Listing of the

Non-Linear Systems Group Seminar
Winter 2005

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Atmospheric Reaction Equations

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January 14

Fairly complicated sets of chemical reactions equations are studied. The equations have constant, linear, and quadratics terms only, somewhat reminiscent of systems describing spread of infectious diseases. The simplest non-trivial case they studied is given by

$$\begin{aligned}
\dot{x_1} &= -k_2 x_1 x_5 + a_1 \\
\dot{x_2} &= -k_1 x_2 - k_3 x_6 x_2 - k_4 x_3 x_2 + k_5 x_4 + a_2 \\
\dot{x_3} &= -k_4 x_3 x_2 + k_5 x_4 - k_6 x_6 x_3 + a_3 \\
\dot{x_4} &= k_4 x_3 x_2 - k_5 x_4 + k_6 x_6 x_3 - k_7 x_5 x_4 \\
\dot{x_5} &= 2k_1 x_2 - k_2 x_5 x_1 + k_3 x_6 x_2 + k_6 x_3 - k_7 x_5 x_6 \\
\dot{x_6} &= -k_2 x_5 x_1 - k_3 x_6 x_2 - k_6 x_6 x_3
\end{aligned}$$

The variables are: $x_1 = CO, x_2 = O_3, x_3 = NO, x_4 = NO_2, x_5 = HO, x_6 = HO_2$.
Parameters: a_1, a_2, a_3, roughly between 10^3 and 10^6. The reaction speeds are on the order of:
$k_1 = 7 \cdot 10^{-8}, k_2 = 2 \cdot 10^{-13}$, $k_3 = 1.5 \cdot 10^{-15}$, $k_4 = 8 \cdot 10^{-15}, k_5 = 4 \cdot 10^{-3}, k_6 = 10^{-11}, k_7 = 1.3 \cdot 10^{-11}$.

Units were not given. The main problem here is: what are the stable equilibria of this system? In general, this means that one has to solve right hand side equals zero (to find the stable and unstable equilibria). This gives a system of coupled quadratic equations. In this case these equations can be fairly analytically easily solved and a stable equilibrium can be determined (though it is unclear if all equilibria in the positive orthant are determined this way). But in general (for more complicated systems), this is a hard non-linear problem. Tierney cited the paper *Basic Principles of Mechanical Theorem Proving* by W. T. Wu (J. Syst. Sc. and Math. Sc., Vol 4, No 3, 207-235, 1984) as using Gröbner bases to reduce the problem to a sort of 'triangular' form. Other suggestions that came up were to use 'monotonocity' à la Hirsch, and an argument recently devised by JJPV to address a similar problem that came up in connection with differential equations describing the growth of certain archaea.

Problems in Public Health

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January 21

Genetic susceptibility to Kidney and Breast Cancers.
Semenza assessed the gene-environment interactions between the two types of cancers and exposure to dietary carcinogens or medications in individuals, stratified by polymorphic variations in the NAT2 genotype for kidney cancer, and estrogen and tobacco smoke metabolism for breast cancer. In both cases, logistic regression and Mantel-Haeszel tests will be employed to assess main effects from environmental exposures and genetic background.

Determinants of the Spatial Distribution of Leukemia in Oregon.
Geocode and GIS are used to process demographic and geographic information, including socioeconomic status, toxic waste dumps, pesticide use by county, and superfund sites. The goal is to identify proximity of Leukemia cases to pollution sources. Spatial and temporal patterns will be explored to investigate disease clustering. Semenza uses the software package ClusterSeer which estimates exposure strength using the inverse of distance to the focus.

Public Health Implications of Coastal Water Pollution in California.
A study is underway to relate the density of Enterococcus bacteria in the coastal waters of Los Angles to GI illness. The difficulty resides in the question of how to factor in a wide range of possible other variables (coastal residents or tourists, industry, military, watershed characteristics, and so on). The purpose is to determine the risk to individual bathers from exposure to sewage and storm drain runoff. The modeling was done using Vensim software based on a health risk model developed by Cabeli (*Swimming Associated Gastroenteritis and Water Quality* Am. J. Epidemiol. 115(4): 606-616, 1982.) and/or Fleischer et al (*Water and Non-Water Related Risk Factors for Gastroenteritis among Bathers Exposed to Sewage Contaminated Waters* Int. J. Epidemiol. 22(4):298-708 1993).

