DYNAMICS OF THE RELATIVE ENTROPY MINIMIZATION PROCESSES

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Abstract
Dynamics of non-stationary processes that minimize the Kullback–Leibler divergence (follow the minimum of the relative entropy principle) are considered. A set of equations describing the system dynamics under the mass conservation and energy conservation constraints is derived. The existence and uniqueness of solution are established, asymptotic stability of the equilibrium is proved. Equations are derived based on the Speed-Gradient (SG) principle originated in the control theory.

Key words
Kullback–Leibler divergence, speed-gradient principle, non-stationary process, convergence.

1 Introduction

In 1951, Solomon Kullback and Richard Leibler [Kullback and Leibler, 1951] introduced a measure of similarity between two discrete probability distributions P and Q as

$$D(P,Q) = \sum_i P(i) \ln\left(\frac{P(i)}{Q(i)}\right). \qquad (1)$$

Typically P represents the actual distribution of data or observations while Q represents a theory, model or approximation of P.

This measure is called Kullback–Leibler (KL) divergence and it is also known as information divergence or relative entropy. It has found numerous applications in many fields of science and sometimes is considered as one of the most general concepts of modern science [Pavon and Ticozzi, 2005].

The KL divergence is used in problems of information theory, mathematical statistics and probability theory (e.g. The Central Limit Theorem [Barron, 1986]). It is also used in crystallography to ensure chemical and structural integrity of the refined models [Murshudov, Skubak and Lebedev, 2011]. In geoscience the KL divergence is applied for automatic labeling of geospatial objects [Akcay and Aksoy, 2008] and for automatic change detection in multitemporal synthetic aperture radar images [Inglada and Mercier, 2007]. It is also actively used in signal processing and pattern recognition [Georgiou, 2002; Georgiou and Lindquist, 2003]. In [Kim and Kang, 2007] the KL divergence is applied for unsupervised texture segmentation problem.

The concept of relative entropy comes from statistical mechanics. The problem of minimizing of the relative entropy has been extended by Solomon Kullback [Kullback, 1959] and Edwin Jaynes [Jaynes, 1989]. Despite a large number of publications studying the minimum of relative entropy, the dynamics of evolution and transient behavior of the physical systems are still not well investigated.

In this paper we propose a hypothesis how a system could evolve to the state with minimum value of the KL divergence (relative entropy). based on the Speed-Gradient (SG) principle [Fradkov, 1991; Fradkov, Miroshnik and Nikiforov, 1999; Fradkov, 2005; Fradkov, 1979] originated in the control theory.

The SG principle has already been successfully applied in [Fradkov, 2008] to derive transient dynamics for a system driven by maximum entropy principle. Applicability of the SG principle is experimentally tested in [Fradkov and Krivtsov, 2010] for the systems of finite number of particles simulated with the molecular dynamics method. Continuous probability distributions are considered in [Fradkov and Shalymov, 2015a]. The dynamics of discrete systems for the Tsallis entropy is discussed in [Shalymov and Fradkov, 2015b]. Continuous Tsallis entropy is investigated in [Shalymov, 2016]. The Rényi entropy is investigated from the SG-principle perspective in [Shalymov and Fradkov, 2016b]. Applicability of SG-principle to general thermodynamic systems is considered in [Khantuleva and Shalymov, 2017]. State-of-the-art of the whole area of cybernetical physics is presented in [Fradkov, 2017].

In this paper an approach proposed in [Fradkov, 2008; Fradkov and Shalymov, 2015a] for Shannon entropy is generalized to the case of relative entropy. A set of equations describing dynamics of non-stationary (transient) states and describing a way and trajectory of the system that minimizes its relative entropy is derived. The evolution law of the system in general form is formulated as:

$$\dot{P}(t) = -\gamma(I - \Psi)A(t), \tag{2}$$

where $A(t) = (\ln \frac{p_1(t)}{p_1^*}, \ldots, \ln \frac{p_m(t)}{p_m^*})^T$, $p_i(t)$ is probability of the system location in state i for time t, p_i^* is desired probability for state i, I is an identity matrix, Ψ is a symmetric matrix that depends on constraints imposed, $\gamma > 0$ is a constant gain.

This paper extends the number of applications of the SG-principle to entropy-driven systems by investigation of the KL divergence.

The paper is organized as follows. The next section briefly formulates the SG-principle The 3th section derives dynamics equation for the mass conservation constraint. The existence and uniqueness of solution is verified, equilibrium stability is proved. The 4th section contains results from 3th section extended to the energy conservation constraint.

