow 000$?

An example over $\mathbb{F}_5$

Consider the following time series in a 3-node local model over $\mathbb{F}_5$:

$$\mathbf{s}_1 = (2,0,0)$$
$$\downarrow$$
$$\mathbf{s}_2 = (4,3,1) = \mathbf{t}_1$$
$$\downarrow$$
$$\mathbf{s}_3 = (3,1,4) = \mathbf{t}_2$$
$$\downarrow$$
$$(0,4,3) = \mathbf{t}_3$$

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

$$\begin{aligned}
\mathbf{s}_1 &= (s_{11}, s_{12}, s_{13}) = (2,0,0)\,, & \mathbf{t}_1 &= (t_{11}, t_{12}, t_{13}) = (4,3,1)\,,\\
\mathbf{s}_2 &= (s_{21}, s_{22}, s_{23}) = (4,3,1)\,, & \mathbf{t}_2 &= (t_{21}, t_{22}, t_{23}) = (3,1,4)\,,\\
\mathbf{s}_3 &= (s_{31}, s_{32}, s_{33}) = (3,1,4)\,, & \mathbf{t}_3 &= (t_{31}, t_{32}, t_{33}) = (0,4,3)\,.
\end{aligned}$$

Note that $\mathbf{s}_1$ differs from $\mathbf{s}_2$ and $\mathbf{s}_3$ in the $\ell = 1$ coodinate, so this ℓ will work for each of r_1, r_2, and r_3.

An example over $\mathbb{F}_5$ (cont.)

Since we are working in $\mathbb{F}_5$, we are taking the remainder of everything modulo 5.

Particularly useful identities are: $0 = 5$, $-1 = 4$, $-2 = 3$, $-3 = 2$, and $-4 = 1$.

Using our formulas for $b_{ij}(\mathbf{x})$, we compute:

$$b_{12}(\mathbf{x}) = (s_{11} - s_{21})^3(x_1 - s_{21}) = (2-4)^3(x_1 - 4) = -8(x_1 + 1) = 2x_1 + 2$$
$$b_{13}(\mathbf{x}) = (s_{11} - s_{31})^3(x_1 - s_{31}) = (2-3)^3(x_1 - 3) = -x_1 + 3 = 4x_1 + 3\,.$$

Therefore, the first r-polynomial is

$$r_1(\mathbf{x}) = b_{12}(\mathbf{x})b_{13}(\mathbf{x}) = (2x_1 + 2)(4x_1 + 3) = 8x_1^2 + 14x_1 + 6 = 3x_1^2 + 4x_1 + 1\,.$$

In-class Exercise

Compute the other two r-polynomials in this example: $r_2(\mathbf{x})$ and $r_3(\mathbf{x})$.

Solution: $r_2(\mathbf{x}) = 3x_1^2 + 3\,,$ $r_3(\mathbf{x}) = 4x_1^2 + x_1 + 2.$

An example over $\mathbb{F}_5$ (cont.)

In summary, we computed the r-polynomials to be:

$$r_1(\mathbf{x}) = b_{12}(\mathbf{x})b_{13}(\mathbf{x}) = (2x_1+2)(4x_1+3) = 8x_1^2+14x_1+6 = 3x_1^2+4x_1+1$$
$$r_2(\mathbf{x}) = b_{21}(\mathbf{x})b_{23}(\mathbf{x}) = (3x_1+4)(x_1+2) = 3x_1^2+10x_1+8 = 3x_1^2+3$$
$$r_2(\mathbf{x}) = b_{31}(\mathbf{x})b_{32}(\mathbf{x}) = (x_1+3)(4x_1+4) = 4x_1^2+16x_1+12 = 4x_1^2+x_1+2$$

