Gradient Dynamical Systems, Bifurcation Theory, Numerical Methods and Applications

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What is this about?

- solution $x_1(y_1, ...c_1, ...c_m, t), ...x_n(y_1, ...c_1, ...c_m, t)$ to

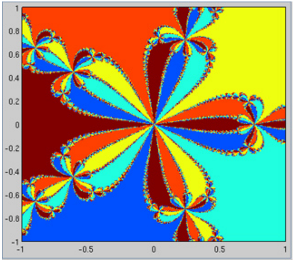
$$F_i\left(x_\alpha ..., c_\beta ... \frac{\partial^k x_j}{\partial y_l^k}, ... \frac{\partial^r x_p}{\partial t^r}, ... \int f_\gamma(x_\delta, ...c_\epsilon, ...y_\zeta)\mathrm{d}y_\zeta, ...\right) = 0$$

- theory of dynamical systems
  - no spatial derivatives
  - no higher order derivatives
  - no integrals
  - first order time derivative separable
- $\frac{\mathrm{d}x_i}{\mathrm{d}t} = f(x_1, ...x_n, c_1, ...c_m, t)$
- bifurcation theory - how the solutions change with c_i
- gradient systems - $\dot{x}_i = \frac{\partial V(x_1,...x_n,c_1,...c_n)}{\partial x_i}$
  - autonomous - right side does not explicitly depend on time
  - gradient - not Hamiltonian systems $p_i = -\frac{\partial H}{\partial q_i}$, $q_i = \frac{\partial H}{\partial p_i}$
- catastrophe theory - one more approximation
  - stationary $\rightarrow$ how solutions to systems of non-linear algebraic equations change with c_i

- not in this presentation

- self-repeating structures - non-integer Haussdorf dimension
- important in dynamical systems but ...
- **discrete** dynamical systems

- in chemistry - basins of attraction



What is a Dynamical System?

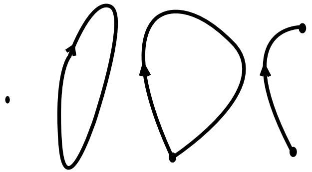
- dynamical system $\{\mathbf{S}, \varphi\}$
- dynamics $\varphi : \mathbf{S} \times \mathbb{R} \rightarrow \mathbf{S}$
  - $\varphi(\sigma, 0) = \sigma$
  - $\varphi(\varphi(\sigma, t), s) = \varphi(\sigma, t + s)$

$$\forall \sigma \in \mathbf{S}$$

- phase flow - in $\mathbb{R}^N$, dynamics given by vector field
- one more condition $\frac{\partial \varphi(\mathbf{x}, t)}{\partial t} = \mathbf{v}(\varphi(\mathbf{x}, t))$
- system of first order ordinary differential equations (SODE)
- if we can evaluate φ fast, we know the dynamics
- no memory
- autonomous
- $\frac{\mathrm{d}x_i}{\mathrm{d}t} = f(x_1, ...x_n, c_1, ...c_m)$

Phase Portrait

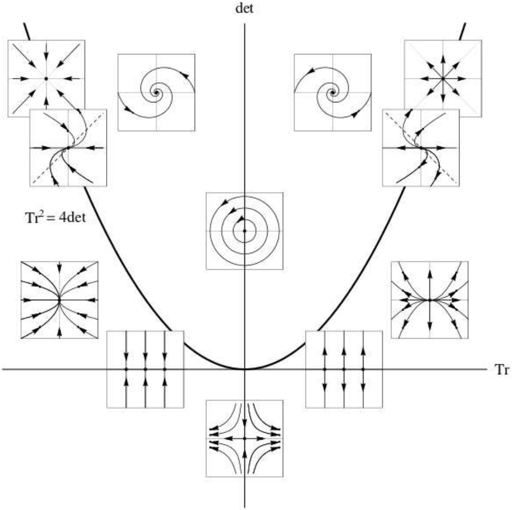
- solution to SODE - touple of functions $(x_1(t), ...x_n(t))$
- trajectories
  - unique (in contrast with configuration space)
  - singular - stationary point, periodic, homoclinic, heteroclinic
- Steady state, periodic, homoclinic, heteroclinic trajectory



