

# **Encyclopedia of Nonlinear Science**

**Alwyn Scott**  
**Editor**

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write

$$\pi(x) = \frac{w(x)q(x)}{\int_{\mathcal{X}} w(x)q(x) dx}$$

and apply importance sampling to both numerator and denominator to yield the following approximation:

$$\hat{\pi}_2(x) = \sum_{i=1}^N \frac{w(X^{(i)})}{\sum_{j=1}^N w(X^{(j)})} \delta(x - X^{(i)}).$$

An approximate sample from  $\pi$  can be obtained by sampling from the discrete distributions  $\hat{\pi}_1$  or  $\hat{\pi}_2$ .

## Applications

The range of applications of Monte Carlo methods is vast. Listed below are some of the more well-known areas.

*Integral equations:* IS methods have been widely used to solve linear systems and integral equations appearing in particle transport problems. The basic idea is to give a probabilistic approximation of operators of the form  $(I - H)^{-1} = \sum_{i=0}^{\infty} H^i$ ; see Sobol (1994) for details.

*Computational physics and chemistry simulation:* Monte Carlo methods are used in physics and chemistry to simulate from Ising models, simulate self-avoiding random walks, and compute the free energy, entropy, and chemical potential over systems; see, for example, Frenkel & Smith (1996).

*Quantum physics:* To compute the dominant eigenvalue and eigenvector of a positive operator, it is possible to use a stochastic version of the power method. This is often applied to the Schrödinger equation; see Melik-Alaverdian & Nightingale (1999) for a recent review.

*Statistics:* Performing inference in complex statistical models invariably requires sampling from high dimensional probability distributions. See Gilks et al. (1996) for applications of MCMC and Doucet et al. (2001) for applications of IS-type methods to such problems.

ARNAUD DOUCET AND BA-NGU VO

See also **Random walks; Stochastic processes**

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## MORPHOGENESIS, BIOLOGICAL

One of the central problems in developmental biology is to understand how patterns and structures are laid down. From the initially almost homogeneous mass of dividing cells in an embryo emerges the vast range of pattern and structure observed in animals. For example, the skeleton is laid down during chondrogenesis when chondroblast cells condense into aggregates that lead eventually to bone formation. The skin forms many specialized structures such as hair, scales, feathers, and glands. Butterfly wings exhibit spectacular colors and patterns, and many animals develop dramatic coat patterns.

Although genes play a key role, genetics say nothing about the actual mechanisms that produce pattern and structure—the process known as morphogenesis—as an organism matures from embryo to adult. Tissue movement and rearrangement are the key features of almost all morphogenetic processes and arise as the result of complex mechanical, chemical, and electrical interactions. Despite the recent vast advances in molecular biology and genetics, little is understood of how these processes conspire to produce pattern and form. There is the danger of falling into the practices of the 19th century, when biology was steeped in the mode of classification and there was a tremendous amount of list-making activity. This was recognized by D'Arcy Thompson, in his classic work first published in 1917 (see Thompson (1992) for the abridged version). He was the first to develop theories for how certain forms arose, rather than simply cataloging different forms, as was the tradition at that time.

At the heart of a number of developmental phenomena is the process of convergence-extension, in which a tissue narrows along one axis while extending along another. This process represents the integration of local cellular behavior that produces forces to change the shape of the cell population. In fact, convergence-extension is essentially responsible for the transformation of the spherical egg into the elongated, bilaterally symmetric vertebrate body axis (Keller et al., 1992).

Cell fate and position within the developing embryo can be strongly influenced by environmental factors. Therefore, to investigate the process of morphogenesis, one must really address the issue of how the embryo organizes the complex spatiotemporal sequence of signalling cues necessary to develop structure in a controlled and coordinated manner. Structure can form through tissue movement and rearrangement. Theoretical studies in this area include the early purse-string model (Odell et al., 1981) for tissue folding in which, in response to a large deformation, cells were proposed to actively contract and, in doing so, cause a large deformation in neighboring cells which, in turn, also contract, setting up a propagating contraction wave which leads to tissue folding. This model was applied to a variety of developmental problems and provided the precursor to the mechanochemical theory of developmental patterning developed by Oster, Murray, and coworkers (for review, see Murray, 2003). This approach emphasized the link between tissue mechanics and chemical regulation and has been applied widely in both developmental biology and medicine.

