

Lecture Guide

CBMS CONFERENCE ON APPLICATIONS OF POLYNOMIAL SYSTEMS

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INTRODUCTION

This guide is designed as a supplement to my lectures at the conference. It serves three main purposes:

- Suggest background readings for the topics covered in the lectures.
- Summarize briefly the content of each lecture.
- Provide complete references for all papers and books mentioned in the lectures.

About a year ago, I wrote a tentative description of the lectures, available at the conference website under the heading *Abstracts of Professor Cox's talks*. However, in the process of writing the lectures, I found them taking on a life of their own that often diverged from my original conception. This guide is based on the actual lectures.

Each day of the conference is devoted to a different topic:

MONDAY: Elimination Theory

TUESDAY: Numerical Algebraic Geometry

WEDNESDAY: Geometric Modeling

THURSDAY: Rigidity Theory

FRIDAY: Chemical Reaction Networks

There will be three lectures per day: two given by me, and the third given by an expert in the field. I am extremely grateful to Carlos D'Andrea, Jon Hauenstein, Hal Schenck, Jessica Sidman, and Alicia Dickenstein for agreeing to be part of the conference. You will enjoy their lectures.

The references at the end of this document fall into two groups:

- Background references, which you might want to look at before the conference begins. These are numbered [B1], [B2], etc.
- References for *all* papers mentioned in my lectures. These are numbered [1], [2], etc.

Besides the five topics listed above, the twin themes *toric varieties* and *algebraic statistics* play a prominent role in the lectures. The papers [B2] and [B7] give the background needed.

MONDAY: ELIMINATION THEORY

Elimination theory has important roles to play in both algebraic geometry and symbolic computation. I will take a historical approach in my lectures on this subject so that you can see how elimination theory has developed over the years.

BACKGROUND READING: [B3, Chapters 2, 3], [B4, Chapters 3, 7], [B9, Sections 1–3].

§1: *Elimination Theory in the 18th and 19th Centuries*. In spite of the title, I will begin in the 17th century with examples from Newton (1666) [93] and Tschirnhaus (1683) [114] to illustrate the geometric and algebraic aspects of elimination. In the 18th century, what we call Bézout's theorem for the plane was well known (e.g., Cramer (1750) [39]) and people, including Bézout (1764) [17], were already thinking about other versions of the theorem.

I will spend some time on Waring’s *Meditationes Algebraicæ* (1772) [122] and Bézout’s *Théorie Générale des Équations Algébriques* (1779) [18]. The latter is 500 pages long and includes many versions of the theorem. In modern terms, Bézout’s formulas are the normalized volumes of certain Newton polytopes. You will see some astonishing pictures. Penchèvre’s article [B9] describes what Bézout did in more detail.

Another important tool was the Poisson formula for the resultant, published in 1802 by Poisson [95]. But it wasn’t until later in the 19th century that the subject exploded with papers and books by Sylvester (1840) [111], Cayley (1864) [30], Brill (1880) [22], Kronecker (1882) [80], Mertens (1886) [87], Netto (1900) [91], Macaulay (1903, 1916) [84, 85], and many others. The 1907 review article of Netto and Le Vasseur [92, pp. 73–169] (97 pages long) and 2006 PhD thesis of Penchèvre (317 pages long) survey the substantial body of the work led to the theory of what we now call the dense or classical resultant. At the same time, people explored various aspects of resultants, which I will illustrate using examples from papers by Minding (1841) [90], Bonnet (1847) [21], and Riemann (1857) [97].

§2: *Elimination Theory in the 20th Century*. I will begin with quotes from Cayley in 1864 [30] and Kronecker in 1882 [80] that establish elimination at the heart of 19th century algebraic geometry. But the century that followed was a roller coaster ride for elimination theory. As noted above, a mature theory of resultants was established in the early 1900s (see [B4, Chapter 3] for a modern treatment). I will explain the intuition behind resultants and discuss the evolution of the *Fundamental Theorem of Elimination Theory*, beginning with proofs by Mertens (1899) [88] using resultants and van der Waerden (1926) [117] using ideals, and ending with the modern theorem that $\mathbb{P}_{\mathbb{Z}}^n \rightarrow \text{Spec}(\mathbb{Z})$ is a proper morphism of schemes (see Hartshorne [62, Thm. II.4.9]).

This evolution began with Severi’s *Principle of Conservation of Number* from 1912 [105]. A rigorous version of this principle requires clear definitions of *generic point*, *specialization* and *multiplicity*. Enriques and Chisini proposed a definition of generic point in 1915 [42]. Van der Waerden gave an algebraic approach to generic points and multiplicity in 1926 and 1927 [116, 118], but many of his proofs still used elimination theory.

In 1946, Weil published *Foundations of Algebraic Geometry* [123], where he famously said that his approach “finally eliminates from algebraic geometry the last traces of elimination theory.” After hearing van der Waerden lecture about this in 1970 [119], Abhyankar wrote a poem that began “Eliminate the eliminators of elimination theory” [2].

Around the time of Abhyankar’s poem, a revival of elimination theory was underway with the development of Gröbner bases by Buchberger in 1965 and 1970 [23, 24] and their application to elimination by Trinks in 1978 [113] (see [B3, Chapters 2 and 3] for an exposition). But resultants were also making a comeback, as I will illustrate using the work of Abhyankar (1976) [3], Giraud (1977) [53], Lazard (1977) [82], Jouanolou (1979) [70] and Sederberg, Anderson and Goldman [101]. I will also mention the book [43] that inspired Sederberg, a geometric modeler, to learn about resultants.

The modern theory of the classical resultant was established by Jouanolou in a series of papers written between 1980 and 1997 that make full use of modern commutative algebra [71, 72, 73, 73, 75]. In 2017, Staglianò wrote a Macaulay2 package to compute the classical resultant [109].

The lecture will conclude with snapshots of resultants, ranging from the Dixon resultant (1909) [40] to the sparse resultants of Gel'fand, Kapranov and Zelevinsky (1994) [52] (see [B4, §7.2] for an exposition), ending with a 2016 example from Botbol and Dickenstein [20].

