The treatment of deautoconvolution as inverse problem, including the multidimensional case

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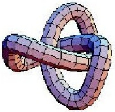

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Outline

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1. Introduction
2. Deautoconvolution for spectra and nanostructures
3. Deautoconvolution in short-term laser optics
4. Variational regularization of deautoconvolution in 2D

In this talk, the **inverse problem of deautoconvolution** means the reconstruction of a quadratically integrable real or complex function x with compact support in the unit n-cube,

$$\mathrm{supp(x)} \subseteq [0,1]^{\mathrm{n}} \subset \mathbb{R}^{\mathrm{n}} \quad (\mathrm{n} \in \mathbb{N}),$$

from noisy data y^δ of its autoconvolution $y = x * x$, or rewritten the solution of the quadratic-type **nonlinear operator equation**

$$F(x) = y \qquad (*)$$

for the **Volterra integral operator** of **autoconvolution**

$$[F(x)](s) := [x * x](s) = \int_{\mathbb{R}^n} x(s-t)\, x(t) dt \qquad (s, t \in \mathbb{R}^n)\,.$$

Here, $F : \mathcal{D}(F) \subseteq X \to Y$ maps between the Hilbert spaces

$$X := L^2([0,1]^n) \quad \text{and} \quad Y := \begin{cases} L^2([0,2]^n) & \text{(full data case)} \\ L^2([0,1]^n) & \text{(limited data case)} \end{cases} .$$

In the **full data case** we observe the autoconvolution function

$$y(s) = \int\limits_{[\max(s-1,0),\min(s,1)]^n} x(s-t)\,x(t)\,\mathrm{d}t \qquad \text{for all } s \in [0,2]^n\,,$$

whereas in the **limited data case** data are available only for

$$y(s) = \int\limits_{[0,s]^n} x(s-t)\,x(t)\,\mathrm{d}t \qquad \text{for all } s \in [0,1]^n\,.$$

In the latter case, non-negativity constraints $\mathcal{D}(F) = \mathcal{D}^+$ with

$$\mathcal{D}^+ := \{x \in X = L^2([0,1]^n) : \; x \geq 0 \text{ a.e. on } [0,1]^n\}$$

play a prominent role. We always assume the data model

$$\|y - y^\delta\|_Y \leq \delta\,, \quad (\delta > 0 \text{ noise lelvel})\,.$$

Note: With x, also $-x$ always solves $(*)$ whenever $\mathcal{D}(F) = X$.

The simplest **application** of deautoconvolution in n dimensions is the recovery of the square integrable **density function** x of an n-dimensional random vector $\mathfrak{X} = (\mathfrak{X}_1, \mathfrak{X}_2, ..., \mathfrak{X}_n)^T$ with support in $[0,1]^n$ from data of the density function $y = x * x$ of $\mathfrak{Y} := \widetilde{\mathfrak{X}} + \widehat{\mathfrak{X}}$, where $\mathfrak{X}, \widetilde{\mathfrak{X}}$ and $\widehat{\mathfrak{X}}$ are assumed to be of i.i.d. type.

If the one-dimensional components $\mathfrak{X}_i$ ($i = 1, 2, ..., n$) are completely **uncorrelated**, then the density is **factored** as

$$x(t_1, t_2, ..., t_n) = x_1(t_1)\, x_2(t_2) \dots x_n(t_n)\,.$$

For analytical and numerical results of 2D-deautoconvolution for factored solutions see:

▷ Y. DENG, B. HOFMANN AND F. WERNER: Deautoconvolution in the 2D case. Paper submitted to ETNA, Oct. 2022, arXiv:2210.14093v1.

Concept of local ill-posedness for operator equations $(*)$:

Definition

The nonlinear operator equation $(*)$ with forward operator $F : \mathcal{D}(F) \subseteq X \to Y$ mapping between the spaces X and Y with domain $\mathcal{D}(F)$ is called **locally ill-posed** at a solution point $x^\dagger \in \mathcal{D}(F)$ if there exist, for all closed balls $\overline{\mathcal{B}_r(x^\dagger)}$ with radius $r > 0$ and center $x^\dagger$, sequences $\{x_k\} \subset \overline{\mathcal{B}_r(x^\dagger)} \cap \mathcal{D}(F)$ such that

$$\|F(x_k) - F(x^\dagger)\|_Y \to 0\,, \quad \text{but} \quad \|x_k - x^\dagger\|_X \not\to 0\,, \quad \text{as} \quad k \to \infty\,.$$

Otherwise, the operator equation is **locally well-posed** at $x^\dagger$.

▷ B.H. AND O. SCHERZER: Factors influencing the ill-posedness of nonlinear problems. *Inverse Problems* **10** (1994), pp. 1277–1297.

