Advanced Detection Schemes for Molecular Communications based on K-Means Clustering Approach

Seminar, MARACAS, CITI

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Outline

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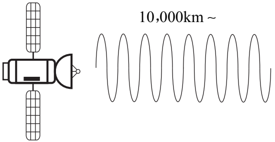
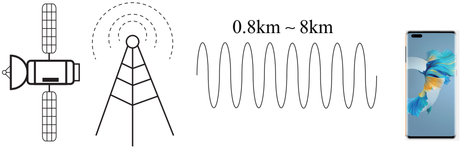
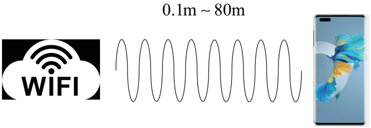
Motivation: Difficulty of EM Wave



(a) Satellite Communications

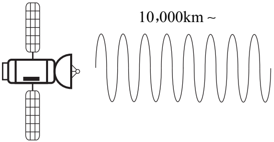


(b) Mobile Communications



(c) Indoor Communications

Figure: Mature Communication Systems



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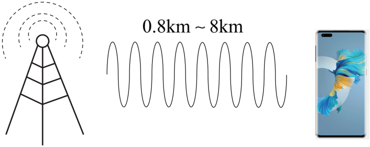

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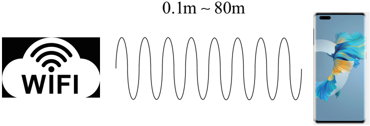

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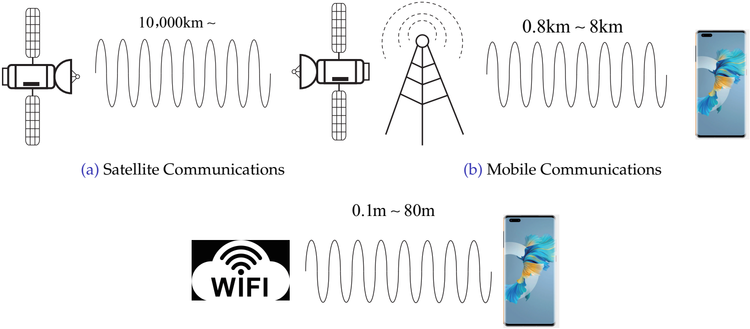
Figure: Mature Communication Systems

- Success of electromagnetic (EM) wave in a variety of systems

Motivation: Difficulty of EM Wave



(a) Satellite Communications (b) Mobile Communications (c) Indoor Communications

Figure: Mature Communication Systems

- 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.

Motivation: Complementary Solution to EM-based Systems

- Solution: Molecular Communications[1]
  Convey information via releasing small particles through aqueous or gaseous medium.

[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/

Motivation: Complementary Solution to EM-based Systems

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- Applications: Micro-robots in blood vessels.

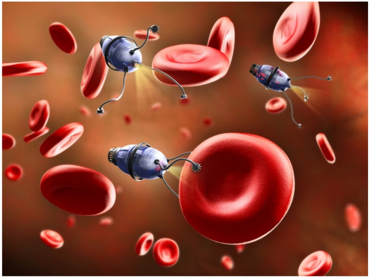

Figure: Micro-robots[2].

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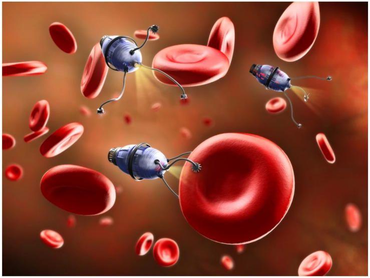

Figure: Micro-robots[2].

How to communicate with these micro-robots?

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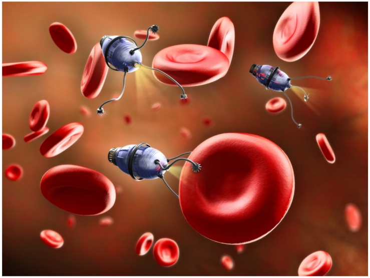

Figure: Micro-robots[2].

How to communicate with these micro-robots? These are the main issues in molecular communications.

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Motivation: Current Progresses

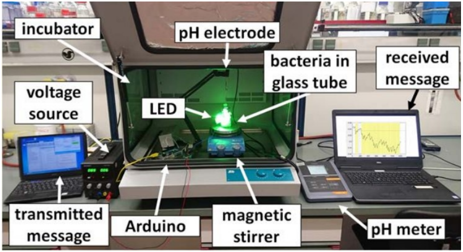


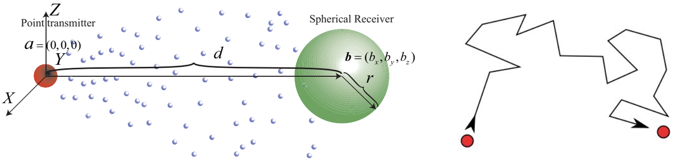
Figure: Optical-to-chemical-signal interface

- Signals can be transmitted by using this optical-to-chemical-signal interface [1].
- Interface of translating chemical signals to electrical signals is on-going.
  - Bacteria-modified receiver
  - Molecule counting receiver

[1] Grebenstein L, Kirchner J, Peixoto RS, Zimmermann W, Irnstorfer F, Wicke W, Ahmadzadeh A, Jamali V, Fischer G, Weigel R, Burkovski A. Biological optical-to-chemical signal conversion interface: A small-scale modulator for molecular communications. IEEE transactions on nanobioscience. 2018 Sep 18;18(1):31-42.

