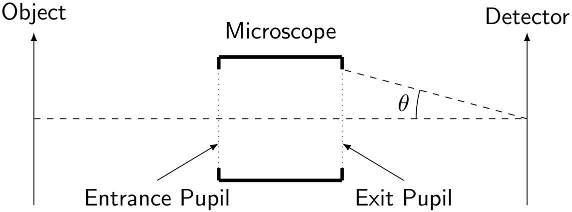
Super-resolution of Positive Sources

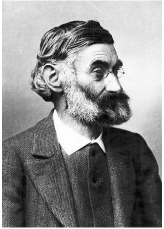
Veniamin I. Morgenshtern

Statistics Department, Stanford

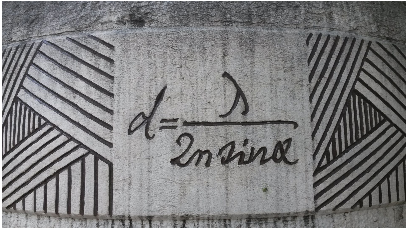
Joint work with Emmanuel Candès

Diffraction limits resolution:

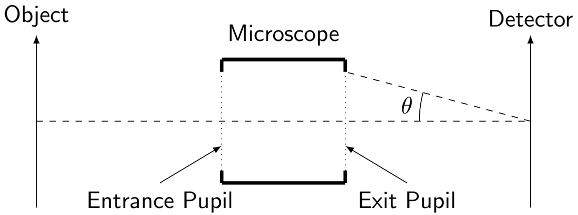


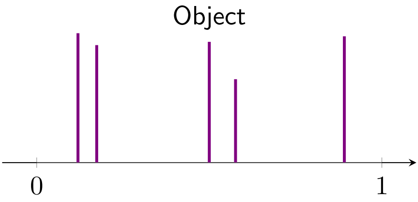


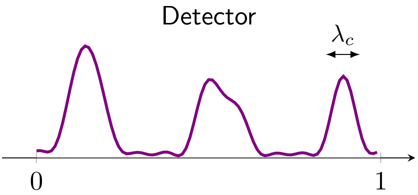
Ernst Abbe

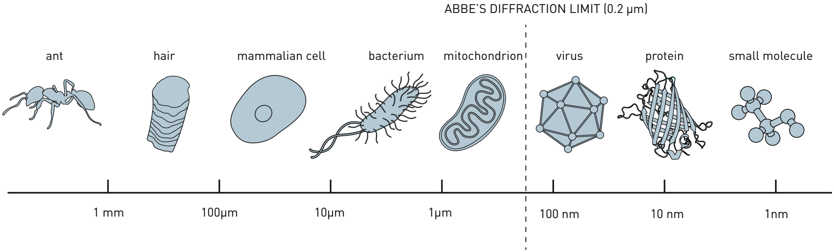


Diffraction limits resolution: $\lambda_c = \frac{\lambda_{\text{LIGHT}}}{2n\sin(\theta)}$



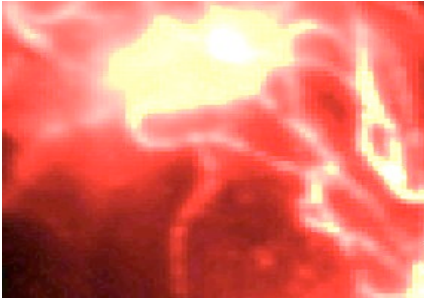






[picture from nobelprize.org]

Looking inside the cell: conventional microscopy



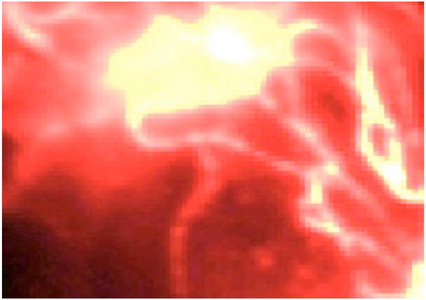
microtubule

Nobel Prize in Chemistry 2014

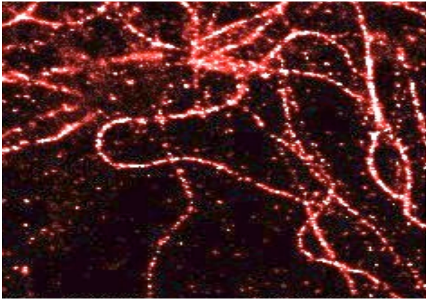
Eric Betzig   Stefan W. Hell   W.E. Moerner

Invention of single-molecule microscopy

Looking inside the cell



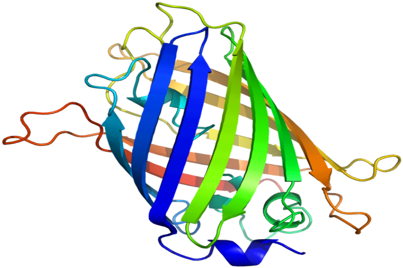
conventional microscopy



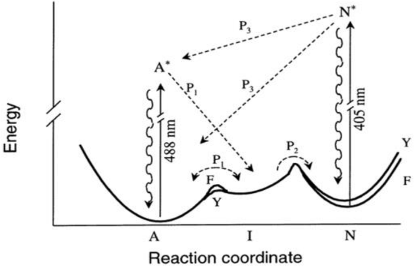
single-molecule microscopy

Single molecule microscopy (basics)

Controlled photoactivation

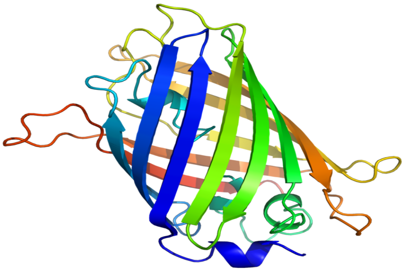


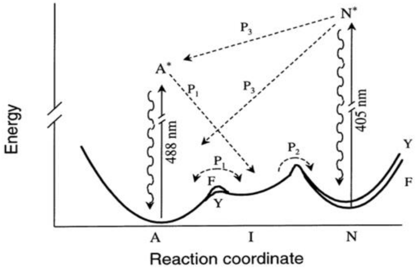
Green fluorescent protein (GFP)



Energy states [Dickson et.al. '97]

Controlled photoactivation



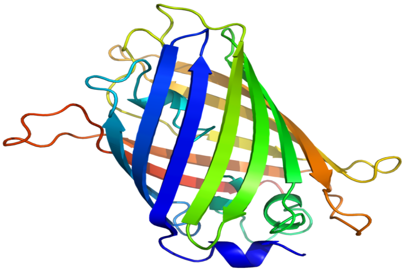


Green fluorescent protein (GFP)

