Advanced Detection and Synchronization Schemes for Molecular Communications

Ph.D. defense

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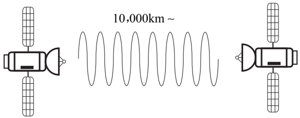
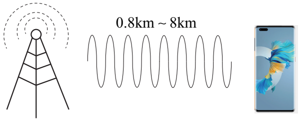
Outline

Motivation

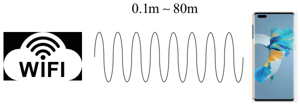
- Success of electromagnetic (EM) wave in a variety of systems
- Difficulties in micro-scale communications
  - Devices are too large.
  - EM wave suffers from severe propagation loss in special medium.
- Solution: Molecular Communications[1]
  Convey information via releasing small particles through aqueous or gaseous medium.
- Applications: Micro-robots in blood vessels.



(a) Satellite Communications



(b) Mobile Communications



(c) Indoor Communications

Figure: Mature Communication Systems

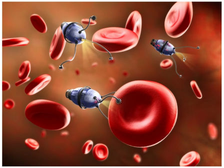
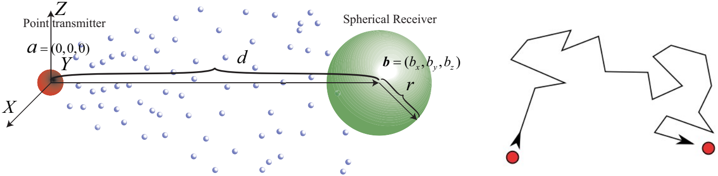


Figure: Micro-robots[2].

[1] Nariman Farsad et al., "A comprehensive survey of recent advancements in molecular communication," IEEE Commun. Surv. Tutor., 18(3): 1887-1919, 2016.

[2] https://newatlas.com/nanobots-blood-drug-delivery/38064/

A Typical Diffusion-based MC System



(a) 3D channel model (b) Diffusion

Figure: A diffusion-based MC system[1]

Diffusion:

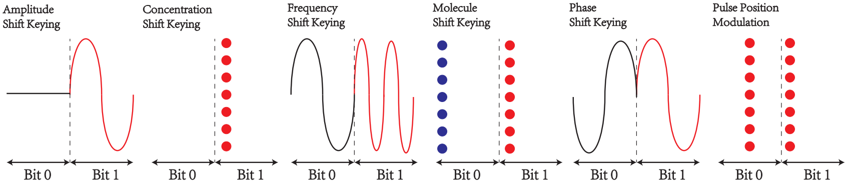
- Net movement from a region of higher concentration to a region of lower concentration
- Movement of each molecule can be modelled by random walk, e.g., Brownian motion, caused by thermal vibrations and collisions
- Characterized by the diffusion coefficient D

Movement of molecules:
Transmitter (high concentration) $\Rightarrow$ Receiver (low concentration)

[1] Nariman Farsad et al., "A comprehensive survey of recent advancements in molecular communication," IEEE Commun. Surv. Tutor., 18(3): 1887-1919, 2016.

A Typical Diffusion-based MC System: Modulation

At the transmitter side: How to modulate symbols?



(a) Concentration Shift Keying (b) Molecule Type Shift Keying (c) Pulse Position Modulation

Figure: Three basic modulation schemes in MC systems and the their counterparts in wireless communications.[1]

Convey information by:

- Molecule number -> Concentration shift keying
- Type of molecule -> Molecular type shift keying
- Release time -> Pulse position modulation

Note: Binary Concentration shift keying is the simplest and most energy-efficient.

[1] Nariman Farsad et al., "A comprehensive survey of recent advancements in molecular communication," IEEE Commun. Surv. Tutor., 18(3): 1887-1919, 2016.

A Typical Diffusion-based MC System: Channel Modelling

The receiver counts the **received molecule number** in each sample duration ϱ.

For each molecule:

- Hitting rate[1] (Probability density function) for reaching to the receiver:

$$f_{hit}(t) = \frac{r(d-r)}{d\sqrt{4\pi D t^3}} e^{-\frac{(d-r)^2}{4Dt}}$$

- Receiving probability in the k-th sample duration:

$$\mathbb{P}_k = \int_{k\varrho}^{(k+1)\varrho} f_{hit}(t) dt$$

Transmitter side: releasing N_{TX} molecules.

Receiver side:
The average received molecule number in the k-th sample duration (k-th average sample) is $\mathbb{C}_k = N_{TX}\mathbb{P}_k$, i.e., the sampled channel response.

The practical received molecule number $r(k)$ in the k-th sample duration (k-th sample) follows Poisson distribution with mean $\mathbb{C}_k$, i.e., $r(k) \sim \text{Poisson}(\mathbb{C}_k)$.

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[1] Yilmaz, H. Birkan, Akif Cem Heren, Tuna Tugcu, and Chan-Byoung Chae. "Three-dimensional channel characteristics for molecular communications with an absorbing receiver." IEEE Communications Letters 18, no. 6 (2014): 929-932.

A Typical Diffusion-based MC System: Signal modelling

Setting: Symbol length $T = M\varrho$, noise mean $\mathbb{C}_n = \bar{\lambda}_0 \varrho$, the ith symbol s_i.
The mth actual and average sample in the ith symbol slot, $r_i(m)$ and $\bar{r}_i(m)$, are

$$r_i(m) = \text{Poisson}(\bar{r}_i(m)), \quad \bar{r}_i(m) = s_i \mathbb{C}_m + \underbrace{\sum_{j=1}^{\infty} s_{i-j} \mathbb{C}_{jM+m}}_{\text{ISI}} + \mathbb{C}_n$$

Table: Simulation parameters

Parameter	Value
$\bar{\lambda}_0$	$100 s^{-1}$
r	45 nm
d	500 nm
D	$4.265 * 10^{-10} m^2/s$
ϱ	5 us
N_{TX}	100,000
M	100
L	5

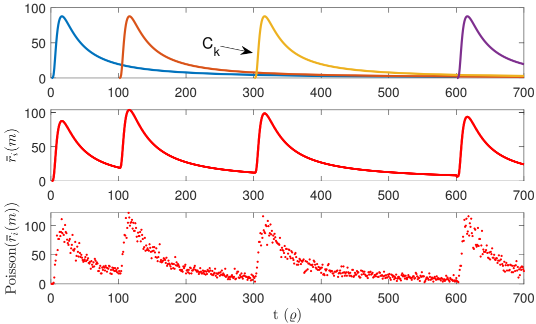

Figure: Sampled channel responses, average samples and actual samples.

Long channel response leads to ISI!

A Typical Diffusion-based MC System: System model

Note: A sum of Poisson random variables is still a Poisson random variable.

The received molecule number in ith symbol duration (ith signal) r_i is

$$r_i = \sum_{m=0}^{M-1} r_i(m) = \text{Poisson}(\bar{r}_i), \quad \bar{r}_i = \sum_{m=0}^{M-1} \bar{r}_i(m) = s_i \sum_{m=0}^{M-1} \mathbb{C}_m + \sum_{j=1}^{\infty} s_{i-j} \sum_{m=0}^{M-1} \mathbb{C}_{jM+m} + M\mathbb{C}_n$$

Let the channel length be L and denote $C_j = \sum_{m=0}^{M-1} \mathbb{C}_{jM+m}$ and $C_n = M\mathbb{C}_n$.

$$\bar{r}_i = s_i C_0 + I_i = s_i C_0 + \sum_{j=1}^{L} s_{i-j} C_j + C_n$$

where $I_i = \sum_{j=1}^{L} s_{i-j} C_j + C_n$.

