Reaction Diffusion Systems

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Animal Skin Patterns
Patterns

- D’Arcy W. Thomson (1860-1948) found that many shapes in nature are deeply rooted in dynamics that follow physical laws.
- Alan Turing studied how chemical systems can generate complex patterns (e.g. leopard skins).
Morphogenesis is one of the most fascinating but also unexplored topics in Biology.

The study of the emergence of complex coatings of animals belongs to this field.

Alan Turing found a general model that can be used to simulate the pattern formation – reaction diffusion systems.
Contents

- Differential Equation Models
  - Ordinary
  - Coupled Systems
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Ordinary differential equations (ODEs)

- \( \frac{dx(t)}{dt} = f(x(t), t) \) ... dx and dt is a differential step in x and t, respectively.

- Examples 1: Racing, constant speed
  - Let \( v \) denote velocity, \( x \) denote length of finished way, and \( t \) denote time
  - \( \frac{dx(t)}{dt} = v \)

- Example 2: Population growth
  - Let \( r_b \) denote reproduction rate/capita, \( r_d \) denote death rate/capita, \( S \) denote population size
  - \( \frac{dS}{dt} = r_b S - r_d S \)
Coupled ordinary differential equations

- \( \frac{dx(t)}{dt} = f_x(x,y,z,t) \)
- \( \frac{dy(t)}{dt} = f_y(x,y,z,t) \)
- \( \frac{dz(t)}{dt} = f_z(x,y,z,t) \)

Multiple coupled ODE’s

Example 1: Predator Prey System

- \( x \): size of prey population, \( y \) size of predator population, death/birth rates: \( d_x, r_x, d_{yx}, r_{xy} \)
- \( \frac{dx}{dt} = r_x x - d_{yx} y x - d_x x \)
- \( \frac{dy}{dt} = r_{xy} y x - d_y y \)
Second order differential equations

- \( \frac{d^2 x}{(dt)^2} = f(x, \frac{dx}{dt}, t) \) (second derivatives)
  ... can be restated as coupled ODE system

Example: Racing with acceleration

- \( \frac{d^2 x}{(dt)^2} = a \frac{dx}{dt} \)
- speed \( v \), location \( x \)
- \( \frac{dx}{dt} = v \)
- \( \frac{dv}{dt} = \frac{d^2 x}{(dt)^2} = a \cdot v \)

Reformulation as coupled system
Example 1: Racing
- $\frac{dx}{dt} = v$
- $dx = v \, dt$ \hspace{10pt} \text{(Separation of variables)}
- $x(t) = C + \int_1^t v \, dt = C + v \, t$ \hspace{10pt} \text{(linear growth)}

Example 2: Population growth
- $\frac{dx(t)}{dt} = v \, x(t)$ \hspace{10pt} \text{(Separation of variables cannot be used)}
- $x(t)=C \, \exp(v \, x(t))$ \hspace{10pt} \text{(Ansatz)}
  Verification: $\frac{d(C' \, \exp(v \, x(t)))}{dt} = C' \, v \, \exp(v \, x(t))$
Initial value problem

- At $t=t_0$ the solution is known
- Then the trajectory of the DE can be computed
- Example:
  - $dx/dt = v$
  - $x(t) = v \cdot t + C$
  - $x(t_0) = v \cdot t_0 + C$ implies $C = (x(t_0) - v \cdot t_0)$
  - implies $x(t) = (x(t_0) - v \cdot t_0) + v \cdot t$
Numerical Solution 1: Euler’s Method

- Euler’s Method: Simulate differential time step
- \( \frac{dx}{dt} = f(x, t) \) implies \( x(t+\Delta t) = x(t) + f(x, t) \Delta t \) (Euler method)

Example 1: Racing with constant speed
- \( x(t+\Delta t) \approx x(t) + v \Delta t \)

Example 2: Population growth
- \( x(t+\Delta t) \approx x(t) + x(t) v \Delta t \)
Euler’s method

