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Էդգար Արայի Վարդանյան

Մոմենտների փակման մոտավորությունը և նրա կիրառությունները մեքենայական ուսուցման և Էվոլյուցիայի մեջ

Ե.13.05 - «Մաթեմատիկական մոդելավորում, թվային մեթոդներ և ծրագրերի

համալիրներ» մասնագիտությամբ տեխնիկական գիտությունների թեկնածուի

գիտական աստիճանի հայցման ատենախոսության

ՍԵՂՄԱԳԻՐ

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Edgar Ara Vardanyan

Moment closure approximation and its applications in machine learning and evolution

SYNOPSIS

of the dissertation for obtaining a Ph.D. degree in Technical Sciences on specialty 05.13.05
''Mathematical modeling, digital methods and program complexes"

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Ատենախոսության թեման հաստատվել է Հայ-ռուսական համալսարանում

Գիտական ղեկավար` ֆիզ.-մաթ. գիտ. դոկտոր Դ.Բ. Սահակյան
Պաշտոնական ընդդիմախոսներ` ֆիզ.-մաթ. գիտ. դոկտոր Է.Մ. Պողոսյան
ֆիզ.-մաթ. գիտ. դոկտոր Օ.Ս. Ռոզանովա
Առաջատար կազմակերպություն` Երևանի Պետական Համալսարան

Ատենախոսության պաշտպանությունը կկայանա 2025թ. հունիսի 16-ին, ժ. 14:00-ին ԳԱԱ Ինֆորմատիկայի և ավտոմատացման պրոբլեմների ինստիտուտում գործող 037 մասնագիտական խորհրդի նիստում հետևյալ հասցեով` Երևան, 0014, Պ. Սևակի 1:

Ատենախոսությանը կարելի է ծանոթանալ ՀՀ ԳԱԱ ԻԱՊԻ գրադարանում:
Սեղմագիրն առաքված է 2025թ. մայիսի 16-ին:

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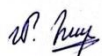քարտուղար ֆիզ.-մաթ. գիտ. դոկտոր`   Մ.Ե. Հարությունյան

The topic of the dissertation was approved at the Russian Armenian University

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Leading organization: Yerevan State University

The dissertation defence will take place on June 16, 2025, at 14:00 at the Specialized Council 037 «Informatics» at the Institute of Informatics and Automation Problems of NAS RA. Address: Yerevan, 0014, P. Sevak 1.

The dissertation is available in the library of IIAP NAS RA.

The abstract is delivered on May 16, 2024.

Scientific Secretary of the Specialized Council, D.Ph.M.S.   M. E. Haroutunian

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Relevance of the topic

Moment closure approximation is a mathematical technique used to simplify complex dynamical systems by reducing an infinite or high-dimensional set of equations to a manageable size, which may allow obtaining analytical equations that approximately predict the dynamics of the stochastic system by estimating the changes of different moments of its variables over time. The core idea is to express different orders of moments and their changes with the moments of other orders, thus obtaining a closed set of equations. If we model the system as discrete time, this set contains ordinary iterative equations, if we model it as continuous time, it will consist of ordinary differential equations. This system of stochastic equations then becomes solvable and tractable after higher orders are ignored, thus, closing the system of equations. The question of which orders will be ignored highly depends on the specifics of the problem. If the setup is such that the distribution of variables under discussion is close to gaussian, we may successfully approximate the system with two moments, if there is a skewness in distributions, we may need three moments, and if the distribution has fatter tails, we may even need higher order moments.

In many stochastic models, each moment (a statistical measure of the system's state) evolves in time and is coupled to other moments, both lower and higher in the most general case. Without approximation, this leads to an endless hierarchy of equations. Moment closure provides an educated guess or formula to truncate this hierarchy, thereby obtaining a finite set of equations that can be analyzed or solved. This approach is crucial in mathematical modeling because many real-world systems are too large or complex to handle exactly. By using approximations, we can capture the essential behavior of these systems without simulating every detail. In summary, moment closure approximations make it possible to analyze complex biological and artificial systems in an analytical way, giving a framework analyze the system without exhaustive simulations. Such approximations are important in complex dynamical systems, as they provide a balanced approach integrating empirical insights and theoretical modeling, allowing researchers to gain insights that might otherwise remain hidden in those complex models.

- **Relevance to population genetics:** In this thesis moment closure approximation has been used as a novel tool in evolutionary biology for modeling dynamics in finite populations where stochastic effects are significant. The quasispecies theory (infinite population size Eigen and Crow-Kimura models) is popular to describe both virus evolution, as well as it is one of the key models of interdisciplinary research, from the virus and cancer to the artificial intelligence [1, 2].
  We solve exactly a series of models, related to the mutator phenomenon. In many classic models such as Eigen or Crow-Kimura an infinitely large population is assumed to simplify analysis, leading to deterministic equations. Moment closure relaxes this assumption by capturing random drift and fluctuations without needing an intractable full stochastic simulation. The key idea is to truncate the hierarchy of

equations for the distribution's moments, focusing on the first few (such as mean and variance) to obtain a closed system. This yields approximate equations for quantities like mean fitness or allele frequency that remain accurate for finite populations.

Using this approach, we can investigate different phenomena that arise in some models of evolutionary dynamics under more realistic conditions. Important factors like mutation rates and recombination are naturally incorporated as hyperparameters that influence the low-order moments of the population's state. For example, in the thesis a moment closure method was applied to the Wright-Fisher model[3] and a finite-population Crow–Kimura model (a quasispecies-type genetics model) with a single-peak fitness landscape[5]. This allowed calculation of finite-population corrections (e.g. to mean fitness) that earlier infinite-population methods could not capture. In general, moment closure provides a way to quantify how random genetic drift interacts with selection and mutation, offering analytical insight into stochastic evolutionary outcomes that would otherwise require intensive simulations.

One notable outcome of the method is the approximation of fixation probabilities in finite populations under the Wright-Fisher model of population genetics. The fixation probability is the chance that a new mutant allele eventually takes over the entire population. Moment closure techniques can accurately approximate this probability across different regimes, effectively bridging the gap between classical infinite-population predictions and the realities of finite, random drift. By obtaining corrections to quantities like mean fitness and fixation likelihoods, the moment closure approximation enriches our understanding of evolutionary dynamics in finite populations and complements more exact (but less tractable) stochastic formulations [4].

