

Support Inference in linear Statistical Inverse Problems

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Outline

- ① Introduction
- ② Theory
- ③ Simulations and real data example
- ④ Conclusion

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- 1 Introduction
- 2 Theory
- 3 Simulations and real data example
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Setting and goal

- \mathcal{X} and \mathcal{Y} Hilbert spaces
- $\{\varphi_i\}_{i \in \mathbb{N}} \subset \mathcal{X}$ a dictionary
- $T : \mathcal{X} \rightarrow \mathcal{Y}$ bounded and linear

Can we identify the active components ($\hat{=}$ 'support') of an unknown f from noisy measurements of Tf ?

More precisely:

Given noisy measurements $Y \approx Tf$ we want to generate a set \mathcal{I}_a such that at a controlled error level all $i \in \mathcal{I}_a$ satisfy $\langle \varphi_i, f \rangle_{\mathcal{X}} > 0$

Support inference?

Special situation: Suppose that

- \mathcal{X} is a space of functions (i.e. $\mathcal{X} = \mathbf{L}^2(\Omega)$),
- and the functions φ_i have compact support (e.g. wavelet dictionary)

Then:

$$\langle \varphi_i, f \rangle_{\mathcal{X}} > 0 \quad \Rightarrow \quad f|_{\text{supp}(\varphi_i)} \not\equiv 0$$

Consequently, we obtain information about the support of f !

Related problems and methods

Suppose f is sparse w.r.t. $\{\varphi_i\}_{i \in \mathbb{N}}$. Then for the recovery of f many methods are used:

- ℓ^1 -penalized Tikhonov regularization / LASSO

$$\hat{f}_\alpha = \operatorname{argmin}_{f \in \mathcal{X}} \left[\|Tf - Y\|_Y^2 + \alpha \sum_{i=1}^{\infty} |\langle \varphi_i, f \rangle_{\mathcal{X}}| \right]$$

- Residual method / Danzig selector

$$\hat{f}_\alpha = \operatorname{argmin}_{f \in \mathcal{X}} \sum_{i=1}^{\infty} |\langle \varphi_i, f \rangle_{\mathcal{X}}| \quad \text{subject to} \quad \|Tf - Y\|_Y \leq \rho$$

- Orthogonal matching pursuit
- ...

But none of these methods can identify the true support at a controlled error level!

Methodology

Inference for a single i :

- compute a function Φ_i such that $\langle \Phi_i, Tf \rangle_{\mathcal{Y}} = \langle \varphi_i, f \rangle_{\mathcal{X}}$, i.e.
 $\varphi_i = T^* \Phi_i$
- compute the (asymptotic) distribution of $\langle \Phi_i, Y \rangle_{\mathcal{Y}}$ (test statistic) under the hypothesis $\langle \varphi_i, f \rangle_{\mathcal{X}} = 0$
- with the $(1 - \alpha)$ -quantile $q_{1-\alpha}$ of this (asymptotic) distribution it holds under $\langle \varphi_i, f \rangle_{\mathcal{X}} = 0$ (asymptotically)

$$\mathbb{P} [\langle \Phi_i, Y \rangle_{\mathcal{Y}} \geq q_{1-\alpha}] \leq \alpha$$

- consequently if $\langle \Phi_i, Y \rangle_{\mathcal{Y}} \geq q_{1-\alpha}$ we have $\langle \varphi_i, f \rangle_{\mathcal{X}} > 0$ with probability $\geq 1 - \alpha$.

Methodology (cont')

Inference for all i :

- if we infer for each i individually, the multiplicity adjustment makes the statements weak (if the statements are true for each single i with probability 90%, then they hold true for two i at the same time only with probability 81% etc.)

↪ remedy: simultaneous testing

- consider the test statistic

$$M = \max_i \left[w_i \left(\frac{\langle \Phi_i, Y \rangle_{\mathcal{Y}}}{\sqrt{\mathbb{V} [\langle \Phi_i, Y \rangle_{\mathcal{Y}}]}} - w_i \right) \right].$$

- compute the asymptotic distribution of M under $f \equiv 0$ and its $(1 - \alpha)$ -quantile $q_{1-\alpha}$
- mark each i for which $\langle \Phi_i, Y \rangle_{\mathcal{Y}} > (q_{1-\alpha}/w_i + w_i) \sqrt{\mathbb{V} [\langle \Phi_i, Y \rangle_{\mathcal{Y}}]}$ as active

Methodology (cont')

- by taking the max in the statistic the statements become uniform in i :

$$\mathcal{I}_\alpha := \left\{ i \mid \langle \Phi_i, Y \rangle_{\mathcal{Y}} > \left(\frac{q_{1-\alpha}}{w_i} + w_i \right) \sqrt{\mathbb{V}[\langle \Phi_i, Y \rangle_{\mathcal{Y}}]} \right\}$$

satisfies (asymptotically)

$$\mathbb{P}[\langle \varphi_i, f \rangle_{\mathcal{X}} > 0 \text{ for all } i \in \mathcal{I}_\alpha] \geq 1 - \alpha.$$

~> we can infer on all i at a controlled level!