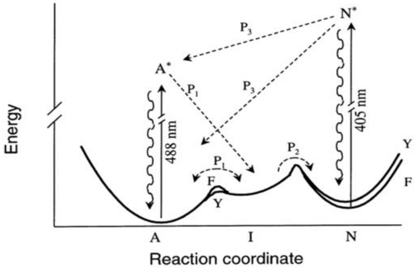
Energy states [Dickson et.al. '97]

- State A is excited to A^* and returns to A upon photon emission

Controlled photoactivation



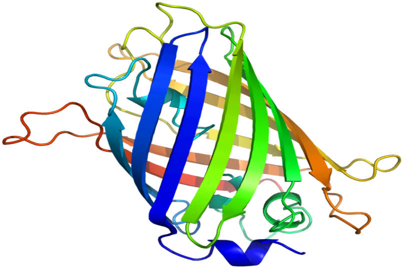
Green fluorescent protein (GFP)



Energy states [Dickson et.al. '97]

- State A is excited to A^* and returns to A upon photon emission
- When I is reached from A there is no fluorescence until I spontaneously moves to A (blinking)

Controlled photoactivation



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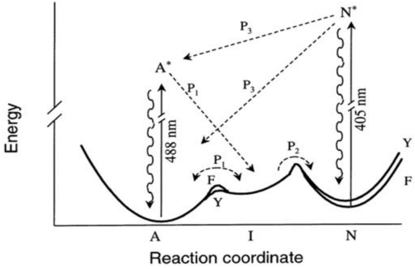
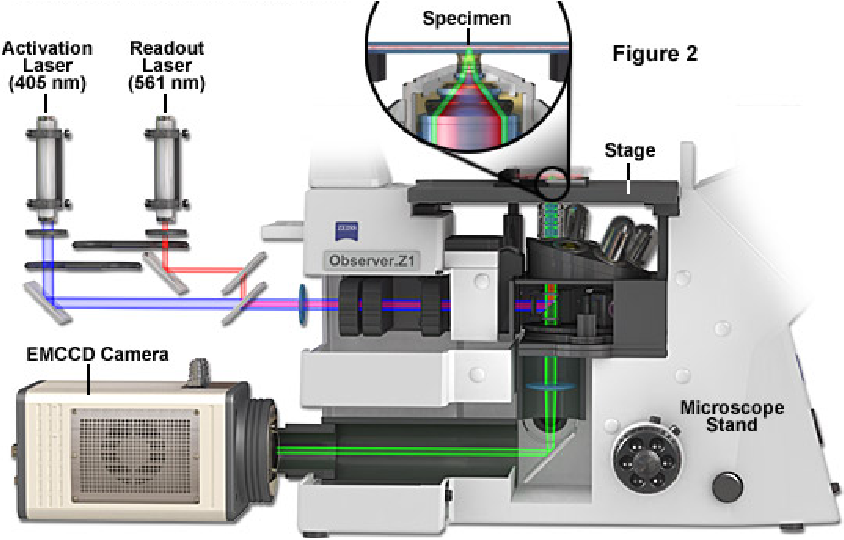


Energy states [Dickson et.al. '97]

- State A is excited to A^* and returns to A upon photon emission
- When I is reached from A there is no fluorescence until I spontaneously moves to A (blinking)
- When I moves to N there is no fluorescence until N is activated by 405nm light and GFP returns to A

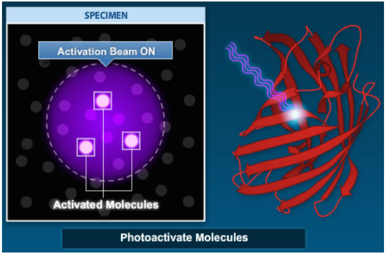
Photoactivated localization microscopy (PALM) Setup



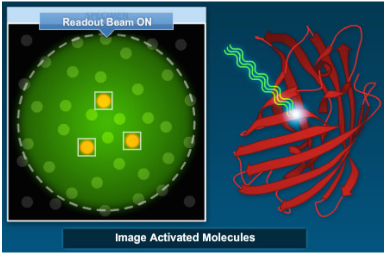
[picture from ZEISS]

PALM Process

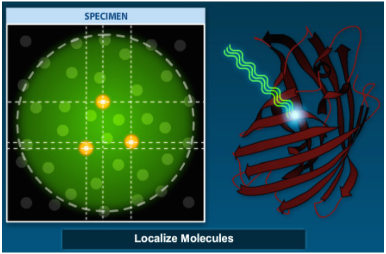
Step 1



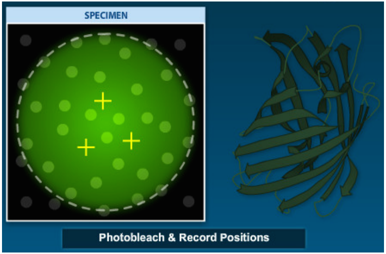
Step 2



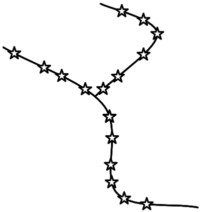
Step 3. Algorithm needed.



Step 4

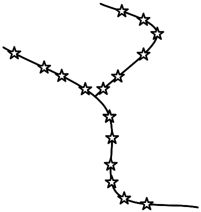


Antibodies: attach fluorescent molecules to the structure

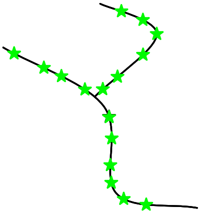


All off

Antibodies: attach fluorescent molecules to the structure

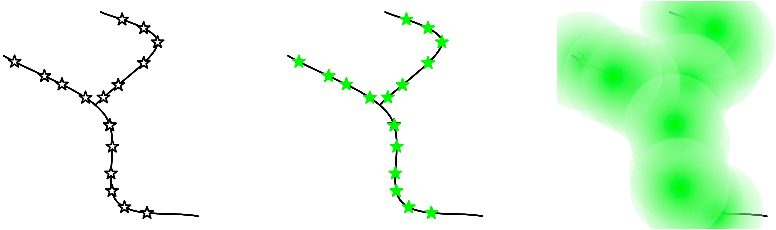


All off



All on

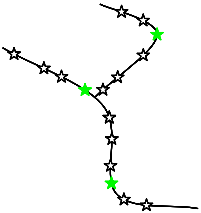
Antibodies: attach fluorescent molecules to the structure



All off　　All on　　Detector

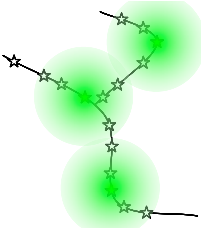
Cannot resolve the structure!

