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

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Big Ideas

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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.

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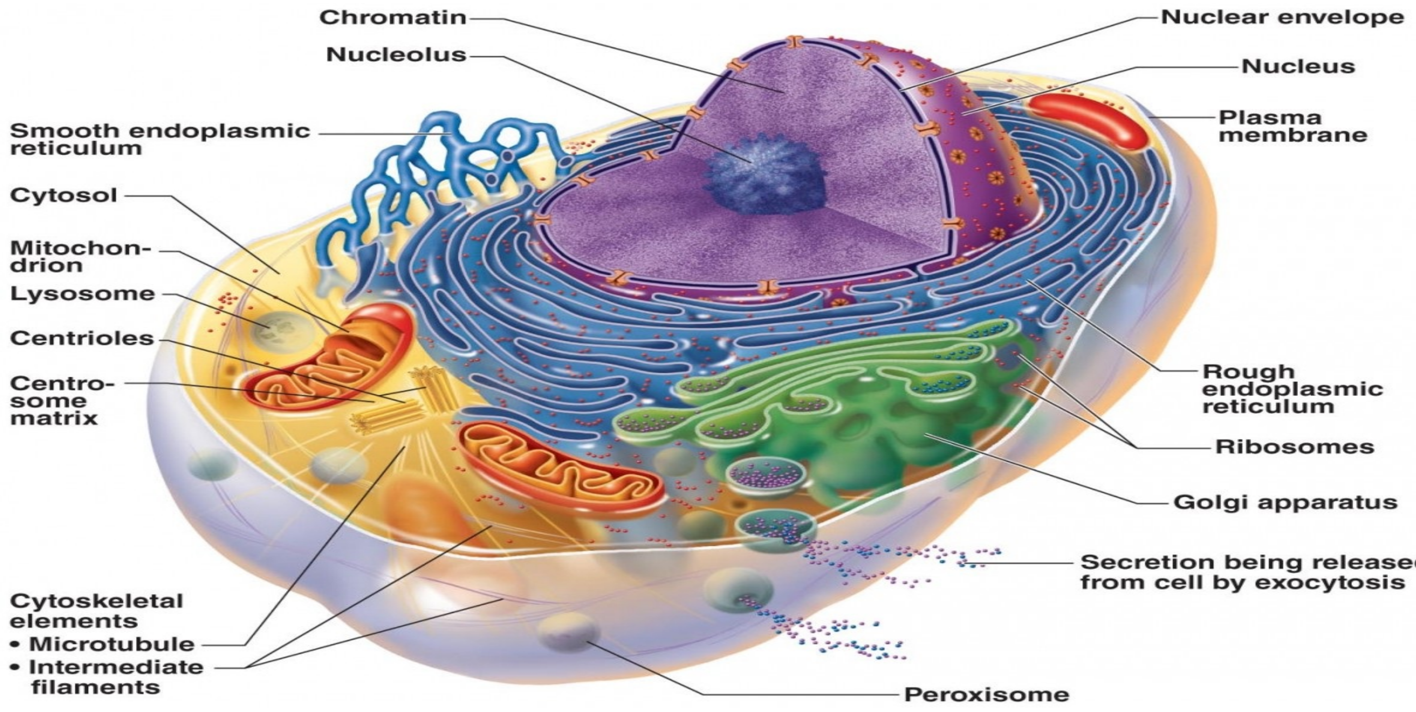

