Exploiting Geometry for High-Resolution Source Localization

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Motivations – New Imaging/Sensing Modalities

New imaging/sensing modalities allow us to probe the nature in unprecedented manners.

The resulting large amount of data brings exciting opportunities that call for new signal processing tools.
How do we break the diffraction limit of optical microscopy?

The Nobel Prize in Chemistry 2014 “for the development of super-resolved fluorescence microscopy”.

E. Betzig  S. W. Hell  W. E. Moerner

Photo credit: https://www.nobelprize.org/nobel_prizes/chemistry/laureates/2014/.
Single-Molecule Fluorescence Microscopy

Single-molecule based superresolution techniques achieve nanometer spatial resolution by integrating the temporal information of the switching dynamics of fluorophores (emitters).

High density implies better time resolution.

Figure credit: "The Nobel Prize in Chemistry 2014 - Popular Information".
Three-dimensional Single-Molecule Imaging

This imaging principle is extended to reconstruct 3-D objects from 2-D images, by modulating the shape of the PSFs along the depth.

Reconstruction is challenging due to the mutually interfering PSF profile.


J. Huang, M. Sun, K. Gumpper, Y. Chi and J. Ma, "3D Multifocus Astigmatism and Compressed Sensing (3D MACS) Based Superresolution Reconstruction”, Biomedical Optics Express, 2015.
Neural Signal Processing

The human brain is the most complicated biological structure in the known universe.

— Francis S. Collins

Spike sorting: to identify and separate the firing times of each neuron from the observed voltage trace at the electrode.

Simultaneous excitation of multiple neurons makes it challenging.

Internet of things and 5G: By 2020, industry analysts predict 50 billion devices will be connected to mobile networks worldwide.

Channel estimation in a multi-user, multi-path environment is the “elephant in the room”.

Blind channel estimation is desirable for reducing overheads.
High-Resolution Source Localization

- **Observations**: Superposition of returns from sources:
\[
y(t) = \sum_{k=1}^{K} \alpha_k g(t - \nu_k) + n(t),
\]
where \(g(t)\) is the point spread function, \(\{\alpha_k\}_{k=1}^{K}\) and \(\{\nu_k\}_{k=1}^{K}\) are the source parameters, and \(n(t)\) is additive noise.

- **Inversion**: Estimate \(\{\alpha_k, \nu_k\}_{k=1}^{K}\), given a set of samples of \(y(t)\).
  - DOA estimation in sensor array processing
  - Frequency and amplitude estimation in spectrum analysis
  - Range, Doppler, and azimuth estimation in radar/sonar
  - Source location estimation in MRI, EEG, NMR spectroscopy
Something Old: Parameter Estimation

**Exploring Physically-meaningful Constraints:** shift-invariance in the frequency domain:

\[
y = g \odot x = g \odot \left( \sum_{k=1}^{K} \alpha_k \begin{bmatrix} e^{j2\pi 2M\tau_k} \\ \vdots \\ 1 \\ \vdots \\ e^{-j2\pi 2M\tau_k} \end{bmatrix} \right).
\]

where \( 2M \) is the cut-off frequency of the PSF.

- Prony’s method [1795]: root-finding.
- Finite rate of innovation [Vetterli’ 2001].

**Performance:** Perfect recovery from (equi-spaced) \( O(K) \) samples. Performance is well understood via estimation-theoretic bounds under Gaussian noise.
Challenges

However, traditional methods no longer apply under more complicated sensing modalities discussed earlier, due to sensitivity to noise, missing data, interference and outliers.

- **Subsampling or missing data:** ultra-wideband signals, channel estimation using fewer pilots.

- **Noise and corruptions:** sensor failures, attacks, outliers, etc.

- **Calibration:** the PSF functions may be unknown and needs to be calibrated.

- **Multi-modality or interference:** the received signal exhibits superpositions of *multiple* PSF functions.
Something New: Compressed Sensing

Exploring Sparsity: Compressed Sensing [Candès and Tao’2006, Donoho’2006] capture the attributes (sparsity) of signals from a small number of samples.

- **Discretize** the parameters and assume a sparse representation over the discretized basis: \( \tau_k \in \mathcal{T}_n = \left\{ \frac{0}{n}, \ldots, \frac{n-1}{n} \right\}; \)

- **Run \( \ell_1 \) minimization** in the discretized parameter space.