2 Speed-Gradient Principle

Let us consider a category of physical systems which dynamics is described by the system of differential equations

$$\dot{x} = f(x, u, t), \tag{3}$$

where $x \in \mathbb{C}^n$ is the system state vector, u is the vector of input (free) variables $t \geq 0$. The problem is to derive the law of variation (evolution) of $u(t)$ that satisfies some criterion of "natural" behavior of the system.

A typical approach to derive such a criterion from variational principles usually starts with specifying some goal functional $Q\,(x(t), t)$ (for example, the action functional of the least action principle [Lanczos, 1962]). Functional minimization defines probable trajectories of the system $\{x(t), u(t)\}$ as points in the corresponding functional space.

The SG law of dynamics is formulated as follows:

$$u = -\Gamma \nabla_u \dot{Q}, \tag{4}$$

where $\dot{Q}$ is a rate of change of the goal functional along the trajectory of the system (3), i.e. the speed $\dot{Q} = \frac{dQ}{dt}$. We use application of the SG principle in the simplest (yet the most important) case where a category of models of the dynamics (3) is specified as the relation:

$$\dot{x} = u. \tag{5}$$

The relation (5) just means that we are deriving the law of change of the state velocities. In accordance with the SG principle, the goal functional $Q\,(x(t), t)$ needs to be specified first. It should be based on physics of a real system and reflect its tendency to decrease the current value. After that, the law of dynamics can be expressed as (4).

3 Minimization of the KL Divergence with the Speed-Gradient Method

Let us consider a discrete system with a set of m possible states $s_1, \ldots, s_m$. The system evolves somehow with probability distribution over states $P(t) = \{p_1(t), \ldots, p_m(t)\}$, where $p_i(t)$ is a probability of the system location in state i. $P^* = \{p_1^*, \ldots, p_m^*\}$ is a desired distribution. Both $P(t)$ and P^* satisfy the normalization conditions:

$$\sum_{i=1}^{m} p_i(t) = 1, \;\; \forall t, \qquad \sum_{i=1}^{m} p_i^* = 1. \tag{6}$$

As a goal functional Q for SG method we use the KL divergence that can be formulated as

$$Q(P, P^*) = D(P(t), P^*) = \sum_{i=1}^{m} p_i(t) \ln \frac{p_i(t)}{p_i^*}. \tag{7}$$

Let us define a law of system dynamics as

$$\dot{x} = u(t), \;\; x = p(t). \tag{8}$$

We have to define a function $u(t)$.

According to the SG principle a rate of the KL divergence change (7) has to be calculated first. Then a gradient of a rate for function u has to be found. And finally, control parameters has to be defined. These parameters are proportional to projection of gradient on a surface of bounds (6).

First we calculate the rate of change for Q:

$$\dot{Q} = \sum_{i=1}^{m} \left(\dot{p}_i(t) \ln \frac{p_i(t)}{p_i^*} + p_i(t) \frac{p_i^*}{p_i(t)} \dot{p}_i(t) \right) = \sum_{i=1}^{m} \dot{p}_i(t) \left(\ln \frac{p_i(t)}{p_i^*} + 1 \right). \tag{9}$$

The constraint (6) implies that

$$\sum_{i=1}^{m} \dot{p}_i(t) = \sum_{i=1}^{m} u_i(t) = 0, \ \ \forall t. \quad (10)$$

Based on (10) we get

$$\dot{Q} = \sum_{i=1}^{m} \dot{p}_i(t) \ln \frac{p_i(t)}{p_i^*} = \sum_{i=1}^{m} u_i(t) \ln \frac{p_i(t)}{p_i^*}.$$

Calculating the speed-gradient of the function we find that $\frac{\partial \dot{Q}}{\partial u_i} = \ln \frac{p_i(t)}{p_i^*}$.

The speed-gradient principle of motion according to (4) forms

$u_i(t) = -\gamma(\ln \frac{p_i(t)}{p_i^*}) + \lambda$, where γ is a positive scalar value and λ is Lagrange multiplier selected to satisfy the constraint (10).

$$\sum_{i=1}^{m} \left(-\gamma \ln \frac{p_i(t)}{p_i^*} + \lambda \right) = 0 \Rightarrow \lambda = \frac{\gamma}{m} \sum_{i=1}^{m} \left(\ln \frac{p_i(t)}{p_i^*} \right). \quad (11)$$

Final system dynamics equation is

$$\dot{p}_i = \gamma \left(-\ln \frac{p_i(t)}{p_i^*} + \frac{1}{m} \sum_{j=1}^{m} \ln \frac{p_j(t)}{p_j^*} \right). \quad (12)$$

Eq. (12) can be represented in more general form

$$\dot{P(t)} = -\gamma (I - \Psi) A(t), \quad (13)$$

where $A(t) = (\ln \frac{p_1(t)}{p_1^*}, \ldots, \ln \frac{p_m(t)}{p_m^*})^T$, $p_i(t)$ is probability of the system location in state i, p_i^* is desired probability for state i, I is an identity matrix, Ψ is a symmetric matrix $m \times m$ where each element is equal to $\frac{1}{m}$, i.e. $\psi_{ij} = \frac{1}{m}$.