§3: *Elimination Theory in the 21st Century* (Carlos D'Andrea). This century finds computational algebraic geometry more in demand for applications and implementations. In his lecture, Carlos will explore “faster” and more tailored methods to perform elimination. This includes more compact types of resultants that have appeared in the last decades (parametric, residual, determinantal, . . .), and also other types of tools, such as elimination matrices, Rees algebras, and homotopy methods.

TUESDAY: NUMERICAL ALGEBRAIC GEOMETRY

In applications, we rarely have the luxury of knowing the exact solutions of a system of polynomial equations; approximations by floating point numbers are the best we can do. In fact, the coefficients of the polynomials are often floating point numbers themselves. Thus numerical issues become important when solving polynomial systems in the real world.

BACKGROUND READING: [B4, Chapters 2, 3], [B13, Parts 1, 2].

§1: *Numerical Polynomials via Linear Algebra*. I will first use MATHEMATICA [125] to illustrate how numerical computations differ from exact computations with examples involving the Binomial Theorem (an example from [120, pp. 44–45]) and Lagrange multipliers (an example from [B3, pp. 99]). I will also introduce paradigms due to Stetter [110] and Sommese and Wampler [107] for dealing with approximate coefficients. All of this is a prelude to the main focus of the lecture, which is the study of polynomial systems via linear algebra.

I will begin with the classical theory of systems $f_1 = \cdots = f_s = 0$ with finitely many solutions in $\mathbb{C}^n$. The Finiteness Theorem gives an algorithmic criterion for determining when this happens. Then the Eigenvalue and Eigenvector Theorems use eigenvalues and eigenvectors of multiplication maps on the finite-dimensional vector space $\mathbb{C}[x_1, \dots, x_n]/\langle f_1, \dots, f_s \rangle$ to get information about the solutions of the system. I will illustrate these results with a simple example. See [11] and [B4, Chapter 2] for precise statements and further examples.

This is where numerical linear algebra comes into the picture. Over the years, powerful numerical methods have been developed to study linear systems. What happens when we apply these methods to the previous paragraph? To answer this question, I will recall the condition number of a matrix and then explore two examples in more detail.

The first example involves generic multiplication maps. Let $f, g \in \mathbb{C}[x, y]$ be generic polynomials of degree d . In this case, we know a monomial basis B of $\mathbb{C}[x, y]/\langle f, g \rangle$ and (after inverting one matrix) we know the matrices of the multiplication maps (this is explained in [B4, §3.6]). These maps were studied recently by Telen and Van Barel [112], who discovered that they can have very large condition numbers. They also give a variant of the QR algorithm from linear algebra to construct a monomial basis B' of $\mathbb{C}[x, y]/\langle f, g \rangle$ with much smaller condition numbers. Although B and B' are both monomial bases, they differ greatly— B is an *order ideal* (it contains all monomials dividing any element of B), while B' is very far from being an order ideal.

The second example involves the joint project *Algebraic Oil* [79] between Shell International and the Universities Genoa and Passau. The goal is to use production data to create a formula that predicts production for all values of the variables. In an example studied by

Baciu and Kreuzer [13], there were seven variables $x_1, \dots, x_7$ and 5500 data points $\mathbb{X} \subseteq \mathbb{R}^7$. In algebraic geometry, there is a standard method (the Buchberger-Möller Algorithm) to find the vanishing ideal (roughly speaking, go from solutions to equations, rather than from equations to solutions). This gives an order ideal consisting of 5500 monomials, so that the production function would be a linear combination of these 5500 monomials. This is useless in practice—a classic example of overfitting.

By using approximate methods (there are two: the Approximate Buchberger-Möller Algorithm and the Approximate Vanishing Ideal [63]), one can reduce to an order ideal consisting of 31 monomials that give a vastly superior model. What’s interesting is that the “generators” of approximate vanishing ideal generate the unit ideal in the algebraic sense. But they still give a useful order ideal that is the basis of the model.

These two examples suggest that if we want to use linear algebra to solve polynomial systems, we need to give something up. In the first example, we had to sacrifice having an order ideal, while in the second, we have an order ideal but have to sacrifice having an ideal in the standard sense.

§2: *Homotopy Continuation and Applications.* Homotopy continuation is a powerful method for solving a polynomial system that uses numerical methods from the theory of ordinary differential equations. The rough idea of homotopy continuation can be found in [B4, §7.5], with full details in [15].

Assume that our system is $f_1 = \dots = f_n = 0$ for $f_i \in \mathbb{C}[x] = \mathbb{C}[x_1, \dots, x_n]$. We call $F = (f_1, \dots, f_n)$ the *target system*, and when F is generic, there are finitely many solutions. For homotopy continuation, we also have a *start system* G whose solutions we know. Then we have the homotopy

$$H(x, t) = tG(x) + (1 - t)F(x).$$

Thus $H(x, 1)$ is the start system and $H(x, 0)$ is the target system. The target system is $t = 0$ since there are more floating point numbers near 0.

Continuation means that we follow solutions of $G = 0$ to solutions of $H = 0$. For a solution p_0 of $G = 0$, assume that $x(t) : [0, 1] \rightarrow \mathbb{C}^n$ satisfies the initial value problem

$$\sum_{i=1}^n \frac{\partial H}{\partial x_i}(x(t), t) x'_i(t) + \frac{\partial H}{\partial t}(x(t), t) = 0, \quad x(1) = p_0.$$

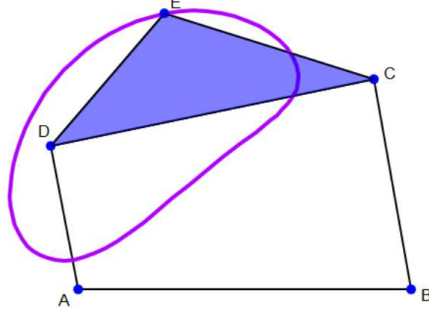
Then $H(x(t), t) = 0$ for all t , so $x(0)$ is a solution of $F = 0$. This is a *path*.