“Blinking” molecules: sparsity



Frame 1

"Blinking" molecules: sparsity



Frame 1

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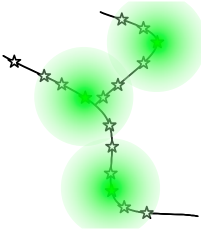
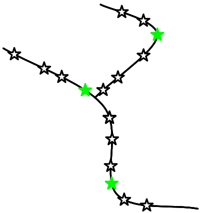


Frame 1

Locate centers of "Gaussian" blobs (parametric estimation)

“Blinking” molecules: sparsity



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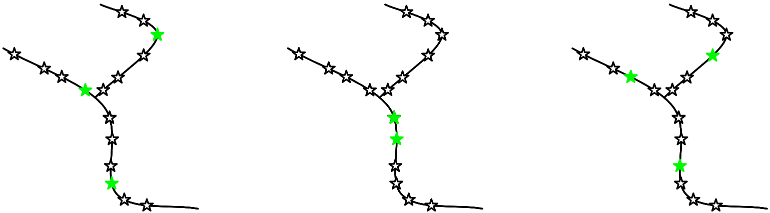
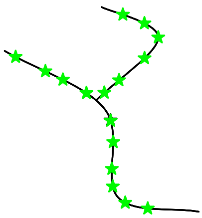


Frame 1 Frame 2 Frame 3

Locate centers of “Gaussian” blobs (parametric estimation)

Combine $\sim$ 10000 frames.

“Blinking” molecules: sparsity



Locate centers of “Gaussian” blobs (parametric estimation)

Combine $\sim$ 10000 frames.

The structure is now resolved!

Next Frontier: image dynamical processes

Imaging ~ 10000 frames is **slow**

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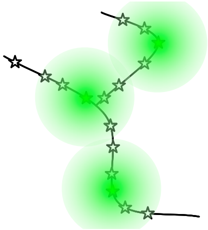
Can we make data acquisition **faster**?

Next Frontier: image dynamical processes

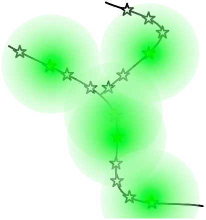
Imaging ~ 10000 frames is **slow**

Can we make data acquisition **faster**?

Image ~ 2500 frames with 4 times more molecules per frame?



parametric estimation works



4 times more active molecules
$\Rightarrow$ parametric estimation
does not work

Next Frontier: image dynamical processes

Imaging ~ 10000 frames is **slow**

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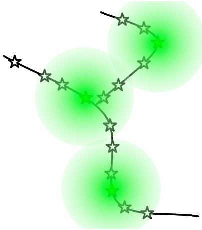
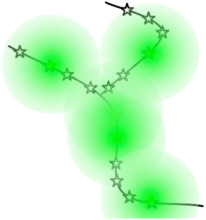
Image ~ 2500 frames with 4 times more molecules per frame?



parametric estimation works



4 times more active molecules
$\Rightarrow$ parametric estimation
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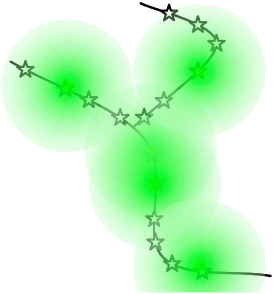
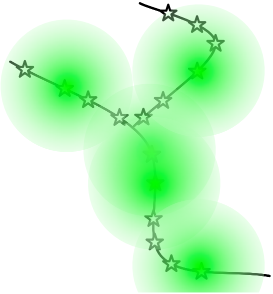
Need powerful super-resolution algorithm!



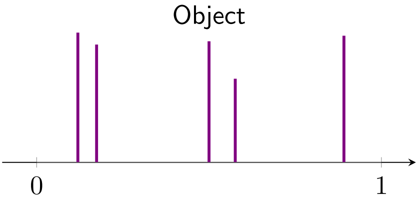
Theory



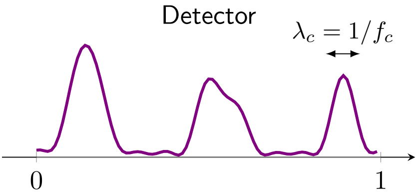
Theory

Which algorithm?
Performance guarantees?
Fundamental limits?

Mathematical model (discrete 1D setup for simplicity)



$$x(t) = \sum_i x_i \delta(t - t_i),\ \ x_i \geq 0$$

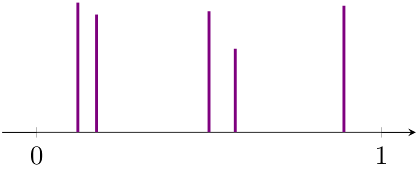


$$s(t) = \int f_{\text{low}}(t - t')x(t')dt'$$

$$f_{\text{low}}(t) = \frac{1}{2f_c}\left(\frac{\sin(2\pi f_c t)}{\pi t}\right)^2$$

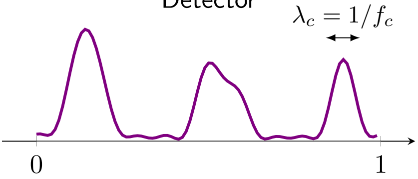
Mathematical model (discrete 1D setup for simplicity)

Object



$$x(t) = \sum_i x_i \delta(t - t_i), \;\; x_i \geq 0$$

Detector



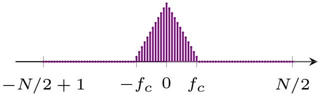
$$s(t) = \int f_{\text{low}}(t - t')x(t')dt'$$

$$\mathbf{x} = [x_0 \cdots x_{N-1}]^\mathsf{T} \geq \mathbf{0}$$

$$\mathbf{s} = \mathbf{P}\mathbf{x} + \mathbf{z}$$

$\mathbf{P} = \mathbf{P}_{\text{tri}}$ is **circulant**

Triangular spectrum



Mathematical model (discrete 1D setup for simplicity)

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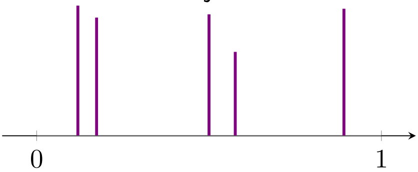
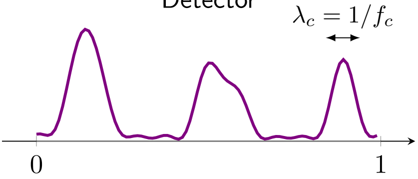


