# Deconvolution by regularization: possible applications at PITZ

## Fredholm Integral Equation of the First Kind

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PPS#777

# Integral Equations

## Integral Equations of the First and Second Kind

$$y(x) - \lambda \int_{\Omega} K(x,s)\, y(s)\, ds = f(x), \quad x \in Q$$

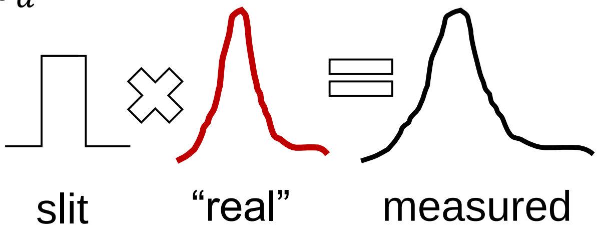
Integral Equations of the Second Kind → in principle, well-posed problem

$$\int_{\Omega} K(x,s)\, y(s)\, ds = f(x), \quad x \in Q$$

Integral Equations of the First Kind→ ill-posed problem! (may not have a perfect solution)

Particular case: deconvolution

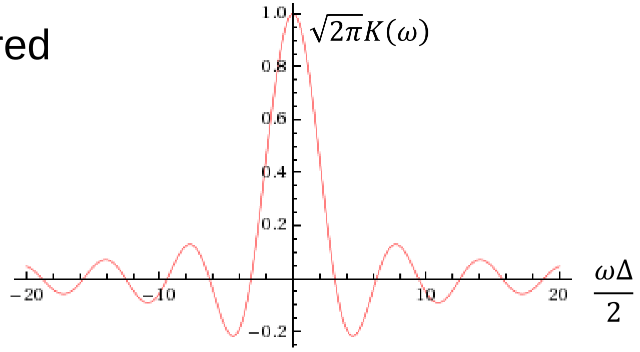
$$\int_a^b K(x-s)y(s)ds = f(x)$$




$$F(\xi) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} f(x) e^{-i\xi x} dx$$

$$K(\xi) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} K(x) e^{-i\xi x} dx$$

$$y(s) = \frac{1}{2\pi} \int_{-\infty}^{\infty} \frac{F(\xi)}{K(\xi)} e^{i\xi s} d\xi$$




e.g. for slit $\Delta \rightarrow K(\omega) = \frac{1}{\sqrt{2\pi}} \text{sinc}\left(\frac{\omega\Delta}{2}\right)$

$$y(s) = \frac{1}{2\pi} \int_{-\infty}^{\infty} \frac{|K(\xi)|^2}{|K(\xi)|^2 + \alpha\xi^{2p}} \cdot \frac{F(\xi)}{K(\xi)} e^{i\xi s} d\xi$$

# Possible applications at PITZ

## Eliminating “apparatus” function from the raw experimental data

1. Charge measurements, especially with rather high noise level (small signal) → deconvolution of the raw signal and noise histograms → more precise information on “pure” signal fluctuations
2. Slit-scan techniques → deconvolution of the slit width from the beamlet profile → “real” divergence local distribution (especially for zoom lens option and tails of the PS)
3. TDS measurements (PST and HEDA2)→ deconvolution of the unstreaked beam profile for more precise temporal shape reconstruction
4. HEDA1 measurements → deconvolution of the vertical beam profile at HIGH1.Scr5 for more precise PZ-projections
5. Image processing → pixel size elimination from the small beam (sharp profiles) → filtering
6. LPS tomography?
7. …

# Integral Equations of the First Kind → Regularization

## **Problem formation** → Tikhonov regularization method

$$A\,y \equiv \int_a^b K(x,s)\,y(s)\,ds = f(x),\quad a \le x \le b$$

$$K(x,s) \longrightarrow G = \{a \le x \le b,\ a \le s \le b\},\quad f(x) \in L_2[a,b],\quad y(s) \in L_2[a,b].$$

$$\|f\|_{L_2}^2 = \int |f(x)|^2 dx$$

Regularization methods (Tikhonov) → smoothing functional for $\alpha$ –regularization:

$$\Phi_\alpha(y) = \|Ay - f\|_{L_2}^2 + \alpha \|y\|_{L_2}^2 \rightarrow \min_{y \in L_2[a,b]}$$

$\alpha > 0$ –regularization parameter

$$\alpha\, y_\alpha(t) + \int_a^b B(t,s)\, y_\alpha(s)\, ds = F(t),\quad a \le t \le b$$

⇨ NB: Integral Equations of the Second Kind → well-posed

$$B(t,s) = \int_a^b K(x,t)\,K(x,s)\,dx \qquad F(t) = \int_a^b K(x,t)\,f(x)\,dx$$

# Regularization (Tikhonov) method

## How to determine the regularization parameter $\alpha$ ?

$$\alpha\, y_\alpha(t) + \int_a^b B(t,s)\, y_\alpha(s)\, ds = F(t), \quad a \le t \le b$$

$$F(t) = \int_a^b K(x,t) f(x) dx$$

$$B(t,s) = \int_a^b K(x,t)\, K(x,s)\, dx$$

$f(x)$ is replaced by $\tilde{f}(x)$: $\left\| f - \tilde{f} \right\|_{L_2} \le \delta$;

choice of α: $\left\| A\, y_\alpha - \tilde{f} \right\|_{L_2} = \delta$ , where $y_\alpha$ - solution of the equation above

Equation w.r.t. $\alpha$ yielding a unique solution

Practical case: $\alpha_i = \theta \alpha_{i-1}, i = 1, \ldots m, 0 < \theta<1$ → for each $\alpha_i$ solution $y_\alpha(t)$ of the equation above

choice of the optimum $\alpha_{opt} \in \{\alpha_i\}$: $\left\| A\, y_{\alpha_i} - \tilde{f} \right\|_{L_2} \approx \delta$

Quasi-optimum choice of the regularization parameter: $\left\| y_{\alpha_i} - y_{\alpha_{i-1}} \right\|_{L_2}$ → min or $\left\| y_{\alpha_i} - y_{\alpha_{i-1}} \right\| / \left\| y_{\alpha_i} \right\|$ → min

# Meshing

## Homogeneous meshes for the problem discretization

$$A\,y \equiv \int_a^b K(x,s)\,y(\mathrm{s})\,ds = f(x),\;\; \mathrm{a} \le x \le b$$

Mesh for $y(s)$ and $K(x,s)$

$$\overline{\omega}_\tau = \{s_j \in [a,b]:\;\; \mathrm{s}_j = a + j\tau,\;\; j = \overline{0,N};\;\; \tau = (b-a)/N\}$$

Mesh for $f(x)$ and $K(x,s)$

$$\overline{\omega}_h = \{x_l \in [a,b]:\;\; x_l = a + lh,\;\; 1 = \overline{0,M};\;\; h = (b-a)/M\}$$

$$\alpha\, y_\alpha(t) + \int_a^b B(t,s)\,y_\alpha(\mathrm{s})\,ds = F(t),\quad a \le t \le b \qquad F(t) = \int_a^b K(x,t)f(x)dx \qquad B(t,s) = \int_a^b K(x,t)\,K(x,s)\,dx$$

$t$-mesh = $s$-mesh

# Discretization

## Using Simpson's rule and assuming parity of $N$ and $M$

Simpson's rule → $A_j^{(N)}$ and $A_l^{(M)}$ → $O(h^4+\tau^4)$

$$\int_a^b P(x)dx \approx \sum_{l=0}^{N} A_l^{(N)} P_l$$

$$y_i \approx y_\alpha(t_i),\quad B_{ij} \approx B(t_i,s_j),\quad F_i \approx F(t_i),\quad i,j=\overline{0,N}$$

$$A_l^{(N)} = \frac{\Delta x}{3}\begin{cases}1 & l=0,N\\ 2 & l-\text{even}\\ 4 & l-\text{odd}\end{cases}$$

$$\alpha\, y_\alpha(t) + \int_a^b B(t,s)\, y_\alpha(s)\, ds = F(t),\quad a \le t \le b$$

$$F(t) = \int_a^b K(x,t) f(x) dx$$

$$B(t,s) = \int_a^b K(x,t)\, K(x,s)\, dx$$

→

$$\alpha y_i + \sum_{j=0}^{N} A_j^{(N)} B_{ij} y_j = F_i,\quad i=\overline{0,N}$$

$$F(t_i) = \sum_{l=0}^{M} A_l^{(M)} K(x_l,t_i) f(x_l) + O(h^4),\quad i,j=\overline{0,N}$$

$$B(t_i,s_j) = \sum_{l=0}^{M} A_l^{(M)} K(x_l,t_i)\, K(x_l,s_j) + O(h^4)$$

# Discretization

**Using Simpson's rule and assuming parity of $N$ and $M$**

$$\alpha y_i + \sum_{j=0}^{N} A_j^{(N)} B_{ij} y_j = F_i, \quad i = \overline{0, N}$$

$$F(t_i) = \sum_{l=0}^{M} A_l^{(M)} K(x_l, t_i) f(x_l) + O(h^4), \quad i, j = \overline{0, N}$$

$$B(t_i, s_j) = \sum_{l=0}^{M} A_l^{(M)} K(x_l, t_i) K(x_l, s_j) + O(h^4)$$

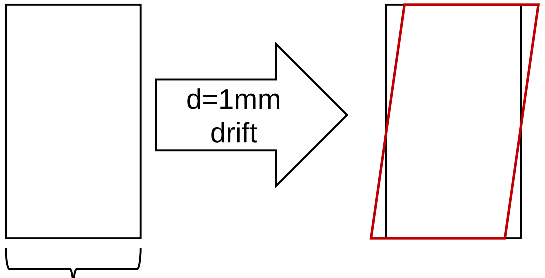
$\Rightarrow$ $y_0, y_1, \dots, y_N$

$$\tilde{y}_\alpha(t) = \frac{1}{\alpha}\left(\sum_{j=0}^{N} A_j^{(N)} B(t, s_j)\, y_j + F(t)\right), \quad a \le t \le b$$

# Beamlet Modeling

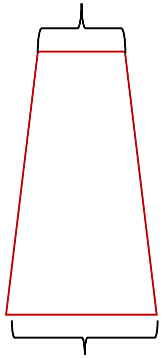
## Deconvolution of the finite slit opening

- 50um slit opening
- f160 → scale~45um → X
- f250 → scale~12um → 4-5 pixel window?
- Rigorously: deconvoluting with trapezium



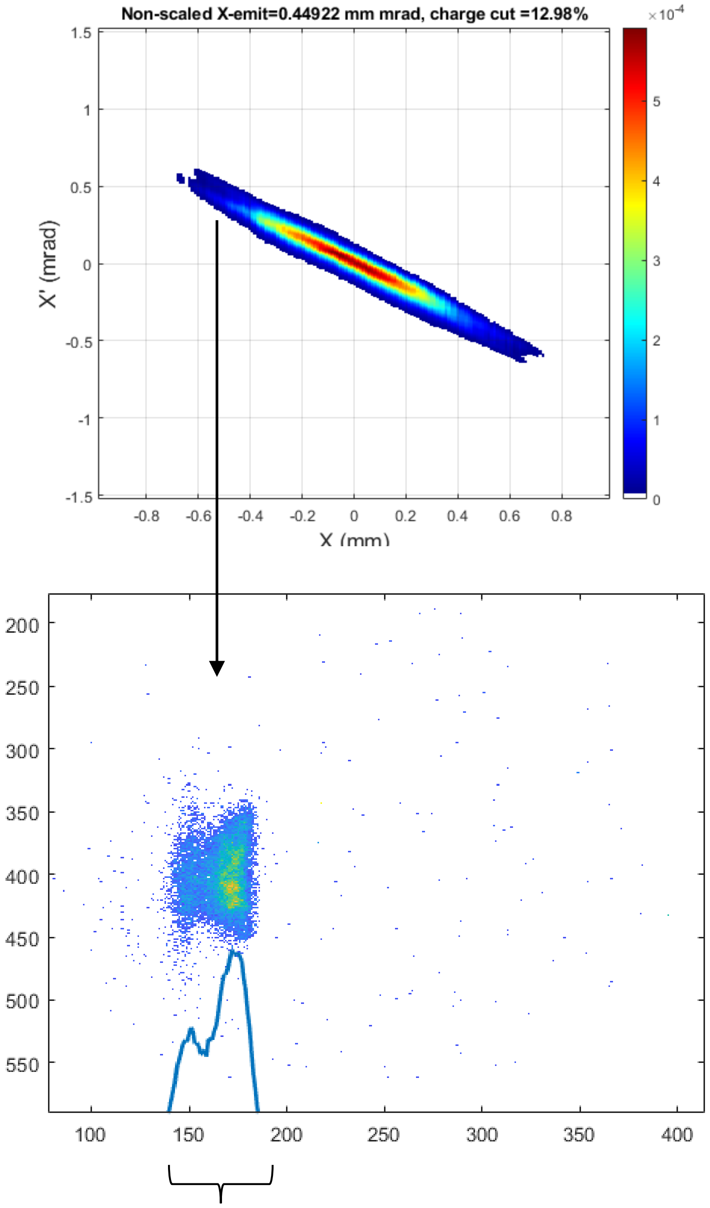

$\Delta_{sl} = 50\mu m$

$\Delta_{sl} - 2\delta$



$$\delta \sim \sigma_{BL} \cdot \frac{d}{L_{drift}}$$

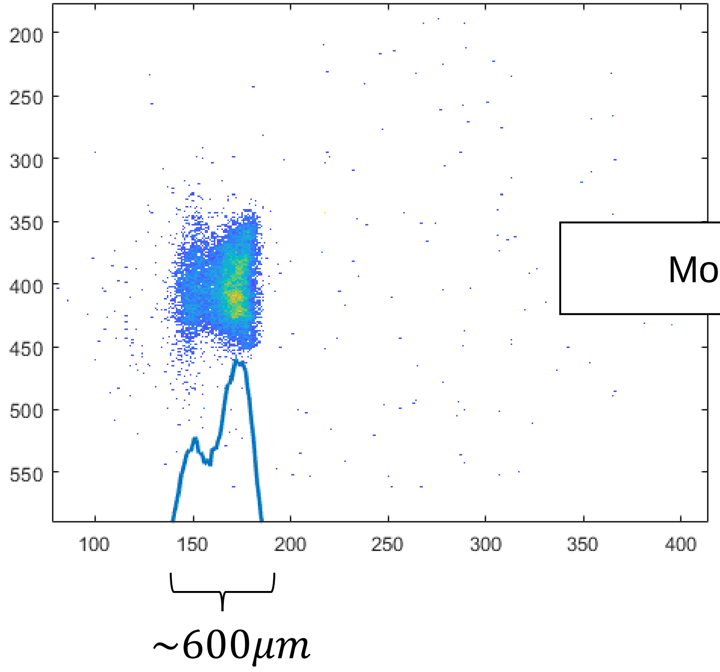
$\Delta_{sl} = 50\mu m$



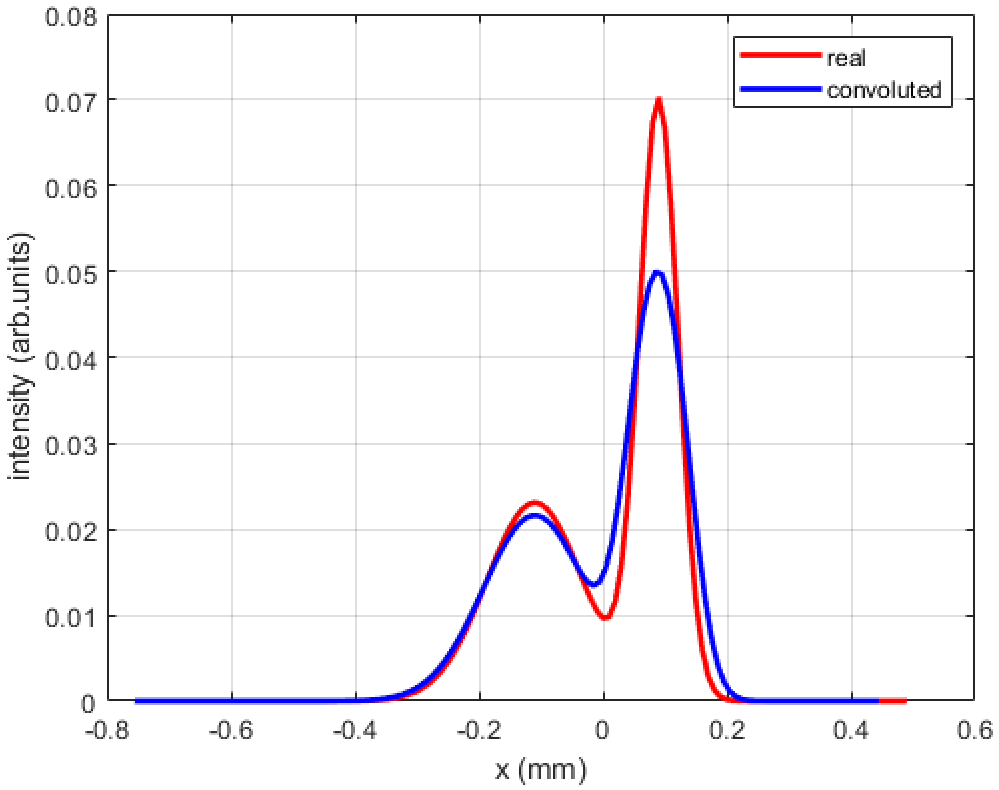

$\sim 600\mu m$

# Beamlet Modeling

## Deconvolution of the finite slit opening




Modeling with 2 Gaussian



# Modeled beamlet profile reconstruction

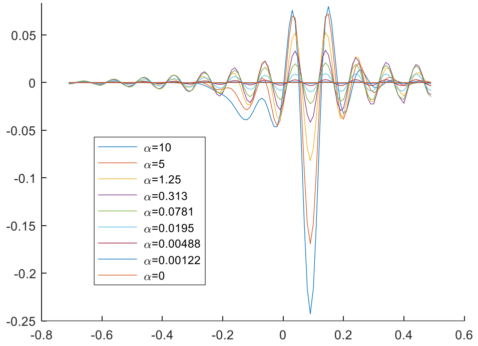
## Deconvolution of the finite slit opening