Outline

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.

At the transmitter side: How to modulate symbols?

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A Typical Diffusion-based MC System: Modulation

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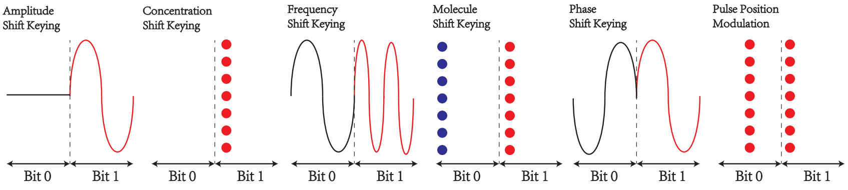

(a) Concentration Shift Keying (b) Molecule Type Shift Keying (c) Pulse Position Modulation

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

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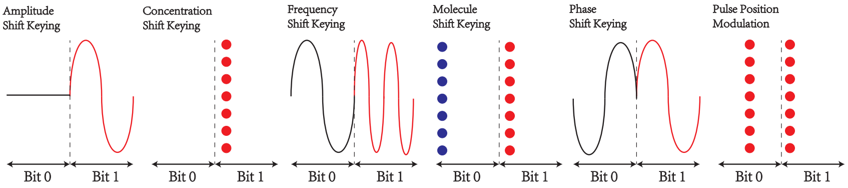

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Note: Binary Concentration shift keying is the simplest and most energy-efficient.

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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., $r(k) \sim \text{Poisson}(\mathbb{C}_k)$.

[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.

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
$\bar{\lambda}_0$	$100s^{-1}$
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

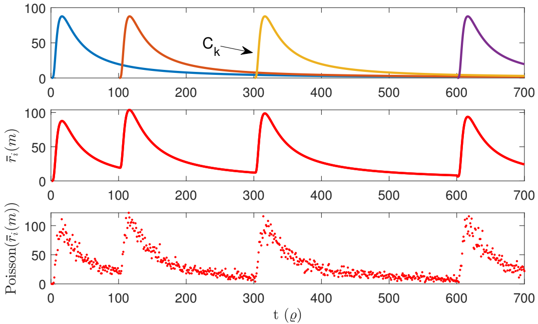

Figure: Sampled channel responses, average samples and actual samples.

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?

[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

How to detect signals r_i?

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

Ideal case[1]

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

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Equivalently, the detection is performed as follows:

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

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]

$$
\begin{aligned}
I_i &\simeq \sum_{j=1}^{K} s_{i-j}C_j + C_n + \sum_{j=K+1}^{L} C_j/2, \quad \Pr_{\text{appro}}(r_i|s_i) = \frac{e^{-(I_i+s_iC_0)}(I_i+s_iC_0)^{r_i}}{r_i!}, \\
\hat{s}_i &= \arg\max_{s_i} \Pr_{\text{appro}}(r_i|s_i) \\
\Rightarrow \hat{s}_i &= \begin{cases} 1 & r_i > \tau|_{s_{i-j},1\le j\le K} \\ 0 & r_i \le \tau|_{s_{i-j},1\le j\le K} \end{cases}, \quad \tau|_{s_{i-j},1\le j\le K} = \frac{C_0}{\ln(1+\frac{C_0}{C_n+\sum_{j=1}^{K} s_{i-j}C_j+\sum_{j=K+1}^{L} C_j/2})}
\end{aligned}
$$

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(1+\frac{C_0}{C_n+\sum_{j=1}^{K} \hat{s}_{i-j}C_j+\sum_{j=K+1}^{L} C_j/2})}
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Outline

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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.

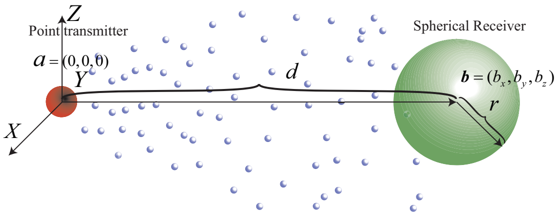

Figure: A diffusion-based MC system

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: An Ideal Case Study

Ideal case: long symbol slot (no ISI)

$$\Pr(r_i|s_i) = \frac{e^{-\bar{r}_i|_{s_i}} (\bar{r}_i|_{s_i})^{r_i}}{r_i!}, \quad \bar{r}_i|_{s_i=1} = C_n + C_0, \quad \bar{r}_i|_{s_i=0} = C_n,$$

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What do signals look like?

