3nd Meeting of

Young Researchers

Modelling Biological Processes

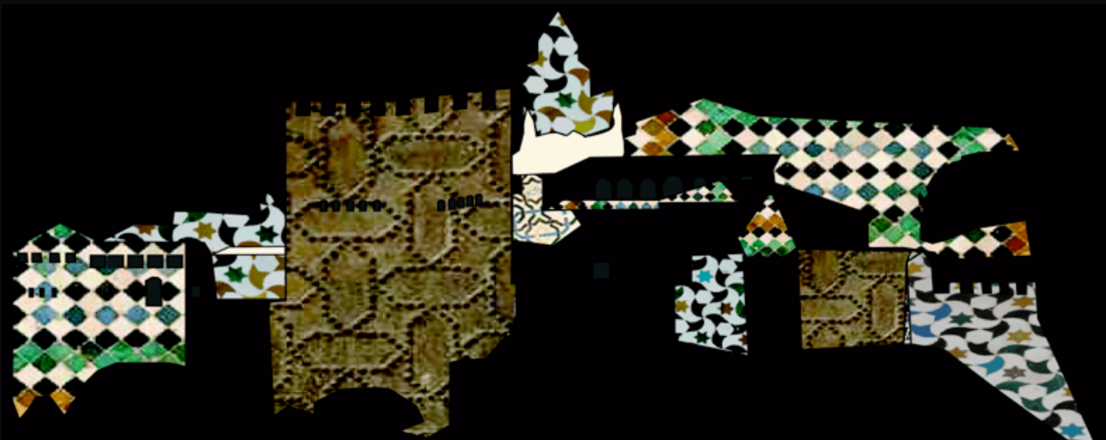
Granada, June 19-20, 2013

BOOK OF ABSTRACTS

BIOMAT 2013

Math 2013

Evolution and cooperation in social sciences and biomedicine



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Notes

1. Average conditions for permanence in N-species nonautonomous competitive systems of PDEs

In this talk we consider a nonautonomous systems of PDEs

$$\begin{cases} \dfrac{\partial u_i}{\partial t} = \mu_i \Delta u_i + f_i(t, x, u_1, \ldots, u_N) u_i, & t > 0,\ x \in \Omega,\ i = 1, \ldots, N \\ \mathcal{B}_i u_i = 0, & t > 0,\ x \in \partial\Omega,\ i = 1, \ldots, N, \end{cases}$$

where Ω is a bounded domain with a sufficiently smooth boundary $\partial\Omega$, Δ is the Laplace operator on Ω and $\mathcal{B}$ is the boundary operator of the Neumann or Dirichlet tpe. Applying the Ahmad and Lazer's definitions of lower and upper averages of a function we give average conditions for the permanence of the system. In the Neumann case we also give a sufficient condition for the system to be globally attractive.

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2. The construction of locally D–optimal designs by canonical forms to an extension for the logistic model

In the literature, it exits a special interest in the construction of optimal designs to the logistic regression models for binary data. Atkinson et al. (1995) consider an experiment based on the dose-response to a fly insecticide in which males and females respond in a different way. The considered model is $\log(\eta(x,q)/(1-\eta(x,q))) = \alpha + \beta x + \gamma q$, being $\eta(x,q)$ the probability of death of an insect, x the dose level and q a indicator variable which scores 0 for males and 1 for females. In this work, it is proposed the use of canonical forms, Ford et al. (1992), in order to compute D-optimal designs.

1. Optimal Design. The used design was an approximated design which suggests the following information matrix to a single observation x on an insect of unknown sex:

$$M(x,\theta) = 0.5\omega_M \begin{pmatrix} 1 & x & x^2 \\ x & x^2 & x \\ 1 & x & 1 \end{pmatrix} + 0.5\omega_F \begin{pmatrix} 1 & x & 0 \\ x & x^2 & 0 \\ 0 & 0 & 0 \end{pmatrix} \text{ with } \omega(x,\theta) = \eta(1-\eta)$$

The chosen criterion was D-optimality whose objetive is to minimize the volume of the confidence ellipsoid of the parameters.

