

Non-Coherent Multiple-Symbol Detection for Diffusive Molecular Communications

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ABSTRACT

Most of the available works on molecular communication (MC) assume that the channel state information (CSI) is perfectly known at the receiver for data detection. In contrast, in this paper, we study non-coherent multiple-symbol detection schemes which do not require knowledge of the CSI. In particular, we derive the optimal maximum likelihood (ML) multiple-symbol (MLMS) detector. Moreover, we propose an approximated detection metric and a sub-optimal detector to cope with the high complexity of the optimal MLMS detector. Numerical results reveal the effectiveness of the proposed optimal and suboptimal detection schemes with respect to a baseline scheme which assumes perfect CSI knowledge, particularly when the number of observations used for detection is sufficiently large.

1. INTRODUCTION

Molecular communication (MC) has recently emerged as a bio-inspired approach for synthetic communication systems over nano/micrometer scale dimensions [3, 8]. Unlike conventional wireless communication systems which employ electromagnetic waves for carrying information, MC systems encode information in the number, type, or time of release of signalling molecules. Calcium signaling of neurons and the exchange of autoinducers in bacteria quorum sensing are among the many examples of MC in nature [3, 4].

In diffusive MC, the channel state information (CSI) is defined as the *means* of the numbers of the signaling and interfering molecules which are observed at the receiver due to the release of a known number of molecules by the transmitter. Most existing works on MC assume that the CSI is perfectly known at the receiver for reliable detection of the transmitted information bits [5, 13, 15]. However, the CSI is not known a priori and has to be estimated. To this end, a training-based CSI estimation framework was developed in [11] and several optimal and suboptimal estimators were proposed. However, the acquisition of the CSI is a suitable option only if the coherence time of the MC channel is sufficiently large such that the corresponding training overhead is tolerable. On the other hand, for the case when the MC channel changes rapidly, accurate CSI estimation entails a large overhead, and reducing the overhead implies a low CSI estimation quality. In this case, directly detecting the data symbols without spending any resources on CSI acquisition is an attractive option which is referred to as *non-coherent* detection.

In this paper, our focus is to design optimal and suboptimal non-coherent multiple-symbol detection schemes which do not require knowledge of the instantaneous CSI. In partic-

ular, we first derive the optimal maximum likelihood (ML) multiple-symbol (MLMS) detector. One of the main challenges in implementing the optimal detector is the computation of the detection metrics, which requires the evaluation of expectations with respect to the probability density function (PDF) of the CSI. The PDF of the CSI depends on the considered MC environment and a general analytical expression is not yet available in the literature. In practice, the PDF of the CSI for a particular MC channel can be obtained using historical measurements of the CSI. In this paper, we propose the Gamma distribution as an approximation for the PDF of the CSI which is shown to accurately match the exact historical distribution for several examples of stochastic MC channels. Moreover, we show that the Gamma distribution yields a closed-form expression for the detection metric. Additionally, we develop a blind suboptimal detector which first estimates the CSI based on the multiple symbols in each detection block (without employing a training sequence) and then performs ML detection based on the estimated CSI. Our numerical results reveal the effectiveness of the proposed optimal and suboptimal non-coherent detectors and show that as the number of observation symbols increases, their performances approach that of the baseline scheme, which assumes perfect CSI.

We note that in contrast to MC, for conventional wireless communication there is a rich literature on non-coherent multiple-symbol detection, see e.g. [6, 16], and the references therein. In particular, in [6], multiple-symbol differential detection without CSI was presented for radio frequency (RF) communications and in [16], non-coherent multiple-symbol detection for a photon-counting receiver was studied for optical communications. We note that the detection problem and the resulting detection strategies developed for conventional wireless communications are not straightforwardly applicable to the corresponding MC detection problem. In the recent paper [12], the authors considered the problem of non-coherent data detection in MC. In particular, it was shown in [12] that the difference in molecule concentration is a stable characteristic of the diffusive MC channel and, based on this fact, a heuristic low-complexity non-coherent symbol-by-symbol detector was proposed. However, to the best of the authors' knowledge, the design of optimal/suboptimal *non-coherent multiple-symbol detectors* has not been considered in the MC literature, yet.

The remainder of this paper is organized as follows. In Section 2, the system model, preliminaries, and assumptions are presented. The proposed optimal/suboptimal detectors are introduced in Section 3. Numerical results are provided in Section 4, and conclusions are drawn in Section 5.



Figure 1: Schematic illustration of the considered MC system where the molecules released by the transmitter in a given symbol interval are shown in green color whereas the noise molecules are shown in red color.

Notations: We use the following notations throughout this paper: $\mathbb{E}_x\{\cdot\}$ denotes expectation with respect to random variable (RV) x and $|\cdot|$ represents the cardinality of a set. Bold letters are used to denote vectors and \mathbf{a}^T represents the transpose of vector \mathbf{a} . $\lfloor \cdot \rfloor$ and $\lceil \cdot \rceil$ denote the floor and ceiling functions which map a real number to the largest previous and the smallest following integer numbers, respectively. Moreover, $\text{Pois}(\lambda)$ denotes a Poisson RV with mean λ , $\text{Bin}(n, p)$ denotes a binomial RV for n trials and success probability p , $\mathcal{N}(\mu, \sigma^2)$ denotes a Gaussian RV with mean μ and variance σ^2 , and $\text{Gamma}(\alpha, \beta)$ denotes a Gamma distributed RV with scale parameter α and rate parameter β .

2. SYSTEM MODEL AND PRELIMINARIES

In this section, we first introduce the adopted MC channel model and state the considered non-coherent detection problem. Subsequently, we provide an example of a stochastic MC channel and a performance upper bound.