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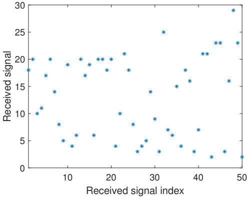

(a) 50 signals

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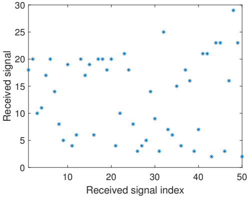

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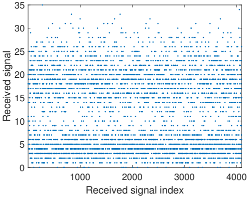

(b) 4096 signals

Ideal case: long symbol slot (no ISI)

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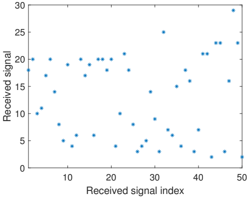

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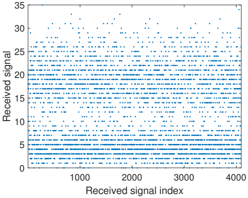

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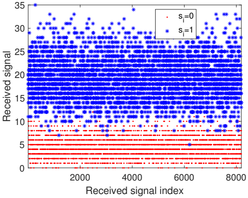

(c) 8192 signals

Figure: Different lengths of signals

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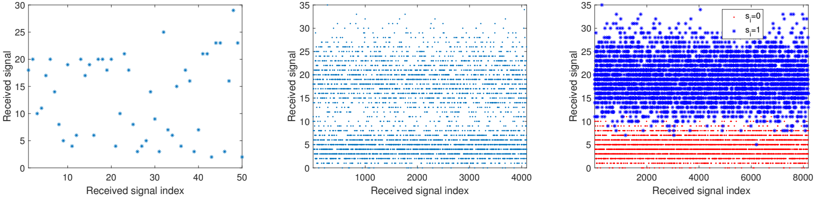

(a) 50 signals

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Figure: Different lengths of signals

From a long sequence of signals, we can obtain some insightful results.

- Two groups of signals with means $C_n + C_0$ (blue markers) and C_n (red markers).
- Separating markers is equivalent to detection.
- The threshold is not the half of the maximum signal. -> $\tau|_{\hat{s}_{i-j}, 1 \le j \le K}$ is necessary.

Problem Formulation: When ISI Exists

Aim: Detection with satisfactory performance under ISI.

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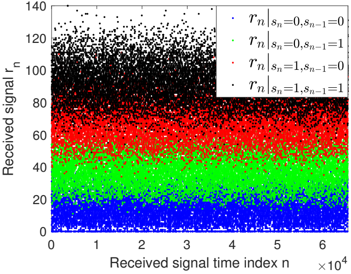

Figure: Four overlapping clusters of received signals (consider the effect of the previous one bit).

Severe ISI leads to more overlapping areas!

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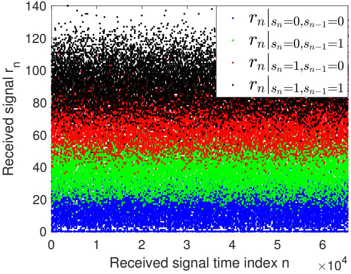

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What can be exploited to compute the threshold except C_j?

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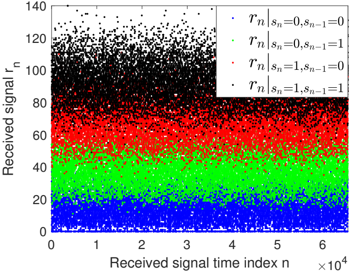

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What can be exploited to compute the threshold except C_j?
What can we infer from these points?

Problem Formulation: When ISI Exists

Observations:

$$\bar{r}_i = s_i C_0 + C_n + \sum_{j=1}^{\mathcal{L}} s_{i-j} C_j + \sum_{j=\mathcal{L}+1}^{L} C_j/2$$

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

Problem Formulation: When ISI Exists

Observations:

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

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 $\bar{r}_i|_{s_i=0, s_{i-j}, 1\leq j\leq \mathcal{L}}$.

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Problem Formulation: When ISI Exists

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$$\bar{r}_i = s_i C_0 + C_n + \sum_{j=1}^{\mathcal{L}} s_{i-j} C_j + \sum_{j=\mathcal{L}+1}^{L} C_j/2$$

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

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

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.

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

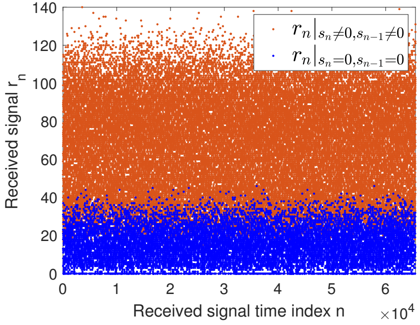

Figure: Comparison of $r_n|_{s_n=0,s_{n-1}=0}$ and other signals.

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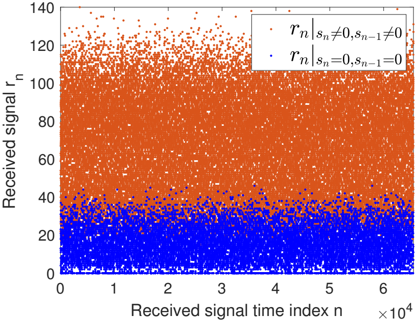

Figure: Comparison of $r_n|_{s_n=0,s_{n-1}=0}$ and other signals.