Gröbner bases and solutions of systems of polynomial equations

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January 28

Given a basis (generating set) for an ideal of a polynomial ring, we try to find a "nicer" basis for the ideal which may, for example, be minimal or might have polynomials of lesser degrees or in less indeterminates. O'halloran discussed the algebraic formalism needed to work with Gröbner bases. The bases will be investigated in more detail in a follow up seminar on February 18.

Given any algebraically closed field F, $F[X] = F[x_1, x_2, ..., x_n]$ is the ring of polynomials over F in n indeterminates x_1 through x_n. The **variety** defined by $f_1, f_2, ..., f_k \in F[X]$ is the set of of common zeros. It is a subset of F^n and is defined as $\mathrm{V}(f_1, f_2, ..., f_k) = \{\alpha \in F^n : f_i(\alpha) = 0, \forall i = 1, ..k\}$.

For a subset S of F^n, the **ideal of *S*** is the set of polynomials that annihilate S: $I(S) = \{f \in F[X] : f(\alpha) = 0, \forall \alpha \in S\}$. The smallest ideal of $F[X]$ containing the set $\{f_1, f_2, ..., f_k\}$ — or the ideal **generated** by $\{f_1, f_2, ..., f_k\}$ — is defined as $\langle f_1, f_2, ..., f_k\rangle = \{\sum_{i=1}^{k} h_i f_i : h_i \in F[X]\}$.

The set $\{f_1, f_2, ..., f_k\}$ is called a **basis** of the ideal $\langle f_1, f_2, ..., f_k\rangle$. For an ideal I of $F[X]$, the **radical of I** is defined as $\sqrt{I} = \{f \in F[X] : f^r \in I \text{ for some non-negative integer } r\}$.

It turns out that

$$V(f_1, f_2, ..., f_k) = V(\sqrt{\langle f_1, f_2, ..., f_k\rangle} \quad \text{and} \quad I(V(f_1, f_2, ..., f_k)) = \sqrt{\langle f_1, f_2, ..., f_k\rangle}) \quad ,$$

and that there is a one to one correspondence between varieties in F^n and radical ideals in $F[X]$. The consequence of this fact is that given two sets $\{f_1, f_2, ..., f_k\}$ and $\{g_1, g_2, ..., g_t\}$,

$$V(f_1, f_2, ..., f_k) = V(g_1, g_2, ..., g_t) \iff \sqrt{\langle f_1, f_2, ..., f_k\rangle} = \sqrt{\langle g_1, g_2, ..., g_t\rangle} \quad .$$

Hence, solutions of equations in one basis will be the same in another satisfying the condition above on the radical ideals. One can go from a given basis to another using the division algorithm, or lexicographical or some other form of total ordering. This can be done using the Euclidean Algorithm: Let f, g, q, r in $F[X]$ such that $f = gq + r$. Then $V(f, g) = V(g, r)$. Thus, since

$$xy^2 = x(y^2 - y) + xy \quad ,$$

we can replace $\langle xy^2, y^2 - y\rangle$ by $\langle xy, y^2 - y\rangle$.

Viral Infections

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February 3

T-cells are highly specialized cells that can detect pathogens when they enter the bloodstream and then attack it. (Their name derives from the small organ behind the sternum that produces them: the thymus.) Any single cell is essentially sensitive to a single pathogen. Thus there are a limited number sensitive to any given pathogen. Once infection occurs and the T-cell comes in contact with the pathogen, they first multiply fast (essentially by cell-division) to create sufficient numbers to

combat the pathogen. Its number increases greatly and then after the infection subsides, decreases, though now with a more substantial permanent presence than before. Another change occurs after contact with the pathogen, namely the T-cell is "promoted" and becomes a "memory" cell instead of a "naive" cell. A memory cell is much more aggressive and effective in combating the infection than a naive cell. However, the organ that produces the T-cells, the thymus (hence the name T-cells), can produce only naive T-cells. The central question is: how does the body regulate the number of T-cells present (on the order of 10^{10} in the human body)?

