Channel Estimation in Diffusion-Based Molecular Communication

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1. Introduction to Molecular Communications
2. Channel Impulse Response
3. Channel Estimation Techniques
4. Training Sequence Design
5. Conclusions and Future Work

- Molecular communication enables communication between nanomachines
- **Definition:** Nanomachines are “machines" whose components have sizes of up to a few hundred nanometer
- Nanomachines may be biological (e.g. cells) or non-biological (e.g. nanosensors)
- Molecular communication is prevalent in "natural" biological systems
- We try to harness molecular communication for man-made communication systems

- Molecular communication enables communication between nanomachines
- **Definition:** Nanomachines are “machines" whose components have sizes of up to a few hundred nanometer
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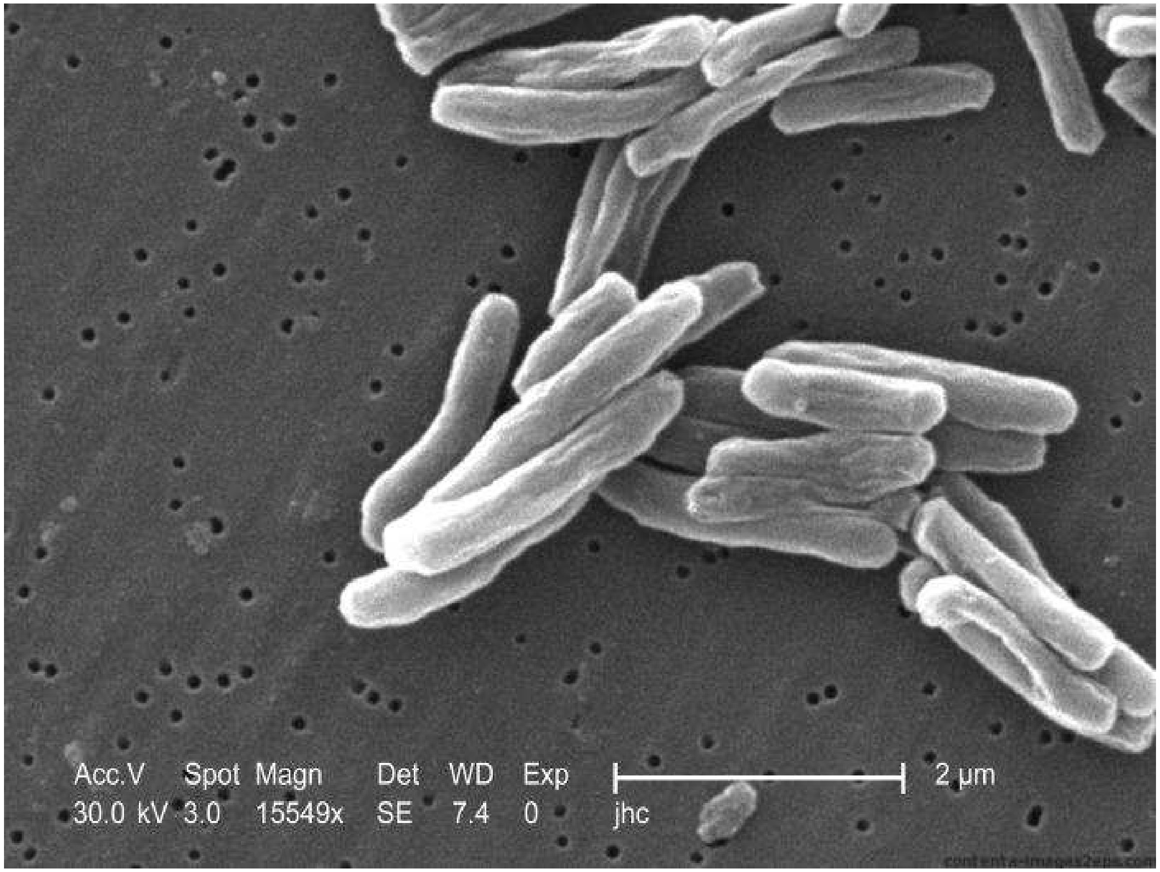
- Molecular communication is prevalent in "natural" biological systems
- We try to harness molecular communication for man-made communication systems
- **We have to develop functionalities that enable man-made molecular communication**
  - Develop “hardware" components for molecular communication
  - Develop pertinent communication-theoretical and signal processing tools

Example for natural nanonetwork (bacteria):



Source: US CDC

Molecular communication presents the following advantages

- Feasibility - regarded as easier to implement than other approaches in the near term
- Scale - appropriate size for nanomachines
- Bio-compatibility - integration with living systems possible (though not guaranteed!)
- Energy efficiency - biochemical reactions have high efficiencies
- Functional complexity - billions of years of evolution

Other advantages depend on the particular implementation and application

Biomedical Applications

- Targeted drug delivery - cooperatively release medication
- Health monitoring - identify presence of toxic substances
- Genetic engineering - Manipulate DNA

Environmental Applications

- Environmental monitoring - detection of pollutants or toxins
- Degradation - safe conversion of undesired materials

Manufacturing

- Quality control - identification of product defects
- Bottom-up formation - precise construction of components
- New functionality - integrate nanonetworks into new products

1959	Richard Feynmans famous lecture "There's Plenty of Room at the Bottom"
1965	Johnson and Knudsen use information theory to explain effects in kidneys
2002	Toby Berger mentioned molecular communication in the 2002 Shannon Lecture
2008	IEEE ComSoc founds Technical Subcommittee on this topic
2010	First issue of Elsevier journal "Nano Communication Networks" appears
2011	New workshops, special sessions, and tracks at various IEEE and ACM conferences (ongoing)
2012	IEEE ComSoc founds "Molecular, Biological, and Multi-Scale Communication Series" in IEEE Journal on Selected Areas in Communications
2013	IEEE founds standardization working group for "Recommended Practice for Nanoscale and Molecular Communication Framework"
2015	New ComSoc journal "IEEE Transactions on Molecular, Biological, and Multi-Scale Communications"

