Experimental Mathematics in dynamical Systems

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Outline

Our point of view and a fast review of our current research

- 1 Numerical techniques to explore complex behaviors
- 2 Experimental mathematics: high-precision and more ...
- 3 Need to mixing techniques (so collaborations): "bailar juntos"
- 4 Need to prove some results: CAP
- 5 Need to use "problem"-specific techniques: kneading plots

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Numerical tools (the need of a lot of techniques ...)



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Experimental Mathematics

What is TIDES?

TIDES: a Taylor series Integrator for Differential EquationS

- Taylor series method using Variable-Stepsize Variable-Order formulation and extended formulas for the variational equations.
- Free numerical software based on extended Taylor series method: TIDES*.
 - *Extremely easy* to use via a MATHEMATICA preprocessor. NOW INCLUDED IN SAGE (2014)!!!
- Automatic construction of Fortran or C codes for solving ODEs
- Automatic construction of C codes for solving solutions of ODEs and variational equations up to any order (and sensitivities with respect to any parameter up to any order)
- Easy to use arbitrary precision (do you need 500 digits?, 1000?)

Where?: http://cody.unizar.es/software or email: tides.taylor@gmail.com, rbarrio@unizar.es

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Experimental Mathematics

^{*}A. Abad, R. Barrio, F. Blesa and M. Rodriguez, "Algorithm 924: TIDES, a Taylor series Integrator for Differential EquationS," ACM Trans. Math. Software, Volume 39(1), 2012

Numerical techniques to explore complex behaviors

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Experimental mathematics in Dynamical Systems

Origin of the discipline in Spain

---> Prof. Carles Simó (Universidad de Barcelona)



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"Experimental mathematics" has emerged in the past 25 years or so to become a competitive paradigm for research in the mathematical sciences.

So what exactly is "experimental mathematics"? While several definitions have been offered, perhaps the most succinct definition is given in the Borwein-Devlin book *The Computer as Crucible*:

Experimental mathematics is the use of a computer to run computations — sometimes no more than trial-and-error tests — to look for patterns, to identify particular numbers and sequences, to gather evidence in support of specific mathematical assertions that may themselves arise by computational means, including search.

Here we should distinguish "experimental mathematics" from "computational mathematics" and "numerical mathematics." While there is no clear delineation, the latter two terms generally encompass computational methods for concrete applied mathematics and engineering applications.

[†]D.H. Bailey, R. Barrio, J.M. Borwein, High-precision computation: Mathematical physics and dynamics, Appl. Math. Comput. 218(20), pp 10106-10121 (2012)

Experimental mathematics: books



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Experimental Mathematics

Progress of Scientific Supercomputers: Data from the Top500 List



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Experimental math: Discovering new mathematical results by computer

- Compute various mathematical entities (limits, infinite series sums, definite integrals) to high precision, typically 100-1000 digits.
- Use algorithms such as PSLQ to recognize these entities in terms of wellknown mathematical constants.
- When results are found experimentally, seek to find formal mathematical proofs of the discovered relations.
- Many results have recently been found using this methodology, both in pure mathematics and in mathematical physics.



Computing: The Third Mode of Scientific Discovery



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- R. Barrio, M. Lefranc, M.A. Martinez, S. Serrano, Symbolic dynamical unfolding of spike-adding bifurcations in chaotic neuron models, Europhysics Letter (EPL), submitted, 2014.
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- R. Barrio, A. Shilnikov, Parameter-sweeping techniques for temporal dynamics of neuronal systems: case study of Hindmarsh-Rose model, The Journal of Mathematical Neuroscience (JMN) 1 (1), 1-22, 2011.

Mathematical neuron models

The Hodgkin-Huxley model is a mathematical model that describes how action potentials in neurons are initiated and propagated.

Alan Lloyd Hodgkin and Andrew Huxley described the model in 1952 to explain the ionic mechanisms underlying the initiation and propagation of action potentials in the squid giant axon. They received the 1963 Nobel Prize in Medicine for this work.



Other mathematical models:

FitzHugh-Nagumo model, Morris-Lecar model, Hindmarsh-Rose model (1984), ...

