On the Capacity of Diffusion Channels for Molecular Communication

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***Abstract*—In the present paper a diffusion channel for molecular communication is investigated. We assume that different amounts of particles are transmitted by an emitter, which diffuse through a medium and are partially absorbed by a receptor. This models biological information exchange, particularly in neural networks. We investigate the capacity of this channel. A novel general representation of mutual information is obtained. Lower and upper bounds for the capacity are derived and their accuracy is numerically assessed. Explicit results are achieved for the truncated Poisson channel, which is a prominent model for biological information exchange, however, notoriously hard to deal with.**

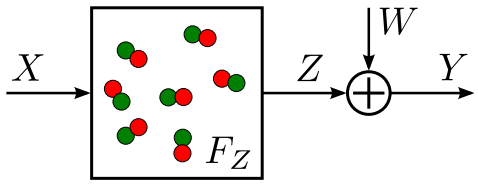

Fig. 1: Molecular communication with input X, transition function F_Z, and additive noise W to yield the output Y.

I. Introduction and Overview

The model used in this paper is inspired by biological information exchange between neurons in the brain. Neurons form a huge network and pass information by axons. Information from connected neurons is collected by the dendritic tree. Information exchange takes place by synapses. Vesicles are transmitted by the axon, which diffuse through the synaptic cleft and are received by receptors of the dendrites. The intensity of the connection varies by controlling the number of vesicles to be transmitted.

In this paper we model and investigate molecular information systems of this type in steady state. Different amounts of particles are transmitted in L bulks with average $x_1, \dots, x_L \in \mathbb{N}$. They form an L-ary alphabet of symbols which are sent over the diffusive channel. The receiver absorbs a certain number of emitted particles, overlaid by noise from other sources. We will keep the stochastic assumptions on the channel model rather general in the present work.

Specific approaches are used in a number of papers on molecular communication and biological information exchange. We briefly cite a view of the most recent ones related to the model used in the present work. A comprehensive overview of contributions to the area of molecular communication as of 2015 with an extensive literature survey is presented in [1]. Following the autors' scheme on different ways of molecular communications, the present work best fits into neurochemical propagation through gap junction where modulation is done by the number of particles. We do not consider error correction and we model the memory of the channel simply through a random number of molecules remaining from previous transmission.

Particle-intensity modulation is considered in [2]. Symbols are encoded by duration of transmission, which translates into the number of particles if the generation rate is constant over time. The authors start with a Bernoulli distribution of particle counts and finally use a Poisson approximation to achieve conditions under which binary input is capacity-achieving.

In order to model past emissions of particles, hence memory of the channel, the authors [3] consider an autoregressive model at the receptor. Using a Poisson approximation for the number of detected particles a training-based channel impulse response estimator is derived under statistical knowledge of the channel. A maximum a-posteriori and a linear mean square error estimator are proposed if no channel knowledge is available.

The main contributions of this work are upper and lower bounds on the capacity of the diffusive channel in general. Most importantly, however, an explicit formula for the capacity of the truncated Poisson diffusion channel is derived. Numerical evaluations give insight into the unexpected behavior of the molecular communication channel.

II. System Model for Molecular Communications

We assume that different amounts of molecular particles, e.g., vesicles are released in discrete time steps. The particles float through a medium to a receptor, which counts the number of received particles per time unit. Messages are encoded in the respective number of particles released. The transport process is by diffusion, hence random. Typical models for this type of information exchange are considered in [4] and [5]. In this work we use a more general system model.

A discrete-time memoryless channel with additive and stochastically independent noise is assumed. The communication system consists of a single transmitter and receiver with a diffusion channel in between. The channel input to the diffusion channel at each time step is described by a discrete random variable X with a finite number $L \in \mathbb{N}$ of pairwise

different and nonnegative support points $\boldsymbol{x} = (x_1, \ldots, x_L)$ and corresponding probabilities $\boldsymbol{p} = (p_1, \ldots, p_L)$. Due to inaccuracies the actual number of particles released into the medium is random governed by a probability mass function (PMF) $f_Z(z)$ with positive support $z \geq 0$. Only a certain rate $0 < \alpha \leq 1$ of emitted particles is received by the receptor, so that the conditional expectation of Z is assumed to be