A Typical Diffusion-based MC System: Detection

How to detect signals r_i?

If the receiver knows: C_j for $0 \leq j \leq L$ and C_n

Ideal case[1]

$$I_i = \sum_{j=1}^{L} s_{i-j} C_j + C_n, \quad \Pr(r_i|s_i) = \frac{e^{-(I_i + s_i C_0)} (I_i + s_i C_0)^{r_i}}{r_i!}, \quad \hat{s}_i = \arg\max_{s_i} \Pr(r_i|s_i)$$

Equivalently, the detection is performed as follows:

$$\hat{s}_i = \begin{cases} 1 & r_i > \tau|_{s_{i-j}, 1 \leq j \leq L} \\ 0 & r_i \leq \tau|_{s_{i-j}, 1 \leq j \leq L} \end{cases}, \quad \tau|_{s_{i-j}, 1 \leq j \leq L} = \frac{C_0}{\ln(1 + \frac{C_0}{C_n + \sum_{j=1}^{L} s_{i-j} C_j})}$$

where $\tau|_{s_{i-j}, 1 \leq j \leq L}$ is obtained by letting $\Pr(r_i|s_i = 1) = \Pr(r_i|s_i = 0)$. s_{i-j} for $1 \leq j \leq L$ are called memory bits.

[1] Mosayebi, R., Arjmandi, H., Gohari, A., Nasiri-Kenari, M., Mitra, U. (2014). Receivers for diffusion-based molecular communication: Exploiting memory and sampling rate. IEEE Journal on Selected Areas in Communications, 32(12), 2368-2380.

A Typical Diffusion-based MC System: Detection

Practical implementation:
The receiver only knows C_j for $0 \le j \le K$ and the value of $C_n + \sum_{j=K+1}^{L} C_j/2$.
Or the receiver only has K memory bits.

Realistic case[1]

$$
\begin{aligned}
I_i &\simeq \sum_{j=1}^{K} s_{i-j} C_j + C_n + \sum_{j=K+1}^{L} C_j/2, \quad \Pr_{\text{appro}}(r_i|s_i) = \frac{e^{-(I_i + s_i C_0)} (I_i + s_i C_0)^{r_i}}{r_i!}, \\
\hat{s}_i &= \arg\max_{s_i} \Pr_{\text{appro}}(r_i|s_i) \\
\Rightarrow \hat{s}_i &= \begin{cases} 1 & r_i > \tau|_{s_{i-j}, 1\le j \le K} \\ 0 & r_i \le \tau|_{s_{i-j}, 1\le j \le K} \end{cases}, \quad \tau|_{s_{i-j}, 1\le j\le K} = \frac{C_0}{\ln\left(1 + \frac{C_0}{C_n + \sum_{j=1}^{K} s_{i-j} C_j + \sum_{j=K+1}^{L} C_j/2}\right)}
\end{aligned}
$$

s_{i-j} for $1 \le j \le L$ are unknown in advance, $\hat{s}_{i-j}$ are used instead.

$$
\hat{s}_i = \begin{cases} 1 & r_i > \tau|_{\hat{s}_{i-j}, 1\le j \le K} \\ 0 & r_i \le \tau|_{\hat{s}_{i-j}, 1\le j \le K} \end{cases}, \quad \tau|_{\hat{s}_{i-j}, 1\le j\le K} = \frac{C_0}{\ln\left(1 + \frac{C_0}{C_n + \sum_{j=1}^{K} \hat{s}_{i-j} C_j + \sum_{j=K+1}^{L} C_j/2}\right)}
$$

[1] Mosayebi, R., Arjmandi, H., Gohari, A., Nasiri-Kenari, M., Mitra, U. (2014). Receivers for diffusion-based molecular communication: Exploiting memory and sampling rate. IEEE Journal on Selected Areas in Communications, 32(12), 2368-2380.

Thesis Problem: Detection without channel information C_j

Solutions with known transmitted symbols:

- Channel estimation[1] .
- Machine learning, especially artificial neural networks(ANN)[2].

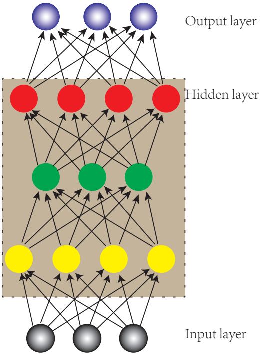

Figure: Typical structure of a feed-forward ANN with fully-connected layers.

Advantages of ANN:

- Easy to implement.
- Possible to emulate every model.
- No need of the channel information.

The model ANN learns:

$$\hat{s}_i = \begin{cases} 1, & \Pr(s_i = 1 | r_i, \hat{s}_{i-j}, 1 \leq j \leq K) > 0.5 \\ 0, & \Pr(s_i = 1 | r_i, \hat{s}_{i-j}, 1 \leq j \leq K) \leq 0.5 \end{cases}$$

Questions: Solved in Part I.

- Which threshold-based receiver has the same performance as the ANN-based receiver?
- How to evaluate the performance of the threshold-based receivers?

[1] V. Jamali, et. al., “Channel estimation for diffusive molecular communications”, IEEE Trans. Commun., vol. 64, no. 10, pp. 4238-4252, Aug. 2016.

[2] N. Farsad, et. al., “Sliding bidirectional recurrent neural networks for sequence detection in communication systems”, IEEE ICASSP, Apr. 2018, pp.2331-2335

Thesis Problem: Detection without channel information C_j

Solutions without known transmitted symbols -> Non-Coherent Detection:

- Exploiting channel response features [1]
  Detection performance to be further improved.
- Strong assumption: no ISI[2].
  Not suitable for high-rate transmission.

To combat ISI and achieve satisfactory detection performance in high-speed transmission, the threshold is necessary.

$$\tau|_{\hat{s}_{i-j},1\leq j\leq K} = \frac{C_0}{\ln(1+\frac{C_0}{C_n+\sum_{j=1}^{K}\hat{s}_{i-j}C_j+\sum_{j=K+1}^{L}C_j/2})}$$

So how to exploit $\tau|_{\hat{s}_{i-j},1\leq j\leq K}$ when C_j are unknown?
Solutions are provided in Part II.

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[1] B. Li, M. Sun, S. Wang, W. Guo, and C. Zhao, "Local convexity inspired low-complexity noncoherent signal detector for nanoscale molecular communications", IEEE Trans. Commun., vol. 64, no. 5, pp. 2079-2091, Mar. 2016.

[2] V. Jamali, N. Farsad, R. Schober, and A. Goldsmith, "Non-coherent detection for diffusive molecular communication systems", IEEE Trans. Commun., vol. 66, no. 6, pp. 2515-2531, Jan. 2018.

Thesis Problem: Synchronization

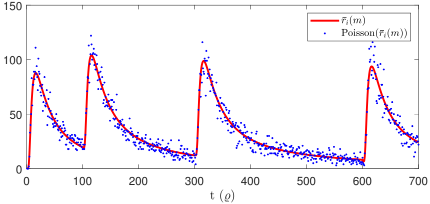

Figure: $\bar{r}_i(m)$ vs $r_i(m)$ for known channel information and symbols.

Synchronization categories:

- Known channel information (known symbols[1] and unknown symbols[2]).
  Maximum likelihood estimation: matching the average samples with the practical samples.
  Limitation: Highly rely on channel information.
- Unknown channel information.
  Too many unknown parameters $\mathbb{C}_k$ -> to be solved in Part III.

