Optimal detector design for molecular communication systems using an improved swarm intelligence algorithm

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Published in Micro & Nano Letters; Received on 4th July 2017; Revised on 7th November 2017; Accepted on 23rd November 2017

The authors optimise the detection process of diffusion-based molecular communication systems utilising the weighted sum detector with appropriate weight values. Interestingly, no optimisation technique has ever been proposed for the calculation of the weights. To this end, they build on the standard particle swarm optimisation (PSO) technique and propose a robust iterative optimisation algorithm, called acceleration-aided PSO (A-APSO). While modified swarm-based optimisation algorithms focus on slight variations of the standard mathematical formulas, in A-APSO, the acceleration variable of the particles in the swarm is also involved in the search space of the optimisation problem. Particularly, they implement the A-APSO algorithm to evaluate the detector’s weights that minimise the closed-form expression of the error probability. Their findings reveal that, when employing the A-APSO weights, the error performance is superior to that achieved by utilising the weight values already existing in the literature or those evaluated with the standard PSO algorithm.

1. Introduction: Nanomachines are devices with functional components on the order of nanometres in size and are capable of performing basic sensing, computing and actuation tasks. Inspired by communication mechanisms naturally occurring in living organisms, molecular communication utilises molecules for the transfer of information among nanomachines [1–3]. The ability of such devices to communicate would enable applications such as cooperative diagnostics, tissue engineering and drug delivery in biomedicine [1, 4]. Particularly, diffusion-based communication is commonly found in cellular systems, when small molecules need to quickly travel short distances relying on the law of diffusion for molecule propagation in the communication fluid environment [5]. Moreover, the receiver is able to recognise and measure some arrival property of the received information molecules. This property can be simply the presence or absence of the information particles, their concentration, time of arrival or any other measurable parameter [2].

The limited processing capabilities of the receiver nanomachine indicate the need for a reliable and low-complexity receiver. To this end, we have adopted the sub-optimal but very promising weighted sum detector, which was introduced in [4] for being physically more realisable and less complex, when using discrete samples [6]. Interestingly, a mechanism similar to this type of detector can be found in neurons, which utilise the inputs of different synapses with proper weights in order to decide whether to fire or not [7]. Given that only two sets of predetermined values for the weights have been proposed so far [4], optimisation-based signal processing techniques need to be employed so as to boost the performance of the weighted sum detector. Among them, swarm intelligence theory seems to be a very promising tool given its widespread use in many scientific fields and applications.

Particle swarm optimisation (PSO) is an effective computational method for optimising continuous non-linear functions [8–10]. The PSO method, originally proposed by Kennedy and Eberhart in [8] and later refined by Shi and Eberhart in [9, 10], has been applied in several scientific fields such as in optimisation analysis, computational intelligence and scheduling applications. More than 30 PSO variants and hybrid algorithms combining PSO with existing techniques have been proposed so far to achieve quickly converging results, just to mention [11–14]. Nevertheless, current algorithms neglect the acceleration factor of the particles in the swarm. Besides, in other techniques inspired from physics-based modelling such as in [15], spring type forces among swarm particles may cause acceleration discontinuities or possible swarm splitting as well as overall anomalies in behaviour.

Hereby, we revisit the standard PSO method by introducing novel swarm equations that involve, among others, the acceleration factor of the particles. We call the proposed optimisation algorithm as the acceleration-aided PSO (A-APSO), inspired by recent advances in signal processing [16]. It is important to note that the abbreviation ‘APSO’ has already been adopted in the literature for modified PSO algorithms, where the terms ‘accelerated’ or ‘acceleration’ characterise the convergence speed of the algorithm [11, 17–20]. However, by utilising fundamental laws of physics, the A-APSO framework introduced here enriches the swarm intelligence theory with the involvement of the acceleration factor of the swarm in the model equations. In this way, the obstacles mentioned in the previous paragraph are avoided, thanks to the refined observation of the swarm.

In this Letter, we apply the A-APSO for the optimal design of the weighted sum detector in diffusive molecular communication systems. More precisely, the A-APSO algorithm evaluates the weight value to be utilised for each discrete sample by the weighted sum detector in order to minimise the error probability. Afterwards, the system error performance utilising the A-APSO weights is compared with the performance achieved when the weights are determined by the standard PSO algorithm as well as by already existing methods, namely (a) all the weights are set equal to one and (b) the so-called matched filter weights are utilised [4]. Interestingly, the A-APSO results outperform all the aforementioned types of weights.

