Support Inference in linear Statistical Inverse Problems

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Outline

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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
- $T : \mathcal{X} \to \mathcal{Y}$ bounded and linear

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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 $\mathcal{I}_\mathrm{a}$ such that at a controlled error level all $i \in \mathcal{I}_\mathrm{a}$ 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:

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

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

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

- Residual method / Danzig selector

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

- Orthorgonal 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. $\varphi_i = T^* \Phi_i$

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- with the $(1-\alpha)$-quantile $q_{1-\alpha}$ of this (asymptotic) distribution it holds under $\langle \varphi_i, f \rangle_{\mathcal{X}} = 0$ (asymptotically)

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

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

- 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 a 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.)

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$\rightsquigarrow$ remedy: simultaneous testing

- consider the test statistic

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

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

Methodology (cont')

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

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

satisfies (asymptotically)

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

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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: $Y_j = (Tf)(x_j) + \xi_j$, $j \in \{1, ..., n\}^d$

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- 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

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

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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

- $\langle \Phi_i, Y \rangle_{\mathcal{Y}}$ is not available, approximate it by

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

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

- 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 ($N(n) \leqslant n^{\kappa}$ for some $\kappa > 0$)
- the smallest scale tends to zero not too fast ($\min_i \min_{\text{entries}} h_i \geqslant \log(n)^p / n$ with some specific p)
- the largest scale tends to zero sufficiently fast ($\max_i \max_{\text{entries}} h_i \leqslant n^{-\delta}$ for some $\delta > 0$)

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Gaussian Approximation

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

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

Gaussian Approximation (cont')

Continuous Gaussian Approximation

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

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

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

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

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 $n \to \infty$

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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 $\mathbb{P}\left[\langle \varphi_i, f \rangle_{\mathcal{X}} > 0\right] \geq 1 - \alpha$.

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

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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

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

uniformly in i.

Special case: deconvolution

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

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

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

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

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

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

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

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$\rightsquigarrow$ 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

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

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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 $h = h(n)$.

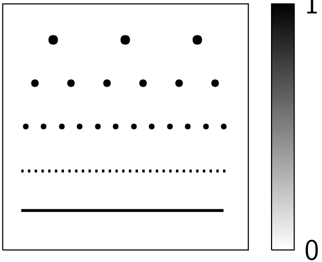
Outline

Considered problem

- T deconvolution problem, i.e.

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

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



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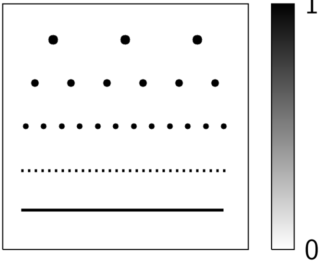
- The kernel k is chosen from the family

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



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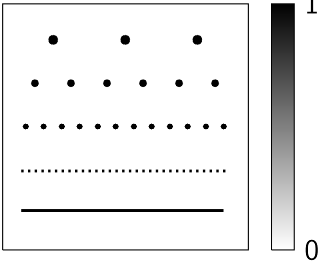

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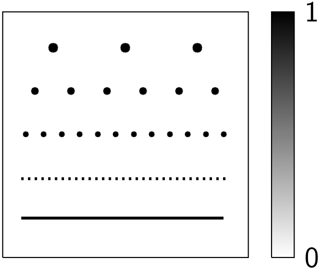
- The mother wavelet φ is chosen to minimize the variance $\|\Phi\|_{L^2}^2$ ($\rightsquigarrow$ Tensor product of Beta-Kernels)

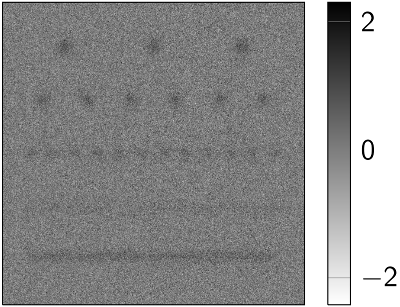


Testfunction f

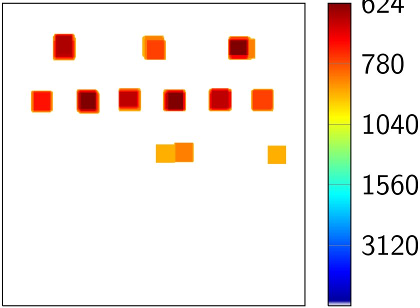
Some empirical levels for $\alpha = 0.1$