Experiments are often done on mice. After the mouse reaches puberty, there is a 10-fold drop in the production of naive cells by its thymus. But other than that, the production of T-cells is not influenced by any factor such as disease (neither does it appear to favor T-cells sensitive to a particular pathogen when the body needs them). The total production is about $2 \cdot 10^6$ cells per day. And the total number of T-cells in a mouse is about 10^8 at any given time.

Memory cells are reported to divide in vitro once every 6 to 8 days. There are theoretical limits on the number of divisions a cell populations can go. Again one has reported 25 to 30 generations as the limit in vitro in the literature. This would imply that the memory cells die out in time (unless the pathogen is present) over time. However, once the individual is exposed to the pathogen the number of memory cells sensitive to that pathogen, remains constant. Früh and his colleagues are interested in modeling the dynamics of a cell population subject to division. It may be necessary to use more parameters which include the influences the naive cells and memory cells have on each other, and the organic surroundings on the T-cells .

Two papers were specifically mentioned: *The rescaling method for the turnover of cell populations* by S. S. Pilyugin et al. J. Theor. Biol., 225, 275-283, 2003 (also available at www.sciencedirect.com), and *Estimating average cellular turnover from ...* by R. J. De Boer et al, Proc. R. Soc. Lond. B, 270, 849-858, 2003.

Analysis of Brain Signals

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February 11

Frogs and toads have an essentially completely permeable skin. When they spend a substantial amount of time on dry land they can lose up to 30 or 40 percent of their weight from dehydration, whereas about 10 percent would be lethal to mammals. Dehydration of the body causes the salt concentration of the bodily fluids to go up drastically (salt does not evaporate with water). If the concentration of particles in the neurons of the frogs would stay the same, these cells would lose water to their surroundings (the "plasma") due the osmosis (the tendency to equalize particle concentration

on both sides of the cell-membrane would drive water out of the cell). The interstice between between two successive neurons — very long cells —, which ideally is on the order of nanometers would thus grow substantially. Signals that travel through the nerve system are of electrical nature while travelling within the neuron, but of chemical nature — and thus much slower — while bridging the interstice between two successive neurons. In the absence of a compensating mechanism, the salted (dehydrated frog) would process signals much slower than his sweet (wet) counterpart.

This compensating mechanism consists of some cellular machinery inside the neuron that, when the outside salt concentration rises, breaks certain proteins available within the cell into much smaller parts, thereby increasing the particle concentration inside the neuron. Thus the osmotic pressure is essentially reduced to zero. It is possible, for example, to measure the time delay between a "click" sound and the onset of the response of the auditory neuronal cells. This is done by putting electrodes on the skin of the frog, so that the response must have travelled through the nerve system before reaching the electrode. It turns out that the performance of the auditory system is maintained under conditions of high plasma salt concentration (as normally occurs when a frog ventures away from water for a day or two). Thus the effectiveness of this mechanism is generally excellent but for unknown reasons slightly different in distinct species of frogs, and in distinct individuals of the same species.

To understand these differences, the time-delays between the (very short) click and the first relevant valley of the auditory response signal is measured with great precision under experimental conditions that control the saltiness of the frog. The outstanding challenge is to design an algorithm that automatically detects the first valley of the response (and thus the delay). It turns out that in the the ideal case this may easily be done, but in general, due to the bad signal to noise ratio, especially in very salty frogs, this can be very hard, and sometimes relies on eye-balling the signals and extensive experience with them. Several methods are currently under investigation. They vary from naive peak detection algorithms, to Fourier Transform, to integrating the signal (and thereby smoothing it), and statistical analysis on a large number of signals where in each successive signal the frog is a little saltier. Currently no single method seems to stand out as universally reliable.