Equations (12) defines the dynamics of the transient regime in the system. Its meaning is the movement of the system state in the direction of the KL divergence minimization (i.e. the equality between $p_i(t)$ and given distribution p_i^*) with maximum possible rate. In equilibrium state the expression $u_i = 0, \ \ \forall i$ is true. It means that $\sum_{i=1}^{m} \ln \frac{p_i(t)}{p_i^*} = m \ln \frac{p_j(t)}{p_j^*}$. This is possible under condition $\frac{p_i(t)}{p_i^*} = \frac{p_j(t)}{p_j^*}$ for $\forall i, j$.

3.1 Solution Existence

Let us show the existence of a solution in (12). We choose $i_0 : \frac{p_{i_0}(0)}{p_{i_0}^*} = \min_i \frac{p_i(0)}{p_i^*}$ and suppose that $\frac{p_{i_0}(0)}{p_{i_0}^*} > 0$. Consider $\frac{d(\frac{p_{i_0}(t)}{p_{i_0}^*})}{dt}$:

$$\frac{\dot{p}_{i_0}(t)}{p_{i_0}^*} = \frac{\gamma}{p_{i_0}^*} \left(\frac{1}{m} \sum_{j=1}^{m} \ln \frac{p_j(t)}{p_j^*} - \ln \frac{p_{i_0}(t)}{p_{i_0}^*} \right) = \frac{\gamma}{m p_{i_0}^*} \left(\ln \frac{\prod_{j=1}^{m} \frac{p_j(t)}{p_j^*}}{\left(\frac{p_{i_0}(t)}{p_{i_0}^*} \right)^m} \right) = \frac{\gamma}{m p_{i_0}^*} \left(\ln \prod_{j=1}^{m} \frac{(\frac{p_j(t)}{p_j^*})}{(\frac{p_{i_0}(t)}{p_{i_0}^*})} \right). \quad (14)$$

Since $\frac{p_j(t)}{p_j^*} / \frac{p_{i_0}(t)}{p_{i_0}^*} \geq 1 \quad \forall j$ is true, then $\frac{\gamma}{m p_{i_0}^*} \left(\ln \frac{\prod_{j=1}^{m} p_j(t)}{\prod_{j=1}^{m} p_j^*} \left(\frac{p_{i_0}^*}{p_{i_0}(t)} \right)^m \right) \geq 0$, i.e. the ratio $\frac{p_{i_0}(t)}{p_{i_0}^*}$ does not decrease and therefore does not tend to zero. Hence the right hand sides of (12) are smooth and bounded the solution of equation (12) exists for all $t > 0$.

3.2 Equilibrium Stability

Let us investigate a stability of obtained equation (12). Consider an entropy-like function of Lyapunov

$$V(p) = Q(p, p^*) - Q_{min}(p, p^*). \quad (15)$$

$V(p) \geq 0$ since the KL divergence is always non-negative [Kullback and Leibler, 1951].

Let us find a derivative of function (15)

$$\dot{V}(p) = \sum_{i=1}^{m} \dot{p}_i(t) \left(\ln \frac{p_i(t)}{p^*} \right) = \frac{\gamma}{m} \left(\left(\sum_{i=1}^{m} \ln \frac{p_i(t)}{p_i^*} \right)^2 - m \sum_{i=1}^{m} \left(\ln \frac{p_i(t)}{p_i^*} \right)^2 \right). \quad (16)$$

We will use the Cauchy-Bunyakovsky-Schwarz (CBS) inequality for vectors $f = (f_1, \ldots, f_m)^T$ and $g = (g_1, \ldots, g_m)^T$:

$$\left(\sum_i f_i g_i \right)^2 \leq \left(\sum_i (f_i)^2 \right) \left(\sum_i (g_i)^2 \right). \quad (17)$$

Taking into account that a scalar value γ is positive and using vectors $f = (\ln \frac{p_1(t)}{p^*}, \ldots, \ln \frac{p_m(t)}{p^*})$ and $g = (1, \ldots, 1)$. we get that $\dot{V}(p) \leq 0$. It is known that equality in the CBS inequality is achieved when multiplicity occurs, i.e. $f = \alpha g$. In our case $\dot{V}(p) = 0$ is true only when $\ln \frac{p_i(t)}{p^*} = \alpha \ \ \forall i$, which means that

$\frac{p_i(t)}{p_i^*} = \frac{p_j(t)}{p_j^*}$ for $\forall i, j$, i.e. in the state of equilibrium. Thus, the law (12) provides a global asymptotic stability for the minimum of KL divergence.