**Performance:** recovery from \( O(K \log n) \) samples, and robust against irregular sampling, noise and outliers enabled by convex optimization.
Sensitivity to Basis Mismatch

**ALERT: Nature does not place the source on the grid!**

![Graphs showing basis mismatch](image)

*Basis mismatch translates a sparse signal into an incompressible signal.*

Our Approach

- Traditional approaches enforce physically-meaningful constraints, but *not* as much sparsity;
- Compressed sensing enforces sparsity, but *not* as much physically-meaningful constraints;

**Geometric Representations:** embed both sparsity and physically-meaningful constraints.

**Convex Relaxations:** enable provable and robust source localization in the presence of non-idealities.

**Applications:** single-molecule fluorescence microscopy.
Geometric Representations
Two-Dimensional Spectral Sparsity Model

• Sampling the **two-dimensional complex harmonic** on a uniform grid, which gives a data matrix $X \in \mathbb{C}^{n_1 \times n_2}$:

\[
X_{\ell_1, \ell_2} = \sum_{k=1}^{K} a_k z_{1,k}^{\ell_1} z_{2,k}^{\ell_2}, \quad 0 \leq \ell_1 < n_1, 0 \leq \ell_2 < n_2
\]

where $z_k = (z_{1,k}, z_{2,k})$ corresponds to the $k$th source location.

• **single-molecule imaging:**
  
  \[ z = e^{-j2\pi\tau}, \quad \tau \in [0, 1]; \]

• **NMR spectroscopy:**
  
  \[ z = \rho e^{-j2\pi\tau}, \quad \rho > 0, \tau \in [0, 1]; \]
Given a data matrix $X$, consider the following matrix enhancement $\mathcal{H}(X)$ [Cadzow, Hua]. Choose two pencil parameters $k_1 = \Theta(n_1)$ and $k_2 = \Theta(n_2)$.

An enhanced form $\mathcal{H}(X)$ is an $k_1 \times (n_1 - k_1 + 1)$ block Hankel matrix:

$$
\mathcal{H}(X) = \begin{bmatrix}
X_0 & X_1 & \cdots & X_{n_1 - k_1} \\
X_1 & X_2 & \cdots & X_{n_1 - k_1 + 1} \\
\vdots & \vdots & \ddots & \vdots \\
X_{k_1 - 1} & X_{k_1} & \cdots & X_{n_1 - 1}
\end{bmatrix},
$$

where each block is a $k_2 \times (n_2 - k_2 + 1)$ Hankel matrix as follows

$$
X_l = \mathcal{H}(X[l,:]) = \begin{bmatrix}
x_{l,0} & x_{l,1} & \cdots & x_{l,n_2 - k_2} \\
x_{l,1} & x_{l,2} & \cdots & x_{l,n_2 - k_2 + 1} \\
\vdots & \vdots & \ddots & \vdots \\
x_{l,k_2 - 1} & x_{l,k_2} & \cdots & x_{l,n_2 - 1}
\end{bmatrix}.
$$
Structured Low-Rank Matrix

- The dimensionality of $\mathcal{H}(X)$ is proportional to $n_1n_2 \times n_1n_2$.
- The enhanced matrix can be decomposed as follows [Hua 1992]:

$$\mathcal{H}(X) = \sum_{k=1}^{K} a_k \left( \begin{array}{c}
1 \\
\hat{z}_{1,k} \\
\vdots \\
\hat{z}_{k_1-1,1}
\end{array} \right) \otimes \left( \begin{array}{c}
1 \\
\hat{z}_{2,k} \\
\vdots \\
\hat{z}_{k_2-1,2}
\end{array} \right) \left( \begin{array}{c}
1 \\
\hat{z}_{1,k} \\
\vdots \\
\hat{z}_{n_1-k_1,1}
\end{array} \right) \otimes \left( \begin{array}{c}
1 \\
\hat{z}_{2,k} \\
\vdots \\
\hat{z}_{n_2-k_2,2}
\end{array} \right) \right)^T,$$

$$u(z_k) \quad v(z_k)^T$$

- The enhanced form $\mathcal{H}(X)$ is decomposed into a sum of rank-one parametric atoms.
  - $\text{rank}(\mathcal{H}(X)) \leq K$
  - Spectral Sparsity $\Rightarrow$ Structured Low-Rank
Promoting Parsimony via Convex Relaxations

\[ x = \sum_{k=1}^{K} c_k a_k, \quad a_k \in \mathcal{A} \]