Are the quantiles $q_{1-\alpha}$ well-defined? How to compute them?

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Specific setting

- $\mathcal{Y} = L^2([0, 1]^d)$, discrete measurements: $Y_j = (Tf)(x_j) + \xi_j$, $j \in \{1, \dots, n\}^d$
- ξ_j are independent, centered ($\mathbb{E}[\xi_j] = 0$) and satisfy a moment condition (especially all moments need to exist)
- the dictionary has at most $N = N(n)$ elements φ_i which satisfy $\varphi_i = T^* \Phi_i$, and there is a transformed mother wavelet Φ such that

$$\{\Phi_i\} = \left\{ \Phi \left(\frac{\cdot - t_i}{h_i} \right) \mid 1 \leq i \leq N(n) \right\}$$

with **scales** $h_i \in [0, 1]^d$ and **positions** $t_i \in [0, 1]^d$

- the function Φ has compact support in $[0, 1]^d$

Test statistic

- $\langle \Phi_i, Y \rangle_Y$ is not available, approximate it by

$$\langle \Phi_i, Y \rangle_n := n^{-d} \sum_{j \in \{1, \dots, n\}^d} Y_j \Phi_i(x_j)$$

- the variance $\sigma_i^2 := \mathbb{V} [\langle \Phi_i, Y \rangle_Y]$ might also be unknown, consider a family of uniformly consistent estimators $\hat{\sigma}_i^2$
- we have to investigate the asymptotic distribution of

$$\mathcal{S}(Y) := \max_i \left[w_i \left(\frac{\langle \Phi_i, Y \rangle_n}{\hat{\sigma}_i} - w_i \right) \right]$$

- the calibration values are only scale-dependent and chosen as

$$w_i = \sqrt{2 \log \left(\frac{C_{\Phi_i}}{\prod h_i} \right)} + C_d \frac{\log \left(\sqrt{2 \log \left(\frac{C_{\Phi_i}}{\prod h_i} \right)} \right)}{\sqrt{2 \log \left(\frac{C_{\Phi_i}}{\prod h_i} \right)}}$$

Gaussian Approximation

Suppose that

- there are only polynomially many probe functions in the dictionary ($N(n) \leq n^\kappa$ for some $\kappa > 0$)
- the smallest scale tends to zero not too fast ($\min_i \min_{\text{entries}} h_i \geq \log(n)^p / n$ with some specific p)
- the largest scale tends to zero sufficiently fast ($\max_i \max_{\text{entries}} h_i \leq n^{-\delta}$ for some $\delta > 0$)

Gaussian Approximation

Then there are i.i.d. standard normal random variables ζ_j such that under $f \equiv 0$ it holds

$$\lim_{n \rightarrow \infty} |\mathbb{P}[\mathcal{S}(Y) > q] - \mathbb{P}[\mathcal{S}(\zeta) > q]| = 0 \quad \text{for all } q$$

Gaussian Approximation (cont')

Continuous Gaussian Approximation

There exists a Brownian sheet W such that $\mathcal{S}(Y)$ can be approximated

$$\mathcal{S}(W) := \max_i \left[w_i \left(\frac{\int \Phi_i(x) dW_x}{\|\Phi_i\|_{L^2}} - w_i \right) \right],$$

i.e. under $f \equiv 0$ it holds

$$\lim_{n \rightarrow \infty} |\mathbb{P}[\mathcal{S}(Y) > q] - \mathbb{P}[\mathcal{S}(W) > q]| = 0 \quad \text{for all } q.$$

Moreover

- $\mathcal{S}(W)$ is a.s. bounded from below and above,
- $\mathcal{S}(W)$ is asymptotically non-degenerate, i.e. does not concentrate to any point,
- $\mathcal{S}(W)$ does not depend on any unknown quantities.

Gaussian Approximation - Implications

This means that we can use quantiles $q_{1-\alpha}$ from

$$\mathcal{S}(\zeta) = \max_i \left[w_i \left(\frac{\langle \Phi_i, \zeta \rangle_n}{\|\Phi_i\|_2} - w_i \right) \right]$$

to hold the asymptotic level.