Notations: In the sequel, Pr{A} stands for the probability of event A and pT denotes the transpose of a vector p.

2. System model: The diffusion-based molecular communication system under study is depicted in Fig. 1 and consists of the
transmitter–receiver pair and the information carrying molecules. We consider an unbounded stationary three-dimensional (3D) environment that has a uniform temperature and is filled with a fluid of certain viscosity. The transmitter is a point source with zero dimensions placed at a distance $d$ from the centre of the receiver. It emits identical molecules that diffuse freely and independently from each other via Brownian motion in the communication medium. Information is embedded in the number of transmitted molecules, where bit-1 corresponds to the emission of $M$ information molecules and bit-0 to no emission (i.e. zero molecules), thus ON–OFF keying modulation is assumed. Besides, the information molecules are emitted instantaneously at the beginning of the symbol interval $T$ and the synchronisation between the transmitter and the receiver is assumed perfect. It should be noted that both transmissions are considered equiprobable, i.e. $\Pr \{x_i = 1\} = \Pr \{x_i = 0\} = 0.5$.

The receiver is a sphere of radius $\rho$ and volume $V$ that works as an ideal passive observer, which does not affect the behaviour of the information molecules reaching its surface, i.e. neither does it react with them nor does it impede their diffusion in any way. Meanwhile, it has the ability to count the number of information molecules reaching its surface, i.e. neither does it react with them nor does it impede their diffusion in any way.

Owing to the random movement of molecules in the communication fluid, the number of observed molecules within the receiver is a random variable (RV) following a Poisson distribution, which can be approximated via a Gaussian distribution [4]. It should be noted that information molecules corresponding to a previous transmission may reach and be observed by the receiver at a later time, thus causing intersymbol interference (ISI) to the current transmission. Therefore, the decision rule of the weighted sum detector, employing single threshold detection with threshold $\theta$, for the estimated value of the $i$th bit, $\hat{x}_i$, can be expressed as

$$\hat{x}_i = \begin{cases} 1 & \text{if } \sum_{k=1}^{M} w_k N_{i,k} \geq \theta \\ 0 & \text{otherwise.} \end{cases}$$  

By approximating the Poisson distribution with a Gaussian and utilising an appropriate continuity correction [4, 42], (44), it can be proved that the average probability of error equals

$$P_e = \left(\frac{1}{2}\right)^{\frac{L}{2}} \sum_{l=1}^{L} \left[ \frac{1}{2} \text{erf} \left( \frac{\theta - 0.5 - \sum_{k=1}^{K} w_k \lambda_k(l, 1)}{\sqrt{2} \sum_{k=1}^{K} w_k^2 \lambda_k(l, 1)} \right) \right] + 1,$$

where $\text{erf}(\cdot)$ stands for the error function, $l$ corresponds to each of the $2^l$ possible bit sequences, $\{u[1], u[2], \ldots, u[L]\}$, while the corresponding mean value $\lambda_k(l, x_i)$ of the $k$th sample time is

$$\lambda_k(l, x_i) = M_x h(z(k)) + \sum_{m=1}^{M} \left[ Mu[m] h(z(k) + mT) \right] + \mu_x.$$  

### 3. Novel A-APSO-based algorithm

From Newton’s second law, and after adopting notation $f' = \beta(t)$ for mapping $l = f(t)$, velocity and position can be written in terms of the acceleration factor $\beta'$ in discrete form as

$$v' = v + \beta t, \quad (7)$$

$$x' = x + v t + \frac{1}{2} \beta t^2. \quad (8)$$

In standard PSO algorithm, let $v' = [v'_1, \ldots, v'_D]^T$ and $x' = [x'_1, \ldots, x'_D]^T$ be the velocity and position vectors of the $j$th particle at iteration $t$, where $D$ is the number of particle dimensions, and $j = 1, 2, \ldots, S$, with $S$ being the size of the swarm. Let now $p_j = [p'_1, \ldots, p'_D]^T$ be the best (position vector) solution obtained from the $j$th particle up to iteration $t$, and $p_b = [p'_b, \ldots, p'_b]^T$ be the best (position vector) solution obtained from $p_j$ in the population at iteration $t$. In this case, we can adjust the velocity and position equations as

$$v'_{j,q} = \omega v_{j,q} + c_1 \xi (p'_j - x'_{j,q}) + c_2 \eta (p'_b - x'_{j,q}), \quad (9)$$

$$x'_{j,q} = x'_{j,q} + v'_{j,q}. \quad (10)$$
where $c_1$, $c_2$ are acceleration coefficients, $\xi$, $\eta$ are random numbers uniformly distributed in the $[0, 1]$ interval, $\omega$ is an inertia weight and $q = 1, 2, \ldots, D_p$ [9].