2.1 System Model

We consider an MC system consisting of a transmitter, a channel, and a receiver, see Fig. 1. At the beginning of each symbol interval, the transmitter releases either N^{Tx} or zero molecules corresponding to the binary bits 1 and 0, respectively, i.e., ON-OFF keying is performed [8]. In this paper, we assume that the transmitter emits only one type of molecule. The released molecules diffuse through the fluid medium between the transmitter and the receiver. We assume that the movements of individual molecules are independent from each other. The receiver counts the number of observed molecules in each symbol interval. We note that this is a rather general model for the MC receiver which includes well-known receivers such as the transparent receiver [13], the absorbing receiver [2], and the reactive receiver [1]. In particular, the number of observed molecules at the receiver in symbol interval k , denoted by $r[k]$, is given by

$$r[k] = c_s[k] + c_n[k], \quad (1)$$

where $c_s[k]$ is the number of molecules observed at the receiver in symbol interval k due to the release of $s[k]N^{\text{Tx}}$ molecules by the transmitter at the beginning of symbol interval k , where $s[k] \in \{0, 1\}$ holds. We assume that the binary information bits are equiprobable, i.e., $\Pr\{s[k] = 1\} = \Pr\{s[k] = 0\} = 0.5$. Moreover, $c_n[k]$ is the number of interfering noise molecules comprising residual inter-symbol interference (ISI), multiuser interference (caused by other MC links), and external noise (originated from natural sources) observed by the receiver in symbol interval k .

The MC channel is dispersive due to the diffusive propagation of the molecules [14]. The ISI-free communication model in (1) implies that the symbol intervals are chosen sufficiently large such that the channel impulse response (CIR) fully decays to zero within one symbol interval. We note

that enzymes [14] and reactive information molecules, such as acid/base molecules [7], may be used to speed up the decaying of the CIR as a function of time. Nevertheless, since the length of the symbol intervals is finite, some residual ISI always exists. Throughout this paper, we assume that the effect of the residual ISI is included in $c_n[k]$ and is sufficiently small compared to the other components in $c_n[k]$ such that $c_n[k]$ is (approximately) independent of the signal component $c_s[k]$.

From a probabilistic point of view, we can assume that each molecule released by the transmitter in a given symbol interval is observed at the receiver in the same symbol interval with a certain probability, denoted by p . Therefore, the probability that n molecules are observed at the receiver due to the emission of N^{Tx} molecules at the transmitter follows a binomial distribution, i.e., $n \sim \text{Bin}(N^{\text{Tx}}, p)$. Moreover, assuming $N^{\text{Tx}} \rightarrow \infty$ while $N^{\text{Tx}}p \triangleq \bar{c}_s$ is fixed, the binomial distribution $\text{Bin}(N^{\text{Tx}}, p)$ converges to the Poisson distribution $\text{Pois}(\bar{c}_s)$ [9]. Another approximation of the binomial distribution $\text{Bin}(N^{\text{Tx}}, p)$ is the Gaussian distribution $\mathcal{N}(N^{\text{Tx}}p, \sqrt{N^{\text{Tx}}p(1-p)})$ which holds for very large N^{Tx} when the success probability p is not close to zero (equivalently when $N^{\text{Tx}}p$ is a large number) [9]. We note that the assumptions for the former case are more justified for MC since the number of released molecules is typically very large and the probability that a molecule released by the transmitter reaches the destination is typically very small. Therefore, we adopt the Poisson approximation in this paper, i.e., $c_s[k] \sim \text{Pois}(\bar{c}_s s[k])$, see [5, 15]. Since the noise molecules originate from interfering natural or syntactic sources, $c_n[k]$ is also modeled as a Poisson RV, i.e., $c_n[k] \sim \text{Pois}(\bar{c}_n)$, where $\bar{c}_n = \mathbb{E}\{c_n[k]\}$. In the remainder of this paper, we refer to the pair (\bar{c}_s, \bar{c}_n) as the CSI of the considered MC system.

REMARK 1. *The channel model in (1) can be generalized to the case of multiple-sample detection if the following sum detector is employed*

$$\begin{aligned} r[k] &= \sum_{m=1}^M y[k, m] \\ &= \sum_{m=1}^M c_s[k, m] + \sum_{m=1}^M c_n[k, m] \triangleq c_s[k] + c_n[k], \quad (2) \end{aligned}$$

where M denotes the number of samples per symbol interval and $y[k, m]$ is the number of molecules observed at the receiver in the m -th sample of symbol interval k . Moreover, $c_s[k, m]$ is the number of molecules observed at the receiver in the m -th sample of symbol interval k due to the release of $s[k]N^{\text{Tx}}$ molecules by the transmitter at the beginning of symbol interval k and $c_n[k, m]$ is the number of noise molecules observed by the receiver in the m -th sample of symbol interval k . Thus, $c_s[k]$ and $c_n[k]$ follow Poisson distributions with means $\bar{c}_s = \sum_{m=1}^M \bar{c}_s^{(m)}$ and $M\bar{c}_n$, respectively, where $\bar{c}_s^{(m)} = \mathbb{E}\{c_s[k, m]\}$ and $\bar{c}_n = \mathbb{E}\{c_n[k, m]\}$. We note that the sum detector in (2) includes the well-known peak observation [15] and energy observation [17] detectors as special cases when only one sample at the peak concentration is taken and (ideally infinitely) many samples per symbol interval are taken, respectively.

REMARK 2. *Unlike the conventional linear input-output model for channels with memory in wireless communications [6], the channel model in (1) is not linear since $s[k]$ does not affect the observation $r[k]$ directly but via Poisson RV $c_s[k]$. However, the expectation of the received signal is linearly*

dependent on the transmitted signal, i.e.,

$$\bar{r}[k] = \mathbb{E} \{r[k]\} = \bar{c}_s s[k] + \bar{c}_n. \quad (3)$$

We note that for a given $s[k]$, in general, the actual number of molecules observed at the receiver, $r[k]$, will differ from the expected number of observed molecules, $\bar{r}[k]$, due to the intrinsic noisiness of diffusion.

2.2 Non-Coherent Detection Problem in MC

Most existing detection schemes in MC assumed that knowledge of the CSI, (\bar{c}_s, \bar{c}_n) , is available at the receiver [5, 13, 15]. In contrast, in this paper, we directly detect a block of multiple transmitted symbols based on the corresponding received observations without spending any resources on CSI acquisition at the receiver.