- **Relevance to evolutionary game theory:** Evolutionary game theory extends population biology concepts to situations where fitness is frequency-dependent – an individual's success depends on interactions (strategies) within the population. In these models, the payoff (fitness) of a strategy changes with its frequency, and classical deterministic approaches lead to the replicator equation for infinite populations. Moment closure approximation proves valuable here by enabling tractable analysis of the stochastic Moran process, a finite-population birth–death model of evolutionary games. Researchers often formulate evolutionary games in finite populations first (capturing randomness in reproduction and death events), and then consider the infinite-population limit for average behavior. The moment closure method allows one to derive equations for the mean frequency of strategies and their variance in the finite setting, providing insight before taking that infinite limit.

  A central concept in evolutionary game dynamics is the fixation probability of a strategy – for instance, the probability that a single mutant strategy will eventually take over a population of individuals playing another strategy. This is analogous to fixation of a mutant allele in genetics, and evolutionary games in finite populations also exhibit such fixation phenomena. Using moment closure, the thesis derived a

second order analytical approximations for the mean number of individuals playing each strategy over time, as well as the probability that a given strategy fixates, under the Moran process dynamics [4]. The method computes second-order corrections to the replicator equation (which describes an infinite population's average behavior) by accounting for finite-population variance. In practical terms, this means we can estimate how likely a strategic behavior is to dominate purely due to stochastic effects, and how the population state fluctuates around the deterministic prediction.

These results have important implications for modeling strategic interactions in finite populations. They show how random drift and finite size can alter the evolutionary outcome of games compared to ideal infinite scenarios. In the thesis, the moment closure-derived strategy dynamics were cross-validated using an independent Hamilton–Jacobi approach, confirming their accuracy. Notably, this was the first application of moment closure techniques in evolutionary game theory, demonstrating high accuracy in capturing the stochastic fixation behavior of strategies. By providing a way to calculate fixation probabilities and trajectory variances, the approach deepens our understanding of frequency-dependent selection in fields ranging from biology to economics. It highlights the broad relevance of moment closure in any domain where game-theoretic interactions are subject to random fluctuations due to finite agent numbers.

- **Relevance to artificial intelligence and Hebbian learning:** Beyond biology, moment closure approximation has been applied in artificial intelligence, particularly to understand learning dynamics in neural networks. Hebbian learning is an unsupervised learning principle inspired by neurobiology, often summarized as "cells that fire together, wire together." It posits that synaptic connections between neurons strengthen when the neurons are active simultaneously. Unlike backpropagation-based learning, Hebbian learning does not require labeled data or an explicit loss function – it is considered a biologically plausible mechanism by which the brain might self-organize to detect patterns. This makes Hebbian models attractive for tasks like pattern recognition, memory modeling, and dimensionality reduction. However, a well-known challenge in basic Hebbian learning rules is unbounded growth of synaptic weights (instability), which requires modifications to keep the system stable.

  Oja's rule is a prominent Hebbian learning model that addresses this instability[6]. It modifies Hebb's rule by normalizing the weight vector, achieved by adding a negative second order regularization term to the update rule: $w_i(t + 1) = w_i(t) + \alpha[x_i(t)y - y^2 w_i(t)]$. It effectively performs a form of principal component analysis (PCA) on the inputs: the network learns a lower dimensional projection that retains maximal input variance.

  In the thesis, moment closure approximation was applied to analyze the stochastic dynamics of Oja's rule in a neural network. By focusing on the first two moments (mean and variance) of the synaptic weight distribution, the analysis derived a closed-form relationship linking the learning parameters to the system's behavior. In particular, a formula was established that connects the steady-state variance of

the synaptic weights to the network's learning rate (for a given data distribution), using moment equations instead of tracking the full weight distribution. This result, validated by simulations, showed explicitly that higher learning rates lead to larger weight variance at equilibrium. In other words, there is a quantitative trade-off: making the learning rate large speeds up learning but also increases the randomness (variability) in the learned weights, which reflects reduced stability.

These findings have practical significance for machine learning algorithms inspired by Hebbian principles. Because Hebbian learning lacks an objective loss function, one cannot directly apply standard adaptive learning-rate schedulers that are common in backpropagation-based networks. The moment closure analysis provides an alternative guideline: by understanding how the learning rate affects outcome variance, one can tune this parameter to ensure stable convergence of the network. For example, if the derived formula predicts that a certain learning rate will blow up the weight variance, one might choose a smaller rate to keep the network in a stable regime. This insight suggests the possibility of designing adaptive learning-rate schedules for Hebbian or PCA-like networks grounded in moment-based variance analysis. Indeed, the thesis proposes that adjusting learning rates based on the variance of synaptic weights (as calculated via a rolling window) could help maintain stability in Hebbian-inspired neural systems. Such an approach is analogous to how learning rate schedulers are used in deep learning, but tailored to unsupervised, self-organizing models.

More broadly, the success of moment closure in analyzing Oja's rule illustrates its utility in AI. It shows that techniques originally developed for population biology can shed light on the dynamics of learning algorithms. In fact, other researchers have applied moment closure methods to reinforcement learning problems as well – for instance, to analyze stochastic multi-agent Q-learning and bandit algorithms, proving that these learning processes can reach a steady state with finite variance. The cross-disciplinary application to Hebbian learning in the thesis further confirms that moment closure approximation is a versatile tool. It enables AI researchers to derive analytical results (like variance formulas or stability criteria) for complex adaptive systems, much as it enables biologists to solve for gene frequency dynamics in finite populations.

Additionally, this approach has relevance for autonomous robotics research, as the windy-gridworld serves as a prototypical environment for exploring how agents adapt to varying and uncertain conditions. By using the moment closure to approximate higher-order effects, we were able to realistically model real-world challenges such as unpredictable wind gusts and the movement of an agent in such environments[7].