4 Total Energy Constraint

Let us consider a system with additional constraint for the total energy conservation. We will consider a conservative case when energy does not depend on a time. The new constraint may be described as

$$E = \sum_{i=1}^{m} p_i(t) E_i, \qquad E = \sum_{i=1}^{m} p_i^* E_i, \tag{18}$$

where E_i is the energy of a system in the state i, E is the common energy of a system.

We consider a system $\dot{p(t)} = u(t)$. For this system the set of constraints can be defined as

$$\sum_{i=1}^{m} u_i E_i = 0, \qquad \sum_{i=1}^{m} u_i = 0. \tag{19}$$

The problem is to find an operator u which satisfies both constraints (6) and (18) at any time t. The evolution law should have the form

$$u_i(t) = -\gamma \left(\ln \frac{p_i(t)}{p_i^*} \right) + \lambda_1 E_i + \lambda_2, \;\; i = 1, \ldots, m, \tag{20}$$

where λ_1, λ_2 are Lagrange multipliers determined by substitution of (20) into (19).

To simplify further equations let us denote $A_i(t) = \ln \frac{p_i(t)}{p_i^*}$. It follows from the condition (6) that $\sum_{i=1}^{m} u_i = 0 \Rightarrow \gamma \sum_{i=1}^{m} A_i(t) = \lambda_1 \sum_{i=1}^{m} E_i + \lambda_2 m \Rightarrow \lambda_2 = \frac{\gamma \sum_{i=1}^{m} A_i(t) - \lambda_1 \sum_{i=1}^{m} E_i}{m}$.

From the second condition (18) we get that

$$- \gamma \sum_{i=1}^{m} A_i(t) E_i + \lambda_1 \sum_{i=1}^{m} E_i^2 + \lambda_2 \sum_{i=1}^{m} E_i = 0 \Rightarrow$$
$$- \gamma \sum_{i=1}^{m} A_i(t) E_i + \lambda_1 \sum_{i=1}^{m} E_i^2 +$$
$$\left(\frac{\gamma \sum_{i=1}^{m} A_i(t) - \lambda_1 \sum_{i=1}^{m} E_i}{m} \right) \sum_{i=1}^{m} E_i = 0 \Rightarrow$$
$$\lambda_1 = \gamma \frac{m \sum_{i=1}^{m} A_i(t) E_i - \sum_{i=1}^{m} A_i(t) \sum_{i=1}^{m} E_i}{m \sum_{i=1}^{m} E_i^2 - \left(\sum_{i=1}^{m} E_i \right)^2}.$$

Now substitute expression for λ_1 into expression for λ_2 obtained from the first constraint (6):

$$\lambda_2 = \frac{\gamma}{m} \sum_{i=1}^{m} A_i(t) -$$
$$\frac{\gamma}{m} \frac{m \sum_{i=1}^{m} A_i(t) E_i + \left(\sum_{i=1}^{m} E_i \right)^2 \sum_{i=1}^{m} A_i(t)}{m \sum_{i=1}^{m} E_i^2 - \left(\sum_{i=1}^{m} E_i \right)^2} \Rightarrow$$
$$\lambda_2 = \gamma \frac{\sum_{i=1}^{m} A_i(t) \sum_{i=1}^{m} E_i^2 - \sum_{i=1}^{m} A_i(t) E_i \sum_{i=1}^{m} E_i}{m \sum_{i=1}^{m} E_i^2 - \left(\sum_{i=1}^{m} E_i \right)^2}.$$

Finally we get for λ_1 and λ_2 :

$$\begin{cases} \lambda_1 = \gamma \frac{m \sum_{i=1}^{m} \ln \frac{p_i(t)}{p_i^*} E_i - \sum_{i=1}^{m} \ln \frac{p_i(t)}{p_i^*} \sum_{i=1}^{m} E_i}{m \sum_{i=1}^{m} E_i^2 - \left(\sum_{i=1}^{m} E_i \right)^2} \\ \lambda_2 = \gamma \frac{\sum_{i=1}^{m} A_i(t) \sum_{i=1}^{m} E_i^2 - \sum_{i=1}^{m} A_i(t) E_i \sum_{i=1}^{m} E_i}{m \sum_{i=1}^{m} E_i^2 - \left(\sum_{i=1}^{m} E_i \right)^2} \end{cases} \tag{21}$$

