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Dynamic Programming based approach for optimal transport by flashing ratchet against a load force

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***Abstract*— Flashing ratchet is a mechanism which employs noise under isothermal and non equilibrium conditions. Its primary is to transport of small particles, possibly against a load force, under the influence of thermal noise and potential energy landscapes that can be realized locally, near the particles position. In this article we present a dynamic programming based approach to analyze and synthesize optimal strategies in the presence of a non-zero load force and finite sampling intervals. We show that it is possible to obtain an order increase in velocity and stalling force, over open-loop strategies. Besides engineered systems, study of such strategy is also important to gain insights on the intra-cellular transport of motor proteins (such as Kinesin and Dynein) on a microtubular track, and on the role of feedback control on their transport.**

Keywords: Flashing ratchets, cellular transport, dynamic programming, stochastic differential equations, switched/hybrid systems

I. Introduction

Noise is often viewed as detrimental to engineered systems. Unlike macro scale systems, for systems at the micro scale or smaller, thermal noise plays an important role and is often the dominant noise component that determines limits of performance of the system. With recent advancements in science and technology it is now possible to observe effects of thermal noise on small-scale systems. Moreover, nanotechnology has facilitated means for altering systems response to thermal noise. Interestingly, several recent experimental breakthroughs ([1]) demonstrate that natural and engineered systems can employ noise beneficially for realizing efficient and robust functionality.

In various schemes [7] under isothermal equilibrium conditions for extracting work from noise using rectifying schemes are shown to violate the laws of thermodynamics. However, work can be realized using rectifiers under non-equilibrium conditions, where noise plays an essential role. A large class of such schemes are termed Brownian rectifiers where typically a particle under the influence of thermal noise can be displaced against a load, where, in the absence of the noise source no transport is possible. Such transport can be achieved even under isothermal conditions.

Brownian rectifiers occur naturally and are fundamental in explaining the functioning of various biological systems which are crucial components of intracellular transport. Intracellular transport is governed by motor proteins (such as *Kinesin* and *Dynein*) which serve as carriers for cellular cargo (in a noisy environment) that influence global aspects of cell biology including establishment of cell polarity, maintenance of genomic stability, regulation of higher brain functions, developmental patterning and suppression of tumorigenesis [10]. Understanding these intracellular phenomena is critical as malfunctioning of such processes underlie a host of medical maladies including neurodegenerative diseases such as Alzheimers [9]. An essential challenge in study of intracellular transport lies in understanding the intrinsic energetics. The possible change in energy landscape due to ATP hydrolysis and presence of high degree of thermal noise in motor protein based transport makes the Brownian rectifier a potential candidate to explain the associated energetics [1]. Here an understanding of how the motor-proteins utilize noise to convert chemical energy into motion will provide valuable insights into natures ways of performing work in an uncertain and complex environment.

Various rectification schemes that are employed toward this end include mainly two classes. First being the *flashing ratchet* where the particle is subjected to a fluctuating energy profile while the second class termed as *changing-force ratchets* involve moving the particle in a periodic potential with a broken symmetry, solely subjected to spatially uniform forces of (temporal or statistical) zero average. Flashing ratchet has found widespread applicability over the latter variant due to

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its ease of analysis and implementation.

One of the main application of flashing ratchet is to enable transport at micron or smaller scale. There are existing schemes that employ feedback to maximize the average velocity [3], [5]. In [3], the strategy described assumes infinite closed loop bandwidth and zero load force condition, none of which correspond to a practical scenario. It has been shown in [4] that the average velocity obtainable by the strategy in [3] degrades with the decrease in closed-loop bandwidth. The strategy described in [5] performs better than [3] under more practical conditions, it is not optimal. Moreover, a limits of performance study is missing from the literature to quantitatively assess the performance of a Brownian ratchet strategy.

In the current paper we present a dynamic programming (DP) based algorithm that yields an optimal strategy to maximize velocity under the constraints of a finite closed-loop bandwidth and non-zero load force. To the best of our knowledge, this is the first-time an optimal strategy encompassing aforementioned issues for maximizing velocity is reported. We comment here that case of a non-zero load force is important, where the maximum power redeemable from the system under given conditions can be quantified. The minimum load under which the particle achieves negligible positive transport is called *stalling force*, which quantifies the maximum power achievable. The dynamic programming approach apart from providing limits on achievable performance, also synthesizes the optimal feedback strategy. We show via Monte Carlo simulations that DP based strategy gives an order of magnitude increase in the velocity and stalling force compared to the open loop scenario.