- $\kappa_{n,s_i=0,s_{i-1}=0}$ 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

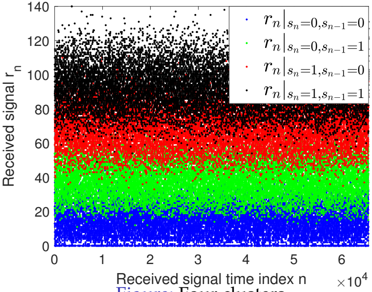

Figure: Four clusters.

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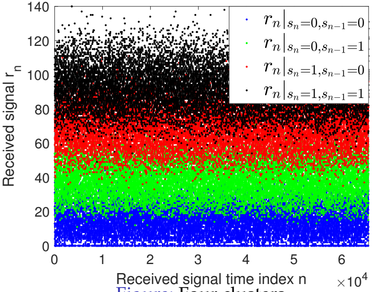
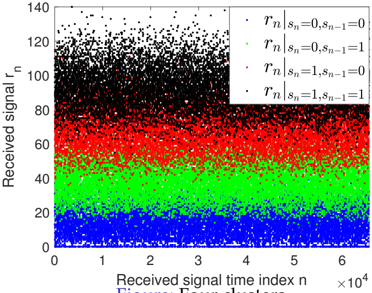


Figure: Four clusters.

- 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.



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Problem summary

Given signals r_n

1. **separate** r_n into several groups (clusters).
2. **compute** the corresponding centroids (arithmetical mean).
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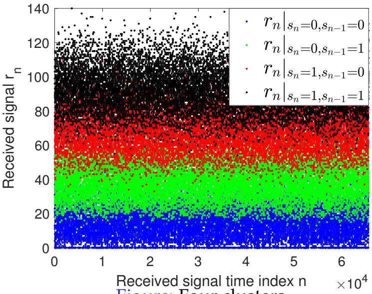

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Note: Separating points into several clusters is called clustering.
A simple clustering algorithm is K-Means clustering algorithm which can solve problem 1 and 2.

Outline

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:

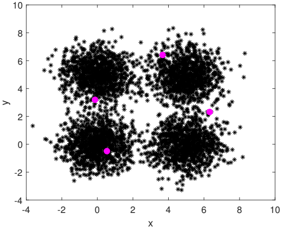
$$\kappa_{n,k} = \begin{cases} 1, & \text{if} \quad k = \arg\min_j \|\boldsymbol{x}_n - \boldsymbol{\mu}_j\|^2 \\ 0, & \text{otherwise} \end{cases}$$

Step II: Update the cluster centroid:

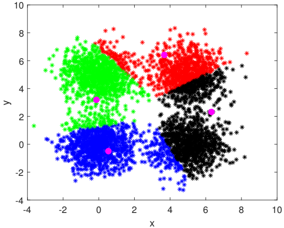
$$\boldsymbol{\mu}_k = \frac{\sum_n \kappa_{n,k} \boldsymbol{x}_n}{\sum_n \kappa_{n,k}}$$

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

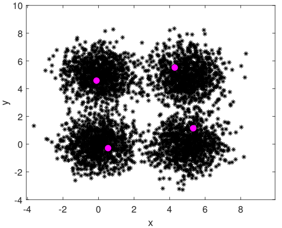
K-Means Clustering Algorithm



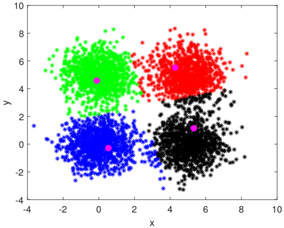
(a) Randomly select initial centroids



(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 $[s_i, s_{i_1}] = [0, 0]$, $[s_i, s_{i_1}] = [0, 1]$, $[s_i, s_{i_1}] = [1, 0]$, $[s_i, s_{i_1}] = [1, 1]$.

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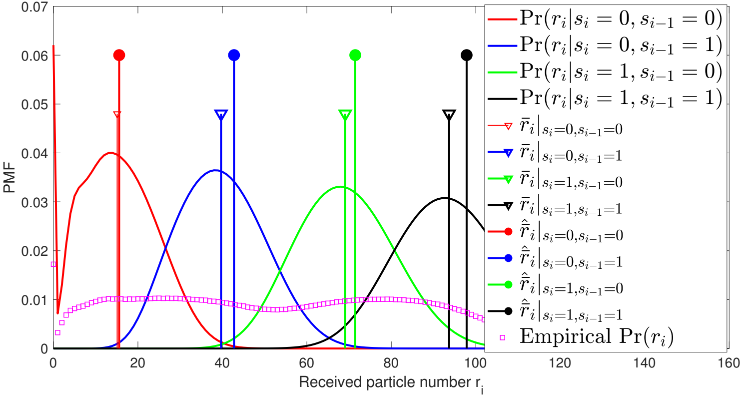

Figure: The positions of $\bar{r}_i|_{s_i,s_{i-1}}$ and $\hat{\bar{r}}_i|_{s_i,s_{i-1}}$ corresponding to the centroids obtained by K-Means algorithm and assuming that the labels $[s_i, s_{i-1}]$ are known) for $T = 30\varrho$

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

Question: How to avoid or **reduce** the overlapping areas of clusters?