Discrete-cell modeling approaches have subsequently been developed in which morphogenesis is hypothesized to occur via mechanical rearrangement of neighbors in an epithelial sheet, and computational finite elements have been developed to test various theoretical explanations for morphogenesis (Weliky et al., 1991; Davidson et al., 1995).

In all these models, individual cell movements within the tissue are determined by the balance of mechanical forces acting on the cell. Such models can exhibit tissue folding, thickening, invagination, exogastrulation, and intercalation, and have been shown to capture many of the key aspects of processes such as gastrulation, neural tube formation, and ventral furrow formation in *Drosophila*. Cells can also sort out depending on their type, and this has led to the theory of differential adhesion and energy minimization (Steinberg, 1970).

Models for tissue motion are not amenable to a mathematical analysis and tend to be highly computation based. However, models for how cells differentiate can be addressed mathematically. Broadly speaking, there are two classes of such models. In one class, the chemical pre-pattern models, it is hypothesized that a chemical signal is set up in some way and cells respond to this signal by differentiating. In the other class, the cell movement models, it is hypothesized that cells respond to mechanochemical cues and form aggregates. Cells in high density aggregates are then assumed to differentiate (see Murray, 2003, for details).

The fact that such models can lead to the generation of spontaneous order was first realized by Alan Turing (1952), who showed that a system of chemicals, stable in the absence of diffusion, could be driven unstable by

diffusion. He proposed that such a spatial distribution of chemicals (which he termed *morphogens*) could set up a pre-pattern to which cells could respond and differentiate accordingly. He was one of the first to postulate the existence of such chemicals, and morphogens have now been discovered. It is still not clear that morphogen patterns in biology are set up by the mechanism proposed by Turing, but Turing patterns have been found in chemistry (see Maini et al., 1997, for a review).

A variety of models based on different biology give rise to mathematical formulations in terms of coupled systems of highly nonlinear partial differential equations. The analysis of these models has, to date, yielded a number of common behaviors. This has led to the idea of using such models to determine developmental constraints. That is, independent of the underlying biology, such models predict that only certain patterns are selected at the expense of others and thus there is a limited variation. This has consequences for evolution. For example, application of mitotic inhibitors to developing limbs produces smaller limbs with reduced elements. Some of the resultant variants look very similar to the pattern of evolution in other species, suggesting that these species may be more closely related than previously thought (Oster et al., 1988). Moreover, the construction rules generated by a study of developmental constraints is another, perhaps more mechanistic, way of describing how different species are related other than the topological deformation approach of D'Arcy Thompson.

Other approaches to morphogenesis and pattern formation include cellular automata models, in which individual entities (cells, for example) behave according to a set of rules. Such models allow one to include much more biological detail and to investigate finer grain patterns than those possible in the continuum approaches discussed above (see, for example, Alt et al., 1997). However, to date they lack a detailed mathematical underpinning.

The recent spectacular advances in molecular genetics raise the issue of how we can combine the enormous amount of data now being generated at this level with the data available from the classical experiments at the cell and tissue level to provide a coherent theory for pattern formation and morphogenesis. This leads to the problem of modeling across a vast range of spatial and temporal scales. The mathematics for this has not yet been developed and is one of the challenges presently being addressed.

PHILIP K. MAINI

*See also* Brusselator; Cellular automata; Pattern formation; Reaction-diffusion systems; Turing patterns

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**MULTIDIMENSIONAL SOLITONS**

Although strict analogs of the Korteweg–de Vries soliton (exponentially localized solution with a specific relation between velocity and amplitude and particular scattering properties) have not been found in the multidimensional context, solvable equations with three or more independent variables exhibit a large variety of soliton-like solutions.