- Lyapunov stability
  - asymptotic

Linear SODE

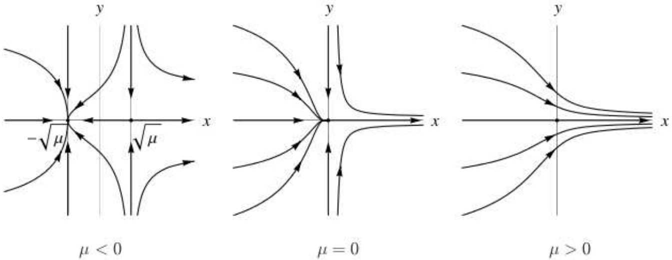
- linear SODE (homogeneous): $\dot{\mathbf{x}} = \mathbf{A}\,\mathbf{x}$
- has an analytical solution: $\varphi(\mathbf{x}_0, \tau) = e^{\mathbf{A}\tau}\mathbf{x}_0$



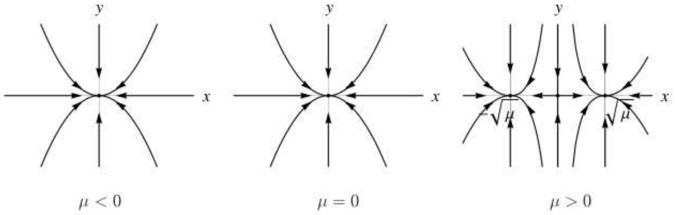
Non-linear SODE

- general system $\dot{x}_i = f_i(x_1, ...x_n, c_1, ...c_m)$
- Grobman-Hartman theorem
  - non-zero Re(eigval)
  - topologically equivalent
- stability by eigenvalues of matrix of linearisation
- qualitative studies of phase portrait
  - identify singular trajectories
  - determine their stability

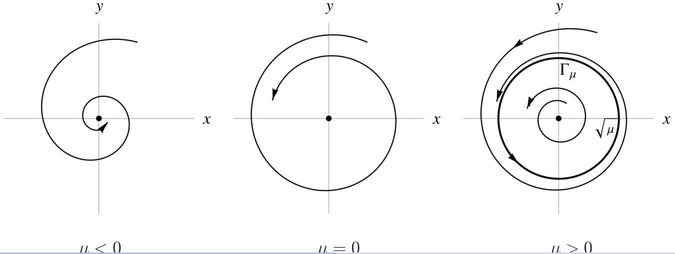
- SODE $\mathbf{x} = \mathbf{v}(\mathbf{x})$ is structurally stable if there is ε, for which all vector fields $\mathbf{u}$ ($|\mathbf{u} - \mathbf{v}| < \varepsilon$) have qualitatively the same phase portraits
- bifurcation - cannot happen in structurally stable systems
  - steady state
  - periodic trajectory
- local bifurcations of 1-parametric system of vector fields
  - saddle-node bifurcation (parameter μ)



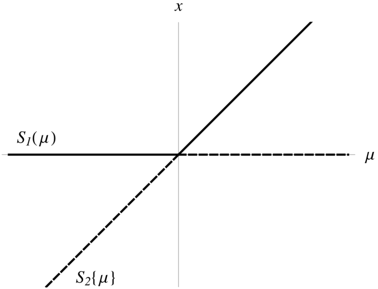
- pitchfork bifurcation

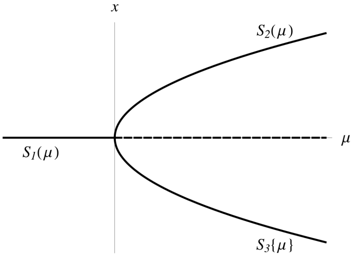


- Hopf bifurcation



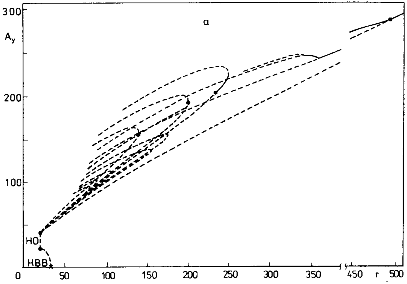
- diagram of stationary solutions
  - a quantity as a function of a parameter
  - branching, critical points, bifurcation points, double, triple BP, HB points