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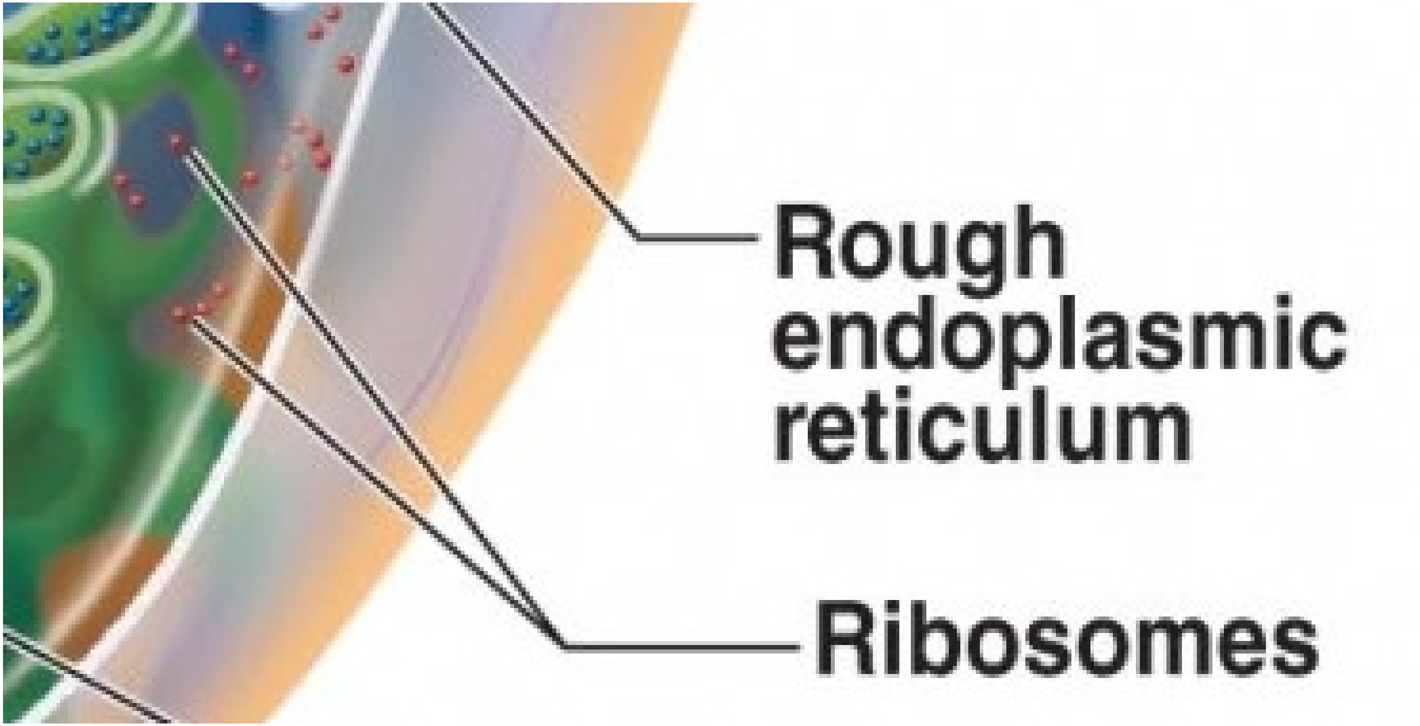

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Ribosome: Protein are made from multiple Amino Acids strung together as a chain.

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.

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,

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Let's say a cell is in need of sodium.

Chemical Reaction Network

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This will signal Kinase to bind with Substrate, begin Phosphorylation, and sodium will start pumping in.

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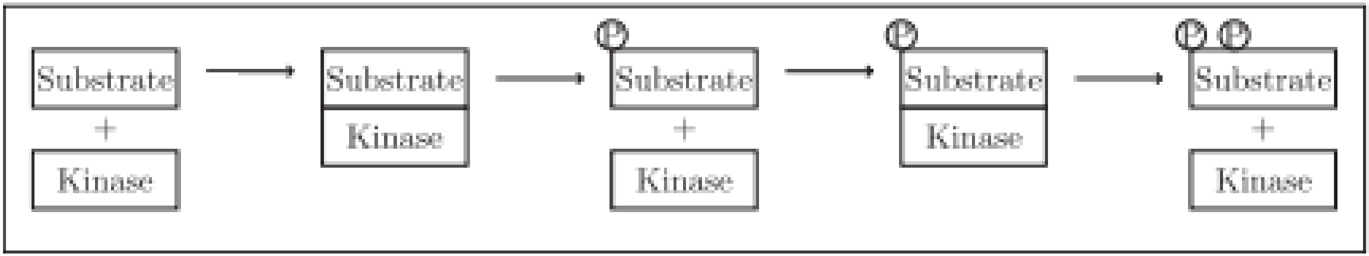
This will signal Kinase to bind with Substrate, begin Phosphorylation, and sodium will start pumping in.

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!

Definition



(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.

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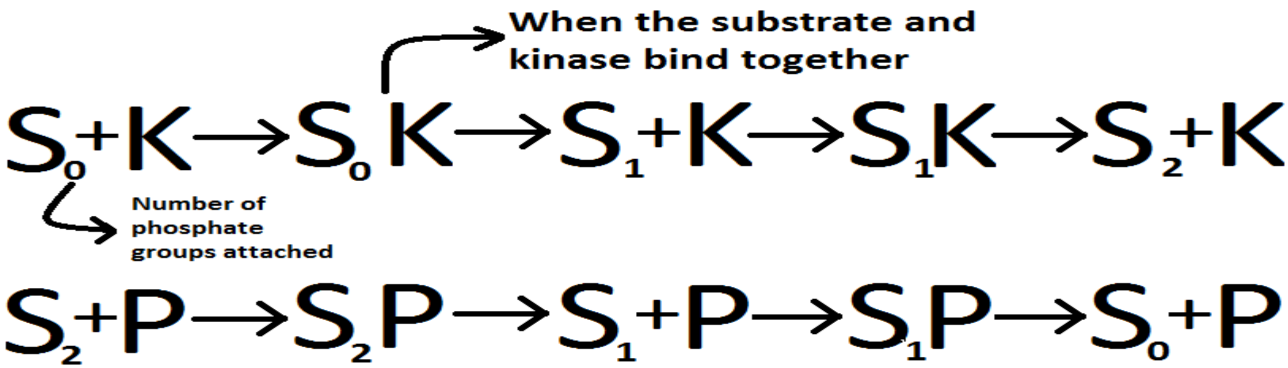

