Binomial Systems

1. Binomial Ideals
   definition and properties
2. Hidden Markov Models
   the maximum likelihood equations
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   decompositing binomial ideals
4. Using Macaulay 2
   running examples with the package Binomials

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Analytic Symbolic Computation
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Binomial Systems

binomial ideals

Consider $\mathbb{K}[\mathbf{x}]$, with $\mathbb{K}^* = \mathbb{K} \setminus \{0\}$.

Typically we will assume that $\mathbb{K}$ is algebraically closed, so $\mathbb{K} = \mathbb{C}$ is our default coefficient field. Then

$$I = \left\langle\, c_{\mathbf{a}} x^{\mathbf{a}} - c_{\mathbf{b}} x^{\mathbf{b}} \mid \mathbf{a}, \mathbf{b} \in \mathbb{N}^n, c_{\mathbf{a}}, c_{\mathbf{b}} \in \mathbb{K}^* \,\right\rangle$$

is a binomial ideal. A polynomial is a binomial if it has exactly two monomials with a nonzero coefficient.

A binomial ideal is generated by binomials.

If the generators are of the form $\mathbf{x}^{\mathbf{a}} - \mathbf{x}^{\mathbf{b}}$, then the binomial ideal is a toric ideal.

toric varieties

Because the exponents determine the structure of the ideal, we then define a toric ideal as

$$I_A = \langle \, \mathbf{x}^{\mathbf{u}} - \mathbf{x}^{\mathbf{v}} \mid \mathbf{u}, \mathbf{v} \in \mathbb{N}^n \text{ and } A\mathbf{u} = A\mathbf{v} \, \rangle.$$

The solution set of a toric ideal is a toric variety.

As an alternative to the ideal description,
a toric variety over $\mathbb{C}$ is defined as

- a complex algebraic variety with an action of $(\mathbb{C}^*)^n$ and
- a dense open subset isomorphic to $(\mathbb{C}^*)^n$ carrying the regular action.

That is: a toric variety is an algebraic torus closure.

In polyhedral homotopies: at ∞ and at 0 are equivalent.

binomial primary decompositions

Binomial ideals have special properties, for instance:

Theorem (Theorem 2.6 in [Eisenbud-Sturmfels, 1996])

If $\mathbb{K}$ is algebraically closed and I is a binomial ideal in $\mathbb{K}[\mathbf{x}]$, then every associated prime of I is generated by binomials.

The condition that $\mathbb{K}$ is algebraically closed is essential:

over $\mathbb{Q}$: $\langle x^3 - 1 \rangle = \langle x - 1 \rangle \cap \langle x^2 + x + 1 \rangle$.

If we extend $\mathbb{Q}$ with $w = e^{(2\pi\sqrt{-1})/3}$, then over $\mathbb{Q}(w)$:

$\langle x^3 - 1 \rangle = \langle x - 1 \rangle \cap \langle x + (1 - \sqrt{-3})/2 \rangle \cap \langle x + (1 + \sqrt{-3})/2 \rangle$.

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computational biology

Consider a sequence of letters over $\{A, C, G, T\}$.

Suppose the sequence was generated rolling four tetrahedral dice, with known probabilities of rolling each letter:

	A	C	G	T
first die	0.15	0.33	0.36	0.16
second die	0.27	0.24	0.23	0.26
third die	0.25	0.25	0.25	0.25

The probabilities of picking which dice is unknown:

1. θ_1 is the probability of using the first die;
2. θ_2 the probability for the second die; and
3. $1 - \theta_1 - \theta_2$ is the probability for the third die.

the likelihood function

The probabilities of each letter showing up in the sequence are then functions of the parameters θ_1 and θ_2.

Denote these functions by p_A, p_C, p_G, and p_T.

The likelihood $L(\theta_1, \theta_2)$ of observing any given sequence is then the product of $p_A^{n_A} p_C^{n_C} p_G^{n_G} p_T^{n_T}$, where n_A, n_C, n_G, and n_T equal the number of times the respective letter A, C, G, and T occur in the sequence.