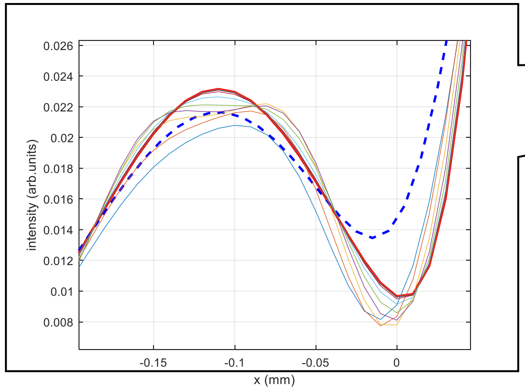
$\alpha_i = \theta \alpha_{i-1}, i = 1, \dots m$

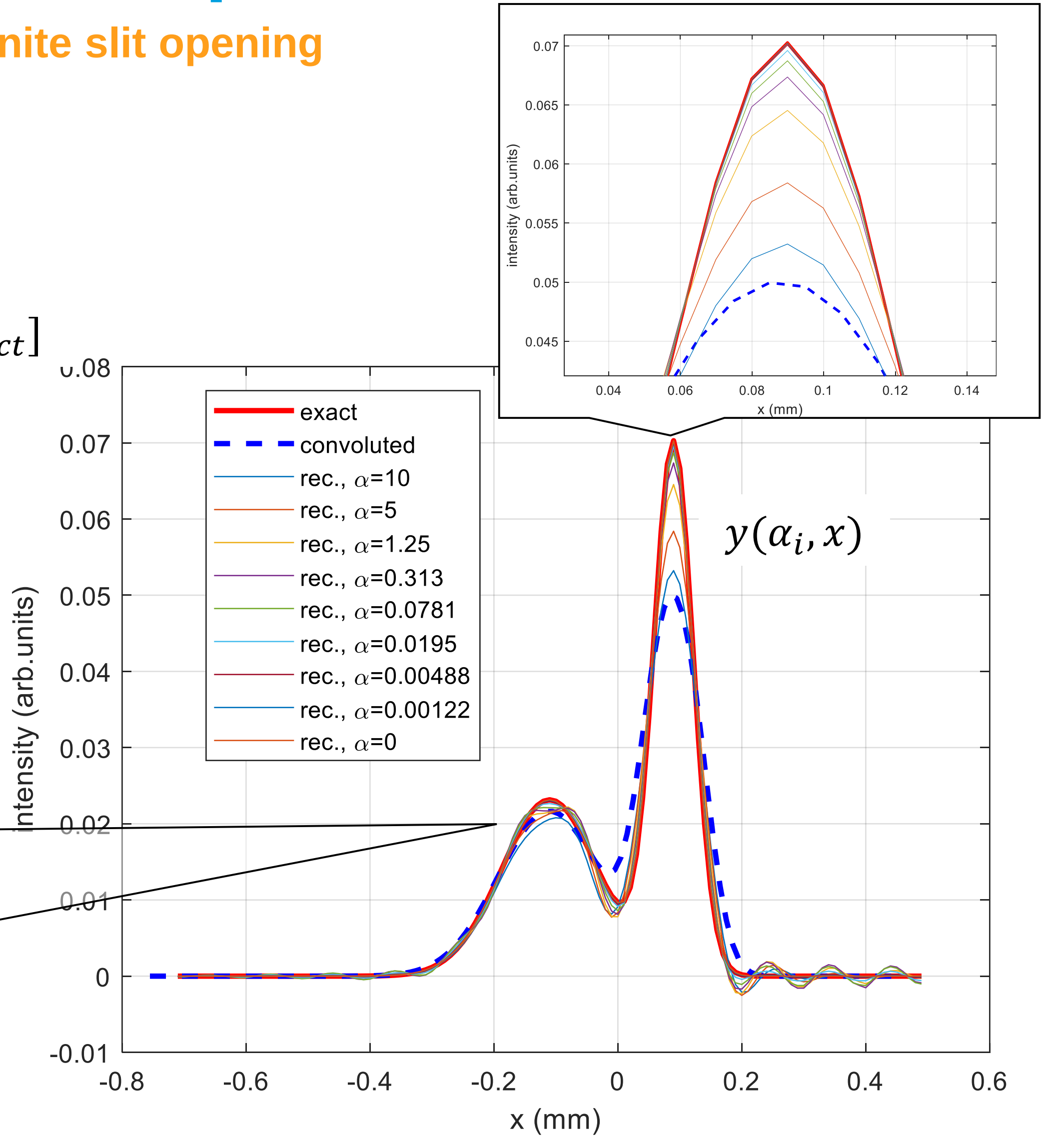
$\alpha_0 = 10$

$\theta = 0.5$

$(y(\alpha_i) - y_{exact})/\max[y_{exact}]$



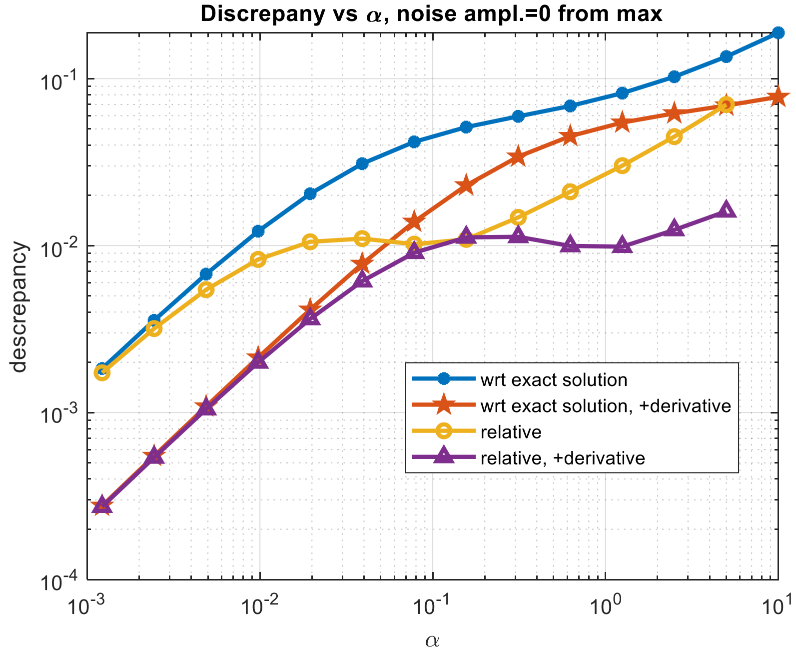




$$\alpha\, y_\alpha(t) + \int_a^b B(t,s)\, y_\alpha(s)\, ds = F(t), \quad a \le t \le b$$

$$B(t,s) = \int_a^{\tilde{b}} K(x,t)\, K(x,s)\, dx \qquad F(t) = \int_a^b K(x,t) f(x) dx$$

$$\Phi_\alpha(y) = \left\| Ay - f \right\|_{L_2}^2 + \alpha \left\| y \right\|_{L_2}^2 \to \min_{y \in L_2[a,b]}$$

Option: 2nd derivative




$$\left\| y_{\alpha_i} - y_{\alpha_{i-1}} \right\| / \left\| y_{\alpha_i} \right\|$$

No noise!

# Modeled beamlet profile reconstruction

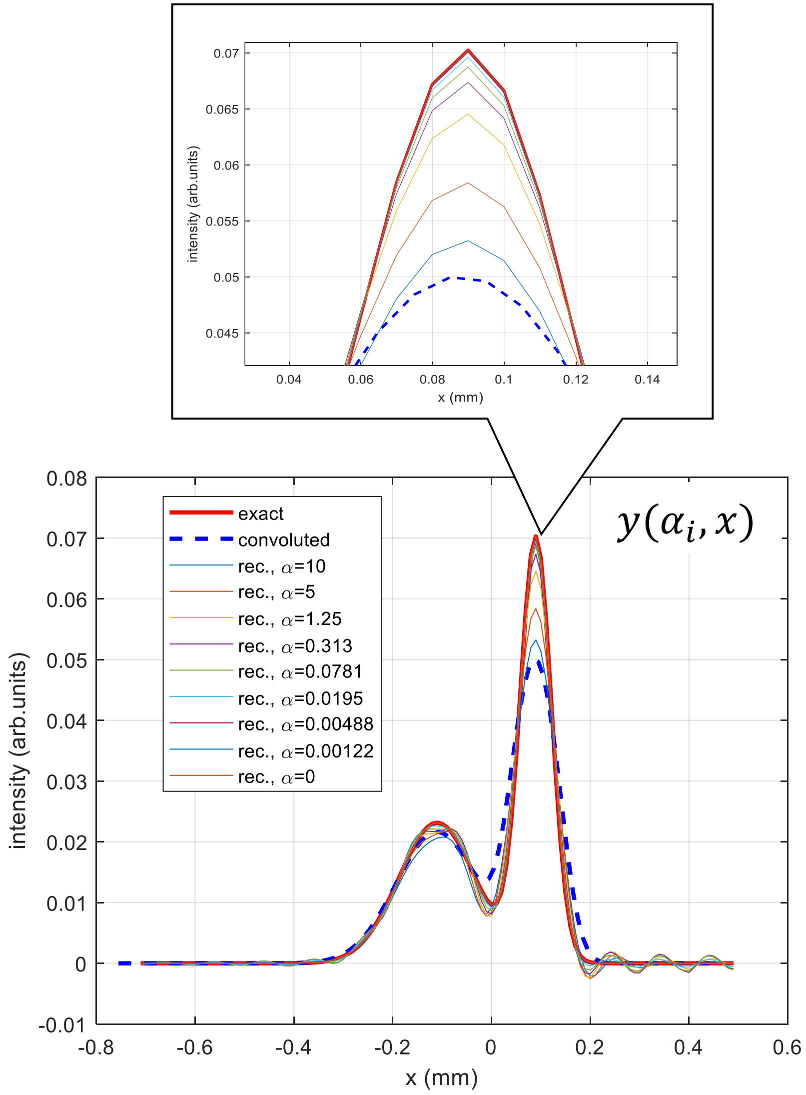
## Deconvolution of the finite slit opening

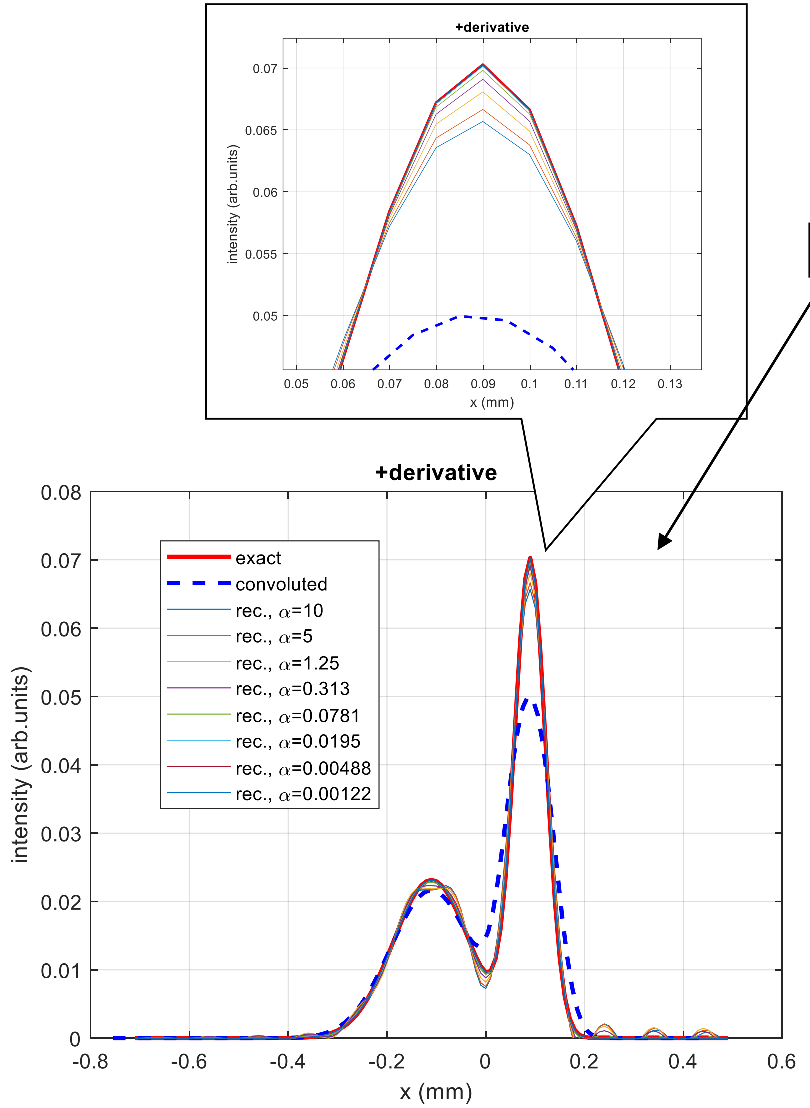
$$\alpha\, y_\alpha(t) + \int_a^b B(t,s)\, y_\alpha(s)\, ds = F(t), \quad a \le t \le b$$

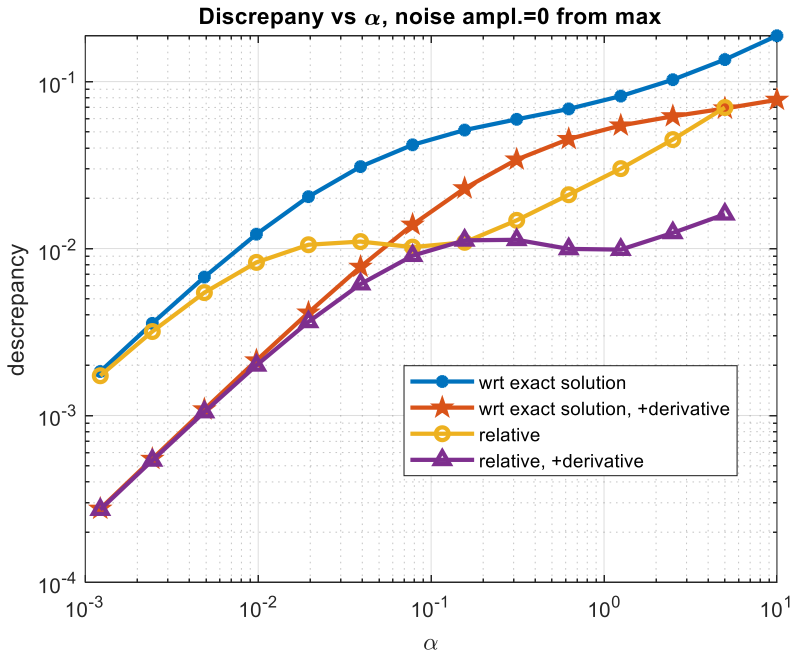
$$B(t,s) = \int_{\vec{a}}^{\vec{b}} K(x,t)\, K(x,s)\, dx \qquad F(t) = \int_a^b K(x,t) f(x) dx$$

$$\Phi_\alpha(y) = \|Ay - f\|_{L_2}^2 + \alpha \|y\|_{L_2}^2 \to \min_{y \in L_2[a,b]}$$