Let $\mathbf{s} = [s[1], s[2], \dots, s[K]]^T$ and $\mathbf{r} = [r[1], r[2], \dots, r[K]]^T$ denote the vectors of the transmitted symbols and the received observations, respectively, over a block of K symbol intervals. Throughout the remainder of the paper, we assume that the CSI remains unchanged over one block of transmitted symbols, but may change from one block to the next (e.g., due to a change of the distance between Tx and Rx). To model this, we assume that CSI (\bar{c}_s, \bar{c}_n) is an RV which takes its values in each block according to PDF $f_{(\bar{c}_s, \bar{c}_n)}(\bar{c}_s, \bar{c}_n)$. Furthermore, we assume that RVs \bar{c}_s and \bar{c}_n are independent, i.e., $f_{(\bar{c}_s, \bar{c}_n)}(\bar{c}_s, \bar{c}_n) = f_{\bar{c}_s}(\bar{c}_s) f_{\bar{c}_n}(\bar{c}_n)$ where $f_{\bar{c}_s}(\bar{c}_s)$ and $f_{\bar{c}_n}(\bar{c}_n)$ are the marginal PDFs of \bar{c}_s and \bar{c}_n , respectively. We note that although the proposed non-coherent detection schemes do not require knowledge of the instantaneous CSI, (\bar{c}_s, \bar{c}_n) , we assume that the statistical CSI, i.e., $f_{(\bar{c}_s, \bar{c}_n)}(\bar{c}_s, \bar{c}_n)$, is available for the design of the proposed optimal non-coherent detector, cf. Theorem 1. Since obtaining the CSI statistics might be difficult for some practical systems, we also propose a suboptimal non-coherent detector which does not require statistical CSI knowledge. For future reference, in the rest of this work, we define $f_{\mathbf{r}}(\mathbf{r}|\bar{c}_s, \bar{c}_n, \mathbf{s}) = \prod_k f_{r[k]}(r[k]|\bar{c}_s, \bar{c}_n, s[k])$ as the PDF of observation vector \mathbf{r} conditioned on both CSI (\bar{c}_s, \bar{c}_n) and transmitted symbol vector \mathbf{s} and $f_{\mathbf{r}}(\mathbf{r}|\mathbf{s}) = \prod_k f_{r[k]}(r[k]|s[k])$ as the PDF of \mathbf{r} conditioned on only \mathbf{s} .

2.3 Example of a Stochastic MC Channel

In this subsection, we present an example for a stochastic MC channel. We will employ this MC channel in Section 4 for the evaluation of the proposed non-coherent detectors. Let us assume a point source with impulsive molecule release, a fully transparent spherical receiver with volume V^{RX} , and an unbounded environment with diffusion coefficient D , where the distance between the transmitter and the receiver is denoted by r . In addition, we assume that there is steady uniform flow (or drift) with parallel and perpendicular velocity components, denoted by v_{\parallel} and v_{\perp} , respectively, with respect to the direction from the transmitter to the receiver. Furthermore, the signaling molecules may react with enzyme molecules, which are present in the MC environment, and degrade into a form that cannot be detected by the receiver. We assume a uniform concentration of the enzyme, denoted by \bar{c}_e , and a first order reaction mechanism between the signaling and enzyme molecules with constant reaction rate κ [15]. Based on the aforementioned assumptions, the expected number of molecules observed at the receiver as a function of time, denoted by $\bar{c}_s(t)$, is given by [15]

$$\bar{c}_s(t) = \frac{N^{\text{TX}} V^{\text{RX}}}{(4\pi D t)^{3/2}} \exp\left(-\kappa \bar{c}_e t - \frac{(r - v_{\parallel} t)^2 + (v_{\perp} t)^2}{4Dt}\right). \quad (4)$$

Furthermore, assuming a peak observation detector, the sample time from the beginning of each symbol interval is chosen as $t^{\text{max}} = \text{argmax}_{t>0} \bar{c}_s(t)$ which leads to $\bar{c}_s = \max_{t>0} \bar{c}_s(t)$.

In practice, however, there may be random variations in the underlying channel parameters which lead to random variations in \bar{c}_s . For instance, the flow velocity components, v_{\parallel} and v_{\perp} , may vary over time or the diffusion coefficient, D , and enzyme concentration, \bar{c}_e , may change due to variations in the environment temperature. To capture these effects, we assume that the channel parameters in each detection block are realizations of RVs according to $z = z^{\text{def}}(1 + \sigma_z \mathcal{N}(0, 1))$, $z \in \{D, v_{\parallel}, v_{\perp}, \bar{c}_e, \kappa, r\}$ where z^{def} denotes the mean value of parameter z and $\sigma_z z^{\text{def}}$ is its standard deviation which determines how much the parameter may deviate from the mean¹. As $\sigma_z \rightarrow 0$, $\forall z$, the respective MC channel becomes deterministic, and for large σ_z , the corresponding MC channel is highly stochastic. Substituting the Gaussian RVs $z \in \{D, v_{\parallel}, v_{\perp}, \bar{c}_e, \kappa, r\}$ into (4) may not lead to a closed-form analytical expression for $f_{\bar{c}_s}(\bar{c}_s)$. Therefore, we employ Monte Carlo simulation to determine the histogram of \bar{c}_s . Furthermore, in Subsection 3.2, we propose an analytical distribution and a strategy to match this analytical distribution to the histogram of \bar{c}_s . We note that since the noise mean \bar{c}_n might also be generated from natural or synthetic noise sources which employ the same type of molecules, the noise mean is also affected by the change in the underlying MC channel parameters. Therefore, in order to obtain $f_{\bar{c}_n}(\bar{c}_n)$, one may also model the variation of \bar{c}_n in a similar manner as discussed above for \bar{c}_s .