Candidate design strategies for communication:

- Free diffusion
- Gap junctions
- Molecular motors
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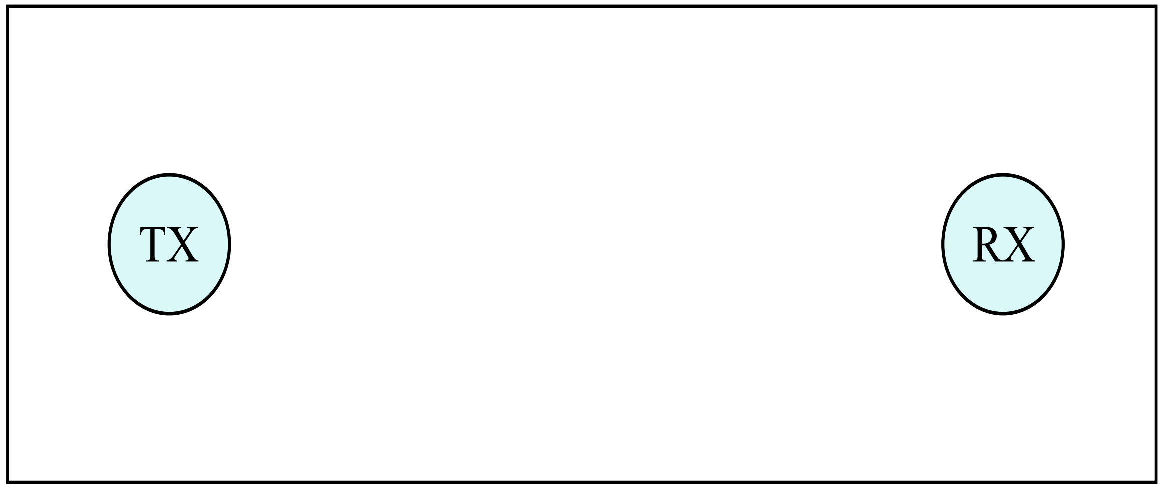
Let's consider a simple modulation scheme



- TX has binary message for RX

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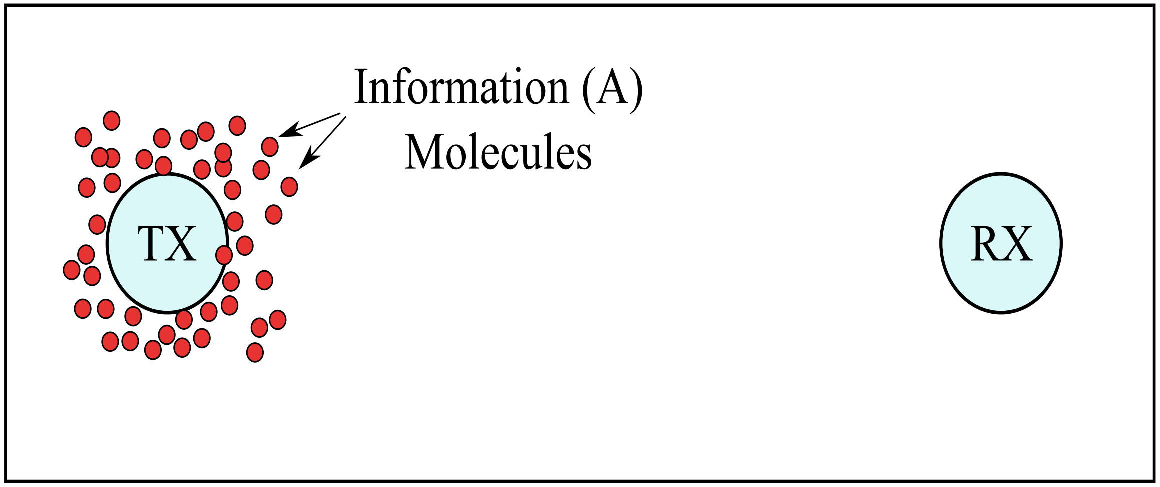

- TX has binary message for RX
- TX uses binary modulation – A molecules are released to indicate a binary 1, no molecules are emitted to represent a binary 0

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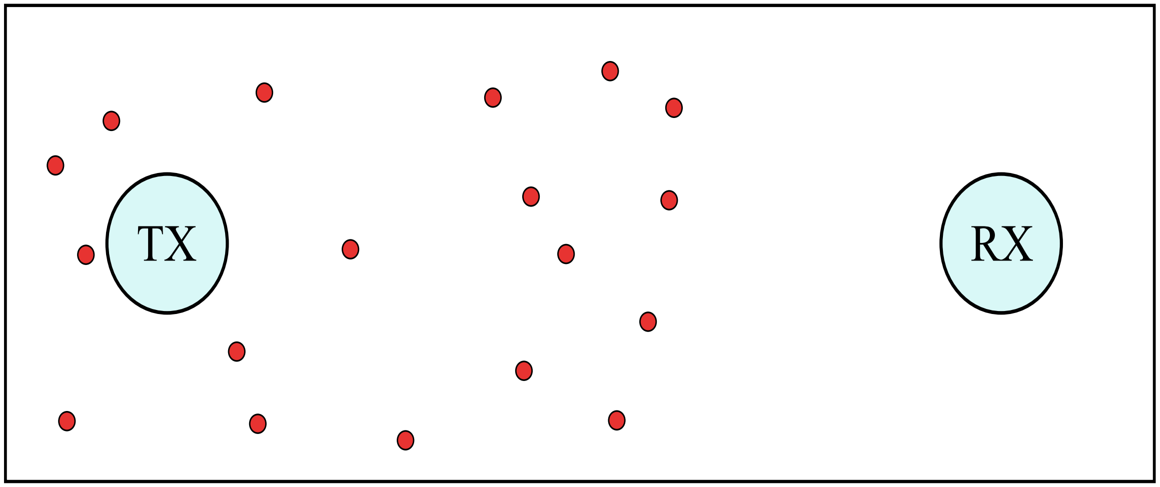