As with the Kadomtsev–Petviashvili equation, wide classes of exact explicit solutions have been constructed for other (2 + 1)-dimensional nonlinear equations solvable by the inverse scattering method. We consider here two basic examples, the first being the Davey–Stewartson (DS) equation

$$i q_t + \frac{1}{2} (\sigma^2 q_{xx} + q_{yy}) + |q|^2 q - q\phi = 0, \quad \phi_{xx} - \sigma^2 \phi_{yy} = 2(|q|^2)_{xx}, \quad (1)$$

where  $q(x, y, t)$  is a complex-valued function,  $\phi$  is a real-valued function, and the parameter  $\sigma^2$  takes two values  $\sigma^2 = \pm 1$ . The DS equation describes propagation of a two-dimensional long surface wave on water

of finite depth. In the one-dimensional limit  $q_y = \phi_y = 0$ , it reduces to the nonlinear Schrödinger equation.

The DS equation (1) has a Lax representation with the two-dimensional Dirac operator as the Lax operator, but it has quite different properties for  $\sigma^2 = 1$  (DS-I equation) and for  $\sigma^2 = -1$  (DS-II equation). In both cases, there are multi-soliton solutions which do not decay in certain directions on the  $x, y$  plane. Similar to the Kadomtsev–Petviashvili equation these solutions describe elastic scattering of line solitons that decay exponentially in the direction of propagation and do not decay in the orthogonal direction. The phase shift can be explicitly calculated.

In addition, the DS equation possesses novel classes of solutions. Thus, the DS-II equation has an infinite set of nonsingular exponential-algebraic solutions, the simplest of which looks like

$$q(x, y, t) = \frac{2\nu \exp \left[ \lambda(x + iy) - \bar{\lambda}(x - iy) - i(\lambda^2 + \bar{\lambda}^2)t \right]}{|x + iy + \mu - 2i\lambda t|^2 + |\nu|^2}, \quad (2)$$

where  $\lambda, \mu$ , and  $\nu$  are arbitrary complex constants. It decays like  $(x^2 + y^2)^{-1}$  as  $x, y \rightarrow \infty$ .

The DS-I equation also possesses solutions for which  $q$  decays exponentially in both space dimensions. The simplest of them is of the form

$$q(x, y, t) = \frac{4\rho\sqrt{\lambda\mu} \exp \left[ \mu(x + y) + \lambda(x - y) + i(\mu^2 + \lambda^2)t \right]}{[1 + e^{2\mu(x+y)}][1 + e^{2\lambda(x-y)}] + |\rho|^2}, \quad (3)$$

where  $\lambda, \mu$  are arbitrary real parameters and  $\rho$  is an arbitrary complex parameter. The function  $\phi$  has the nontrivial boundary values as  $x, y \rightarrow \infty$ . Called dromions, such solutions exhibit not only a two-dimensional phase shift during interaction but also a change of the form. Basically, these solutions are driven by the boundary conditions on the function  $\phi$ .

Our second example—the Ishimori equation—is of the form

$$\begin{aligned} S_t + S \times (S_{xx} + \sigma^2 S_{yy}) + \phi_x S_y + \phi_y S_x &= 0, \\ \phi_{xx} - \sigma^2 \phi_{yy} + 2\sigma^2 S \cdot (S_x \times S_y) &= 0, \end{aligned} \quad (4)$$

where  $S = (S_1, S_2, S_3)$  is a unit vector  $S^2 = 1$ ,  $\sigma^2 = \pm 1$ , and  $\phi$  is a scalar real-valued function. It represents an integrable (2 + 1)-dimensional generalization of the Heisenberg Ferromagnet model equation  $S = S \times S_{xx}$ . An important feature of the Ishimori equation is that its solutions can be characterized by the topological invariant