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[1] V. Jamali, A. Ahmadzadeh, and R. Schober, "Symbol synchronization for diffusion-based molecular communications", IEEE Trans. Nanobiosci., vol. 16, no. 8, pp. 873-887, Dec. 2017.

[2] H. ShahMohammadian, G. G. Messier, and S. Magierowski, "Blind synchronization in diffusion-based molecular communication channels", IEEE Commun. Lett., vol. 17, no. 11, pp. 2156-2159, Oct. 2013.

Part I: Molecular Communications: Model-Based and Data-Driven Receiver Design and Optimization

Motivation

Aim: Test if the conventional threshold-based receiver can achieve the same performance as the corresponding ANN-based receiver.

Zero-bit memory threshold: model-based

$$\hat{s}_i = \begin{cases} 1 & r_i > \tau \\ 0 & r_i \leq \tau \end{cases}, \quad \tau = \frac{C_0}{\ln(1 + \frac{C_0}{C_n + \sum_{j=1}^{L} C_j/2})}$$

Corresponding model ANN learns: data-driven

$$\hat{s}_i = \begin{cases} 1, & \Pr(s_i = 1|r_i) > 0.5 \\ 0, & \Pr(s_i = 1|r_i) \leq 0.5 \end{cases}$$

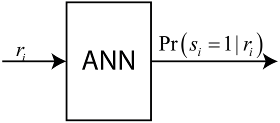


Figure: ANN-based zero-bit memory receiver

Table: Parameters for generating signals

Parameter	Value
λ_0	$100s^{-1}$
r	45 nm
d	500 nm
D	$4.265 * 10^{-10} m^2/s$
ϱ	9 us
T	30ϱ
L	5

Training datum structure:
$\{r_i, \Pr(s_i = 1|r_i) = s_i\}$

Motivation

Table: ANN parameters

Parameter	Value
Number of layers	1
Number of neurons	10
Learning rate	0.01
Training epoch	200
Number of training bits	1000
Replication times	50

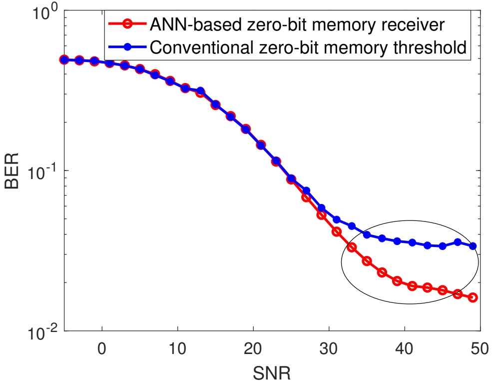


Figure: ANN-based zero-bit memory receiver vs. conventional zero-bit memory threshold

- There exists detection performance gap. There must be another threshold that can achieve the same performance as the ANN-based receiver.
- How to evaluate the performance of the threshold-based receivers?

Optimal Zero-Bit Memory Receiver

What's wrong with the derivation of the conventional threshold?

Conventional zero-bit memory threshold

$$I_i \simeq C_n + \sum_{j=1}^{L} C_j/2, \mathrm{Pr}_{\mathrm{appro}}(r_i|s_i) = \frac{e^{-(I_i+s_iC_0)}(I_i+s_iC_0)^{r_i}}{r_i!}, \hat{s}_i = \arg\max_{s_i} \mathrm{Pr}_{\mathrm{appro}}(r_i|s_i)$$

$$\Rightarrow \hat{s}_i = \begin{cases} 1 & r_i > \tau \\ 0 & r_i \leq \tau \end{cases}, \quad \tau = \frac{C_0}{\ln\left(1 + \frac{C_0}{C_n + \sum_{j=1}^{L} C_j/2}\right)}$$

$\mathrm{Pr}_{\mathrm{appro}}(r_i|s_i)$ is an approximated probability and is not exactly $\mathrm{Pr}(r_i|s_i)$!

One may ask: How to obtain a better threshold?
$\Rightarrow$ What is the optimal threshold?

Optimal Zero-Bit Memory Receiver

The optimal threshold: leading to the minimum BER !

Aim: Formulate the BER $P_e(\tau)$ as a function of threshold τ (performance analysis).

$$P_e(\tau) = \frac{1}{2^L} \sum_{\mathbf{s}_{i-1}} P_e(\mathbf{s}_{i-1}, \tau)$$

where

$$P_e(\mathbf{s}_{i-1}, \tau) = \frac{1}{2}(\underbrace{P(r_i \geq \tau | \mathbf{s}_{i-1}, s_i = 0)}_{\text{False alarm probability}} + \underbrace{P(r_i < \tau | \mathbf{s}_{i-1}, s_i = 1)}_{\text{Miss detection probability}}), \quad \mathbf{s}_{i-1} = \{s_{i-1}, ..., s_{i-L}\}$$

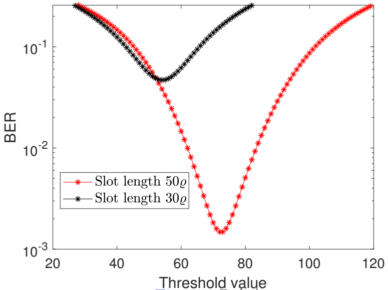


Figure: $P_e(\tau)$

- An optimal value of τ does exist that minimizes the BER and depends on the time slot duration T.
- Due to the analytical complexity of $P_e(\tau)$, it is not possible to compute explicitly.

Optimal Zero-Bit Memory Receiver Design (Model-based Design)

The optimal threshold that minimizes the BER of the zero-bit memory receiver is:

$$(\tau^*, P_e^*) = \arg\min_{\tau} \quad P_e(\tau)$$

Difference between conventional threshold and the optimal threshold:

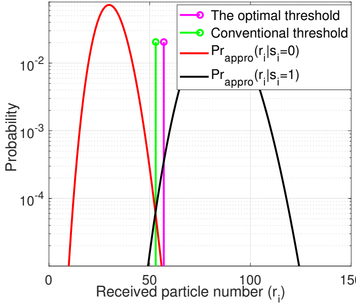


Figure: $\mathrm{Pr}_{\mathrm{appro}}(r_i|s_i = 0) = \mathrm{Pr}_{\mathrm{appro}}(r_i|s_i = 1)$.

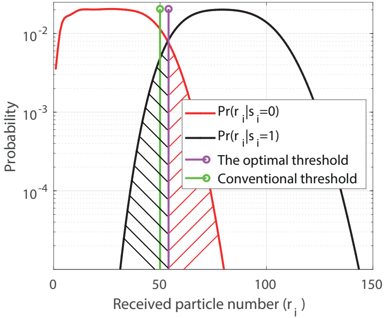


Figure: $\arg\min_{\tau} P_e(\tau)$.

Optimal Zero-Bit Memory Receiver: Simulation Results

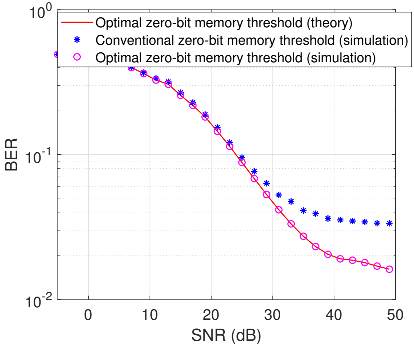


Figure: BER of optimal vs. conventional zero-bit memory receiver - $T = 30\varrho$.