Gröbner bases and solutions of systems of polynomial equations II

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February 18

Given a basis (generating set) for an ideal of a polynomial ring, we try to find a "nicer" basis for the ideal which may, for example, be minimal or might have polynomials of lesser degrees or in less

indeterminates. This seminar is a sequel to the one given on January 28 (see above).

A **graded lexicographical ordering** on a set of polynomials is defined as follows: $x_1^{s_1}x_2^{s_2}...x_n^{s_n} < x_1^{t_1}x_2^{t_2}...x_n^{t_n}$ if $\sum s_i < \sum t_i$ or if $\sum s_i = \sum t_i$ and $s_i = t_i, i = 1, 2, ..., r$ and $s_r < t_r$ for some r between 1 and n inclusive. (Order by total degree, and within polynomials of the same degree apply the dictionary ordering.)

A set of polynomials $\{g_1, g_2, ..., g_r\}$ in $F[X]$ is a **Gröbner Basis** for an ideal I of $F[X]$ if for each nonzero $f \in I, \exists i$ such that the leading term (monomial term highest in the ordering) of g_i, $LT(g_i)$, divides the leading term, $LT(f)$, of f .

A Gröbner Bases is **reduced** if: i) The leading coefficient of $g_i = 1$ for all i. ii) For each g_i, no monomial of g_i is in the ideal $\langle LT(g_1), ..., LT(g_{i-1}), LT(g_{i+1}), \cdots, LT(g_r)\rangle$.

The main theorem is this area states that given an ideal and an ordering, there is a unique reduced Gröbner basis. This basis can in principle be calculated in finitely many steps. These calculations are done for two main reasons, namely to identify when two ideals are identical or not, and to simplify the calculation of the set of common zeros of an ideal (the variety).

For example, consider $I = \langle x^3 - 2xy, x^2y - 2y^2 + x\rangle \subset \mathbf{R}[X]$. The set $\{x^3 - 2xy, x^2y - 2y^2 + x\}$ is not a Gröbner basis of I relative to the graded lexicographical ordering since $x(x^2y - 2y^2 + x) - y(x^3 - 2xy) = x^2$ is in I, but the leading term of the two polynomials, namely x^2y and x^3, do not divide (the leading term of) x^2. So we may add x^2 to the basis. However, since we are interested in radical ideals (see January 28), we add x instead. By considering combinations of the first polynomial and x we see that we can add y to the basis as well. All these polynomials can be generated by the 'smaller' elements x and y, and so we get $\{x, y\}$ as a basis for I after excluding the redundant elements. It can be checked that this last set is in fact a reduced Gröbner basis for I. Note that the variety consists of the point $(x, y) = (0, 0)$, something that was not initially obvious.

In general, it is difficult to figure out how a a given basis may be "beefed up" so that the resulting set at the end is indeed a Gröbner or a reduced Gröbner basis. However, the effort is worthwhile since given an ideal I and an ordering on monomials, there exist a *unique* Gröbner basis for I. O'Halloran mentioned the book *Ideals, varieties, and algorithms* by Cox, Little, and O'Shea as a good reference for algorithms that construct Gröbner bases.

Iterated Function Systems

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February 25

An Iterated Function System is a (finite) collection $\mathcal{F}$ of affine contracting maps $\{f_i : \mathbb{R}^d \to \mathbb{R}^d\}_{i=1}^n$. For simplicity just assume that $d = 2$. Clearly $\mathcal{F}$ itself is not a function from $\mathbb{R}^2$ to itself. However,

it is not hard to see that $\mathcal{F}$ maps a compact set in $\mathbb{R}^2$ to another compact set. So we can consider $\mathcal{F}$ as a map from the space of compact sets in $\mathbb{R}^2$ to itself. The Hausdorff distance between two sets S_1 and S_2 is the infimum of the numbers ϵ such that the ϵ neighborhood of S_1 contains S_2 and vice versa. The collection of compact sets with this notion of distance becomes a metric space. And $\mathcal{F}$ is a contraction in that space. The Contracting Mapping Theorem implies that $\mathcal{F}$ has a unique fixed point, that is: there is a unique set S such that $S = \cup_i \, f_i S$.