The leech heart interneuron model[‡]

[‡]Weaver, A.L., Roffman, R.C., Norris, B.J., Calabrese, R.L. A role for compromise: synaptic inhibition and electrical coupling interact to control phasing in the leech heartbeat CpG. Frontiers in behavioral neuroscience. 2010.

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The leech heart interneuron model

- Onion-like structures.
- Spike-adding bifurcations \longrightarrow UPOs foliated in the attractor \longrightarrow ??

The Hindmarsh and Rose model (1984)

A phenomenological system of ODEs for modeling bursting and spiking oscillatory activities in isolated neurons:

$$\dot{x} = y - ax^3 + bx^2 - z + I \dot{y} = c - dx^2 - y$$

$$\dot{z} = \varepsilon(s(x - x_0) - z)$$

$$(1)$$

- x is treated as the membrane potential, while y and z describe some fast and slow gating variables for ionic currents.
- Slow "activation" of z is due to the small parameter $0 < \varepsilon \ll 1$.
- The parameters are typically set as a = 1, c = 1, d = 5, s = 4, $x_0 = -1.6$ and $\varepsilon = 0.01$.
- A key parameter is the external applied current *I*.

Fast-slow decomposition

Fast-slow decomposition

Bursting classification (Rinzel-Izhikevich)

		bifurcations of limit cycles				
		saddle-node on invariant circle	saddle homoclinic orbit	supercritical Andronov- Hopf	fold limit cycle	
turcations of equilibria	saddle-node (fold)	fold/ circle	fold/ homoclinic	fold/ Hopf	fold/ fold cycle	
	saddle-node on invariant circle	circle/ circle	circle/ homoclinic	circle/ Hopf	circle/ fold cycle	
	supercritical Andronov- Hopf	Hopf/ circle	Hopf/ homoclinic	Hopf/ Hopf	Hopf/ fold cycle	
ā	sub critical Andronov- Hopf	subHopt/ circle	subHopf/ homoclinic	subHopf/ Hopf	subHopf/ fold cycle	

Square-wave bursting (fold/hom bursting)

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But ... why and where is the chaotic behavior?

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Scheme of the macroscopic chaotic structures $(\forall \varepsilon)$

The Hindmarsh and Rose model: bifurcation analysis

Codimension-two homoclinic bifurcation points

• Inclination flip

• Inclination flip + orbit flip homoclinic bifurcations

The Hindmarsh and Rose model

Hindmarsh and Rose: bifurcation sketch

Given a three-dimensional (3D) hyperbolic chaotic flow Φ_t , Birman and Williams define the following equivalence relation which identifies points of the invariant set Λ having the same asymptotic future:

$$\forall x, y \in \Lambda, \quad x \sim y \Leftrightarrow \lim_{t \to \infty} ||\Phi_t(x) - \Phi_t(y)|| = 0$$

The Birman-Williams theorem states:

- In the set of equivalence classes, the hyperbolic flow Φ_t induces a semi-flow Φ_t on a branched manifold *K*. The pair (Φ_t, *K*) is called a *template*, or knot-holder
- Unstable periodic orbits of Φ_t in Λ are in one-to-one correspondence with unstable periodic orbits of (Φ_t in *K*). Moreover, every link of unstable periodic orbits of (Φ_t, Λ) is isotopic to the corresponding link of (Φ_t, *K*).

Topological templates

Left: two periodic orbits of periods 1 and 4 embedded in a strange attractor; Right: a link of two knots that is equivalent to the pair of periodic orbits up to continuous deformations without crossings.

Topological templates: subtemplates

The Hindmarsh and Rose model: chaotic attractors

Topological templates: Hindmarsh and Rose model

Topological templates: Hindmarsh and Rose model

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Topological templates: Hindmarsh and Rose model

The templates follows the "onion" structure.

Proper grammar of the symbolic sequences

 \longrightarrow (forbidden symbolic sequences)

Topological templates: successive Cantor structures

Theoretical framework for the "onion-bulb" chaotic structures

Numerical techniques to explore complex behaviors

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- R. Barrio, A. Martinez, S. Serrano, D. Wilczak, When chaos meets hyperchaos, submitted for publication, 2014.
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- R. Barrio, A. Dena and W. Tucker, *A data-base of rigorous and high-precision periodic orbits of the Lorenz model*, submitted for publication (2014).