Not all paths behave nicely, as I will illustrate with pictures over $\mathbb{R}$. By working over $\mathbb{C}$, many of these problems go away, but serious smarts are needed to create good software. I will say a few words about the issues to consider and list the main software packages:

- BERTINI [16], named for the Bertini Theorems.
- PHCPACK [124], for Polyhedral Homotopy Continuation package.
- NAGM2 [83], for Numerical Algebraic Geometry for MACAULAY2.
- HOM4PS [31], for Homotopy for Polynomial Systems.

I will then discuss higher dimensional solution sets, where one uses a *witness set* as a numerical replacement for a generic point of an irreducible variety. My point of view will be Noether normalization. By a 1979 result of Harris [59], the resulting Galois group equals the monodromy group of the witness set. This leads to an algorithm for the *numerical irreducible decomposition* of the solution set. The classical Bertini Theorems are also relevant here [76].

The lecture will end with four extended examples. The first will revisit the Lagrange multipliers example from the previous lecture and will introduce the idea of a *parameter homotopy*. This will illustrate how the program BERTINI handles numerical coefficients. The second example is the classic four-bar mechanism:



If we fix the points A, B and the lengths AD, BC, DC, DE, CE , then point E traces out the curve shown above as we spin AD about the point A . This system has nine degrees of freedom (four for A, B and five for the five lengths). It follows that if we fix nine points, there should be a finite number of mechanisms that give a curve that goes through the nine points. Computing the number of solutions of this *nine-point problem* was one of the early successes of numerical algebraic geometry. Besides the original 1992 article [121] by Wampler, Morgan and Sommese, the nine-point problem is also treated in the books [15] and [107]. For this example, the resulting system of equations has some interesting Bézout numbers, one of which involves a toric variety whose Bézout number can be computed using POLYMAKE [6].

The third example is an HIV model studied by Gross, Davis, Ho, Bates, and Harrington [56] that leads to a system of differential equations whose steady states form a variety. A computation in MACAULAY2 [55] reveals an extinction component and a main component with a more interesting biological behavior. For the main component, I will explain how numerical algebraic geometry can be used to estimate one of the parameters used in this model. This is our first encounter with biochemical reaction networks, the main topic of Friday's lectures.

The fourth example is a maximum likelihood estimation problem from algebraic statistics. Following Kosta and Kubjas [77], consider a root and three leaves, with probabilities π_0, π_1 at the root and transition matrices P_1, P_2, P_3 along the edges:

$$\begin{array}{c}
 (\pi_0, \pi_1) \\
 \begin{array}{ccc}
 P_1 & & P_3 \\
 & \nearrow & \searrow \\
 & P_2 & \\
 & \nwarrow & \nearrow \\
 & &
 \end{array}
 \end{array}
 \quad
 P_i = \begin{pmatrix} \frac{1}{2} + \frac{1}{2}e^{-2t_i} & \frac{1}{2} - \frac{1}{2}e^{-2t_i} \\ \frac{1}{2} - \frac{1}{2}e^{-2t_i} & \frac{1}{2} + \frac{1}{2}e^{-2t_i} \end{pmatrix}, \quad t_i \geq 0$$

The probabilities at the leaves are $p_{000}, \dots, p_{111}$, where

$$p_{ijk} = \pi_0(P_1)_{0i}(P_2)_{0j}(P_3)_{0k} + \pi_1(P_1)_{1i}(P_2)_{1j}(P_3)_{1k}.$$

The p_{ijk} that occur satisfy the obvious restrictions $p_{ijk} \geq 0$ and $p_{000} + \dots + p_{111} = 1$, and

- three quadratic equations.
- seven strict linear inequalities.
- four quadratic weak inequalities.

Analyzing this example via numerical algebraic geometry reveals the surprising result that for some data, the maximum likelihood estimate fails to exist.

The four examples hint at the range of applications of numerical algebraic geometry. The third and fourth examples are our first glimpses of algebraic statistics, which will reappear in different guises on Wednesday, Thursday and Friday.

§3: *Applications of Sampling in Numerical Algebraic Geometry* (Jon Hauenstein). The central data structure to represent a variety in numerical algebraic geometry is a witness set. From a witness set, one is able to move the corresponding linear slice to sample points on the variety. In his lecture, Jon will explore several recent methods in numerical algebraic geometry that have been developed using the ability to sample points. Some highlights include new approaches for solving semidefinite programs in optimization, deciding algebraic and topological properties of a variety, and computing real points on the variety. Jon will conclude by turning this computation around to use sampling with the aim of constructing a witness set which permits one to statistically estimate the degree of a variety when it is too large to compute directly. Examples will be used to demonstrate all of these methods.

WEDNESDAY: GEOMETRIC MODELING

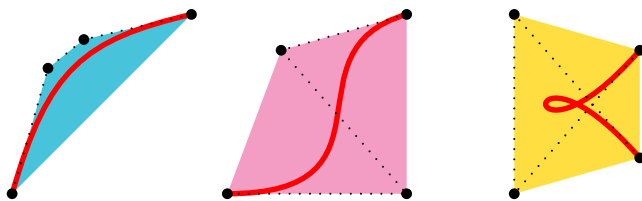
The interactions between geometric modeling, algebraic geometry, and commutative algebra are rich and varied. The geometry has compelling pictures and applications, and the algebra is equally interesting.

BACKGROUND READING: [B1], [B8, Sections 1–4], [B10, Chapters 2, 15].

§1: *Geometry*. I will start with the classic Bézier curves (see [B10, Chapter 2]). The *blending functions* $\binom{n}{i}t^i(1-t)^{n-i}$ and *control points* $P_0, \dots, P_n \in \mathbb{R}^d$ give the Bézier Curve

$$\Phi(t) = \sum_{i=0}^n \binom{n}{i} t^i (1-t)^{n-i} P_i, \quad t \in [0, 1].$$

Here are some Bézier cubics that illustrate the *convex hull* property:

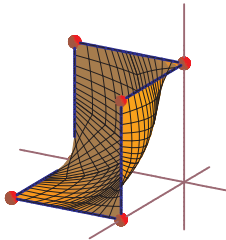


I will discuss tangent lines and curvature and use a webpage from Autodesk Alias [9] to illustrate how geometric modelers use *curvature combs* rather than osculating circles to visualize curvature.