- The atomic set \( \mathcal{A} \) can be finite, countably infinite, or continuous.
- **Decompose** the signal \( x \) into the fewest number of atoms in an atomic set \( \mathcal{A} \): combinatorial!

\[ \|x\|_{\mathcal{A},0} = \min\{K : x = \sum_{k=1}^{K} c_k a_k, \ a_k \in \mathcal{A}\} \]

- **Relax** by the convex surrogate, yielding the **atomic norm**:

\[ \|x\|_{\mathcal{A}} = \inf \left\{ t > 0 : x \in t\text{conv}(\mathcal{A}) \right\} = \inf \left\{ \sum_i |c_i| : x = \sum_i c_i a_i, \ a_i \in \mathcal{A} \right\} \]

Consequence for Localization

**Identify** activated atoms (source localization) via the dual solution \( q \):

\[
\max \langle x, q \rangle \quad \text{subject to} \quad \|q\|_A^* \leq 1
\]

- Relaxation is tight (recover the decomposition), when:

  - **Strict boundeness:** \( |\langle a, q \rangle| < 1, \quad q \in A \backslash \{a_k\} \)
  - **Interpolation:** \( \langle a_k, q \rangle = \text{sign}(c_k) \),

![Graph showing the function and points identified by the dual solution](image)

Example if \( A \) is parameterized over \([0, 1]\)
Choosing atoms as rank-1 matrices: Nuclear Norm

\[ \mathcal{H}(X) = \sum_{k=1}^{K} a_k \begin{pmatrix} 1 \\ z_{1,k} \\ \vdots \\ z_{k-1,k} \\ z_{1,k} \\ \vdots \\ z_{n-1,k} \end{pmatrix} \otimes \begin{pmatrix} 1 \\ z_{2,k} \\ \vdots \\ z_{k-1,k} \\ z_{2,k} \end{pmatrix} \begin{pmatrix} 1 \\ z_{1,k} \\ \vdots \\ z_{n-1,k} \\ z_{2,k} \end{pmatrix} \begin{pmatrix} 1 \\ z_{2,k} \\ \vdots \\ z_{k-1,k} \\ z_{2,k} \end{pmatrix}^T, \]

\[ u(z_k) \]

\[ v(z_k)^T \]

- Set \( \mathcal{A} = \{ \text{rank-one matrices} \} = \{ uv^T, \|u\| = \|v\| = 1 \} \) leads to the nuclear norm:

\[ \|\mathcal{H}(X)\|_* = \inf \left\{ \sum_i |c_i| \left\| \mathcal{H}(X) = \sum_i c_i uv^T, \|u\| = \|v\| = 1 \right\} \]

which is a semidefinite program that promotes \textit{structured low-rank}.  

- The large atomic set handles not only damping modes, but more general LTI systems identification.
Choosing atoms as sinusoids: Atomic Norm

$$\mathcal{H}(X) = \sum_{k=1}^{K} a_k \left( \begin{bmatrix} 1 \\ z_{1,k} \\ \vdots \\ z_{k_1-1,k} \\ z_{1,k} \\ \vdots \\ z_{k_2-1,k} \end{bmatrix} \otimes \begin{bmatrix} 1 \\ z_{2,k} \\ \vdots \\ z_{k_1-1,k} \\ z_{1,k} \\ \vdots \\ z_{n_2-k_2,2} \end{bmatrix} \right) \begin{bmatrix} 1 \\ u(z_k) \\ \vdots \\ v(z_k) \end{bmatrix}^{T},$$

- Set $\mathcal{A} = \{\text{complex sinusoids}\} = \{u(e^{-j2\pi\tau})v(e^{-j2\pi\tau})^{T}\}$ leads to the atomic norm:

$$\|X\|_{\mathcal{A}} = \inf \left\{ \sum_{i} |c_i| \left| \mathcal{H}(X) = \sum_{i} c_i u(e^{-j2\pi\tau})v(e^{-j2\pi\tau})^{T}, \ \tau \in [0, 1) \right| \right\}$$

which is a semidefinite program that promotes structured low-rank.