Multi-Dimensional Clustering

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Solution: Construct multi-dimensional elements.

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

Multi-Dimensional Clustering

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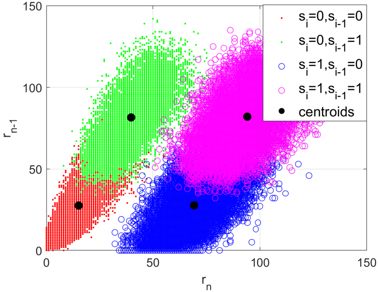
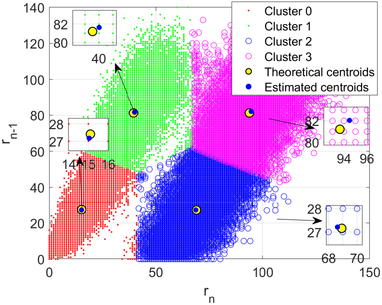
Case Study: One memory bit implies 2-D clustering for points $[r_n, r_{n-1}]$.



(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.

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- 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 $\max(\boldsymbol{r})$.

Setup of the Initial Centroids

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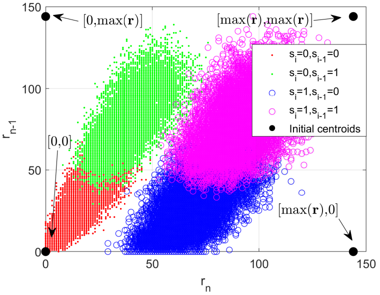

Figure: The customized initial centroids and the corresponding clusters ($T = 30\varrho$)

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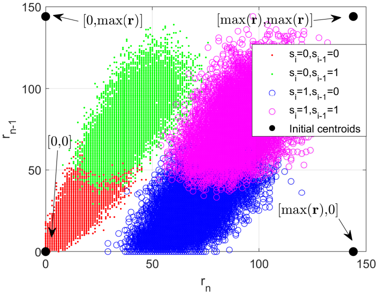

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Example 1: $[0, \max(\boldsymbol{r})]$ corresponds to the label $[s_i, s_{i-1}] = [0, 1]$ and the estimated centroid is $[\hat{\bar{r}}_i|_{s_i=0,s_{i-1}=1}, \hat{\bar{r}}_{i-1}|_{s_{i-1}=1}]$.

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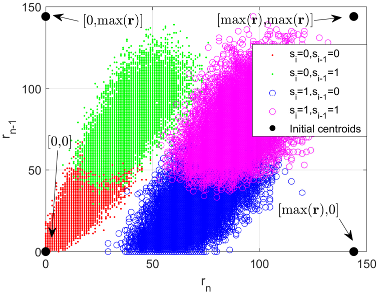

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Remark

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** $\hat{s}_n$.

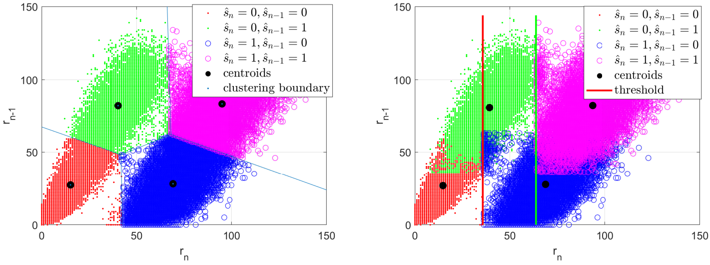
Algorithm 1: Direct clustering-based inference

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

Simulations and Analysis: : One-Bit Information

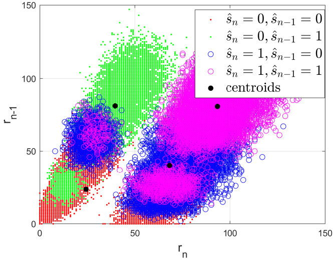


(a) Direct clustering-based inference (b) Clustering-plus-threshold detection

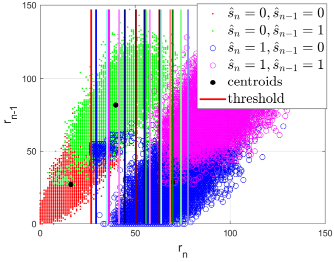
Figure: Distribution of $[r_n, r_{n-1}]|_{\hat{s}_n, \hat{s}_{n-1}}$ and estimated centroids ($\mathcal{L} = 1$ and $T = 30\varrho$).

- 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.
- $[r_n, r_{n-1}]|_{\hat{s}_n, \hat{s}_{n-1}}$ denotes one point and the corresponding estimated label while $[r_n, r_{n-1}]|_{s_n, s_{n-1}}$ denotes the point with the correct label.
- 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.