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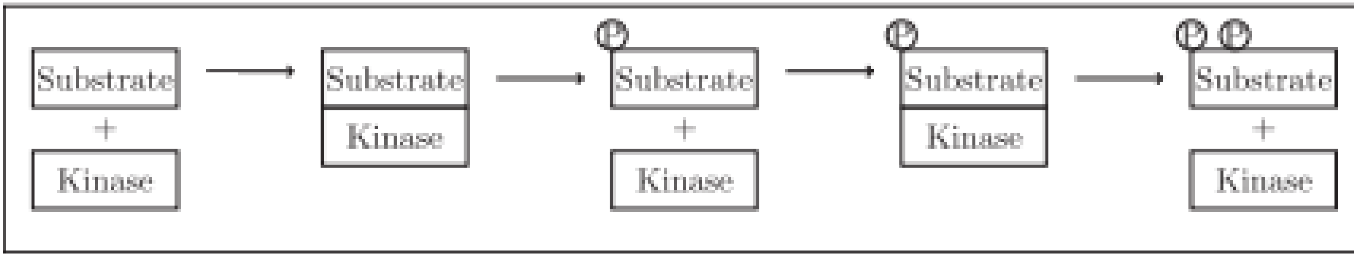

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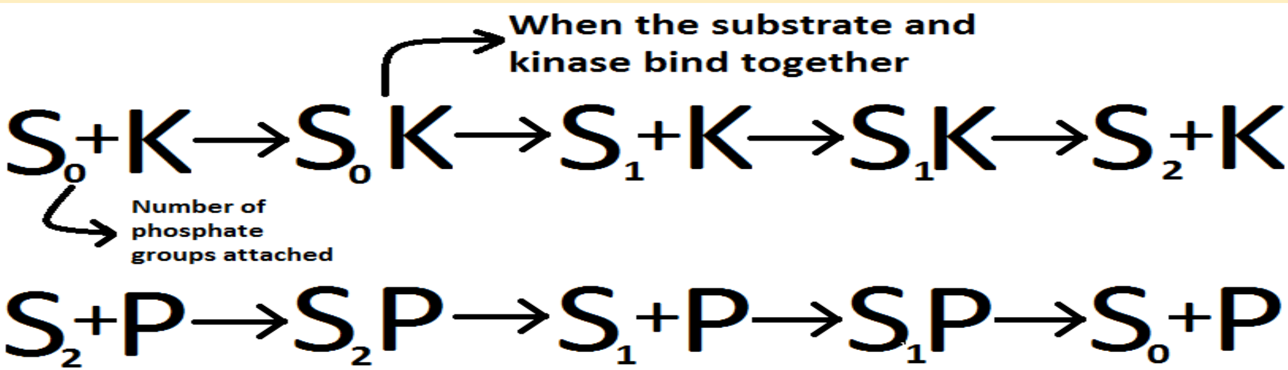

Chemical Reaction Network

$$S_0 + K \xrightarrow{K_1} S_0K \xrightarrow{K_2} S_1 + K \xrightarrow{K_3} S_1K \xrightarrow{K_4} S_2 + K$$

$$S_2 + P \xrightarrow{K_5} S_2P \xrightarrow{K_6} S_1 + P \xrightarrow{K_7} S_1P \xrightarrow{K_8} S_0 + P$$

Chemical Reaction Network - 3 Major Components

Chemical Reaction Network

$$S_0 + K \xrightarrow{K_1} S_0K \xrightarrow{K_2} S_1 + K \xrightarrow{K_3} S_1K \xrightarrow{K_4} S_2 + K$$