Detector



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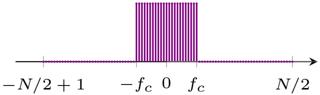
$$\mathbf{x} = [x_0 \cdots x_{N-1}]^{\mathsf{T}} \geq \mathbf{0}$$

$$\mathbf{s} = \mathbf{P}\mathbf{x} + \mathbf{z}$$

$\mathbf{P} = \mathbf{P}_{\text{flat}}$ is **circulant**

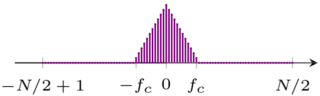
Flat spectrum



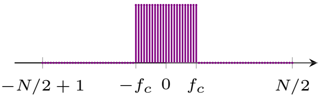
Super-resolution factor and stability

$$\mathbf{x} = [x_0 \cdots x_{N-1}]^\mathsf{T}$$

Triangular spectrum



Flat spectrum



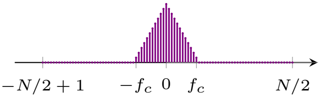
$$\mathbf{s} = \mathbf{P}\mathbf{x} + \mathbf{z}$$

$$\mathrm{SRF} \triangleq N/(2f_c)$$

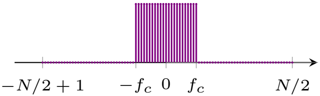
Super-resolution factor and stability

$$\mathbf{x} = [x_0 \cdots x_{N-1}]^\mathsf{T}$$

Triangular spectrum



Flat spectrum

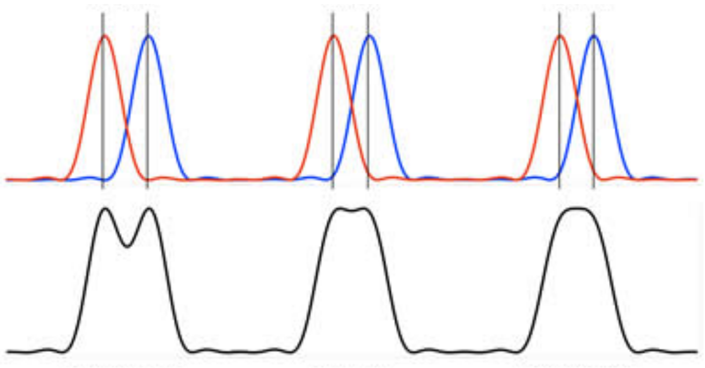


$$\mathbf{s} = \mathbf{P}\mathbf{x} + \mathbf{z}$$

$$\mathrm{SRF} \triangleq N/(2f_c)$$

Stability: $\|\mathbf{x} - \hat{\mathbf{x}}\| \overset{?}{\leq} \|\mathbf{z}\| \cdot$ (amplification factor)

Classical resolution criteria: separation is about λ_c



$1.22\lambda_c$
Rayleigh criterion

λ_c
Abbe criterion

$0.94\lambda_c$
Sparrow criterion

Rayleigh-regularity: $\mathbf{x} \in \mathcal{R}(d, r)$

$\mathbf{x}$ has fewer than r spikes in every $\lambda_c d$ interval $[\lambda_c \triangleq 1/f_c]$

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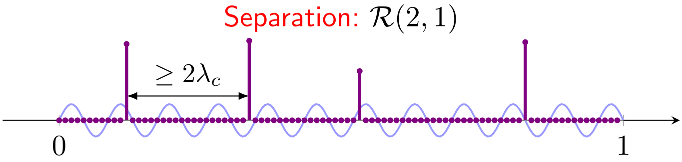

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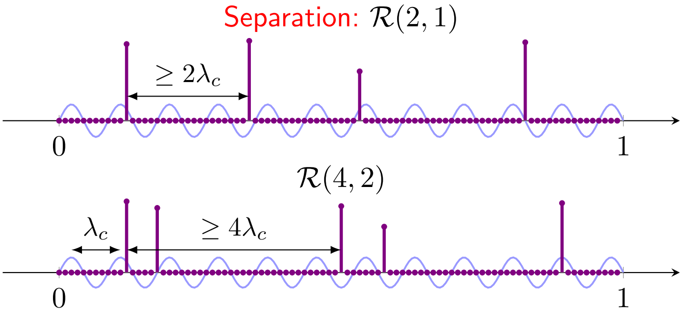

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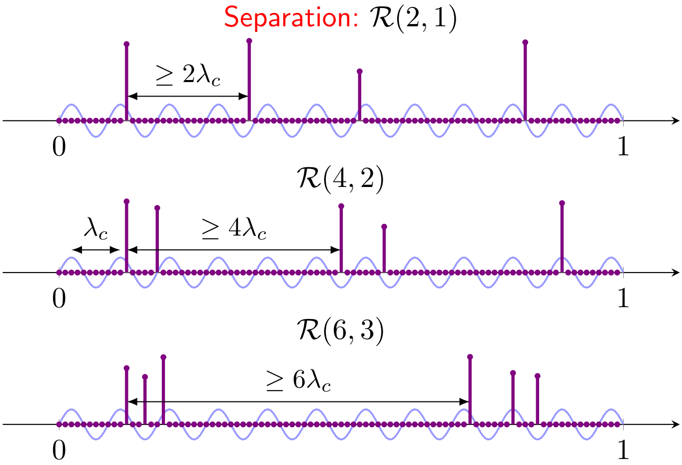


Key contribution

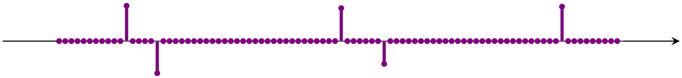
[Prony'1795]

$\mathbf{x} \in \mathbb{C}^N$

no stability

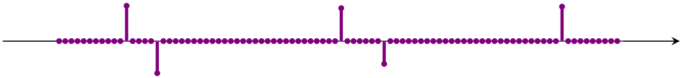
–

efficient



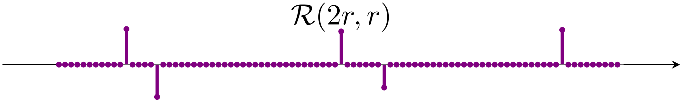
Key contribution

[Prony'1795]	**MUSIC, ESPRIT**
$\mathbf{x} \in \mathbb{C}^N$	$\mathbf{x} \in \mathbb{C}^N$
no stability	stability not understood
–	–
efficient	efficient



Key contribution

[Prony'1795]	MUSIC, ESPRIT	[Donoho'92]
$\mathbf{x} \in \mathbb{C}^N$	$\mathbf{x} \in \mathbb{C}^N$	$\mathbf{x} \in \mathbb{C}^N$
no stability	stability not understood	stability
–	–	Rayleigh-regularity
efficient	efficient	combinatorial