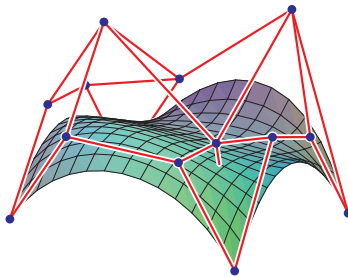
I will also introduce weighted versions of Bézier curves and preview the connection to toric geometry. When you have multiple Bézier curves, I will use Autodesk Alias [9] to explain the continuity conditions that describe how curves meet and give an example.

I then turn to surfaces, where I begin with Bézier surface patches (see [B10, Chapter 15]). I will give some examples of how these surface patches are used, including another image from Autodesk Alias [10].

In 2002, Krasauskas [78] defined *toric patches*, which include Bézier curves and surfaces. See [B8] for an introduction. A classic example due to Sottile [108] is



The data for a toric patch includes a weight assigned to each control point. By changing the weights, one gets a family of toric patches that have interesting degenerations. I will use this to explain the variation diminishing property of Bézier curves (Schoenberg 1930 [100]) and also explain the image



due to García-Puente, Sottile and Zhu [47].

The lecture will end with a discussion of the concept of *linear precision*. In the toric context, this leads to *rational linear precision*, defined by García-Puente and Sottile in 2009 [46]. I will give an example using a trapezoid and discuss a theorem from [46] that relates rational linear precision to maximum likelihood estimates in algebraic statistics.

§2: *Algebra*. I will begin with plane curves and work projectively. From this point of view, a curve parametrization becomes a map $\varphi : \mathbb{P}^1 \rightarrow \mathbb{P}^2$ whose image is a curve $C \subseteq \mathbb{P}^2$. After recalling the degree formula for φ , we turn to our first main topic, the implicitization problem, which seeks to find the defining equation of C , often called the *implicit equation*. One can use Gröbner bases, as explained in [B3, Chapter 3] or in the recent work of Abbott, Bigatti and Robbiano [1].

However, we will instead focus on a different approach to implicitization that uses syzygies. If we write $\varphi = (a, b, c)$, where $a, b, c \in \mathbb{C}[s, t]$ are relatively prime homogeneous polynomials of degree n , then we get the ideal

$$I = \langle a, b, c \rangle \subseteq R = \mathbb{C}[s, t].$$

By the Hilbert Syzygy Theorem, I has a free resolution

$$0 \longrightarrow R(-n - \mu_1) \oplus R(-n - \mu_2) \longrightarrow R(-n)^3 \xrightarrow{(a,b,c)} I \longrightarrow 0$$

with $\mu_1 + \mu_2 = n$. This was proved by Meyer in 1887 [89] and vastly generalized in 1890 by Hilbert [65]. This exact sequence tells us that the *syzygy module* of I is free, with generators of degrees

$$\mu = \min(\mu_1, \mu_2) \leq \max(\mu_1, \mu_2) = n - \mu.$$

In geometric modeling, Sederberg, Anderson and Goldman used resultants to find the implicit equation in 1984 [101]. In 1995, Sederberg and Chen [103] considered moving lines that follow the parametrization. This led them to an equation of the form $Aa + Bb + Cc = 0$, which says that (A, B, C) is in the syzygy module of a, b, c .

This is where I got involved in geometric modeling. In 1998, Sederberg, Chen and I published [34], which introduced the idea of a μ -basis. As I will explain, this gives a lovely geometric way to think about syzygies and curve parametrizations. We will also see that the resultant of a μ -basis gives the implicit equation.

I will then turn to the Rees algebra, which for the ideal $I \subseteq R$ is the graded R -algebra $\mathcal{R}(I) = \bigoplus_{m=1}^{\infty} I^m e^m \subseteq R[e]$. Since $I = \langle a, b, c \rangle$, $(x, y, z) \mapsto (ae, be, ce)$ induces a surjection $R[x, y, z] \rightarrow \mathcal{R}(I)$. Generators of the kernel K are called *defining equations* of $\mathcal{R}(I)$.

In 1997, Sederberg, Goldman, Du [102] generalized moving lines to *moving curves* that follow the parametrization. These lie in the kernel K , which means that the geometric modeling community independently discovered the defining equations of $\mathcal{R}(I)$ without any idea of the connection to commutative algebra. The paper [102] also described minimal generators when a, b, c are generic of degree 4. I gave a rigorous proof of this in 2008 [32]. In the same year, Hoffman, Wang and I [33] found the defining equations for arbitrary n when $\mu = 1$. Many people have worked in the area, including Busé, Cortadellas, D’Andrea, Hong, Jia, Kustin, Madsen, Simis, Polini, Song, Vasconcelos, Ulrich and others.

Next come surfaces. The commutative algebra becomes more complicated, due in part to the presence of basepoints, a new feature of the surface case. This complicates the degree formula, which now involves the Hilbert-Samuel multiplicities of the basepoints.

In the affine case, one can show that the syzygy module is free of rank three. Geometrically, this gives *moving planes* p, q, r that give a basis of the syzygy module. However, there is no natural notion of minimal basis in the affine case, so that the resultant $\text{Res}(p, q, r)$ has an imperfect relation to the implicit equation of the parametrized surface—there may be *extraneous factors*, some coming from basepoints and some coming from ∞ .

I will give an intuitive analysis of how basepoints affect $\text{Res}(p, q, r)$, including an explanation of why it vanishes identically in the presence of a really bad basepoint. When the basepoints are worst local almost complete intersections, Busé, Chardin and Jouanolou [27] showed in 2009 that

$$(1) \quad \text{Res}(p, q, r) = F^{\deg(\varphi)} \times \prod_{e_p > d_p} L_p^{e_p - d_p} \times \underbrace{\text{extraneous factor from } \infty}_{\text{described in [27]}}$$

where $F = 0$ is the implicit equation, L_p is a linear form, and $e_p - d_p$ measures how far the basepoint p is from being a local complete intersection. So there is clearly some lovely algebra and geometry going on here.