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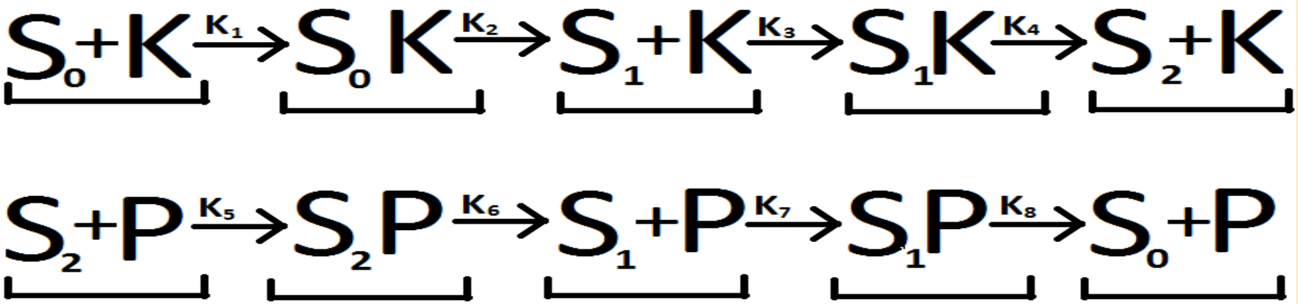
Reactions: Represented by arrows in the graph and labeled by the reaction rate constants.

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



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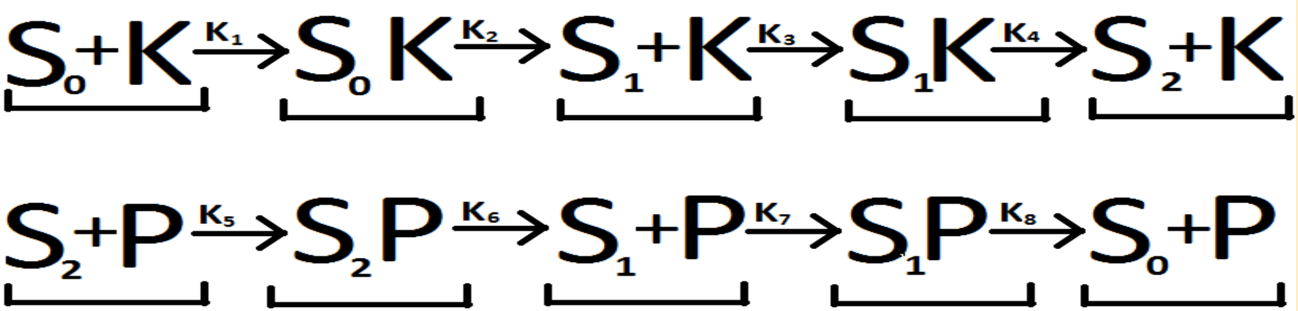

Complexes: The vertices in the graph and the chemical compound formed by the union of species.
These are defined by:
$S_0 + K, S_0K, S_1 + K, S_1K, S_2 + K, S_2 + P, S_2P,$
$S_1 + P, S_1P, S_0 + P$

Chemical Reaction Network

$$\underset{X_1}{S_0} + \underset{X_8}{K} \xrightarrow{K_1} \underset{X_4}{S_0K} \xrightarrow{K_2} \underset{X_2}{S_1} + \underset{X_8}{K} \xrightarrow{K_3} \underset{X_5}{S_1K} \xrightarrow{K_4} \underset{X_3}{S_2} + \underset{X_8}{K}$$

$$\underset{X_3}{S_2} + \underset{X_9}{P} \xrightarrow{K_5} \underset{X_7}{S_2P} \xrightarrow{K_6} \underset{X_2}{S_1} + \underset{X_9}{P} \xrightarrow{K_7} \underset{X_6}{S_1P} \xrightarrow{K_8} \underset{X_1}{S_0} + \underset{X_9}{P}$$

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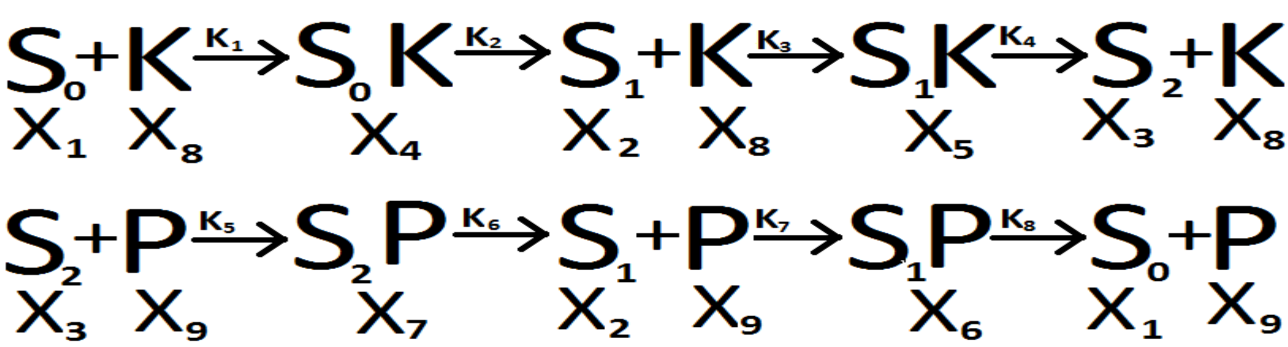

Species: The molecules undergoing the reactions that make up the components of the complexes.

