Error Probability Optimization for Non-Orthogonal Multiple Access in DBMC Networks

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***Abstract*—Non-orthogonal multiple access (NOMA) represents a promising option for differentiating multiple transmitters using only a single molecule type in a future diffusion-based molecular communication (DBMC) network. This paper addresses the bit error probability optimization of a DBMC-NOMA network with bio-nano-machines incapable of complex computations for classical optimization methods. We propose a pilot-symbol-based algorithm to approximate the optimal detection threshold and emitted number of transmitter molecules. Our solution is based on two algorithms for the separate optimization of thresholds and the number of molecules, which are applied alternatingly. Our Monte-Carlo simulation results show that the algorithm reliably approaches the global optimum parameter values regardless of initial values and signaling-molecule-to-noise ratio. Since it is composed of only a few basic operations, such as comparisons and additions, there is potential for an implementation using stochastic chemical reaction networks in future work.**

***Index Terms*—Molecular communication, non-orthogonal multiple access, optimization algorithm, bit error probability**

I. Introduction

DIFFUSION-BASED molecular communication (DBMC) is envisioned to play a significant role in nanoscale and biological communication networks due to its advantages over electromagnetic communication with respect to bio-compatibility, size constraints, and energy efficiency. To enable complex use cases such as targeted drug delivery and other advanced medical applications in a future internet of bio-nano-things (IoBNT) [1], bio-nano-machines (BNMs) must be able to cooperate and communicate. Individual BNMs are expected to perform only simple tasks such as emission of and reaction to surrounding molecules [1]. One step towards the communication between a large number of BNMs is enabling multiple access (MA). Multiple approaches to MA for DBMC have been investigated, such as time-division, molecule-division, and non-orthogonal multiple access (NOMA). NOMA based on successive interference cancellation (SIC) was proposed as an option for DBMC networks since it allows for concurrent transmission from multiple transmitters (TXs) to a receiver (RX) using a single molecule type [2]. DBMC-NOMA was shown to match the performance of orthogonal schemes like molecule-division MA for the optimal choice of communication parameters [3]. Therefore, optimizing the system to achieve the lowest possible bit error probability (BEP) is crucial, but in [3] only an exhaustive search of the analytical formula was considered. Related work on parameter optimization for DBMC networks exists, for example, also focused on analytical solutions [4], or using global optimization algorithms like gradient descent optimization [5], or data-driven machine learning (ML) approaches [6]. While these methods reliably achieve the optimum value, they could be infeasible in an IoBNT framework, where we have to optimize parameters on low-capability BNMs. Stochastic chemical reaction networks have been proposed to capture the resulting constraints on possible computation procedures in DBMC systems more accurately, and implement simple heuristic methods based on pilot symbols and thresholds [7].

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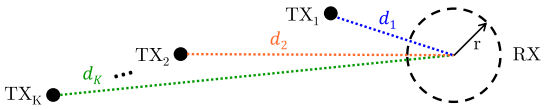

Fig. 1. DBMC scenario with K point transmitters at distances d_1, d_2 ... d_K from a spherical receiver.

In this paper, we propose a pilot-symbol-based heuristic optimization algorithm targeted towards the BEP minimization in a DBMC network using NOMA. In contrast to previous work on NOMA for DBMC in [2], [3] that assumes accurate channel estimation to facilitate SIC, we frame the SIC procedure as threshold detection with multiple thresholds per TX. This allows for simple systematic optimization without explicit channel estimation. The presented algorithm alternatingly adjusts the detection threshold and emitted number of molecules per TX across multiple iterations based on decision rules derived from the mechanisms behind NOMA in a DBMC network found in [3]. The algorithm works without any knowledge of initial values or the underlying analytical function and its derivatives as opposed to analytical or gradient descent methods in previous work [4], [5]. Additionally, considering the limited capabilities of future BNMs, the algorithm uses only elementary operations as opposed to ML methods, which rely on large computational power [6]. We investigate the convergence of the algorithm for different choices of initial values and different levels of background noise. Lastly, we investigate its robustness to changes in channel conditions during run-time.