**Option: 2nd derivative**



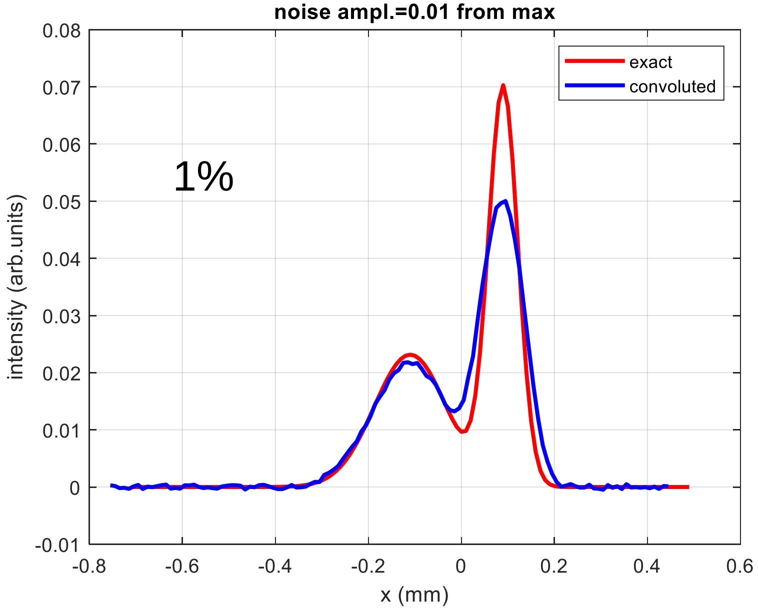



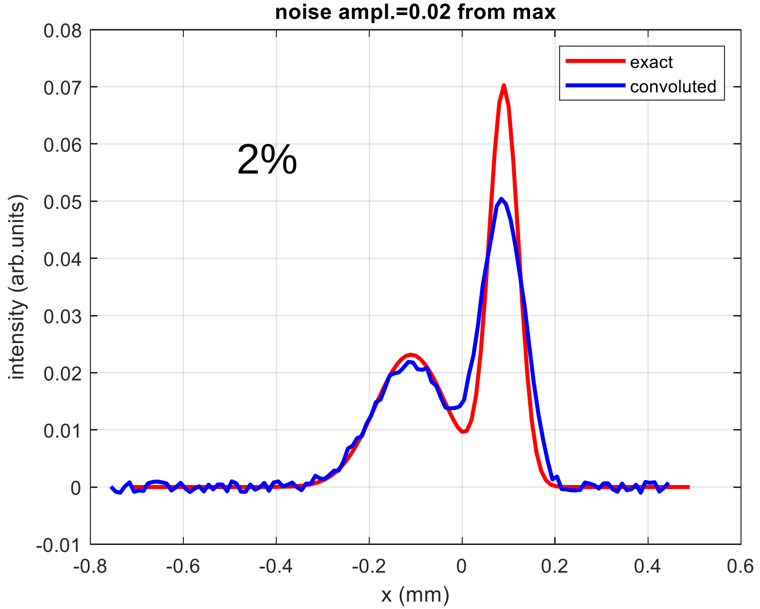



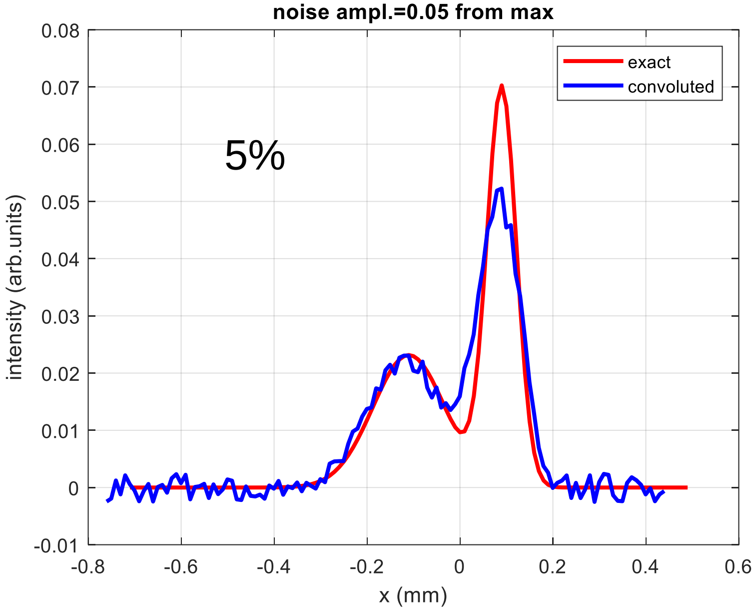

$$\|y_{\alpha_i} - y_{\alpha_{i-1}}\| / \|y_{\alpha_i}\|$$

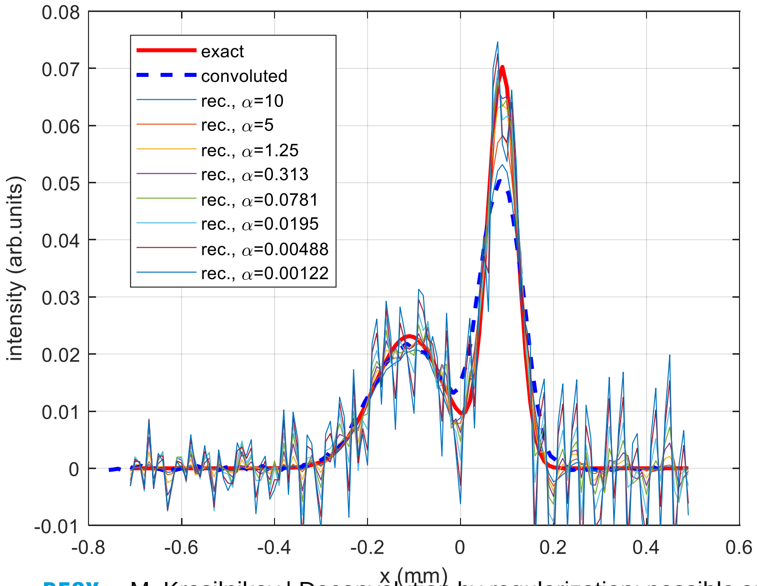
No noise!

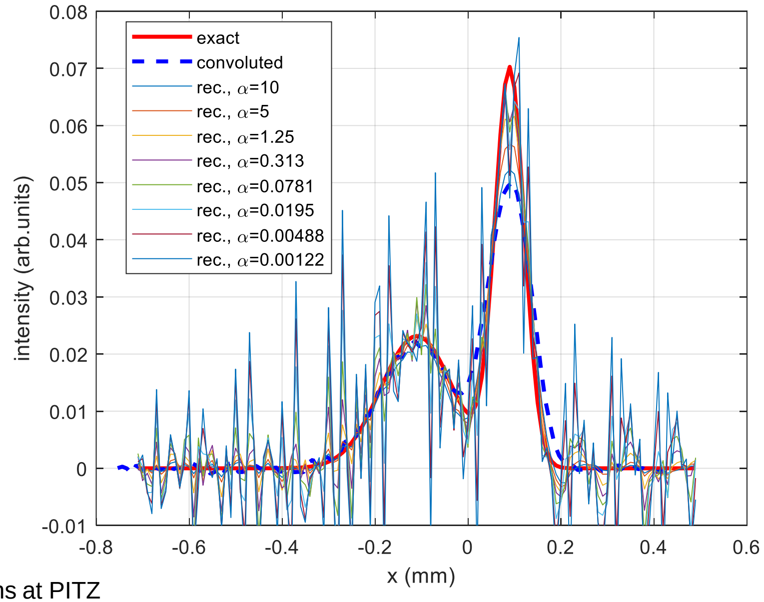
# Modeled beamlet profile reconstruction additive white Gaussian random noise

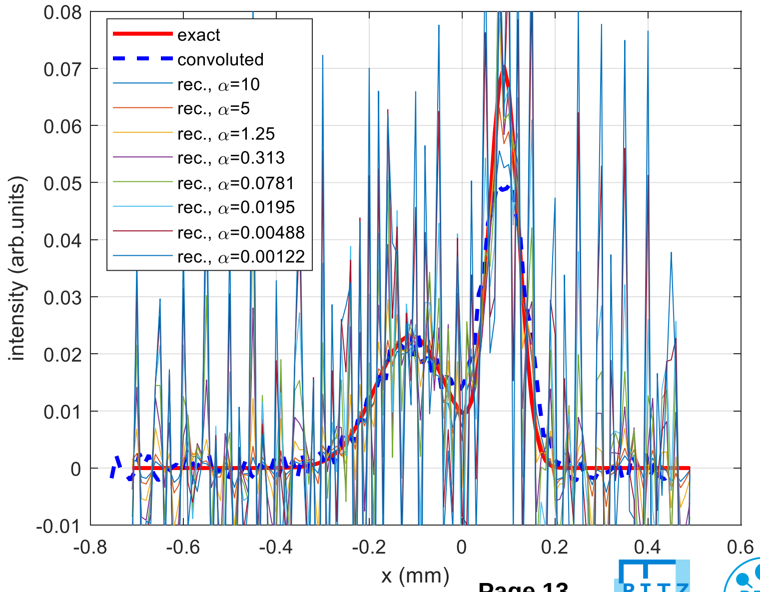


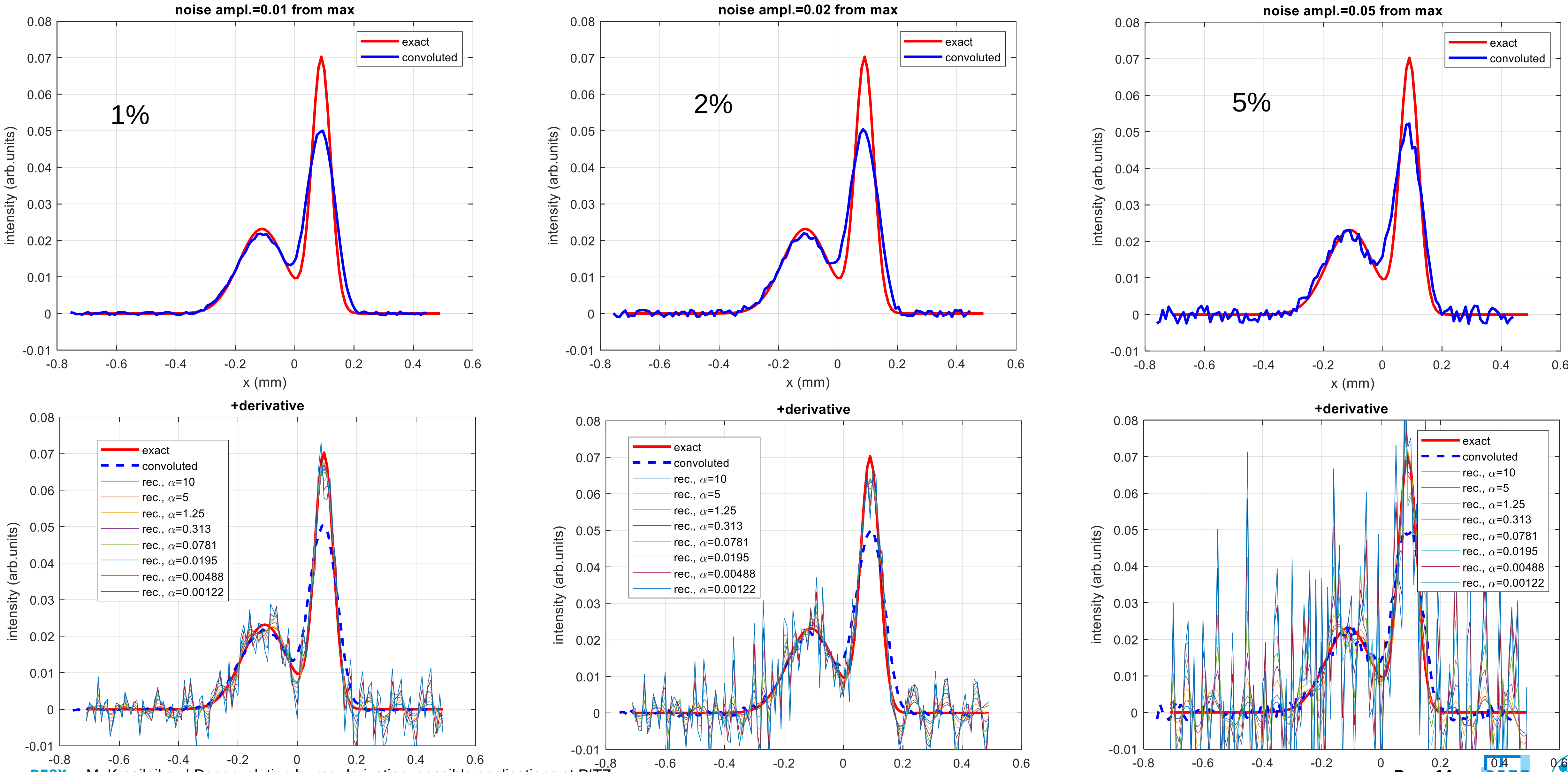



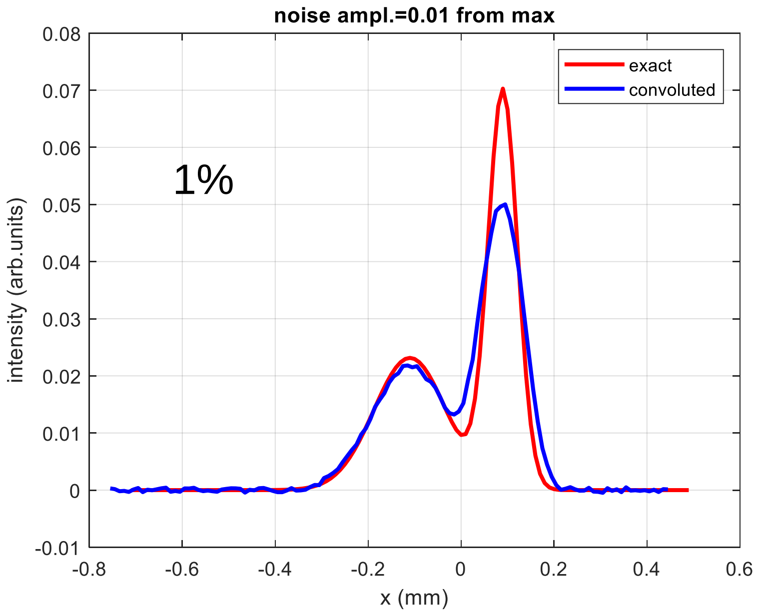



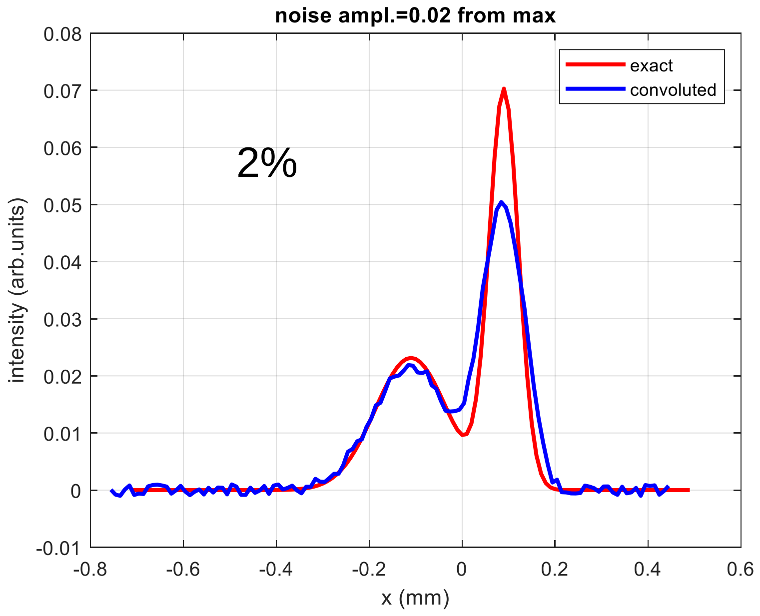
# Modeled beamlet profile reconstruction