- The smaller atomic set allows a tighter convex relaxation for complex sinusoids.

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Case Studies
Robustness to Missing Data

**Missing data:** a subset of entries is observed in an index set $\Omega$, where $m = |\Omega| \ll n = n_1 n_2$.

$$Y_{i,j} = X_{i,j}, \quad (i,j) \in \Omega.$$ 

**EMaC (Enhanced Matrix Completion)**

$$\min_{M \in \mathbb{C}^{n_1 \times n_2}} \| \mathcal{H}(M) \|_* \quad \text{subject to} \quad M_{i,j} = Y_{i,j}, \quad \forall (i,j) \in \Omega$$

Enhancement
• **Gram matrix** of the source via Dirichlet kernel:

\[ G_{i,j} = D(z_i - z_j) \]

• **Incoherence** is defined as smallest \( \mu \) that

\[ \sigma_{\text{min}}(G) \geq \frac{1}{\mu}. \]

• \( \mu = \Theta(1) \) for many scenarios.
Theorem (Chen and Chi, TIT 2014)

If $\Omega$ is sampled uniform at random, EMaC recovers $X$ perfectly with high probability if

$$m \gtrsim \mu K \log^4 n.$$ 

- **Near-optimal** sample complexity as long as $\mu = \Theta(1)$ up to logarithmic factors.
- RHS: Phase transition when $n_1 = n_2 = 15$.
- Reconstruction is robust to additional bounded noise and sparse outliers, by adding additional regularizations.

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Robustness to Multi-Modalities

Multi-Modalities (two PSFs):

\[
y(t) = \sum_{k=1}^{K_1} \alpha_{1,k} g_1(t - \tau_{1,k}) + \sum_{k=1}^{K_2} \alpha_{2,k} g_2(t - \tau_{2,k})
\]

or equivalently in the **frequency domain**:

\[
y = g_1 \odot x_1 + g_2 \odot x_2,
\]

where \( x_1 \) and \( x_2 \) are spectrally-sparse.

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**AtomicDemix**

\[
\min_{x_1, x_2} \|x_1\|_A + \|x_2\|_A \quad \text{subject to} \quad y = g_1 \odot x_1 + g_2 \odot x_2.
\]

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Success Conditions

- **Separation condition (source):** for each component, define the minimum separation between point sources as

  \[ \Delta_i = \min_{k \neq j} |\tau_{ik} - \tau_{ij}| \geq \frac{1}{M}; \]

- **Random signs (source):** The signs of the coefficients \( \alpha_{ik} \)'s are i.i.d. generated from a symmetric distribution on the complex unit circle.

- **Incoherence condition (PSF):** Each entry of the PSF sequence \( g_i \)'s is generated i.i.d. from a uniform distribution on the complex unit circle.

  - The PSF functions should be incoherent across components
Performance Guarantees of AtomicDemix

**Theorem (Li and Chi, ACHA 2017+)**

Let $M \geq 4$. With probability at least $1 - \delta$, AtomicDemix recovers $\{x_1, x_2\}$ perfectly as long as

$$M \lesssim (K_1 + K_2) \log \left( \frac{K_1 + K_2}{\delta} \right) \log \left( \frac{M}{\delta} \right).$$

- **Near-optimal** sample complexity up to logarithmic factors.
- The reconstruction is also stable in the presence of noise.
Robustness to Unknown PSF

**Blind deconvolution:** estimating the source when \( g(t) \) is *unknown*:

\[
y(t) = \sum_{k=1}^{K} \alpha_k g(t - \tau_k).
\]

- **In the frequency domain:** bilinear form

\[
y = g \odot x = \text{diag}(g)x
\]

No. of unknowns \( > \) No. of equations!
Bilinear Inverse Problem and Lifting

- **Subspace assumption:** We assume the sequence $g$ lies in some known low-dimensional subspace:

$$ g = Bh \in \mathbb{C}^{4M+1}, $$

where $B = [b_{-2M}, \cdots, b_{2M}]^T \in \mathbb{C}^{(4M+1) \times L}$, and $h \in \mathbb{C}^L$.