- $\mathcal{S}(\zeta)$ is 'distribution free', i.e. it depends only on known quantities
 \rightsquigarrow quantiles can be simulated easily
- quantiles are meaningful as $n \rightarrow \infty$

If $\langle \Phi_i, Y \rangle_n > \left(\frac{q_{1-\alpha}}{w_i} + w_i \right) \hat{\sigma}_i$ mark i as active (i.e. $i \in \mathcal{I}_a$)!

Detection properties

So far: whenever $i \in \mathcal{I}_a$, then asymptotically $\mathbb{P}[\langle \varphi_i, f \rangle_{\mathcal{X}} > 0] \geq 1 - \alpha$.

But how large must $\langle \varphi_i, f \rangle_{\mathcal{X}}$ be to be detected?

Lower detection bound

If $\langle \varphi_i, f \rangle_{\mathcal{X}} \geq 2 \left(\frac{q_{1-\alpha}}{w_i} + w_i \right) \sigma_i$, then

$$\lim_{n \rightarrow \infty} \mathbb{P}[i \in \mathcal{I}_a] \geq 1 - \alpha$$

uniformly in i .

Special case: deconvolution

- Suppose $d = 2$ and T is a convolution operator, i.e.

$$(Tf)(y) = (k * f)(y) := \int_{[0,1]^2} k(x - y) f(y) \, dy.$$

↪ This implies that if we choose $\{\varphi_i\}$ of Wavelet-type we obtain

$$\{\Phi_i\} = \left\{ \tilde{\Phi}_{h_i} \left(\frac{\cdot - t_i}{h_i} \right) \mid 1 \leq i \leq N(n) \right\}$$

where $\tilde{\Phi}_h$ depends on h .

- Suppose the Fourier transform of the kernel k has a polynomial decay, i.e.

$$\underline{c}(1 + \|\xi\|_2^2)^{-a} \leq |\mathcal{F}k(\xi)| \leq \overline{C}(1 + \|\xi\|_2^2)^{-a}.$$

↪ This implies that the functions φ_i can be chosen such that they are **non-negative** and have **compact support**, and $\|\tilde{\Phi}_h\|_{L^2}$ behaves like $\max_{\text{entries}} h^{2a}$.

Special case: deconvolution (cont')

- $\mathcal{S}(Y)$ can be approximated by a Gaussian version which is a.s. bounded and non-degenerate
- ↪ whenever $i \in \mathcal{I}_a$, then asymptotically $\mathbb{P}[\langle \varphi_i, f \rangle_{\mathcal{X}} > 0] \geq 1 - \alpha$.
- If $\langle \varphi_i, f \rangle_{\mathcal{X}}$ is sufficiently large, then i will be detected with probability $\geq 1 - \alpha$.

Optimality of the lower detection bound

In $d = 1$ this lower detection bound is optimal in the sense that no estimator for a β -Hölder-continuous function f can distinguish between $f|_{[t, t+h]} = 0$ and $f|_{[t, t+h]} \geq h^\beta$ at a faster rate in $h = h(n)$.

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Considered problem

- T deconvolution problem, i.e.

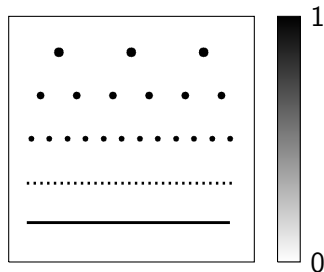
$$Y_j = (k * f)(x_j) + \xi_j, \quad j \in \{1, \dots, n\}^2$$

with an equidistant grid $\{x_j\}$ on $[0, 1]^2$.

- The kernel k is chosen from the family

$$(\mathcal{F}k_{a,b})(\xi) = (1 + b^2 \|\xi\|_2^2)^{-a}, \quad \xi \in \mathbb{R}^2.$$

- The variance is considered to be known.
- The mother wavelet φ is chosen to minimize the variance $\|\Phi\|_{L^2}^2$
(\leadsto Tensor product of Beta-Kernels)