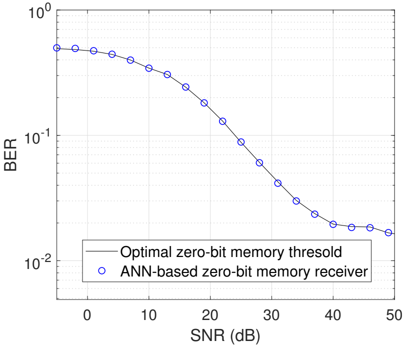


Figure: The ANN-based receiver achieves the same BER performance as the optimal zero-bit receiver - $T = 30\varrho$.

- The detection threshold that minimizes the BER provides us with better performance than the conventional threshold.
- Simulation results match with the analytical framework.
- ANN-based receiver achieves the same performance as the optimal threshold.

Optimal Zero-Bit Memory Receiver: Simulation Results

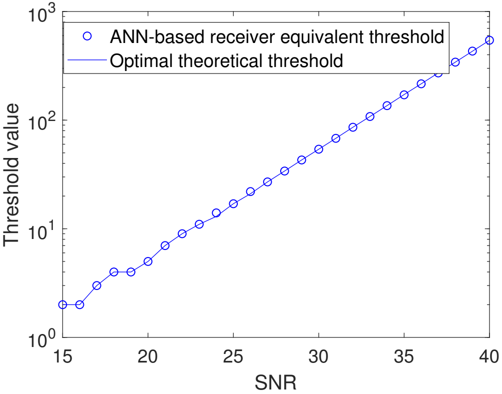


Figure: $\arg\min_\tau P_e(\tau)$ vs. $\Pr(s_i = 1|\tau_{ANN}) = 0.5$ -$T = 30\varrho$.

The ANN-based implementation is capable of learning the demodulation threshold in a very accurate manner.

Summary of Contribution

- The performance disparity between the conventional threshold and the corresponding ANN-based receiver is analysed and explained.
- The optimal threshold is proposed based on the analysis.
- The performance analysis framework is proposed.

Part II: K-Means Clustering-Aided Non-Coherent Detection for Molecular Communications

Motivation

Realistic scenarios:

- The channel model may be unknown to the receiver.
- Channel parameters change with time or temperature.
- The receiver may not know the pilot symbols of the transmitter.

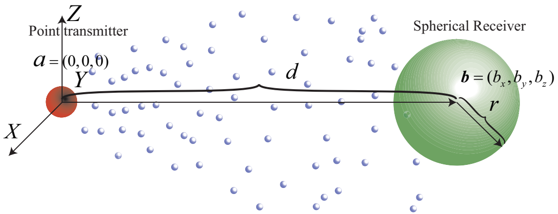


Figure: A diffusion-based MC system

Imagine a receiver just moves to the range of the transmitter, it does not know the channel information or the pilot symbols.

How to detect signals?

Problem Formulation

Aim: Detection with satisfactory performance under ISI. **Solution**: Threshold.

Threshold with analytical expression:

$$\tau|_{s_{i-j},1\leq j\leq \mathcal{L}} = \frac{C_0}{\ln(1+\frac{C_0}{C_n+\sum_{j=1}^{\mathcal{L}} s_{i-j}C_j+\sum_{j=\mathcal{L}+1}^{L} C_j/2})}$$

What can be exploited to compute the threshold except C_j?

Observations:

$$\bar{r}_i = s_i C_0 + \sum_{j=1}^{L} s_{i-j}C_j + C_n$$

In $\tau|_{s_{i-j},1\leq j\leq \mathcal{L}}$, $C_n + \sum_{j=1}^{\mathcal{L}} s_{i-j}C_j + \sum_{j=\mathcal{L}+1}^{L} C_j/2$ is exactly equal to $\bar{r}_i|_{s_i=0,s_{i-j},1\leq j\leq \mathcal{L}}$.
In the meantime, $\bar{r}_i|_{s_i=1,s_{i-j},1\leq j\leq \mathcal{L}} = C_0 + \bar{r}_i|_{s_i=0,s_{i-j},1\leq j\leq \mathcal{L}}$.

$$\tau|_{s_{i-j},1\leq j\leq \mathcal{L}} = \frac{\bar{r}_i|_{s_i=1,s_{i-j},1\leq j\leq \mathcal{L}} - \bar{r}_i|_{s_i=0,s_{i-j},1\leq j\leq \mathcal{L}}}{\ln(\frac{\bar{r}_i|_{s_i=1,s_{i-j},1\leq j\leq \mathcal{L}}}{\bar{r}_i|_{s_i=0,s_{i-j},1\leq j\leq \mathcal{L}}})}$$

As long as $\bar{r}_i|_{s_i=0,s_{i-j},1\leq j\leq \mathcal{L}}$ and $\bar{r}_i|_{s_i=1,s_{i-j},1\leq j\leq \mathcal{L}}$ are obtained, the threshold can be used.
$\bar{r}_i|_{s_i,s_{i-j},1\leq j\leq \mathcal{L}}$ are the intermediate variables to be obtained.

Analysis:

$$\bar{r}_i|_{s_i,s_{i-1}} = E[r_i|_{s_i,s_{i-1}}] = \lim_{K\to\infty} \frac{\sum_{n=0}^{K} r_n \kappa_{n,s_i,s_{i-1}}}{\sum_{n=0}^{K} \kappa_{n,s_i,s_{i-1}}}$$

where $\kappa_{n,s_i,s_{i-1}} = 1$ if $[s_n, s_{n-1}] = [s_i, s_{i-1}]$ and $\kappa_{n,s_i,s_{i-1}} = 0$ otherwise.

Example: Signals r_n for $0 \le n \le K-1$ with $s_n = s_{n-1} = 0$ are marked by blue dots. Other signals are marked by brown dots.

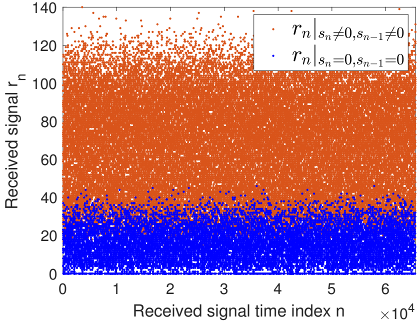


Figure: Comparison of $r_n|_{s_n=0,s_{n-1}=0}$ and other signals.

- $\kappa_{n,s_i=0,s_{i-1}=0}$ are used to identify the blue dots.
- $\bar{r}_i|_{s_i=0,s_{i-1}=0}$ is estimated by the average of blue dots.
- We call $[0, 0]$ as the label of the blue dots.

A Case Study: How To Estimate $\bar{r}_i|_{s_i,s_{i-1}}$ Without Pilot Symbols

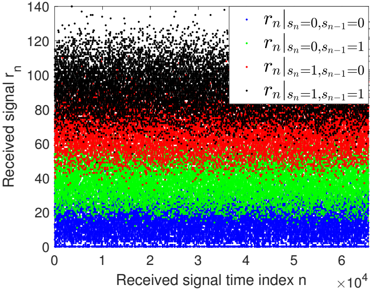


Figure: Four clusters.

- Four groups of signals: $r_n|_{s_n=0,s_{n-1}=0}$, $r_n|_{s_n=0,s_{n-1}=1}$, $r_n|_{s_n=1,s_{n-1}=0}$ and $r_n|_{s_n=1,s_{n-1}=1}$.
- Signals r_n following the same condition $[s_n, s_{n-1}] = [s_i, s_{i-1}]$ form a group.
- $[s_i, s_{i-1}]$ is the label of the group of signals.
- $\bar{r}_i|_{s_i,s_{i-1}}$ is the arithmetical mean (centroid) of that group of points.