Local ill-posedness everywhere for deautconvolution:

Theorem

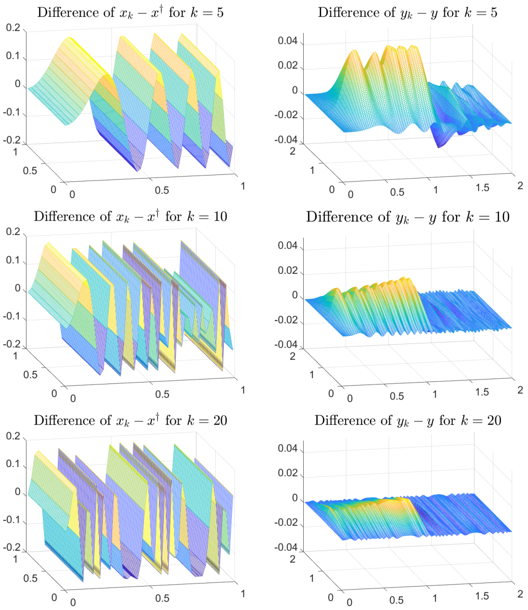
The operator equation $(*)$ of deautoconvolution with forward operator $F : \mathcal{D}(F) \subseteq X \to Y$ is **locally ill-posed everywhere** on $\mathcal{D}(F)$ for both cases, namely the
full data case: $X = L^2([0,1]^n)$, $Y = L^2([0,2]^n)$ and $\mathcal{D}(F) = X$, as well as the
limited data case: $X = L^2([0,1]^n)$, $Y = L^2([0,1]^n), \mathcal{D}(F) = \mathcal{D}^+$.

The complete proofs for **real spaces** $L^2([0,1]^n)$ $L^2([0,2]^n)$ and arbitrary dimensions $n \in \mathbb{N}$ will be published soon in

$\triangleright$ B.H., F. WERNER AND Y. DENG: On uniqueness and ill-posedness for the deautoconvolution problem in the multidimensional case. In preparation, Fall 2022.

Proof for the full data case ($n = 1$, complex-valued functions): see the next but one section.

Illustration for the full data case ($n = 2$, real-valued functions): see the next slide.



$x_k(t_1,t_2) := x^\dagger(t_1,t_2) + \frac{\sqrt{2}}{8}\sin(k^2 t_1^2), \qquad x^\dagger(t_1,t_2) = \frac{2\pi}{3(2+\pi)}(t_1+1)(\cos((t_2-\frac{1}{2})\pi)+1), \qquad y_k - y = x_k * x_k - x^\dagger * x^\dagger$

Outline

Deautoconvolution of **real functions** over $[0, 1]$ is required for the verification of

Appearance potential spectra (APS) in spectroscopy:

▷ J. BAUMEISTER: Deconvolution of appearance potential spectra. In: Direct and inverse boundary value problems, Oberwolfach, 1989, Vol. 37 of *Methoden Verfahren Math. Phys.*, Peter Lang, Frankfurt am Main, 1991, pp. 1–13.

and **Solid surfaces structures and Nanostructures**:

▷ Z. DAI: Local regularization methods for inverse Volterra equations applicable to the structure of solid surfaces. *J. Integral Equations Appl.* **25** (2013), pp. 223–252.

Analytical basics and regularization for this case:

▷ R. GORENFLO AND B.H.: On autoconvolution and regularization. *Inverse Problems* **10** (1994), pp. 353–373.

A glimpse of the limited data case $F: L^2(0,1) \to L^2(0,1)$:

The operator

$$[F(x)](s) := \int_0^s x(s-t)x(t)dt \quad (0 \le s \le 1)$$

is **not compact**, but has a **compact** Fréchet derivative $F'(x)$

$$[F'(x)\,h](s) = 2\int_0^s x(s-t)h(t)dt \quad (0 \le s \le 1)$$

satisfying the **nonlinearity condition**

$$\|F(x) - F(x^\dagger) - F'(x^\dagger)(x - x^\dagger)\|_{L^2(0,1)} \le \|x - x^\dagger\|^2_{L^2(0,1)}.$$

No condition of **tangential cone type**

$$\|F(x) - F(x^\dagger) - F'(x^\dagger)(x - x^\dagger)\|_{L^2(0,1)} \le \sigma(\|F(x) - F(x^\dagger)\|_{L^2(0,1)})$$

with index function σ could be shown.