It is not easy to compute the moving planes p, q, r , and the extraneous factor at ∞ is annoying. A better approach is to use *matrix representations*, which are easy-to-construct matrices that drop rank on the surface. As we learned on Monday, van der Waerden used this idea in 1926 [117] in his proof of the Fundamental Theorem of Elimination Theory.

In the situation here, again needs to worry about basepoints, and with the same hypothesis as in (1), the paper [27] constructs a matrix that represents $F^{\deg(\varphi)} \times \prod_{e_p > d_p} L_p^{e_p - d_p}$. Although the matrix is easy to describe, the proof uses the *approximation complexes* defined by Herzog,

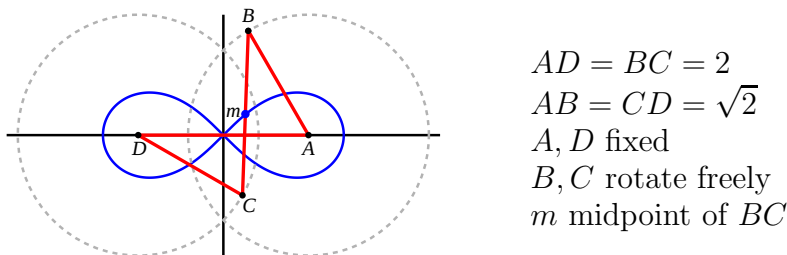
Simis and Vasconcelos in 1982 [64]. These complexes were first applied to geometric modeling and elimination theory in 2003 by Busé and Jouanolou [26].

When combined with numerical linear algebra, matrix representations lead to some nice applications, such as the papers of Ba, Busé, Mourrain [12] on curve-surface intersections in 2009 and Busé and Ba (2012) [25] on surface-surface intersections in 2012. I will conclude by revisiting the example from Botbol and Dickenstein [20] presented on Monday.

§3: *Rees Algebras, Syzygies, and Computational Geometry* (Hal Schenck). Rees and symmetric algebras are fundamental topics in commutative algebra, and have recently entered the toolkit of computational geometers. In his lecture, Hal will begin with an overview of the basic machinery. Then he will introduce and develop some of the more specialized tools used in the area, including Fitting ideals, the determinant of a complex, approximation complexes, and the McRae invariant. Hal will focus on applying these tools to several examples of interest in geometric modeling.

THURSDAY: RIGIDITY THEORY

This fascinating topic involves the study of frameworks built from bars and joints in $\mathbb{R}^2$ and $\mathbb{R}^3$. Here is a version of a framework introduced by James Watt in 1784:

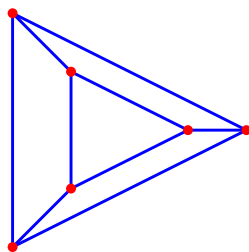


In this picture, the point m traces out the lemniscate shown above. Given a bar and joint framework, a key question is whether it is rigid, and if not, what motions are possible. Studying these questions involves Euclidean geometry, algebraic geometry, and combinatorics.

Background reading: [B11, Chapters 1, 2], [B12].

§1: *Geometry of Rigidity*. A *framework* for a simple graph $G = (V, E)$ in $\mathbb{R}^d$ consists of points $\mathbf{q}_i \in \mathbb{R}^d$ for $i \in V$ (the joints) and line segments $\overline{\mathbf{q}_i \mathbf{q}_j}$ for $ij \in E$ (the bars). Not surprisingly, we called this a *bar-and-joint framework*. While these frameworks are the main focus of my lectures, I will also say a few words about *bar-and-body frameworks*, which are important in many applications. In particular, I will mention Stewart-Gough platforms and discuss a splendid image created by Arnold and Wampler in 2006 [5].

I will then give careful definitions of motion and local rigidity. The special Euclidean group $SE(d)$ plays a prominent role here. I will use Gröbner bases to study the framework:



We will see that this framework is locally rigid but not infinitesimally rigid. I will also mention a 1979 theorem of Asimow and Roth [8] which states that infinitesimal rigidity implies local rigidity (so the converse fails by the above example).

Given a framework $\mathbf{q} = \{\mathbf{q}_i\}_{i \in V}$ in $\mathbb{R}^d$ for $G = (V, E)$, one can define a *rigidity matrix* $R_{G,\mathbf{q}}$ which allows us to characterize infinitesimal rigidity in terms of the rank of $R_{G,\mathbf{q}}$. We will use this to derive some inequalities that relate $m = |E|$ to the number $dn - \binom{d+1}{2}$ (the binomial coefficient is the dimension of $\text{SE}(d)$). I will then discuss various flavors of rigidity, which include local rigidity, infinitesimal rigidity, as well as global rigidity. And each of these have minimal and generic versions.

For the remainder of the lecture, I take a more algebro-geometric point of view. If we fix the edge lengths, then all frameworks for G form a *configuration variety* in $(\mathbb{R}^d)^n$, where $n = |V|$. Furthermore, this variety is smooth of dimension $dn - m$ at frameworks $\mathbf{q}$ where the rigidity matrix $R_{G,\mathbf{q}}$ has rank $m = |E|$.

As an application of these ideas, consider a 3-dimensional convex polytope $P \subseteq \mathbb{R}^3$. Its edges give a graph G , and its vertices $\mathbf{q} \in (\mathbb{R}^3)^n$ form a framework for G . I will prove a 1978 theorem of Asimow and Roth [7] which states that $\mathbf{q}$ is locally rigid for G if and only if every face of P is a triangle. The proof uses a 1975 result of Gluck [54] and a classic result of Cauchy whose proof is in THE BOOK [4].