Problem summary

Given signals r_n

1. **separate** r_n into several groups (clusters).
2. **compute** the corresponding centroids.
3. **associate** the centroid with correct label $[s_i, s_{i-1}]$.

Note: Separating points into several clusters is called clustering.
A simple clustering algorithm is K-Means clustering algorithm which can solve problem 1 and 2.

K-Means Clustering Algorithm

Setting: Given a data set $\{\boldsymbol{x}_1, \boldsymbol{x}_2, ...\boldsymbol{x}_N\}$ of N observations and each element is a $\mathbb{D}$-dimensional vector $\boldsymbol{x}_n$.

Iterative procedures:
Initialization: Set the initial centroids (randomly selected or predefined)
Step I: Assign $\boldsymbol{x}_n$ to the closest cluster (initial, if this is the first iteration) centroid:

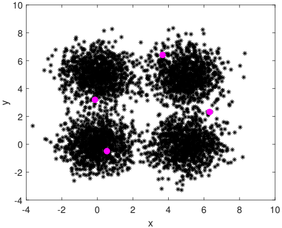
$$\kappa_{n,k} = \begin{cases} 1, \quad \textit{if} \quad k = \arg\min_j \|\boldsymbol{x}_n - \boldsymbol{\mu}_j\|^2 \\ 0, \qquad\qquad \text{otherwise} \end{cases}$$

Step II: Update the cluster centroid:

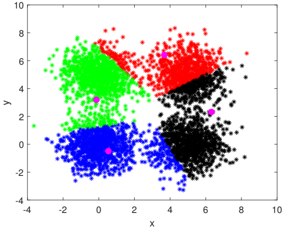
$$\boldsymbol{\mu}_k = \frac{\sum_n \kappa_{n,k} \boldsymbol{x}_n}{\sum_n \kappa_{n,k}}$$

where $\sum_n \kappa_{n,k}$ is the number of points in the kth cluster.

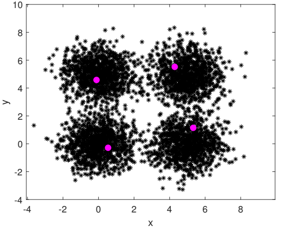
K-Means Clustering Algorithm



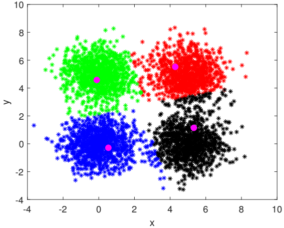
(a) Randomly select initial centroids



(b) Assign points to the closest centroids



(c) Update centroids



(d) Assign points to the closest centroids

Figure: Illustration of the K-Means clustering (The magenta circles denote the centroids).

Single-Dimensional Clustering: Challenges and Limitations

Objective: Clustering the received signals $\{r_1, ..., r_n, ..., r_K\}$ into four clusters that correspond to labels $[s_i, s_{i_1}] = [0,0]$, $[s_i, s_{i_1}] = [0,1]$, $[s_i, s_{i_1}] = [1,0]$, $[s_i, s_{i_1}] = [1,1]$.

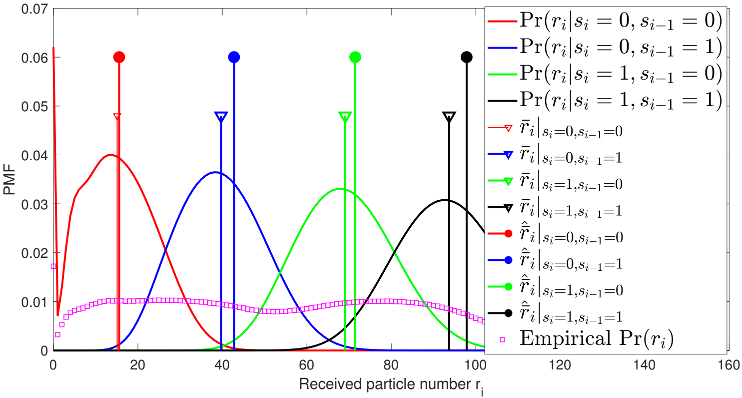


Figure: The positions of $\bar{r}_i|_{s_i,s_{i-1}}$ and $\hat{\bar{r}}_i|_{s_i,s_{i-1}}$ corresponding to the centroids obtained by K-Means algorithm and assuming that the labels $[s_i, s_{i-1}]$ are known) for $T = 30\varrho$

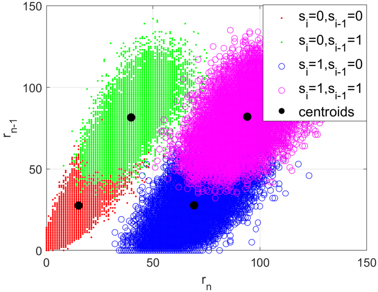
Limitations: Non-negligible estimation error
Reason: Each cluster **overlaps** with other clusters.

Multi-Dimensional Clustering

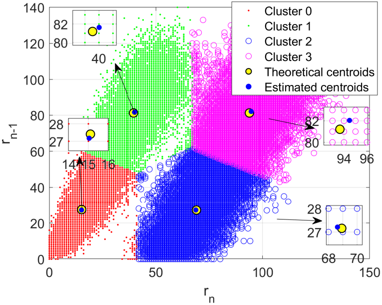
Question: How to avoid or **reduce** the overlapping areas of clusters?
Solution: Construct multi-dimensional elements.

$$\boldsymbol{r}_n = [r_n, r_{n-1}, ..., r_{n-\mathcal{L}}]$$

Case Study: One memory bit implies 2-D clustering for points $[r_n, r_{n-1}]$.



(a) Points $[r_n, r_{n-1}]$ and theoretical centroids. In this case, the labels are assumed to be known a priori



(b) Theoretical (yellow circles) vs. estimated (blue circles) centroids obtained by using the K-means algorithms

Figure: Theoretical and estimated centroids obtained from clustering the data vector $[r_n, r_{n-1}]$ $(T = 30\varrho)$

Setup of the Initial Centroids

Solution to problem 3: Assign correct labels to the centroids.

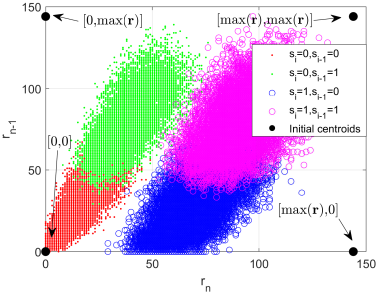


Figure: The customized initial centroids and the corresponding clusters ($T = 30\varrho$)

- Assign the correct labels to the initial centroids.
- The association between the estimated centroids and the correct labels does not change when applying the K-means clustering algorithm.
- Initial centroids are constructed based on the maximum received signal $\max(\boldsymbol{r})$.

Example 1: $[0, \max(\boldsymbol{r})]$ corresponds to the label $[s_i, s_{i-1}] = [0, 1]$ and the estimated centroid is $[\hat{\hat{r}}_i|_{s_i=0,s_{i-1}=1}, \hat{\hat{r}}_{i-1}|_{s_{i-1}=1}]$.

Remark

If the observation vector $[r_n, r_{n-1}]$ belongs to the cluster with label $[s_i, s_{i-1}]$, we believe $[s_n, s_{n-1}] = [s_i, s_{i-1}]$ i.e., if $\kappa_{n,k} = 1$, $\hat{s}_n = s_i$.

Direct Clustering-Based Inference and Clustering-plus-Threshold Detection

Important: $\kappa_{n,k}$ can be used to **infer** $\hat{s}_n$.