II. System Model

Figure 1 depicts a communication scenario with K TXs TX_i at distances $d_1 \leq d_2 \leq \cdots \leq d_K$ from a central spherical, passive RX with radius r. The TXs are modeled as points emitting instantaneous pulses of molecules. The received signal $n_{\mathrm{RX}}(t)$ is the number of molecules within the RX volume at time t. With $N_{\mathrm{TX},i}$, the number of molecules

emitted by TX_i per pulse, V_{RX}, the RX volume, and the diffusion coefficient D, the impulse response between one TX_i and the RX can be modeled as a Poisson-distributed random variable $n_{\mathrm{RX}}(t) \sim \mathcal{P}(\lambda_i(t))$ [8] with time-varying mean

$$\lambda_i(t) = \frac{N_{\mathrm{TX},i} V_{\mathrm{RX}}}{(4\pi D t)^{\frac{3}{2}}} \exp\left(-\frac{d_i^2}{4Dt}\right). \tag{1}$$

Eq. (1) is valid under the uniform concentration assumption [8], and if $n_{\mathrm{RX}}(t)$ is sufficiently small in comparison to a sufficiently large $N_{\mathrm{TX},i}$ [9]. If additionally $\lambda_i(t)$ is sufficiently large, the received signal can be further approximated by a Gaussian distribution $n_{\mathrm{RX}}(t) \sim \mathcal{N}(\mu_i, \sigma_i^2)$ with mean $\mu_i(t) = \lambda_i(t)$ and variance $\sigma_i^2(t) = \lambda_i(t)$ [9].

The TXs use on-off-keying, where a pulse of $N_{\mathrm{TX},i}$ molecules is emitted for a '1' and nothing for a '0' with both symbols equally likely. The emitted number of molecules is limited by a maximum molecule budget $N_{\mathrm{TX,max}}$ per symbol per TX. We assume that the system is fully synchronized and that the symbol period T is sufficiently large such that inter-symbol interference (ISI) is negligible. Therefore, we consider only the current symbol, where all TX_i send a pulse of $s_i N_{\mathrm{TX},i}$ molecules at $t = 0$, with the symbol from TX_i denoted by $s_i \in \{0, 1\}$. For decoding, the RX takes one sample per time slot at the peak time t_{p} of the received signal.

In this paper, we implement the DBMC-NOMA scheme described in [3]. Therefore, with respect to the current time slot, all TXs transmit simultaneously using the same molecule type. The overall received signal at t_{p} is a sum of multiple independent random variables. For Poisson variables, the sum can be modeled as a single Poisson distribution with combined mean and variance $\lambda_{\mathrm{NOMA}} = \lambda_{\mathrm{n}} + \sum_{i=1}^{K} s_i \lambda_i(t_{\mathrm{p}})$, where $\lambda_i(t_{\mathrm{p}})$ represents the expected value of the contribution from TX_i and λ_{n} is an additive noise term. The sample at the RX is a realization of the Poisson distribution $n_{\mathrm{s}} \sim \mathcal{P}(\lambda_{\mathrm{NOMA}})$.

To differentiate the symbols from each TX at the RX, successive interference cancellation (SIC) is used. TXs are considered for detection by the RX one by one from the highest expected signal value $\lambda_i(t_{\mathrm{p}})$ to the lowest. Going forward, we assume that the TX indexing is ordered according to the values of $\lambda_i(t_{\mathrm{p}})$, i.e., $\lambda_1(t_{\mathrm{p}}) \geq \lambda_2(t_{\mathrm{p}}) \geq \cdots \geq \lambda_K(t_{\mathrm{p}})$. Usually, for NOMA in classical communications as well as for DBMC, it is assumed that the contribution of the currently considered TX to the received signal is removed from the sample value n_{s} after each detection using channel estimation information [3]. In this paper, we propose to model SIC as threshold detection with multiple thresholds per TX instead. To detect the symbol sent by TX_i, the RX employs threshold detection on the sample n_{s} with the decision rule

