Modeling of Belousov-Zhabotinsky reaction

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Aims

- To see how the system of the reaction reacts on the different shapes or size of Petri dish
- Trying to describe the structure of expanding wave of the system and compare it with models in computer modelations
- Test software for the calculation system’s structure (Entropy calculator)
History of the discovering

• The discovery of the phenomenon is credited to B. P. Belousov in 1959 (A periodic reaction and its mechanism)

• Later, in 1961, a graduate student named A. M. Zhabotinsky rediscovered this reaction sequence and described its mechanism (Periodic processes of malonic acid oxidation in a liquid phase)

• Results of this work was presentation to the West in a Prague conference in 1968.
Using reagents:

- sodium bromate (NaBrO3);
- sulphuric acide (H2SO4);
- sodium bromide (NaBr);
- malonic acide (HOOCCH2COOH);
- phenanthroline ferrous complex – ferroin (C36H24FeN6^{2+})
Chemical mechanism

1. \( \text{NaBrO}_3 + \text{H}_2\text{O} \xrightarrow{\text{H}_2\text{SO}_4} \text{HBrO}_3 + \text{NaOH} \)
2. \( \text{NaBr} + 2\text{H}_2\text{O} \xrightarrow{} \text{BrOH} + \text{NaOH} + 2\text{H}^+ \)
3. \( \text{HBrO}_3 + \text{Br}^- + \text{H}^+ \xrightarrow{} \text{Br}_2 + \text{H}_2\text{O} \)
4. \( \text{BrO}_2^- + \text{Fe(phen)}_3^{2+} \xrightarrow{} \text{HBrO}_2 + \text{Fe(phen)}_3^{3+} \)
5. \( \text{BrO}_3^- + \text{CH}_2(\text{COOH})_2 \xrightarrow{} \text{HCOOH} + \text{CO}_2 + \text{HBrO}_2 + \text{H}^+ \)
Belousov-Zhabotinsky reaction
mechanism

HBrO₃

Fe(phen)₃²⁺

HBrO₂

Fe(phen)₃³⁺

Br⁻

ferroine

The Belousov-Zhabotinsky reaction is a chemical reaction that produces oscillations in concentration over time. The reaction involves the oxidation of bromide ions to bromine, with ferroine as the catalyst. The reaction is characterized by a series of waves in concentration, which can be observed over time (t).
CellMarkerSci

- Cutting images and separation into 3 colour channels RGB
Image processing – Information entropy

Sum of the individual information weighted by the probabilities of their occurrences. For maximal information gain from images we used information entropy based on Rényi equation:

$$I_\alpha = \lim_{\rho \to 0} \frac{1}{1 - \alpha} \ln \sum_{i=1}^{n} p_i^\alpha$$

- By changing parameter $\alpha$ we emphasize different part of image:
  - $\alpha=0.5$
  - $\alpha=1.0$
  - $\alpha=2.5$
  - original image
It is also known as a projection method, because it takes information carried by the original variables and projects them onto a smaller number of latent variables called Principal Components (PC). Each PC explains a certain amount of the total information contained in the original data and the first PC contains the greatest source of information in the data set. Each subsequent PC contains, in order, less information than the previous one.

\[ X = T \cdot P + E, \]  
where:

- \( T \) - is the scores matrix
- \( P \) - the loadings matrix
- \( E \) - the error matrix
Nonhierarchical clustering (K-clustering) is an unsupervised method which works iteratively to group samples based on their similarity based on some measured variables. The analysis involves starting with a collection of samples that one attempts to group them into $k$ Number of clusters based on certain specific distance measurements.
Data analysis

Cross calculation method

Whole calculation method
Still image length - 0.15s
Time between shootings - 10 s
Still image length - 0.15s
Time between shootings - 10 s
Still image length - 0.15s
Time between shootings - 10 s
Conclusions

- Shapes determine structure of the waves, also size of the dishes determine number of the wave sources.
- Evolution of the system is determined not only by chemical factors but also by physical factors.
- We tested software for calculation of system’s structure.
- Entropy calculation approach could be used for recognizing the structure of the self-organized system (chemical reactions, living cells...) but some improvement are needed.
Thank you for attention!

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