- TX has binary message for RX
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- A molecules diffuse freely in unbounded environment

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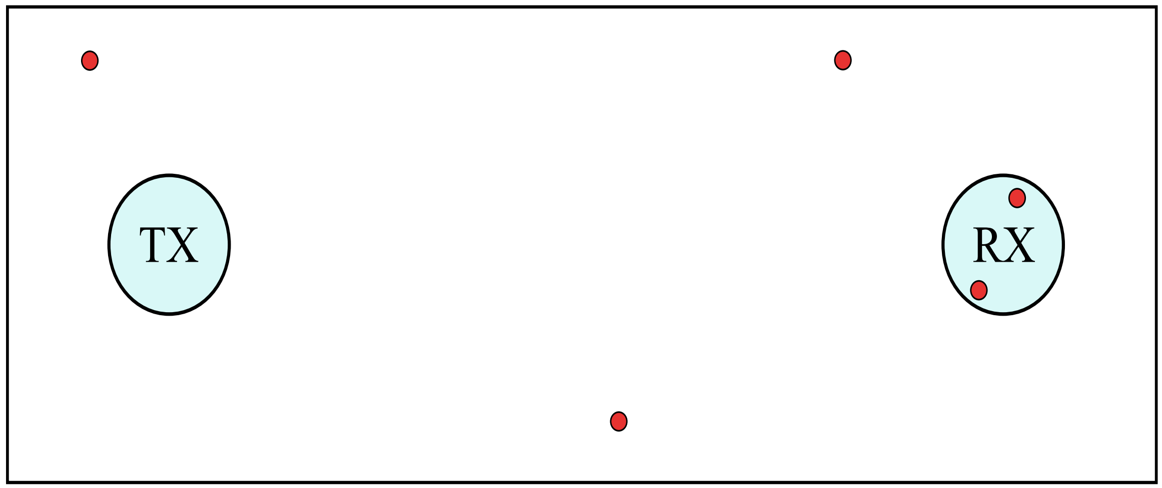

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(Diffusive) molecular communication presents the following challenges

- Design and modelling of components of communication system
- Processing capabilities may be limited and vastly different from other types of communication systems
- Modulation and coding schemes have to be developed
- Detection and equalization are necessary to extract information from received signal
- Synchronization between transmitting and receiving nodes has to be established
- Channel between TX and RX has to be learned at RX

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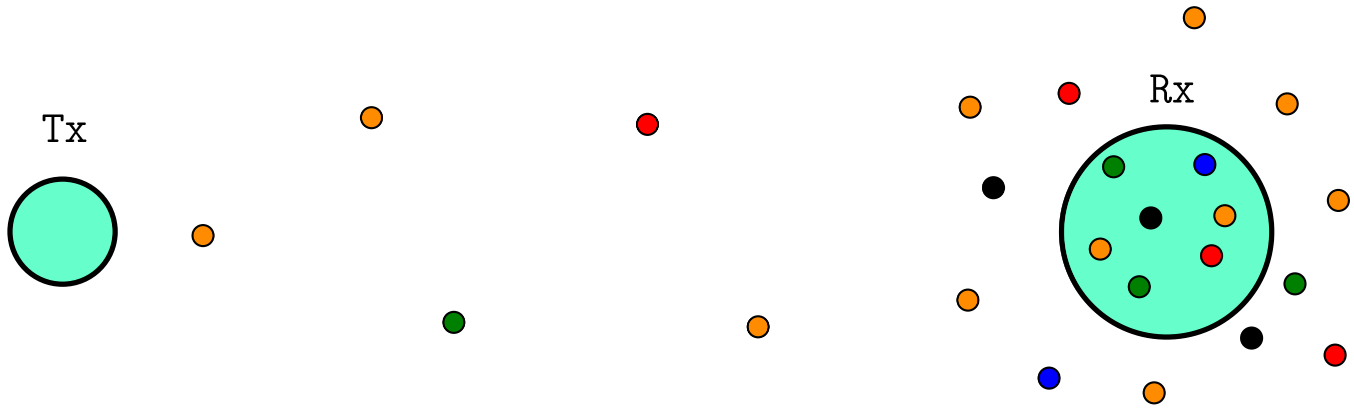


- Transmitter: Releases 0 or N information molecules at the beginning of each signalling interval
- ON/OFF keying: Number of emitted molecules $Ns[k]$, $s[k] \in \{0, 1\}$
- Receiver: Received (random) signal