2. Canonical Forms. Assuming known the insect sex, the change of variable $z = \alpha + \beta x$ involves a linear transformation in the information matrix so that $M_x(\xi) = B^{-1} M_z(\xi) B$. Due to the D-optimal criterion does not vary by non-singular linear transformations of the design space, the maximization problem of $M_x(\xi)$ determinant reduces to maximize $M_z(\xi)$.

Reformulating the problem and operating conveniently, the information matrix to n dose levels $z_1, z_2, ..., z_n$ and considering unknown sex results: $M_{z_1,z_2,...,z_n}(\xi) = 0.5 \sum_{k=1}^{2n} \xi(z_k) f_i(z_k) f_j(z_k)$. Written thereby, several formulas can be used to obtain an expression of the determinant.

3. Results. The developed work is based on experiments with two and three design points. Explicit expressions of the optimal weights are achieved from the above determinant formula for both. These are $p^* = \frac{2F-E\pm\sqrt{F^2-EF+E^2}}{3(F-E)}$ and $p^* = \frac{-B\pm\sqrt{B^2-3AC}}{3F}$ for two and three points respectively (considering in the last case a symetric design). The optimal design points are obtained by maximization routine to the determinant expression. The considered designs will be locally D-optimal in sene that they will depend on the estimations of the parameters in the model. The resuls are shown in the incoming table:

$\alpha = 1.804$, $\beta = 1.1757$				
$\gamma = -1$	x_i^*	-1.757	-0.018	
	p_i^*	0.5	0.5	
$\gamma = -2.599$	x_i^*	-1.347	-0.287	0.772
	p_i^*	0.375	0.250	0.375
$\gamma = -3$	x_i^*	-1.378	-0.173	1.032
	p_i^*	0.339	0.322	0.339
$\gamma = -5$	x_i^*	-1.349	0.396	2.141
	p_i^*	0.316	0.368	0.316

Table 1: locally D-optimal designs

An extension of the equivalence theorem let us to validate the optimal designs proposed in this work.

[1] Atkinson, A.C., Demetrio, C.G.B. and Zochhi, S.S., *Optimun Dose Levels when Males and Females Differ en Response*, Appl. Statist. **44(2)**, (1995), 213-226.

[2] Ford, I., Tosney, B. and Wu, C.F.J. , *The use of a canonical form in the construction of locally optimal designs for non-linear problems*, J. R. Statist. Soc. B.,**54 (2)**, (1992), 569-583.

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3. Evolutionary dynamics of populations with genotype–phenotype map

There is a complex relationship between genotype and phenotype. One of the outstanding features of this map is that is not a one-to-one map, because many genotypes are compatible with the same phenotype. Whereas genes are the entities passed on from one generation to the next and their frequencies measured over populations (the remit of population genetics), selection acts at the level of phenotypes. Thus, assigning fitness values to genes (mutant variants, different alleles, etc.) is not, in general, the valid approach. We are trying to put forward some of new properties we may expect to emerge when the genotype- phenotype difference is taken into account, both in a general setting and in particular cases related to disease. We have been focused on formulating models of evolutionary dynamical processes with genotype-phenotype map, give a definition of phenotype based on the attractors of simple models of the dynamics gene regulatory networks, and simulate it in order to ascertain its dynamical properties. We have introduced a bipartite network to study genotype and phenotype together and their structural relationship. Also a way to understand their structure is to study their clustering coeficient, existence of communities, which are related to phenotypic robustness, or connectivity between communities (it means, innovation).

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4. A kinetic theory approach to the modeling of crowd dynamics

This presentation deals with a kinetic theory approach to the modeling of crowd dynamics with the aim of showing how the dynamics at the micro-scale is transferred into collective behaviors. Time and space dynamics of the distribution function over the microscopic state of pedestrians, which includes position, velocity and activity variables is studied by the approach of the kinetic theory of active particles. In details, we show the model developed in [1, 2], which takes into account the complexity features of pedestrian crowds, that are related to the ability of individuals to develop a strategy based on that of the surrounding individuals. A qualitative analysis of the initial value problem follows, while some simulations that are developed by computational schemes based on splitting methods [2].

[1] N. Bellomo, A. Bellouquid, *On the modeling of crowd dynamics: looking at the beautiful shapes of swarms*, Networks and heterogeneous media **6(3)**, (2011), 383399.