R. Barrio, M. Rodriguez, F. Blesa, *Computer-assisted proof of skeletons of periodic orbits*, Computer Physics Communications 183 (1), 80-85, 2012.

Classical hyperchaos was invented by Sinai (around 1978). He showed that billiards colliding in 3D produce maximal chaos, that is, possess n - 1 positive Lyapunov characteristic exponents.

Ya.G. Sinai, Appendix to the translation of S. Krylov, Works on the Foundations of Statistical Physics, Princeton University Press, Princeton, 1980.

For simple dissipative system with hyperchaos, that is, more than one direction of divergence of trajectories the first system was introduced by O. Rössler (1979).

O. E. Rossler, An equation for hyperchaos, Physics Letters A, 71, 155-157, 1979.

The occurrence of hyperchaotic behavior has been found in an electronic circuit (Matsumoto et al, 1986), NMR laser (Stoop et al, 1988), in a semi-conductor system (Stoop et al, 1989) and in a chemical reaction system (Eiswirth et al, 1992).

M. Eiswirth, Th.-M. Kruel, G. Ertl and F. W. Schneider, Hyperchaos in a chemical reaction, Chemical Physics Letters, 193 (4), 305, 1992.

T. Matsumoto, L. O. Chua and K. Kobayashi, Hyperchaos: laboratory experiment and numerical confirmation, 'IEEE Transactions on Circuits and Systems, CAS-33 (11), 1143-1147, 1986.

R. Stoop, J. Peinke, J. Parisi, B. Rohricht and R. P.Hubener, A p-Ge semiconductor experiment showing chaos and hyperchaos,

Physica D, 35, 425-435, 1989.

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Experimental Hyperchaos

Electronic circuits

T. Kapitaniak, L. Chua, G. Zhong, Experimental Hyperchaos in Coupled Chua's Circuits, IEEE Transactions on Circuits and Systems, 41 (7), 1994.

Fig. 1. Five identical coupled Chua's circuits forming a ring.

Fig. 2. Experimental two-dimensional projections of hyperchaotic attractors: $K_{1-5} = 0.01$; (a) $v_0^{(1)}$ versus $v_{01}^{(2)}$. Horizontal axis is $v_{01}^{(2)}$. Views versus $v_{01}^{(2)}$, Horizontal axis is $v_{02}^{(2)}$, werse $v_{02}^{(2)}$, werse $v_{02}^{(2)}$, Horizontal axis is $v_{02}^{(2)}$, 200 mVdiv, (e) $v_{02}^{(2)}$ werses $v_{02}^{(2)}$. Horizontal axis is $v_{02}^{(2)}$, 200 mVdiv, (e) $v_{02}^{(2)}$ werses $v_{02}^{(2)}$. Horizontal axis is $v_{02}^{(2)}$, 200 mVdiv, (e) $v_{02}^{(2)}$ werses $v_{02}^{(2)}$. Horizontal axis is $v_{02}^{(2)}$.

- So, chaotic?
- Hyperchaotic?
- WHAT?

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Experimental Mathematics

 $^{^{\}S}$ P. Rech, Chaos and hyperchaos in a Hopfield neural network, Neurocomputing, 2011.

Biparametric study of the 4D Rössler system

$$\dot{x} = -(y+z), \dot{y} = x + ay + w, \dot{z} = b + xz, \dot{w} = -cz + dw,$$

where we fix the values of parameters b=3.0 and d=0.05, and we allow the values of *a* and *c* change.