Thus, the following functions fit the data:

$$\begin{aligned} f_1(\mathbf{x}) &= t_{11}r_1(\mathbf{x}) + t_{21}r_2(\mathbf{x}) + t_{31}r_3(\mathbf{x}) \\ &= 4(3x_1^2+4x_1+1) + 3(3x_1^2+3) + 0(4x_1^2+x_1+2) \\ &= x_1^2+x_1+3 \end{aligned}$$

$$\begin{aligned} f_2(\mathbf{x}) &= t_{12}r_1(\mathbf{x}) + t_{22}r_2(\mathbf{x}) + t_{32}r_3(\mathbf{x}) \\ &= 3(3x_1^2+4x_1+1) + 1(3x_1^2+3) + 4(4x_1^2+x_1+2) \\ &= 3x_1^2+x_1+4 \end{aligned}$$

$$\begin{aligned} f_3(\mathbf{x}) &= t_{13}r_1(\mathbf{x}) + t_{23}r_2(\mathbf{x}) + t_{33}r_3(\mathbf{x}) \\ &= 1(3x_1^2+4x_1+1) + 4(3x_1^2+3) + 3(4x_1^2+x_1+2) \\ &= 2x_1^2+2x_1+4 \end{aligned}$$

Comments on this? [Note that only the variable x_1 appears.]

An example over $\mathbb{F}_5$ (cont.)

Recall that the ideal I is the set of polynomials that vanish on all $\mathbf{s}_i$:

$$I = I(\mathbf{s}_1) \cap I(\mathbf{s}_2) \cap I(\mathbf{s}_3) \qquad \mathbf{s}_1 = (2,0,0)\,, \quad \mathbf{s}_2 = (4,3,1)\,, \quad \mathbf{s}_3 = (3,1,4)\,.$$

These are precisely the sets

$$I(\mathbf{s}_1) = \langle x_1 - 2, x_2, x_3 \rangle = \{(x_1-2)g_1(x) + x_2 g_2(x) + x_3 g_3(x)\}$$
$$I(\mathbf{s}_2) = \langle x_1 - 4, x_2 - 3, x_3 - 1 \rangle = \{(x_1-4)g_1(x) + (x_2-3) g_2(x) + (x_3-1) g_3(x)\}$$
$$I(\mathbf{s}_3) = \langle x_1 - 3, x_2 - 1, x_3 - 4 \rangle = \{(x_1-3)g_1(x) + (x_2-1) g_2(x) + (x_3-4) g_3(x)\}.$$

As before, we compute the vanishing ideal I in Macaulay2:

```
R=ZZ/5[x1,x2,x3] / ideal(x1^5-x1, x2^5-x2, x3^5-x3);
I1 = ideal(x1-2, x2, x3);
I2 = ideal(x1-4, x2-3, x3-1);
I3 = ideal(x1-3, x2-1, x3-4);
I = intersect{I1,I2,I3};
G = gens gb I
```

This says that a Gröbner basis for I under the default monomial ordering **GrRevLex** is

$$\mathcal{G} = \{x_1 - 2x_2 - x_3 - 2,\ x_3^2 + 2x_2 - 2x_3,\ x_2x_3 + 2x_2 + x_3,\ x_2^2 + x_3\}.$$

For a slightly different format, try the command: `flatten entries gens gb I`

An example over $\mathbb{F}_5$ (cont.)

Let us enter the functions that we reverse-engineered into Macaulay2:

```
f1=x1*x1+x1+3;
f2=3x1^2+x1+4;
f3=2x1^2+2x1+4;
```

The following command will reduce each function modulo I:

```
p1=f1%I;
p2=f2%I;
p3=f3%I;
(p1,p2,p3)
```

The output is

$$(p_1, p_2, p_3) = (-x_3 - 1,\ x_2 - 2,\ -2x_3 + 1).$$

The polynomial p_j is called the normal form of f_j with respect to the Gröbner basis $\mathcal{G}$.

Using a different monomial order will (likely) give a different Gröbner basis, and thus a different reduction modulo I.

To use the **Lex** monomial ordering, repeat the above commands but using

```
R=ZZ/5[x1,x2,x3,MonomialOrder=>Lex] / ideal(x1^5-x1, x2^5-x2, x3^5-x3);
```

Also try the **GrLex** monomial ordering.