$$r[k] = \sum_{l=1}^{L} c_l[k] + c_{\mathrm{n}}[k]$$

Receiver: Received (random) signal

$$r[k] = \sum_{l=1}^{L} c_l[k] + c_\mathrm{n}[k]$$

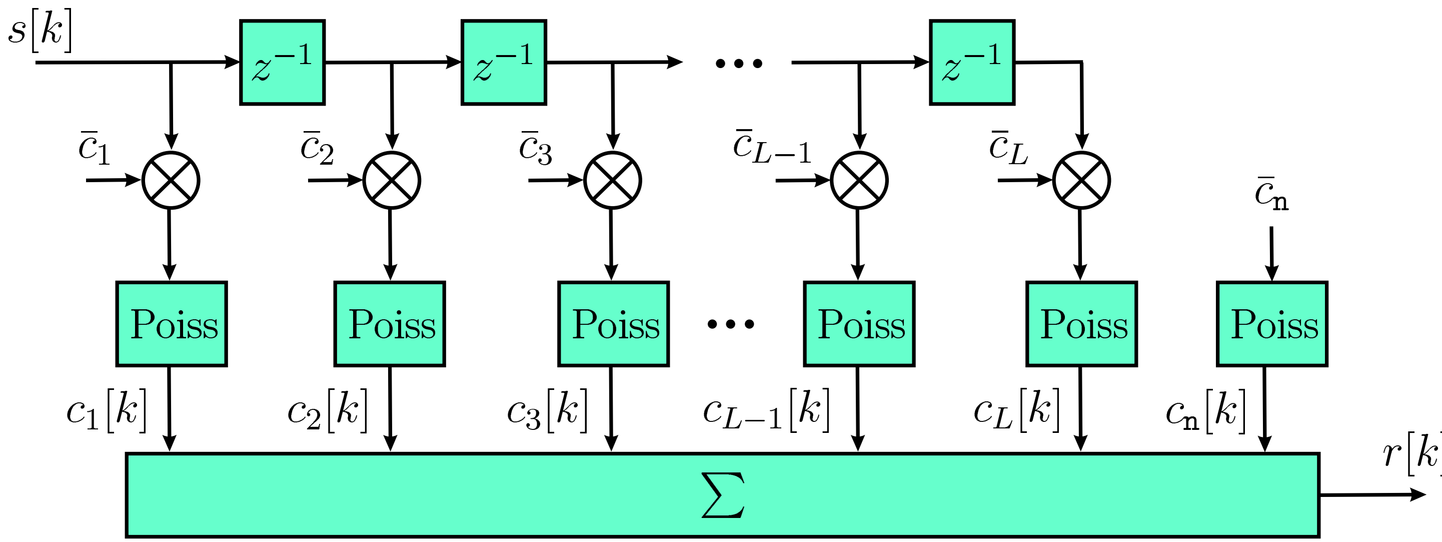
- $c_l[k]$ is the random number of molecules observed at Rx in symbol interval k due to emission of $Ns[k-l+1]$ molecules at Tx in symbol interval $k-l+1$
- $c_l[k]$ follows a Binomial distribution
- $c_l[k]$ is well approximated by a Poisson random variable with mean $\bar{c}_l s[k-l+1]$

$$c_l[k] \sim \mathrm{Poiss}\left(\bar{c}_l s[k-l+1]\right)$$

- $c_\mathrm{n}[k]$ is noise originating from other sources and modelled as

$$c_\mathrm{n}[k] \sim \mathrm{Poiss}\left(\bar{c}_\mathrm{n}\right)$$

where $\bar{c}_\mathrm{n} = \mathcal{E}\left\{c_\mathrm{n}[k]\right\}$.



- Observation: We are not dealing with a conventional linear time-invariant system
- Challenge 1: $c_l[k]$ changes independently from symbol interval to symbol interval
  $\Rightarrow$ Estimating $c_l[k]$ would be pointless
- Challenge 2: Mean $\bar{c}_l$ is constant but $r[k]$ does not depend linearly on $\bar{c}_l$

Solution: Consider *expected* received signal

$$\bar{r}[k] = \mathcal{E}\left\{r[k]\right\} = \sum_{l=1}^{L} \bar{c}_l s[k-l+1] + \bar{c}_{\mathtt{n}}.$$

- The above equation characterizes a linear time-invariant system with input $s[k]$ and output $\bar{r}[k]$
- $\bar{c}_l$, $l \in \{1, \ldots, L\}$, may be considered as the impulse response of this system
- In a slight abuse of notation, we will refer to

  $$\bar{\mathbf{c}} = [\bar{c}_1, \bar{c}_2, \ldots, \bar{c}_L, \bar{c}_{\mathtt{n}}]^T$$

  as channel impulse response (CIR) in the following.
- Knowledge of CIR is needed for detection, channel estimation, inferring properties of channel, ...

CIR depends on

- Shape and properties of TX: Point source, spherical source, ...
- Shape and properties of RX: Transparent receiver, absorbing receiver, ...
- Properties of environment: Diffusion coefficient, flow, molecule degradation, distance between TX and RX, ...
- Simple example: Point source, fully transparent receiver, infinite environment

$$\bar{c}(t) = \iiint_{\mathbf{x} \in V^{\mathtt{rec}}} \bar{\mathcal{C}}(\mathbf{x}, t) \mathrm{d}x \mathrm{d}y \mathrm{d}z.$$

with

$$\bar{\mathcal{C}}(\mathbf{x}, t) = \frac{N}{(4\pi D t)^{3/2}} \exp\left(-\frac{|\mathbf{x}|^2}{4Dt}\right)$$

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Problem Statement

- Objective: Estimation of CIR $\bar{\mathbf{c}}$
- Given:
  - Training sequence emitted by Tx:
  $$\mathbf{s} = [s[1], s[2], \ldots, s[K]]^T$$
  - (Random) observations at receiver
  $$\mathbf{r} = [r[L], r[L+1], \ldots, r[K]]^T$$
  - Potentially, probability density function (PDF) of $\bar{\mathbf{c}}$, $f_{\bar{\mathbf{c}}}(\bar{\mathbf{c}})$
- Known: Conditional PDF

$$f_{\mathbf{r}}(\mathbf{r}|\bar{\mathbf{c}}, \mathbf{s}) = \prod_{k=L}^{K} \frac{\left(\bar{\mathbf{c}}^T \mathbf{s}_k\right)^{r[k]} \exp\left(-\bar{\mathbf{c}}^T \mathbf{s}_k\right)}{r[k]!}.$$

Performance Bounds

- Cramer Rao (CR) Bound: The estimation error variance of any *unbiased* estimator $\hat{\bar{\mathbf{c}}}$ is lower bounded by the CR bound
- Classical CR Bound: Considering $\bar{\mathbf{c}}$ as a *deterministic* parameter, the variance of the estimation error $\mathbf{e} = \bar{\mathbf{c}} - \hat{\bar{\mathbf{c}}}$ is bounded as

$$\mathcal{E}_{\mathbf{r}|\bar{\mathbf{c}}}\left\{\|\mathbf{e}\|^2\right\} \geq \mathrm{tr}\left\{\mathbf{I}^{-1}\left(\bar{\mathbf{c}}\right)\right\} = \mathrm{tr}\left\{\left[\sum_{k=L}^{K}\frac{\mathbf{s}_k\mathbf{s}_k^T}{\bar{\mathbf{c}}^T\mathbf{s}_k}\right]^{-1}\right\}$$

  where $\mathbf{I}\left(\bar{\mathbf{c}}\right)$ is the Fisher information matrix and $\mathbf{s}_k = [s[k], s[k-1], \dots, s[k-L+1], 1]^T$.