$$\hat{s}_i = \begin{cases} 1 & n_{\mathrm{s}} \geq \tau_i^{\underline{\hat{s}}_{i-1}} \\ 0 & n_{\mathrm{s}} < \tau_i^{\underline{\hat{s}}_{i-1}} \end{cases}, \tag{2}$$

where $\hat{s}_i$ is the detected symbol for TX_i, and $\underline{\hat{s}}_{i-1} = [\hat{s}_1, \ldots, \hat{s}_{i-1}]$ is the vector of all previously detected symbols for the TXs up to and including TX_{i-1}. Thereby, we end up with a set $\mathcal{T}_i = [\tau_i^{0\ldots000}, \tau_i^{0\ldots001}, \tau_i^{0\ldots010}, \ldots, \tau_i^{1\ldots110}, \tau_i^{1\ldots111}]$ of 2^{i-1} different possible thresholds for TX_i.

We will evaluate the performance of the network using the system bit error probability (BEP), i.e., the average BEP across all TXs, denoted as $P_{\mathrm{e,sys}}$, derived for a DBMC-NOMA system in [3]. For the sake of the scalability of our Monte Carlo simulations (MCSs), we approximate the Poisson distribution with the Gaussian as described at the beginning of the section. Otherwise, the calculations are exactly the same. To introduce the notion of channel quality and noise, we use the signaling-molecule-to-noise ratio (SNR): $\mathrm{SNR} = \frac{\max_i \lambda_i(t_{\mathrm{p}})}{\lambda_n}$.

III. Pilot-Symbol-Based BEP Optimization

The BEP of a DBMC-NOMA system depends on many different parameters. The detection thresholds and the emitted number of molecules from each TX are two primary factors due to their effect on the detection performance and the received number of molecules, respectively, as shown in [3]. Therefore, we will also focus on the optimal choice of detection thresholds $\tau_i^{\underline{\hat{s}}_{i-1}}$ and the emitted number of molecules $N_{\mathrm{TX},i}$ for the proposed algorithms.

Analytical solutions and global optimization algorithms [3]–[5] can often lead us to the optimal values. However, these methods require capabilities from the nodes in the network, such as accurate channel estimation, storage of pre-computed solutions, or computation of functions or their derivatives, for example, for a gradient descent algorithm. Compared to the current and even future capabilities of synthetic cells that will act as BNMs in DBMC networks, these tasks are very complex. Therefore, we aim to find possibly greedy heuristics that rely on simpler operations. Previously, pilot-symbol-based approaches have been shown to work together with stochastic chemical reaction networks to approximate a real-world implementation of DBMC using simple operations like threshold comparisons [7].

We propose pilot-symbol-based optimization algorithms, first separately for the detection thresholds and the number of molecules. Ultimately, we combine the two for a joint optimization of the BEP in a DBMC-NOMA system. In the following, for the sake of brevity and simplicity of the depicted algorithms, we will assume a network with 2 TXs, i.e., $K = 2$.

A. Optimizing the Detection Thresholds

For the design of the algorithm optimizing the detection thresholds, we assume that the number of molecules $N_{\mathrm{TX},i}$ is static. The scheme is based on a sequence of pilot symbols from $\mathcal{S}_{\mathrm{pilot}} = \{\underline{s} = [s_1 s_2]; s_j \in \{0, 1\}\}$, which is known to both TXs and the RX. As with the DBMC-NOMA scheme, all symbols in each pilot symbol vector $\underline{s}$ are sent simultaneously from all TXs. Starting from a set of initial values $\left[\tau_{1,\mathrm{init}}, \tau_{2,\mathrm{init}}^0, \tau_{2,\mathrm{init}}^1\right]$, the thresholds are adjusted after the transmission, sampling, and decoding of a pilot symbol $\underline{s}$ as defined in Section II. The detected symbols are then compared to the correct symbols in the pilot sequence. If the symbol is detected correctly, the threshold stays the same. If the symbol is incorrectly detected as a '1', the threshold is increased to make the detection of a '0' more likely. Consequently, the threshold is decreased for a symbol incorrectly detected as '0'. Note that for a certain pilot symbol vector $\underline{s}$, only the applicable threshold is altered for TX_2, for example, τ_2^1 in the case $s_1 = 1$. Importantly, we apply $\tau_2^{s_1}$ for the detection of