Noise scenario	Parameters	false positives %
Gaussian noise		8.8
	$\nu = 3$	100
	$\nu = 6$	94.7
	$\nu = 7$	72.3
Student's t noise	$\nu = 11$	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 $\mathcal{N}\left(0, \sigma^2\right)$	$t = 100,\ b = 0.005, \sigma = 0.01$	14.5

Support recovery - result



data ($\sigma = 0.5$)



90% significance map

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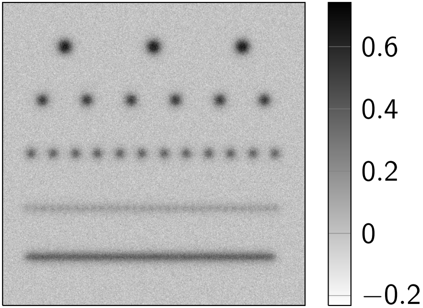
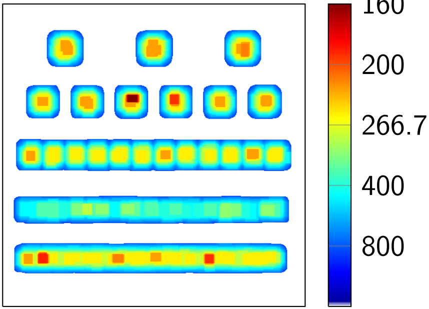


data ($\sigma = 0.05$)



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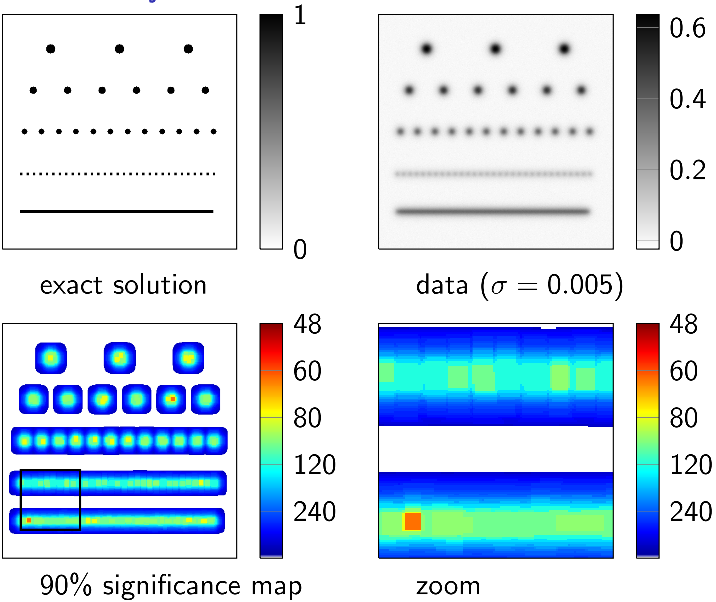
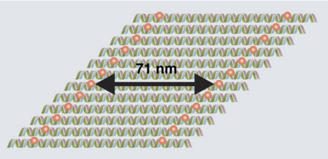
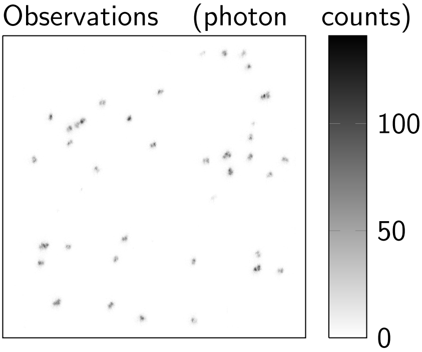