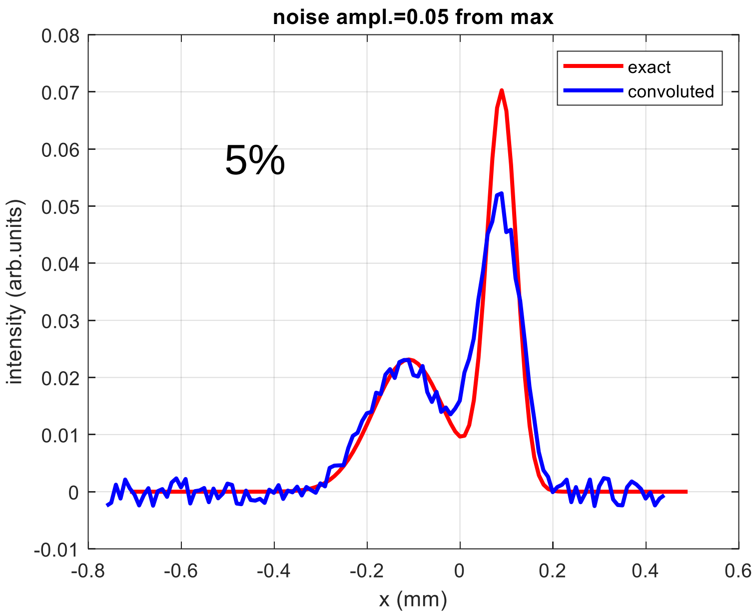
**Option: $2^{nd}$ derivative**

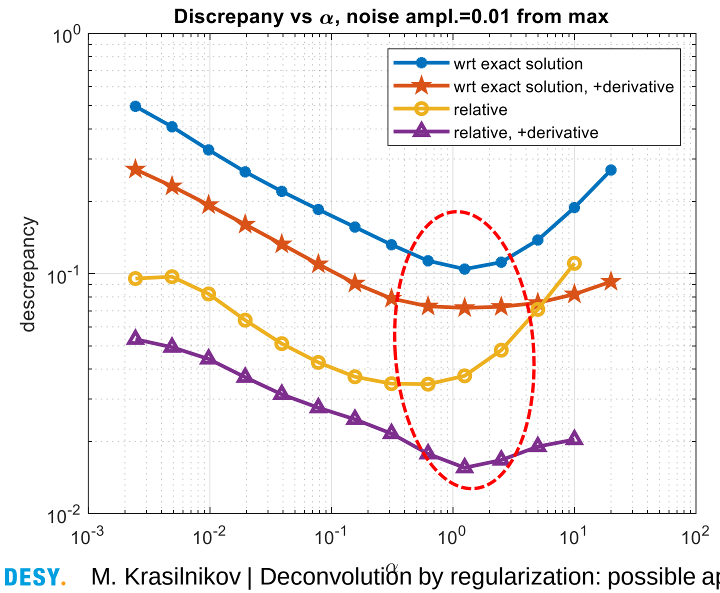


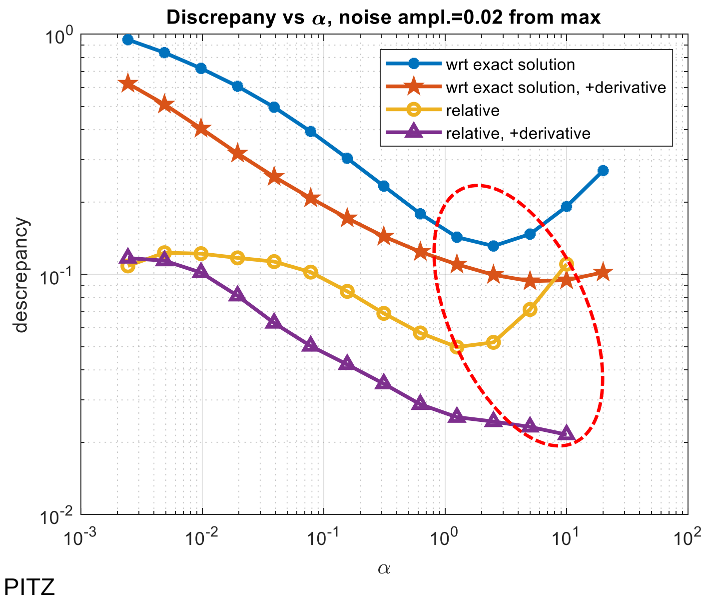
# Modeled beamlet profile reconstruction additive white Gaussian random noise

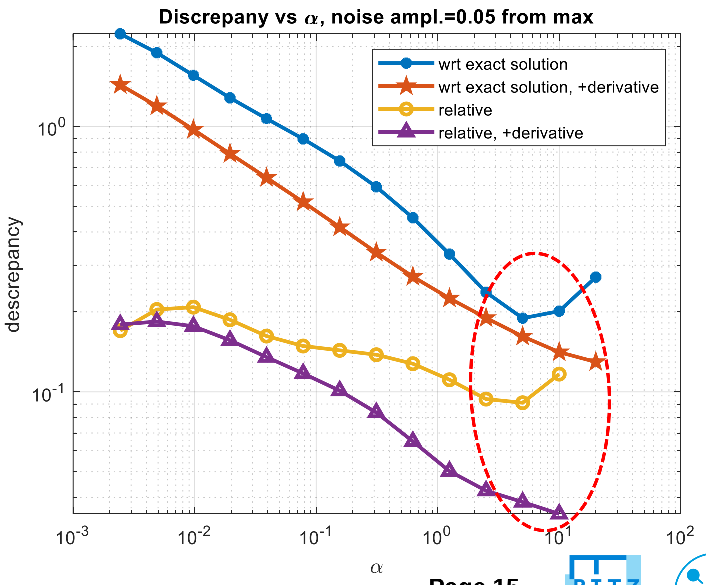


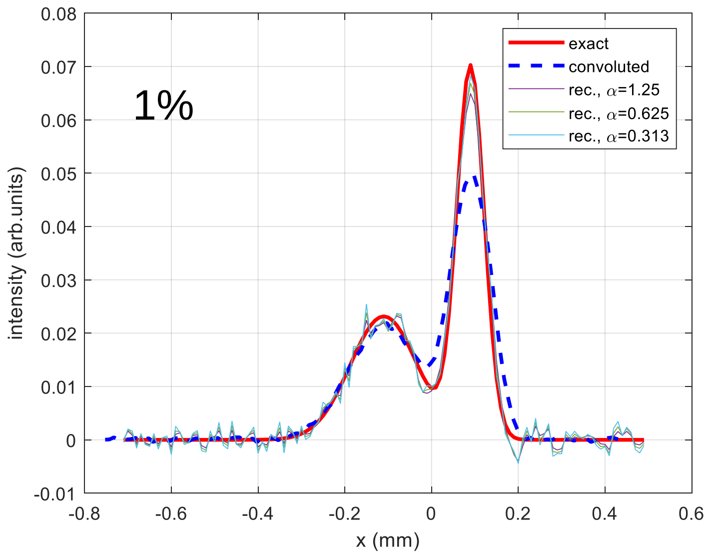



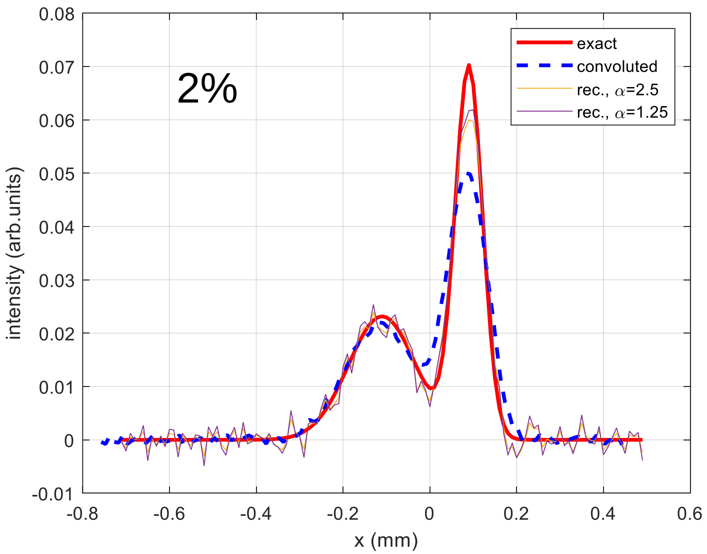



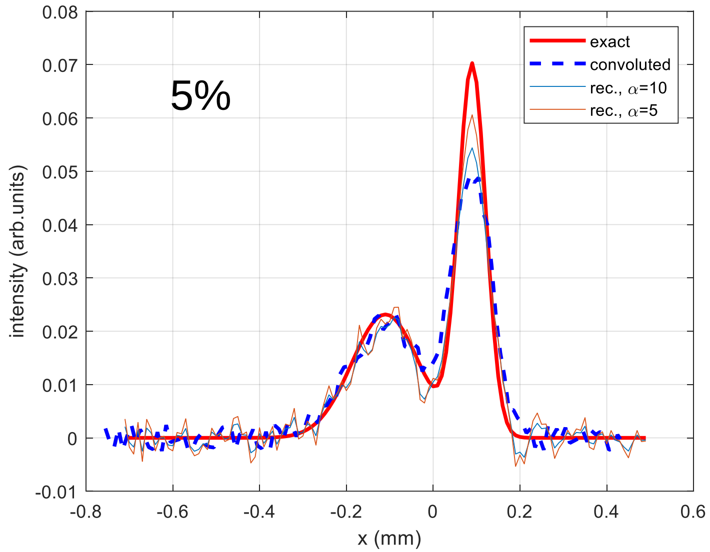



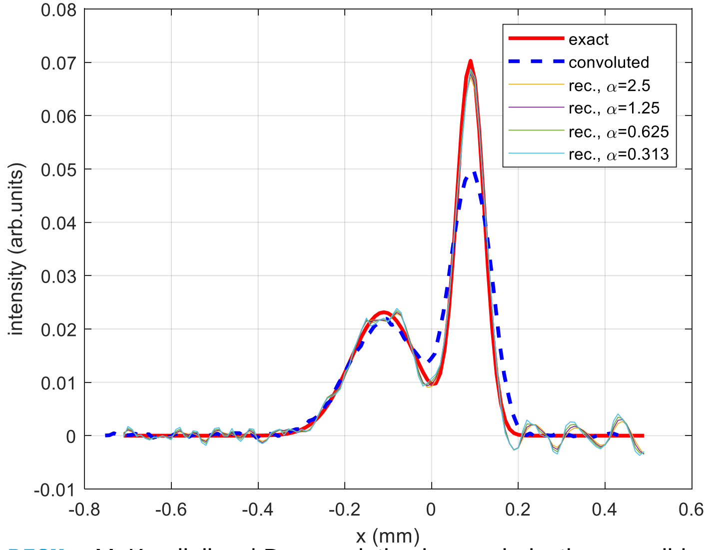
# Modeled beamlet profile reconstruction

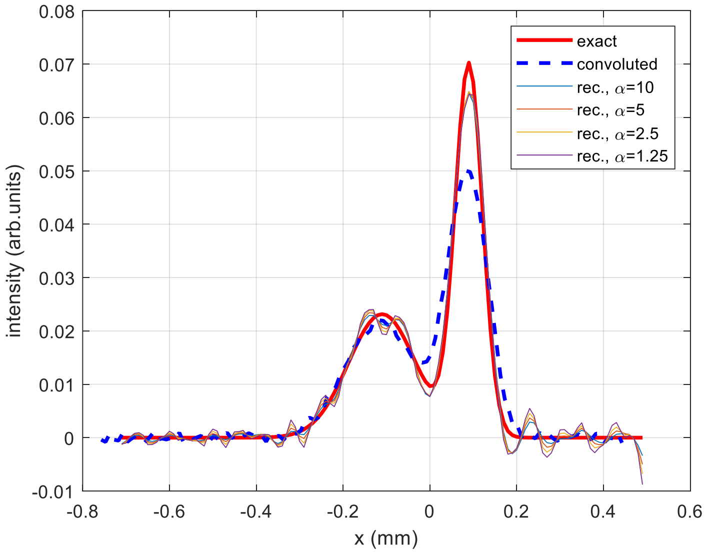
“best” cases

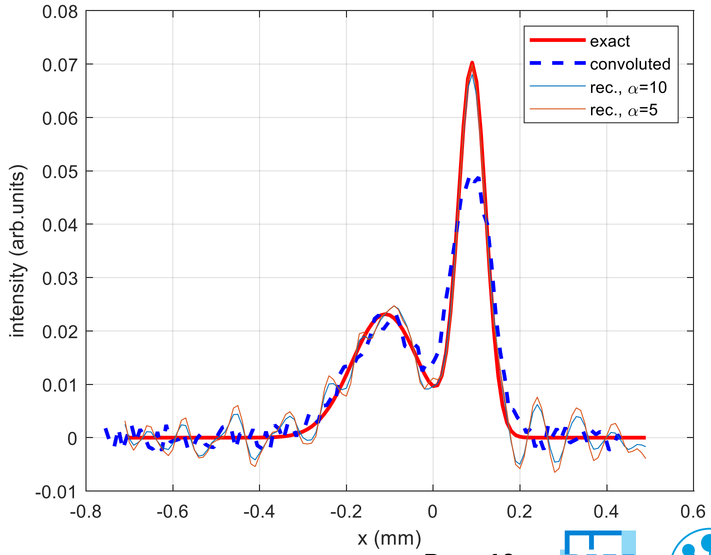


# Discussion

## Deconvolution of the finite slit opening by regularization

- It might be relevant especially for high
  - camera zoom (pixel size at BL collector screen << slit opening)
  - small beam / beamlets or beams with structure comparable with ppixel size
- Regularization parameter choice and optimum solution:
  - very case sensitive
  - very dependent on noise level → accurate filtering is important
  - Oscillatory solutions for principally positive function? ➔ another approach → exponential (Gaussian) fit