The statistical principles of maximal likelihood presumes that those values for θ_1 and θ_2 were used which make the likelihood of observing the sequence as large as possible.

Maximizing $L(\theta_1, \theta_2)$ is equivalent to maximizing

$$\ell(\theta_1, \theta_2) = \log(L(\theta_1, \theta_2)).$$

maximal likelihood

A straightforward solution to this optimization problem is to search for the critical points, and solving the system defined by the rational functions $\frac{\partial \ell}{\partial \theta_1} = 0$ and $\frac{\partial \ell}{\partial \theta_2} = 0$.

$\ell(\theta_1, \theta_2) = n_A \log(p_A) + n_C \log(p_C) + n_G \log(p_G) + n_T \log(p_T)$, the system is

$$\left\{ \begin{array}{l} \frac{\partial \ell}{\partial \theta_1} = \frac{n_A}{p_A}\frac{\partial p_A}{\partial \theta_1} + \frac{n_C}{p_C}\frac{\partial p_C}{\partial \theta_1} + \frac{n_G}{p_G}\frac{\partial p_G}{\partial \theta_1} + \frac{n_T}{p_T}\frac{\partial p_T}{\partial \theta_1} = 0 \\ \frac{\partial \ell}{\partial \theta_2} = \frac{n_A}{p_A}\frac{\partial p_A}{\partial \theta_2} + \frac{n_C}{p_C}\frac{\partial p_C}{\partial \theta_2} + \frac{n_G}{p_G}\frac{\partial p_G}{\partial \theta_2} + \frac{n_T}{p_T}\frac{\partial p_T}{\partial \theta_2} = 0. \end{array} \right.$$

Only solutions in $[0, 1]$ are interesting.

A hidden Markov model is a polynomial map from the parameter space to the probability space.
Via maximum likelihood, this hidden model is reconstructed.

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cellular ideals

Consider $\mathcal{E} \subseteq \{1, 2, \ldots, n\}$ and
denote the algebraic torus corresponding to $\mathcal{E}$ by

$$(\mathbb{K}^*)^{\mathcal{E}} = \{ \mathbf{x} \in \mathbb{K}^n \mid x_i \neq 0 \text{ for } i \in \mathcal{E} \text{ and } x_j = 0 \text{ for } j \not\in \mathcal{E} \}.$$

The central definition is

Definition

A proper binomial ideal I in $\mathbb{K}[\mathbf{x}]$ is *cellular* if each variable x_i is either a nonzerodivisor or nilpotent modulo I.

Primary ideals I are cellular as every element in $\mathbb{K}[\mathbf{x}]/I$ is either nilpotent or a nonzerodivisor.

characterizing cellular ideals

We have a characterization for an ideal I being cellular in the following lemma.

Lemma

A proper binomial ideal I in $\mathbb{K}[\mathbf{x}]$ is cellular if and only if there exists a set $\mathcal{E} \subseteq \{1, 2, \ldots, n\}$ of indices of variables in $\mathbf{x}$ such that

1. $I = \left(I : \left(\prod_{i \in \mathcal{E}} x_i \right)^\infty \right)$*; and*
2. *For every $i \not\in \mathcal{E}$, there exists an integer $d_i \geq 0$ such that $\langle x_i^{d_i} \mid i \not\in \mathcal{E} \rangle$ is contained in I.*

an algorithm

The `Binomials` package in Macaulay 2 provides an implementation of the following recursive algorithm:

Algorithm [cellular decomposition]

Input: a binomial ideal I.
Output: a cellular decomposition of I.

1. If I is cellular, then return I.
2. Choose x_i that is a zerodivisor but not nilpotent modulo I.
3. Determine the power m such that $(I : x_i^m) = (I : x_i^\infty)$.
4. Call the algorithm on $(I : x_i^m)$ and $I + \langle x_i^m \rangle$.

solving toric ideals

Input: a zero dimensional toric ideal I.
Output: roots of unity to extend $\mathbb{Q}$ and solutions in $V(I)$.