$\hat{s}_2$ based on the pilot symbol s_1, not the detected symbol $\hat{s}_1$. Thereby, for the purposes of the threshold optimization, we assume correct detection for all previous TXs. The scheme is described in detail in Algorithm 1.

Algorithm 1 Detection Threshold Optimization Algorithm

INPUT: $\tau_1, \tau_2^0, \tau_2^1$
for $i = 1$ to $\mathrm{N_{pilot}}$ **do**
  CHOOSE: $\underline{s} \leftarrow [s_1, s_2] \in \mathcal{S}_{\mathrm{pilot}}$
  TRANSMIT: $\mathrm{TX}_1 \rightarrow s_1 N_{\mathrm{TX},1}$, $\mathrm{TX}_2 \rightarrow s_2 N_{\mathrm{TX},2}$
  RECEIVE: $n_{\mathrm{s}} \leftarrow n_{\mathrm{RX}}(t_{\mathrm{p}}) \sim \mathcal{N}(\lambda_{\mathrm{NOMA}}, \lambda_{\mathrm{NOMA}})$
  DECODE TX_1: Use τ_1 to obtain $\hat{s}_1$, Eq. (2)
  if $\hat{s}_1 \neq s_1$ **AND** $s_1 = 0$ **then**
    $\tau_1 \leftarrow \tau_1 + \Delta\tau$
  else if $\hat{s}_1 \neq s_1$ **AND** $s_1 = 1$ **then**
    $\tau_1 \leftarrow \tau_1 - \Delta\tau$
  DECODE TX_2: Use $\tau_2^{s_1}$ to obtain $\hat{s}_2$, Eq. (2)
  if $\hat{s}_2 \neq s_2$ **AND** $s_2 = 0$ **then**
    $\tau_2^{s_1} \leftarrow \tau_2^{s_1} + \Delta\tau$
  else if $\hat{s}_2 \neq s_2$ **AND** $s_2 = 1$ **then**
    $\tau_2^{s_1} \leftarrow \tau_2^{s_1} - \Delta\tau$
OUTPUT: $\tau_1, \tau_2^0, \tau_2^1$

B. Optimizing the Emitted Number of Molecules

Similarly to Algorithm 1, we now assume that the detection thresholds are static and the number of molecules is adjusted based on the transmission, sampling, and decoding of a pilot sequence known to both TXs and RX. Here, we assume to know the order in which the RX will decode the TXs and, therefore, also the order of the magnitude of their contribution λ_i to the received signal. This could, for example, be achieved by a preliminary step involving pilot symbols from each TX with a specified amplitude to order them at the RX. As a result, it is possible to assign the maximum molecule budget per TX $N_{\mathrm{TX,max}}$ as $N_{\mathrm{TX},1}$ and focus on optimizing $N_{\mathrm{TX},2}$ relative to that maximum starting from an initial value $N_{\mathrm{TX,init}}$. After detecting the symbols from both TXs, we propose to use a set of decision rules determining the adjustment of $N_{\mathrm{TX},2}$. Firstly, there is only a reason for changing $N_{\mathrm{TX},2}$, if $s_2 = 1$. Otherwise it stays the same. If $s_2 = 1$, we will now describe two example cases to illustrate the rationale behind the decision rules. If $\hat{s}_1 \neq s_1 = 0$, and $\hat{s}_2 = s_2 = 1$, this means that we should decrease $N_{\mathrm{TX},2}$ since we observed enough molecules to classify $s_2 = 1$, but there were too many molecules such that we incorrectly crossed the threshold for TX_1. If $\hat{s}_1 = s_1 = 0$, and $\hat{s}_2 \neq s_2 = 1$, it means that we should increase $N_{\mathrm{TX},2}$ since we incorrectly did not observe enough molecules to cross the threshold for TX_2, but the detection for TX_1 is still not affected by too much interference from TX_2. We make one important additional assumption: there is a feedback mechanism from the RX back to the TX_2 to communicate the necessary adjustment, for example, via a separate control signaling molecule, which we do not explicitly model. The details of the scheme can be found in Algorithm 2.