Simulations and Analysis: Multi-Bit Information



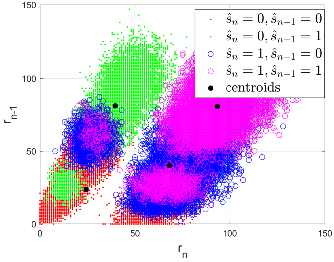
(a) Direct clustering-based inference



(b) Clustering-plus-threshold detection

Figure: Distribution of $[r_n, r_{n-1}]|_{\hat{s}_n, \hat{s}_{n-1}}$ and estimated centroids ($\mathcal{L} = 4$ and $T = 30\varrho$).

- If more clusters are considered (large $\mathcal{L}$), Algorithm 1 is worse mainly due to mis-clustering errors in high dimension.
- Threshold can help reduce detection errors.



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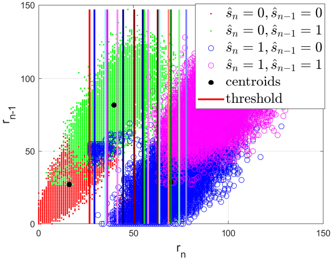

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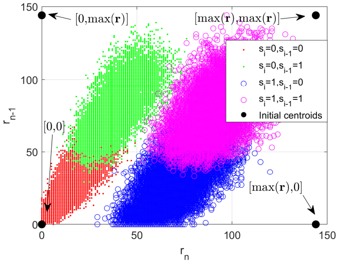
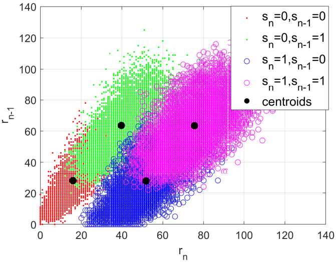
- If more clusters are considered (large $\mathcal{L}$), Algorithm 1 is worse mainly due to mis-clustering errors in high dimension.
- Threshold can help reduce detection errors.
- Preferable detection scheme: large $\mathcal{L}$, threshold.

A Case Study: When ISI is Severe (Short Symbol Slot)



(a) Initial centroids using $\max(\boldsymbol{r})$ in long symbol slot case

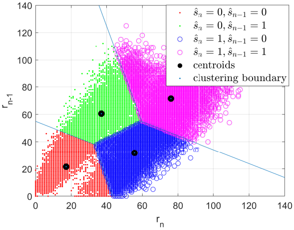


(b) Short symbol slot case

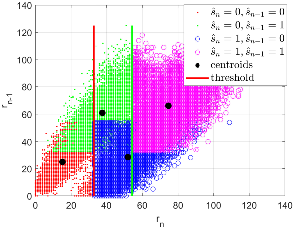
Figure: Distribution of $[r_n, r_{n-1}]|_{s_n, s_{n-1}}$ and exact labels.

- Under severe ISI, there will be more overlapping area.
- Initial centroids constructed using $\max(\boldsymbol{r})$ may lead to more errors.

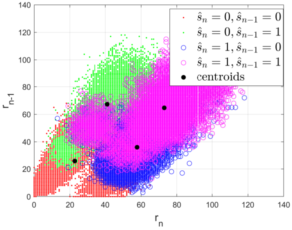
A Case Study: When ISI is Severe (Short Symbol Slot)



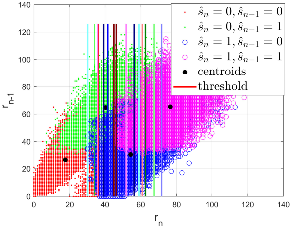
(a) Direct clustering-based inference $\mathcal{L} = 1$



(b) Clustering-plus-threshold detection $\mathcal{L} = 1$



(c) Direct clustering-based inference $\mathcal{L} = 4$



(d) Clustering-plus-threshold detection $\mathcal{L} = 4$

Figure: Distribution of $[r_n, r_{n-1}]|_{\hat{s}_n, \hat{s}_{n-1}}$, estimated centroids and clustering boundaries/thresholds ($T = 20\ \Delta T$).

Outline

Iterative Algorithm for Computing the Initial Centroids

From the above case study, $\hat{\hat{r}}_m|_{s_{m-j}=s_{i-j},0\leq j\leq \mathcal{L}}$ are not accurate enough.
-> The initial centroids using $\max(\boldsymbol{r})$ are not close to theoretical centroid sufficiently.

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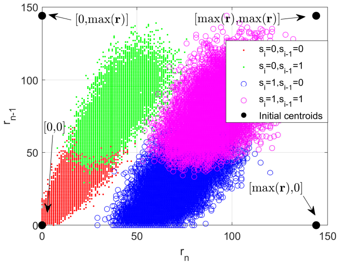

(a) Initial centroids using $\max(\boldsymbol{r})$

Observation: Algorithm 1 and 2 exploit 0 and $\max(\boldsymbol{r})$.