Algorithm Direct clustering-based inference

First Step: Clustering

1: Set $\mathcal{L}$
2: Construct the data $\boldsymbol{r}_n$ via $\boldsymbol{r}_n = [r_n, r_{n-1}, ..., r_{n-\mathcal{L}}]$
3: Construct the initial centroids $\boldsymbol{\mu}_k$
4: Cluster the $\boldsymbol{r}_n$ using the K-means algorithm with the initial centroids $\boldsymbol{\mu}_k$

Second Step: Inference

5: Infer $\hat{s}_n$ from the indicator variables $\kappa_{n,k}$

Algorithm Clustering-plus-threshold detection

First Step: Clustering

1: Set $\mathcal{L}$
2: Construct the data $\boldsymbol{r}_n$ via $\boldsymbol{r}_n = [r_n, r_{n-1}, ..., r_{n-\mathcal{L}}]$
3: Construct the initial centroids $\boldsymbol{\mu}_k$
4: Cluster the $\boldsymbol{r}_n$ using the K-means algorithm with the initial centroids $\boldsymbol{\mu}_k$

Second Step: Detection

5: Obtain $\hat{\bar{r}}_i|_{\hat{s}_{i-j}, 0 \leq j \leq \mathcal{L}}$ from the estimated centroids $\hat{\boldsymbol{\mu}}_k$
6: Compute the detection thresholds using $\hat{\bar{r}}_i|_{\hat{s}_{i-j}, 0 \leq j \leq \mathcal{L}}$
7: Detect the symbols using $\hat{\bar{\tau}}|_{\hat{s}_{i-j}, 1 \leq j \leq \mathcal{L}}$

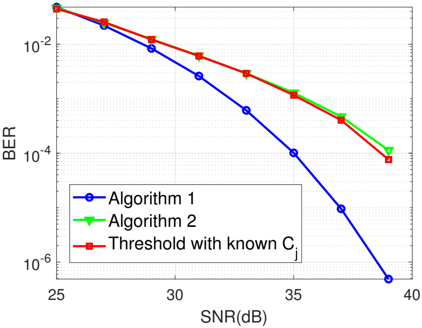
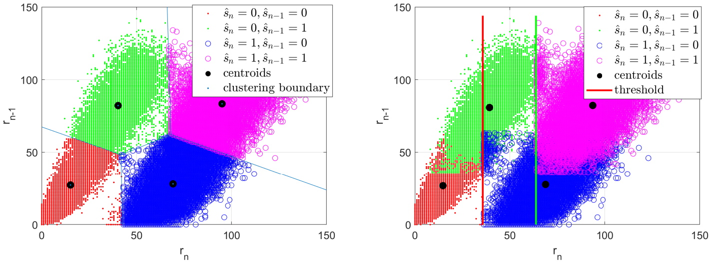


Figure: BER comparison of the proposed algorithms (mild ISI, $\mathcal{L} = 1$ and $T = 30\varrho$)

- Algorithm 2 achieves the similar performance as the ideal threshold with known C_j as the estimated intermediate variables $\hat{\hat{r}}_i|_{s_i,s_{i-1}}$ are accurate enough.
- The algorithm that exploits only the indicator variables $\kappa_{n,k}$ achieves better BER performance.



(a) Direct clustering-based inference

(b) Clustering-plus-threshold detection

Figure: Distribution of $[r_n, r_{n-1}]|_{\hat{s}_n, \hat{s}_{n-1}}$ and estimated centroids ($\mathcal{L} = 1$ and $T = 30\varrho$).

- After estimating the symbol $\hat{s}_n$, all points $[r_n, r_{n-1}]$ with $[\hat{s}_n, \hat{s}_{n-1}] = [0, 0]$, $[\hat{s}_n, \hat{s}_{n-1}] = [0, 1]$, $[\hat{s}_n, \hat{s}_{n-1}] = [1, 0]$, and $[\hat{s}_n, \hat{s}_{n-1}] = [1, 1]$ are depicted in red, green, blue, and magenta colors, respectively.
- Dots represent $\hat{s}_n = 0$ and circles represent $\hat{s}_n = 1$.
- Algorithm 1 takes $[r_n, r_{n-1}]$ into account and algorithm 2 only compare r_n with the threshold.

Summary of Contribution

- The threshold is reformulated by using the intermediate variables that can be estimated from received signals.
- Intermediate variables are obtained by applying K-Means clustering algorithm and predefining the initial centroids to the multi-dimensional data.
- Two algorithms are proposed and analysed for better understanding the non-coherent detection and proposing better algorithms.

Part III: Synchronization for Constant-Threshold-based Receivers in Diffusive Molecular Communication Systems

Motivation

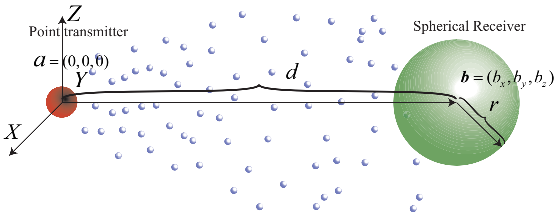


Figure: A diffusion-based MC system

When a receiver moves to the range of the transmitter, it does not know the channel information. Even knowing the pilot symbols, synchronization is a tough problem.

Task of Synchronization: Find or design a metric function whose maximum value corresponds to the optimal synchronization point.

No matter what rule is exploited. Just find one useful rule or conclusion to design the metric function.

System Model

The aim of synchronization: -> To decide the start point of a symbol duration.

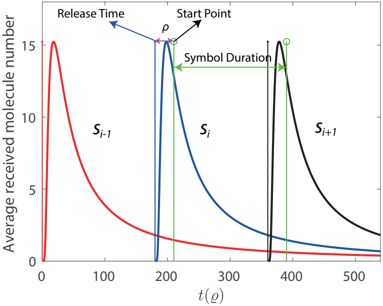


Figure: Start point may not be the release time.

Table: Simulation parameters

Parameter	Value
λ_0	$100s^{-1}$
Receiver radius r	45 nm
Distance d	500 nm
Diffusion coefficient D	$4.265 \times 10^{-10} m^2/s$
Sample duration ϱ	4.5 us
Slot length	180ϱ
Channel length L	7

- The receiver may wait ρ sample durations and start to regard the following samples to the ith received signal.
- s_{i+1} may have effect on the ith signal.

System Model

- Assume the start point is ρ, the t-th average sample in the i-th symbol slot is:

$$\bar{r}_i(t,\rho,s_{i+1},s_i,...,s_{i-L}) = \sum_{j=-1}^{L} s_{i-j}\mathbb{C}_{jM+\rho+t} + \mathbb{C}_n$$

- The i-th average signal is

$$\bar{r}_i(\rho,s_{i+1},s_i,...,s_{i-L}) = \sum_{t=0}^{M-1} \bar{r}_i(t,\rho,s_{i+1},s_i,...,s_{i-L})$$
$$= C_n + \sum_{j=-1}^{L} s_{i-j} \sum_{t=0}^{M-1} \mathbb{C}_{jM+\rho+t} = C_n + \sum_{j=-1}^{L} s_{i-j} C_j(\rho)$$

where $C_n = M\mathbb{C}_n$ and $C_j(\rho) = \sum_{t=0}^{M-1}\mathbb{C}_{jM+\rho+t}$.