2.4 Performance Bound

As a performance upper bound, we consider the optimal detection scheme for perfect CSI knowledge. Moreover, since the observations in different symbol intervals are independent, without loss of optimality, the considered benchmark scheme performs symbol-by-symbol data detection. Thereby, the optimal ML detector is given by

$$\begin{aligned} \hat{s}^{\text{ML}}[k] &= \underset{s[k] \in \{0, 1\}}{\text{argmax}} f_{r[k]}(r[k]|\bar{c}_s, \bar{c}_n, s[k]) \\ &= \underset{s[k] \in \{0, 1\}}{\text{argmax}} \frac{(\bar{c}_s s[k] + \bar{c}_n)^{r[k]} \exp(-\bar{c}_s s[k] - \bar{c}_n)}{r[k]!}, \end{aligned} \quad (5)$$

where $f_{r[k]}(r[k]|\bar{c}_s, \bar{c}_n, s[k])$ is the Poisson distribution function. The aforementioned ML detector can be rewritten in the form of a threshold-based detector as follows

$$\hat{s}^{\text{ML}}[k] = \begin{cases} 1, & \text{if } r[k] \geq \xi^{\text{ML}} \\ 0, & \text{otherwise} \end{cases} \quad (6)$$

where $\xi^{\text{ML}} = \frac{\bar{c}_s}{\ln(1 + \frac{\bar{c}_s}{\bar{c}_n})}$.

3. MULTIPLE-SYMBOL DETECTION

In this section, we first derive the optimal non-coherent MLMS detector. Subsequently, we propose an approximate detection metric and a low-complexity suboptimal detector to cope with the high complexity of the MLMS detector.

3.1 Optimal Multiple-Symbol Detector

¹We note that a Gaussian RV may assume negative values whereas D , \bar{c}_e , and r are non-negative parameters. Therefore, we assume small values for σ_D , $\sigma_{\bar{c}_e}$, and σ_r and omit those realizations for which $z \in \{\bar{c}_e, D, r\}$ is negative.

The MLMS detector is mathematically given by

$$\begin{aligned}
\hat{\mathbf{s}}^{\text{MLMS}} &= \underset{\mathbf{s} \in \mathcal{A}}{\operatorname{argmax}} f_{\mathbf{r}}(\mathbf{r}|\mathbf{s}) \\
&= \underset{\mathbf{s} \in \mathcal{A}}{\operatorname{argmax}} \int_{\bar{c}_s \geq 0} \int_{\bar{c}_n \geq 0} f_{\mathbf{r}}(\mathbf{r}|\bar{c}_s, \bar{c}_n, \mathbf{s}) f_{(\bar{c}_s, \bar{c}_n)}(\bar{c}_s, \bar{c}_n) d\bar{c}_s d\bar{c}_n \\
&= \underset{\mathbf{s} \in \mathcal{A}}{\operatorname{argmax}} \int_{\bar{c}_s \geq 0} \int_{\bar{c}_n \geq 0} \prod_{k=1}^K \frac{(\bar{c}_s s[k] + \bar{c}_n)^{r[k]} \exp(-\bar{c}_s s[k] - \bar{c}_n)}{r[k]!} \\
&\quad \times f_{\bar{c}_s}(\bar{c}_s) f_{\bar{c}_n}(\bar{c}_n) d\bar{c}_s d\bar{c}_n, \tag{7}
\end{aligned}$$

where \mathcal{A} is the set of all 2^K possible binary sequences of length K . In (7), we employ the multivariate Poisson distribution function $f_{\mathbf{r}}(\mathbf{r}|\bar{c}_s, \bar{c}_n, \mathbf{s})$ and exploit the facts that the observations in different symbol intervals are independent and that RVs \bar{c}_s and \bar{c}_n are independent. Before presenting the MLMS detector as a solution of (7) in the following theorem, we introduce some auxiliary variables. For a given hypothetical sequence \mathbf{s} , let \mathcal{K}_1 and \mathcal{K}_0 denote the sets of indices k for which $s[k] = 1$ and $s[k] = 0$ holds, respectively. Additionally, for a given observation vector \mathbf{r} , we define $n_1 = \sum_{k \in \mathcal{K}_1} r[k]$ and $n_0 = \sum_{k \in \mathcal{K}_0} r[k]$.

THEOREM 1. *The non-coherent MLMS detector for ON-OFF keying modulation in diffusive MC selects a sequence whose “1” elements correspond to the k_{thr} largest elements of \mathbf{r} . Moreover, the optimal threshold k_{thr}^* is obtained as*

$$k_{\text{thr}}^* = \underset{k_{\text{thr}} \in \{0, 1, \dots, K\}}{\operatorname{argmax}} \Lambda(\mathbf{s}), \tag{8}$$

where $\Lambda(\mathbf{s})$ is the MLMS detection metric and is given by

$$\Lambda(\mathbf{s}) = \sum_{i=0}^{n_1} \binom{n_1}{i} \mathbb{E}_{\bar{c}_s} \left\{ \bar{c}_s^{n_1-i} e^{-k_{\text{thr}} \bar{c}_s} \right\} \mathbb{E}_{\bar{c}_n} \left\{ \bar{c}_n^{n_0+i} e^{-K \bar{c}_n} \right\}. \tag{9}$$

Furthermore, as $K \rightarrow \infty$, we obtain $k_{\text{thr}}^* \rightarrow \frac{K}{2}$.

PROOF. Please refer to the Appendix. \square

In other words, for MLMS detection, we may first sort all elements of \mathbf{r} in a decreasing manner in a new vector denoted by $\tilde{\mathbf{r}} = [\tilde{r}[1], \tilde{r}[2], \dots, \tilde{r}[K]]^T$, i.e., $\tilde{r}[1] \geq \tilde{r}[2] \geq \dots \geq \tilde{r}[K]$. Second, for each $k_{\text{thr}} \in \{0, 1, \dots, K\}$, we set the elements of the candidate MLMS detection sequence \mathbf{s} corresponding to the first k_{thr} elements of $\tilde{\mathbf{r}}$ to “1” and the remaining elements of \mathbf{s} to “0”. Among the $K + 1$ candidate MLMS detection sequences corresponding to $k_{\text{thr}} \in \{0, 1, \dots, K\}$, we choose that \mathbf{s} which maximizes the MLMS detection metric $\Lambda(\mathbf{s})$ given in (9).

