Geometry of $\mathbb{R}$ roots of $9 \times 9$ Polynomial Systems: Analyzing Chemical Reaction Networks

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- These Chemical Reactions can be modeled by Chemical Reaction Networks.
Big Ideas

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- Modeling Phosphorylation and using Mass Action Kinetics to generate a $9 \times 9$ system of equations.
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• Interested in equilibria: when do they occur, where, and why?
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Use Discriminant Varieties to see what type of coefficients give us equilibria.

Use Linear Programming to see which of these regions are actually feasible.
Chemical Reaction Network

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Chemical Reaction Network

Phosphorylation: the enzyme-mediated edition of a phosphate group to a protein substrate.

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Protein make up the DNA/RNA of a cell which control most of the major functions of the cell.

Phosphorylation then activates certain functions of the cell by adding Phosphate groups to the protein Substrate.
Proteins being used in our case: Kinase, Phosphatase, and a Protein Substrate.
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Kinase: Protein that has the function of starting Phosphorylation.
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Kinase: Protein that has the function of starting Phosphorylation.

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Kinase: Protein that has the function of starting Phosphorylation.

Phosphatase: Protein that has the function of starting Dephosphorylation.

Protein Substrate: Holds a protein so that phosphate groups can be added and a function can take place.
For example,
For example,

Let’s say a cell is in need of sodium.
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This will signal Kinase to bind with Substrate, begin Phosphorylation, and sodium will start pumping in.
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This will signal Kinase to bind with Substrate, begin Phosphorylation, and sodium will start pumping in.

Once the cell has enough sodium, Phosphatase will be signaled to bind with a Substrate, begin Dephosphorylation, and sodium will stop pumping in.

Once Dephosphorylation stops, we get an equilibrium!
(1) A Protein Substrate with no Phosphate groups and a Kinase Protein are floating around.
(2) The Substrate and Kinase attach and bind together.
(3) The Kinase is absorbed and a Phosphate group is attached.
(4) The new (modified) Substrate with ONE Phosphate group and a new Kinase are floating around again, waiting to bind together.
(5) Process repeats.
Chemical Reaction Network: A weighted directed graph with complexes as the vertices and arrows labeled by reaction rate constants as the edges.
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When the substrate and kinase bind together:

\[ S_0 + K \rightarrow S_0 K \rightarrow S_1 + K \rightarrow S_1 K \rightarrow S_2 + K \]

Number of phosphate groups attached:

\[ S_2 + P \rightarrow S_2 P \rightarrow S_1 + P \rightarrow S_1 P \rightarrow S_0 + P \]
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Chemical Reaction Network - 3 Major Components

Chemical Reaction Network

\[ S_0 + K \xrightarrow{K_1} S_0 \xrightarrow{K_2} S_1 + K \xrightarrow{K_3} S_1 \xrightarrow{K_4} S_2 + K \]

\[ S_2 + P \xrightarrow{K_5} S_2 \xrightarrow{K_6} S_1 + P \xrightarrow{K_7} S_1 \xrightarrow{K_8} S_0 + P \]
Chemical Reaction Network - 3 Major Components

Reactions: Represented by arrows in the graph and labeled by the reaction rate constants.
Reaction Rate Constants: Give the rate at which each reaction happens.
These are defined by: $K_1, K_2, K_3, K_4, K_5, K_6, K_7, K_8$
Chemical Reaction Network - 3 Major Components

Complexes: The vertices in the graph and the chemical compound formed by the union of species. These are defined by:

- $S_0 + K \xrightarrow{K_1} S_0 K \xrightarrow{K_2} S_1 + K \xrightarrow{K_3} S_1 K \xrightarrow{K_4} S_2 + K$
- $S_2 + P \xrightarrow{K_5} S_2 P \xrightarrow{K_6} S_1 + P \xrightarrow{K_7} S_1 P \xrightarrow{K_8} S_0 + P$