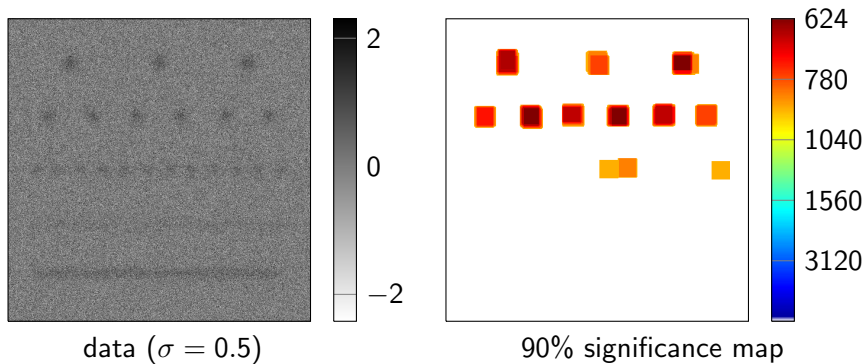


Testfunction f

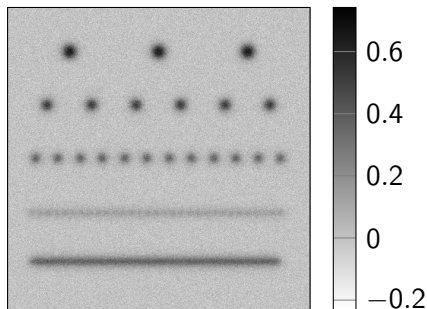
Some empirical levels for $\alpha = 0.1$

Noise scenario	Parameters	false positives %
Gaussian noise		8.8
Student's t noise	$\nu = 3$	100
	$\nu = 6$	94.7
	$\nu = 7$	72.3
	$\nu = 11$	21.8
	$\nu = 15$	15.7
	$\nu = 19$	13.0
	$\nu = 23$	13.3
CCD noise (Sneyder '93, '95):	$t = 100, b = 0.5, \sigma = 0.01$	9.8
obs. time t , background b ,	$t = 1000, b = 0.005, \sigma = 0.01$	8.1
read-out errors $\mathcal{N}(0, \sigma^2)$	$t = 100, b = 0.005, \sigma = 0.01$	14.5

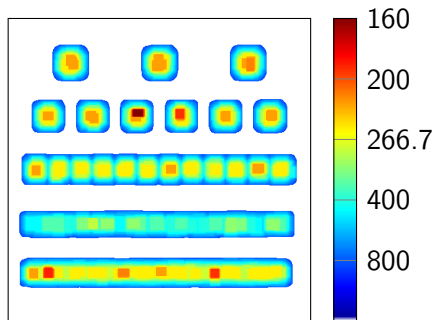
Support recovery - result



Support recovery - result

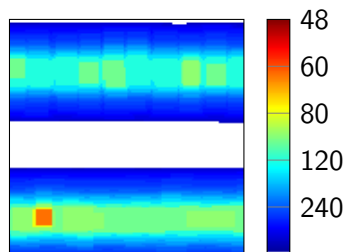
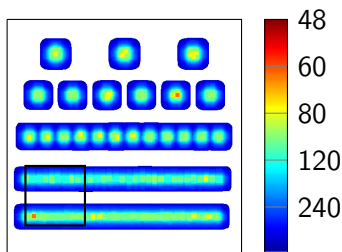
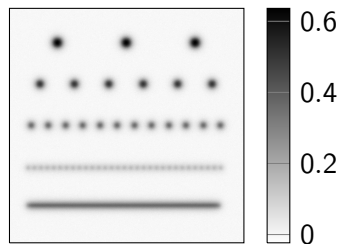
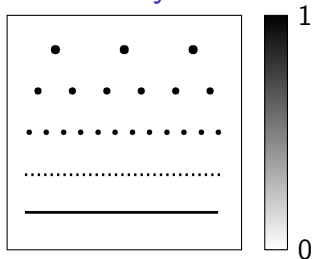


data ($\sigma = 0.05$)



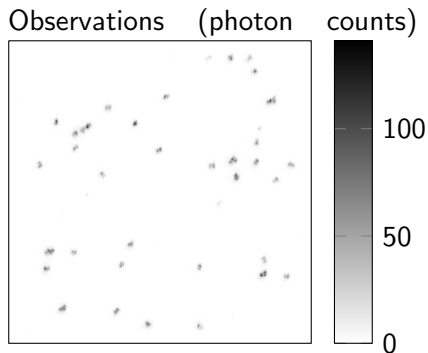
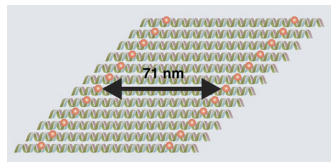
90% significance map

Support recovery - result



Real data example - Setup

- we analyze fluorescent dyes on single DNA Origami
- imaging is performed by a STED microscope
- each of the two strands can at most hold 12 markers