# Charge measurements

## From “pure” signal-noise to raw signal-noise

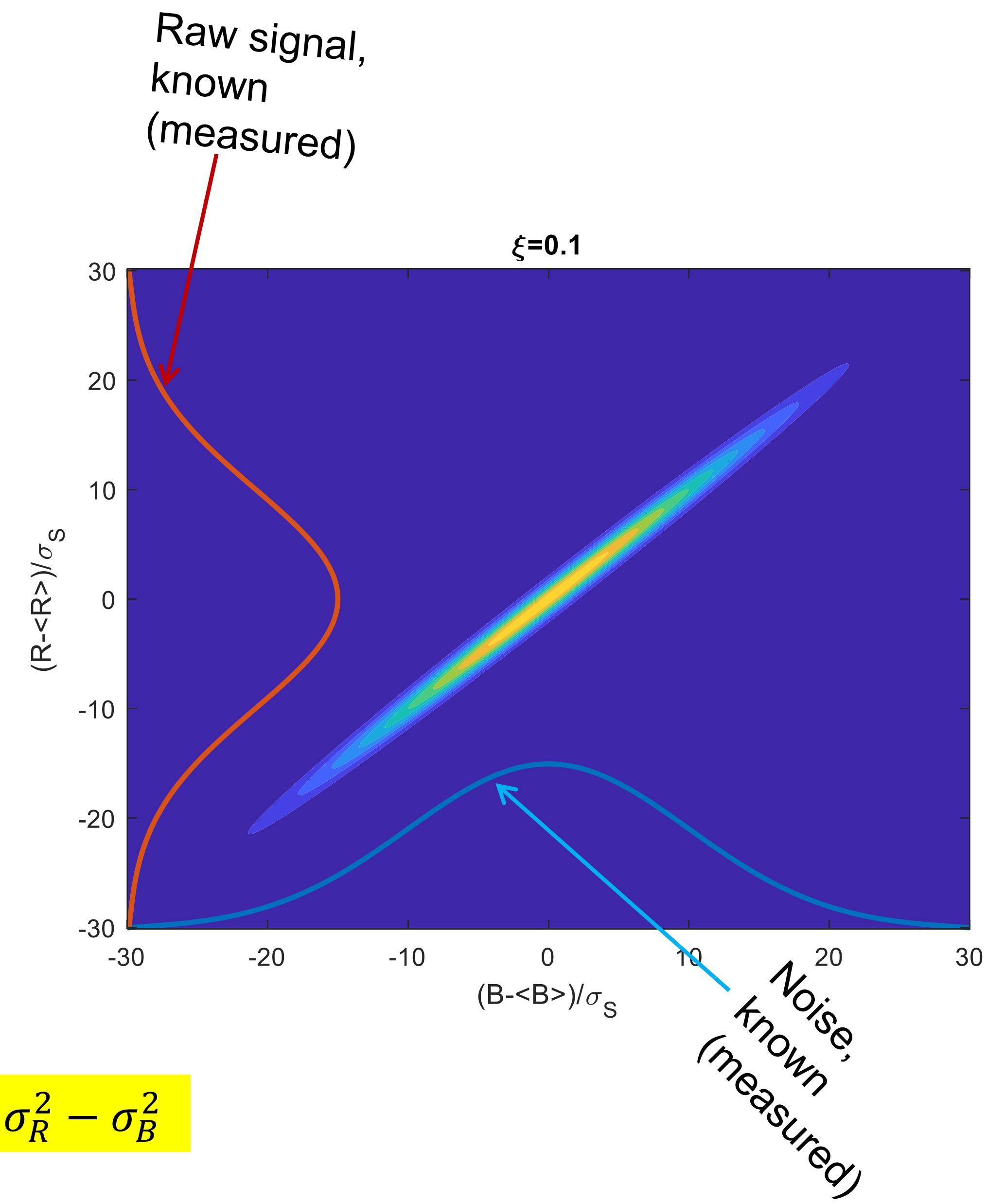
$$P_{s+n}(S,B) = \frac{1}{2\pi\sigma_S\sigma_B}\exp\left[-\frac{(S-\langle S\rangle)^2}{2\sigma_S^2}-\frac{(B-\langle B\rangle)^2}{2\sigma_B^2}\right]$$

$$R = S + B$$

$$\langle R\rangle = \langle S\rangle + \langle B\rangle$$

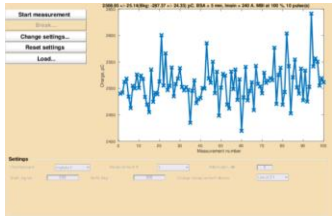
$$P_{r+n}(R,B) = \frac{1}{2\pi\sigma_S\sigma_B}\exp\left[-\frac{(R-B-\langle R\rangle+\langle B\rangle)^2}{2\sigma_S^2}-\frac{(B-\langle B\rangle)^2}{2\sigma_B^2}\right]$$

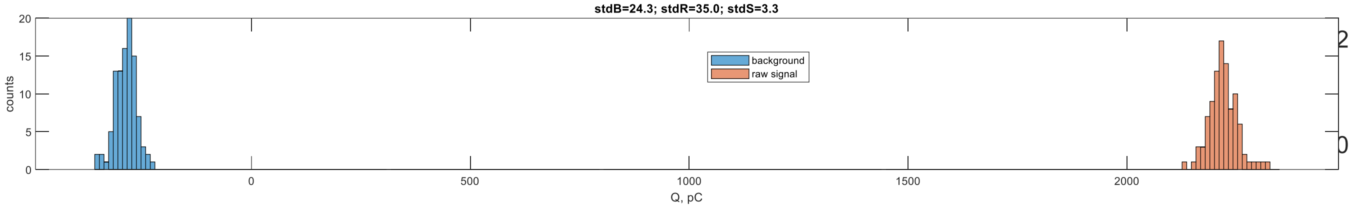
$$\sigma_R^2 = \iint_{-\infty}^{\infty}(R-\langle R\rangle)^2 P_{r+n}(R,B)\,dR\,dB = \sigma_S^2+\sigma_B^2 \;\Longrightarrow\; \sigma_S^2 = \sigma_R^2 - \sigma_B^2$$

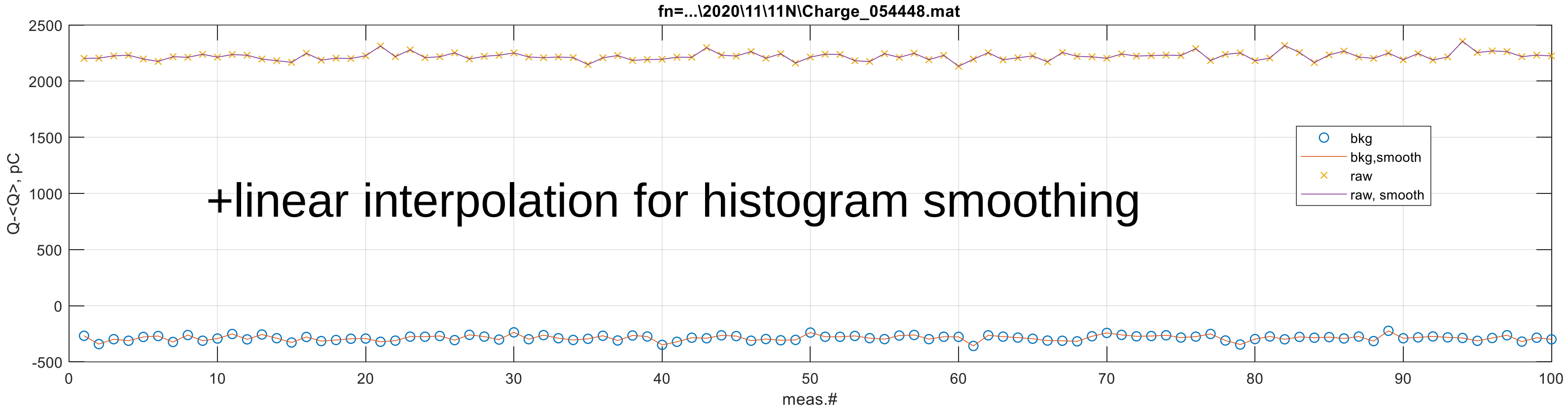


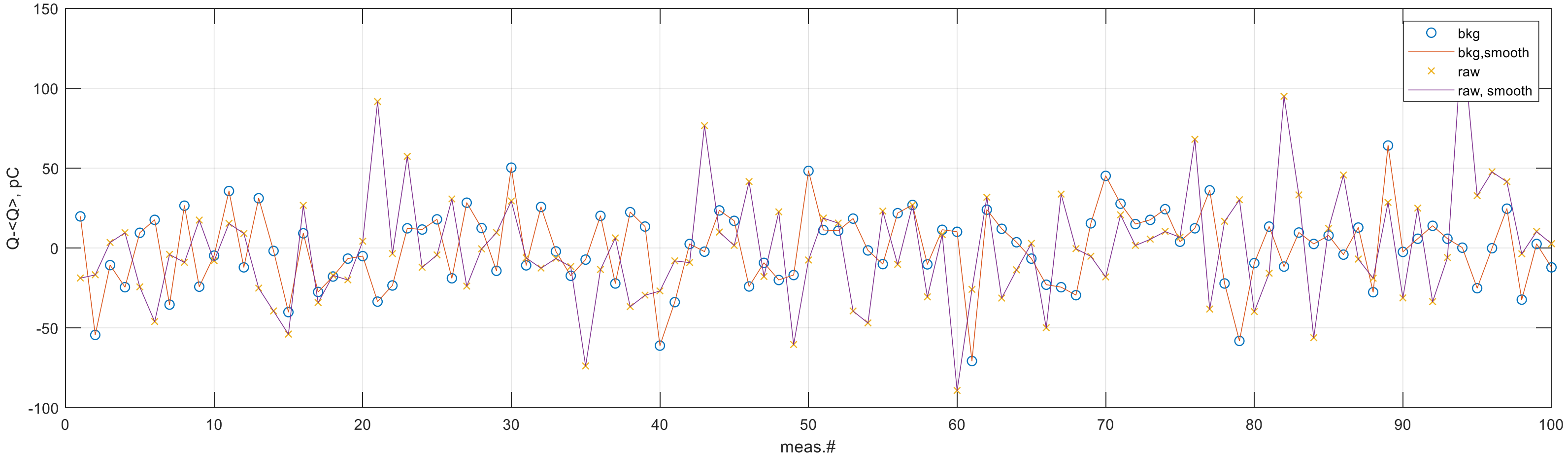
# Charge measurement

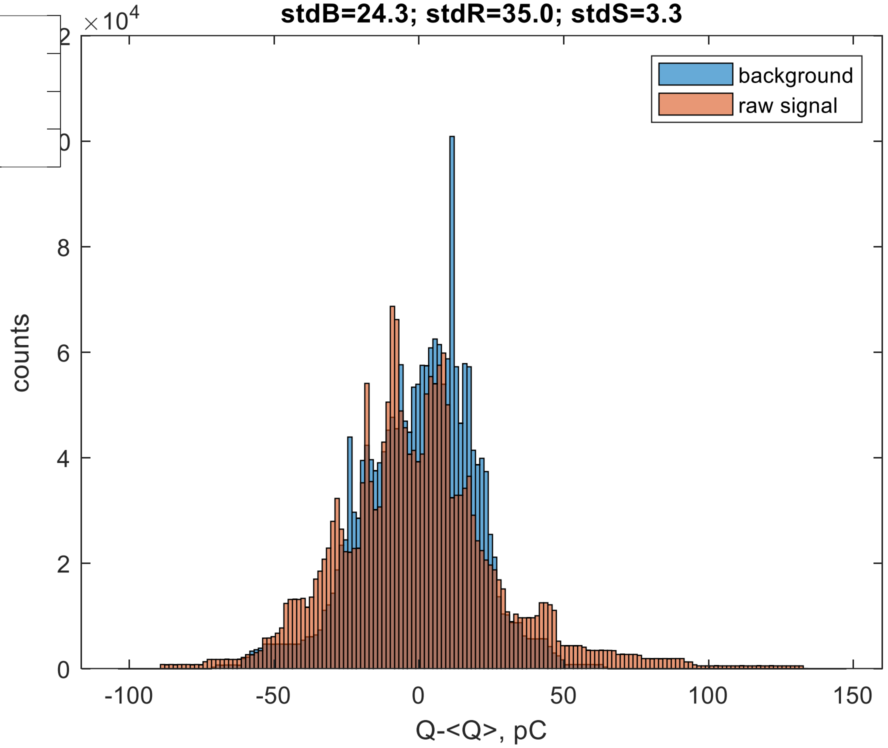
## Typical measurements at PITZ + linear interpolation applied for more detailed histograms



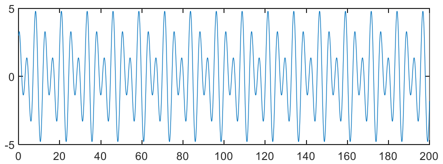


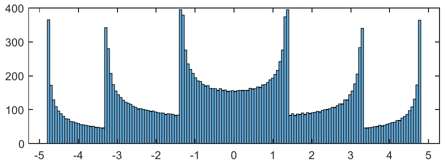



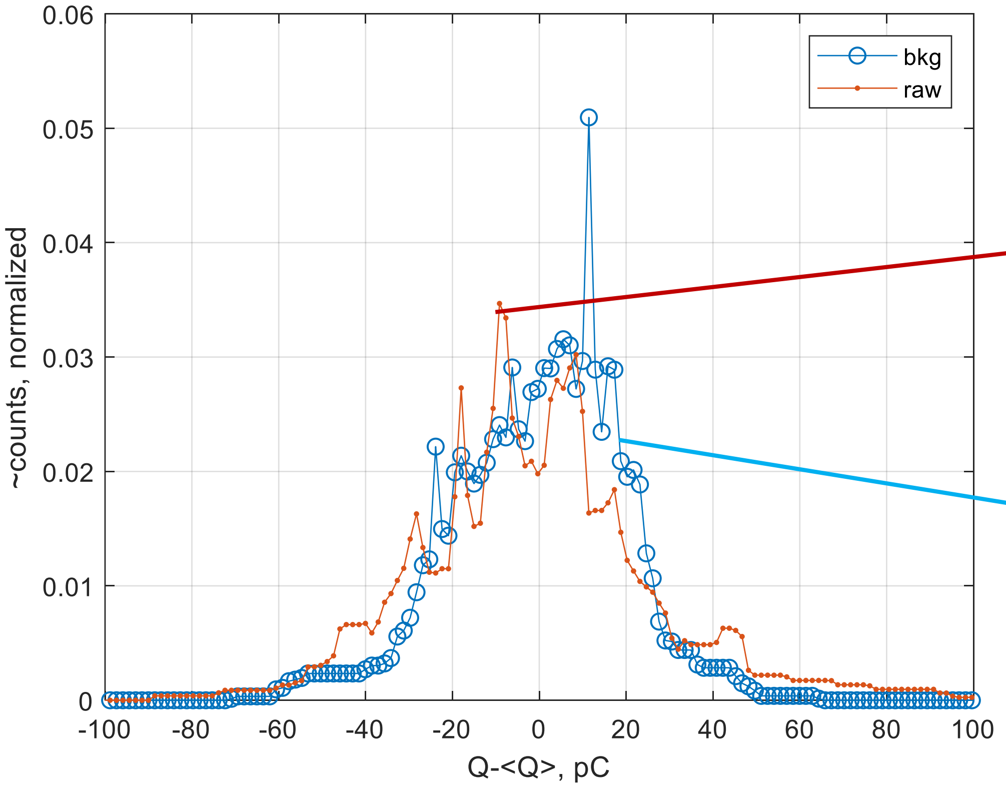

Spikes & bumps = Signatures of oscillatory terms?

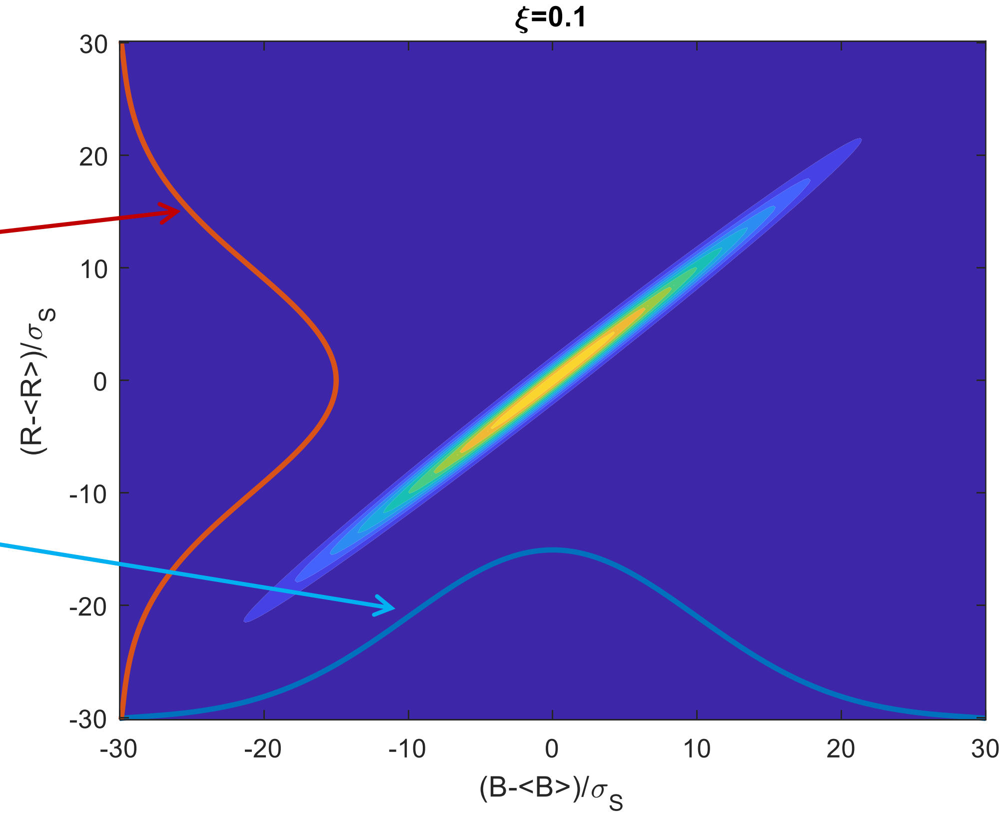




# Charge measurements

## “Pure” charge histogram reconstruction



# Charge histogram reconstruction

## Using regularization

$$\alpha\, y_\alpha(t) + \int_a^b B(t,s)\, y_\alpha(s)\, ds = F(t), \quad a \le t \le b$$