I will conclude with Cayley-Menger varieties, which record the relations among the edge lengths of frameworks $\mathbf{q} \in (\mathbb{R}^d)^n$ for the complete graph K_n . Cayley determined these relations in 1841 [29]. A change of variables relates this to variety of $(n-1) \times (n-1)$ symmetric matrices of rank $\leq d$. The degree of this variety was determined in 1905 by Gambelli [45], with rigorous proofs given in 1982 by Jósefiak, Lascoux and Pragacz [69] and independently in 1984 by Harris and Tu [60]. In 2004, Borcea and Streinu [19] used this to prove that if $\mathbf{q}$ has generic edge lengths, then up to congruence, the number of frameworks for G with the same edge lengths as $\mathbf{q}$ is bounded by

$$\prod_{\ell=0}^{n-d-2} \frac{\binom{n-1+\ell}{n-d-1-\ell}}{\binom{2\ell+1}{\ell}}.$$

I will also mention a 2018 paper by Capco, Gallet, Grasegger, Koutschan, Lubbes and Schicho [28] and a 2018 preprint by Bartosz, Emir, Legerský and Tsigaridas [14].

§2: *Combinatorics of Rigidity*. I will begin with two examples of *matroids*: the linearly independent subsets of a finite set of vectors (a linear matroid) and the algebraically independent subsets of a finite set of elements in a field extension (an algebraic matroid). With these examples in mind, the definition of matroid in terms of *independent sets* follows easily. See [B11, Chapter 3] for more on matroids.

For us, a central object is the *rigidity matroid* $\mathcal{R}_d(n)$ of complete graph K_n in dimension d . I will give two descriptions of $\mathcal{R}_d(n)$. The first is that $\mathcal{R}_d(n)$ is the linear matroid given by the rows of the rigidity matrix $R_{K_n,\mathbf{q}}$, where $\mathbf{q} \in (\mathbb{R}^d)^n$ is a suitably generic framework for K_n .

The reason for using K_n is that its rows of $R_{K_n,\mathbf{q}}$ correspond to edges of K_n , so picking a subset E of rows gives a graph $G(E)$ with edges E and vertices determined by the endpoints of E . Furthermore, if $\mathbf{q}_E$ are the elements of $\mathbf{q} \in (\mathbb{R}^d)^n$ indexed by $V(E)$, then rearranging

the columns of $R_{K_n, \mathbf{q}}$ gives

$$\text{rows of } R_{K_n, \mathbf{q}} \text{ indexed by } E = (R_{G(E), \mathbf{q}_E} \mid 0).$$

This allows us to relate local rigidity, infinitesimal rigidity and independence. For example, if $|V(E)| \geq d + 1$, then any two of the following imply the third:

- E is independent in $\mathcal{R}_d(n)$.
- E is locally rigid.
- $|E| = d|V(E)| - \binom{d+1}{2}$.

I will then discuss a classic result proved by Gerard Laman [81] in 1970, which states that a generic framework in $\mathbb{R}^2$ for G is minimally locally rigid if and only if

$$|E| = 2|V| - 3 \text{ and } |F| \leq 2|V(F)| - 3 \text{ for all } \emptyset \neq F \subseteq E.$$

(Minimally locally rigid means that the framework is locally rigid but ceases to be so when any edge is removed.) I will also mention the recent discovery of a 1927 paper by Hilda Pollaczek-Geiringer [96] that proves the same result.

This will be followed by a second description of the rigidity matroid $\mathcal{R}_d(n)$ as the algebraic matroid of the Cayley-Menger variety defined in the previous lecture.

I will finish with an application of $\mathcal{R}_d(n)$ to algebraic statistics, following the 2018 paper *The maximum likelihood threshold of a graph* by Gross and Sullivant [57]. After recalling the Gaussian normal distribution, I will define a *Gaussian graphical model* $\mathcal{N}(0, \Sigma)$ on $\mathbb{R}^n$, where the variables are indexed by the vertices of $G = (V, E)$ and the model is determined by a $n \times n$ symmetric positive definite matrix Σ with $(\Sigma^{-1})_{ij} = 0$ for $i \neq j$ and $ij \notin E$.

A key question for a Gaussian graphical model is how many observations $X^{(1)}, \dots, X^{(d)} \in \mathbb{R}^n$ are needed in order to ensure the existence of a maximum likelihood estimate with probability 1. It is straightforward to show that the MLE exists when $d \geq n$.

A 2012 theorem of Uhler [115] gives the following sufficient condition for the existence of the MLE. If $I_{n,d} \subseteq \mathbb{C}[x_{ij} \mid 1 \leq i \leq j \leq n]$ is the ideal defining the variety $\text{Sym}_d(n)$ of $n \times n$ symmetric matrices of rank $\leq d$, then the MLE exists with probability 1 for $G = (V, E)$ and d observations whenever

$$I_{n,d} \cap \mathbb{C}[x_{ii}, x_{ij} \mid i \in V, ij \in E] = \{0\}.$$

This can be interpreted as saying that $\{x_{ii}, x_{ij} \mid i \in V, ij \in E\}$ is an independent set in the algebraic matroid of $\text{Sym}_d(n)$ relative to the x_{ij} !

In the previous lecture, we noted a relation between symmetric matrices and Cayley-Menger varieties. This relation does not preserve the matroid structure, but in [57], Gross and Sullivant give a variant of this relation that leads to an isomorphism of matroids. This gives several interesting results. My favorite, which I will prove in detail, states that if G is a planar graph with n vertices, then the MLE of the Gaussian graphical model for G exists for $d \geq 4$ observations (with probability 1).

§3: *Polynomial Methods and Rigidity Theory* (Jessica Sidman). In combinatorial rigidity theory, linearized constraint equations are used to study a generic framework associated to a given graph G . In this setting, White and Whiteley defined a “pure condition,” a polynomial that vanishes for embeddings of G that are “special” or singular. In her lecture, Jessica will explain how this circle of ideas generalizes to other frameworks, including systems of constraints that arise in common CAD software packages.

Returning to bar-and-joint frameworks, Jessica will contrast polynomial methods with the linear-combinatorial ones. In particular, she will discuss rigidity of a framework in terms of various algebraic matroids associated to it.

FRIDAY: CHEMICAL REACTION NETWORKS

A system of chemical or biochemical reactions gives a system of differential equations by the law of mass action. These systems have a lovely structure whose analysis involves graph theory and toric varieties.