Algorithm 1: The proposed A-APSO-based algorithm

(i) Set $t = 0$ and randomly generate $v_{j,q} \in [-v_{\text{max}}, v_{\text{max}}]$ and $x_{j,q} \in [0, 1]$, where $j = 1, 2, \ldots, S$, $q = 1, 2, \ldots, D_p$ and $v_{\text{max}}$ is the maximum selected velocity.

(ii) Compute FV for each particle in the swarm and set $p_j^t = [x_{j,1}^t, \ldots, x_{j,D_p}^t]^T$ and $p_k^t = [x_{k,1}^t, \ldots, x_{k,D_p}^t]^T$, where $b$ is the index of the particle with the best FV value.

(iii) Set $t = t + 1$ and update velocity $v_{j,q}$ according to (12). If $v_{j,q} > v_{\text{max}}$, then $v_{j,q} = v_{\text{max}}$, while if $v_{j,q} < -v_{\text{max}}$, then $v_{j,q} = -v_{\text{max}}$.

(iv) Define acceleration factor as in (11).

(v) Update position $x_{j,q}$ according to (13).

(vi) Compute the FV for each particle in the population.

(vii) For the $j$th particle, if its FV is less than the FV of $p_j^{t-1}$, then set $p_j^t = [x_{j,1}^t, \ldots, x_{j,D_p}^t]^T$, else $p_j^t = p_j^{t-1}$.

(viii) If the $j$th particle’s FV is less than the FV of $p_k^{t-1}$, then set $p_k^t = [x_{k,1}^t, \ldots, x_{k,D_p}^t]^T$. Else, if there is no particle with FV less than the FV of $p_k^{t-1}$, then set $p_k^t = p_k^{t-1}$.

(ix) If $t$ equals the maximum iteration, terminate, else go to (iii).

After comparison of the original PSO equations and the updated ones, we note the absence of the acceleration factor, which we define now as

$$a_{j,q}^t = c_1 \xi \left( p_{j,q}^{t-1} - x_{j,q}^t \right) + c_2 \eta \left( p_k^{t-1} - x_{j,q}^t \right), \quad (11)$$

where $a_{j,q}^t = [a_{j,1}^t, \ldots, a_{j,D_p}^t]^T$ is the acceleration vector of the $j$th particle at iteration $t$. It is worth mentioning that the two terms on the right-hand side of (11), which represent the cognitive and social components [15], respectively, are similar to elastic forces (Hooke’s law).

Therefore, the velocity and position equations, considering also $t = 1$ in (7) and (8), can now be expressed as

$$v_{j,q}^t = \omega v_{j,q}^{t-1} + a_{j,q}^t, \quad (12)$$

$$x_{j,q}^t = x_{j,q}^{t-1} + v_{j,q}^t + \frac{1}{2} a_{j,q}^t. \quad (13)$$

The proposed A-APSO is described in detail in Algorithm 1, where the exact computation of the fitness values (FVs) depends on the targeted application. For illustration purposes, we consider here that the objective function is to be minimised.

In step (iv) of Algorithm 1, we can introduce further constraints on the acceleration behaviour of swarm particles. Particularly, in Fig. 2, the mean acceleration of the swarm particles is plotted with respect to the number of iterations. This is in agreement with past studies that introduced randomness in acceleration coefficients according to the pseudo-code [10]

$$\left\{ \begin{array}{ll}
   c_1 = c_1 + (\text{rand}(1, 1) - \text{rand}(1, 1)) \times \text{maxit} / \text{maxit} \\
   c_2 = c_2 + (\text{rand}(1, 1) - \text{rand}(1, 1)) \times \text{maxit} / \text{maxit} \\
   \left[-a_{\text{max}}, a_{\text{max}}\right] = [-2, 2]
\end{array} \right. \quad (14)$$