Iterative Algorithm for Computing the Initial Centroids

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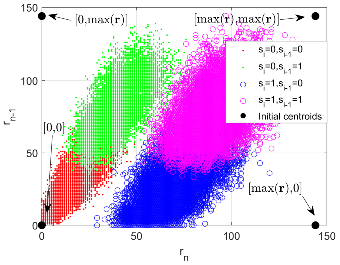

(a) Initial centroids using $\max(\boldsymbol{r})$

Idea: Can other values a and b be exploited with $0 < a < b < \max(\boldsymbol{r})$?
-> New initial centroids $[a, a]$, $[a, b]$, $[b, a]$ and $[b, b]$.
-> One dimension clustering ($a = \hat{\hat{r}}_m|_{s_m=0}$ and $b = \hat{\hat{r}}_m|_{s_m=1}$)

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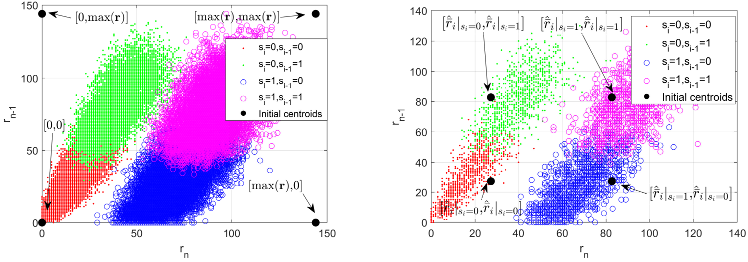

(a) Initial centroids using $\max(\boldsymbol{r})$

(b) Initial centroids using $\hat{\hat{r}}_i|_{s_i}$

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

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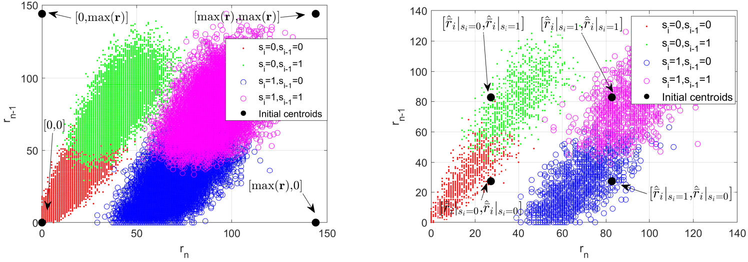

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-> One dimension clustering ($a = \hat{\hat{r}}_m|_{s_m=0}$ and $b = \hat{\hat{r}}_m|_{s_m=1}$)

After 2-D clustering, the initial centroids are updated via:

$$\boldsymbol{\mu}_k = [\hat{\hat{r}}_m|_{s_{m-j}=s_{i-j},0\leq j\leq l-1}, \hat{\hat{r}}_m|_{s_{m-j}=s_{i-1-j},0\leq j\leq l-1}, \hat{\hat{r}}_{m-1}|_{s_{m-j}=s_{i-1-j},1\leq j\leq l-1}, \ldots, \hat{\hat{r}}_{m-l+1}|_{s_{m-l+1}=s_{i-l}}]$$

Iterative Algorithm for Computing the Initial Centroids

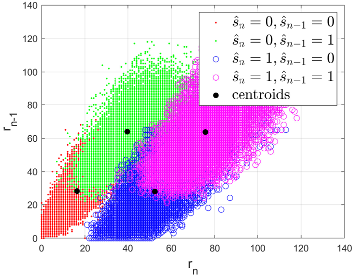
Algorithm 3: Iterative clustering-based inference

Set the initial centroids $\boldsymbol{\mu}_0 = 0$ and $\boldsymbol{\mu}_1 = \max(\boldsymbol{r})$
for $l = 1$ to $\mathcal{L}+1$ **do**
    Construct the data $\boldsymbol{r}_n = [r_n, ..., r_{n-l+1}]$
    Cluster $\boldsymbol{r}_n$ using the K-means algorithm with the initial centroids $\boldsymbol{\mu}_k$
    Set the new initial centroids to $\boldsymbol{\mu}_k$ by using (36)
end for
Infer $\hat{s}_n$ from the indicator variables $\kappa_{n,k}$

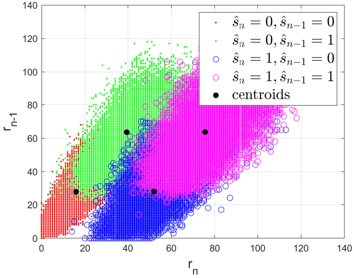
Algorithm 4: Iterative clustering-plus-threshold detection

Set the initial centroids $\boldsymbol{\mu}_0 = 0$ and $\boldsymbol{\mu}_1 = \max(\boldsymbol{r})$
for $l = 1$ to $\mathcal{L}+1$ **do**
    Construct the data $\boldsymbol{r}_n = [r_n, ..., r_{n-l+1}]$
    Cluster $\boldsymbol{r}_n$ using the K-means algorithm with the initial centroids $\boldsymbol{\mu}_k$
    Set the new initial centroids to $\boldsymbol{\mu}_k$
end for
Obtain $\hat{\bar{r}}_i|_{\hat{s}_{i-j},0\le j\le\mathcal{L}}$ from the estimated centroids $\hat{\boldsymbol{\mu}}_k$
Compute the detection thresholds using $\hat{\bar{r}}_i|_{\hat{s}_{i-j},0\le j\le\mathcal{L}}$
Detect the symbols using $\hat{\bar{\tau}}|_{\hat{s}_{i-j},1\le j\le\mathcal{L}}$