REMARK 3. *The complexity of the proposed MLMS detector in Theorem 1 is significantly smaller than that of the original search given in (7). In particular, the complexity of the search in (7) grows exponentially in K , i.e., $|\mathcal{A}| = 2^K$, whereas the complexity of the search in Theorem 1 is linearly increasing in K , i.e., there are $K + 1$ possibilities. Furthermore, for each search step, we have to calculate metric $\Lambda(\mathbf{s})$ which is a function of the statistical CSI, but not the instantaneous CSI, since \bar{c}_s and \bar{c}_n are averaged out in $\Lambda(\mathbf{s})$, cf. (9). Moreover, all the terms in the MLMS detection metric are in the form of $\mathbb{E}_x \{x^a e^{-bx}\}$ where $x \in \{\bar{c}_s, \bar{c}_n\}$ and a and b are constants. Therefore, if these expectations for all required a and b can be computed offline, they can be stored at the receiver and used for online data detection.*

3.2 Suboptimal Detection Metric

The main challenge of the optimal detector in Theorem 1 is the calculation of the detection metric in (9). In particular, the metric in (9) is in the form of expectations over the PDF of the CSI, i.e., $f_x(x)$, $x \in \{\bar{c}_s, \bar{c}_n\}$. These PDFs depend on the considered MC environment and general analytical expressions for $f_x(x)$, $x \in \{\bar{c}_s, \bar{c}_n\}$ are not yet available in the literature. In practice, for a particular MC channel, these PDFs can be obtained using historical measurements of \bar{c}_s and \bar{c}_n . However, the historical PDFs might not lend themselves to a simple analytical form. Therefore, a common convenient approach for mathematical derivation of the detection metric in (9) is to assume a particular parametric model for $f_x(x)$ and to adjust the parameters of the model to match the simulation/experimental data. Using this approach, the parametric model for the PDF of the CSI has to satisfy the following criteria:

- The PDF $f_x(x)$ has to be supported only over the non-negative range, i.e., $f_x(x) = 0$ for $x < 0$, since \bar{c}_s and \bar{c}_n assume only non-negative values.
- A flexible parametric model is desirable such that by varying its parameters, it is able to accurately approximate the exact distribution. This goal can be achieved if PDF $f_x(x)$ has several parameters which can be adjusted for accurate approximation.
- The adopted PDF $f_x(x)$ has to be analytically tractable and, for the purpose of this paper, effectively lead to a sufficiently simple detection metric.

Considering the above criteria, we have investigated several well-known distributions, including chi-square, Nakagami, log-normal, Weibull, and Levy distributions [10], and found that the Gamma distribution, given in (10) below, is an accurate approximation of $f_x(x)$, $x \in \{\bar{c}_s, \bar{c}_n\}$, for the considered stochastic MC channel introduced in Subsection 2.3. In particular, the Gamma distribution is given by

$$f_x^{\text{gamma}}(x) = \begin{cases} \frac{\beta^\alpha x^{\alpha-1} e^{-\beta x}}{\Gamma(\alpha)}, & \text{if } x \geq 0 \\ 0, & \text{otherwise} \end{cases} \tag{10}$$

where $\Gamma(\cdot)$ is the Gamma function, and $\alpha, \beta > 0$ are the parameters of the Gamma distribution [10]. As we will show in Section 4, the Gamma distribution can effectively capture the randomness of the CSI introduced by the random variations of the underlying MC channel parameters, e.g., the flow velocity, the enzyme concentration, the diffusion coefficient, etc. Note that the terms in the detection metric in (9) are of the form $\mathbb{E}_x \{x^a e^{-bx}\}$ where $x \in \{\bar{c}_s, \bar{c}_n\}$ and a and b are constants. Therefore, using the Gamma distribution, $\mathbb{E}_x \{x^a e^{-bx}\}$ can be expressed as

$$\begin{aligned}
\mathbb{E}_x \{x^a e^{-bx}\} &= \int_{x=0}^{\infty} x^a e^{-bx} \times \frac{\beta^\alpha x^{\alpha-1} e^{-\beta x}}{\Gamma(\alpha)} dx \\
&= \frac{\beta^\alpha}{\Gamma(\alpha)} \int_{x=0}^{\infty} x^{a+\alpha-1} e^{-(b+\beta)x} dx \\
&= \frac{\beta^\alpha \Gamma(a+\alpha)}{\Gamma(\alpha)(b+\beta)^{a+\alpha}} \underbrace{\int_{x=0}^{\infty} \frac{(b+\beta)^{a+\alpha} x^{a+\alpha-1} e^{-(b+\beta)x}}{\Gamma(a+\alpha)} dx}_{=1} \\
&= \frac{\Gamma(a+\alpha)\beta^\alpha}{\Gamma(\alpha)(b+\beta)^{a+\alpha}}. \tag{11}
\end{aligned}$$

The parameters α and β have to be properly chosen such that the resulting Gamma distribution well approximates the exact distribution or the histogram of the measurement data. To this end, we adopt the weighted min square error

as a criterion to be minimized for the optimal choice of α and β . In particular, the optimal α^* and β^* are obtained as

$$(\alpha^*, \beta^*) = \underset{\alpha, \beta > 0}{\operatorname{argmin}} \int_{x=0}^{\infty} w(x) |f_x(x) - f_x^{\text{gamma}}(x)|^2 dx, \quad (12)$$

where $w(x) \geq 0$, $\forall x$, is an appropriately chosen weight function which can be used to give priority for accurate matching of a specific range of x . Using the Gamma distribution with the optimized parameters, the metric required in Theorem 1 is given in closed form based on (11).