Key contribution

[Prony'1795]
$\mathbf{x} \in \mathbb{C}^N$
no stability
–
efficient

MUSIC, ESPRIT
$\mathbf{x} \in \mathbb{C}^N$
stability not understood
–
efficient

[Donoho'92]
$\mathbf{x} \in \mathbb{C}^N$
stability
Rayleigh-regularity
combinatorial

[Donoho et al.'90]
$\mathbf{x} \geq \mathbf{0}$
no stability
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Key contribution

[Prony'1795]
$\mathbf{x} \in \mathbb{C}^N$
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efficient

MUSIC, ESPRIT
$\mathbf{x} \in \mathbb{C}^N$
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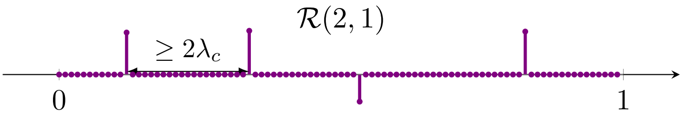
Works:



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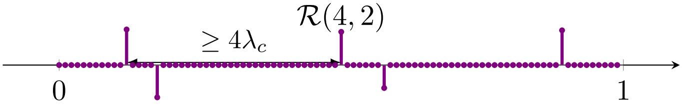
Breaks:



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[Donoho et al.'90]	[Candès & F.-Granda'12]	This work
$\mathbf{x} \geq \mathbf{0}$	$\mathbf{x} \in \mathbb{C}^N$	$\mathbf{x} \geq \mathbf{0}$
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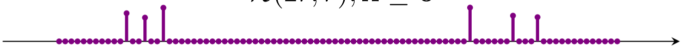
$\mathcal{R}(2r, r), \mathbf{x} \geq \mathbf{0}$

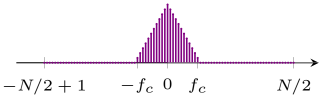


Main results

Recall:

$$\mathbf{s} = \mathbf{P}\mathbf{x} + \mathbf{z}$$

spectrum



Solve:

$$\text{minimize } \|\mathbf{s} - \mathbf{P}\hat{\mathbf{x}}\|_1 \quad \text{subject to} \quad \hat{\mathbf{x}} \geq 0$$

Theorem: [V. Morgenshtern and E. Candès, 2014]

Take $\mathbf{P} = \mathbf{P}_{\text{tri}}$ or $\mathbf{P} = \mathbf{P}_{\text{flat}}$. Assume $\mathbf{x} \geq 0$, $\mathbf{x} \in \mathcal{R}(2r, r)$. Then,

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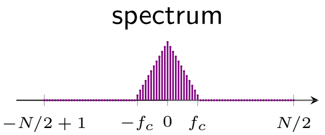

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Converse: [V. Morgenshtern and E. Candès, 2014]

For $\mathbf{P} = \mathbf{P}_{\text{tri}}$, no algorithm can do better than $c \cdot \|\mathbf{z}\|_1 \cdot \left(\frac{N}{2f_c}\right)^{2r-1}$.

Key ideas

→ **Duality theory:** to prove stability we need a low-frequency trigonometric polynomial that is "curvy"

- **[Dohono, et al.'92]** construct trigonometric polynomial that is not "curvy"
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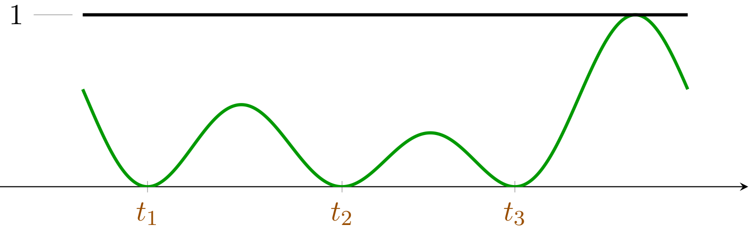

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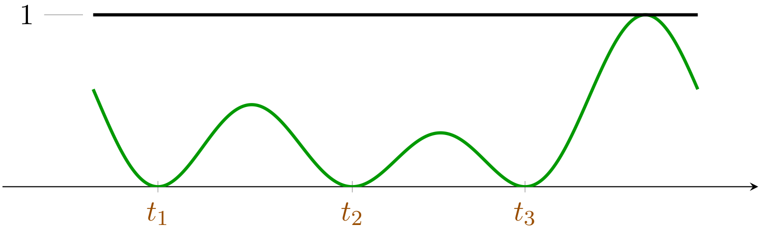
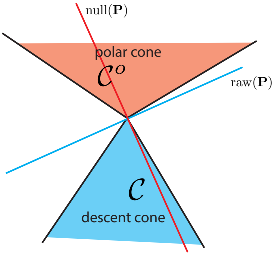


- Then, $\hat{\mathbf{x}} = \mathbf{x}$.

Connection to LASSO ($\mathbf{x}$ can be negative here)

$$\text{minimize} \quad \|\hat{\mathbf{x}}\|_1 \quad \text{subject to} \quad \mathbf{s} = \mathbf{P}\hat{\mathbf{x}}$$



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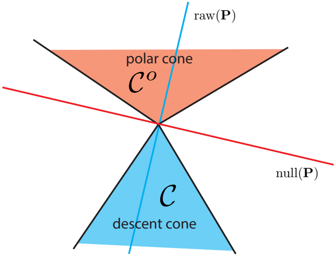

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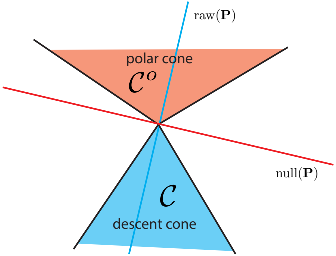

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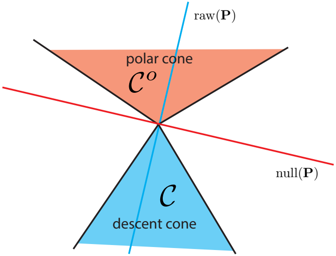

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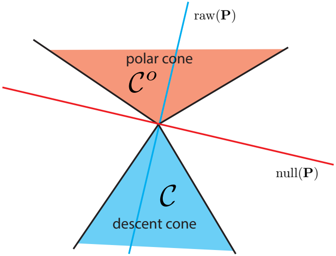
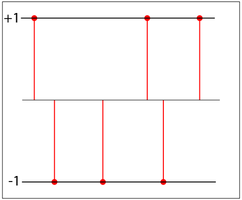
- $\mathbf{q} \in \partial\|\mathbf{x}\|_1 \Leftrightarrow$
  $$\begin{cases} q(t_i) = \mathrm{sign}(x_i) & x_i \neq 0 \\ |q(t_i)| \leq 1 & x_i = 0 \end{cases}$$