- Assuming the start point ρ, the practical ith signal $r_i(\rho)$ follows:

$$\Pr(r_i(\rho)|\bar{r}_i(\rho,s_{i+1},s_i,...,s_{i-L})) = \frac{e^{-\bar{r}_i(\rho,s_{i+1},s_i,...,s_{i-L})}\left[\bar{r}_i(\rho,s_{i+1},s_i,...,s_{i-L})\right]^{r_i(\rho)}}{r_i(\rho)!}$$

Optimal Start Point

Note: Optimal start point will give the smallest BER!

Start from the simplest receiver, zero-bit memory receiver that has the analytical BER expression.

The BER $P_e(\rho, \tau)$, a function of ρ and τ, can be formulated analytically and optimized:

$$P_e(\rho, \tau) = \frac{1}{2}(\Pr(r_i(\rho) > \tau | s_i = 0, \rho) + \Pr(r_i(\rho) \leq \tau | s_i = 1, \rho))$$

$$(P_e^*, \rho^*, \tau^*) = \min_{\rho, \tau} P_e(\rho, \tau)$$

where

$$\Pr(r_i(\rho) > \tau | s_i = 0, \rho) = \frac{1}{2^{L+1}} \sum_{s_i=0} \Pr(r_i(\rho) > \tau | \bar{r}_i(\rho, s_i, s_{i-1}, ..., s_{i-L}, s_{i+1}))$$

$$\Pr(r_i(\rho) \leq \tau | s_i = 1, \rho) = \frac{1}{2^{L+1}} \sum_{s_i=1} \Pr(r_i(\rho) \leq \tau | \bar{r}_i(\rho, s_i, s_{i-1}, ..., s_{i-L}, s_{i+1}))$$

Problem: $P_e(\rho, \tau)$ can only be evaluated numerically.

Solution:

- Original probability:

$$\Pr(r_i(\rho)|\bar{r}_i(\rho, s_{i+1}, s_i, ..., s_{i-L})) = \frac{e^{-\bar{r}_i(\rho, s_{i+1}, s_i, ..., s_{i-L})}[\bar{r}_i(\rho, s_{i+1}, s_i, ..., s_{i-L})]^{r_i(\rho)}}{r_i(\rho)!}$$

- Approximation using Gaussian distributions by assuming large N_{TX}:

$$\Pr(r_i(\rho)|\bar{r}_i(\rho, s_i, s_{i-1}, ..., s_{i-L}, s_{i+1})) = \Pr(r_i(\rho)|\mu_i(\rho, k)) = \frac{1}{\sqrt{2\pi\mu_i(\rho, k)}} e^{-\frac{(r_i(\rho)-\mu_i(\rho,k))^2}{2\mu_i(\rho,k)}}$$

where $\mu_i(\rho, k) = \bar{r}_i(\rho, s_i, s_{i-1}, ..., s_{i-L}, s_{i+1})$ and $[s_i, s_{i-1}, ..., s_{i-L}, s_{i+1}]$ is the binary expression of k. For $k < 2^{L+1}$, $s_i = 0$ and for $k \geq 2^{L+1}$, $s_i = 1$.

- Reformulated $P_e(\rho, \tau)$:

$$P_e(\rho, \tau) = \frac{1}{2}\left(\int_{\tau}^{+\infty} \Pr(r_i(\rho)|s_i = 0)dr_i(\rho) + \int_{-\infty}^{\tau} \Pr(r_i(\rho)|s_i = 1)dr_i(\rho)\right)$$

where

$$\Pr(r_i(\rho)|s_i = 0) = \sum_{k=0}^{2^{L+1}-1} \frac{\Pr(r_i(\rho)|\mu_i(\rho, k))}{2^{L+1}}, \quad \Pr(r_i(\rho)|s_i = 1) = \sum_{k=2^{L+1}}^{2^{L+2}-1} \frac{\Pr(r_i(\rho)|\mu_i(\rho, k))}{2^{L+1}}$$

Task: Find the region of ρ and τ for small $P_e(\rho, \tau)$ to find out the condition ρ^* follows.

Optimal Start Point

$$P_e(\rho,\tau) = \frac{1}{2^{L+2}} \sum_{k=0}^{2^{L+1}-1} \int_{\tau}^{+\infty} \Pr(r_i(\rho)|\mu_i(\rho,k))dr_i(\rho) + \int_{-\infty}^{\tau} \Pr(r_i(\rho)|\mu_i(\rho,2^{L+1}+k))dr_i(\rho)$$

$$= \frac{1}{2^{L+2}} \sum_{k=0}^{2^{L+1}-1} \operatorname{erfc}\left(\frac{\tau-\mu_i(\rho,k)}{\sqrt{2\mu_i(\rho,k)}}\right) + \operatorname{erfc}\left(\frac{\mu_i(\rho,2^{L+1}+k)-\tau}{\sqrt{2\mu_i(\rho,2^{L+1}+k)}}\right)$$

where $\operatorname{erfc}(z) = 1 - \frac{2}{\sqrt{\pi}} \int_0^z e^{-t^2} dt$.

Assumption: The symbol duration $M\varrho$ is not too short and N_{TX} is large.
Approximation:

$$P_e(\rho,\tau) \simeq \frac{1}{2^{L+2}} \left(\operatorname{erfc}\left(\frac{\tau-\mu_i(\rho,2^{L+1}-1)}{\sqrt{2\mu_i(\rho,2^{L+1}-1)}}\right) + \operatorname{erfc}\left(\frac{\mu_i(\rho,2^{L+1})-\tau}{\sqrt{2\mu_i(\rho,2^{L+1})}}\right) \right)$$

Asymptotic Optimal Start Point

With the approximated BER in hand,

$$P_e(\rho,\tau) \simeq \frac{1}{2^{L+2}} \left(\mathrm{erfc}\Big(\frac{\tau - \mu_i(\rho, 2^{L+1}-1)}{\sqrt{2\mu_i(\rho, 2^{L+1}-1)}}\Big) + \mathrm{erfc}\Big(\frac{\mu_i(\rho, 2^{L+1}) - \tau}{\sqrt{2\mu_i(\rho, 2^{L+1})}}\Big) \right)$$

By letting $\dfrac{dP_e(\rho,\tau)}{d\tau} = 0$

Lemma

The asymptotic optimal threshold is

$$\tau^*(\rho) = \sqrt{\mu_i(\rho, 2^{L+1})\mu_i(\rho, 2^{L+1}-1)[1 + \frac{\ln(\mu_i(\rho, 2^{L+1})) - \ln(\mu_i(\rho, 2^{L+1}-1))}{\mu_i(\rho, 2^{L+1}) - \mu_i(\rho, 2^{L+1}-1)}]} \simeq \sqrt{\mu_i(\rho, 2^{L+1})\mu_i(\rho, 2^{L+1}-1)}$$

Substituting $\tau^*(\rho)$ into $P_e(\rho,\tau)$,

Lemma

The optimal start point ρ^* maximizes $\mu_i(\rho, 2^{L+1}) = C_0(\rho)$ where $C_0(\rho) = \sum_{t=0}^{M-1} \mathbb{C}_{\rho+t}$.

Proposed Data-Aided Synchronization Scheme

Analysis: Find a function $F(\rho)$ to imitate $C_0(\rho)$, the optimal start point maximizes $F(\rho)$.