- The Euler that have a linear solution
- In case of a non-linear solution an error is accumulated
- The error is smaller, if stepsize $\Delta t$ is small
- Runge Kutta Method is more precise
Runge Kutta Method

- More precise solution of \( \frac{dx}{dt} = f(x,t) \)
- Common 4th order Runge Kutta Method

\[
x(t+\Delta t) = f(x,t) + \frac{1}{6}(k_1 + 2k_2 + 2k_3 + k_4)
\]

\[
k_1 = \Delta t \ f(x,t) \quad \text{... with } x \text{ we mean } x(t)
\]

\[
k_2 = \Delta t \ f(x + \frac{1}{2} k_1 , t + \frac{1}{2} \Delta t)
\]

\[
k_3 = \Delta t \ f(x + \frac{1}{2} k_2 , t + \frac{1}{2} \Delta t)
\]

\[
k_4 = \Delta t \ f(x + k_3 , t + \Delta t)
\]
Solution of coupled systems

- Replace $x$ by vector, e.g. $x=(x,y,z)$
- Euler’s method
  
  $x(t+\Delta t) = x(t)+\Delta t \ f(x(t),t), \ x \ \text{in} \ \mathbb{R}^n$

- Runge Kutta
  
  $x(t+\Delta t) = f(x(t),t)+1/6(k_1+2k_2+2k_3+k_4)$

  compute $k_i$ using vector $x$ and not scalar $x$
Partial differential equations (PDEs)

- Not only temporal, but also spatial derivatives (changing rates)
- Let $x, y, z$ denote spatial coordinates, and $t$ denote the time
- Then $\frac{df(x,y,z,t)}{dx}$, $\frac{df(x,y,z,t)}{dy}$, $\frac{df(x,y,z,t)}{dz}$, and $\frac{df(x,y,z,t)}{dt}$ are called partial derivatives
- PDEs are formulated based on these
Example?: Gradient diffusion

- Let $\mathbf{x}(t) = (x(t), y(t), z(t))$ is position of particle
  $\frac{d\mathbf{x}}{dt} = -(\frac{dP}{dx}, \frac{dP}{dy}, \frac{dP}{dz})$, where $P(x, y, z)$ is a potential function or energy function
- $(\frac{dP}{dx}, \frac{dP}{dy}, \frac{dP}{dz})$ is also denoted as gradient of $P$ or in short notation $\nabla P$
- The gradient $\nabla P(x, y, z)$ points in the direction of steepest ascent of $P$ at $(x, y, z)^T$.

This is not a PDE but a coupled system of ODEs.

Why? Where does gradient diffusion move the particle?
Diffusion PDEs

- Diffusion in one dimension:
- Let \( c(x) \) denote the concentration of a substance in position \( x \), and \( D \) denote diffusivity (‘diffusion speed’)
- \( \frac{dc(x)}{dt} = D \frac{d^2c(x)}{(dx)^2} \)

(Fick’s second law)

... this is a (one-dimensional) PDE. Why?

Diffusion Equation in 3D

- Fick’s law in three dimensions:
  we write \( \frac{c(x,y,z,t)}{dx}, \frac{c(x,y,z,t)}{dy}, \frac{c(x,y,z,t)}{dz} \)
  with \( \nabla = (1/dx, 1/dy, 1/dz) \) as
  \( \nabla c(x,y,z,t) \) or simply \( \nabla c \)

- Now Fick’s law can be formulated as:
  \( \frac{dc(x,y,z,t)}{dt} = \nabla (D \nabla c(x,y,z,t)) = D \nabla^2 c(x,y,z,t) \)
Simulation of Diffusion Equation

- **Boundary condition**
  - A proper formulation of a differential equation problem for PDE’s needs to state initial values: \( c_0(x,y,z,t) \) for \( t_0 \) and all \( x,y,z \)
  - Often a boundary condition is stated, for instance \( c(x,y,z,t) \equiv 0 \) for \( x,y,z \) at the boundary of a shape or at a sink node or \( c(x,y,z,t) \equiv C (>0) \) at a source node.
Simulation of PDE, Euler’s method