$\mathrm{sign}(x) \quad (x \neq 0)$

Dual certificate (noisy case)

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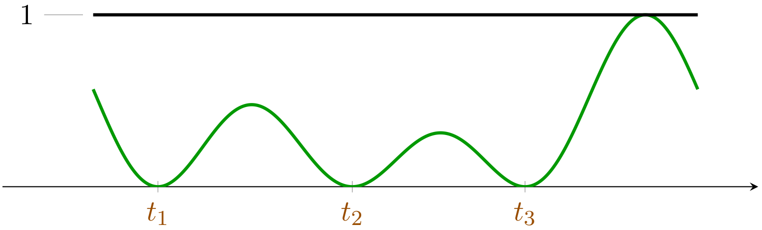

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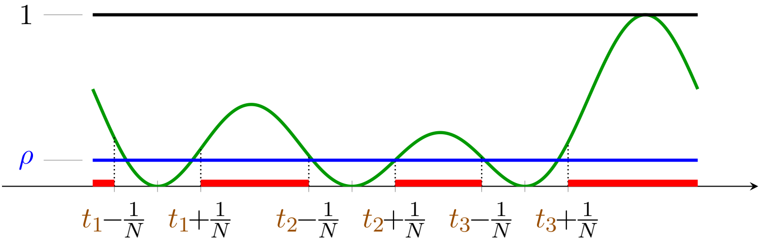

- Then, $\|\hat{\mathbf{x}} - \mathbf{x}\|_1 \le 4\|\mathbf{z}\|_1/\rho$.

Key ideas

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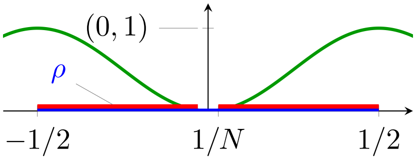
[Dohono, et al.'92]: "Classical" q(t)

$$q(t) = \prod_{t_0 \in \mathcal{T}} \frac{1}{2} \left[\cos(2\pi(t + 1/2 - t_0)) + 1\right].$$

No separation required

Low curvature!

$$q(t - t_0) \approx (t - t_0)^2 \Rightarrow \|\mathbf{x} - \hat{\mathbf{x}}\|_1 \leq \|\mathbf{z}\|_1 \cdot N^2$$



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[Candès, Fernandez-Granda'12]: "Curvy" $q(t)$

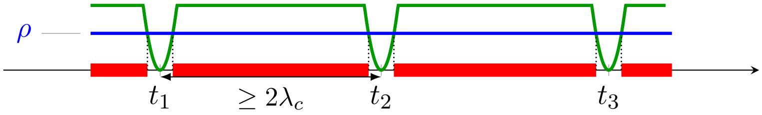
$$q(t) = \sum_{t_j \in \mathcal{T}} a_j K(t - t_j) + \text{corrections},$$

$K(t) \ldots$ low-frequency and "curvy"

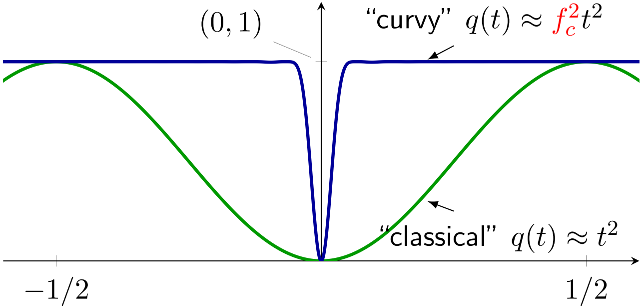
Separation between zeros required: $\mathcal{T} \in \mathcal{R}(2, 1)$

High curvature!

$$q(t - t_i) \approx f_c^2 (t - t_i)^2 \Rightarrow \|\mathbf{x} - \hat{\mathbf{x}}\|_1 \leq c \cdot \|\mathbf{z}\|_1 \cdot \left(\frac{N}{2 f_c}\right)^2$$



Comparison of Trigonometric Polynomials



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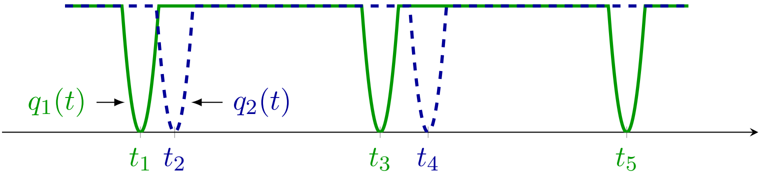
New construction: curvature without separation

Partition support: $\mathcal{T} = \mathcal{T}_1 \cup \mathcal{T}_2, \quad r = 2$

Regularity: $\mathcal{T} \in \mathcal{R}(2 \cdot 2, 2) \Rightarrow \mathcal{T}_i \in \mathcal{R}(4, 1)$



$$q(t; f_c) = q_1(t; f_c/2) \times q_2(t; f_c/2)$$

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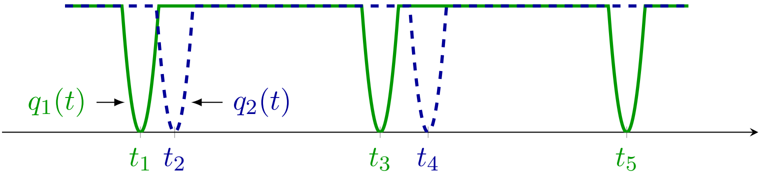

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Summation vs. multiplication

Remember: $q(t)$ must be frequency-limited to f_c!

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This work:

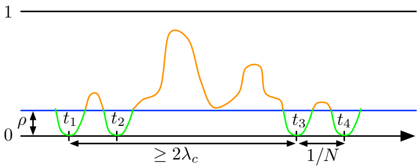
$$q(t) = \prod_{k=1}^{r} \sum_{t_{jk} \in \mathcal{T}_k} \underbrace{a_{jk} K(t - t_{jk})}_{\text{frequency } f_c/r}$$

Complex vs. positive signals

Why do we need $\mathbf{x} \geq \mathbf{0}$?

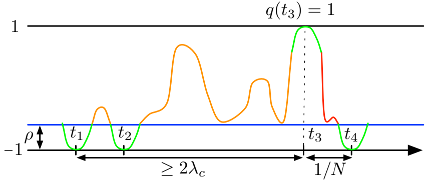
$\mathbf{x} \geq \mathbf{0}$

Interpolate **zero** on supp. of $\mathbf{x}$



$\mathbf{x} \in \mathbb{C}^N$

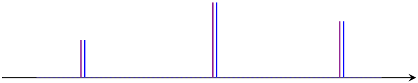
Interpolate $\operatorname{sign}(\mathbf{x})$ on supp. of $\mathbf{x}$



Does not exist! (Bernstein Th.)