These are defined by the following with X_i representing the concentration of each species:

$X_1 := S_0, X_2 := S_1, X_3 := S_2, X_4 := S_0K, X_5 := S_1K,$
$X_6 := S_1P, X_7 := S_2P, X_8 := K, X_9 := P$

Mass Action Kinetics

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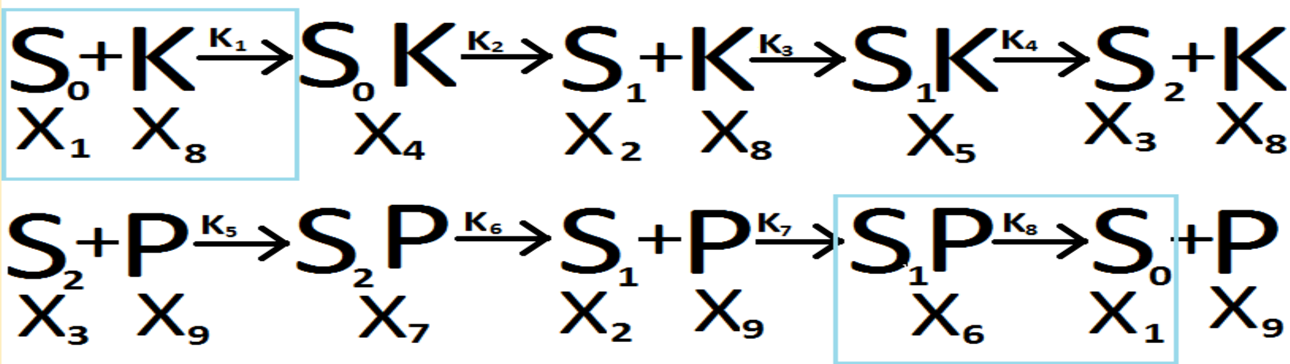
In other words, we are going to look at the graph, and for each species, we will combine the rate of the reaction of that species each time it undergoes a reaction.

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

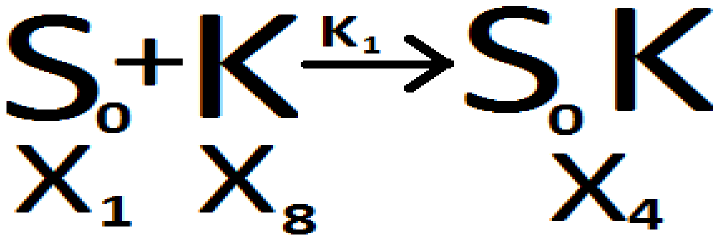


Mass Action Kinetics

$$S_0 + K \xrightarrow{K_1} S_0K$$

$$\underset{X_1}{S_0} \quad \underset{X_8}{K} \qquad \underset{X_4}{S_0K}$$

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.

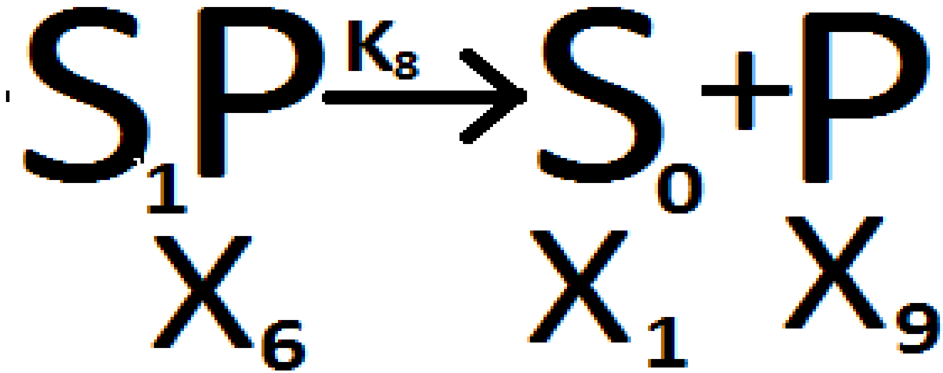
Since S_0 is being lost as its own species in the reaction, the reaction rate becomes negative. This results in the first case of X_1 to look like:

$$-K_1 \cdot X_1 \cdot X_8$$

Mass Action Kinetics

$$\underset{X_6}{S_1P} \xrightarrow{K_8} \underset{X_1}{S_0} + \underset{X_9}{P}$$