[2] N. Bellomo, A. Bellouquid, D. Knopoff, *From the micro–scale to collective crowd-dynamics*, Multiscale modeling and simulations, (2013), submitted. arXiv:1301.5574 [math-ph].

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5. On quantum models of excitation energy transfer in photosynthesis

This contribution is devoted to introduce and compare some mathematical models for excitation energy transfer (EET), which are very useful in Chemistry and Biology. Also, EET processes are being increasingly studied because they constitute a key point to understand the dynamics of solar light harvesting ocurring in photosynthesis. In order to describe the pigment-pigment interaction, quantum coherence must be taken into account, and also it reveals essential to optimize the efficiency of the energy transmision. The interaction among pigments and the sorrounding protein inside the photosyntethic complexes, though, contributes to soothe such quantum effects. We discuss a suitable formalism to describe this situation as well as several models for EET, which have proved to be applicable in different real photosyntethic complexesm for instance, the well known Fenna–Matthews–Olsen complex.

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6. Rewards and coordination for public goods

Changes in global systems inevitably affect all things on earth. Voluntary cooperation to prevent global risk suffers from self–interested behaviours. Exploiters can free-ride on others efforts. In game–theoretical studies, such social dilemmas have often been investigated by using public good games. It has turned out that cooperation can be sustained by combining public good games with rewards, which are selective incentives for cooperative behaviour [1]. The previous model considered three strategies: to be (a) a cooperator or (b) a defector in the standard public goods game, or to be (c) a rewarder, who contributes both to the public good and to a fund that rewards players who contribute during the game. Only those who contribute in the public good game can be invited into the center of the charmed circle [2] with rewards. They can spread even in a population of the defectors, since these are excluded from the rewards. The incentive system itself, however, is voluntary and costly. Thus, this scheme can easily be subvert by cooperators who contribute to the public good, but not to the rewards; in the next step, since contribution to the public good game itself is costly, too, cooperators will be eliminated by the first-order-freeriding defectors. As a result, the replicator dynamics for the three strategies can exhibit a rock-scissors-paper cycle [1]. Here we discuss an extensive application of reward funds to a public good game with a provision threshold. Such models have recently drawn much at- tention, and are used to explore collective-risk social dilemmas, such as issues of climate changes. We show when and how a cooperative equilibrium can be selected in the collective-risk dilemma game, irrespective of the initial state, by using the reward fund as a mechanism for providing positive incentives.

[1] T. Sasaki, T. Unemi, Replicator dynamics in public goods games with reward funds, *Journal of Theoretical Biology* **287**, (2011), 109114.

[2] M. Olson, *The Logic of Col lective Action: Public Goods and the Theory of Groups*, Cambridge, MA: Harvard University Press, (1965), p. 61.

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7. Accurate and robust finite element solvers for chemotaxis–dominated partial differential equations

Up to the present, many scientists encouraged themselves in modelling complex chemotaxis systems of PDEs by introducing kinetic terms, incorporating certain quorum-sensing or volume-filling mechanisms or even extend the system to multiple species/chemical agents. However most of this research lacks of a very important issue, the implementation of a numerically well elaborated solver. From numerical point of view this is far from being trivial. Even for the minimal model it is numerically challenging to tackle the chemotaxis term. Almost comparable with convection-dominated flows in the CFD world, the main task is to guarantee positivity and mass conservation, which necessitates special stabilization techniques. We developed a Finite Element based solver for chemotaxis PDEs incorporating various finite elements in 2D and 3D, a variety of boundary conditions, a large selection of iterative sub-solvers, a FCT/TVD stabilization technique and arbitrary user-prescribed model parameters. Its applicability on serveral models, like blowing up solutions and pattern formation, has already verified the reliability of this solver, [1, 2]. Moreover integrating already developed paradigms, like parallelization, fast multigrid solvers and r- and h-adaptivity, will extend the application to a level which enables to tackle even fully coupled multi-species systems of chemotaxis.

[1] R. Strehl, A. Sokolov, D. Kuzmin and S. Turek, A flux-corrected finite element method for chemotaxis problems, *CMAM* **10**, (2010), 118131.

[2] R. Strehl, A. Sokolov, D. Kuzmin, D. Horstmann and S. Turek, A positivity-preserving finite element method for chemotaxis problems in 3D, *Journal of Computational and Applied Mathematics* **239**, (2013), 290303.

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