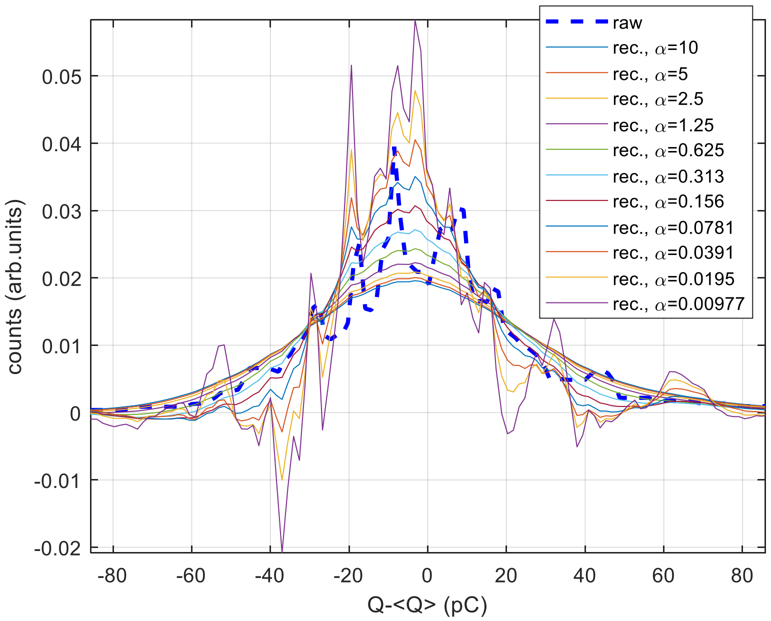
$$B(t,s) = \int_a^{\tilde{b}} K(x,t)\, K(x,s)\, dx \qquad F(t) = \int_a^b K(x,t) f(x) dx$$

$$\Phi_\alpha(y) = \|Ay - f\|_{L_2}^2 + \alpha \|y\|_{L_2}^2 \rightarrow \min_{y \in L_2[a,b]}$$

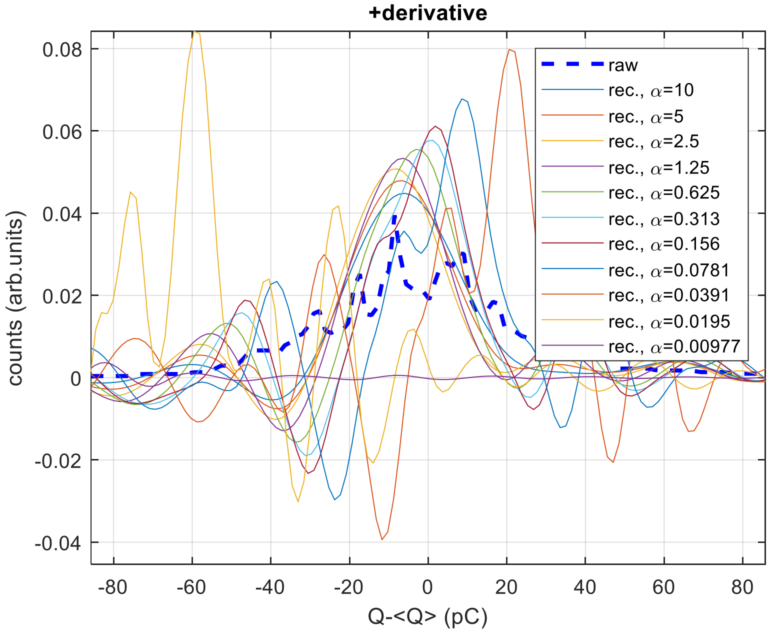
Option: 2nd derivative

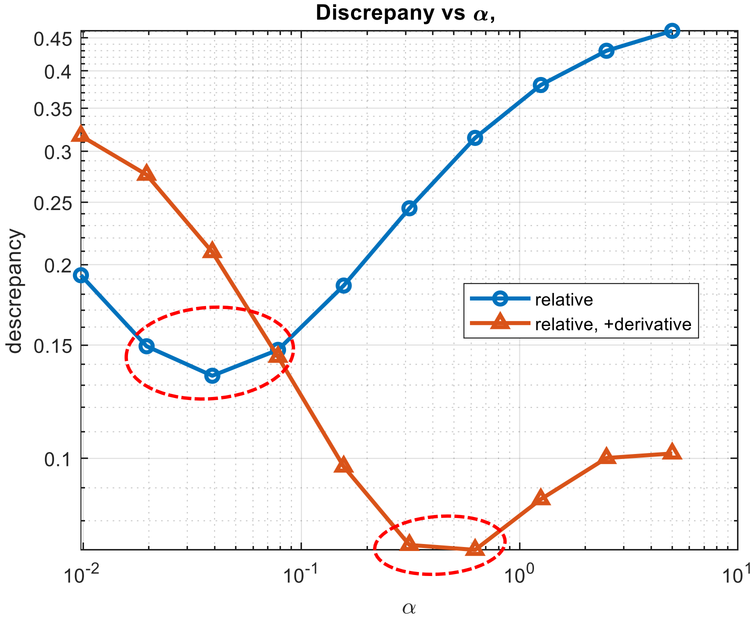
$$\alpha_i = \theta \alpha_{i-1}, i = 1, \dots m$$
$$\alpha_0 = 10$$
$$\theta = 0.5$$

$y(\alpha_i, Q)$




$y(\alpha_i, Q)$, incl. 2nd derivative




$$\left\| y_{\alpha_i} - y_{\alpha_{i-1}} \right\| / \left\| y_{\alpha_i} \right\|$$

# Charge histogram reconstruction

## Using regularization

$$\alpha\, y_\alpha(t) + \int_a^b B(t,s)\, y_\alpha(s)\, ds = F(t), \quad a \le t \le b$$

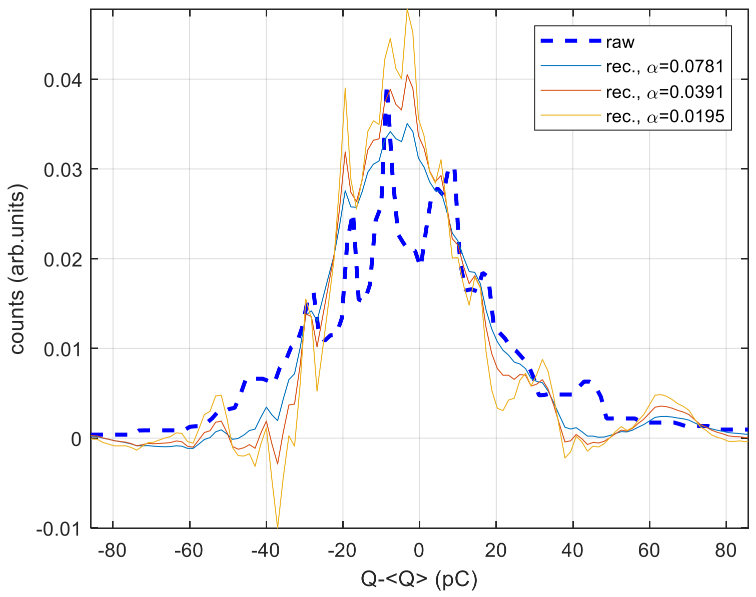
$$B(t,s) = \int_a^{\tilde{b}} K(x,t)\, K(x,s)\, dx \qquad F(t) = \int_a^b K(x,t) f(x) dx$$

$$\Phi_\alpha(y) = \left\|Ay - f\right\|_{L_2}^2 + \alpha \left\|y\right\|_{L_2}^2 \to \min_{y \in L_2[a,b]}$$

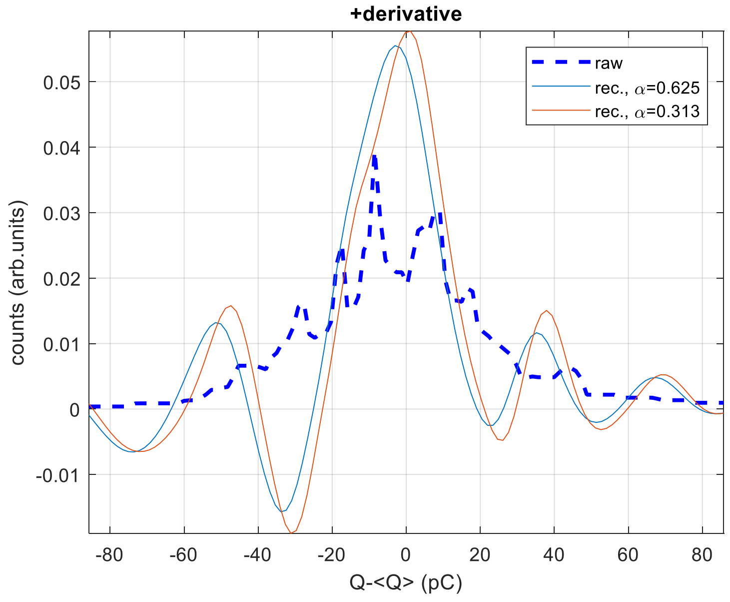
Option: 2$^{nd}$ derivative

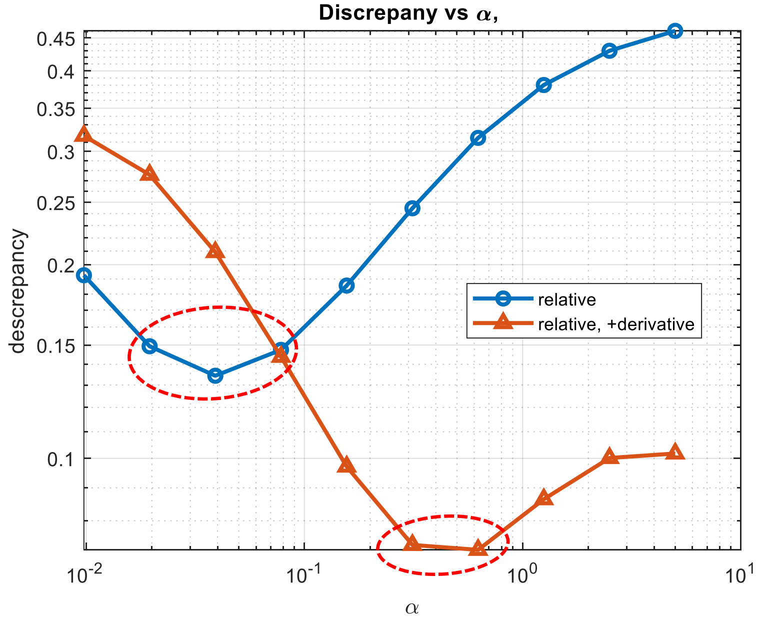
$\alpha_i = \theta \alpha_{i-1}, i = 1, \ldots m$
$\alpha_0 = 10$
$\theta = 0.5$