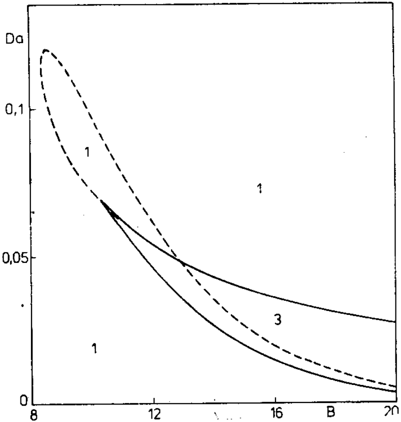




- bifurcation diagram
  - more than 1 parameter
  - curves of bifurcation points

- **LEFT** diagram of stationary states - periodic trajectories for lorenz model





- **RIGHT** - bifurcation diagram for CSTR1EXO model

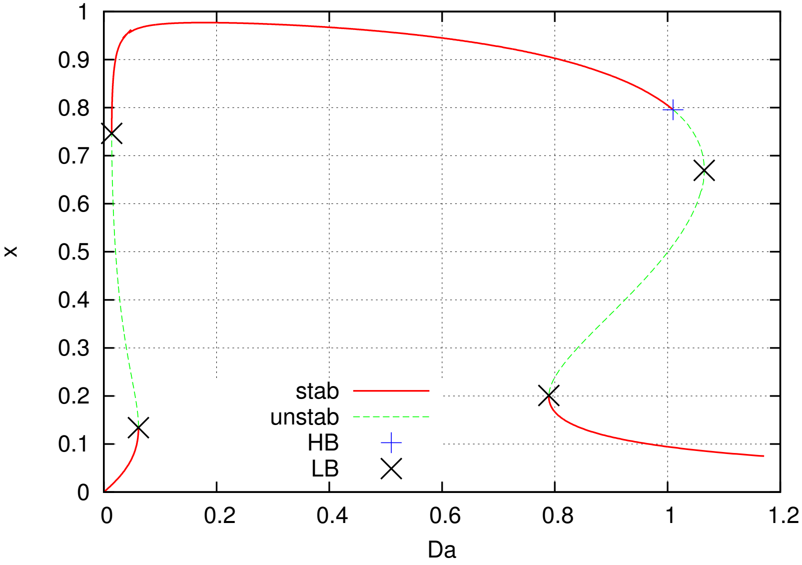
- finding stationary solutions
- parameter mapping
  - not efficient
- DERPAR
  - introducing an artificial parameter (parametrisation of the curve in the diagram of stationary solutions)
  - $\sum_{i=1}^{n} \left(\frac{\mathrm{d}x_i}{\mathrm{d}z}\right)^2 + \left(\frac{\mathrm{d}\alpha}{\mathrm{d}z}\right)^2 = 1$
  - in stationary point $\frac{\mathrm{d}f_i}{\mathrm{d}z} = 0$
  - $\frac{\partial f_i}{\partial \alpha}\frac{\mathrm{d}\alpha}{\mathrm{d}z} + \sum_{j=1}^{n} \frac{\partial f_i}{\partial x_j}\frac{\mathrm{d}x_j}{\mathrm{d}z} = 0$
  - underdetermined system
  - Gauss-Jordan elimination using maximum pivot
  - algorithm must remember signs of derivatives
- predictor-corrector
  - can continuate the whole curve
  - cannot find isolated curve of solutions
- periodic trajectories - DERPER

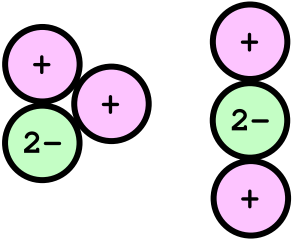
- stirred tank reactor with an exothermic reaction
- toy system for bifurcation analyses with connection to chem eng reality