C. Alternating Joint Optimization of the BEP

Given Algorithm 1 and Algorithm 2, we need either knowledge of the optimal number of molecules or detection thresholds, respectively, to arrive at the joint optimal solution. Therefore, we propose a joint BEP optimization scheme in Algorithm 3 based on alternating between Algorithms 1 and 2 using arbitrary initial values for both detection thresholds and number of molecules. Both partial optimization algorithms are run once for $\mathrm{N_{pilot}}$ pilot symbols, and this is repeated for $\mathrm{N_{iter}}$ iterations. After each set of pilot symbols, the algorithm output is used as the input for the other algorithm.

Algorithm 2 Number of Molecules Optimization Algorithm

INPUT: $N_{\mathrm{TX},2}$
for $i = 1$ to $\mathrm{N_{pilot}}$ **do**
  CHOOSE: $\underline{s} \leftarrow [s_1, s_2] \in \mathcal{S}_{\mathrm{pilot}}$
  TRANSMIT: $\mathrm{TX}_1 \rightarrow s_1 N_{\mathrm{TX},1}$, $\mathrm{TX}_2 \rightarrow s_2 N_{\mathrm{TX},2}$
  RECEIVE: $n_{\mathrm{s}} \leftarrow n_{\mathrm{RX}}(t_{\mathrm{p}}) \sim \mathcal{N}(\lambda_{\mathrm{NOMA}}, \lambda_{\mathrm{NOMA}})$
  DECODE TX_1: Use τ_1 to obtain $\hat{s}_1$, Eq. (2)
  DECODE TX_2: Use $\tau_2^{s_1}$ to obtain $\hat{s}_2$, Eq. (2)
  if $s_2 = 1$ **then**
    if $s_1 = 0$ **AND** $\hat{s}_1 \neq s_1$ **AND** $\hat{s}_2 = s_2$ **then**
      $N_{\mathrm{TX},2} \leftarrow N_{\mathrm{TX},2} \cdot (1 - \alpha_N)$
    if [$s_1 = 0$ **AND** $\hat{s}_1 = s_1$ **AND** $\hat{s}_2 \neq s_2$]
      OR [$s_1 = 1$ **AND** $\hat{s}_1 \neq s_1$ **AND** $\hat{s}_2 \neq s_2$]
      OR [$s_1 = 1$ **AND** $\hat{s}_1 = s_1$ **AND** $\hat{s}_2 \neq s_2$] **then**
      $N_{\mathrm{TX},2} \leftarrow N_{\mathrm{TX},2} \cdot (1 + \alpha_N)$
OUTPUT: $N_{\mathrm{TX},2}$