Aim of the work

The thesis proposes a novel approximation technique by specifying the approach in previously more loosely defined moment closure approximation that is particularly helpful in

stochastic Markov processes studied in the thesis. The identified objectives around which significant results were achieved are the following:

- Developing a versatile moment closure method for analyzing stochastic dynamics in finite-population evolutionary models.
- Bridging finite and infinite population approaches by deriving corrections to classic deterministic models and validating them numerically.
- Extending the approximation to evolutionary games, capturing fixation probabilities under frequency-dependent selection.
- Applying the developed method to AI, particularly Hebbian learning (Oja's rule), to study weight variance and stability in unsupervised models.

Highlighting interdisciplinary potential, demonstrating how a single mathematical framework can inform both biological and machine learning research.

The practical significance of the work

The results presented in this thesis have potential applications in diverse areas of both theoretical and applied research. On the evolutionary side, moment closure approximation can help develop more precise genetic algorithms by modeling stochastic effects and finite-population corrections, which are often neglected in classic large-population assumptions. These refined algorithms can be beneficial in problems such as industrial optimization, drug discovery, and bioinformatics, where adaptive search strategies must account for random drift or strong selection.

In evolutionary game theory, the approach clarifies how strategies may fixate under realistic conditions, informing economic, ecological, and computational models of multi-agent interactions. This can be especially relevant for studies of social networks and public goods games, where population sizes are not trivially large and strategic decisions evolve dynamically, and can also have applications in the study of cancer development where healthy cells are in competition with the cancer cells.

In artificial intelligence, the methodology has already shown promise by connecting the stability parameters of the network with the tunable hyperparamers in Hebbian learning. A precise understanding of learning rate effects and parameter fluctuations can guide the design of neural architectures that avoid can more robustly adapt to changing inputs and can self-optimize the learning rate during the learning process itself. We have also shown that the method can have practical application in robotics where it can help us predict the trajectory of an agent in a stochastic environment.

Methods of investigation

Diverse methods have been used while developing this study coming from different fields, including but not limited to probability theory, mathematical analysis, linear algebra, stochastic processes, machine learning, neural networks, theoretical physics and other related fields.

All analytical results have been validated by comparison with computer simulations. Python with respective libraries have been used for developing this study for the simulations of stochastic processes and the trainings of neural networks.

Publications

All results represented in the thesis have been published in peer reviewed journals. The results are published in 7 articles (5 were published in international journals included in the lists of Scopus and Web of Science, and 2 were published in local journals). The complete list of the publications is given at the end of the synopsis.

Approbation of the results

The results were presented in the "XVIII International Annual Scientific Conference of Russian-Armenian University" and in a scientific seminar organized by Institute for Informatics and Automation Problems of NAS RA.

Structure of the work

The thesis has an introduction, 4 chapters, conclusion and bibliography.
1. Introduction describes the models that have been studied in the thesis, main challenges that arise during the mathematical modeling of their dynamics and the aim of the thesis.
2. Chapter 1 introduces quasispecies models, and the work we did for solving the cases of randomly changing fitness landscape with recombination and the mutator model with asymmetric transitions.
3. Sections 2.1-2.4 discuss the Wright-Fisher finite population evolution model and the work we did for estimating the fixation probability under this model for static and randomly changing fitness landscapes.
4. Section 2.5 introduces our proposed form of moment closure approximation that utilizes the master equation.
5. Sections 2.6-2.13 discuss our solutions to the dynamics of Wright-Fisher model and finite population version of Crow-Kimura model. The results are discussed for both two and three allele models, and the cases of small selective coefficients and single peak fitness Crow-Kimura model are described separately.

6. Chapter 3 introduces out results in finite population evolution games. Both the moment-closure approach and Hamilton-Jacobi approach for the Moran model are discussed.
7. Sections 4.1-4.4 describe our work done on the scope of Hebbian learning. This part of the thesis derives the closed form solution that connects the steady-state variance of the models parameters with the learning rate with the help of a simple linear equation.
8. Section 4.5 the modeling of the movement of an agent in a stochastic environment with the moment-closure approach.

Main results of the work

Each chapter the thesis focuses on a specific application domain and presents the core results achieved. Below is a summary of the main results from the thesis:

- **Analytical Corrections for Finite Populations:** One of the primary results is the successful application of moment closure to finite population genetic models, yielding analytical insights that go beyond classic infinite-population theories. We begin by constructing a moment closure scheme for the Wright-Fisher model [5], which allows us to account for finite-population sampling effects without resorting to a full-blown stochastic treatment. First, we write down the **master equation** that governs how allele frequencies change over each iteration. We introduce the probability distribution functions $P_{j_1,..j_L}(n)$ having the given set of integers at n-th moment of time.

$$P_{j_1,...j_L}(n+1) =$$
$$\sum_{i_1,,i_L} P_{i_1,...i_L}(n) M(i_1, ... i_L; j_1, .. j_L),$$
$$M(i_1, ... i_L; j_1, ... j_L) =$$
$$\frac{N!}{j_1! .. j_L! (N - j_1 - \cdots j_L)!} \eta_1^{j_1} ... \eta_1^{j_L} (1 - \eta_1 - \cdots \eta_L)^{N-j_1...-j_L}$$
$$\eta_j = \frac{\sum_l i_l r_l m_{lj}}{\sum_l i_l r_l}$$

(1)

Here m_{lj} is the mutation probabilities from the l-th to j states, while r_i are the fitnesses. $M(i_1, ... i_L; j_1, .. j_L)$ is the final transition probability of going from the state described by integers $i_1, ... i_L$, to the described by integers $j_1, ... j_L$ during a single iteration. Then, instead of trying to solve the master equation exactly, we

calculate the first two (and sometimes three) moments—namely, the mean, variance, and skewness of the allele distribution—and approximate higher moments in terms of these lower ones. Doing so, we get an iterative rule for the first and second degree moments of the variables in the system.