$y(\alpha_i, Q)$




$y(\alpha_i, Q)$, incl. 2nd derivative

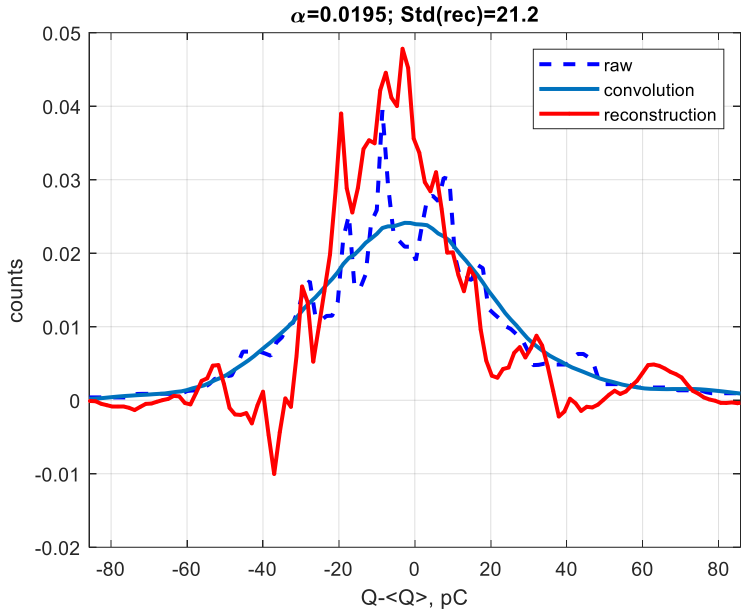


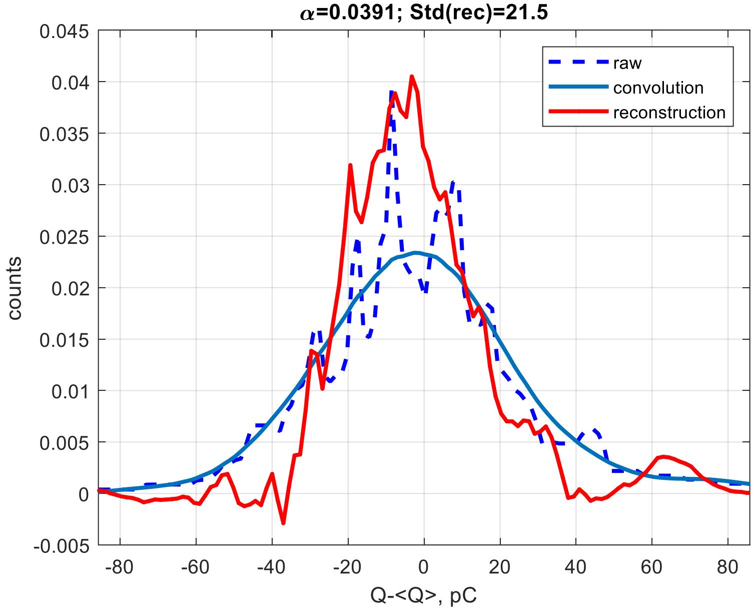



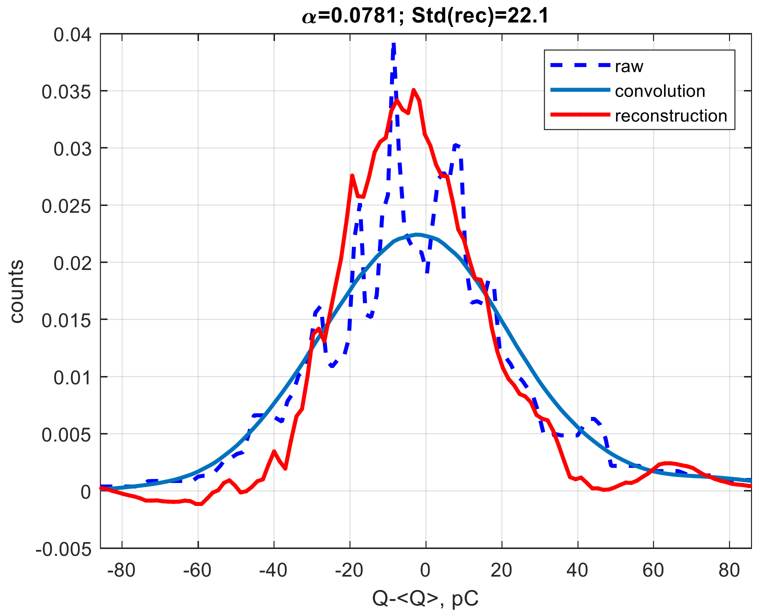

$$\left\|y_{\alpha_i} - y_{\alpha_{i-1}}\right\| / \left\|y_{\alpha_i}\right\|$$

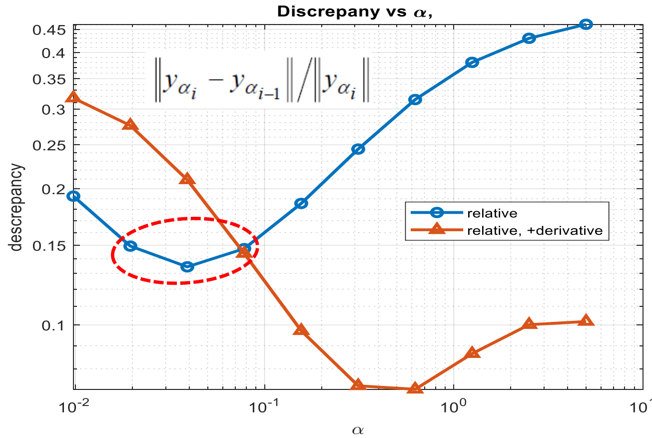
# Charge histogram reconstruction

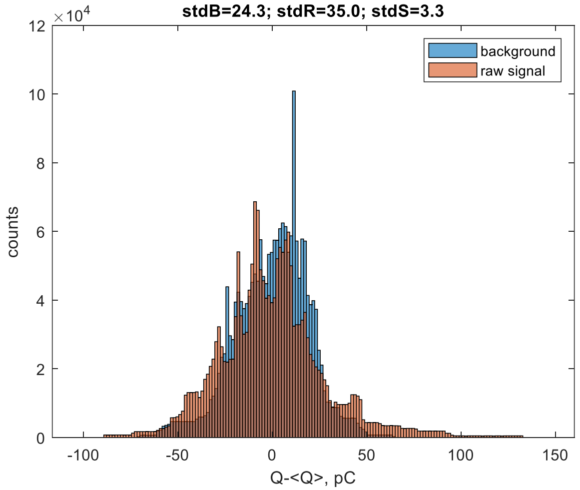
## Using regularization



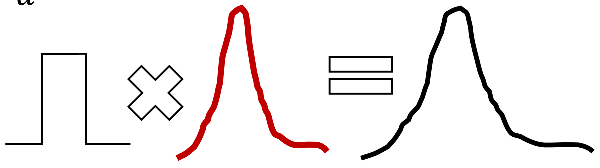

$\sigma_S^2 = \sigma_R^2 - \sigma_B^2$ ⇨ $\sigma_S$ =3.3pC

reconstruction ⇨ $\sigma_S$ =22pC

# Deconvolution by Fourier Transformation

## Optimized Wiener filter concept

$$\int_a^b K(x-s)y(s)ds = f(x)$$

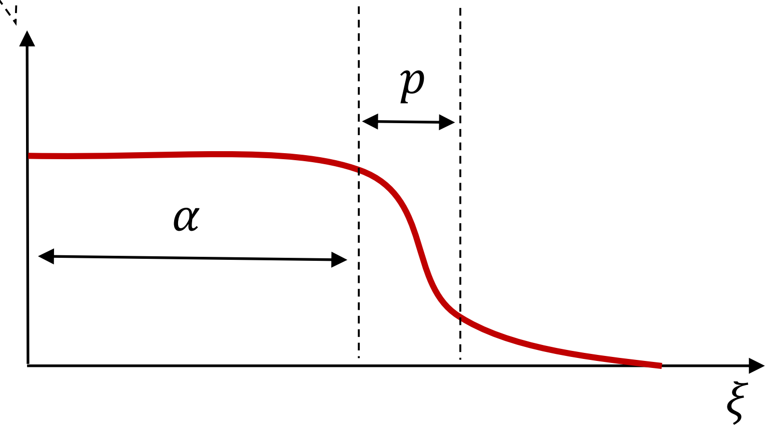



$$y(s) = \frac{1}{2\pi}\int_{-\infty}^{\infty}\frac{F(\xi)}{K(\xi)}e^{i\xi s}d\xi$$

$$F(\xi) = \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty} f(x)e^{-i\xi x}dx$$

$$K(\xi) = \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty} K(x)e^{-i\xi x}dx$$

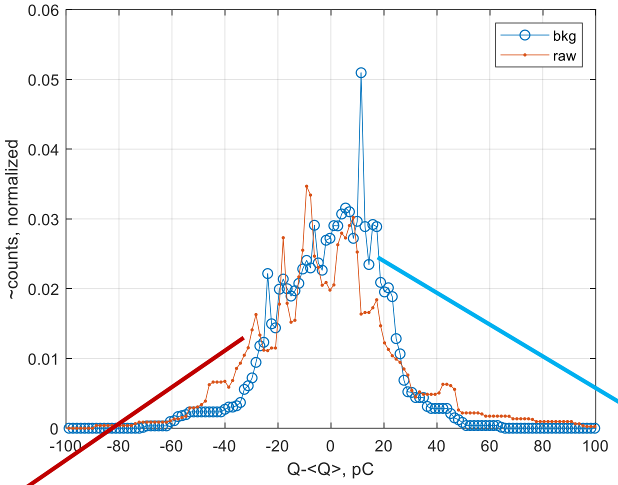
$$y(s) = \frac{1}{2\pi}\int_{-\infty}^{\infty}\frac{|K(\xi)|^2}{|K(\xi)|^2+\alpha\xi^{2p}}\cdot\frac{F(\xi)}{K(\xi)}e^{i\xi s}d\xi$$

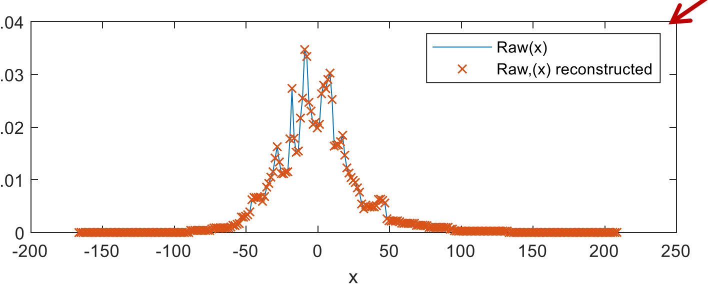


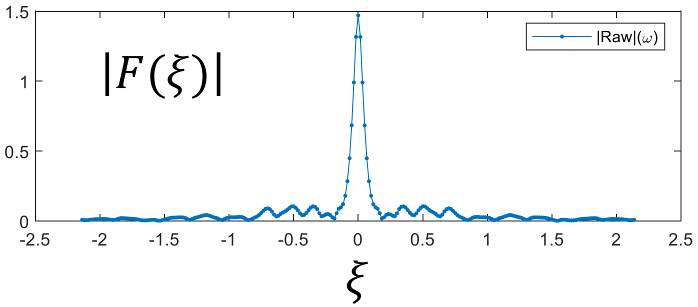
# Charge measurements: Deconv by Fourier Transformation

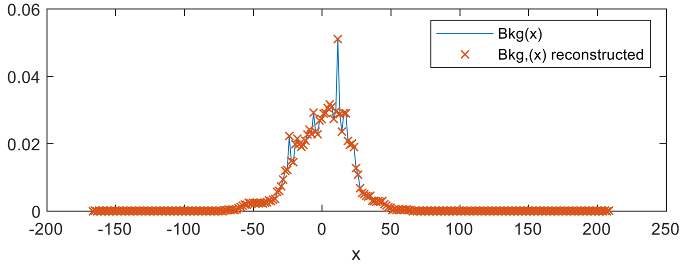
## Fourier transformations

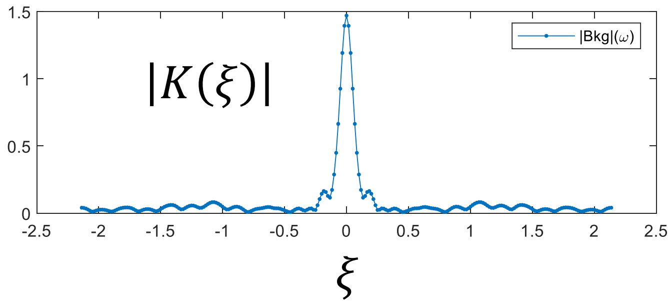
$$y(s) = \frac{1}{2\pi}\int_{-\infty}^{\infty} \frac{|K(\xi)|^2}{|K(\xi)|^2 + \alpha\xi^{2p}} \cdot \frac{F(\xi)}{K(\xi)} e^{i\xi s} d\xi$$



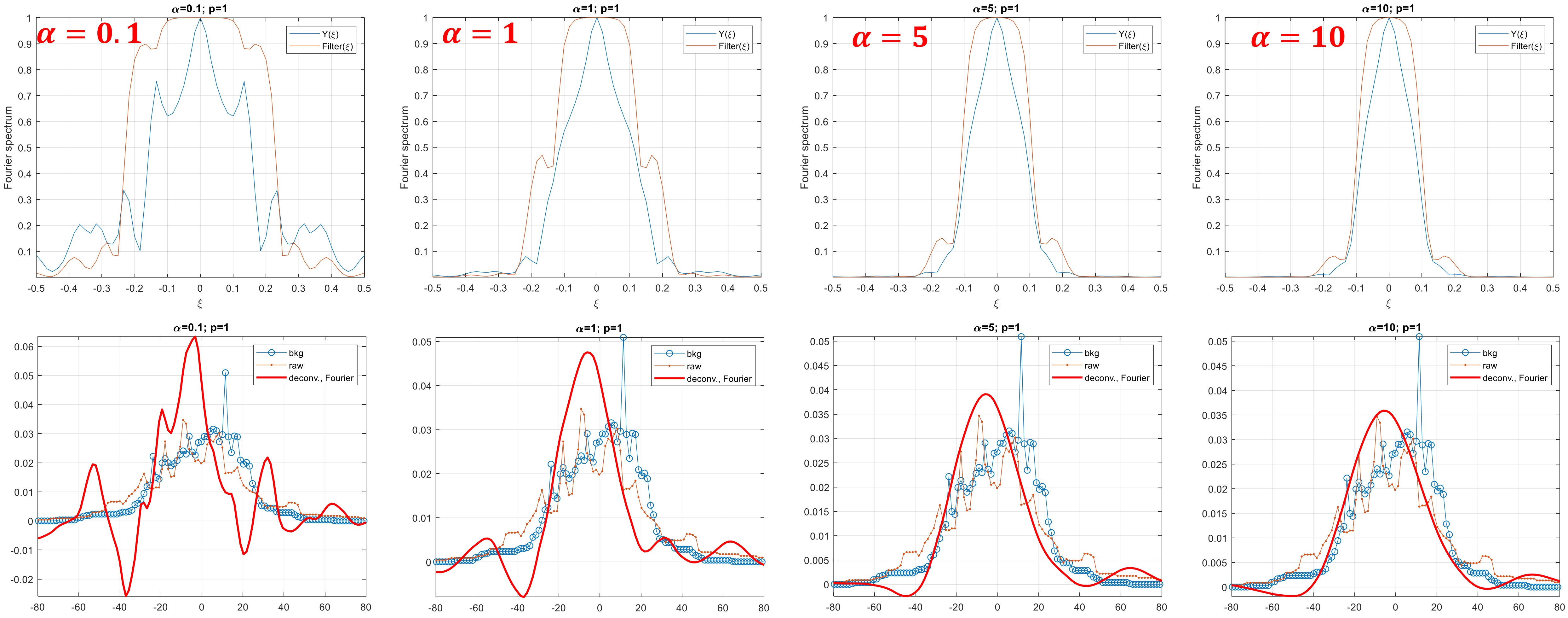



# Charge measurements: Deconv by Fourier Transformation

## Fourier transformations

$p = 1$

$$y(s) = \frac{1}{2\pi}\int_{-\infty}^{\infty} \frac{|K(\xi)|^2}{|K(\xi)|^2 + \alpha\xi^{2p}} \cdot \frac{F(\xi)}{K(\xi)} e^{i\xi s} d\xi$$

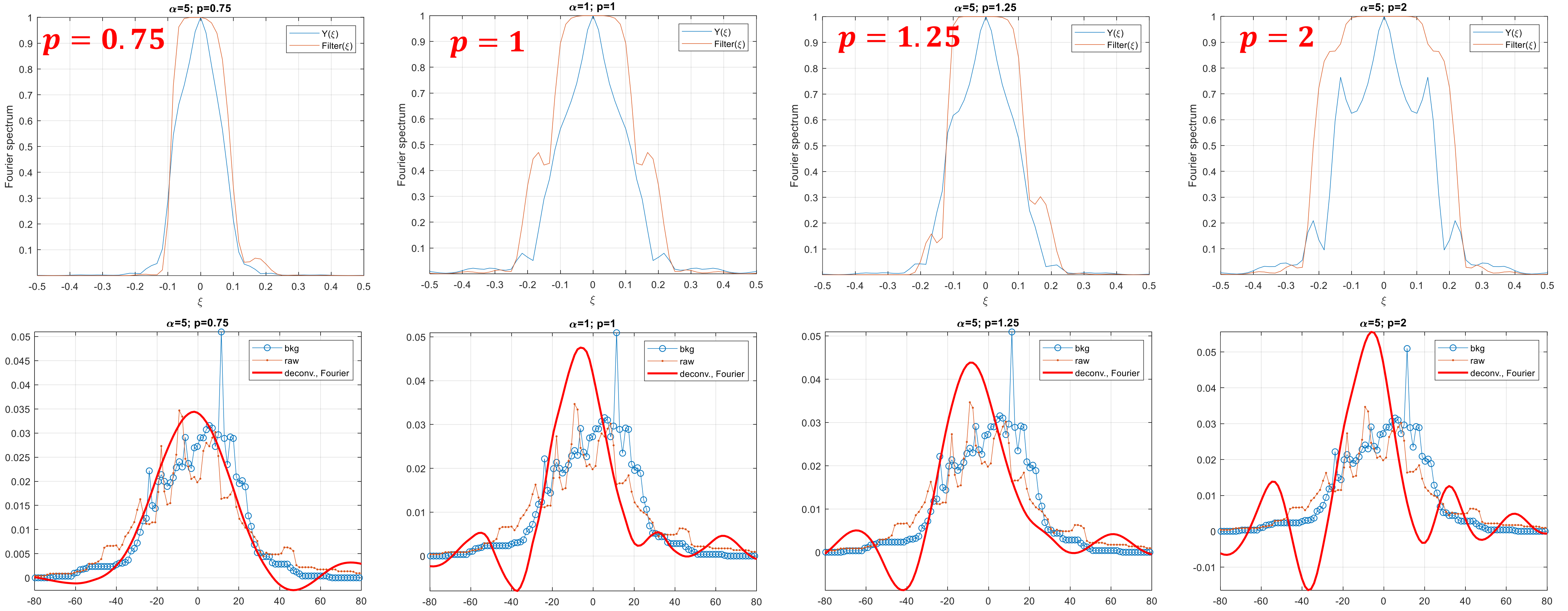


# Charge measurements: Deconv by Fourier Transformation

## Fourier transformations

$\boldsymbol{\alpha = 5}$

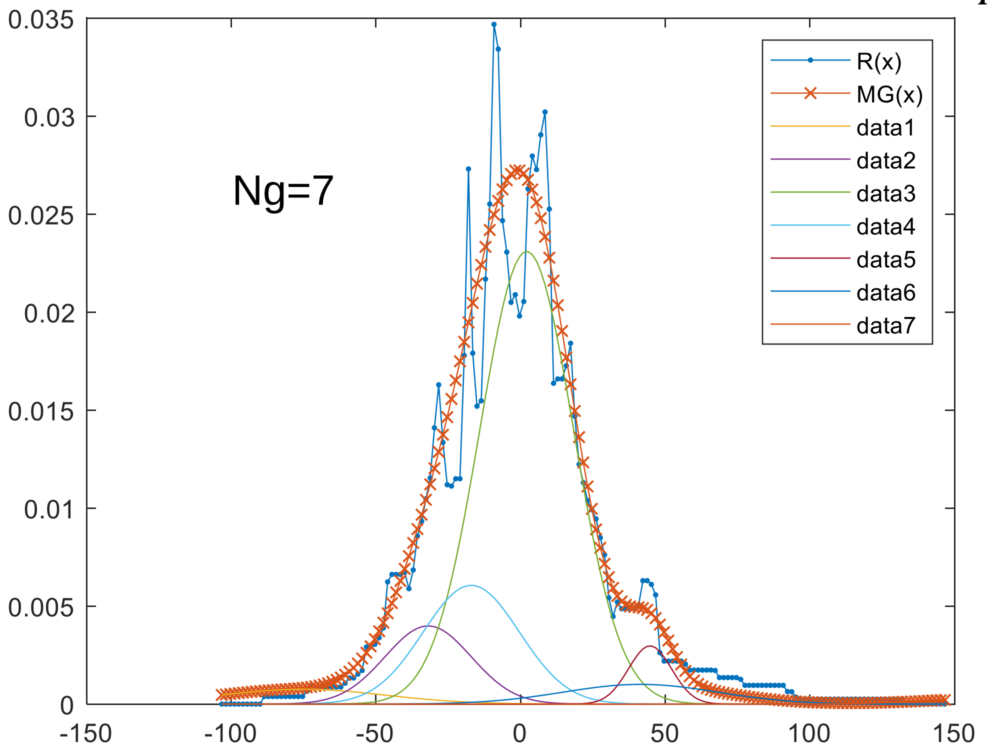
$$y(s) = \frac{1}{2\pi}\int_{-\infty}^{\infty} \frac{|K(\xi)|^2}{|K(\xi)|^2 + \alpha\xi^{2p}} \cdot \frac{F(\xi)}{K(\xi)} e^{i\xi s} d\xi$$