Given (21) we obtain the common equation of system dynamics based on (20):

$$u_i(t) = -\gamma \left(\ln \frac{p_i(t)}{p_i^*} \right) +$$
$$\left(\gamma \frac{m \sum_{i=1}^{m} \ln \frac{p_i(t)}{p_i^*} E_i - \sum_{i=1}^{m} \ln \frac{p_i(t)}{p_i^*} \sum_{i=1}^{m} E_i}{m \sum_{i=1}^{m} E_i^2 - \left(\sum_{i=1}^{m} E_i \right)^2} \right) E_i +$$
$$\gamma \frac{\sum_{i=1}^{m} A_i(t) \sum_{i=1}^{m} E_i^2 - \sum_{i=1}^{m} A_i(t) E_i \sum_{i=1}^{m} E_i}{m \sum_{i=1}^{m} E_i^2 - \left(\sum_{i=1}^{m} E_i \right)^2}. \tag{22}$$

Equations (22) are defined when $m \sum\limits_{i=1}^{m} E_i^2 - \left(\sum\limits_{i=1}^{m} E_i \right)^2 \neq 0$. It is not true only if all energies E_i are equal (a confluent case). The existence of solution for (22) is possible to show by the similar way as it was shown for the case of one constraint.

Law of evolution (22) can be represented in abbreviated form:

$$\dot{P} = -\gamma (I - \Psi) A(t), \tag{23}$$

where $A(t) = (\ln \frac{p_1(t)}{p_1^*}, \ldots, \ln \frac{p_m(t)}{p_m^*})^T$, $p_i(t)$ is probability of the system location in state i, p_i^* is desired probability for state i, I is an identity operator, Ψ is a symmetric $m \times m$ matrix defined as follows

$$\psi_{ij} = \frac{1}{m} + \frac{\tilde{E}_i \tilde{E}_j}{\|\overline{E}\|^2 - \frac{1}{m}(\mathbf{1}\overline{E})^2},$$

where $\tilde{E}_i = E_i + \frac{1}{m} \sum_{i=1}^{m} E_i$, $\mathbf{1} = (1, \ldots, 1)^T$ and $\overline{E} = (E_1, \ldots, E_m)^T$ is a vector of energies.

4.1 Stability of Equilibrium

Further we examine the equilibrium of obtained equation (22). Let us find the equilibrium state of the system (20) and investigate its stability. In the state of equilibrium it is true that:
$\gamma(-\ln \frac{p_i(t)}{p_i^*}) + \lambda_1 E_i + \lambda_2 = 0, i = 1, \dots, m.$
Thus,

$$p_i(t) = Ce^{-\mu E_i}, \tag{24}$$

where $\mu = \frac{-\lambda_1 E_i}{\gamma}$ and $C = p_i^* exp(\frac{\lambda_2}{\gamma})$. After substitution λ_1 and λ_2 multiplier γ is reduced, i.e. state of equilibrium does not depend on γ. Value of C satisfies the normalization condition $C^{-1} = m \sum_{i=1}^{m} e^{-\mu E_i}$. It is possible to show that the obtained value delivers the minimum of the KL divergence.

Let us show that function $V(p)$ (15) is the Lyapunov function for the system (22) and that the state of equilibrium is the only one stable state in the non-confluent case. We calculate the derivative of functional (15) for the system (22):

$$\dot{V} = \sum_{i=1}^{m} u_i A_i(t) =$$
$$\sum_{i=1}^{m} \left(-\gamma A_i(t)^2 + \lambda_1 E_i A_i(t) + \lambda_2 A_i(t)\right) =$$
$$-\sum_{i=1}^{m} \gamma A_i(t)^2 +$$
$$\left(\gamma \frac{\sum_{i=1}^m A_i(t) \sum_{i=1}^m E_i^2 - \sum_{i=1}^m A_i(t) E_i \sum_{i=1}^m E_i}{m \sum_{i=1}^m E_i^2 - \left(\sum_{i=1}^m E_i\right)^2}\right)$$
$$\left(\sum_{i=1}^{m} E_i A_i(t) + \sum_{i=1}^{m} A_i(t)\right).$$