$$\mathrm{E}(Z \mid X = x_\ell) = \alpha\, x_\ell.$$

Furthermore, the number of particles Y that are absorbed by the receptor is subject to additive random noise W with PMF $\phi(w)$ and nonnegative support $w \geq 0$. The noise W accounts for the number of particles left over in the medium from past transmissions not yet being absorbed. This simplifies the elobarate assumptions of an autoregressive process as considered in [3]. We assume that the number of left-over particles has a finite first and second moment, $\mathrm{E}(W) < \infty$ and $\mathrm{E}(W^2) < \infty$, so that they are vanishing at a constant rate by absorption. In summary, the system model reads as

$$Y = Z(X) + W,$$

as depicted in Fig. 1.

A common assumption for the counting processes is the Poisson distribution, which leads to

$$f_{Z|X=x}(z) = \frac{\alpha^z x^z}{z!}\,\mathrm{e}^{-\alpha x} \text{ and } \phi(w) = \frac{\lambda^w}{w!}\,\mathrm{e}^{-\lambda}$$

$z, w \in \mathbb{N}_0$ and $\lambda > 0$ being the noise intensity. Poissonian models of this type are the starting point for the work [4], [5], [6]. Other distributions like the geometric or binomial are conceivable and have been investigated in the literature, confer, e.g., [2], [3], [7], [8].

III. Mutual Information of the Molecular Channel

We set out to obtain a convenient expression for the mutual information which will allow determining capacity by maximizing over all input distributions. With the probabilities[1]

$$\begin{aligned}\Pr(Y = k \mid X = x_\ell) &= \Pr(Z + W = k \mid X = x_\ell)\\ &= \sum_z f_{Z|X=x_\ell}(z)\,\phi(k-z)\end{aligned}$$

and

$$\begin{aligned}\Pr(Y = k) &= \Pr(Z + W = k)\\ &= \sum_{\ell=1}^{L} p_\ell \sum_z f_{Z|X=x_\ell}(z)\,\phi(k-z)\end{aligned}$$

[1]The logarithm of $q > 0$ with respect to the base $a > 1$ is denoted by $\log_a(q)$ and the self-information of $q \geq 0$ by $\rho_a(q) = -q\log_a(q)$. It holds for the first derivative that $\rho_a'(q) = -\log_a(\mathrm{e}\,q)$, where e is the Euler's number. The discrete entropy of a probability vector $\boldsymbol{q} = (q_1, \ldots, q_n)$ is then defined as $h_a(\boldsymbol{q}) = \sum_{i=1}^{n} \rho_a(q_i)$. If the base is $a = \mathrm{e}$, we write in short $\ln(q)$, $\rho(q)$ and $h(\boldsymbol{q})$.

mutual information $I(X;Y)$ between input X and output Y may be written as

$$\begin{aligned}I(X;Y) &= H(Y) - H(Y \mid X)\\ &= \sum_{k=0}^{\infty}\Bigg[\rho_a\Big(\sum_{\ell=1}^{L} p_\ell \sum_z f_{Z|X=x_\ell}(z)\phi(k-z)\Big)\\ &\qquad - \sum_{\ell=1}^{L} p_\ell\,\rho_a\Big(\sum_z f_{Z|X=x_\ell}(z)\phi(k-z)\Big)\Bigg].\end{aligned} \tag{1}$$

Using the notation $\Delta_k(x_\ell) = \sum_z f_{Z|X=x_\ell}(z)\,\phi(k-z)$ a concise representation of (1) is obtained as

$$I(X;Y) = \sum_{k=0}^{\infty}\Bigg[\rho_a\Big(\sum_{\ell=1}^{L} p_\ell \Delta_k(x_\ell)\Big) - \sum_{\ell=1}^{L} p_\ell\,\rho_a\big(\Delta_k(x_\ell)\big)\Bigg]. \tag{2}$$

It holds that $\Delta_k(x_\ell) = \big(f_{Z|X=x_\ell} * \phi\big)(k)$ is the convolution of the conditional PMF $f_{Z|X=x_\ell}$ and ϕ. Hence, $\Delta_k(x_\ell)$ is a PMF with respect to k such that $\Delta_k(x_\ell) \geq 0$ for all k, ℓ and $\sum_{k=0}^{\infty}\Delta_k(x_\ell) = 1$ for all ℓ. However, $\Delta_k(x)$ is not necessarily increasing nor decreasing in x.