- Bayesian CR Bound: Considering $\bar{\mathbf{c}}$ as a *stochastic* parameter with PDF $f_{\bar{\mathbf{c}}}(\bar{\mathbf{c}})$, the variance of the estimation error is bounded as

$$\mathcal{E}_{\mathbf{r},\bar{\mathbf{c}}}\left\{\|\mathbf{e}\|^2\right\} \geq \mathrm{tr}\left\{\left[\mathcal{E}_{\bar{\mathbf{c}}}\left\{-\nabla^2_{\bar{\mathbf{c}}\bar{\mathbf{c}}}\ln\{f_{\bar{\mathbf{c}}}(\bar{\mathbf{c}})\} + \sum_{k=L}^{K}\frac{\mathbf{s}_k\mathbf{s}_k^T}{\bar{\mathbf{c}}^T\mathbf{s}_k}\right\}\right]^{-1}\right\}$$

Maximum-likelihood (ML) Estimation:

- Definition:

$$\hat{\bar{\mathbf{c}}}^{\mathtt{ML}} = \underset{\bar{\mathbf{c}} \geq \mathbf{0}}{\operatorname{argmax}} \; f_{\mathbf{r}}(\mathbf{r}|\bar{\mathbf{c}}, \mathbf{s}).$$

- Solution: Leads to a nonlinear system of equations.

Least Sum of Squared Errors (LSSE) Estimation:

- Definition:

$$\hat{\bar{\mathbf{c}}}^{\mathtt{LSSE}} = \underset{\bar{\mathbf{c}} \geq \mathbf{0}}{\operatorname{argmin}} \; \|\boldsymbol{\epsilon}\|^2$$

where $\boldsymbol{\epsilon} = \mathbf{r} - \mathcal{E}\left\{\mathbf{r}\right\} = \mathbf{r} - \mathbf{S}\bar{\mathbf{c}}$ where $\mathbf{S} = \left[\mathbf{s}_L, \mathbf{s}_{L+1}, \ldots, \mathbf{s}_K\right]^T$.

- Candidate solution:

$$\bar{\mathbf{c}}^{\mathtt{LSSE}} = \mathbf{F}^{\mathtt{LSSE}}\mathbf{r}$$

where $\mathbf{F}^{\mathtt{LSSE}} = \left(\mathbf{S}^T\mathbf{S}\right)^{-1}(\mathbf{S})^T$. Additional similar problems have to be solved if $\bar{\mathbf{c}}^{\mathtt{LSSE}} \geq \mathbf{0}$ does not hold.

Maximum a Posteriori (MAP) Estimation:

- Definition:

$$\hat{\bar{\mathbf{c}}}^{\mathtt{MAP}} = \underset{\bar{\mathbf{c}} \geq \mathbf{0}}{\mathrm{argmax}} \; f_{\bar{\mathbf{c}}}(\bar{\mathbf{c}}|\mathbf{r},\mathbf{s}) = \underset{\bar{\mathbf{c}} \geq \mathbf{0}}{\mathrm{argmax}} \; f_{\mathbf{r}}(\mathbf{r}|\bar{\mathbf{c}},\mathbf{s}) f_{\bar{\mathbf{c}}}(\bar{\mathbf{c}})$$

- Solution: Leads to a nonlinear system of equations.

Minimum Mean Square Error (MSSE) Estimation:

- Definition:

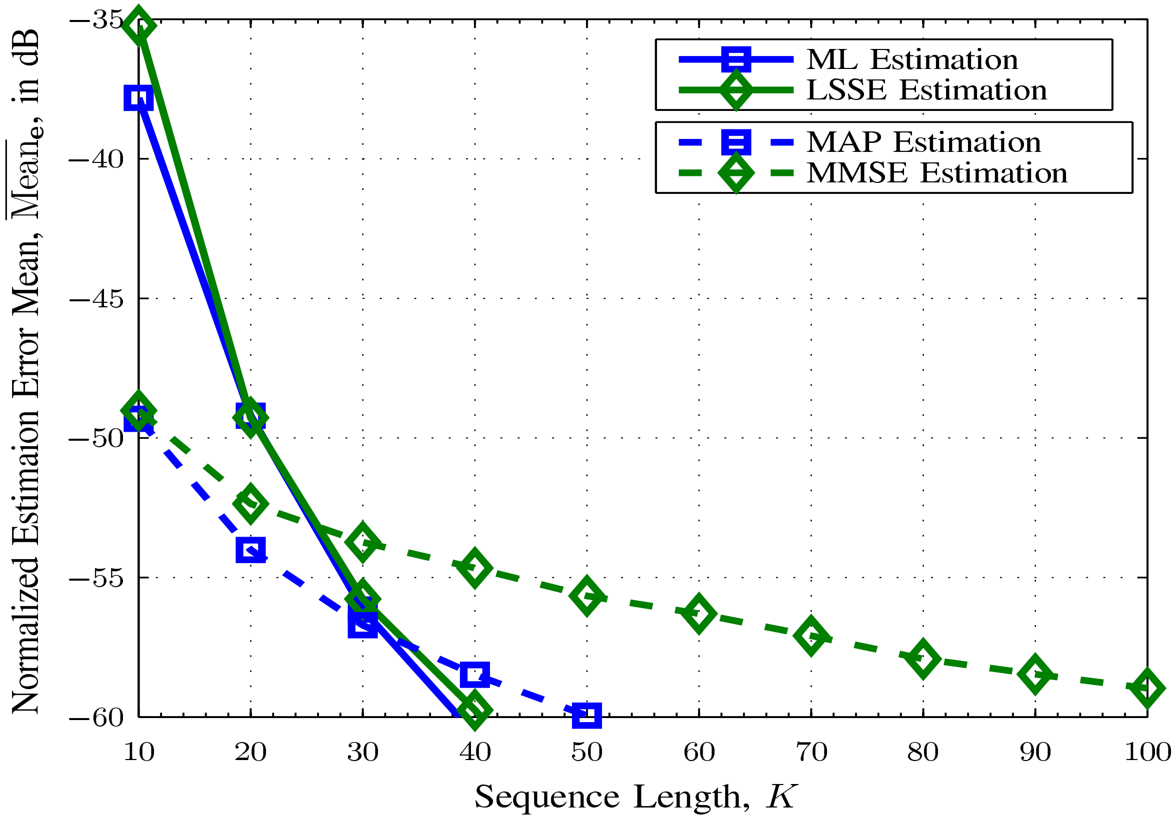
$$\mathbf{F}^{\mathtt{MMSE}} = \underset{\mathbf{F}}{\mathrm{argmin}} \; \mathcal{E}_{\mathbf{r},\bar{\mathbf{c}}} \left\{ \|\mathbf{e}_{\mathrm{up}}^{\mathtt{MMSE}}\|^2 \right\}$$