1. Compute a cellular decomposition of I.
2. For each cellular component do
2.1 Set the noncell variables to zero and determine the product $D := \prod_{i \notin \mathcal{E}} d_i$ of the minimal powers of the noncell variables.
2.2 Compute a lexicographic Gröbner basis and solve the lattice ideal of the cellular component, adjoining roots of unity.
2.3. Save each solution D times.
3. Compute the least common multiple m of the powers of the adjoined roots of unity and construct the cyclotomic field $\mathbb{Q}(w_m)$.
4. Return the list of solutions as elements in $\mathbb{Q}(w_m)$.

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running Binomials

The package `Binomials` of Thomas Kahle is in Macaulay 2 version 1.4.

```
i1 : S = QQ[x,y,z];
i2 : I = ideal(x^2-y,y^3-z,x*y-z);
i3 : loadPackage "Binomials";
i4 : binomialSolve I
BinomialSolve created a cyclotomic field
of order 3

o4 = {{1, 1, 1}, {- ww  - 1, ww , 1},
                       3        3
    {ww , - ww  - 1, 1},
       3      3
    {0, 0, 0}, {0, 0, 0}, {0, 0, 0}}
i5 : degree I
o5 = 6
```

binomial primary decomposition

```
i6 : BPD I
Running cellular decomposition:
cellular components found: 1
cellular components found: 2
Decomposing cellular components:
Decomposing cellular component: 1 of 2
1 monomial to consider for this cellular component
BinomialSolve created a cyclotomic field of order 3
done
Decomposing cellular component: 2 of 2
3 monomials to consider for this cellular component
done
Removing redundant components...
4 Ideals to check
3 Ideals to check
2 Ideals to check
1 Ideals to check
0 redundant ideals removed.
Computing mingens of result.
```

the result

The primary decomposition of $\langle x^2 - y, y^3 - z, xy - z \rangle$ is

```
o6 = {ideal (z - 1, y - 1, x - 1),

   ideal (z - 1, y - ww , x + ww  + 1),
                       3        3

   ideal(z - 1, y + ww  + 1, x - ww ),
                      3             3


                2         2
   ideal (z, y , x*y, x  - y)}
```

associated prime

We consider the last ideal in the primary decomposition

```
i7 : I = ideal(z,y^2,x*y,x^2 - y);

i8 : binomialAssociatedPrimes I
3 monomials to consider for this cellular
component

o8 = {ideal (z, y, x)}
```

cellular decompositions

```
i2 : S = QQ[x1,x2,x3,x4,x5];
i3 : I = ideal(x1*x4^2-x2*x5^2,
 x1^3*x3^3-x2^4*x4^2, x2*x4^8-x3^3*x5^6);
i4 : I
                 2         2    3  3      4  2
o4 = ideal (x1*x4  - x2*x5 , x1 x3  - x2 x4 ,
          8     3  6
     x2*x4  - x3 x5 )

i5 : BCD I
```

the output of BCD I

```
cellular components found: 1
redundant component
redundant component
cellular components found: 2
                  2        2    3  3     4  2
o5 = {ideal (x1*x4  - x2*x5 , x1 x3  - x2 x4 ,
    3  4     2  3  2
  x2 x4  - x1 x3 x5 ,
   2  6      3  4     2  3  2
 x2 x4  -  x2 x4  - x1 x3 x5 ,
   2  6         3  4       8     3  6
 x2 x4  -  x1*x3 x5 , x2*x4  - x3 x5 ),
          2       2        2    5
 ideal (x1 , x1*x4  - x2*x5 , x2 ,
    6    4  2    8
  x5 , x2 x4 , x4 )}
```

Summary + Exercises

Binomial ideals are an interesting class of problems.

Exercises:

1. Install version 1.4 of Macaulay 2 and explore the package Binomials.
2. Explore the capabilities in CoCoA for handling binomial ideals.