where $\text{maxit}$ corresponds to the current iteration, $\text{maxit}$ is the maximum preselected iterations, $a_{\text{max}}$ is the maximum selected acceleration and rand $(1, 1)$ denotes a single uniformly distributed random number within $[0,1]$. Snapshots in Fig. 3 illustrate swarm movement during four different instances (i.e. at the initial state, the 25th, the 50th and the 100th iteration) in 3D space. Of course, this is a pseudo-3D display since the original problem lies in $D_p$ dimensions, and therefore it cannot be realistically attributed. Still, the convergence of the particles toward the best vector is obvious. A uniform distribution has been used for initialisation, while the swarm size parameter $S$ has been set equal to 50. Actually, this is a typical value for $S$ that gives a good tradeoff between optimisation performance and complexity, as revealed by our studies. Besides, $v_{\text{max}}$ has been set equal to 5, in order to increase the range of possible values and, thus, enhance the derived results. Finally, $\omega$ is set equal to 1 and the initial values of both $c_1$ and $c_2$ are selected equal to 2.

4. Problem formulation and simulation setup: In the following, we have implemented the A-APSO algorithm in the molecular communication system described in Section 2 in order to determine the weights $w = [w_k, \ldots, w_s]^T$ that minimise the probability of error. Thus, we have solved the optimisation problem expressed as follows:

$$w = \arg \min_{w} P_e \quad \text{s.t.} \quad w_k \geq 0 \quad \text{for} \quad k = 1, 2, \ldots, K. \quad (15)$$

Using the mean error probability expressed in (5) as the objective function, it holds that $D_p = K$ and $w = p_k^t$ when $t$ equals the maximum iteration.

Hereby, we note that the evaluated weights should be non-negative numbers. Nevertheless, the A-APSO algorithm may result in one or more negative weight values. In this case, the negative values are substituted with zeros for the evaluation of the error probability. Moreover, we emphasise that the detection for each weight vector is implemented utilising the optimal threshold value, which is computed numerically in all assumed scenarios. Thus, the FV values computed in the A-APSO algorithm application, correspond to the error probability values when the weight vector is substituted with the position vector stated in the specific step of the algorithm and the optimal threshold value is utilised. Finally, the number of iterations that should be performed in order to calculate the weight vector highly depends on the molecular communication system parameters and the number of samples assumed at the weighted sum detector.

Regarding the simulation parameters, we have assumed a 3D environment with a diffusion coefficient $D = 4.365 \times 10^{-10}$ m$^2$/s and a spherical receiver with radius $r = 45$ nm at a distance $d = 300$ nm from the receiver. Moreover, the instantaneous
emission of $M = 5000$ molecules corresponds to bit-1 and the symbol duration is equal to $T = 200$ μs. The selection of the symbol duration has been influenced by the need for ISI mitigation along with a high transmission rate. Specifically, for the considered parameters, the maximum number of molecules is expected to be observed at the receiver 34.36 μs after their emission, thus, selecting a symbol duration that is adequately higher than this value satisfies the aforementioned tradeoff [4].

To ease the time required for simulations and derive tractable results, we have assumed that only one previous symbol causes ISI to the current transmission, i.e. $I = 1$, unless otherwise stated. More precisely, systems with higher levels of ISI, i.e. $I = 2$ and $3$, have been also examined in the following section.

Furthermore, the system performance resulting from the use of the weights extracted by the A-APSO algorithm has been compared in terms of error probability with the following cases:

(i) equal weights for all the samples, i.e. $w_k = 1$, for $k = 1, 2, \ldots, K$;

(ii) matched filter weights, i.e. $w_k = M h(\tau(k))$, for $k = 1, 2, \ldots, K$; and

(iii) weights evaluated with the standard PSO algorithm.

It should be mentioned that the matched filter weights are considered optimal in the case, where the ISI effect is negligible and the external additive noise follows the Gaussian distribution [4].

5. Results and discussion: In this section, we refer to the error probability simply as bit error rate (BER) and compare the theoretical values of BER calculated from (5) with those derived from Monte Carlo simulations. Interestingly, as will be mentioned in the sequel, the simulation results are lower than the theoretical ones. This can be explained by the fact that the theoretical closed-form expression of BER is an approximation. Nevertheless, it can be considered as an upper bound of the actual BER, which is extremely useful as the real system’s performance is expected to be superior to the theoretical one.