$$Q_i = N\left(\eta_i(\vec{Q}) + \sum_{i,j} \eta''_{i;j,l}\frac{v_{jl}}{2}\right)$$

$$Q_{ii} = N^2\left(\sum_{jl}\left((\eta'_{i;j}\eta'_{i;l} + \eta_i\eta''_{i;j,l})\left(1 - \frac{1}{N}\right) + \frac{\eta''_{i,l,l}}{N}\right)v_{jl}\right) \tag{2}$$

$$Q_{ij} = N^2\left(\eta_i\eta_j\left(1 - \frac{1}{N}\right) + \right.$$

$$\left(1 - \frac{1}{N}\right)\left(\sum_{l,n}(\eta'_{i,l}\eta'_{j,n} + \eta''_{i;l,n}\eta_j + \eta''_{j;l,n}\eta_i)v_{ln}\right)$$

Where the moments are defined as

$$Q_i \equiv <i> = N<\eta_i>$$

$$Q_{ii} \equiv <i^2> = N^2<(\eta_i)^2>\left(1 - \frac{1}{N}\right) + \eta_iN, \tag{3}$$

$$Q_{ij} \equiv <ij> = N^2<\eta_i\eta_j>\left(1 - \frac{1}{N}\right)$$

In equation (2) we used the following forms for partial derivatives:

$$\eta_{i;j} = \frac{\partial\eta_i(q_1 \ldots q_L)}{\partial q_j}$$

$$\eta_{i;j,l} = \frac{\partial\eta_i(q_1 \ldots q_L)}{\partial q_j \partial q_l}$$

These results were validated by comparison with numerical results obtained with the help of computer simulations of the Wright-Fisher process. The comparison with the numerical results for the 2 allele case can be found in Figure 1 and Figure 2. The results for the 3 allele case are represented in the thesis.

The same form of the moment closure approximation is also tested and validated for the finite population Crow-Kimura model.
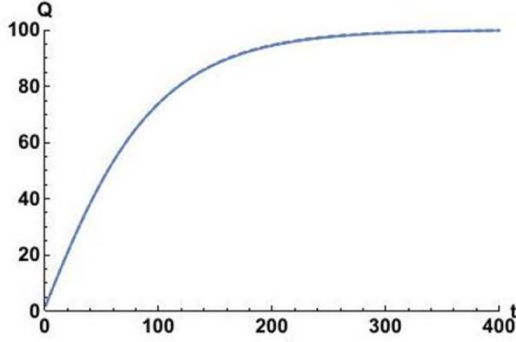
Figure 1: Two allele Wright-Fisher model given by Eqs. (1), $w_i \equiv w(x) = \frac{x(1+s)+u(1-x)}{1+xs}, x = i/N, u$ is the mutation rate to the mutant, $(1+s)$ is the mutant fitness. The average number of mutants $Q = <i>$ versus the time for two allele model with $N = 100, u = 0.01, s = 0.01$, numerical result and the result obtained with the moment closure approach.

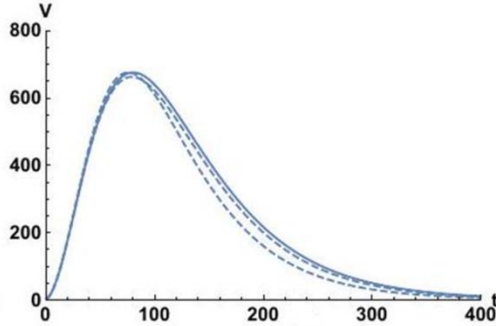Figure 2: Two allele Wright-Fisher model given my Eqs. (1), $w_i \equiv w(x) = \frac{x(1+s)+u(1-x)}{1+xs}, x = i/N, u$ is the mutation rate to the mutant, $(1+s)$ is the mutant fitness. The variance versus the time for two allele model with $N = 100, u = 0.01, s = 0.01$, the low dashed line corresponds to the second degree moment closure approximation, the high dashed line-to three moment approximation. The smooth line corresponds to the numerical results obtained with the help of computer simulations.
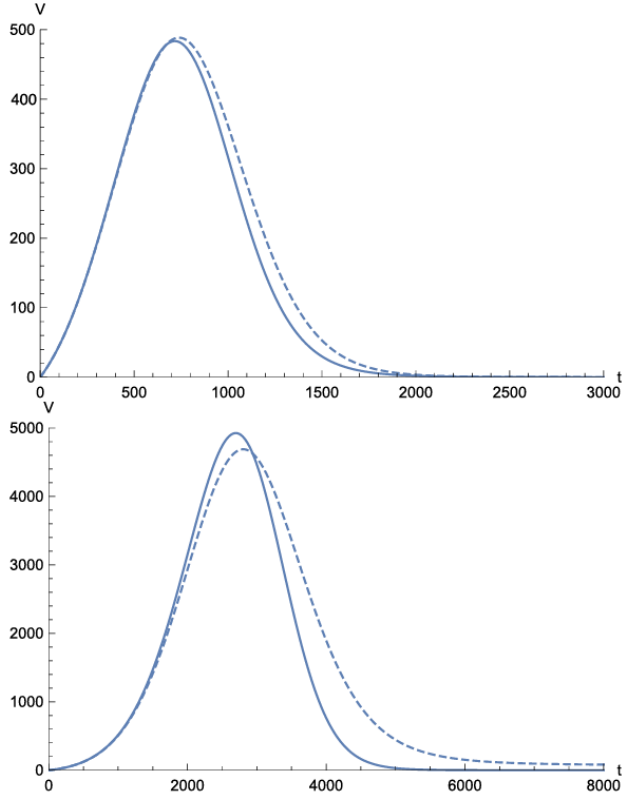
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Figure 3: The dynamics of variance for the Prisoners Dilemma game with constant payoff matrix $(a, b, c, d) = (0.5, 1.5, 0, 1)$ with $w = 0.9$, but different number of replicators and initial conditions. The first plot is for $N = 200, i_0 = 40$, the second one is for $N = 400$, $i_0 = 20$ with N being the number of all replicators, and i_0 being the initial number of replicators with the first strategy. The solid line represents the numerical result while the dashed line is the result obtained with the moment closure approximation.