Mass Action Kinetics



The second case is:

$$K_8 \cdot X_6$$

Mass Action Kinetics

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 × 9 Polynomial System

$$\dot{X}_1 = -K_1X_1X_8 + K_8X_6$$
$$\dot{X}_2 = K_2X_4 - K_3X_2X_8 + K_6X_7 - K_7X_2X_9$$
$$\dot{X}_3 = K_4X_5 - K_5X_3X_9$$
$$\dot{X}_4 = K_1X_1X_8 - K_2X_4$$
$$\dot{X}_5 = K_3X_2X_8 - K_4X_5$$
$$\dot{X}_6 = K_7X_2X_9 - K_8X_6$$
$$\dot{X}_7 = -K_5X_3X_9 - K_6X_7$$
$$\dot{X}_8 = -K_1X_1X_8 + K_2X_4 - K_3X_2X_8 + K_4X_5$$
$$\dot{X}_9 = -K_5X_3X_9 + K_6X_7 - K_7X_2X_9 + K_8X_6$$

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 9×9

$$0 = \dot{X}_1 + \dot{X}_2 + \dot{X}_3 + \dot{X}_4 + \dot{X}_5 + \dot{X}_6 + \dot{X}_7$$
$$0 = \dot{X}_4 + \dot{X}_5 + X_8$$
$$0 = \dot{X}_6 + \dot{X}_7 + \dot{X}_9$$

Reducing the 9×9

$$
\begin{aligned}
0 &= -K_1X_1X_8 + K_8X_6 \\
0 &= K_4X_5 - K_5X_3X_9 \\
0 &= K_1X_1X_8 - K_2X_4 \\
0 &= K_3X_2X_8 - K_4X_5 \\
0 &= K_7X_2X_9 - K_8X_6 \\
0 &= -K_5X_3X_9 - K_6X_7
\end{aligned}
$$

Reducing the 9×9

$$X_1 = \frac{K_7}{K_1} X_2 X_9$$

$$X_3 = \frac{K_3}{K_5} X_2 X_8$$

$$X_4 = \frac{K_7}{K_2} X_2 X_9$$

$$X_5 = \frac{K_3}{K_4} X_2 X_8$$

$$X_6 = \frac{K_7}{K_8} X_2 X_9$$

$$X_7 = \frac{K_3}{K_6} X_2 X_8$$

All functions of (X_2, X_8, X_9)

Reducing the 9×9

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

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

$$P_{TOT} = \frac{K_7}{K_8} X_2 X_9 + \frac{K_3}{K_6} X_2 X_8 + X_9$$

Reducing the 9×9

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

2×2 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:

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

A-Discriminant Varieties

Example:

$f(x) = c_0 + c_1 x + c_2 x^2$

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$$\nabla_A = \{[c_0 : c_1 : c_2] \in \mathbb{P}^2_{\mathbb{C}} \mid \{ \begin{array}{l} c_0 + c_1x + c_2x^2 = 0 \\ c_1 + 2c_2x = 0 \end{array} \} \text{ has a root}\}$$

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After simplifying these equations,

$$\nabla_A = \{[c_0 : c_1 : c_2] \in \mathbb{P}^2_{\mathbb{C}} \mid c_1^2 - 4c_0c_2 = 0\}$$

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A-Discriminant Polynomial Δ_A: $c_1^2 - 4c_0c_2$

Thus, ∇_A is the zero set of a polynomial.

Why is finding the Discriminant important?

A-Discriminant Varieties - Motivation

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The Discriminant divides the coefficient space into regions with constant topology.

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The Discriminant divides the coefficient space into regions with constant topology.

We want to see which orthants ∇_A touches.

A-Discriminant Varieties - Motivation

What orthants does ∇_A touch?

- Let $C :=$ cone over∇_A
- In coefficient space, $\mathbb{R}^t \backslash C$ is a union of connected regions where the number of positive roots of our system is constant

A-Discriminant Varieties - Motivation

What orthants does ∇_A touch?