where $\mathbf{e}_{\mathrm{up}}^{\mathtt{MMSE}} = \bar{\mathbf{c}} - \hat{\bar{\mathbf{c}}}_{\mathrm{up}}^{\mathtt{MMSE}}$ and $\hat{\bar{\mathbf{c}}}_{\mathrm{up}}^{\mathtt{MMSE}} = \mathbf{F}\mathbf{r}$.

- Solution:

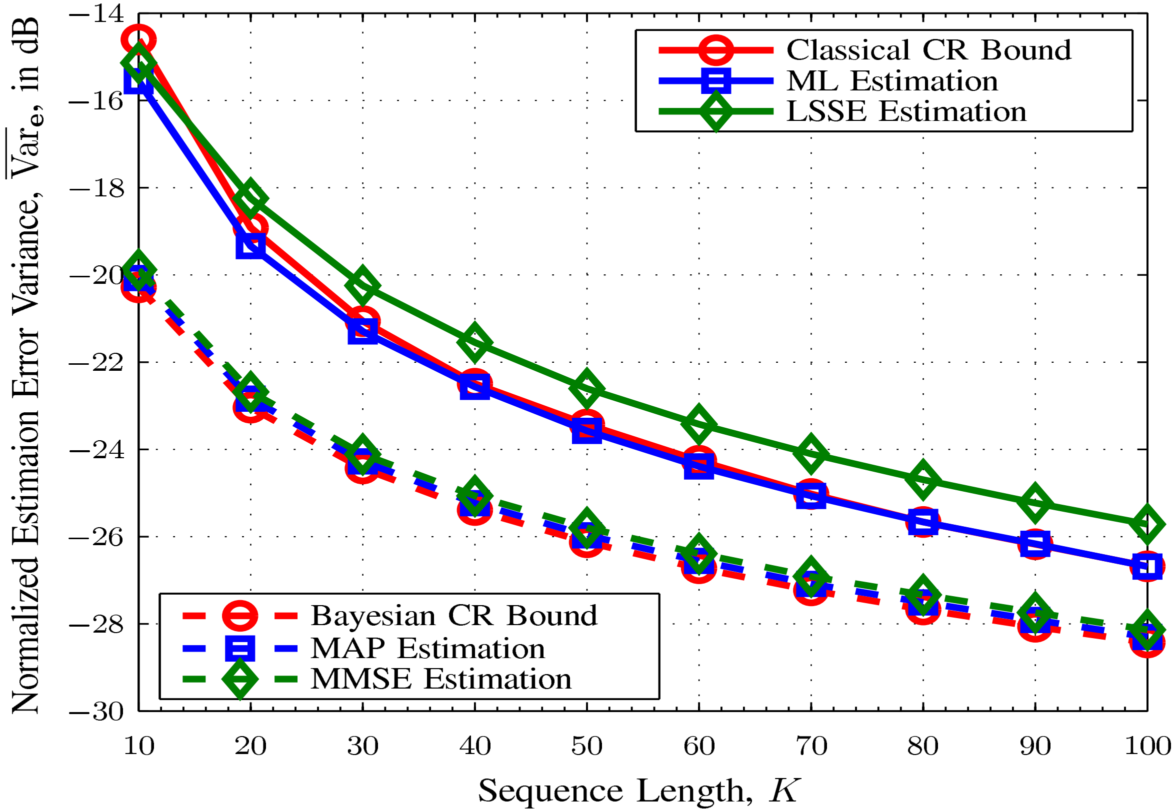
$$\mathbf{F}^{\mathtt{MMSE}} = \mathbf{\Phi}_{\bar{\mathbf{c}}\bar{\mathbf{c}}}^{T} \mathbf{S}^{T} \left(\mathbf{S}\mathbf{\Phi}_{\bar{\mathbf{c}}\bar{\mathbf{c}}}\mathbf{S}^{T} + \mathrm{diag}\left\{\mathbf{S}\boldsymbol{\mu}_{\bar{\mathbf{c}}}\right\} \right)^{-1}$$

where $\boldsymbol{\mu}_{\bar{\mathbf{c}}} = \mathcal{E}_{\bar{\mathbf{c}}}\{\bar{\mathbf{c}}\}$ and $\mathbf{\Phi}_{\bar{\mathbf{c}}\bar{\mathbf{c}}} = \mathcal{E}_{\bar{\mathbf{c}}}\left\{\bar{\mathbf{c}}\bar{\mathbf{c}}^{T}\right\}$. The MMSE estimate is $\hat{\bar{\mathbf{c}}}^{\mathtt{MMSE}} = \left[\mathbf{F}^{\mathtt{MMSE}}\mathbf{r}\right]^{+}$.