A very well-known Iterated Function System is given by the collection of contractions in $\mathbb{R}^2$:

$$\{ \, f_1(x) = \frac{x}{2} \, , \; f_2(z) = \frac{z}{2} + \frac{1}{2} \, , \; f_3(x) = \frac{x}{2} + \frac{1}{2} e^{i\pi/3} \, \} \quad ,$$

in complex notation. Starting with any initial point x_0 in $\mathbb{R}^2$ (the 'seed'), and apply f_{i_1} to it to get x_1, then f_{i_2} to x_1 to get x_2 and so on. The previous paragraph now implies that after very few iterates the points of the sequence will lie very close to the fixed points set. This fixed point set is the well-known Sierpinski gasket. If we chose $\{i_j\}_{j=1}^N$ to be a random sequence in $\{1,2,3\}^N$ then the sequence $\{x_j\}_{j=1}^N$ will sample random regions of the gasket (after it converges to it). The points of this sequence (except the first) thus trace out a picture of the gasket.

Devaney presented this Iterated Function System in the form of a game known as the *chaos game*. The computer chooses an initial point x_0 and a region of the fractal. The player is supposed to give a sequence of N contractions such that x_N lies in the interior of the specified region. The player that can do that in the smallest number of moves, wins. Similar games can be played for more complicated Iterated Function Systems consisting of 4 or 5 , or more contractions, and the contractions themselves may involve rotations, or may not be conformal. The shapes of the invariant set get more and more complicated (the famous 'fern' for example) and the corresponding chaos game will be harder to play.

(As an amusing note we remark that another way to create the Sierpinski gasket is to write the binomial coefficients as a Pascal triangle. If an entry in the triangle is odd then it is part of the gasket otherwise it is not.)

Dynamics of Accumulation of Chemicals in Living Systems

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March 04

The majority of the advisories regarding pollutants in the United States are issued for Mercury, PCB's, Chlorodane, Dioxins, and DDT metabolites. These pollutants accumulate in living organisms through breathing, diet and other interactions of an organism with the environment. This process

is known as bio-accumulation. For example, methyl-mercury enters lakes and rivers by way of industrial waste disposal. It contaminates organisms that live in this environment. The fish that eat these organisms (and also live in the environment) are thus contaminated from two sources. In this way the offending material works it self through the food web and may accumulate in certain organism more than others. Thus in a given environment certain organisms may be very hazardous to humans while others are less so.

The model discussed is a "food web bio-accumulation model". These models are *compartmental*, that is: they assume that the distribution of a chemical in any single compartment is uniform. Depending on how many details the model contains, the individual compartments could be the different species in a certain food chain, or the different individuals present in the area, or even the different organs in one fish. An example of a model where each compartment is a species, was presented. It is based on: *F. A. P. C. Gobas, "A Model for Predicting the Bio-accumulation of Hydrophobic Organic Chemicals in Aquatic Food-Webs: Application to Lake Ontario", Ecological Modelling 69, 1-17, 1993.* The species taken into account are several types of Aquatic Macrophytes (aquatic plants), and several types of Benthic (bottom dwelling) Invertebrates, and Fish (the Spotted Gar). This results in a set (five) of linear first order ordinary differential equations of the following type.

$$\dot{x} = Ax + b$$

where A is a five by five matrix and b is a constant vector, and the components of x are the concentration of the chemical in each of the species. The desired information is the value and stability type of the equilibrium (which is $(I - A)^{-1}b$ if $(I - A)$ is invertible).