The paper is organized as follows: in Section II we derive a mathematical model of ratchet based transport of particles that turns off and on in a predefined periodic manner. In Section III, we cast the problem of maximizing transport for a particle in an optimization framework. The realized framework is solved with the help of dynamic programming in Section IV and the corresponding computational complexity is further discussed. Simulation results demonstrating the advantages of the developed close-loop strategy over open-loop are presented in Section V. Further insights and discussions of the model, its solution, and its extension for multiple particles are provided in section VI.

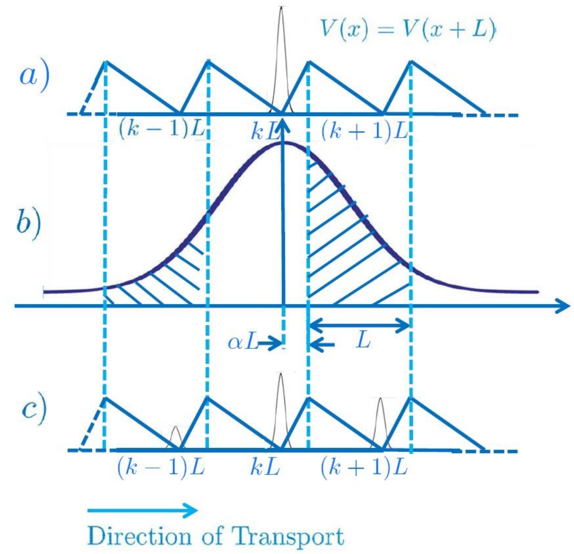


Fig. 1. (a) describes a periodic potential with spatial period L. (b) shows a Gaussian pdf with mean kL and variance t_{off}. Consider a particle which initially at time $t = 0$ is at the well $x = kL$. The corresponding pdf at time $t = 0$ is shown in (a). The potential is absent for time $[0, t_{off}]$. The probability of finding the particle in the region $x > (k+\alpha)L$ is much higher than finding the particle in the region $x < (k-1+\alpha L)L$ after a time t_{off}. If the potential is turned on at time t_{off} probability of having the particle move in the well at $(k+1)L$ is much higher than having the particle move to the well at $(k-1)L$ thus achieving transport to the right. (c) illustrates the evolved pdf of the particle after one flash.

II. Modeling

As already mentioned, Brownian ratchets provide a mechanism to realize transport of a particle undergoing diffusive motion (for example due to thermal noise forcing). In a simple version of a Brownian ratchet, a spatially periodic potential (see Figure 1(a)) is switched on and off in an alternating manner for time intervals t_{on} and t_{off} respectively. Consider for example, the potential shown in Figure 1(a), that illustrates a potential with a positive slope (the corresponding force, $-\frac{\partial V}{\partial x}$, will be negative) in the interval $(kL, (k+\alpha)L]$ and a negative slope (the corresponding force will be positive) in the interval $((k-1+\alpha)L, kL]$ of the kth spatial period. Suppose that the potential is off in the time interval $[0, t_{off}]$. During this time interval, the particle motion is described by Brownian motion where the probability density function (pdf) of the particle's position x at time t given that it is at $x = kL$ at $t = 0$ (see Figure 1(a)) is described by