Lacey Eagan Department of Mathematics, Texas A& Geometry of $\mathbb{R}$ roots of 9x9 Polynomial Systems: Analysis...
Chemical Reaction Network

Complexes: The vertices in the graph and the chemical compound formed by the union of species. These are defined by:

$S_0 + K, S_0K, S_1 + K, S_1K, S_2 + K, S_2 + P, S_2P, S_1 + P, S_1P, S_0 + P$
Chemical Reaction Network - 3 Major Components

Species: The molecules undergoing the reactions that make up the components of the complexes. These are defined by the following with $X_i$ representing the concentration of each species:

- $X_1 := S_0$
- $X_2 := S_1$
- $X_3 := S_2$
- $X_4 := S_0 K$
- $X_5 := S_1 K$
- $X_6 := S_1 P$
- $X_7 := S_2 P$
- $X_8 := S_3 P$
- $X_9 := S_4 P$

Geometry of $\mathbb{R}$ roots of 9x9 Polynomial Systems: Analysis
Species: The molecules undergoing the reactions that make up the components of the complexes. These are defined by the following with $X_i$ representing the concentration of each species:

$X_1 := S_0$, $X_2 := S_1$, $X_3 := S_2$, $X_4 := S_0 K$, $X_5 := S_1 K$,
$X_6 := S_1 P$, $X_7 := S_2 P$, $X_8 := K$, $X_9 := P$
MAK: The rate of an elementary reaction is proportional to the product of the concentrations of the species in the reactant.
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We use Mass Action Kinetics to obtain a system of Ordinary Differential Equations that model the Chemical Reaction Network.
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We use Mass Action Kinetics to obtain a system of Ordinary Differential Equations that model the Chemical Reaction Network.

In other words, we are going to look at the graph, and for each species, we will combine the rate of the reaction of that species each time it undergoes a reaction.

Since we have 9 species, we are looking for 9 rate equations represented by $\dot{X}_i = \frac{d}{dt} X_i$
Mass Action Kinetics

Chemical Reaction Network

\[
S_0 + K \xrightarrow{k_1} S_0 + K \xrightarrow{k_2} S_1 + K \xrightarrow{k_3} S_1 + K \xrightarrow{k_4} S_2 + K
\]

\[
S_2 + P \xrightarrow{k_5} S_2 + P \xrightarrow{k_6} S_1 + P \xrightarrow{k_7} S_1 + P \xrightarrow{k_8} S_0 + P
\]
Mass Action Kinetics

In the first case, the product of the concentrations is shown through the variables corresponding to the species $S_0$ and $K$.

Since $S_0$ is being lost as its own species in the reaction, the reaction rate becomes negative. This results in the first case of $X_1$ to look like:

$$-K_1 \cdot X_1 \cdot X_8 \cdot X_4$$
In the first case, the product of the concentrations is shown through the variables corresponding to the species $S_0$ and $K$.

Since $S_0$ is being lost as its own species in the reaction, the reaction rate becomes negative. This results in the first case of $X_1$ to look like:

$$-K_1 \cdot X_1 \cdot X_8$$
The second case is:

\[
S_1 P \xrightarrow{K_8} S_0 + P \\
X_6 \quad X_1 \quad X_9
\]
The second case is:

\[ K_8 \cdot X_6 \]
To get the final product for $\dot{X}_1$, combine the first and second cases together, resulting in the following equation:

$$-K_1 \cdot X_1 \cdot X_8 + K_8 \cdot X_6$$
Our 9 $\times$ 9 Polynomial System

\[
\begin{align*}
\dot{X}_1 &= -K_1 X_1 X_8 + K_8 X_6 \\
\dot{X}_2 &= K_2 X_4 - K_3 X_2 X_8 + K_6 X_7 - K_7 X_2 X_9 \\
\dot{X}_3 &= K_4 X_5 - K_5 X_3 X_9 \\
\dot{X}_4 &= K_1 X_1 X_8 - K_2 X_4 \\
\dot{X}_5 &= K_3 X_2 X_8 - K_4 X_5 \\
\dot{X}_6 &= K_7 X_2 X_9 - K_8 X_6 \\
\dot{X}_7 &= -K_5 X_3 X_9 - K_6 X_7 \\
\dot{X}_8 &= -K_1 X_1 X_8 + K_2 X_4 - K_3 X_2 X_8 + K_4 X_5 \\
\dot{X}_9 &= -K_5 X_3 X_9 + K_6 X_7 - K_7 X_2 X_9 + K_8 X_6
\end{align*}
\]
Conservation Laws