For a fixed transition distribution f_Z, mutual information (2) is hence a function of the amount of input molecules $\boldsymbol{x} = (x_1, \ldots, x_L)$ and their probabilities $\boldsymbol{p} = (p_1, \ldots, p_L)$, which motivates the notation $I(\boldsymbol{p}, \boldsymbol{x})$ instead of $I(X;Y)$. Since ρ_a is a strictly concave function, mutual information $I(\boldsymbol{p}, \boldsymbol{x})$ is also strictly concave as a function of $\boldsymbol{p}$. Despite concavity maximization over $\boldsymbol{p}$ seems to be very hard.

In the special case that $f_{Z|X}$ and ϕ are Poisson distributions the sum $Z + W$ conditional on $X = x_\ell$ is also Poisson distributed with parameter $\gamma_\ell = \alpha x_\ell + \lambda$. Hence,

$$\Delta_k(x_\ell) = \frac{\gamma_\ell^k}{k!}\,\mathrm{e}^{-\gamma_\ell}$$

and mutual information for the Poissonian diffusion channel reads as

$$I(\boldsymbol{p}, \boldsymbol{\gamma}) = \sum_{k=0}^{\infty}\Bigg[\rho_a\Big(\sum_{\ell=1}^{L} p_\ell \tfrac{\gamma_\ell^k}{k!}\,\mathrm{e}^{-\gamma_\ell}\Big) - \sum_{\ell=1}^{L} p_\ell\,\rho_a\big(\tfrac{\gamma_\ell^k}{k!}\,\mathrm{e}^{-\gamma_\ell}\big)\Bigg]. \tag{3}$$

Equation (3) may also be written as the difference between the entropy of a mixture of Poisson distributions and the weighted sum of the entropies of Poissonians:

$$I(\boldsymbol{p}, \boldsymbol{\gamma}) = h\Big(\sum_{\ell=1}^{L} p_\ell \mathrm{Poi}(\gamma_\ell)\Big) - \sum_{\ell=1}^{L} p_\ell h\big(\mathrm{Poi}(\gamma_\ell)\big).$$

After some algebra and using the explicit form of the entropy of a Poisson distribution the following interesting representation is obtained

$$I(\boldsymbol{p}, \boldsymbol{\gamma}) = 1 - \sum_{\ell=1}^{L} p_\ell \gamma_\ell (1 - \ln \gamma_\ell) - D\Big(\sum_{\ell=1}^{L} p_\ell \mathrm{Poi}(\gamma_\ell)\Big\|\mathrm{Poi}(1)\Big),$$

where $D(\cdot\|\cdot)$ denotes the Kullback-Leibler divergence.

IV. Optimization of Mutual Information

Maximizing mutual information (2) w.r.t. $\boldsymbol{p}$ subject to the constraints $p_\ell \geq 0$ and $\sum_{\ell=1}^{L} p_\ell = 1$ leads to the following Karush-Kuhn-Tucker (KKT) conditions. A solution $\boldsymbol{p}$ is optimal iff it satifies for all $i = 1, \ldots, L$

$$0 \leq p_i \,, \tag{4a}$$

$$0 \leq \mu_i \,, \tag{4b}$$

$$0 = \mu_i \, p_i \,, \tag{4c}$$

$$1 = \sum_{\ell=1}^{L} p_\ell \,, \tag{4d}$$

$$\mu_i = \tilde{\lambda} + \sum_{k=0}^{\infty} \Delta_k(x_i) \log_a\Big(\mathrm{e} \sum_{\ell=1}^{L} p_\ell \Delta_k(x_\ell)\Big) + \rho_a\big(\Delta_k(x_i)\big), \tag{4e}$$

where $\boldsymbol{\mu}$ and $\tilde{\lambda}$ are Lagrangian multipliers. For any optimal $p_i^\star > 0$ it follows $\mu_i^\star = 0$ from (4c) and by (4e) we obtain