REMARK 4. *In Section 4, we perform an exhaustive search to find the optimal α^* and β^* . However, since the feasible sets of α and β are semi-infinite, i.e., $\alpha, \beta \in (0, +\infty)$, a full search is not possible. To overcome this challenge, we first note that there exists a unique Gamma distribution $f_x^{\text{gamma}}(x)$ which has the same mean and variance as the exact distribution $f_x(x)$. The parameters of this Gamma distribution, denoted by $(\bar{\alpha}, \bar{\beta})$, as a function of the mean and the variance of the exact distribution, denoted by μ_x and σ_x^2 , respectively, are given by*

$$(\bar{\alpha}, \bar{\beta}) = \left(\frac{\mu_x^2}{\sigma_x^2}, \frac{\mu_x}{\sigma_x^2} \right). \quad (13)$$

Since the optimal parameters (α^*, β^*) are expected to lead to a Gamma distribution which has a mean and a variance that are close to those of the exact distribution, we can efficiently limit the search to intervals $\alpha \in [(1 - \delta)\bar{\alpha}, (1 + \delta)\bar{\alpha}]$ and $\beta \in [(1 - \delta)\bar{\beta}, (1 + \delta)\bar{\beta}]$, where $\delta \geq 0$ determines how large the search intervals are.

3.3 Suboptimal Detector Based on Blind CSI Estimation

The optimal MLMS detector requires *statistical* knowledge of the CSI which might be difficult to be acquired for some practical MC systems. Therefore, in the following, we propose a suboptimal detector which does not need statistical CSI knowledge. The main idea behind the simple detector which we propose in this subsection is to first estimate the CSI based on the symbols in the detection block in order to approximate the optimal ML threshold which is denoted by $\xi_{\text{BL}}^{\text{ML}}$. Subsequently, symbol-by-symbol detection can be performed based on the approximated threshold $\xi_{\text{BL}}^{\text{ML}}$. We note that the channel estimator is blind since no training sequence is used.

For a given observation block \mathbf{r} , let $\tilde{\mathcal{K}}_1$ ($\tilde{\mathcal{K}}_0$) denote the sets of indices k for the $\lceil \frac{K}{2} \rceil$ -th largest ($\lfloor \frac{K}{2} \rfloor$ -th smallest) $r[k]$ in the block. The proposed suboptimal detector is formally presented in the following.

Proposed Blind ML-Based Detector: *The proposed blind ML-based detector for ON-OFF keying modulation in diffusive MC is given by*

$$\hat{s}_{\text{BL}}^{\text{ML}}[k] = \begin{cases} 1, & \text{if } r[k] \geq \xi_{\text{BL}}^{\text{ML}} \\ 0, & \text{otherwise} \end{cases} \quad (14)$$

where $\xi_{\text{BL}}^{\text{ML}} = \frac{\hat{c}_s}{\ln(1 + \frac{\hat{c}_s}{\hat{c}_n})}$ is the blind detection threshold. Hereby,

the CIR estimates \hat{c}_s and \hat{c}_n are obtained as

$$\hat{c}_s = \frac{1}{\lceil \frac{K}{2} \rceil} \sum_{k \in \tilde{\mathcal{K}}_1} [r[k] - \hat{c}_n] \quad (15a)$$

$$\hat{c}_n = \frac{1}{\lfloor \frac{K}{2} \rfloor} \sum_{k \in \tilde{\mathcal{K}}_0} r[k]. \quad (15b)$$

Table 1: Default Values of the Numerical Parameters [4, 15].

Variable	Definition	Value
N^{rx}	Number of released molecules	10^4 molecules
V^{rx}	Receiver volume	$\frac{4}{3}\pi 50^3 \text{ nm}^3$ (a sphere with radius 50 nm)
r	Distance between the transmitter and the receiver	500 nm
D	Diffusion coefficient for the signaling molecule	$4.365 \times 10^{-10} \text{ m}^2 \cdot \text{s}^{-1}$
\bar{c}_e	Enzyme concentration	$10^7 \text{ molecule} \cdot \mu\text{m}^{-3}$ (approx. 1.66 micromolar)
κ	Rate of molecule degradation reaction	$2 \times 10^{-19} \text{ m}^3 \cdot \text{molecule}^{-1} \cdot \text{s}^{-1}$
$(v_{\parallel}, v_{\perp})$	Components of flow velocity	$(10^{-3}, 10^{-3}) \text{ m} \cdot \text{s}^{-1}$

The CSI estimates \hat{c}_s and \hat{c}_n in (15) correspond to simple averaging over the expected positions of $s[k] = 1$ and $s[k] = 0$, respectively. Since the noise molecules are always present whereas the signal molecules are present only when $s[k] = 1$ holds, the *expected* number of molecules observed at the receiver in positions with $s[k] = 1$ is higher than that in positions with $s[k] = 0$. Based on this fact and since $s[k] = 1$ and $s[k] = 0$ are equiprobable, we assume that the $\lceil \frac{K}{2} \rceil$ -th largest elements of \mathbf{r} correspond to $s[k] = 1$ and the remaining elements ($\lfloor \frac{K}{2} \rfloor$ -th smallest elements of \mathbf{r}) correspond to $s[k] = 0$. Thus, we first compute \hat{c}_n directly from (15b) and then calculate \hat{c}_s from (15a). Having the estimated CSI (\hat{c}_s, \hat{c}_n) , we then compute the ML threshold $\xi_{\text{BL}}^{\text{ML}}$ and perform the ML detection based on (14).

4. NUMERICAL RESULTS

In this section, we first present the considered stochastic MC channel and the adopted system parameters. Subsequently, we use this model to evaluate the performances of the optimal and suboptimal detectors.

4.1 Stochastic MC Channel Model

We assume the stochastic MC channel model introduced in Subsection 2.3. We use this channel model to obtain the “true” distribution of the CSI and to verify the effectiveness of the proposed Gamma distribution to approximate the true distribution. However, we emphasize that the proposed detection framework is not limited to the transmitter, channel, and receiver models presented in Subsection 2.3. The default values of the channel parameters are given in Table 1. We allow random variations of channel parameters D , v_{\parallel} , v_{\perp} , and \bar{c}_e . To this end, we consider the following three scenarios: Scenario 1: $(D, \sigma_{v_{\parallel}}, \sigma_{v_{\perp}}, \sigma_{\bar{c}_e}) = (0.1, 0.5, 0.5, 0.1)$, Scenario 2: $(D, \sigma_{v_{\parallel}}, \sigma_{v_{\perp}}, \sigma_{\bar{c}_e}) = (0.2, 1, 1.5, 0.1)$, and Scenario 3: $(D, \sigma_{v_{\parallel}}, \sigma_{v_{\perp}}, \sigma_{\bar{c}_e}) = (0.1, 1.5, 0.5, 0.2)$.