\[ S_{TOT} = X_1 + X_2 + X_3 + X_4 + X_5 + X_6 + X_7 \]
\[ K_{TOT} = X_4 + X_5 + X_8 \]
\[ P_{TOT} = X_6 + X_7 + X_9 \]
Reducing the $9 \times 9$

\[0 = \dot{X}_1 + \dot{X}_2 + \dot{X}_3 + \dot{X}_4 + \dot{X}_5 + \dot{X}_6 + \dot{X}_7\]
\[0 = \dot{X}_4 + \dot{X}_5 + X_8\]
\[0 = \dot{X}_6 + \dot{X}_7 + \dot{X}_9\]
Reducing the $9 \times 9$

\begin{align*}
0 &= -K_1 X_1 X_8 + K_8 X_6 \\
0 &= K_4 X_5 - K_5 X_3 X_9 \\
0 &= K_1 X_1 X_8 - K_2 X_4 \\
0 &= K_3 X_2 X_8 - K_4 X_5 \\
0 &= K_7 X_2 X_9 - K_8 X_6 \\
0 &= -K_5 X_3 X_9 - K_6 X_7
\end{align*}
Reducing the $9 \times 9$

\[
X_1 = \frac{K_7}{K_1} X_2 X_9 \\
X_3 = \frac{K_3}{K_5} X_2 X_8 \\
X_4 = \frac{K_7}{K_2} X_2 X_9 \\
X_5 = \frac{K_3}{K_4} X_2 X_8 \\
X_6 = \frac{K_7}{K_8} X_2 X_9 \\
X_7 = \frac{K_3}{K_6} X_2 X_8
\]

All functions of $(X_2, X_8, X_9)$
Reducing the $9 \times 9$ polynomial systems:

\[ S_{TOT} - K_{TOT} - P_{TOT} = \frac{K_7}{K_1} X_2 X_9 + X_2 + \frac{K_3}{K_5} X_2 X_8 - X_8 - X_9 \]

\[ K_{TOT} = \frac{K_7}{K_2} X_2 X_9 + \frac{K_3}{K_4} X_2 X_8 + X_8 \]

\[ P_{TOT} = \frac{K_7}{K_8} X_2 X_9 + \frac{K_3}{K_6} X_2 X_8 + X_9 \]
Reducing the $9 \times 9$

\[ c_1 X^2_8 + c_2 X_8 X_9 + c_3 X_8 + c_4 X_9 + c_5 = 0 \]
\[ c_6 X^2_9 + c_7 X_8 X_9 + c_8 X_8 + c_9 X_9 + c_{10} = 0 \]

$2 \times 2$ Quadratic Pentanomial System!
A-Discriminant Varieties

Definition:

If $A = [a_1, \cdots, a_t] \in \mathbb{Z}^{1 \times t}$ and $f(x) := c_1 x^{a_1} + \cdots + c_t x^{a_t}$ (with the $a_i$ distinct), the A-Discriminant Variety is:

$$\nabla_A := \{[c_1 : \cdots : c_t] \in \mathbb{P}_{\mathbb{C}}^{t-1} | f \text{ has a degenerate root in } \mathbb{C}\backslash\{0\}\}$$
Example:

\[ f(x) = c_0 + c_1 x + c_2 x^2 \]
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\[ \nabla_A = \{ [c_0 : c_1 : c_2] \in \mathbb{P}_2^\mathbb{C} | \{ \begin{array}{l} c_0 + c_1 x + c_2 x^2 = 0 \\ c_1 + 2c_2 x = 0 \end{array} \} \text{ has a root} \} \]
Example:

\[ f(x) = c_0 + c_1 x + c_2 x^2 \]

\[ \nabla_A = \{ [c_0 : c_1 : c_2] \in \mathbb{P}_\mathbb{C}^2 | \begin{cases} c_0 + c_1 x + c_2 x^2 = 0 \\ c_1 + 2c_2 x = 0 \end{cases} \} \text{ has a root} \}

After simplifying these equations,

\[ \nabla_A = \{ [c_0 : c_1 : c_2] \in \mathbb{P}_\mathbb{C}^2 | c_1^2 - 4c_0c_2 = 0 \} \]
A-Discriminant Varieties

Example:

\[ f(x) = c_0 + c_1 x + c_2 x^2 \]

\[ \nabla_A = \{ [c_0 : c_1 : c_2] \in \mathbb{P}_\mathbb{C}^2 \mid \begin{cases} c_0 + c_1 x + c_2 x^2 = 0 \\ c_1 + 2c_2 x = 0 \end{cases} \} \text{ has a root} \]

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A-Discriminant Polynomial \( \Delta_A: c_1^2 - 4c_0 c_2 \)
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A-Discriminant Polynomial \( \Delta_A: c_1^2 - 4c_0 c_2 \)

Thus, \( \nabla_A \) is the zero set of a polynomial.
Why is finding the Discriminant important?
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The Discriminant divides the coefficient space into regions with constant topology.
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We want to see which orthants $\nabla_A$ touches.
What orthants does $\nabla_A$ touch?

- Let $C := \text{cone over } \nabla_A$
- In coefficient space, $\mathbb{R}^t \setminus C$ is a union of connected regions where the number of positive roots of our system is constant
What orthants does $\nabla_A$ touch?

- If $\nabla_A$ does not intersect a particular orthant, then the number of positive roots is constant on the whole orthant.

Ex: $-1 - cx + x^2$ always has exactly 1 positive root if $c > 0$.
What orthants does $\nabla A$ touch?

- If $\nabla A$ intersects a particular orthant, then the number of positive roots can change.

Ex: If $a, b > 0$ then

$$x^6 + ay^3 - y$$
$$y^6 + bx^3 - x$$

can have 1, 3, or 5 positive roots!
Definition:

Given \( A = \{a_1, \cdots, a_m\} \subset \mathbb{Z}^N \) with \( \nabla_A \) a hypersurface, the discriminant locus \( \nabla_A \) is the closure of:

\[
\{ [u_1 \lambda^{a_1} : \cdots : u_m \lambda^{a_m}] \mid u \in \mathbb{C}^m, Au = 0, \sum_{i=1}^{m} u_i = 0, \lambda \in (\mathbb{C}^*)^n \}
\]

Thus, the null space of a \((n + 1) \times m\) matrix, \( \hat{A} \), provides a parametrization of \( \nabla_A \)
Horn-Kapranov Uniformization

\[
A = \begin{bmatrix}
0 & 1 & 0 & 4 & 1 \\
0 & 0 & 1 & 1 & 4
\end{bmatrix}
\]

\[c_1 + c_2 x + c_3 y + c_4 x^4 y + c_5 x y^4 \quad \text{and} \quad \nabla A \subset \mathbb{P}^4_{\mathbb{C}}\]

We can rescale by a polynomial, \(x\), or \(y\)!
Horn-Kapranov Uniformization

\[ A = \begin{bmatrix} 0 & 1 & 0 & 4 & 1 \\ 0 & 0 & 1 & 1 & 4 \end{bmatrix} \]

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We can rescale by a polynomial, x, or y!