- **Results for quasispecies models:** In addition to this, we also developed and solved evolutionary quasispecies models that incorporate mutator genes, asymmetric mutation rates, and recombination on fluctuating fitness landscapes. We proposed a two-state quasispecies model in which a special gene switches between a normal

(wild-type) and a mutator allele [2], leading to different mutation rates and fitness functions. Employing a Hamilton–Jacobi equation approach, we analytically derived the population's mean fitness and steady-state distribution for large genome length. A key outcome is the emergence of a mutator phase, in which a high-mutation allele persists and alters the system's phase structure. We also found an interesting phenomenon where sufficiently large genomes exhibit oscillatory and non-smooth dynamics, indicating a transition that undermines the single-equation approximation.

We also extended this study to include recombination and random switching in the fitness landscape [1]. By combining Crow–Kimura-like dynamics with recombination, we derived near-exact steady-state solutions under various symmetry conditions, sometimes mapping the system onto a simpler effective fitness model. We showed that recombination may raise or lower mean fitness depending on the epistatic properties of the effective landscape: negative epistasis favors recombination, whereas non-negative epistasis can diminish its benefit.

- **Derivation of Finite-Population Strategy Dynamics:** In the context of evolutionary game theory, we presented the first application of moment closure approximation to stochastic game dynamics in finite populations. Focusing on the Moran process (a common model for finite-population evolution of strategies, where individuals are randomly replaced over time proportional to fitness), the work derived **second-order analytical approximations** for the trajectory of game strategy frequencies [4]. In practical terms, this means the thesis obtained iterative equations that describe how the expected number of individuals playing each strategy changes over time, along with how those numbers vary due to random drift.

The equations were setting iterative rules for the first and second order moments of the process variables at timestamp n, denoted by Q and $Q_{2,n}$ respectively and had the following form.

$$
Q_n = \sum P_i(n)\frac{l}{N},
$$
$$
Q_{2,n} = \sum_i P_i(n)\left(\frac{i}{N}\right)^2
$$

(4)

$$
Q_{n+1} = Q + \frac{(F(Q) - B(Q))}{N} + +(F''(Q) - B''(Q))\frac{V}{2N}
$$

$$
Q_{2,n+1} = Q_{2,n} + F(Q)\left(\frac{2Q}{N} + \frac{1}{N^2}\right) + B(Q)\left(-\frac{2Q}{N} + \frac{1}{N^2}\right) + (F''(Q) + B''(Q))\frac{V}{2N^2} +
$$

$$
\left(2(F'(Q) - B'(Q)) + Q(F''(Q) - B''(Q))\right)\frac{V}{N}
$$

(5)

where $F(Q)$ and $B(Q)$ are the probabilities of increase and decrease in the numbers of the replicators of the first type respectively

These equations can be seen as a corrected version of the replicator equation for finite populations: they reduce to the classical replicator dynamics in the infinite population limit, but include additional terms (of order $1/N$, where N is population size) that account for stochastic fluctuations.

The accuracy of these moment-closure based equations for evolutionary games was rigorously tested. The process was simulated using numerical methods and the numerically estimated moments for different parameters of the model was compared with the moments obtained through the iterative rule. The comparison of analytical results obtained by equation (5) and numerical results obtained by computer simulations is represented in Figure (3).

- **Analyzing Stochastic Hebbian Learning:** Moving to the domain of machine learning, the thesis applied moment closure to analyze the learning dynamics of Oja's rule, which is a classic model of Hebbian learning. Oja's rule is an iterative algorithm where a synaptic weight vector is adjusted in proportion to the neuron's output and input (Hebb's principle), with a normalization term that ensures the weight vector length remains constant (preventing unbounded growth). When Oja's rule is used on streaming data (inputs coming in one by one, possibly with some noise), the update process is inherently stochastic. The main result here was the derivation of a closed-form relationship linking the learning parameters to the long-term behavior of the system, using a moment closure approximation.

By considering the first two moments of the weight distribution (mean and variance of the weights) and closing the system at the second moment, the thesis obtained an analytical expression for the steady-state variance of the synaptic weights as a function of the learning rate and the properties of the input data (correlation of the input features) [6].

$$\hat{V} = \alpha \frac{1 - \rho^2}{8|\rho|} \tag{6}$$

In simpler terms, this result quantitatively describes how "noisy" or variable the learned weights will be after a long training time, depending on how aggressively the network is learning. The analysis showed explicitly that if you increase the learning rate in Oja's rule, the variance of the weight values at equilibrium becomes larger linearly. This makes intuitive sense — a higher learning rate means bigger jumps with each update, leading to more fluctuation — but the thesis provided a precise formula for this relationship. The result was backed by simulations of Oja's rule: the theoretical predictions of weight variance matched the empirical variance observed in simulations across different learning rates,

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confirming the validity of the moment closure approach in this context. The numerical simulations were carried out by training the model on a synthetic data using Python programming language.

To validate the result of (6), we have created a simple experimental setup. Initially, we set $w_1 = 0$ and $w_2 = 1$. At each iteration, we generate a new data point from the bi-variate Gaussian distribution. Then we train for sufficiently long iterations until the steady state distribution is reached. We repeat this training process from scratch 500 times, save the final weights after each training process and calculate the variance of these 500 weights. Since the sign of the steady state solution depends on the initial weights every time we set the same value for the weights at the beginning. The same variance will be obtained for other initial conditions as well, while the mean steady state value may differ in sign. Then we repeat this same process for different learning rates to capture the relation between the final variance of the weights and the learning rate α.

This same process is repeated for different sets of data points generated from multivariate normal distribution with different correlation coefficients ρ to check the dependence of variance on correlation found in (6). Comparisons of the variances with the analytic values obtained in the previous section are represented in Figure. In those figures we can see that for values of learning rate which are in the range conventionally used in practical applications our equation (4.10) very accurately describes the variance of the parameters of the model at the steady state of the system after sufficiently long process of training.

Understanding the trade-off between learning speed and stability is a key insight from the above result. The thesis highlighted that while a larger learning rate allows the network to adapt faster to data, it also injects more randomness into the weight updates, potentially causing the weights to bounce around a noisier equilibrium (which could be seen as a form of *instability* in learning). This insight is significant for practitioners of machine learning who use Hebbian-like learning rules or other stochastic methods without a clear objective function.