Background reading: [B5, Sections 1, 2] and [B6, Lectures 1, 2].

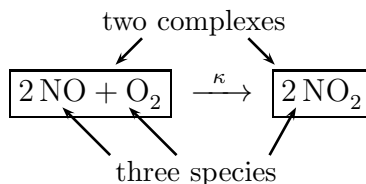
§1: *The Classical Theory of Chemical Reactions*. The standard way of writing a chemical reaction leads to a system of ODEs. An example involving nitrogen N and oxygen O is



with reaction rate κ . Applying the law of mass action leads to the system of ODEs

$$(3) \quad \begin{aligned} \frac{d[\text{NO}]}{dt} &= -2\kappa[\text{NO}]^2[\text{O}_2] \\ \frac{d[\text{O}_2]}{dt} &= -\kappa[\text{NO}]^2[\text{O}_2] \\ \frac{d[\text{NO}_2]}{dt} &= 2\kappa[\text{NO}]^2[\text{O}_2] \end{aligned} \quad \text{or} \quad \frac{d}{dt} \begin{pmatrix} [\text{NO}] \\ [\text{O}_2] \\ [\text{NO}_2] \end{pmatrix} = \underbrace{\begin{pmatrix} 2 & 0 \\ 1 & 0 \\ 0 & 2 \end{pmatrix}}_Y \underbrace{\begin{pmatrix} -\kappa & 0 \\ \kappa & 0 \end{pmatrix}}_{A_\kappa} \underbrace{\begin{pmatrix} [\text{NO}]^2[\text{O}_2] \\ [\text{NO}_2]^2 \end{pmatrix}}_\Phi,$$

where $[\dots]$ denotes concentration, Φ consists of monomials in the concentrations coming from the law of mass action, A_κ is the transposed Laplacian of the weighted directed graph $\bullet \xrightarrow{\kappa} \bullet$ underlying (2), and Y is the *stoichiometric matrix* that records the integer coefficients appearing in (2). We also have *species* and *complexes*:



In this lecture, I will begin with the law of mass action (including its subtleties [58]) and the general form of (3) for the vector of concentrations $\mathbf{x}$, which following [B6] is given by

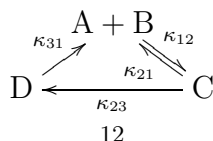
$$(4) \quad \frac{d\mathbf{x}}{dt} = Y A_\kappa \Phi(\mathbf{x}).$$

The steady states of such a system satisfy

$$(5) \quad Y A_\kappa \Phi(\mathbf{x}) = \mathbf{0}.$$

For chemists and biologists, the steady states of interest are positive. Since reaction rates for individual reactions are typically unknown, they are usually regarded as parameters, similar to the numerical polynomial systems discussed on Tuesday.

We often write a reaction network as a directed graph, such as



Note that the vertices are the complexes. If the directed graph is $G = (V, E)$, then the system (4) can be written

$$\frac{dx}{dt} = \sum_{i \rightarrow j \in E} \kappa_{i \rightarrow j} x^{y_i} (y_j - y_i), \quad x = (x_1, \dots, x_n)^t,$$

where the y_i are the columns of the stoichiometric matrix Y . This implies that solutions lie on translates of the *stoichiometric subspace* $S = \text{Span}(y_j - y_i \mid i \rightarrow j \in E)$. Intersecting these translates with the positive orthant gives *stoichiometric compatibility classes*.

As a more substantial example of the biochemical reaction network, I will revisit the HIV model presented on Tuesday. I will then pose some general questions about steady state solutions that involve *multistationarity* and whether solutions are locally or globally attracting within their stoichiometric compatibility class. This is also a good time to mention the creators of this theory, Fritz Horn, Roy Jackson and Martin Feinberg. Among their many papers are [44, 66, 67, 68].

I will conclude with complex balancing and the Deficiency Zero Theorem, proved by Horn in 1972 [66]. A network is *complex balanced* when it has a positive steady state solution $\mathbf{x}_*$ of (5) that is a solution at the level of the complexes, i.e., $A\Phi(\mathbf{x}_*) = \mathbf{0}$, $\mathbf{x}_* > 0$. In 1972, Feinberg [44] defined the *deficiency* of a network to be

$$\delta = m - \ell - s,$$

where m = number of complexes, ℓ = number of connected components of the underlying graph, and s = dimension of the stoichiometric subspace S . The Deficiency Zero Theorem states that a chemical reaction network is complex balanced for *every* set of positive reaction rates κ if and only if it has deficiency zero and is *weakly reversible* (meaning that every connected component of the underlying graph is strongly connected as a directed graph).

When the Deficiency Zero Theorem applies, the steady states are really nice:

- For *any* rate constants and *any* stoichiometric compatibility class, there is a *unique* positive steady state solution x_* .
- The solution x_* is *complex balanced* and *locally attracting*.

The (still open) *Global Attractor Conjecture* asserts that x_* is globally attracting.

§2: *Toric Dynamical Systems*. In 2009, Craicun, Dickenstein, Shiu and Sturmfels proposed the name *toric dynamical system* for differential equations of the form (4) that have a positive complex balanced steady state solution, i.e., $A_\kappa \Psi(\mathbf{x}_*) = \mathbf{0}$, $\mathbf{x}_* > 0$. There are two main reasons for the new name: the connection with toric varieties (more on this below) and the fact that many systems of the form (4) have nothing to do with chemistry. I will give examples from epidemiology and population genetics.

I will then use the example



to illustrate the Matrix Tree Theorem and show that we get a toric dynamical system if and only if $K_1 K_3 = K_2^2$, where

$$K_1 = \kappa_{21}\kappa_{31} + \kappa_{23}\kappa_{31} + \kappa_{32}\kappa_{21}$$

$$K_2 = \kappa_{12}\kappa_{32} + \kappa_{13}\kappa_{32} + \kappa_{31}\kappa_{12}$$

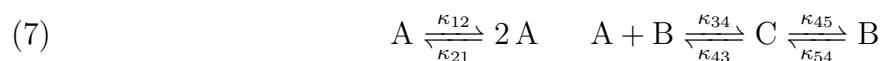
$$K_3 = \kappa_{13}\kappa_{23} + \kappa_{12}\kappa_{23} + \kappa_{21}\kappa_{13}.$$

It follows easily that (6) is a toric dynamical system when $K_1 K_3 = K_2^2$, which defines a toric variety when we use K_1, K_2, K_3 as coordinates. We will see that this is no accident.