Continuous setup

f_c fixed, $N \to \infty \Rightarrow \mathrm{SRF}_{\mathrm{OLD}} \to \infty$

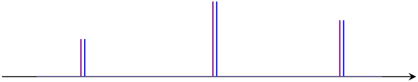


Is the problem hopeless?

f_c fixed, $N \to \infty \Rightarrow \mathrm{SRF}_{\mathrm{OLD}} \to \infty$

$x(t)$

$x(t)$ and $\hat{x}(t)$



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No: we need to be less ambitions!

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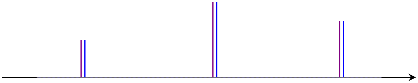

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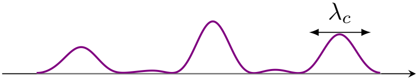

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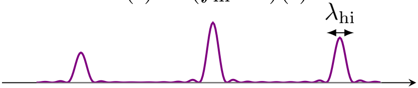

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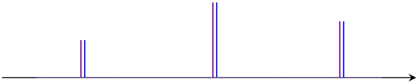

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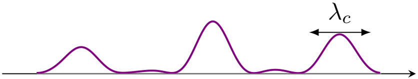

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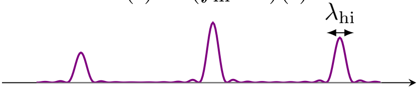

Error$=\| f_{\mathrm{hi}} \star (x - \hat{x}) \|_1$

$$\mathrm{SRF}_{\mathrm{NEW}} = \lambda_c / \lambda_{\mathrm{hi}}$$

Need new tools

Theorem: [V. Morgenshtern and E. Candès, 2014]

Assume $x(t) \geq 0$, $x(t) \in \mathcal{R}(2r, r)$. Then,

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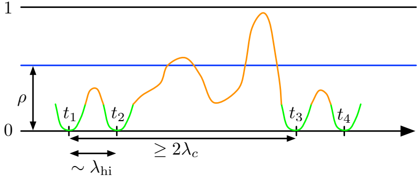
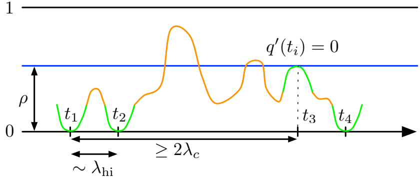
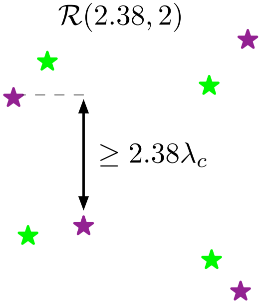
Can do: all zeros



Need: arbitrary pattern $\{0, +\rho\}$



2D Super-resolution



Theorem: [V. Morgenshtern and E. Candès, 2014]

Take $\mathbf{P} = \mathbf{P}_{\text{tri,2D}}$ or $\mathbf{P} = \mathbf{P}_{\text{flat,2D}}$. Assume $\mathbf{x} \geq 0$, $\mathbf{x} \in \mathcal{R}(2.38r, r)$. Then,

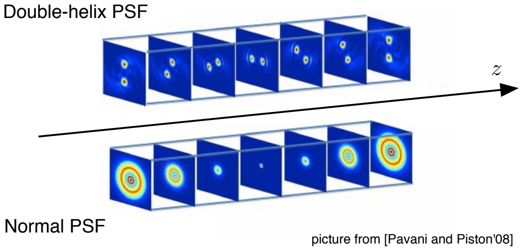
$$\|\hat{\mathbf{x}} - \mathbf{x}\|_1 \leq c \cdot \left(\frac{N}{2f_c}\right)^{2r} \delta.$$

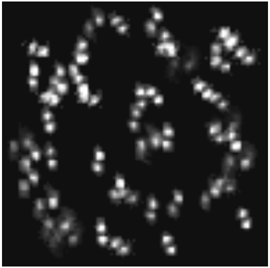
New: number of spikes is linear in the number of observations

Improving microscopes

Collaboration with Moerner Lab, C.A. Sing-Long, E. Candès

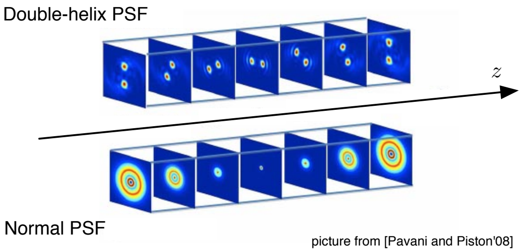
Reconstruction of 3D signals from 2D data

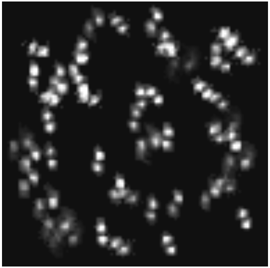




2D double-helix data

Reconstruction of 3D signals from 2D data

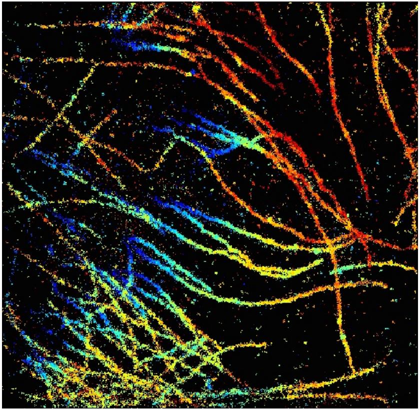




2D double-helix data

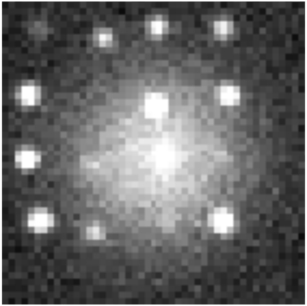
$$\begin{aligned} &\text{minimize} \quad \frac{1}{2}\|\mathbf{s} - \mathbf{P}\hat{\mathbf{x}}\|_2^2 + \lambda\sigma\|\operatorname{diag}(\mathbf{w})\hat{\mathbf{x}}\|_1 \\ &\text{subject to} \quad \hat{\mathbf{x}} \geq 0 \end{aligned}$$

Preliminary result: 4 times faster than state-of-the-art



10000 CVX problems solved
TFOCS first order solver
millions of variables

Flexible framework: smooth background separation



minimize	$\frac{1}{2}\|\mathbf{s} - \mathbf{P}(\hat{\mathbf{x}} + \mathbf{b})\|_2^2 + \lambda\sigma\|\hat{\mathbf{x}}\|_1$
subject to	$\hat{\mathbf{x}} \geq 0$
	$\mathbf{b}$ low freq. trig. polynomial (background)