In the simulation results provided in the following, we assume that the variation of the mean of the noise \bar{c}_n is modeled similarly as the variation of the mean \bar{c}_s . In particular, we assume $\bar{c}_n \sim \text{SNR}^{-1} \bar{c}_s$ where $\text{SNR} = \frac{\mathbb{E}_{\bar{c}_s} \{\bar{c}_s\}}{\mathbb{E}_{\bar{c}_n} \{\bar{c}_n\}}$ is a constant analogous to the signal-to-noise ratio (SNR) in conventional wireless systems. Furthermore, if $\bar{c}_s \sim \text{Gamma}(\alpha, \beta)$ holds, we obtain $\bar{c}_n \sim \text{Gamma}(\alpha, \text{SNR}\beta)$ [10]. Hereby, we keep the mean of the noise fixed and change the number of molecules released by the transmitter to obtain different SNRs.

REMARK 5. *We note that the non-coherent detector in [12] was designed assuming an additive white Gaussian noise (AWGN) channel model. As discussed in Subsection 2.1, the Poisson distribution for the observed number of molecules at the receiver is a more accurate model for the diffusive MC channel than the Gaussian distribution. Additionally, the signal model assumed in [12] is different from that considered in this paper. Therefore, we have not included the detection*

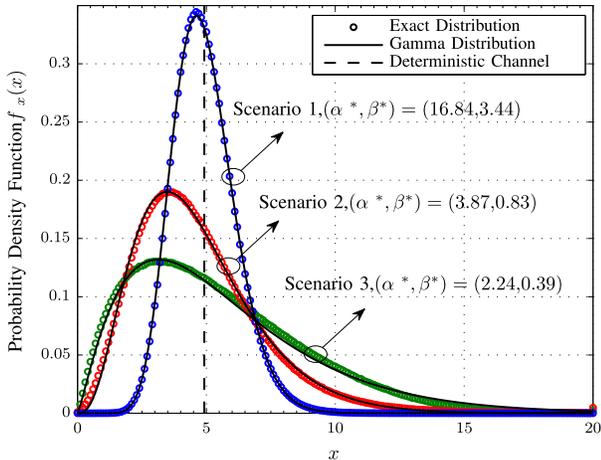


Figure 2: The exact PDF and the approximated Gamma PDF for Scenarios 1-3.

scheme in [12] as a benchmark in this section as a direct comparison would not be fair.

4.2 Performance Evaluation

Fig. 2 shows the exact PDF obtained by Monte Carlo simulation of the CSI, \bar{c}_s , and the approximated Gamma PDF for the three considered stochastic scenarios. Additionally, the result for the case when all the underlying channel parameters in (4) assume their nominal values given in Table 1, i.e., the channel is deterministic, is shown. The optimal parameters of the Gamma distribution are also shown in Fig. 2 and found using the search procedure presented in Subsection 3.2 and Remark 4 with $w(x) = 1, \forall x$, and $\delta = 0.5$. We observe a perfect match between the true PDF and the approximated Gamma PDF for all three scenarios. Moreover, we observe that as the underlying channel parameters become more random, i.e., Scenario 3 compared to Scenario 1, the mean of the CSI decreases and its variance increases.

In Fig. 3, we show the bit error rate (BER) versus the length of the detection block K for the three considered scenarios and SNR = 10 dB. As a lower bound on the BERs of the proposed detectors, we include the coherent ML detector which requires perfect CSI. Note that the actual CSI in (4) is used for simulation whereas the approximated Gamma distribution is employed to calculate the selection metric for the proposed MLMS detector in (9) by using (11). We observe from Fig. 3 that the BERs of the proposed optimal and suboptimal detectors converge to the lower bound as $K \rightarrow \infty$. Furthermore, the gap between the BER of the MLMS detector and the lower bound is small for reasonably large K , which reveals the effectiveness of the optimal MLMS detector, although no resources are spent for training and CSI acquisition. The gap between the BER of the proposed optimal MLMS detector and the proposed suboptimal detector decreases for larger values of K and also from Scenario 1 to Scenario 3.

In Fig. 4, we plot the BER versus the SNR in dB for Scenario 2 and $K \in \{6, 10, 20\}$. In this figure, we observe that as the SNR increases, the BER improves for all considered detectors. We note that as SNR $\rightarrow \infty$, the BER of the proposed suboptimal detector saturates to a certain error floor. This is due to the fact that for the *blind* CSI estimator in (15), we assumed that the percentages of the ones and the zeros in a given detection block are exactly 50% which is not always

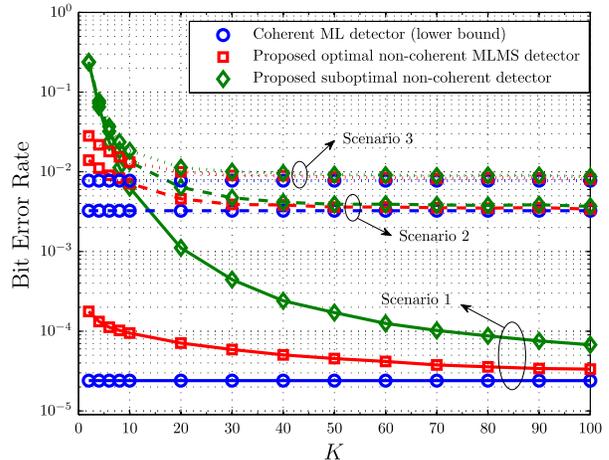


Figure 3: Bit error rate versus the length of the detection block for Scenarios 1-3 and SNR = 10 dB.