\[ 1 + \alpha x + \beta y + x^4 y + x y^4 \] where this is reduced to 2 parametrics

\[ \varphi : \mathbb{P}_R^1 \rightarrow \mathbb{R}^2 \]
Theorem

The number of connected components of the real zero set of

\[ f(x) = \sum_{i=1}^{T} c_i x^{a_i} \] (suitably compactified) is constant when

\[ [c_1 : \cdots : c_T] \] ranges over a fixed connected component of

\[ \mathbb{P}^{T-1}_\mathbb{R} \setminus \nabla A \]

Ex: \( A = [0,1,2] \): when evaluating the connected components and the sign of \( \Delta_A \) is constant, the number of \( \mathbb{R} \) roots is 1 or 2, respectively.
Reduced A-Discriminant Contour

Example:

\[ A = [0, 1, 2, 3] \Rightarrow f(x) = c_1 + c_2 x + c_3 x^2 + c_4 x^3 \]

\[ \hat{A} = \begin{bmatrix} 1 & 1 & 1 & 1 \\ 0 & 1 & 2 & 3 \end{bmatrix} \Rightarrow B = \begin{bmatrix} 1 & 2 \\ -2 & -3 \\ 1 & 0 \\ 0 & 1 \end{bmatrix} \]

\[ C = \text{Reduced A-Discriminant Contour} = \{ (\log|\lambda_1: \lambda_2|) : B \subset \mathbb{R}^2 \} \]

This is NOT the same as the Discriminant Variety and loses information because of the absolute value signs. It takes away information about the coefficients.
Reduced A-Discriminant Contour

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\[ C = \text{Reduced A-Discriminant Contour} = \{ (\log|\lambda_1 : \lambda_2|B^T)B \subset \mathbb{R}^2 \} \]

This is NOT the same as the Discriminant Variety and loses information because of the absolute value signs. It takes away information about the coefficients.
We can fix the signs of $\sigma = (\text{sign}(c_1), \cdots, \text{sign}(c_4))$ to get $C_\sigma = \text{a piece of } C$ corresponding to $\nabla_A \cap \mathbb{P}_{\mathbb{R}}^{t-1}$ with $[c_1 : \cdots : c_4]$ having sign $\neq \sigma$.
We can fix the signs of $\sigma = (\text{sign}(c_1), \cdots, \text{sign}(c_4))$ to get $C_\sigma = \nabla_A \cap \mathbb{P}^{t-1}_\mathbb{R}$ with $[c_1 : \cdots : c_4]$ having sign $\neq \sigma$
Looking at Horn-Kapranov, we have...

\[
[c_1 : c_2 : c_3 : c_4] \in \mathbb{P}^3_\mathbb{R} \Rightarrow \text{sign}(\lambda_1 + 2\lambda_2) = \sigma_1 \text{ or } -\sigma_1 \\
\text{sign}(-2\lambda_1 - 3\lambda_2) = \sigma_2 \text{ or } -\sigma_2 \\
\text{sign}(\lambda_1) = \sigma_3 \text{ or } -\sigma_3 \\
\text{sign}(\lambda_2) = \sigma_4 \text{ or } -\sigma_4
\]
In the projective space...
In the projective space...
We are able to see how the roots behave depending on the coefficients using our A-Discriminant Varieties.

To get a more accurate version of this, we have to pay attention to the signs of the coefficients.

The different combinations of signs will tell us where the orthants of constant $\mathbb{R}$ roots are.

Our $2 \times 2$ system has 1024 sign combinations

Linear Programming will run through all 1024 possibilities and tell us which ones are feasible.
By Horn-Kapranov, the $\mathbb{P}^{t-1}_\mathbb{R} \cap \nabla A$ is given by:
$$(\text{vector of linear forms})^{\text{rational powers}} \ldots$$