$$p(x, t|kL, 0) = \frac{1}{\sqrt{4\pi t}} e^{\frac{-(x-kL)^2}{4t}}, \tag{1}$$

whose mean at $x = kL$ does not change with time, while the variance increases linearly with time t. The particle diffuses according to the above pdf for a time t_{off} at the end of which its pdf is described by (1) with $t = t_{off}$. The probability of finding the particle in the region $x > (k+\alpha)L$ and $x < (k-1+\alpha)L$ are given by $\int_{(k+\alpha L)}^{\infty} p(x,t|kL,0)dx$ and $\int_{-\infty}^{(k-1+\alpha)L} p(x,t|kL,0)dx$ respectively. Since the length αL is smaller than the length $(1-\alpha)L$, at time $t = t_{\text{off}}$ there is greater probability of finding the particle (using (1)) in the region $x > (k+\alpha)L$ than finding it in the region $x < (k-1+\alpha)L$. Thus when the ratchet potential is turned on (at $t = t_{off}$), there is a higher probability of finding the particle under the influence of a positive force, and if t_{on} is long enough, the particle will more likely settle in the well whose minimum is at $x = (k+1)L$ or stay at the current well (at $x = kL$) (see Figure 1(c)). In contrast the probability of finding the particle inside the well with a minimum at $(k-1)L$ is considerably smaller. *Thus on average, the particle will move to the right*. The evolved pdf of the particle's position after the potential is turned back *on* is shown in Figure 1(c).

The above description provides the essence of the principle on which the flashing ratchets and their variants[14] operate. Note that it is evident that there will be no effective transport when the ratchet is kept *on* (or *off*) for all the time or when the ratchet potential is symmetric within a period (i.e. $\alpha = 1/2$). Also the asymmetric potential in the absence of noise cannot lead to any transport (the particle will be stuck at the current well). Only when the asymmetric potential is used *together* with the thermal noise based fluctuations is it possible to achieve directed motion *even against an opposing force*. Furthermore, we require that $V_0 >> k_B T$ to ensure that thermal noise is not high enough to overcome the potential barrier and thus the particle will stay in its current valley when the potential is *on*.

III. Problem Formulation

There are a number of theoretical studies of Brownian ratchets in the literature [3], [1], [8], [5], [12]. However, there is a paucity of emphasis on obtaining optimal strategies for maximizing transport. Here we synthesize an optimal closed-loop strategy with the objective of maximizing velocity with constraints that incorporates the availability of measurements only at sampled intervals . The underlying principles can be viewed as laying the framework for analysis and synthesis of optimal Brownian ratchets.

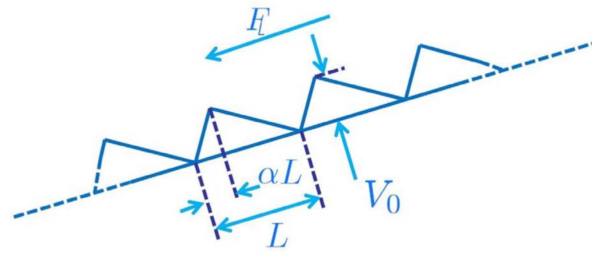


Fig. 2. The effective potential felt by a particle under the influence of a load force F_L opposing the motion and a periodic potential as shown in Fig. 1(a).

Consider a particle under Brownian ratchet described by the piecewise linear potential shown in Figure 1 and a stochastic forcing. The stochastic differential equation (SDE) governing Brownian ratchet dynamics is given by

$$\gamma dx = f(x,\theta)dt + \sqrt{D}dW(t), \tag{2}$$

where $x(t)$ is the position of the particle, γ is the viscous drag coefficient of the medium, $\theta \in \{0,1\}$ is the switch parameter, $D = \frac{K_B T}{\gamma}$([11]) is the Diffusion constant, K_B is the Boltzman constant, T is the absolute temperature, and $W(t)$ is the Wiener process. The force $f(x,\theta)$, acting on the particle switches (or flashes) between two functions, one defined for each θ in $\{0,1\}$.

Depending on the application, the evolution of the switch-trigger parameter can be deterministic or stochastic. Since feedback is typically implemented by sampled-data systems, a discrete-time system that describes the evolution of the expected value of the position is considered. The SDE based model is easy to implement numerically and particularly useful for simulation studies. Also since it represent directly the dynamics of the particle position, system theoretic tools developed for ODEs (such as optimal control [2]) can be extended to such system. We also assume a load force F_L being exerted on the particle. We adopt the SDE modeling framework of (2) where

$$f(x,\theta) = -F_L - \theta(t)V'(x) \tag{3}$$

resulting in

$$\gamma dx = -F_L dt - \theta(t)V'(x)dt + \sqrt{D}dW(t), \tag{4}$$

where the force $V'(x)$ arising from the piece-wise linear potential (see Figure 2) is given by

$$V'(x) = \begin{cases} \dfrac{V_0}{\gamma\alpha L} & \text{for } \mathrm{Mod}(x,L) < \alpha L \\ -\dfrac{V_0}{\gamma(1-\alpha)L} & \text{for } \mathrm{Mod}(x,L) \geq \alpha L. \end{cases} \tag{5}$$