- \( c(x,y,z,t+\Delta t) = c(x,y,z,t)+f(c(x,y,z,t),t)\Delta t \)  
  (Taylor approximation, 1st order)

- \( f(c(x,y,z,t),t) = D\nabla^2 c(x,y,z,t) \)

\( \nabla_{\text{approx}}^c(\ldots) = \left( \frac{c(x-\Delta x,y,z,t)+c(x+\Delta x,y,z,t)}{2\Delta x}, \right. \)
\( \frac{c(x,y-\Delta y,z,t)+c(x,y+\Delta y,z,t)}{2\Delta z}, \)
\( \frac{c(x,y,z-\Delta z,t)+c(x,y,z+\Delta z,t)}{2\Delta y} \) \)

\( \nabla^2_{\text{approx}}^c(\ldots) = \left( \frac{1}{\Delta x}, \frac{1}{\Delta y}, \frac{1}{\Delta z} \right)^T \cdot \nabla_{\text{approx}}^c(\ldots) \)  
  (scalar product)
The reaction diffusion PDE

- Parabolic PDE of the form:
  \[ \frac{dc}{dt} = D \nabla^2 c + r(c) \]

diffusion term
reaction term

generated by Dr. H. U. Bödeker
Coupled Reaction diffusion system of Turing type

\( u \): concentration of pigment, \( v \): concentration of inhibitor, 
\( \text{D}_u \): diffusion of \( u \), \( \text{D}_v \) diffusion of \( v \),  
\( f_u, f_v, g_u, \) and \( g_v \): reaction speeds

Instead of \( \frac{dF(x_1, \ldots, x_i, \ldots, x_n)}{dx_i} \) we write \( F_{xi} \)

\[
\frac{\partial u}{\partial t} = f(u, v) + D_u \nabla^2 u \\
\frac{\partial v}{\partial t} = g(u, v) + D_v \nabla^2 v,
\]

linearization

\[
\frac{\partial \tilde{u}}{\partial t} = f_u \tilde{u} + f_v \tilde{v} + D_u \nabla^2 \tilde{u} \\
\frac{\partial \tilde{v}}{\partial t} = g_u \tilde{u} + g_v \tilde{v} + D_v \nabla^2 \tilde{v}.
\]

Turing Condition 1: \( f_u g_v - f_v g_u > 0 \)

Turing Condition 2: \( f_u + g_v < 0 \)

Turing Condition 3: \( f_u D_v + g_v D_u > 0 \)

Turing Condition 4: \( f_u D_v + g_v D_u > 2\sqrt{D_u D_v (f_u g_v - f_v g_u)} \)
Turing type conditions, interpreted

- Fast diffusion term
- Autocatalytic reaction (self-amplifying) of pigment
Plausibility of reaction diffusion system

Once the activator $X$ starts spreading from a point source, inhibitor $Y$ is created, which diffuses faster, and halts the spread of $X$ when it has diffused farther than $X$. 
BZ Reaction

(a) propagating wavefronts

(b) spiral formations
Bacterial growth patterns

Patterns formed by chemotaxis in *Dictyostelium discoideum*. Image courtesy of The National Academy of Sciences of the USA.
Summary and Outlook

- Differential equations are models for continuous dynamical systems.
- Can be simulated with Euler’s method or more accurately with Runge Kutta.
- Coupled differential equations can model interacting systems.
- Partial differential equations model dependency on spatial components.
Summary and Outlook

- Diffusion model: PDE using Fick’s second law via concentration gradient
- Reaction Diffusion systems introduce diffusion term
- Turing established conditions, under which complex pattern formation takes place
- Various patterns in biology and chemistry can be simulated by RD systems of Turing type
RD Demo

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