Real data example - Setup

- 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



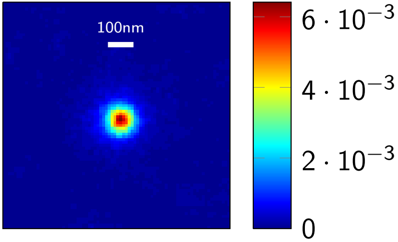


Modeling

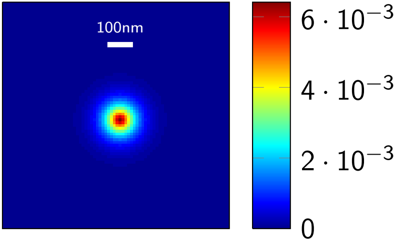
The observations can perfectly modeled by

$$Y_j \overset{\text{independent}}{\sim} \mathrm{Bin}\left(t, \left(k * f\right)\left(x_j\right)\right), \qquad j \in \{1, ..., n\}^2 .$$

- $\mathrm{Bin}(t, p)$: 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

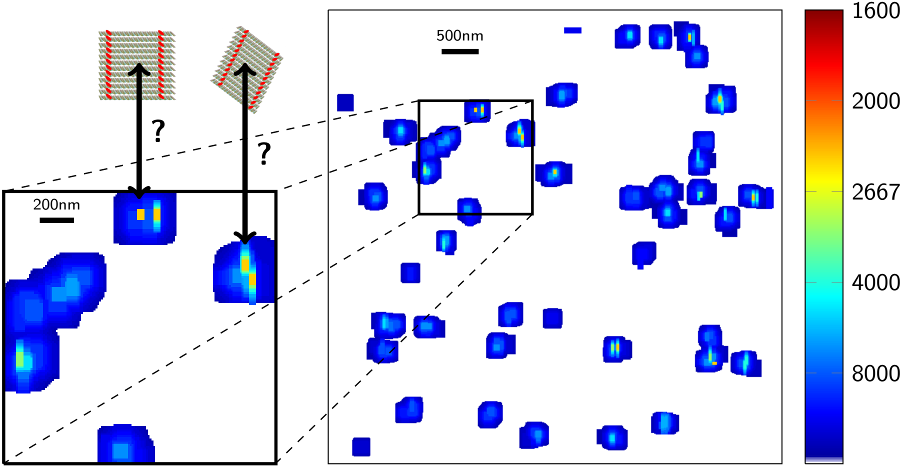


experimental kernel

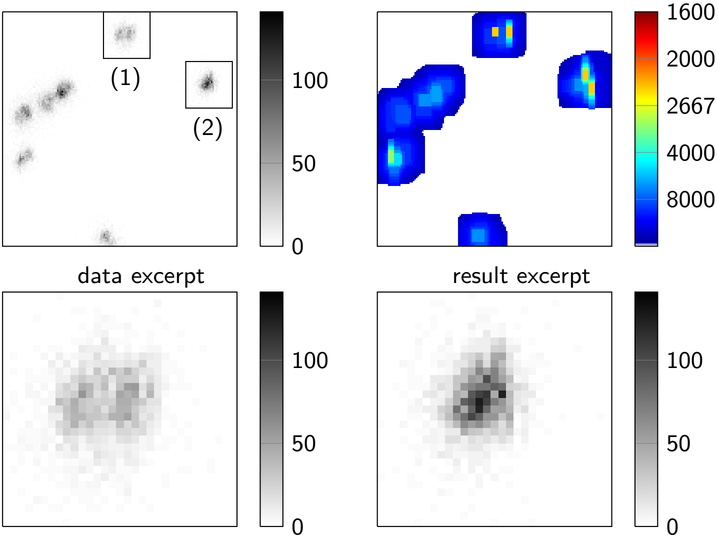


$k_{2,0.016}$

Result



Comparison of the result with the data



data excerpt

result excerpt

zommed data (1)

zommed data (2)

Outline

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

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Thank you for your attention!