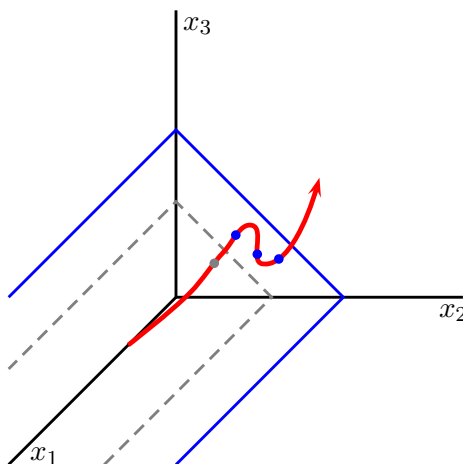
I will then spend some time on the paper [37], defining toric ideals T_G and M_G and showing how the latter leads algebraic equations generalizing $K_1 K_3 = K_2^2$ that characterize which rate constants give a toric dynamical system. I will also explain how the codimension of the variety defined by M_G reveals the intrinsic meaning of the deficiency defined in the previous lecture. This will give an immediate proof of the Deficiency Zero Theorem!

The next portion of the lecture will be devoted to the work of Karin Gatermann, whose papers [48, 49, 50, 51] published between 2001 and 2005 pioneered the use to toric methods in the study of chemical reaction networks. I will quote part of Maurice Rojas's Math Review [98] of one of her last papers before her tragic death in 2005.

To give of the flavor of what Gatermann did, I will follow a classic example



due to Edelstein in 1970 [41]. Feinberg studied this example in his 1979 lectures [B6] and gave a nice picture to illustrate how multistationarity can occur:

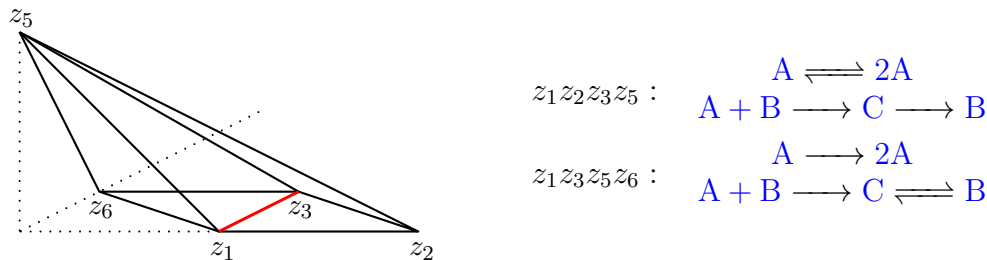


In 1989, Melenk, Möller and Neun [86] studied the steady states using Gröbner basis methods, and this example also appears in Gatermann's papers [49] (with Huber) and [50] (with Wolfrum). To get a sense of the depth of Gatermann's contributions, I will discuss the treatment of (7) in [50]. For this example, Gatermann and Wolfrum introduce *reaction coordinates* $z_1, \dots, z_6$ since (7) has six reactions. This leads to the *deformed toric ideal*

$$\langle z_4 - \alpha z_5, z_2 z_6 - \beta z_1 z_3 \rangle \subseteq \mathbb{Q}(\kappa)[z_1, \dots, z_6], \quad \alpha = \frac{\kappa_{43}}{\kappa_{45}}, \quad \beta = \frac{\kappa_{21}\kappa_{54}}{\kappa_{12}\kappa_{34}},$$

which has four Gröbner bases corresponding to *regular triangulations* of the polytope $P = \text{Conv}(y_1, y_2, y_3, y_4, y_4, y_5)$ (we think of these in terms of *edges*, so y_4 gets repeated). Here

is one of the triangulations, which shows how each simplex picks four vertices that give a simpler reaction network:



Geometrically, these simpler systems correspond to Gröbner deformations. An important observation of [50] is that multistationarity in one of these simpler systems can persist to the whole system. This idea underlies the recent research of Shiu and de Wolff [106] on classifying small networks. I should also note that in (7), the complex C is an example of an *intermediate*. A recent paper by Sadeghimanesh and Feliu [99] explores how intermediates influence the Gröbner basis of the network.

This is all very rich material, but there is a further surprise in store, for the expression

$$\sum_{i \rightarrow j} \underbrace{\kappa_{ij}}_{\text{weights}} \underbrace{x^{y_i}}_{\text{blending functions}} \underbrace{(y_j - y_i)}_{\text{control points}}$$

has a natural interpretation in geometric modeling. In fact, Gheorges Craicun, one of the authors of *Toric Dynamical Systems* [37], wrote a geometric modeling paper with García-Puente and Sottile [38] that relates Gröbner deformations (such as above) to the toric degenerations we saw on Wednesday. Craicun also wrote a paper with Feinberg [36] and posted an incomplete proof of the Global Attractor Conjecture in 2015 [35].

I will end by listing some further interesting topics about chemical reaction networks.

§3: *Algebraic Methods for the Study of Biochemical Reaction Networks* (Alicia Dickenstein). In recent years, techniques from computational and real algebraic geometry have been successfully used to address mathematical challenges in systems biology. The algebraic theory of chemical reaction systems aims to understand their dynamic behavior by taking advantage of the inherent algebraic structure in the kinetic equations, and does not need a priori determination of the parameters, which can be theoretically or practically impossible.

In her lecture, Alicia will describe general results based on the network structure. In particular, she will explain a general framework for biological systems, called MESSI systems, that describe *Modifications of type Enzyme-Substrate or Swap with Intermediates*, and include many post-translational modification networks. Alicia will also outline recent methods to address the important question of multistationarity.

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