Note:

$$\bar{r}_i(\rho, s_{i+1}, s_i, ..., s_{i-L}) = s_i C_0(\rho) + s_{i+1} C_{-1}(\rho) + \sum_{j=1}^{L} s_{i-j} C_j(\rho) + C_n$$

$$\bar{r}_i(\rho, s_i = 1) - \bar{r}_i(\rho, s_i = 0) = C_0(\rho)$$

Analysis: $E[N_{s_i=1}] = E[N_{s_i=0}] = K/2$.

$$\lim_{K\to\infty} \sum_{m=0}^{K-1} r_m(\rho, s_m = 1, ..., s_{m-L}, s_{m+1}) = \frac{K}{2} \bar{r}_i(\rho, s_i = 1)$$

$$\lim_{K\to\infty} \sum_{m=0}^{K-1} r_m(\rho, s_m = 0, ..., s_{m-L}, s_{m+1}) = \frac{K}{2} \bar{r}_i(\rho, s_i = 0)$$

Synchronization metric function:

$$F(\rho) \quad = \quad \sum_{m=0}^{K-1} r_m(\rho, s_m = 1..., s_{m-L}, s_{m+1}) - \sum_{m=0}^{K-1} r_m(\rho, s_m = 0..., s_{m-L}, s_{m+1})$$

where $\lim_{K\to\infty} F(\rho) = \frac{K}{2} C_0(\rho)$ and $E[F(\rho)] = \frac{K}{2} C_0(\rho)$.

Proposed Data-Aided Synchronization Scheme

$$E[F(\rho)] = \frac{K}{2} C_0(\rho)$$

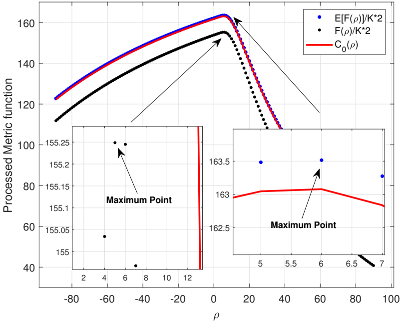


Figure: Comparison of $\frac{E[F(\rho)]}{K/2}$, $\frac{F(\rho)}{K/2}$ and $C_0(\rho)$ (SNR is 30 dB and $K = 64$)

- On average, $\frac{E[F(\rho)]}{K/2}$ is very close to $C_0(\rho)$.
- In one trial, $\hat{\rho}_s^*$ still close to ρ^*.

K-Means-based Non-Data-Aided (Blind) Synchronization Scheme

What if the transmitted symbols s_n are unknown?

Recall:

$$\bar{r}_i(\rho, s_i = 1) - \bar{r}_i(\rho, s_i = 0) = C_0(\rho)$$

Inspiration:
$\bar{r}_i(\rho, s_i = 1)$ is the expectation of signals $r_n(\rho)$ with $s_n = 1$.
-> $\bar{r}_i(\rho, s_i = 1)$ is an arithmetic mean -> centroid -> intermediate variable!

The proposed non-coherent detection: estimating intermediate variables by exploiting K-Means clustering algorithm.

Solution: K-Means clustering algorithm
Assuming the start point ρ, applying K-Means clustering algorithm to the signals $r_n(\rho)$ gives two centroid values. As $\bar{r}_i(\rho, s_i = 1) > \bar{r}_i(\rho, s_i = 0)$, the larger centroid value corresponds to $\hat{\bar{r}}_i(\rho, s_i = 1)$ and the smaller centroid value corresponds to $\hat{\bar{r}}_i(\rho, s_i = 0)$.

Synchronization metric function:

$$G(\rho) = \hat{\bar{r}}_i(\rho, s_i = 1) - \hat{\bar{r}}_i(\rho, s_i = 0)$$

$$G(\rho) = \hat{\hat{r}}_i(\rho, s_i = 1) - \hat{\hat{r}}_i(\rho, s_i = 0)$$

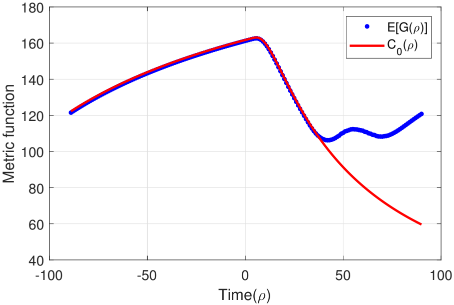


Figure: Comparison of $E[G(\rho)]$ and $C_0(\rho)$ (SNR is 30 dB)

The $E[G(\rho)]$ is in accord with $C_0(\rho)$ around the ρ^* and the estimated optimal start point $\tilde{\rho}^*$ is close to ρ^*

Simulations

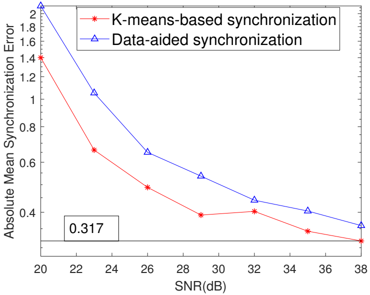


Figure: The absolute mean synchronization error comparison $|E_s(\hat{\rho}_s^* - \rho^*)|$ ($M = 180$ and $K = 64$).

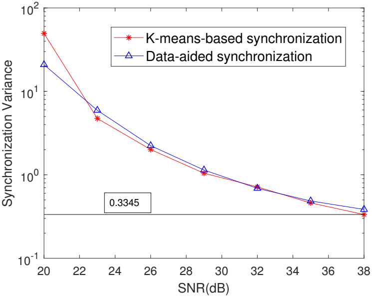


Figure: The synchronization variance comparison $E|\hat{\rho}_s^* - \rho^*|^2$ ($M = 180$ and $K = 64$).

180 samples in each symbol duration!

Summary of Contribution

- The condition the asymptotic start point follows has been proposed.
- The data-aided and non-data-aided synchronization metric functions are proposed.

Conclusion

- Optimal threshold-based receiver and the performance analysis framework are proposed, as well as designing the ANN-based receiver.
- Novel non-coherent receivers are designed by applying K-Means clustering to obtain the key parameters used in reformulated thresholds.
- Data-aided and non-data-aided synchronization metric functions are proposed based on the condition the asymptotic optimal start point follows.

Future Work

- Exploit the probabilistic graphical model (an interpretable methodology for designing ANN based on Bayesian inference) by applying the proposed optimal threshold.
- Apply code theory to non-coherent detection in order to further improve detection performance.
- Investigate the synchronization system using multi-memory-bit-aided thresholds.
- Do experiments to verify the proposed schemes and algorithms.

Publications

- J1 **X. Qian**, M. Di Renzo, A. Eckford, “Molecular Communications: Model-Based and Data-Driven Receiver Design and Optimization”, *IEEE Access*, April, 2019.
- J2 **X. Qian**, M. Di Renzo, A. Eckford, “K-Means Clustering-Aided Non-Coherent Detection for Molecular Communications”, *IEEE Transactions on Communications*, under review, August, 2020.
- J3 **X. Qian**, M. Di Renzo, A. Eckford, “Synchronization for Constant-Threshold-based Receivers in Diffusive Molecular Communication Systems”, *IEEE Transactions on Communications*, in Submission, 2020.
- C1 **X. Qian**, M. Di Renzo,“Receiver Design in Molecular Communications: An Approach Based on Artificial Neural Networks”, *IEEE International Symposium on Wireless Communication Systems*, pp. 1-5, Lisbon, Portugal, 2018.

Publications Outside the Scope of the Thesis

J1 **X. Qian**, M. Di Renzo, J. Liu, A. Kammoun, and M. S. Alouini,"Beamforming Through Reconfigurable Intelligent Surfaces in Single-User MIMO Systems: SNR Distribution and Scaling Laws in the Presence of Channel Fading and Phase Noise", *IEEE Wireless Communications Letters*, accepted, Sep., 2020.

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Thank you!