Biparametric study of the 4D Rössler system (Lyapunov exponents based)

Biparametric study of the 4D Rössler system (Lyapunov exponents based)

... and now with a long transient time + larger precision +

Extensive numerical studies yield us to find many approximate periodic orbits for *P*. For some pairs of these orbits we could find approximate heteroclinic connections on which we will built chaotic dynamics.

p ₁ ⁸	=	(-104.32937253702462, 0.028756669726685443, 44.645081351998819),
p ₂ ⁸	=	(-104.26664163365506, 0.028773972266421831, 44.640115482927115),
p_{3}^{8}	=	(-104.42324539012806, 0.028730815749171541, 44.678254866134068),
p ₄ ¹⁶	=	(-104.39575243552828, 0.028738382959034744, 44.666264617071981),
q ₁ ¹²	=	(-103.69667754570543, 0.028932144798038389, 44.407870627484129),
q_{2}^{14}	=	(-103.37098255164607, 0.029023312473829044, 44.284349486019579).

The points p_i^j are approximate periodic points for *P* of period *j* with one-dimensional unstable manifold. The points q_i^j are approximate periodic points of period *j* with two-dimensional unstable manifold.

This numerical study \longrightarrow generates hypothesis and conjectures

Now it is time to state results :-)

• Defining the Poincaré section

$$\Pi = \{ (x, 0, z, w) \in \mathbb{R}^3; \dot{y} = x + z < 0 \}$$

and $P : \Pi \rightarrow \Pi$, the associated Poincaré map, and fixing the parameter values a = 0.27857, b = 3, c = 0.3 and d = 0.05.

 Using rigorous ODE solvers for the systems and variational equations (CAPD library[¶] of the CAPD group (Krakow))

¶Free-software: http://http://capd.ii.uj.edu.pl/

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Theorem

For each $u^{j} \in \{p_{1}^{8}, p_{2}^{8}, p_{3}^{8}, p_{4}^{16}, q_{1}^{12}, q_{2}^{14}\}$ there is a unique periodic orbit v for P of the principal period j in the ball $B(u^{j}, 10^{-8})$ in the maximum norm. Moreover, the resulting periodic points close to p_{i}^{j} have one-dimensional unstable manifold and those corresponding to q_{i}^{j} have two-dimensional invariant manifold.

Proof Let us fix $u^j \in \{p_1^8, p_2^8, p_3^8, p_4^{16}, q_1^{12}, q_2^{14}\}$ and define $F : \Pi^j \to \Pi^j$ by

$$F_j(v_1, v_2, \ldots, v_j) = (v_1 - P(v_j), v_2 - P(v_1), \ldots, v_j - P(v_{j-1})).$$

Solutions to $F_j(v_1, v_2, ..., v_j) = 0$ correspond to *j*-periodic orbits for *P* provided $v_i \neq v_c$ for $i \neq c$. Put

$$z_0 = (v_1, v_2, \ldots, v_j) = (u^j, \hat{P}(u^j), \hat{P}^2(u^j), \ldots, \hat{P}^{j-1}(u^j)),$$

where by $\hat{P}(u)$ we denote an approximate value of P(u) obtained by nonrigorous numerical method. Let $Z = B(z_0, 10^{-8})$ be the ball centered at z_0 in the maximum norm. Using rigorous solvers for ODEs and variational equations from the CAPD library we computed the interval Newton operator

$$N(F_j, Z, z_0) = z_0 - [DF_j(Z)]^{-1} \cdot F_j(z_0)$$

and obtained that $N(F_j, Z, z_0) \subset int(Z)$. This proves that F_j has unique zero (v_1, \ldots, v_j) in Z. Moreover, this zero belongs to $N(F_j, Z, z_0)$ which in most cases had diameter less than 10^{-9} . From these estimation we could conclude that u^j has principal period *j*.

... and now some theorems (CAP)

Then we computed rigorous bounds for $DP^{j}(v_{1}) \in DP^{j}(B(u^{j}, 10^{-10}))$ and we could check the hyperbolicity type of u^{j} by analysis of the spectrum of the obtained interval matrix. The actual bounds for eigenvalues $\{\lambda_{1}, \lambda_{2}, \lambda_{3}\}$ are the following