Iterative Algorithm for Computing the Initial Centroids



(a) Iterative clustering-based inference

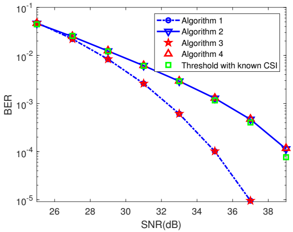


(b) Iterative clustering-plus-threshold detection

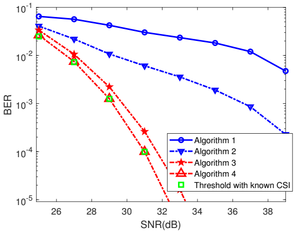
Figure: Distribution of $[r_n, r_{n-1}]|_{\hat{s}_n, \hat{s}_{n-1}}$ and estimated centroids ($\mathcal{L} = 4$, $T = 20\Delta T$).

- The iterative algorithms yield better detection performance even under severe ISI.

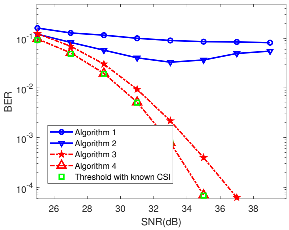
Simulations and Analysis



(a) $\mathcal{L} = 1$ and $T = 30\ \Delta T$ (mild ISI)



(b) $\mathcal{L} = 4$ and $T = 30\ \Delta T$ (mild ISI)



(c) $\mathcal{L} = 4$ and $T = 20\ \Delta T$ (severe ISI)

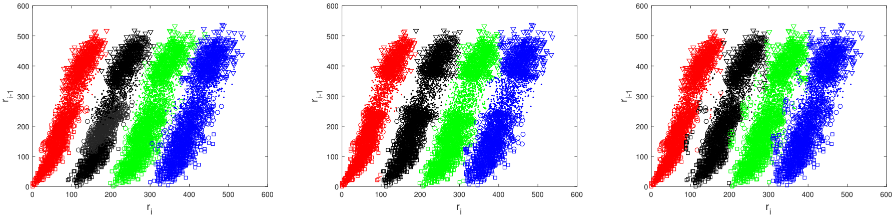
Figure: BER comparison of the proposed algorithms

Outline

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.
- Four algorithms are proposed and analysed for better understanding the non-coherent detection and proposing better algorithms.

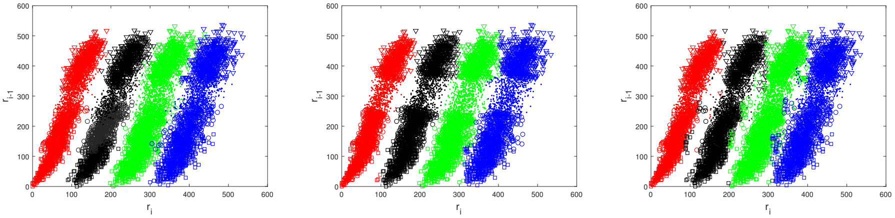
Application to multi-level molecular communications



(a) Exact distribution (b) Algorithm 3 (c) Algorithm 4

Figure: Distribution of $[r_n, r_{n-1}]|_{\hat{s}_n, \hat{s}_{n-1}}$

Application to multi-level molecular communications



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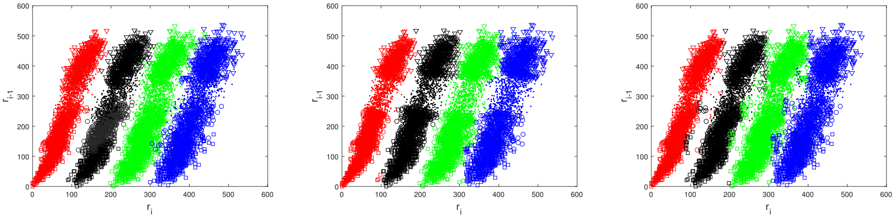
Application to other modulation schemes, e.g., Molecular type shift keying, Pulse position modulation

Future work

Application to multi-level molecular communications



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Application to mobile molecular communications

Future work

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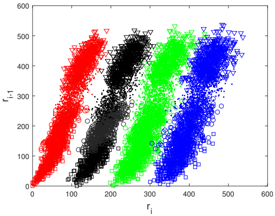
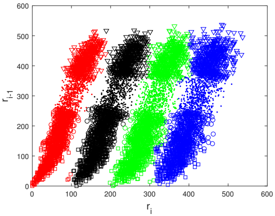
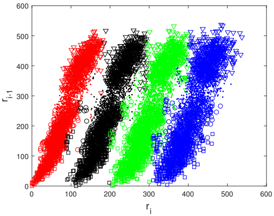


(a) Exact distribution



(b) Algorithm 3



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Thanks!
Q & A