$\theta(t)$ is 0 if the ratchet is *off* and 1 if it is *on*. We assume that the time horizon T is finite which is divided into N stages and that a decision whether to switch the ratchet potential on or off has to be made every $T_s = T/N$ seconds. We denote by x_k the state at time kT_s that is $x_k := x(kT_s)$. It follows that the sampled dynamics is given by

$$x_{k+1} = x_k + f_k(x_k, u_k) + w_k;\ \ u_k \in U_k \tag{6}$$

where u_k is the control action at stage k, deciding whether the potential is applied or not, $U_k = \{\text{On,Off}\}$, w_k is the thermal noise and $f_k(x_k, u_k)$ is described by

$$f_k(x_k, u_k) = \begin{cases} -\dfrac{F_L}{\gamma}T_s & u_k = \text{ Off} \\ -\dfrac{F_L}{\gamma}T_s + \int_0^{T_s} V'(x(t))dt & u_k = \text{ On.} \end{cases} \tag{7}$$

The problem of maximizing the average velocity of the particle can be addressed by finding an optimal strategy to maximize the expected distance that is traveled in the time horizon T. The related optimization strategy can be obtained from the solution of

$$\underset{u_0,\ldots,u_{N-1}}{\text{arg max}} \underset{w_0,\ldots,w_N}{E}[x_N]\,. \tag{8}$$

In next section, a dynamic programming based approach is outlined to solve the problem in (8).

IV. Solution Methodology and Computational Cost

For the open-loop problem, the decision variables $u_0, \ldots, u_{N-1}$ are decided without regard to any measurement available and thus the best static sequence of on and off is determined that maximizes the expected value of the terminal distance x_N [13]. However, in the above setup, $u_k \in \{on,\ off\}$ can be decided based on the measurement of the position x_k of the particle at the k^{th} stage. Thus assuming perfect measurement of the position, $u_k := \mu_k(x_k)$ will be determined as a solution of the above problem, which provides an optimal closed-loop strategy. We remark that it is possible that the distance traveled is not positive for high enough load forces. The associated task is to determine the *stalling force* which is the minimum load under which the particle achieves negligible positive transport.

The DP steps entail defining the cost $g_k(s_k, u_k, w_k)$ of stage k incurred where s_k defines the state for the DP problem. For the problem (8) the state s_k is the position of the particle x_k with the cost at the k^{th} stage given by

$$g_k(x_k, u_k, w_k) = \begin{cases} 0 & \text{for } k < N \\ x_N & \text{for } k = N. \end{cases} \tag{9}$$

where $g_N(x_N)$ is the terminal cost. Here we set intermediate costs to zero as we are only interested in maximizing the final distance traveled. Let $J_k(x_k)$ be the cost to go defined as

$$J_k(x_k) = \max_{u_k,\ldots,u_{N-1}} \underset{w_k,\ldots,w_{N-1}}{E}[g_N(x_N) + \sum_{i=k}^{N-1} g_i(x_i, u_i, w_i)] \tag{10}$$

with $J_N(x_N) = g_N(x_N) = x_N$. Using the DP principle [2], we can show that

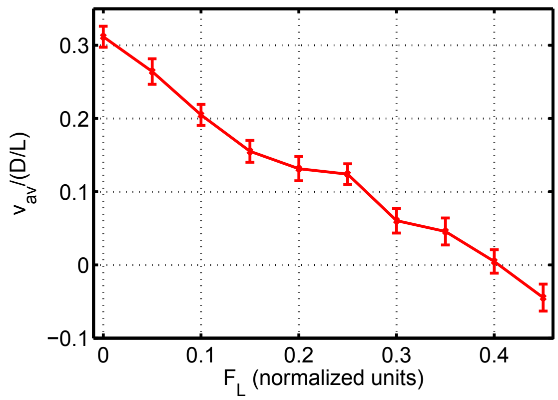
$$J_k(x_k) = \max_{u_k\in\{off,on\}} \underset{w_k}{E}[g_k(x_k, u_k, w_k) + J_{k+1}(x_{k+1})]. \tag{11}$$

Thus we can propagate the recursion backward: given $J_{k+1}(x_{k+1})$, we determine $J_k(x_k)$ for every feasible x_k.