Algorithm 3 Joint BEP Optimization Algorithm

INITIALIZE $\left[\tau_1[0], \tau_2^0[0], \tau_2^1[0]\right] \leftarrow [\tau_{1,\mathrm{init}}, \tau_{2,\mathrm{init}}^0, \tau_{2,\mathrm{init}}^1] = \underline{\tau}_{\mathrm{init}}$
$N_{\mathrm{TX},1} \leftarrow N_{\mathrm{TX,max}}, N_{\mathrm{TX},2}[0] \leftarrow N_{\mathrm{TX,init}}$
for $it = 1$ to $\mathrm{N_{iter}}$ **do**
  RUN: **Algorithm 1** for $\mathrm{N_{pilot}}$ symbols
    INPUT: $\tau_1[it-1], \tau_2^0[it-1], \tau_2^1[it-1]$
    OUTPUT: $\tau_1[it], \tau_2^0[it], \tau_2^1[it]$
  RUN: **Algorithm 2** for $\mathrm{N_{pilot}}$ symbols
    INPUT: $N_{\mathrm{TX},2}[it-1]$
    OUTPUT: $N_{\mathrm{TX},2}[it]$

IV. Numerical Results

In the following, the proposed algorithm will be evaluated using Monte Carlo simulations (MCSs) based on the Gaussian stochastic channel model described in Section II. The optimization process with $\mathrm{N_{iter}}$ iterations of Algorithm 3 is repeated 100 times. An overview of the simulation parameters can be found in Table I.

Firstly, Figure 2 depicts the development of all parameters for two choices of the initial number of molecules, either $N_{\mathrm{TX,init}} = 1$ or $N_{\mathrm{TX,init}} = N_{\mathrm{TX,max}} = 10^6$. The results show that the BEP is reliably optimized without any knowledge of the current or optimal BEP itself. There is a convergence towards the optimal parameters τ_i^{s*}, $N_{\mathrm{TX},2}^*$ (obtained separately via exhaustive search) and therefore also the optimal BEP, $P_{\mathrm{e,sys}}^*$. Additionally, the difference for an initial value at either end of the applicable spectrum is visible but does not disturb

TABLE I

Parameter	Symbol	Values (Default)
TX distances	$\{d_1, d_2\}$	$\{\underline{10}, 11, 12\}$ µm
RX radius	r	1 µm
Diffusion coefficient	D	$10^{-9}\,\mathrm{m^2\,s^{-1}}$
Signaling-molecule-to-noise ratio	SNR	$\{\underline{\infty}, 3.16\}$
Molecule budget per TX	$N_{\mathrm{TX,max}}$	10^6 molecules
Number of pilot symbols	N_{pilot}	1000
Number of iterations	N_{iter}	1000
Threshold step	$\Delta\tau$	1 molecule
Number of molecules multiplier	α_N	0.1
Initial thresholds	$\underline{\tau}_{\mathrm{init}}$	$[1, 1, 1]$ molecules
Initial number of molecules	$N_{\mathrm{TX,init}}$	$\{1, \underline{10^6}\}$ molecules

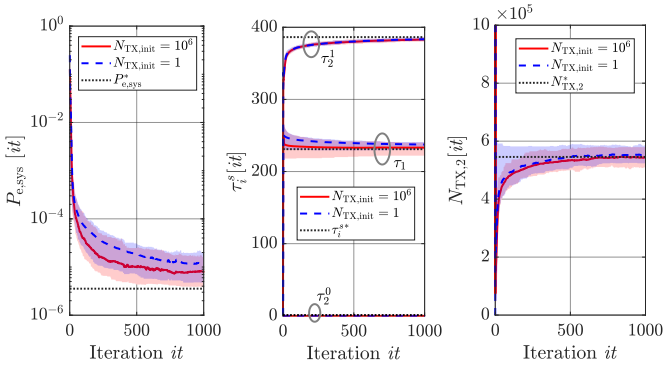

Fig. 2. Performance of Algorithm 3 for two choices of initial value $N_{\mathrm{TX,init}}$. Median (bold line) and 5th–95th percentile (shaded area) of bit error probability $P_{\mathrm{e,sys}}$, detection thresholds τ_i^s, and emitted number of molecules from TX_2 $N_{\mathrm{TX},2}$ shown across 1000 iterations repeated 100 times.