In Fig. 4, the theoretical BER is plotted against the number of samples within a symbol interval for different assumptions regarding the additive noise and the weight values. As expected, utilising more samples enhances the system performance, while, on the other hand, increases the receiver complexity which is generally undesirable in molecular communication applications. Furthermore, the weights derived from the A-APSO algorithm lead to superior performance when compared with both the cases of unity and matched filter weights. This finding reveals that the A-APSO is suitable for the optimal design of the weighted sum detector in diffusive molecular communications systems. Interestingly, the gap between the error rates, evaluated when the matched filter and the A-APSO-based weights are utilised, decreases as the additive noise increases. Thus, the A-APSO is proved more advantageous when the additive noise is low. Besides, it becomes evident that a small increase in the mean value of the additive noise results in a
tremendous decrease of the system performance. Finally, the benefit derived from the A-APSO is higher when more time samples are considered.

In Fig. 5, the matched filter weights and those determined by the A-APSO algorithm have been employed in simulating the molecular communication system. It can be easily observed that the theoretical BER values correspond to an upper bound on the molecular communication system performance, especially in the A-APSO case. Therefore, using the closed-form expression for the BER ensures that the actual performance of the system will be better. Once more, it is obvious that when the additive noise increases, the implementation of A-APSO weights does not result in a significant BER improvement when compared with the matched filter weights case. Besides, in the marginal case where \( \mu_s = 5 \), which corresponds to a system experiencing high additive noise, we observe that all the curves tend to coincide.

From Fig. 6, we conclude that higher levels of ISI deteriorate the error performance, though not as much as by increasing the additive noise. Furthermore, as ISI increases, the BER performance enhancement due to the A-APSO decreases. Therefore, selecting an appropriate symbol duration can ensure the beneficial effect of the A-APSO algorithm, given that increasing the symbol duration results in a reduction of the experienced ISI.

In Fig. 7, the proposed A-APSO is compared with the standard PSO algorithm, when \( K = 10 \) equally spaced time samples and additive noise of mean \( \mu_s = 0 \) and 2 are considered. Obviously, the A-APSO algorithm converges to a lower BER value for a given complexity level, i.e. number of iterations, while the gap between the BERs for the two algorithm cases decreases as the number of iterations increases.

Regarding the weights, it should be mentioned that the evaluated weight values with the A-APSO algorithm are neither unique nor always the same for an assumed system model. Interestingly, it has been found that, different weight vectors can lead to the same error performance. Moreover, the required number of iterations for the A-APSO algorithm increases when more samples are considered and, thus, more weights need to be calculated. Interestingly, we have concluded that the first sample should be multiplied by a zero weight, i.e. \( w_1 = 0 \), for \( K \geq 20 \), since the A-APSO results in a negative value for the first weight. Meanwhile, both the first and the second weights should be set equal to 0 when \( K \geq 40 \). This behaviour can be explained by the fact that the first observations are the ones that suffer most from ISI. Particularly, the earlier in time an observation is made, the more of the observed molecules come from previous transmissions than from the current one.

Motivated by the previous conclusion, we propose the utilisation of the A-APSO algorithm along with an optimal timing of the observations made at the receiver. Optimising the number and timing of the samples at the receiver and implementing the A-APSO algorithm for the weight determination is expected to further enhance the error performance of the system while reducing the receiver’s complexity at the same time.

6. Conclusion: In this Letter, we considered an improved version of the standard PSO algorithm, called A-APSO, which takes into account the acceleration factor of the swarm particles in the associated model equations. The novel swarm intelligence algorithm has been implemented in a diffusion-based molecular communication system in order to evaluate the weight values for the weighted sum detector of a passive receiver. The results revealed that the A-APSO algorithm is a promising tool for optimal detection in molecular communication systems, providing a lower probability of error than the standard PSO algorithm for a given complexity level (i.e. number of iterations). Finally, the evaluated weights using the A-APSO algorithm are proved more advantageous in terms of error performance than the commonly adopted in the literature so far, namely unity and matched filter weights. Before closing, we would like to indicate as future work the extension of the proposed system model by considering a...
communication environment with a steady uniform flow and/or enzymes.

7. Acknowledgments: The research works of Georgia D. Ntouni and George K. Karagiannidis have been supported by the ‘Research Projects for Excellence IKY/Siemens’. The authors thank Prof. Traianos V. Yioultsis from the Aristotle University of Thessaloniki, Department of Electrical and Computer Engineering, for his useful discussion.

8 References