Comparison of super-resolution algorithms

Work in progress:

- Need to carefully compare super-resolution algorithms in practice
  - Naive matched-filters
  - Algebraic methods: MUSIC, ESPRIT, ...
  - Convex-optimization algorithms with different regularizers
- Realistic physical model
  - Noise: quantum noise and out-of-focus background
  - Point-spread function $(\mathbf{P})$ uncertainty and variation
  - Rotation of single molecules
  - ...
- Test images (phantoms):
  - Different densities of sources
  - Different spacial distributions
  - **Correct answer should always be known**
- Create a database of test cases for quick algorithm assessment

Conclusion

Convex optimization is a near-optimal method
for super-resolution of positive sources

- Flexibility and good practical performance
- Non-asymptotic precise stability bounds
- Rayleigh-regularity is fundamental: separation between spikes is only one part of the picture

Lots of questions remain

- What is the best regularizer in the presence of stochastic noise?
- Fast parallel solver exploiting the structure of the problem
- Theory for Double-Helix reconstruction: 3D signal from 2D observations
- Tractable near-optimal algorithm for complex-valued signals?

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- What is the best regularizer in the presence of stochastic noise?
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- Theory for Double-Helix reconstruction: 3D signal from 2D observations
- Tractable near-optimal algorithm for complex-valued signals?
- **Sparse regression where the design matrix has highly correlated columns:**
  - $\mathbf{A} = [\mathbf{a}_1, \ldots, \mathbf{a}_N]$
  - Shift-invariance: $\langle \mathbf{a}_k, \mathbf{a}_l \rangle = \langle \mathbf{a}_{k+r}, \mathbf{a}_{l+r} \rangle$
  - $\langle \mathbf{a}_k, \mathbf{a}_{k+r} \rangle$ is large for small r
  - $\langle \mathbf{a}_k, \mathbf{a}_{k+r} \rangle$ decays quickly with r
  - Minimum separation likely needed in general
  - If all elements in $\mathbf{A}$ are nonnegative and the signal is nonnegative, regularity might be enough

Acknowledgements

- Swiss National Science Foundation Fellowship
- Simons Foundation
- Theory: collaboration with E. Candès
- Motivation and applications: collaboration with W.E. Moerner, C.A. Sing-Long, M.D. Lew, A. Backer, S.J. Sahl
- Helpful discussions and related work: C. Fernandez-Granda, M. Soltanolkotabi, R. Heckel

Thank you

Backup slides

Proof of Lemma

- Set: $\mathbf{h} = \hat{\mathbf{x}} - \mathbf{x}, \quad \mathcal{T} = \{l/N : h_l < 0\}$

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- Dual vector $q_l = q(l/N)$ satisfies:

$$\mathbf{P}_{\text{flat}}\mathbf{q} = \mathbf{q}, \quad \|\mathbf{q}\|_\infty = 1, \quad \text{and} \quad \begin{cases} q_l = 0, & l/N \in \mathcal{T} \\ q_l > \rho, & \text{otherwise.} \end{cases}$$

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$$\begin{aligned} |\langle \mathbf{q} - \rho/2, \mathbf{h}\rangle| &= |\langle \mathbf{P}(\mathbf{q} - \rho/2), \mathbf{h}\rangle| = |\langle \mathbf{q} - \rho/2, \mathbf{P}\mathbf{h}\rangle| \\ &\le \|\mathbf{q} - \rho/2\|_\infty \|\mathbf{P}\mathbf{h}\|_1 \le \|\mathbf{P}\mathbf{x} - \mathbf{s} + \mathbf{s} - \mathbf{P}\hat{\mathbf{x}}\|_1 \\ &\le \|\mathbf{P}\mathbf{x} - \mathbf{s}\|_1 + \|\mathbf{s} - \mathbf{P}\hat{\mathbf{x}}\|_1 \\ &\le 2\|\mathbf{P}\mathbf{x} - \mathbf{s}\|_1 \le 2\|\mathbf{z}\|_1. \end{aligned}$$

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- Combining: $\|\mathbf{h}\|_1 \le 4\|\mathbf{z}\|_1/\rho$.

Connection to Bernstein theorem

Consider: $q(t) = \sum_{k=-f_c}^{f_c} \hat{q}_k e^{-\mathrm{i}2\pi kt}$ with $\|q\|_\infty \leq 1$
Then: $\|q'\|_\infty \leq 2f_c$

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"Curvy" $q(t)$ has best possible curvature!

Since

$$q(t_i) = 0$$
$$q'(t_i) = 0$$
$$\|q\|_\infty \leq 1$$

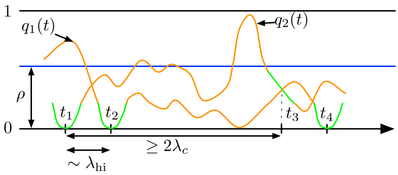
We conclude:

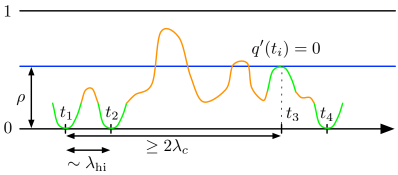
$$\begin{aligned} \|q'\|_\infty \leq 2f_c &\Rightarrow \|q''\|_\infty \leq (2f_c)^2 \\ &\Rightarrow q(t - t_i) \leq (2f_c)^2 (t - t_i)^2 \\ &\Rightarrow q(t_i + 1/N) \leq \frac{(2f_c)^2}{N^2} = \frac{1}{\mathrm{SRF}^2} \end{aligned}$$

New tools

1. Control behavior on separated set
2. **Multiply**

$$q(t) = q_1(t) \times q_2(t)$$
$$0 = q'(t_3) = q_1'(t_3)q_2(t_3) + q_1(t_3)q_2'(t_3)$$





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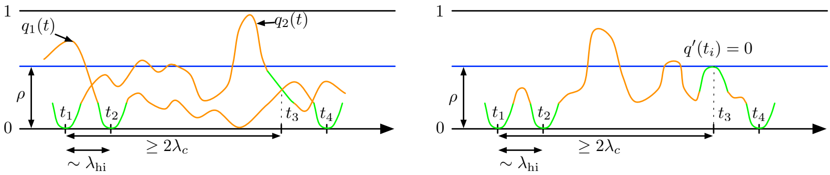

3. **Sum**

$$q(t) = \sum_{r} \prod_{k=1}^{r} \sum_{t_{jk} \in \mathcal{T}_k} \underbrace{a_{jk} K(t - t_{jk})}_{\text{frequency } f_c/r}$$