$$\lambda^\star = -\sum_{k=0}^{\infty} \bigg[\Delta_k(x_i) \log_a\Big(\sum_{\ell=1}^{L} p_\ell^\star \Delta_k(x_\ell)\Big) + \rho_a\big(\Delta_k(x_i)\big) \bigg], \tag{5}$$

where $\lambda^\star = \tilde{\lambda}^\star + \log_a(\mathrm{e})$. Multiplying the previous equation by $p_i^\star$ and summing up over all i yields

$$\lambda^\star = \sum_{k=0}^{\infty} \bigg[\rho_a\Big(\sum_{\ell=1}^{L} p_\ell^\star \Delta_k(x_\ell)\Big) - \sum_{\ell=1}^{L} p_\ell^\star \rho_a\big(\Delta_k(x_\ell)\big) \bigg], \tag{6}$$

which is identical to the objective function (2). Hence, the maximum value of the mutual information is given by $I(\boldsymbol{p}^\star, \boldsymbol{x}) = \lambda^\star$, i.e.,

$$\begin{aligned} I(\boldsymbol{p}^\star, \boldsymbol{x}) &= -\sum_{k=0}^{\infty} \Delta_k(x_i) \log_a\Big(\sum_{\ell=1}^{L} p_\ell^\star \Delta_k(x_\ell)\Big) + \rho_a\big(\Delta_k(x_i)\big) \\ &= \sum_{k=0}^{\infty} \Delta_k(x_i) \log_a\bigg(\frac{\Delta_k(x_i)}{\sum_{\ell=1}^{L} p_\ell^\star \Delta_k(x_\ell)}\bigg) \end{aligned} \tag{7}$$

for any i with $p_i^\star > 0$. The optimal values of the input probabilities $p_\ell^\star$ cannot be determined in closed form, however, they can be computed numerically using (5). Once the optimal input probabilities are known, equation (7) describes the channel capacity for molecular communication for a given support $\boldsymbol{x}$. The maximization of $I(\boldsymbol{p}, \boldsymbol{x})$, or even of $I(\boldsymbol{p}^\star, \boldsymbol{x})$, over $\boldsymbol{x}$ is extremely challenging. Both $I(\boldsymbol{p}, \boldsymbol{x})$ and $I(\boldsymbol{p}^\star, \boldsymbol{x})$ are neither convex nor concave functions of $\boldsymbol{x}$.

Identity (7) shows that the maximum value is equal to the Kullback-Leibler divergence between the probabilities $\Delta_k(x_i)$ and $\sum_{\ell=1}^{L} p_\ell^\star \Delta_k(x_\ell)$ over k. Using the notations

$$\boldsymbol{u}_i = \big(\Delta_0(x_i), \Delta_1(x_i), \Delta_2(x_i), \ldots\big) \tag{8}$$

and

$$\boldsymbol{v} = \bigg(\sum_{\ell=1}^{L} p_\ell^\star \Delta_0(x_\ell), \sum_{\ell=1}^{L} p_\ell^\star \Delta_1(x_\ell), \sum_{\ell=1}^{L} p_\ell^\star \Delta_2(x_\ell), \ldots\bigg) \tag{9}$$

a compact characterization of the optimum is obtained by (7) and the Kullback-Leibler divergence, i.e., $D(\boldsymbol{u}_i \| \boldsymbol{v}) = \lambda^*$ for all i such that $p_i^\star > 0$.

V. Capacity Bounds for the Molecular Channel

The formula for the unknown channel capacity in (7) can be used to develop lower and upper bounds on the capacity. Any $\boldsymbol{p}$ substituted in (7) yields a lower bound on the capacity.

An easy upper bound can be found with the aid of [9, p. 41, Lemma 3.11], which states that $D(\boldsymbol{u}_i \| \boldsymbol{v}) \leq D(\tilde{\boldsymbol{u}}_i \| \tilde{\boldsymbol{v}})$ for any row stochastic matrix $\boldsymbol{A}$ with $\boldsymbol{u}_i = \tilde{\boldsymbol{u}}_i \boldsymbol{A}$ and $\boldsymbol{v} = \tilde{\boldsymbol{v}} \boldsymbol{A}$ for all i. Without loss of generality we can assume that all probabilities are positive, i.e., $p_\ell^\star > 0$ for all $\ell = 1 \ldots L$. The $L \times \infty$ matrix