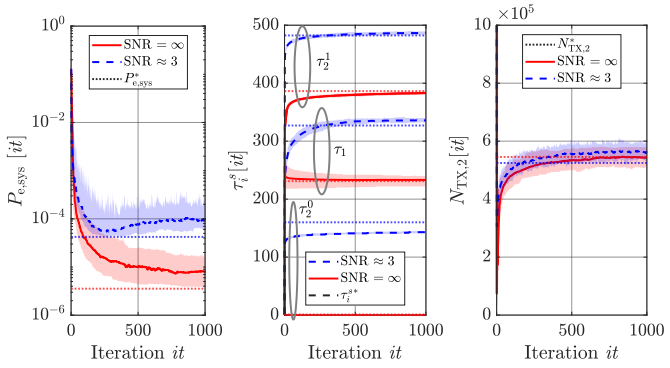

Fig. 3. Performance of Algorithm 3 for two different values of SNR. Median (bold line) and 5th–95th percentile (shaded area) of bit error probability $P_{\mathrm{e,sys}}$, detection thresholds τ_i^s, and emitted number of molecules from TX_2 $N_{\mathrm{TX},2}$ shown across 1000 iterations repeated 100 times.

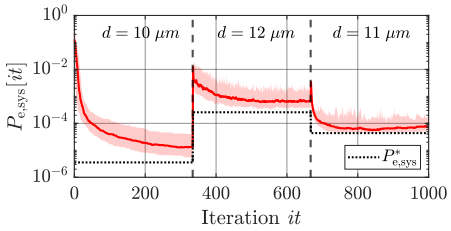

Fig. 4. Median (bold line) and 5th–95th percentile (shaded area) of bit error probability $P_{\mathrm{e,sys}}$ for 100 runs of 1000 iterations of Algorithm 3. After 333 and 666 iterations the distance of the TXs to the RX was changed from 10 μm to 12 μm and again to 11 μm, respectively.

the overall convergence. This shows the robustness of the algorithm towards the choice of initial value. We also observe that when the thresholds and $N_{\mathrm{TX},i}$ are far from the optimum at the beginning, there are a lot of errors and, therefore, a lot of adjustments to the values by the algorithm, causing more drastic changes, followed by smaller adjustments as we approach the optimum.

Secondly, in Figure 3, we also look at the performance of the algorithm under varying levels of background noise, comparing the results for $\mathrm{SNR} = \infty$ to $\mathrm{SNR} \approx 3$. The plots show that the optimization also works for the case with noise. Crucially, the optimal values are significantly influenced by the added noise, but the algorithm approximates them without knowledge of the noise level. We can observe some increased variability and jitter in the median and percentiles, and it seems as if the algorithm slightly overestimates both the optimal threshold and the number of molecules for the case of added noise. A rigorous investigation of the underlying reasons is left for further work.

Lastly, Figure 4 evaluates the reaction of the algorithm to changes in the channel conditions during run-time. The sequence of 1000 iterations is split into three parts, where after every 333 iterations, the distance of both TXs is changed from $10\,\mu\mathrm{m}$ to $12\,\mu\mathrm{m}$ and subsequently to $11\,\mu\mathrm{m}$. We can observe that although the instantaneous BEP jumps up at the time of the change, the subsequent speed of the optimization is quick. Especially for the first few iterations after the change, the BEP is reduced by orders of magnitude towards the optimum. This shows the potential of this type of algorithm to work in a running DBMC system.

V. Conclusion

In this paper, we proposed a BEP optimization algorithm for a DBMC network using NOMA based on the transmission of pilot symbols. We have shown that the algorithm can reliably approximate the optimal values for the detection threshold and the number of molecules in a system with 2 TXs and 1 RX, requiring no prior knowledge of the initial values. This provides a promising perspective for the use of MA schemes in a real MC network. Additionally, the algorithm deliberately uses simple steps without the computation of more complex functions. We plan to address the implementation of the algorithm using stochastic chemical reaction networks in future work. A more detailed analysis of the effect of the step size and the necessary synchronization and feedback mechanisms will be considered, and a generalization to more transmitters will be conducted.

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