orbit	λ_1	λ_2	λ_3	return time
p_{1}^{8}	2.7 ⁶	-0.16_{4}^{6}	$[-1, 1] \cdot 10^{-11}$	56.585531937_{00}^{57}
p_{2}^{8}	-3.9^{91}_{89}	-0.54_{4}^{7}	$[-5,5] \cdot 10^{-12}$	56.59832252_{61}^{73}
p_{3}^{8}	$-1.^{91}_{88}$	0.36 ⁶ ₄	$[-1, 1] \cdot 10^{-11}$	56.593931 ⁹¹ 89
p_{4}^{16}	[-3.30, -2.96]	[-0.05, 0.26]	+ [-0.13, 0.13] <i>i</i>	113.1853 ⁶¹ 59
q_1^{12}	$-22.^{31}_{28}$	$-3.^{14}_{06}$	$[-8,8] \cdot 10^{-11}$	85.0883812 ³⁶
q_2^{14}	$-4.^{47}_{39}+5.^{48}_{36}i$	$-4.^{47}_{39}-5.^{48}_{36}i$	$[-5,5] \cdot 10^{-11}$	99.2973738 ⁵³ ₃₄

We have also proved that:

- there is an explicitly given trapping region B ⊂ Π for P, i.e.
 P(B) ⊂ B,
- the maximal invariant set A =inv(P, B) contains three invariant sets, say S₁, S₂, S₃, on which the dynamics is Σ₂ chaotic, i.e. it is semiconjugated to the Bernoulli shift on two symbols,
- S₁ is hyperchaotic set with two positive Lyapunov exponents,
- S_2 and S_3 are chaotic sets with one positive Lyapunov exponent,
- there is a countable infinity of heteroclinic connections linking S₁ with S₂, S₂ with S₃ and S₁ with S₃,
- there is countable infinity of periodic orbits and heteroclinic/homoclinic orbits inside each horseshoe.

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References

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The Lorenz model

The Lorenz model

$$\frac{dx}{dt} = -\sigma x + \sigma y, \quad \frac{dy}{dt} = -xz + r x - y, \quad \frac{dz}{dt} = xy - b z,$$

Three dimensionless control parameters:

- *σ* Prandtl number,
- **b** a positive constant,
- r relative Rayleigh number.

The Saltzman values: $\sigma = 10, b = 8/3, r = 28$

The Lorenz model: Three-parametric analysis

Theorem

For a given fixed r > 1 the region where chaos is possible is bounded in b, and if $b \ge \epsilon > 0$ then the region is bounded in σ too. To be precise, outside a bounded region every positive semiorbit of the Lorenz system converges to an equilibrium.

The Lorenz model: bifurcation analysis

(L.P. Shilnikov, 1980)

More T-points: the Lorenz model

Location of T-points in the Lorenz system is a quite complex task. And, what about locating *all* the T-points automatically?

In this case, the T-points are a kind of codimension-two heteroclinic loop. It connects a homoclinic curve with another spiral homoclinic curve.

The Lorenz model: T-points

A new computer technique: more and more T-points

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The Lorenz model: T-points

A new computer technique: more and more T-points

Kneading sequence $\{\kappa_n(O^+)\}$ defined (Milnor and Thurston, 1980)

$$\kappa_n(O^+) = \begin{cases} +1, & \text{if } T^n(O^+) > 0, \\ -1, & \text{if } T^n(O^+) < 0, \\ 0, & \text{if } T^n(O^+) = 0; \end{cases}$$

here $T^n(O^+)$ is the *n*-th iterate of the right separatrix O^+ of the origin. The condition $T^n(O^+) = 0$ is interpreted as a homoclinic loop, i.e. the separatrix returns to the origin after *n* steps.

The kneading invariant for the separatrix is defined in the form of a formal

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Figure 2: Sketch of a partial bifurcation unfolding of a Bykov T-point (from [Bykov, 1980]) corresponding to a codimensiontwo heteroclinic connection between a saddle of the (2,1)-type and a saddle-focus of the (1,2)-type. It features the characteristic spirals corresponding to homoclinic bifurcations of the saddle. Turning points (labeled by M's) on the spiral are codimensiontwo points of inclination-switch bifurcations giving rise to stable periodic orbits through saddle-node and period-doubling bifurcations (l_m -curves) and subsequent spiral structures of smaller scales between spiral's scrolls.

The Shimizu-Morioka model: more and more T-points

The Shimizu-Morioka model: fractal structure (Bykov)

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• Fractal structure: our "open-air" homoclinic mines