$$\boldsymbol{A} = \begin{pmatrix} \Delta_0(x_1) & \Delta_1(x_1) & \Delta_2(x_1) & \ldots \\ \Delta_0(x_2) & \Delta_1(x_2) & \Delta_2(x_2) & \ldots \\ \Delta_0(x_3) & \Delta_1(x_3) & \Delta_2(x_3) & \ldots \\ \vdots & \vdots & \vdots & \\ \Delta_0(x_L) & \Delta_1(x_L) & \Delta_2(x_L) & \ldots \end{pmatrix} \tag{10}$$

with the vectors[2]

$$\tilde{\boldsymbol{u}}_i = \boldsymbol{e}_i \tag{11}$$

and

$$\tilde{\boldsymbol{v}} = \big(p_1^\star, p_2^\star, p_3^\star, \ldots, p_L^\star\big) \tag{12}$$

satisfy the assumptions and we obtain $D(\tilde{\boldsymbol{u}}_i \| \tilde{\boldsymbol{v}}) = -\log_a(p_i^\star)$. Since the previous equation holds for all i, a simple upper bound is obtained as

$$I(\boldsymbol{p}^\star, \boldsymbol{x}) \leq D(\tilde{\boldsymbol{u}}_i \| \tilde{\boldsymbol{v}}) \leq -\log_a\big(\tfrac{1}{L}\big) = \log_a(L) \,. \tag{13}$$

This upper bound is sharp whenever the distance between any two mass points is much greater than the standard deviation of the noise. In this case the input probabilities will converge to the uniform distribution and the mass points are equidistant.

For finding sharper upper bounds more effort is needed. By the aid of [10, Theorem F] the inequality

$$D(\boldsymbol{u} \| \boldsymbol{v}) \leq \log_a\Big(\frac{1-\eta}{-\ln(\eta)}\Big) - \frac{\log_a(\eta)}{1-\eta} - \log_a(\mathrm{e}) \tag{14}$$

holds for arbitrary $\boldsymbol{u}$ and $\boldsymbol{v}$ with $\eta = \frac{\min_k v_k/u_k}{\max_k v_k/u_k}$. From this inequality an upper bound for the molecular channel is obtained by

$$D(\boldsymbol{u}_i \| \boldsymbol{v}) \leq \min_j \bigg\{ \log_a\Big(\frac{1-\eta_j}{-\ln(\eta_j)}\Big) - \frac{\log_a(\eta_j)}{1-\eta_i} - \log_a(\mathrm{e}) \bigg\} \tag{15}$$

for all i and for all j with $p_j^\star > 0$ and $\eta_j = \frac{m_j}{M_j}$, where

$$m_j = \min_k \frac{\sum_{\ell=1}^{L} p_\ell^\star \Delta_k(x_\ell)}{\Delta_k(x_j)} \text{ and } M_j = \max_k \frac{\sum_{\ell=1}^{L} p_\ell^\star \Delta_k(x_\ell)}{\Delta_k(x_j)} \,.$$

Since the right hand side of (14) is decreasing in η, we can eliminate the influence of $\boldsymbol{p}^\star$ by replacing each η_j by

$$\check{\eta}_j = \frac{\min\limits_k \frac{\min_\ell \Delta_k(x_\ell)}{\Delta_k(x_j)}}{\max\limits_k \frac{\max_\ell \Delta_k(x_\ell)}{\Delta_k(x_j)}} \leq \eta_j \,, \tag{16}$$

since

$$m_j \geq \min_k \frac{\min_\ell \Delta_k(x_\ell)}{\Delta_k(x_j)} \text{ and } M_j \leq \max_k \frac{\max_\ell \Delta_k(x_\ell)}{\Delta_k(x_j)} \tag{17}$$

[2]The canonical unit vectors are denoted by $\boldsymbol{e}_1$, $\boldsymbol{e}_2$, $\boldsymbol{e}_3$ and so on.