One practical proposition emerging from this work is the idea of an adaptive learning-rate strategy for Hebbian learning. Since the moment closure analysis provides a way to calculate or estimate the current variance of weight changes, one could design the learning algorithm to adjust its learning rate on the fly: if the variance (instability) grows beyond a certain threshold, the learning rate could be reduced to stabilize learning. Conversely, if the variance is very low (indicating perhaps slow learning or convergence), the learning rate might be increased slightly to speed up progress.
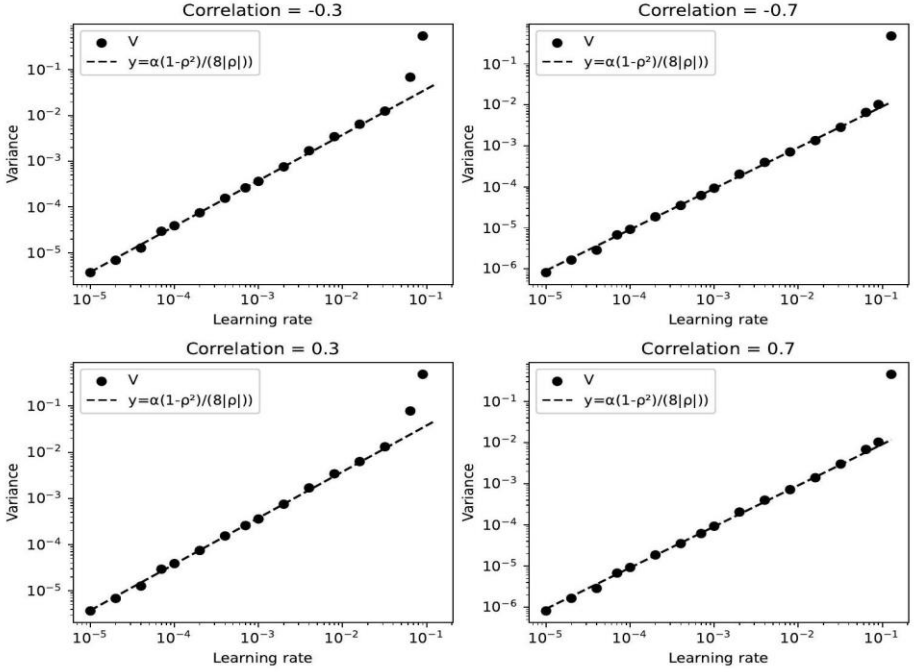
Figure 4: If we train the system from scratch many times and calculate the variance of the final weight w_1, it will be very close to the analytically calculated value of (6) for learning rates that are sufficiently small for converging. Here it is checked for 4 different correlation coefficients, both positive and negative, thus showing the robustness of the result.

- **Analyzing the movement of an agent in a stochastic environment:** In addition, the thesis demonstrates an application of the moment closure method in the windy-gridworld problem, a well-known benchmark in reinforcement learning [7]. In this environment, an agent navigates a grid where "wind" exerts a stochastic influence on its movements, causing random drifts that deviate the agent from its intended path. By formulating the agent's position distribution and velocity increments through the master equation framework, the moment closure approximation yields efficient estimates of both mean trajectories and higher-order statistics. These analytical results are validated against simulation data, showing that second-order approximations can capture critical features of the environment's randomness more accurately than simple first-order or deterministic models.

  The implications for robotics are significant, as windy-gridworld environments model the type of stochastic disturbances common to real-world robotic applications—such as aerial drones subject to sudden gusts or ground robots

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navigating uneven terrain. Employing a moment closure approach enables one to calculate closed-form updates for positions, velocities, or control signals without extensive sampling.

In addition to estimating the dynamics of the second moment (variance) with the help of the moment-closure technique, we also validated that the usage of the second moment in the equations also significantly improves the estimation of the first moment yielded by the first order approximation. This is an important result, further indicating that including higher order terms in the closed set of equations also improves the accuracy of the estimation of lower order moments. See Table 1 for the comparison.

N	n_{steps}	1st degree approximation MAE	2nd degree approximation MAE
3	18	$6.79*10^{-3}$	**$4.01*10^{-4}$**
4	24	$7.67*10^{-3}$	**$5.11*10^{-4}$**
5	30	$7.43*10^{-3}$	**$4.05*10^{-4}$**
10	60	$8.41*10^{-3}$	**$4.74*10^{-4}$**
20	120	$8.30*10^{-3}$	**$8.08*10^{-4}$**
50	300	$8.59*10^{-3}$	**$1.11*10^{-3}$**
100	600	$9.00*10^{-3}$	**$9.11*10^{-4}$**

Table 1: Here for different values of N (size of the grid in of the stochastic environment) Mean Absolute Errors for first and second degree approximations are compared with one another. As can be seen, second degree approximation significantly outperforms the first degree approximation across different scales of N.

Conclusion

In conclusion, the thesis "Moment Closure Approximation and its Applications in Machine Learning and Evolution" brings forward a unifying framework to address complexity in systems across biology and artificial intelligence. The moment closure approximation, as developed and applied in this work, proved to be a powerful tool for deriving analytical insights into stochastic processes that were previously tractable only via computer simulation or not at all. By achieving the aims – from evolutionary genetics models to game-theoretic dynamics and neural learning rules – the research demonstrated that a single mathematical approach can illuminate diverse phenomena.

One of the common threads linking the findings is that finite-size and randomness matter greatly in real systems, and that we can account for them in a systematic way. In

evolutionary theory, the work shows how finite populations deviate from ideal infinite ones, quantifying those deviations and enriching evolutionary predictions. In evolutionary game theory, it highlights how chance can tip the balance of strategy competitions, providing tools to calculate those odds. In machine learning, it reveals how the parameters of a learning process influence stability, offering a way to balance learning speed and reliability. Together, these results not only solve specific problems in their respective fields but also collectively expand our methodological toolkit for scientific inquiry. Crucially, the thesis underscores an important insight: mathematical techniques developed in one domain (like moment closure in chemical models) can be adapted to seemingly unrelated domains (like population genetics, game theory and neural networks) to great effect. Such cross-pollination of ideas is increasingly important in modern science, where complex systems research, data science, biology, and AI often intersect. The findings of this work encourage a more integrated view of complex system analysis. By bridging theoretical gaps between fields, the thesis opens the way for future research to build on its moment closure methods – whether that means exploring new evolutionary scenarios (e.g. co-evolution, epidemiological models), new game-theoretic models (networked games, fluctuating environments), or new machine learning algorithms (reinforcement learning dynamics, adaptive systems).