- If ∇_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 $c > 0$

A-Discriminant Varieties - Motivation

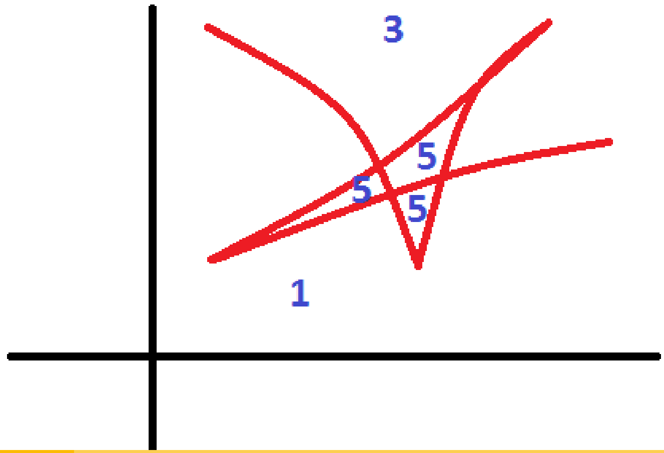
What orthants does ∇_A touch?

- If ∇_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!



Horn-Kapranov Uniformization

Definition:

Given $A = \{a_1, \cdots, a_m\} \subset \mathbb{Z}^N$ with ∇_A a hypersurface, the discriminant locus ∇_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 ∇_A

Horn-Kapranov Uniformization

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

$c_1 + c_2 x + c_3 y + c_4 x^4 y + c_5 x y^4$ and $\nabla_A \subset \mathbb{P}^4_{\mathbb{C}}$

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

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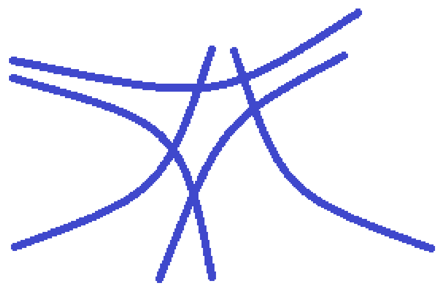
We can rescale by a polynomial, x, or y!

$1 + \alpha x + \beta y + x^4 y + x y^4$ where this is reduced to 2 parametrics
$\varphi : \mathbb{P}^1_{\mathbb{R}} \to \mathbb{R}^2$



Horn-Kapranov Uniformization

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 $\mathbb{P}_{\mathbb{R}}^{T-1} \backslash \nabla_A$

Ex: A = [0,1,2] : when evaluating the connected components and the sign of Δ_A is constant, the number of $\mathbb{R}$ roots is 1 or 2, respectively.

Reduced A-Discriminant Contour

Example:

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Example:

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

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 = 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.

Signed Reduced A-Discriminant Contour

We can fix the signs of $\sigma = (\text{sign}(c_1), \cdots, \text{sign}(c_4))$ to get $C_\sigma =$ a piece of C corresponding to $\nabla_A \cap \mathbb{P}^{t-1}_{\mathbb{R}}$ with $[c_1 : \cdot : c_4]$ having sign $\neq \sigma$

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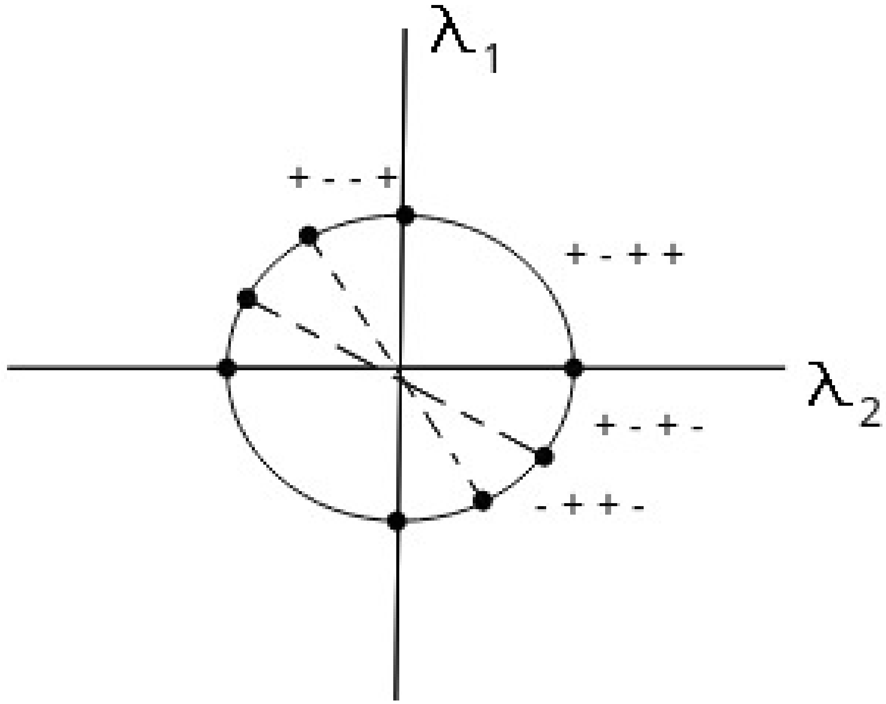
Looking at Horn-Kapranov, we have...