- $\bar{\mathbf{c}}$ is assumed Gaussian distributed, random training sequence
- Normalized mean estimation error $\overline{\text{Mean}}_{\mathbf{e}} = \|\mathcal{E}\{\mathbf{e}\}\|^2 / \|\mathcal{E}\{\bar{\mathbf{c}}\}\|^2$
- All estimators are asymptotically unbiased

3. Channel Estimation Techniques - Results (2)



- $\bar{\mathbf{c}}$ is assumed Gaussian distributed, random training sequence
- Normalized estimation error variance $\overline{\text{Var}}_{\mathbf{e}} = (\mathcal{E}\left\{\|\mathbf{e}\|^2\right\} - \|\mathcal{E}\left\{\mathbf{e}\right\}\|^2)/\|\mathcal{E}\left\{\bar{\mathbf{c}}\right\}\|^2$
- Low-complexity suboptimal estimators perform well

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Problem Statement

- Objective: Find the training sequence $\mathbf{s}$ which minimizes estimation error

- Here: Minimize error for LSSE estimator

$$\mathcal{E}_{\mathbf{r},\bar{\mathbf{c}}}\left\{\|\mathbf{e}^{\mathrm{LSSE}}\|^2\right\} = \mathcal{E}_{\mathbf{r},\bar{\mathbf{c}}}\left\{\mathrm{tr}\left\{\left(\bar{\mathbf{c}} - \left(\mathbf{S}^T\mathbf{S}\right)^{-1}\mathbf{S}^T\mathbf{r}\right)\left(\bar{\mathbf{c}} - \left(\mathbf{S}^T\mathbf{S}\right)^{-1}\mathbf{S}^T\mathbf{r}\right)^T\right\}\right\}$$

- Solution:

$$\mathbf{s}^{\mathrm{LSSE}} = \underset{\mathbf{s}\in\mathcal{S}}{\mathrm{argmin}}\ \mathrm{tr}\left\{\mathbf{S}^T\mathrm{vdiag}\left\{\mathbf{S}\left(\mathbf{S}^T\mathbf{S}\right)^{-2}\mathbf{S}^T\right\}\boldsymbol{\mu}_{\bar{\mathbf{c}}}^T\right\}$$

ISI-Free Training Sequence Design

- Objective: Find a suboptimal training sequence which leads to a low-complexity estimator

- Solution: Insert at least L zeros between any two ones in $\mathbf{s}$

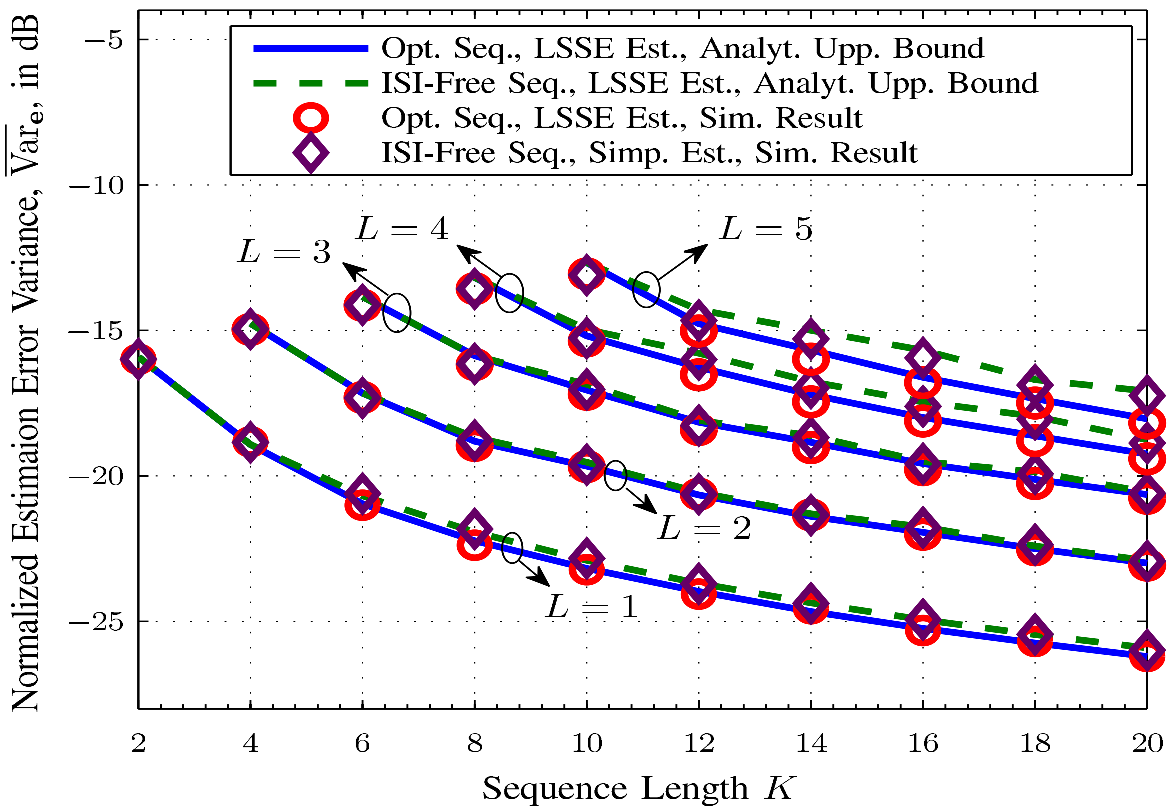
- Corresponding estimator:

$$
\begin{aligned}
\hat{c}_l^{\mathtt{ISIF}} &= \frac{1}{|\mathcal{K}_l|}\Big[\sum_{k\in\mathcal{K}_l}\left[r[k]-\hat{c}_{\mathtt{n}}^{\mathtt{ISIF}}\right]\Big]^{+}, \quad l=1,\dots,L \\
\hat{c}_{\mathtt{n}}^{\mathtt{ISIF}} &= \frac{1}{|\mathcal{K}_{\mathtt{n}}|}\sum_{k\in\mathcal{K}_{\mathtt{n}}} r[k]
\end{aligned}
\tag{1}
$$

- For large K, we can show $\hat{\mathbf{c}}^{\mathtt{ML}} = \hat{\mathbf{c}}^{\mathtt{LSSE}} = \hat{\mathbf{c}}^{\mathtt{MAP}} = \hat{\mathbf{c}}^{\mathtt{MMSE}} = \hat{\mathbf{c}}^{\mathtt{ISIF}}$.