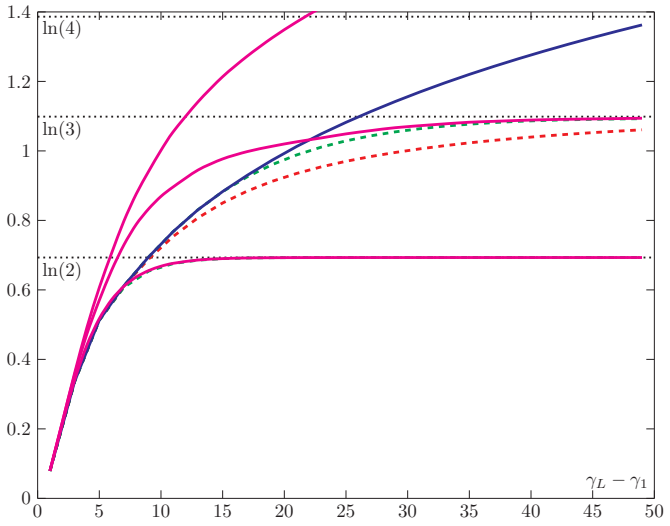

Fig. 2: Capacity of the molecular channel with both Poissonian diffusion and noise distribution.

for all j. Hence, we obtain the upper bound

$$I(\boldsymbol{p}^\star, \boldsymbol{x}) \leq \min_j \left\{ \log_a\Big(\frac{1-\check{\eta}_j}{-\ln(\check{\eta}_j)}\Big) - \frac{\log_a(\check{\eta}_j)}{1-\check{\eta}_j} - \log_a(\mathrm{e}) \right\} \quad (18)$$

for which we only need to determine the terms $\check{\eta}_j$ from (16) for all j with $p_j^\star > 0$. The upper bound in (18) still depends on the input constellation $\boldsymbol{x}$ and the knowledge of the index of positive probabilities. Since the extreme mass-points x_1 and x_L always have positive probabilities, we obtain a looser upper bound as

$$I(\boldsymbol{p}^\star, \boldsymbol{x}) \leq \min_{j\in\{1,L\}} \left\{ \log_a\Big(\frac{1-\check{\eta}_j}{-\ln(\check{\eta}_j)}\Big) - \frac{\log_a(\check{\eta}_j)}{1-\check{\eta}_j} - \log_a(\mathrm{e}) \right\}. \quad (19)$$

We can further relax this upper bound to eliminate the position of the input symbols by replacing each $\tilde{\eta}_j$ by

$$\hat{\eta} = \frac{\min\limits_k \frac{\min_{x\in[x_1,x_L]} \Delta_k(x)}{\max_{x\in[x_1,x_L]} \Delta_k(x)}}{\max\limits_k \frac{\max_{x\in[x_1,x_L]} \Delta_k(x)}{\min_{x\in[x_1,x_L]} \Delta_k(x)}} \leq \check{\eta}_j \quad (20)$$

for all j. This yields the ultimative upper bound

$$I(\boldsymbol{p}^\star, \boldsymbol{x}) \leq \log_a\Big(\frac{1-\hat{\eta}}{-\ln(\hat{\eta})}\Big) - \frac{\log_a(\hat{\eta})}{1-\hat{\eta}} - \log_a(\mathrm{e})\,. \quad (21)$$

The attraction of both bounds (13) and (21) is that they do not depend on the distribution of the mass points and their probabilities. While (13) only depends on the number L of mass points, the upper bound (21) is depending on the span $x_L - x_1$.

VI. Numerical Results

In this section we discuss some numerical results regarding the capacity and the upper bounds on the capacity of a diffusion channel. In Fig. 2 we show some results that are obtained for the case of Poissonian diffusion and noise distribution. All the curves are showing the throughput over the span $\gamma_m - \gamma_1 = \max_i\{x_i\} - \min_i\{x_i\}$ The solid blue curve is the true capacity, obtained by numerically maximizing mutual information over $\boldsymbol{p}$ and $\boldsymbol{x}$. The solid purple curves are the upper bounds on the capacity if the number of input symbols is limited by 2, 3, and 4, respectively. The dashed curves are the most interesting results. The dashed red curve is the maximum mutual information for the case that the number of input symbols are limited by 3 and the input symbols are equidistantly arranged. The dashed green curve, which is located above the dashed red curve, shows the results for the same scenario whith the exception that the maximum mutual information is further maximized over the position of the input symbols. For $L = 2$ input symbols the dashed green curve nearly coincides with the dashed red curve.

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