- reduction of parameters by using dimensionless quantities
- x - conversion, Θ - temperature
- Da - Damköhler number - flow
- Θ_c - temp of cooling medium, γ - activation energy, β - heat exchange param, Λ - recycle, B - heat production param

$$\frac{\mathrm{d}x}{\mathrm{d}t} = -\Lambda x + \mathrm{Da}(1-x)e^{\frac{\Theta}{1+\Theta/\gamma}}$$
$$\frac{\mathrm{d}\Theta}{\mathrm{d}t} = -\Lambda\Theta + \mathrm{Da}B(1-x)e^{\frac{\Theta}{1+\Theta/\gamma}} - \beta(\Theta - \Theta_c)$$

Case 1 - Results



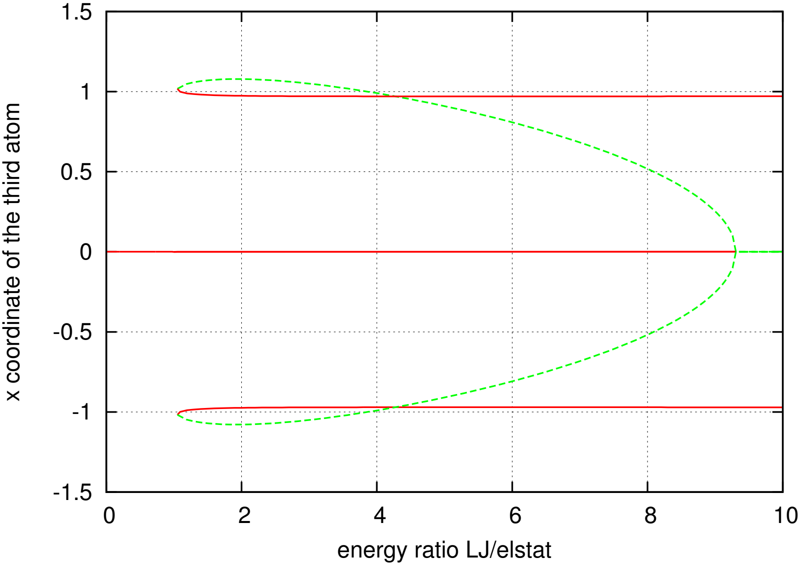


- gradual increase of LJ energy
  - $x_1 = y_1 = x_2 = 0$
  - $r_{13} = \sqrt{x_3^2 + y_3^2}$
  - $r_{23} = \sqrt{x_3^2 + (y_3 - y_2)^2}$

- SODE (6-dimensional phase space):

$$\dot{y}_2 = vy_2$$
$$\dot{x}_3 = vx_3$$
$$\dot{y}_3 = vy_3$$
$$\dot{vy}_2 = -\left[\frac{2}{y_2^2} - \frac{y_2 - y_3}{r_{23}^3} + 6\epsilon\left(-\frac{2}{y_2^{13}} - \frac{2(y_2 - y_3)}{r_{23}^{14}} + \frac{1}{y_2^7} + \frac{(y_2 - y_3)}{r_{23}^8}\right)\right]$$
$$\dot{vx}_3 = -\left[\frac{2x_3}{r_{13}^3} - \frac{x_3}{r_{23}^3} + 6\epsilon x_3\left(-\frac{2}{r_{13}^{14}} - \frac{2}{r_{23}^{14}} + \frac{1}{r_{13}^8} + \frac{1}{r_{23}^8}\right)\right]$$
$$\dot{vy}_3 = -\left[\frac{2y_3}{r_{13}^3} - \frac{y_3 - y_2}{r_{23}^3} + 6\epsilon\left(-\frac{2y_3}{r_{13}^{14}} - \frac{2(y_3 - y_2)}{r_{23}^{14}} + \frac{y_3}{r_{13}^8} + \frac{(y_3 - y_2)}{r_{23}^8}\right)\right]$$

Case 2 - Results



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