Let us denote the expression $m \sum_{i=1}^m E_i^2 - \left(\sum_{i=1}^m E_i\right)^2 = B$. Then we get

$$\dot{V} = \frac{\gamma}{B} \left(\sum_{i=1}^m E_i\right)^2 \sum_{i=1}^m A_i(t)^2$$
$$- \frac{\gamma}{B} \left(m \sum_{i=1}^m E_i^2 \sum_{i=1}^m A_i(t)^2 + m \left(\sum_{i=1}^m A_i(t) E_i\right)^2\right)$$
$$-\frac{\gamma}{B} 2 \sum_{i=1}^m A_i(t) \sum_{i=1}^m E_i \sum_{i=1}^m A_i(t) E_i +$$
$$\frac{\gamma}{B} \left(\left(\sum_{i=1}^m A_i(t)\right)^2 \sum_{i=1}^m E_i^2\right). \tag{25}$$

Now let us multiply (25) by $\frac{m}{m}$ and for the expression in parentheses add and subtract a new member $\left(\sum_{i=1}^m E_i\right)^2 \left(\sum_{i=1}^m A_i(t)\right)^2$:

$$\dot{V} = \frac{\gamma}{m * B} \left(m \sum_{i=1}^m E_i A_i(t) - \sum_{i=1}^m E_i \sum_{i=1}^m A_i(t)\right)^2$$
$$-\frac{\gamma}{m * B} \left(m \sum_{i=1}^m A_i(t)^2 - \left(\sum_{i=1}^m A_i(t)\right)^2\right)$$
$$\left(m \sum_{i=1}^m E_i^2 - \left(\sum_{i=1}^m E_i\right)^2\right). \tag{26}$$

Let us introduce a new scalar product function for two vectors $f = (f_1, \dots, f_m)^T$ and $g = (g_1, \dots, g_m)^T$ as

$$\langle f, g \rangle = m \sum_i^m f_i g_i - \sum_i^m f_i \sum_i^m g_i \tag{27}$$

Properties of the scalar product (27) with proofs are provided in section A.

As (27) is scalar product then the CBS inequality (17) is true for it:

$$\langle f, g \rangle^2 \le \langle f, f \rangle \langle g, g \rangle \tag{28}$$

Due to the properties of (27) (see section A) it can be shown that an equality in (28) takes place only when $\exists \lambda, \mu \in \mathbb{R} : f = \lambda g + \mu$.

Using inequality (28) for vectors $f = (A_1, \dots, A_m)^T$ and $g = (E_1, \dots, E_m)^T$ we get for (26) that $\dot{V}(\beta) \le 0$. And $\dot{V}(\beta) = 0$ occurs for the only one case when $\exists \lambda, \mu \in \mathbb{R} : A_i = \lambda E_i + \mu$ for all i. Due to (20) at the equilibrium state of the system the following equalities hold:

$$\gamma(-A_i(t)) + \lambda_1 E_i + \lambda_2 = 0, \quad i = 1, \dots, m. \tag{29}$$

Which means that for equilibrium state the final distribution of points satisfy the equation

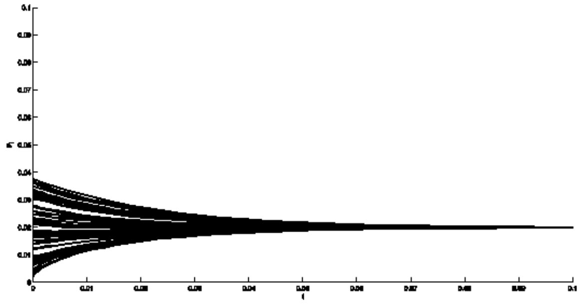
$$A_i(t) = \lambda E_i + \mu,$$

where $\lambda = \frac{\lambda_1}{\gamma}$, $\mu = \frac{\lambda_2}{\gamma}$ for λ_1 and λ_2 defined in (21).

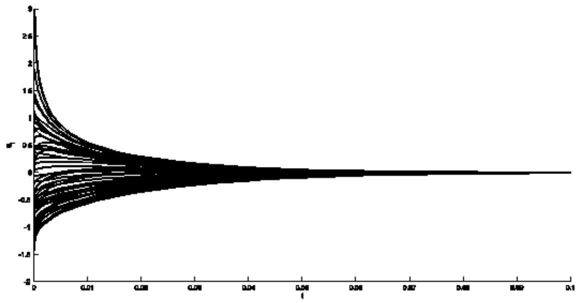
It follows that there is only one distribution which corresponds to the equilibrium state of the system (20).