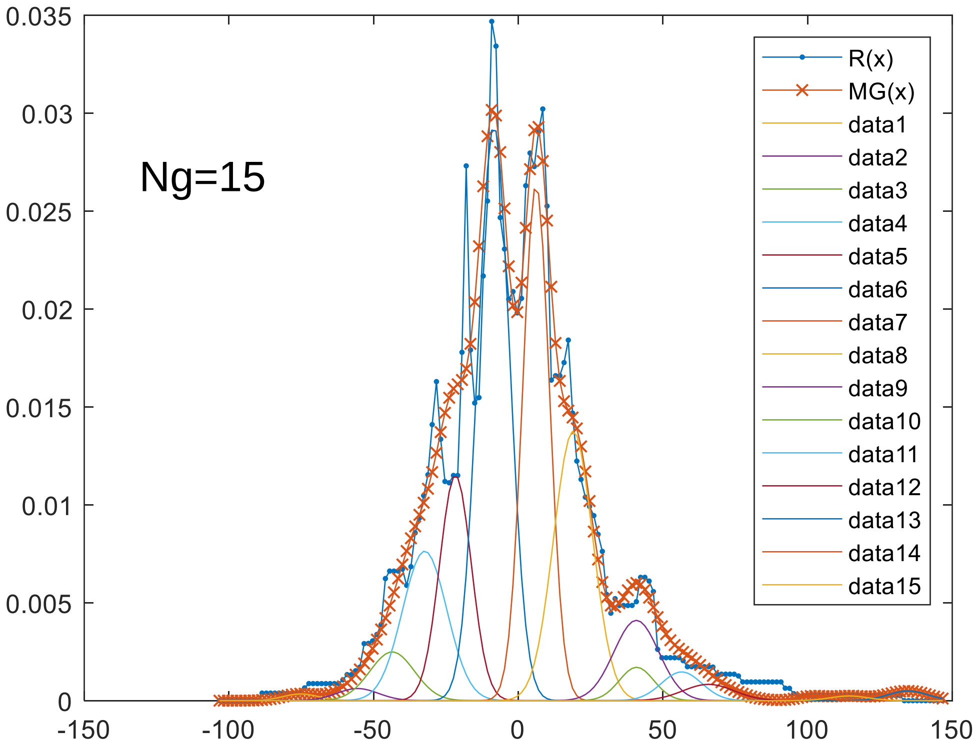


# Multi-gaussian fit ~> Gaussian Wavelets

## Approximation of positive (smooth enough) functions → e.g. Raw (charge+noise) histogram

$$R(x) = \sum_{n=1}^{N_g} e^{c_{n0}+c_{n1}x+c_{n2}x^2}$$




$$\hat{C} = \begin{pmatrix} c_{10} & c_{11} & c_{12} \\ c_{20} & c_{21} & c_{22} \\ \cdots & \cdots & \cdots \\ c_{N_g0} & c_{N_g1} & c_{N_g2} \end{pmatrix}$$

# Reconstruction by multi-Gaussian optimization

## Multidimensional optimization to fit background histogram convolution to the measured raw histogram

$$\hat{C} = \begin{pmatrix} c_{10} & c_{11} & c_{12} \\ c_{20} & c_{21} & c_{22} \\ \cdots & \cdots & \cdots \\ c_{N_g0} & c_{N_g1} & c_{N_g2} \end{pmatrix}$$

$$S(t) = \sum_{n=1}^{N_g} e^{c_{n0}+c_{n1}t+c_{n2}t^2}$$ → positive functions only

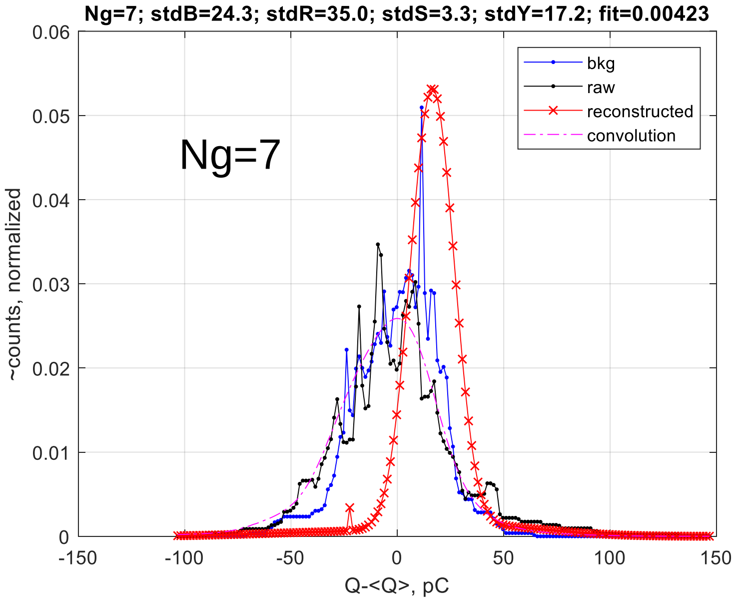
$$\Phi(\hat{C}) = \int_{q_{min}}^{q_{max}} dq \left[ Raw(q) - \int_{q_{min}}^{q_{max}} \Delta Bkg(q-t)\, S(t) dt \right]^2$$

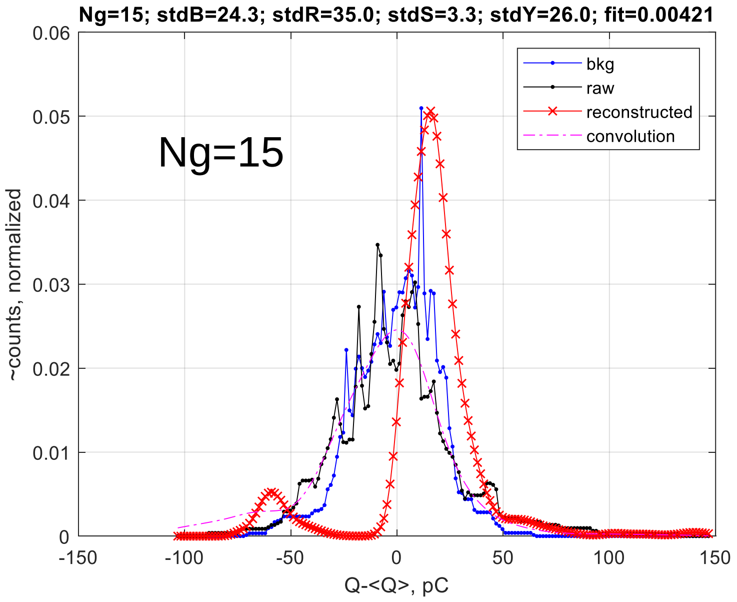
$$\check{S}(t) = \min \Phi(\hat{C})$$ → optimization in $3*N_g$ space

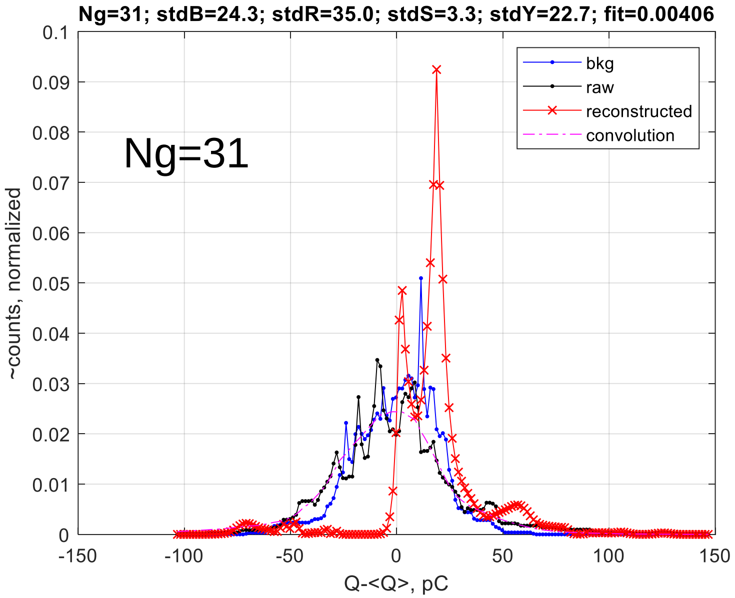
Normalized variables used in the optimization (*fminsearch*): $v_{nm} = \frac{c_{nm}-c_{nm}^0}{dc_m} \cdot 0.00025$

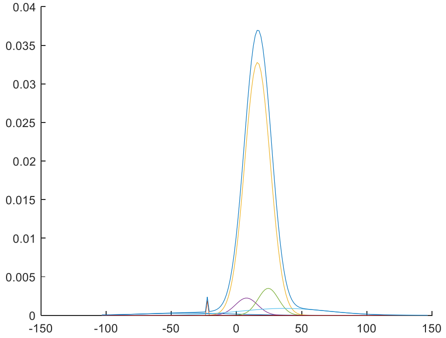
# Reconstruction by multi-Gaussian optimization

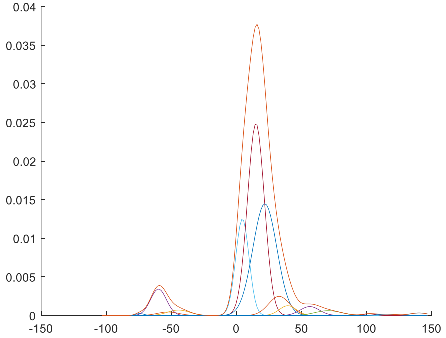
## Multidimensional optimization to fit backgroung histogram convolution to the measured raw histogram

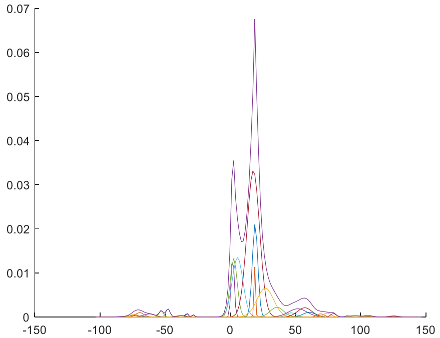






# Discussion

## Charge measurements

- Fourier → oscillating solutions (<0 ) → needs thorough filter tuning
- Regularization needs tuning as well
- Multi-Gaussian (Gaussian wavelets) might be more straightforward
- Asymmetric rms errors are possible, also with statistical fraction

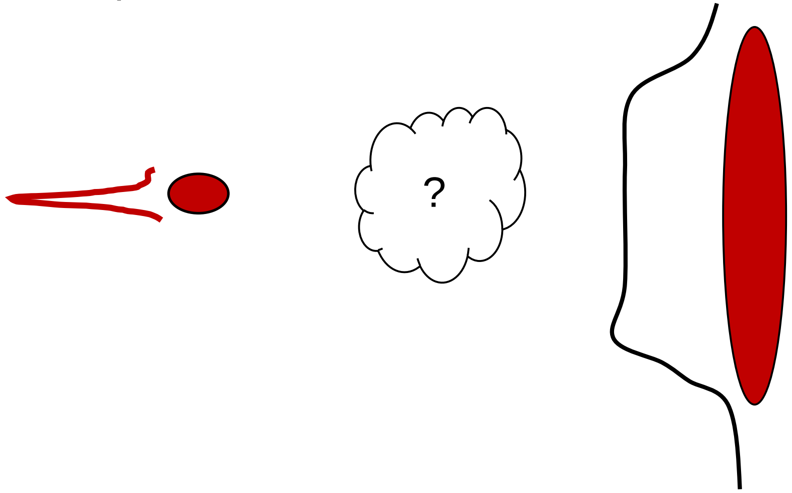
- Experimental data:
  - More statistics is desirable
  - Noise has to be reduced, periodical fluctuations have impact (spikes and bumps in histograms)

# Deconvolution for TDS measurements

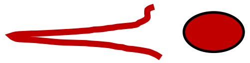
## Idea ( $s$– coordinate within bunch, ~time)

$$\int_{\Omega} K(x,s)\, y(s)\, ds = f(x), \quad x \in Q$$

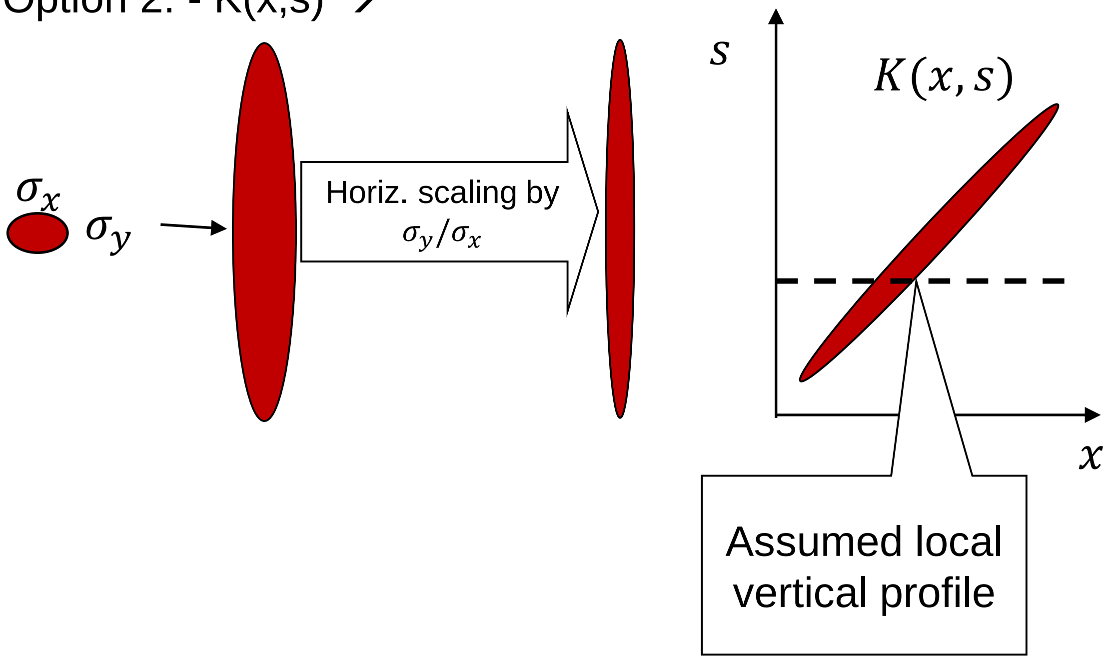
- $K(x,s)$ ⇩ Measured (vertically unstreaked) profile
- $y(s)$ ⇩ Real temporal profile
- $f(x)$ ⇩ Measured (vertically streaked) profile




Option 1: - convolution K(x-s) →



Option 2: - K(x,s) →



D.Yuan, X. Zhang, An overview of numerical methods for the first kind Fredholm integral equation, SN Applied Sciences (2019) 1:1178 | https://doi.org/10.1007/s42452-019-1228-3

# Outlook

## Overview of numerical methods for the 1st kind Fredholm integral equation

- Regularization method:
  - Tikhonov regularization
  - Projective iterative (collocation) and pure iterative (Friedmann)
  - Constructing regularizers for more homogeneous convergence
- Wavelet method
  - Gaussian wavelet, CAS (cosine and sine) wavelet, Legendre wavelet, Chebyshev wavelet, Coifnan wavelet, Haar wavelet, …
  - Especially for 2D case…(?LPS Tomo)
- Multilevel iteration method
  - Multiscale fast algorithm for the 2nd kind Fredholm equations (by applying Tikhonov regularization algorithm ) combined with Galerkin method
- Smooth factor solution method
  - Based on adding some “regularity” or “smoothness” constraints, and by adjusting the corresponding parameters to find the stable solution of the equation
- Other methods
  - discrete kernel method, optimal homotopy asymptotic method, algebraic method, Lagrange polynomial interpolation method, trust region algorithm, slow solution, collocation method, sinc collocation method, etc.

# Conclusions

## Deconvolution by regularization: possible applications at PITZ

- Deconvolution could/should be used to reconstruct accurate data from the experimental raw measurements
- It could be applied to several basic measurements at PITZ
  - Charge
  - Beamlets
  - TDS
  - …
- Many methods could be used → rather case dependent (?)

# Histograms from periodic signals

## To the charge histograms