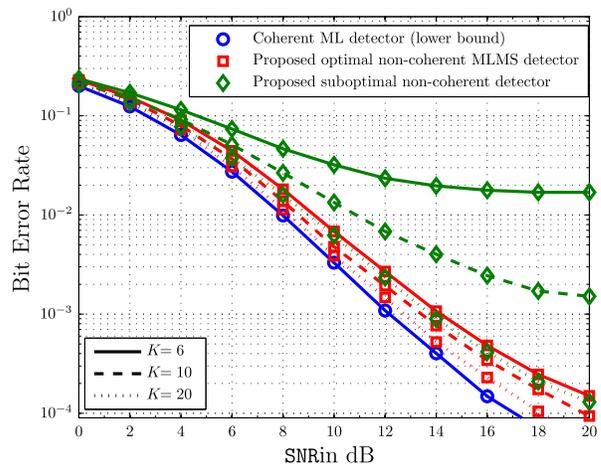


Figure 4: Bit error rate versus the SNR in dB for Scenario 2 and $K \in \{6, 10, 20\}$.

true especially for small values of K . This introduces an inherent CSI estimation error and leads to the aforementioned error floor for the proposed suboptimal detector. Note that as K increases, the BER of the proposed optimal detector decreases and approaches the lower bound. We can also observe from Fig. 4 that the proposed optimal MLMS detector outperforms the proposed suboptimal detector particularly for small K , but the gap between the BERs of these two detectors decreases as K increases.

5. CONCLUSIONS

We have derived the optimal non-coherent multiple-symbol detector which does not require instantaneous CSI knowledge. In order to alleviate the complexity of the proposed optimal detector, we also developed an approximate detection metric and a low-complexity suboptimal detector. Numerical results showed that the proposed optimal detector outperformed the suboptimal detector, particularly for small detection block lengths. However, as the length of the detection block increases, the performances of the proposed optimal and suboptimal detectors converge to that of the baseline scheme which requires perfect CSI. This demonstrates

the effectiveness of the proposed detection schemes.

APPENDIX

Using sets \mathcal{K}_1 and \mathcal{K}_0 , (7) can be simplified to

$$\mathbf{s}^{\text{MLMS}} = \underset{\mathbf{s} \in \mathcal{A}}{\text{argmax}} \int_{\bar{c}_s \geq 0} \int_{\bar{c}_n \geq 0} (\bar{c}_s + \bar{c}_n)^{\sum_{k \in \mathcal{K}_1} r[k]} \bar{c}_n^{\sum_{k \in \mathcal{K}_0} r[k]} \exp(-|\mathcal{K}_1| \bar{c}_s - K \bar{c}_n) f_{(\bar{c}_s, \bar{c}_n)}(\bar{c}_s, \bar{c}_n) d\bar{c}_s d\bar{c}_n, \quad (16)$$

where the term $r[k]!$ in (7) is removed in (16) since it does not affect the MLMS detection result. Moreover, the MLMS detector can be written equivalently in expectation form as

$$\mathbf{s}^{\text{MLMS}} = \underset{\mathbf{s} \in \mathcal{A}}{\text{argmax}} \mathbb{E}_{(\bar{c}_s, \bar{c}_n)} \left\{ \underbrace{(\bar{c}_s + \bar{c}_n)^{\sum_{k \in \mathcal{K}_1} r[k]} \bar{c}_n^{\sum_{k \in \mathcal{K}_0} r[k]}}_{A(\mathbf{s})} \times \underbrace{\exp(-|\mathcal{K}_1| \bar{c}_s - K \bar{c}_n)}_{B(\mathbf{s})} \right\}. \quad (17)$$

We can conclude the following properties from the MLMS detection metric $\Lambda(\mathbf{s}) = \mathbb{E}_{(\bar{c}_s, \bar{c}_n)} \{A(\mathbf{s})B(\mathbf{s})\}$. First, with respect to the data sequence \mathbf{s} , term $B(\mathbf{s})$ is only a function of the number of ones in \mathbf{s} . Second, for a given number of ones in \mathbf{s} , term $A(\mathbf{s})$ is maximized if the ones in \mathbf{s} correspond to the largest elements of the observation vector \mathbf{r} . Note that these two properties hold for any given CSI (\bar{c}_s, \bar{c}_n) . Hence, they also hold after the expectation operation with respect to (\bar{c}_s, \bar{c}_n) , i.e., $\mathbb{E}_{(\bar{c}_s, \bar{c}_n)} \{A(\mathbf{s})B(\mathbf{s})\}$. Therefore, we can avoid searching over all $\mathbf{s} \in \mathcal{A}$, and instead, find the optimal threshold $k_{\text{thr}} \in \{0, 1, \dots, K\}$ which sets the elements of \mathbf{s} corresponding to the k_{thr} -th largest elements of \mathbf{r} to one and the remaining elements to zero. Moreover, we can further simplify the MLMS detection metric in (17) as

$$\Lambda(\mathbf{s}) \stackrel{(a)}{=} \mathbb{E}_{(\bar{c}_s, \bar{c}_n)} \left\{ \left[\sum_{i=0}^{n_1} \binom{n_1}{i} \bar{c}_s^{n_1-i} \bar{c}_n^i \right] \bar{c}_n^{n_0} \exp(-|\mathcal{K}_1| \bar{c}_s - K \bar{c}_n) \right\} \\ \stackrel{(b)}{=} \sum_{i=0}^{n_1} \binom{n_1}{i} \mathbb{E}_{\bar{c}_s} \left\{ \bar{c}_s^{n_1-i} e^{-k_{\text{thr}} \bar{c}_s} \right\} \mathbb{E}_{\bar{c}_n} \left\{ \bar{c}_n^{n_0+i} e^{-K \bar{c}_n} \right\}, \quad (18)$$

where in equality (a), we employ the Binomial expansion and in equality (b), we use $k_{\text{thr}} = |\mathcal{K}_1|$ and the assumption that RVs \bar{c}_s and \bar{c}_n are independent. The MLMS detection metric in (18) is given in Theorem 1 in both expectation and integration forms. Furthermore, recalling that $\Pr\{s[k] = 1\} = \Pr\{s[k] = 0\} = 0.5$ holds, the optimal threshold k_{thr}^* approaches $K/2$ as $K \rightarrow \infty$. This concludes the proof.

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