5 Numeric Experiments

Consider a discrete system which consists of N identical particles distributed over m cells. Particles can migrate from one cell to another. In case when the mass



a. Dynamics of distributions



b. Dynamics of control variables

Figure 1: Dynamics of the system with 50 states and uniform desired distribution

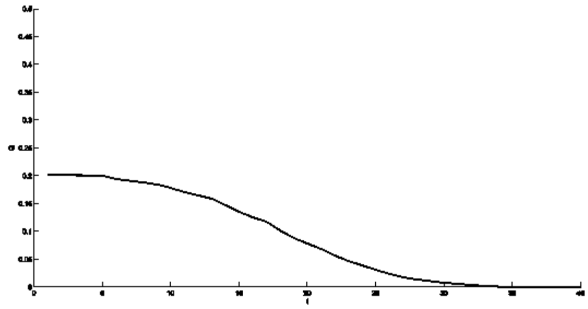


Figure 2: KL Divergence dynamics of the system with 50 states and uniform desired distribution

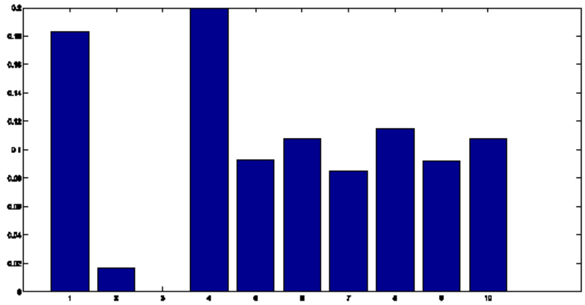


Figure 3: Initial distribution for 10 states

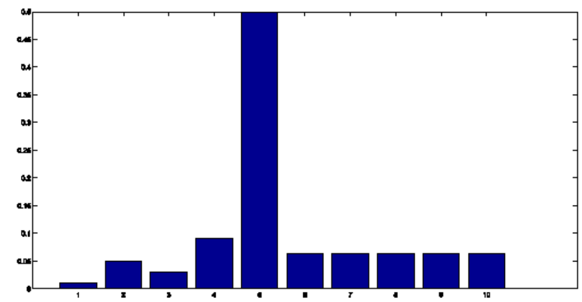


Figure 4: Initial distribution for 10 states

conservation constraint holds it is true that $\sum_{i=1}^{m} N_i$, which can be normalized as $\sum_{i=1}^{m} \frac{N_i}{N} = 1$. State s_i of this system denotes a number of particles contained in the cell with number i.

Energy conservation constraint can also be represented as

$$\sum_{i=1}^{m} \frac{N_i}{N} E_i = E.$$

Our goal is to control the behavior of the system so as to achieve the desired (given apriori) distribution in a finite time. In Sections 3 and 4 we have derived equations (12) and (22) which describe dynamics of the system under a given set of constraints.

Consider a system with two constraints where desired distribution is set as uniform distribution and the number of states (cells) is set as 50. As initial distribution we take any non-degenerate one. En example of initial distribution for the system with 10 states is shown in Figure (3). Energy levels are set as $E_i = i$.

Evolution dynamics of corresponding distributions (i.e. how the number of particles contained in one cell change in time) is shown on Figure (1.a).

Figure (1.b) shows evolution of control variables.

Diagram of the KL Divergence changing in time is shown in Figure (2).

From Figures (1) and (2) we see that the KL Divergence goes to zero together with control variables as the desired (goal) distribution is reached.

Consider the system with 10 states and initial (non-uniform) distribution shown in Figure (3).

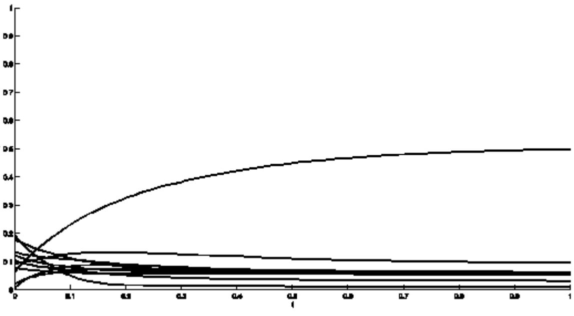
Let us set the desired distribution as non-uniform distribution shown in Figure (4). Dynamics of system for this desired distribution is shown in Figures (5) and (6).

Diagram of the KL Divergence changing in time for non-uniform initial distribution is shown in Figure (6).

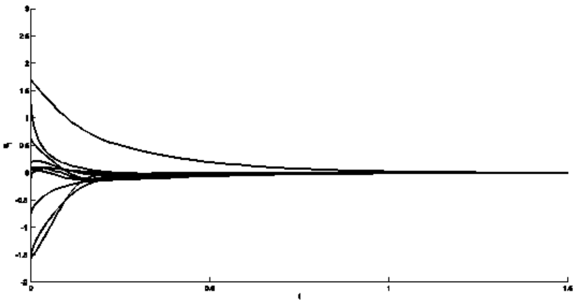
These experiments with artificial data confirm theoretical results obtained in Sections 3 and 4. Results for the case when the system evolves under only one constraint (i.e. the energy constraint is not considered) are almost the same.