In summary, this work is significant both for the specific results it delivers and for the broader perspective it provides. It demonstrates that moment closure approximation can be a cornerstone technique for analyzing and understanding the behavior of stochastic systems without needing infinite models or exhaustive simulations. The practical implications range from more accurate evolutionary computations to more stable learning algorithms. By tying together the fields of evolution and machine learning through a common analytical approach, the thesis contributes to a vision of science where universal principles and tools help unravel the complexity of the natural and artificial worlds.

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[6] E. A. Vardanyan, "Analyzing steady state Variance in Hebbian Learning: A Moment Closure Approach," *Mathematical Problems of Computer Science,* vol. 62, pp. 82-93, 2024

[7] E. A. Vardanyan. "Second order approximations for "Windy Gridworld" models," Вестник Российско-Армянского (Славянского) университета (серия: физико-математические и естественные науки). 2024(2):7-14.

<p style="text-align:center">**Ամփոփում**</p>
<p style="text-align:center">Էդգար Արայի Վարդանյան</p>

Մոմենտների փակման մոտավորությունը և նրա կիրառությունները մեքենայական ուսուցման և Էվոլյուցիայի մեջ

Ատենախոսությունում ներկայացված է միասնական մոտեցում, որը հիմնված է մոմենտների փակման մոտարկման վրա և հնարավորություն է տալիս անալիտիկ կերպով ուսումնասիրել բարդ ստոխաստիկ համակարգեր Էվոլյուցիոն կենսաբանության և արհեստական բանականության բնագավառներում։ Այս մոտեցումը թույլ է տալիս ստանալ մաթեմատիկական մոտարկումներ այնպիսի պրոցեսների դինամիկայի վերաբերյալ, որոնք նախկինում պահանջել են անսահման մեծ պոպուլյացիայի ենթադրություններ կամ մեծածավալ համակարգչային սիմուլյացիաներ։ Մեթոդը կիրառվել է տարբեր ոլորտներում՝ վերջավոր պոպուլյացիաների գենետիկայում, Էվոլյուցիոն խաղերի տեսությունում, Հեբբյան ուսուցման նեյրոնային ցանցերում և գործակալի ստոխաստիկ նավիգացիայի խնդիրներում։ Աշխատանքում ցույց է տրված, որ միասնական մաթեմատիկական մոտեցումը թույլ է տալիս հաշվի առնել վերջավոր համակարգերի էֆեկտները և պատահական տատանումները, ստանալով ավելի ճշգրիտ կանխատեսումներ Էվոլյուցիոն դինամիկայում և կայուն վիճակը նկարագրող արդյունքներ ուսուցման ալգորիթմների համար։

Ատենախոսության հիմնական նպատակը ստոխաստիկ դինամիկական համակարգերի վերլուծության համար ընդհանուր կիրառելի մեթոդի մշակումն ու կիրառումն է՝ հիմնված մոմենտների փակման մոտարկման վրա։ Կոնկրետ նպատակներն են՝

- Ստեղծել վերջավոր պոպուլյացիաների Էվոլյուցիոն մոդելների վերլուծության ունիվերսալ մեթոդ։
- Դետերմինիստական մոդելների մեջ շոկումների հաշվարկ և դրանց թվային հաստատում՝ կապելով վերջավոր և անսահման պոպուլյացիաների դինամիկան։
- Մեթոդի կիրառումը Էվոլյուցիոն խաղերի տեսությունում՝ հաշվի առնելով պատահականության ազդեցությունը վերջավոր պոպուլյացիաներում։
- Մեքենայական ուսուցման ոլորտում (Հեբբյան ուսուցում) մեթոդի կիրառումը՝ ուսուցման պարամետրերի և երկարաժամկետ կայունության միջև կապի ուսումնասիրության և մոդելների զուգամիտության վերլուծության համար։
- Մեթոդի միջդիսցիպլինար կիրառելիության ցուցադրում՝ Էվոլյուցիոն կենսաբանության և արհեստական բանականության խնդիրներում։

Հիմնական արդյունքները

- **Պոպուլյացիոն գենետիկայում** մոմենտների փակման մեթոդը կիրառվել է վերջավոր պոպուլյացիաների գենետիկական մոդելների դեպքում (Ռայթ-Ֆիշերի և վերջավոր Կրոու-Կիմուրայի մոդելներում): Ստացվել են անալիտիկ բանաձևեր ալելային հաճախականությունների դինամիկայի համար (միջին արժեք և դիսպերսիա՝ ընտրության և մուտացիաների ազդեցությամբ), որոնք արտացոլում են վերջավոր պոպուլյացիաների շեղումները դասական անսահման պոպուլյացիաների մոդելներից: Արդյունքները թվային սիմուլյացիաներով հաստատվել են, ապահովելով մեծ ճշգրտություն:

- **Քվազիտեսականների մոդելներում** ստացվել են անալիտիկ լուծումներ՝ ներառելով մուտատոր գեներ և ռեկոմբինացիա փոփոխական ֆիթնես լանդշաֆտների դեպքում: Հայտնաբերվել է նոր՝ «մուտատոր փուլ», երբ բարձր մուտացիոն ակտիվությամբ ալելը երկարաժամկետ պահպանվում է պոպուլյացիայում և զգալիորեն փոխում է էվոլյուցիոն ելքերը:

- **Էվոլյուցիոն խաղերի տեսությունում** մեթոդը առաջին անգամ կիրառվել է վերջավոր պոպուլյացիաների էվոլյուցիոն խաղերի ստոխաստիկ դինամիկայի վրա (Մորանի գործընթաց): Ամfraնցvel է ռեպլիկատորային դինամիկայի շտկված տարբերակը, որն արտացոլում է վերջավոր պոպուլյացիաների պատահական էֆեկտները և սահմանային դեպքում համընկնում է դասական ռեպլիկատորային դինամիկային: Ստացված անալիտիկ արդյունքները ստուգվել և հաստատվել են սիմուլյացիաներով՝ դառնալով նոր գործիք էվոլյուցիոն խաղերի անալիտիկ հետազոտության համար:

- **Հերքյան ուսուցման մեջ** Օյայի կանոնի համար կիրառվել է մոմենտների փակման մեթոդը, ստացվել է ուսուցման արագության և սինապտիկ կշիռների կայուն վիճակի դինամիկայի միջև անալիտիկ կապ: Ցույց է տրվել, որ ուսուցման ավելի մեծ արագությունը հանգեցնում է կշիռների մեծ դիսպերսիայի, ինչպ հավաստվել է սիմուլյացիաներով: Այս արդյունքը հիմքեր է տալիս Հերքյան ցանցերի համար ուսուցման արագության ադապտիվ կարգավորումների հետազոտությունների համար:

- **Գործակալի ստոխաստիկ նավիգացիայի խնդրում** մեթոդը ընդլայնվել է («քամու ցանցային աշխարհ»): Ստացվել են գործակալի միջին դիրքի և դիրքի դիսպերսիայի անալիտիկ կանխատեսումներ՝ հաշվի առնելով պատահական քամու ազդեցությունը: Երկրորդ կարգի մոմենտի (դիսպերսիայի) հաշվառումը զգալիորեն բարելավել է կանխատեսումների ճշգրտությունը:

Այսպիսով, աշխատանքը վկայում է, որ մոմենտների փակման մոտարկման մեթոդը արդյունավետ գործիք է ստոխաստիկ համակարգերի անալիտիկ հետազոտության համար, ապահովում է ճշգրիտ կանխատեսումներ և կարևորում մեթոդի կիրառելիությունը տարբեր ոլորտներում՝ կենսաբանությունից մինչ արհեստական բանականություն:

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Заключение
Варданян Эдгар Араевич

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Приближение замыкания моментов и его приложения в машинном обучении и эволюции

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В диссертации представлен единый подход, основанный на методе замыкания моментов, позволяющий проводить аналитический анализ сложных стохастических систем в областях эволюционной биологии и искусственного интеллекта. Метод решает задачу получения аналитических решений для процессов, ранее требовавших предположений о бесконечно больших популяциях или масштабных компьютерных симуляций. Применяя замыкание моментов в различных областях – таких как генетика конечных популяций, эволюционные игры, Хеббовское обучение в нейронных сетях и стохастическая навигация агентов – работа связывает теоретические модели с реальной изменчивостью. Диссертация показывает, что единая математическая схема может учитывать эффекты конечного размера системы и случайные флуктуации, обеспечивая улучшенные прогнозы эволюционной динамики и критерии устойчивости для алгоритмов обучения.

Главной задачей работы было разработать и применить универсальную методику замыкания моментов для анализа стохастических динамических систем. Конкретные цели включали:

- Создание универсального подхода замыкания моментов для эволюционных моделей конечных популяций.
- Выведение и численное подтверждение поправок к классическим детерминистским моделям, связывающим динамику конечных и бесконечных популяций.
- Распространение метода на эволюционную теорию игр с учётом влияния случайности в конечных популяциях.
- Применение подхода к задачам машинного обучения (Хеббовское обучение) для анализа связи параметров обучения с долгосрочной устойчивостью и сходимостью моделей.
- Демонстрация междисциплинарного потенциала метода на примерах задач эволюции и искусственного интеллекта.

Диссертация получает результаты в различных областях:

- **Популяционная генетика:** Метод замыкания моментов применён к генетическим моделям конечных популяций (например, модели Райта–Фишера и конечнопопуляционной модели Кроу–Кимуры). Получены аналитические формулы для динамики аллельных частот (среднее значение и дисперсия), которые количественно описывают отклонения реальных (конечных) популяций от классических бесконечнопопуляционных

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прогнозов. Эти формулы позволяют точнее оценивать вероятность фиксации мутаций и среднюю приспособленность. Численные симуляции подтвердили высокую точность этих аналитических результатов.

- **Модели квазивидов:** Получены аналитические решения для моделей квазивидов, включающих сложные элементы, такие как гены-мутаторы и рекомбинация в условиях изменяющихся ландшафтов приспособленности. Выявлена новая «мутаторная фаза», при которой в популяции стабильно сохраняется аллель с повышенной скоростью мутаций, существенно изменяющая эволюционные сценарии.

- **Эволюционная теория игр:** Впервые применён подход замыкания моментов к стохастической динамике эволюционных игр в конечных популяциях (на примере процесса Морана). Выведена скорректированная репликаторная динамика, учитывающая случайные эффекты конечного размера популяции и сходящаяся к классической репликаторной динамике в пределе бесконечной популяции. Аналитические результаты (траектории частот стратегий и вероятности их фиксации) были тщательно проверены и подтверждены численными экспериментами, что предоставляет новый аналитический инструмент для изучения эволюционных игр.

- **Хеббовское обучение:** Метод замыкания моментов применён к правилу Ойя (стабилизированному варианту Хеббовского обучения). Выведена аналитическая зависимость между скоростью обучения и стационарной дисперсией синаптических весов нейросети. Показано, что более высокие скорости обучения приводят к большему разбросу весов, что отражает компромисс между скоростью обучения и стабильностью. Результаты подтверждены численными симуляциями и предлагают теоретическую основу для адаптивной настройки скорости обучения в Хеббовских нейросетях.

- **Стохастическая навигация агентов:** Расширение метода на задачу стохастической навигации агента («ветреный сеточный мир») позволило вывести аналитические уравнения для средней траектории и дисперсии положения агента в условиях случайных возмущений (ветра). Включение моментов второго порядка (дисперсии) существенно улучшило точность прогнозов по сравнению с подходом, учитывающим только средние значения.

Таким образом, диссертация демонстрирует, что подход замыкания моментов является инструментом для аналитического анализа стохастических систем, обеспечивающим точные прогнозы и глубокое понимание процессов, ранее доступных лишь с помощью численных методов. Результаты работы способствуют дальнейшему развитию методов моделирования сложных адаптивных систем и имеют широкое практическое применение как в биологии, так и в задачах искусственного интеллекта.