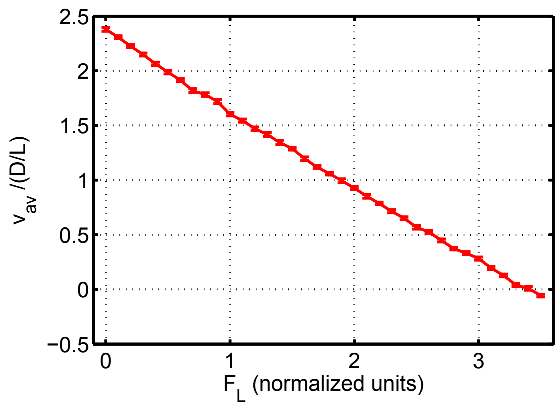
Computational Complexity: We here provide an analysis for the computational cost. As x_k is a real variable, the problem of determining the function J_k (from J_{k+1} using (11)) is infinite dimensional. To overcome this problem, we will grid the state x_k by bounding the maximum forward and backward distance that is most likely to be traveled.

The displacement due to thermal noise can be assumed to be bounded by $2\sigma = 2\sqrt{2DT_s}$ in each direction with an error of 5%. Suitable bounds for the maximum forward distance and backward distance that can be traveled in one stage can be obtained as $d_F = F_P T_s + 2\sigma$ and $d_B = F_N T_s + 2\sigma$, respectively. Here $F_N = \dfrac{V_0}{\gamma\alpha L} + \dfrac{F_L}{\gamma}$ and $F_P = \dfrac{V_0}{\gamma(1-\alpha)L} - \dfrac{F_L}{\gamma}$ are position-dependent forces in negative and positive direction respectively. For the state at stage k, we grid the interval $[-kd_B, kd_F]$ into intervals of size Δ and evaluate $J_k(x_k)$ for values of x_k at the grid values. This would entail km values of x_k, where $m = \dfrac{(d_F + d_B)}{\Delta}$, for which $J_k(x_k)$ has to be determined. Two computations for a given x_k have to be performed to solve (11) corresponding to two actions of $u_k = on$ and $u_k = off$ and the one yielding higher cost is chosen. At the k^{th} stage there are thus $2km$ computations of the expectation to be performed in evaluating (11). The total number of evaluations for all the stages is $\sum_{k=1}^{N} 2km = 2mk(k+1)/2$. Thus the problem scales as the square of the number of time stages in the DP, which is dependent on the time horizon T and the grid size on the time axis given by T/T_s. This computational cost is certainly tractable as independent computations in a stage can be easily evaluated in parallel.

V. Simulation Results



(a)



(b)

Fig. 3. Monte Carlo simulation results for (a) open loop; stalling force $\approx$ 0.4 (normalized units)(b) closed loop; stalling force $\approx$ 3.4 (normalized units). Curves in both figures shows a decrease in average velocity with increase in load force. Clearly, from (b) the average velocity and the stalling force in close loop are an order of magnitude higher than in open loop.

For simulating the performance of DP based feedback strategy, as mentioned in the previous section, position attainable by the particle at the stage k was bounded by kd_{span}, where $x_{span} = d_B + d_f$, is the span of the displacement, the particle can experience in any stage. Conforming with our assumption of perfect measurement of the state, decision table depending on discretized position at each stage k was determined implementing the dynamic programming strategy. This table is used as the control strategy while performing Monte Carlo simulations. Simulation are run for 100 sample paths for each load force for both open-loop and closed-loop case. Simulation time and average velocity were normalized such that $v_{av,norm} = \frac{v_{av}}{(D/L)}$ and $T_{s,norm} = \frac{T_s}{(L^2/D)}$.