6 Conclusions

The KL divergence is widely used in information theory, signal processing, pattern recognition and many



a. Dynamics of distributions



b. Dynamics of control variables

Figure 5: Dynamics of the system with 10 states and non-uniform desired distribution

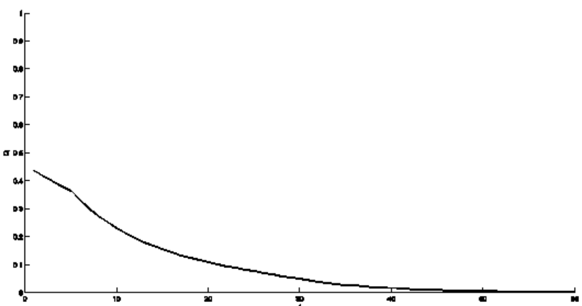


Figure 6: KL Divergence dynamics of the system with 10 states and non-uniform desired distribution

other areas. We have derived a set of equations that determine the dynamics of non-stationary (transient) states and describe a way and trajectory of the system that tends to the state with minimum of the KL divergence (i.e. relative entropy).

The key point of our approach is using the SG-method with the goal function chosen as the relative entropy of the process. The results are formulated in Eq. (12), (22) and in a more general form in (13),(23). We have shown the existence of solution for the system (12). We have established the stability of equilibrium and have proved that there is only one distribution that corresponds to the state of equilibrium. Mass conservation and energy conservation constraints were considered.

The physical meaning of obtained laws of system's dynamics is moving along the direction of the KL divergence minimization with the highest possible rate. These laws allow forecasting the direction of evolution of the system and can be useful to study dynamics of non-equilibrium systems of both macroscopic and microscopic world.

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APPENDIX

A Extra Materials

Here we provide several properties of the functional $\langle f, g\rangle$ for two vectors $f = (f_1, \dots, f_m)^T$ and $g = (g_1, \dots, g_m)^T$ from the section 4.1:

$$\langle f, g\rangle = m\sum_i^m f_i g_i - \sum_i^m f_i \sum_i^m g_i. \qquad (30)$$

Property 1. *Linearity in the first argument*
$\forall f, g, h \in \mathbb{R}^m,\ \forall \lambda \in \mathbb{R}\ \langle \lambda f + g, h\rangle = \langle \lambda f, h\rangle + \langle g, h\rangle$.

Proof Using the linearity of the sum we obtain

$$\begin{aligned}\langle \lambda f + g, h\rangle &= m\sum_i^m(\lambda f_i + g_i)h_i \\ &- \sum_i^m(\lambda f_i + g_i)\sum_i^m h_i = \\ &= \left(m\sum_i^m \lambda f_i h_i - \sum_i^m \lambda f_i \sum_i^m h_i\right) \\ &+ \left(m\sum_i^m g_i h_i - \sum_i^m g_i\sum_i^m h_i\right) = \\ &= \langle \lambda f, h\rangle + \langle g, h\rangle.\end{aligned}$$

Property 2. *Symmetry*
$\forall f, g \in \mathbb{R}^m\ \langle f, g\rangle = \langle g, f\rangle$.

Proof

$$\begin{aligned}\langle f, g\rangle = m\sum_i^m f_i g_i - \sum_i^m f_i \sum_i^m g_i = \\ m\sum_i^m g_i f_i - \sum_i^m g_i\sum_i^m f_i = \langle g, f\rangle.\end{aligned} \qquad (31)$$

Property 3. *Positiveness and the condition of zero value*
$\forall f \in \mathbb{R}^m\ \langle f, f\rangle \geq 0,\ \langle f, f\rangle = 0 \Leftrightarrow f = \mu = const.$

Proof Let us consider a scalar multiplication. CBS (17) comes true for it: $|(f, g)|^2 \leq (f, f)(g, g)$ and $|(f, g)|^2 = (f, f)(g, g) \Leftrightarrow \exists\mu \in \mathbb{R} : f = \mu g$. Substituting $g = (1, \dots, 1)^T$ we get

$$\left|\sum_i^m f_i\right|^2 \leq (f, f)\sum_i^m 1 = m\sum_i^m f_i^2.$$

Thereby it is true that $\langle f, f\rangle = m\sum_i^m f_i^2 - \left(\sum_i^m f_i\right)^2 \geq 0$. Moreover $\langle f, f\rangle = 0 \Leftrightarrow \left|\sum_i^m f_i\right|^2 = (f, f)(\mathbf{1}, \mathbf{1}) \Leftrightarrow \exists\mu \in \mathbb{R} : f = \mu\mathbf{1}$, i.e. $f = \mu$.