	Criterion	$K = 10$	$K = 20$
$L = 1$	LSSE-based	$\mathbf{s}^* = [1001101110]^T$	$\mathbf{s}^* = [00101110111010101111]^T$
	MMSE-based	$\mathbf{s}^* = [1111000111]^T$	$\mathbf{s}^* = [11011110101100010111]^T$
$L = 3$	LSSE-based	$\mathbf{s}^* = [1100001001]^T$	$\mathbf{s}^* = [10101101101101100000]^T$
	MMSE-based	$\mathbf{s}^* = [0001101011]^T$	$\mathbf{s}^* = [00110101100000111011]^T$
$L = 5$	LSSE-based	$\mathbf{s}^* = [1000001000]^T$	$\mathbf{s}^* = [11111110000100001000]^T$
	MMSE-based	$\mathbf{s}^* = [0000010110]^T$	$\mathbf{s}^* = [00000011001010100111]^T$

- Examples for optimal LSSE/MMSE sequences
- $\bar{\mathbf{c}}$ is assumed Gaussian distributed
- Blue sequence is ISI free



- $\bar{\mathbf{c}}$ is assumed Gaussian distributed, random training sequence
- Normalized estimation error variance $\overline{\mathrm{Var}}_{\mathbf{e}} = (\mathcal{E}\left\{\|\mathbf{e}\|^2\right\} - \|\mathcal{E}\left\{\mathbf{e}\right\}\|^2)/\|\mathcal{E}\left\{\bar{\mathbf{c}}\right\}\|^2$
- Low-complexity ISI-free designs perform well

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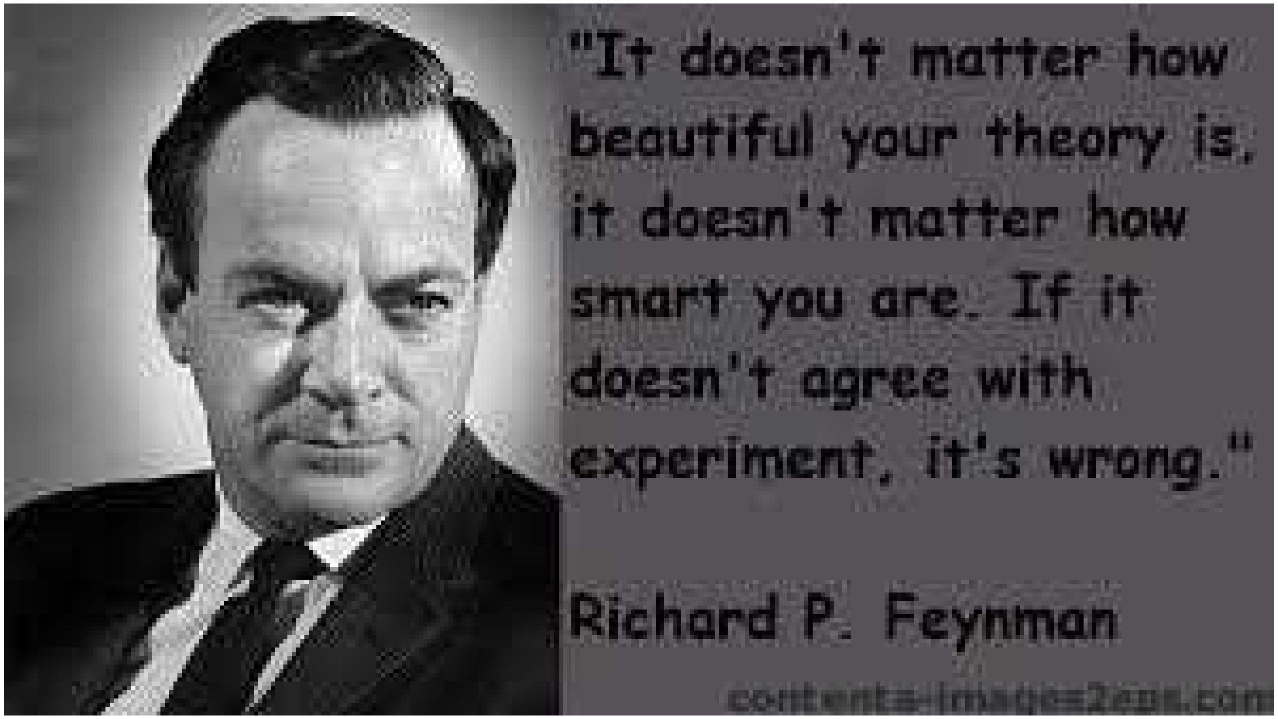
- Knowledge of CIR is required at Rx for data detection and equalization $\Rightarrow$ Channel estimation is necessary
- Nature of estimation problem is different from conventional wireless communication
- Efficient training-based channel estimation schemes for the cases with and without statistical channel knowledge were proposed
- Optimal and suboptimal training sequence designs were investigated
- Low-complexity design achieve close-to-optimal performance


"It doesn't matter how beautiful your theory is, it doesn't matter how smart you are. If it doesn't agree with experiment, it's wrong."
Richard P. Feynman

- **Big Picture**
  - Very young research area $\Rightarrow$ Many open problems
  - Accurate and generally accepted mathematical models are needed
  - More experimental work is needed to advance field

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Channel Estimation

- Experimental verification
- Non-training based (blind) approaches
- Non-coherent detection schemes