What complicates the analysis is that the model contains many parameters. Most of these are evaluated as composites of yet other parameters. Actual data on values of these last parameters are in most cases scarce and sometimes non-existent (and very hard to measure). Furthermore it is not unreasonable to suppose that many of these parameters vary from place to place (distance to the sewer etcetera) and even from time to time. In these cases one can use a statistical model to determine error bars on the value of the equilibrium that reflect our current knowledge. The suggestion also came up to run the the naive model based on the above differential equation for all the measured parameter values and determine error bars hat way (the simulation takes a fraction of a millisecond and there are relatively few data-points).

Monotone Dynamical Systems

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March 11

Monotone systems are common in biology, chemistry, control theory, and other fields. Such systems have in common that there is a field of 'positive cones' that is mapped into itself by the forward time map. This forces the ω-limit sets of the dynamics to be (geometrically) simple sets. This holds for maps, ordinary differential equations, as well as partial differential equations (hence the Banach space formulation below).

A *semiflow* is a map Φ from $X \times R_+ \to X$ with

$$\Phi_0 = id_X \quad \text{and} \quad \Phi_s \circ \Phi_t(X) = \Phi_{st}(X) \quad .$$

The notation $\Phi_t(x)$ simply means the position after time t of the orbit that started at x at time 0. The *orbit* of a point x is defined as $O(x) = \{\Phi_t(x) : t \geq 0\}$. The set of *equilibria* is the set $E = \{x : O(x) = \{x\}\}$.The *ω-limit set* of x is $\omega(x) = \bigcap_{t\geq 0} \overline{\cup_{s\geq t} \Phi_s(x)}$.

For a given Banach Space X (a complete normed linear space), define the *positive cone* K as a set which is non-empty and closed, and

$$\begin{aligned} R_+K &\subset K \\ K + K &\subset K \\ K \cap (-K) &= \{0\} \quad . \end{aligned}$$

For example, in $\mathbb{R}^2$, the positive quadrant R^2_+ is a positive cone. For partial differential equations, a more appropriate example of a Banach space is $L^2(X, \mu)$, the space of square integrable functions, or $C^0(X)$, the space of continuous functions. In the latter, the set of functions f so that $f(x) \geq 0$ almost everywhere is a positive cone. With respect to this cone a partial order in the Banach space can be defined:

$$x \geq y \quad \Longleftrightarrow \quad x - y \in K \quad .$$

Thus, in the first example, $x \geq y$ if and only if $x_1 \geq y_1$ and $x_2 \geq y_2$.

A *Monotone System* satisfies the condition that

$$x \geq y \quad \Longrightarrow \quad \Phi_t \geq \Phi_y \quad .$$

Here is one of the main results:
Convergence criterion: If $\overline{O(x)}$ is compact and if $\Phi_T(x) \geq x$ for some $T > 0$, then $\omega(x)$ consists of a T-periodic orbit. It follows that if $\Phi_t(x) \geq x$ for some t in some non-empty open subset of $(0, \infty)$, then $\Phi_t(x) \to p \in E$ (an equilibrium point) as t goes to ∞.
Slightly sharper version maybe obtained when one assumes a little more: strict monotonicity, or strong monotonicity.

Traditional applications of this theory are cooperative systems and competitive systems. These are systems of ordinary differential equations $\dot{x}_i = F_i(x)$ where $\frac{\partial}{\partial x_j} F_i(x)$ is always positive (in the first case) or always negative (in the latter case). For example the competitive system

$$\begin{aligned} \dot{x}_1 &= x_1(1 - x_1 - a_1 x_2) \\ \dot{x}_2 &= x_2(1 - x_2 - a_2 x_1) \quad , \end{aligned}$$

where the parameters are positive, is monotone in the positive quadrant. Unfortunately, while monotonicity with respect to one the standard orthants can be checked via combinatorial argument, there is no simple criterion to check in general whether a system is monotone. In the case of the deceptively simple competitive system in $\mathbb{R}^2$, the lines $1 - x_1 - a_1 x_2 = 0$ and $1 - x_2 - a_2 x_1$ cut the positive quadrant in 4 components. In each of these components the positivity cone is different!