So the possible signs of the coordinates of $\nabla A$ are described by:
$$(\text{sign}(\beta_1 \cdot \lambda), \ldots, \text{sign}(\beta_t \cdot \lambda))$$
where the null space $B$ looks like

$$B = \begin{bmatrix}
\beta_1 \\
\cdot \\
\cdot \\
\beta_T
\end{bmatrix}$$
In other words,
A choice of sign $\sigma := (\sigma_1, \cdots, \sigma_t) \in \{\pm 1\}^t$
occurs $\iff \exists \lambda = (\lambda_1, \cdots, \lambda_{t-n-1}) \in \mathbb{R}^{t-n-1}$
with $\text{sign}(\lambda \cdot \beta_1) = \sigma_1 \cdots \text{sign}(\lambda \cdot \beta_t) = \sigma_t$

So, for LP feasibility, we want to see if
$\lambda \cdot \beta_1 + \cdots + \lambda_{t-n-1} \cdot \beta_{t-n-1} \geq 0$
Linear Programming - Steps

\[ c_1X_8^2 + c_2X_8X_9 + c_3X_8 + c_4X_9 + c_5 = 0 \]
\[ c_6X_9^2 + c_7X_8X_9 + c_8X_8 + c_9X_9 + c_{10} = 0 \]

(1) Find the Cayley Embedding
(2) Find the corresponding B matrix
(3) Solve the following 1024 LP Feasibility problems to see which signs occur:

\[ \lambda \cdot \beta_1 > 0 \]
\[ \lambda \cdot \beta_1 < 0 \]
\[ \vdots \]
\[ \lambda \cdot \beta_{10} > 0 \]
\[ \lambda \cdot \beta_{10} < 0 \]
Step One: Cayley Embedding

\[ c_1 X_8^2 + c_2 X_8 X_9 + c_3 X_8 + c_4 X_9 + c_5 = 0 \]
\[ c_6 X_9^2 + c_7 X_8 X_9 + c_8 X_8 + c_9 X_9 + c_{10} = 0 \]

\[
A = \begin{bmatrix}
1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 \\
2 & 1 & 1 & 0 & 0 & 0 & 1 & 1 & 0 & 0 \\
0 & 1 & 0 & 1 & 0 & 2 & 1 & 0 & 1 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 1 & 1 & 1 & 1 & 1 \\
\end{bmatrix}
\]
Linear Programming

Step Two: Corresponding B Matrix

\[ B = \begin{bmatrix}
1 & 1 & -1 & -1 & 0 & 0 \\
-1 & 0 & 1 & 2 & 1 & 2 \\
-1 & -2 & 0 & -1 & -1 & -2 \\
1 & 0 & 0 & 0 & 0 & 0 \\
0 & 1 & 0 & 0 & 0 & 0 \\
0 & 0 & -1 & -1 & -1 & -1 \\
0 & 0 & 1 & 0 & 0 & 0 \\
0 & 0 & 0 & 1 & 0 & 0 \\
0 & 0 & 0 & 0 & 1 & 0 \\
0 & 0 & 0 & 0 & 0 & 1 
\end{bmatrix} \]
Linear Programming

Step Three: Solve the following 1024 LP Feasibility problems to see which signs occur

Standard Form LP:
Maximize $c \cdot x$ such that $Ax = b, x \geq 0$

Does there exist $\lambda$ such that

$$\lambda_1 \cdot \beta_1 + \cdots + \lambda_{t-n-1} \cdot \beta_{1,t-n-1} > 0$$

$$\cdots$$

$$\lambda_1 \cdot \beta_t + \cdots + \lambda_{t-n-1} \cdot \beta_{t,t-n-1} \leq 0$$

$$\lambda \beta^t \geq 0?$$
What does this tell us?

- 674 sign combinations where the inequalities are feasible
- Forced $c_5$ and $c_{10}$ to be positive, found 151 sign combinations where the inequalities are feasible
- 151 sign combinations that give us regions without constant $\mathbb{R}$ roots
- The rest of the sign combinations will give us constant $\mathbb{R}$ roots
- We are able to draw what the roots look like and see exactly which sign combinations give us what number of roots
- We will see error when our system has a sign combination in the group of 151 since these roots will vary