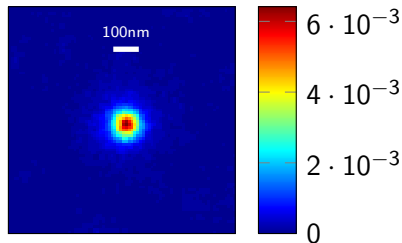


Modeling

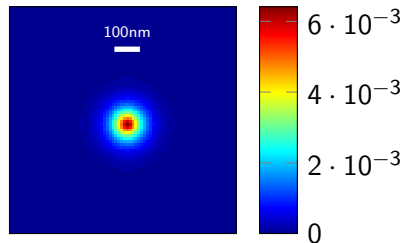
The observations can perfectly modeled by

$$Y_j \stackrel{\text{independent}}{\sim} \text{Bin}(t, (k * f)(x_j)), \quad j \in \{1, \dots, n\}^2.$$

- $\text{Bin}(t, p)$: Binomial distribution with parameters $t \in \mathbb{N}$ and $p \in [0, 1]$
- $f(x)$: probability that a photon emitted at grid point x is recorded at the detector in a single excitation pulse

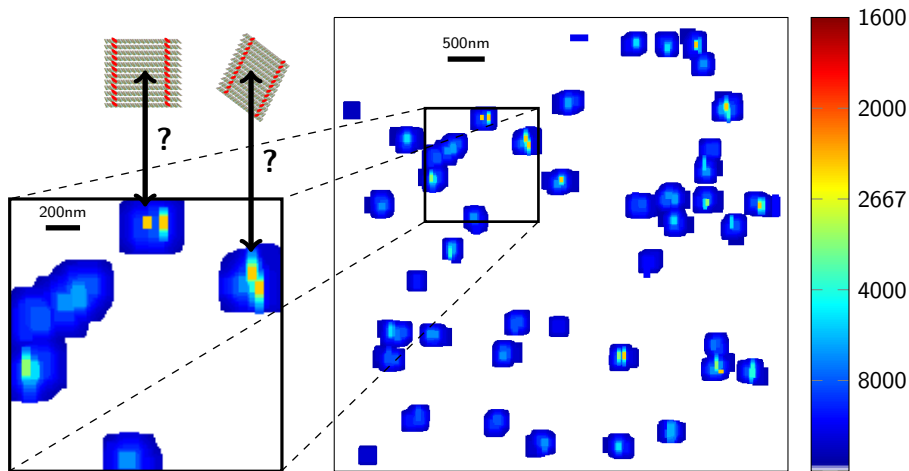


experimental kernel

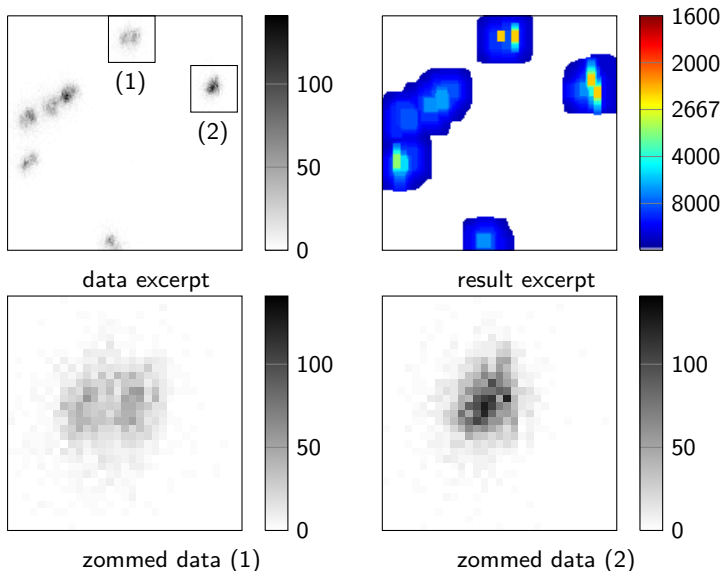


$k_{2,0.016}$

Result



Comparison of the result with the data



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Outlook

- Methodology and theory:
 - inference on active coefficients $\langle \varphi_i, f \rangle_{\mathcal{X}}$ w.r.t. a dictionary $\{\varphi_i\}$
 - techniques from multiscale testing yield uniform inference at a controlled (asymptotic) error level
 - detection power is optimal in a suitable sense
- Application:
 - the method can be used to determine the support of a function observed in a convolution model
 - performs well in a real data example

Thank you for your attention!