- **The lifting trick:**

  $\begin{bmatrix} y \\ \hline B \\
 h \end{bmatrix} \odot \begin{bmatrix} x \\ \hline x^T \end{bmatrix} = \chi \left( \begin{bmatrix} x \\ \hline x^T \end{bmatrix} \right)$

  $$ y = \chi(Z) \in \mathbb{C}^{4M+1}, \quad \text{where} \quad Z = xh^T. $$

  _Translates a bilinear problem to an underdetermined linear one!_
\( Z \) can be regarded as a **spectrally-sparse ensemble** with the same set of frequencies:

\[
Z = x h^T = [h_1 x, h_2 x, \ldots, h_L x].
\]

whose structure can be motivated by the **atomic norm** using the multiple measurement vector (MMV) model [Li and Chi, TSP 2016]:

\[
\|Z\|_A = \min_{s, W} \left\{ \frac{1}{2} \text{Tr}(\text{Toep}(s)) + \frac{1}{2} \text{Tr}(W) \left| \begin{bmatrix} \text{Toep}(s) & Z \\ Z^H & W \end{bmatrix} \right| \leq 0 \right\}
\]

\[
\hat{Z} = \arg\min_Z \|Z\|_A \quad \text{subject to} \quad y = \mathcal{X}(Z).
\]

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Success Conditions of AtomicLift

- **Separation condition (source):** define the minimum separation between point sources

\[ \Delta = \min_{k \neq j} |\tau_k - \tau_j| \geq \frac{1}{M}; \]

- **Random signs (source):** The signs of the coefficients \( \alpha_{ik} \)'s are i.i.d. generated from a symmetric distribution on the complex unit circle.

- **Incoherence condition (PSF):** Each row of the subspace \( B \) is i.i.d. from a population \( F \), i.e. \( b_n \sim F \):
  - **Isometry property:**
    \[ \mathbb{E}bb^H = I_L, \quad b \sim F. \]
  - **Spreadness property:** for \( b = [b_1, \ldots, b_L]^T \)
    \[ \mu \text{ is the smallest number that} \]
    \[ \max_{1 \leq i \leq L} |b_i|^2 \leq \mu \]
Performance Guarantee of AtomicLift

**Theorem (Chi, JSTSP 2016)**

Let $M \geq 4$. With probability at least $1 - \delta$, AtomicLift recovers $Z$ perfectly, as long as

$$M \gtrsim \mu KL \log^2 \left( \frac{M}{\delta} \right).$$

- When the coherence parameter $\mu = \Theta(1)$, $O(KL)$ samples suffice.
  - $O(K)$ samples suffice when PSF is known.
- This requirement is larger than $O(K + L)$.
- The reconstruction is robust to noise.

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Applications
Super-Resolution Microscopy Imaging

With my student Jiaqing Huang (PhD 2016), in collaboration with OSU Davis Heart and Lung Research Institute, we have developed several algorithms for super-resolution imaging.
Super-Resolution Microscopy Imaging

**3DMACS (BOE 2015):** A multi-camera approach that leverages diversity to improve resolution in CSSTORM.

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**J. Huang, M. Sun, K. Gumpper, Y. Chi, and J. Ma,** “3D Multifocus Astigmatism and Compressed Sensing (3DMACS) Based Supper-resolution Reconstruction,” Biomedical Optics Express, vol. 6, pp. 902-917, 2015.
**Super-Resolution Microscopy Imaging**

**MempSTORM (OL 2015):** a fast and cheap method for 2D super-resolution imaging using truncated SVD-based spectral estimation that is much faster than state-of-the-art CSSTORM.

Upper: CSSTORM; Lower: MempSTORM

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Super-Resolution Microscopy Imaging

TVSTORM (TCI 2017, in press): measure optimization for 3-D image reconstruction under Poisson noise that achieves better performance than state-of-the-art CSSTORM.

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Summary

**Geometric Representations:** embed both sparsity and physically-meaningful constraints for source localization.

**Convex Relaxations:** enable provable and robust source localization in the presence of missing data, outliers, multiple modalities, and mis-calibrations.

**Imaging Applications:** fast algorithms are developed for super-resolution image reconstruction in single-molecule fluorescence microscopy.
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Thank you for listening!

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