A closer analysis of the dynamic programming table which provides feedback control strategy for different states shows that the one part of the strategy is to switch the potential on when the particle is on the positive side ($\text{Mod}(x_k, L) \geq \alpha L$) of the ratchet potential. Another interesting observation seen from the dynamic programming table is that when particle is on the negative side ($\text{Mod}(x_k, L) < \alpha L$) of the potential (negative slope) but within $\frac{F_L}{\gamma}T_S$ of the valley, it is optimal to switch the potential on. An intuition for this strategy is that as in this case if the potential is switched off, particle will travel $\frac{F_L}{\gamma}T_S$ distance toward the negative direction on an average. But if the potential is switched on, then the average *maximum* distance it can travel toward negative direction is the amount the particle is away from the valley, is smaller than $\frac{F_L}{\gamma}T_S$. Once reaching the valley, it will be trapped. Thus found threshold based switching strategy was used for Monte Carlo simulations. To summarize, the DP look-up table that provides the feedback value for every discretized particle position, was used to infer more "global" feedback rules that are not look-up tables and are thus much easier to implement.

Figure 3(a) and (b) shows the normalized average velocity achieved with varying load forces for open loop and closed loop methods; bars shows the *variance* for each load force. It is clear from Figure 3 that an order of magnitude increase in the transport velocity is achieved with closed-loop strategy. It is worth mentioning that the stalling force against which the particle can move for closed loop strategy is also increased an order of magnitude with respect to the open loop case. Parameters used in Monte Carlo simulation are:

- normalized sampling time $T_{s,norm} = 1e - 2$,
- $\alpha = \frac{1}{3}$,
- $L = 1$, $\gamma = 1$, $k_BT = 1$ and
- $V_0 = 5K_BT$.

VI. Analysis and Discussion

In this article, we have studied the flashing ratchet mechanism which can be used to perform useful work utilizing noise. In particular we presented an optimal feedback strategy to maximize transport for a particle for non-zero load force while incorporating realistic constraints of measurement system. The strategy shows an order of increase in the *stalling force* compared to the open loop strategy[1], [13].

In experimental setups, it is easier to implement controllers on digital platforms like FPGAs or DSPs, which inherently have a finite sampling time. Even the sensors involved for position sensing have digitally sampled output in many cases. Different state-of-the-art optimal feedback strategies to maximize transport [3] make unrealistic assumptions like infinite closed loop bandwidth and infinite sampling frequency. All the aforementioned issues thus render these strategies unfeasible for physical application. Other strategies [5], [6] that address these assumptions are based on ad-hoc methods and are not proven to be optimal. Also, to the best of our knowledge, no feedback strategy exists hitherto that incorporates the effect of a non-zero load force.

To address the aforementioned issues, the dynamic programming formulation was used numerically to find an optimal feedback strategy maximizing the transport. In this formulation, we incorporated the effect of finite sampling time and non-zero load force. After scrutiny of the computed decision table, we were able to extract a threshold based closed loop switching strategy, thus obviating the need for high computational cost of construction and storage of dynamic programming based decision tables for different scenarios. This DP based framework can also be used to derive an optimal strategy when there are various delays (actuator, sensor, etc.) in the feedback loop.

The approach adopted in this paper can be extended to the case of multiple particles. For transport of multiple particles, the dynamics of each particle is independent of each other. However, all the particles will be under the same potential. Thus the control action (whether the potential is *on* or *off*) is the same for all particles and has to incorporate the position of all the particles. Here the transport objective plays an important role in the computational cost. Natural objectives can be posed in terms of the mean and variance of the positions of the particles (for example, it might be desired to move the centroid beyond a certain distance). If the objective is so fine that it poses separate objectives for each of the many particles the complexity can grow as $P!$ where P is the number of particles. Given the factorial dependence, it can be shown that the problems involving as many as 30 particles can be suitably handled by DP with computing units having more than 100 cores of GHz processors. This type of supercomputing units can be used to compute and store such decision tables that can be used during real-time applications, which constitutes our future work.

The presented study apart from discerning the motor protein based transport, will also provide efficient methods to transport nano-scale particles in engineered systems.

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