$$[c_1 : c_2 : c_3 : c_4] \in \mathbb{P}^3_{\mathbb{R}} \Rightarrow \begin{aligned} &\text{sign}(\lambda_1 + 2\lambda_2) = \sigma_1 \text{ or } -\sigma_1 \\ &\text{sign}(-2\lambda_1 - 3\lambda_2) = \sigma_2 \text{ or } -\sigma_2 \\ &\text{sign}(\lambda_1) = \sigma_3 \text{ or } -\sigma_3 \\ &\text{sign}(\lambda_2) = \sigma_4 \text{ or } -\sigma_4 \end{aligned}$$

Signed Reduced A-Discriminant Contour

In the projective space...



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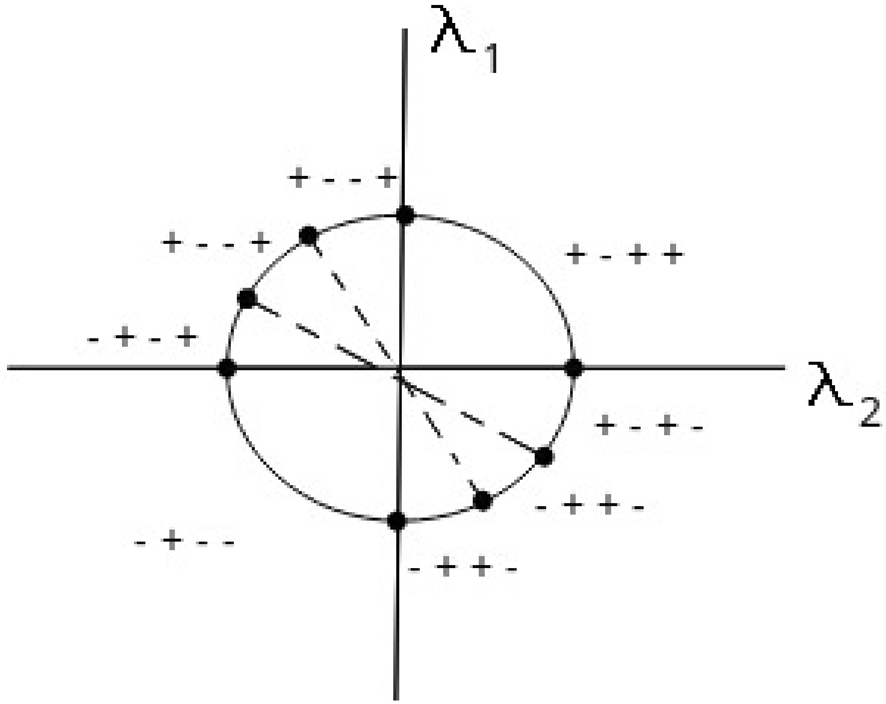

Linear Programming - Motivation

- 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 2×2 system has 1024 sign combinations
- Linear Programming will run through all 1024 possibilities and tell us which ones are feasible.

Linear Programming

By Horn-Kapranov, the $\mathbb{P}^{t-1}_{\mathbb{R}} \cap \nabla_A$ is given by:
$((\text{vector of linear forms})^{rationalpowers} \ldots)$

So the possible signs of the coordinates of ∇_A are described by:
$(sign(\beta_1 \cdot \lambda), \cdots, sign(\beta_t \cdot \lambda))$ where the null space B looks like

$$B = \begin{bmatrix} \beta_1 \\ \cdot \\ \cdot \\ \cdot \\ \beta_T \end{bmatrix}$$

Linear Programming

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

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

Linear Programming - Steps

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

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

$$\lambda \cdot \beta_1 \gtrless 0$$

$$\vdots$$

$$\lambda \cdot \beta_{10} \gtrless 0$$

Linear Programming

Step One: Cayley Embedding

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

$$A = \begin{bmatrix} 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 \\ 2 & 1 & 1 & 0 & 0 & 0 & 1 & 1 & 0 & 0 \\ 0 & 1 & 0 & 1 & 0 & 2 & 1 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 & 1 & 1 & 1 & 1 \end{bmatrix}$$

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 λ such that

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

$$\vdots$$

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

$\lambda \beta^t \substack{> \\ <} 0$?

Linear Programming - Conclusion

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