The theory by ENGL/KUNISCH/NEUBAUER 1989 yields for

$$T_\alpha^\delta(x) := \|F(x) - y^\delta\|^2_{L^2(0,1)} + \alpha\, \|x - \bar{x}\|^2_{L^2(0,1)}$$

the convergence rate

$$\|x_\alpha^\delta - x^\dagger\|_{L^2(0,1)} = \mathcal{O}(\sqrt{\delta}) \quad \text{as} \quad \delta \to 0$$

under the benchmark source condition

$$x^\dagger(t) = \bar{x}(t) + \int_t^1 x^\dagger(s-t)v(s)ds \quad (0 \le t \le 1,\ v \in L^2(0,1))\ (\$)$$

and the smallness condition

$$\|v\|_{L^2(0,1)} < 1\,. \qquad (\$\$)$$

Proposition

In the case, $\overline{x} = 0$ there is no $x^\dagger \neq 0$ which satisfies ($) – ($$). Apart from the trivial case $\overline{x} = x^\dagger$, the conditions ($) – ($$) can only hold if $x^\dagger \neq 0$ and if the reference element $\overline{x} \in L^2(0,1)$ is chosen such that

$$\frac{\|x^\dagger - \overline{x}\|_{L^2(0,1)}}{\|x^\dagger\|_{L^2(0,1)}} < 1,$$

where $x^\dagger - \overline{x}$ is a cont. function on $[0,1]$ with $\overline{x}(1) = x^\dagger(1)$. A proper choice of $\overline{x}$ and the value $x^\dagger(1)$ must be known.

For more details see:

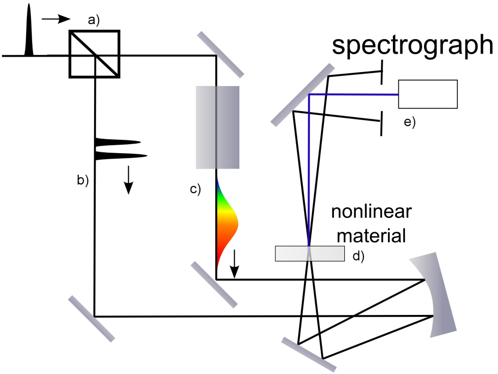
▷ S. BÜRGER AND B.H.: About a deficit in low order convergence rates on the example of autoconvolution. *Applicable Analysis* **94** (2015), pp. 231–243.

Outline

Deautoconvolution in short-term laser optics ($n = 1$)

SPIDER = Spectral Phase Interferometry for Direct Electric Field Reconstruction

Special version **Self-Diffraction (SD) SPIDER** was developed by **Max Born Institute for Nonlinear Optics, Berlin**



The physical model leads to an **autoconvolution problem**

$$\int_{\max(s-1,0)}^{\min(s,1)} k(s,t)x(s-t)x(t)dt = y(s) \quad (0 \le s \le 2) \quad (*)$$

with the corresponding **nonlinear forward operator**

$$F : X = L^2_{\mathbb{C}}(0,1) \to Y = L^2_{\mathbb{C}}(0,2).$$

The **complex-valued** function $x(t) = A(t)\, e^{i\varphi(t)}$ $(0 \le t \le 1)$ characterizing a short-term (femtosecond) laser pulse) is to be determined from complex-valued measurement data of y, where the complex-valued continuous kernel k is available.

▷ D. GERTH, B.H., S. BIRKHOLZ, S. KOKE AND G. STEINMEYER: Regularization of an autoconvolution problem in ultrashort laser pulse characterization. *Inverse Probl. Sci. Eng.* **22** (2014), pp. 245–266.

▷ S. W. ANZENGRUBER, S. BÜRGER, B.H. AND G. STEINMEYER: Variational regularization of complex deautoconvolution and phase retrieval in ultrashort laser pulse characterization. *Inverse Problems* **32** (2016), 035002 (27pp).

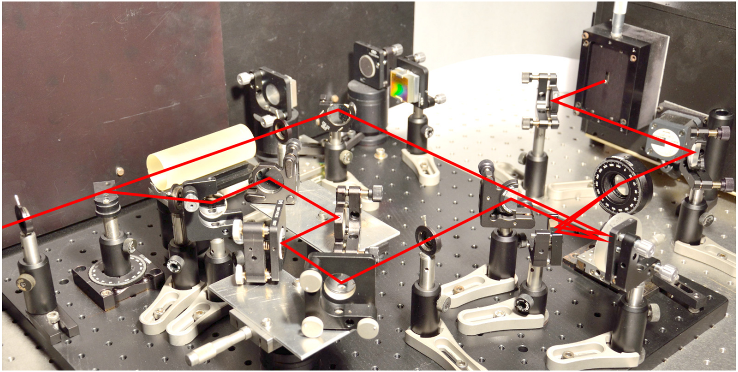


Figure: Measurement setup in self-diffraction spectral interferometry.

▷ J. Flemming: *Variational Source Conditions, Quadratic Inverse Problems, Sparsity Promoting Regularization. New Results in Modern Theory of Inverse Problems and an Application in Laser Optics*. Frontiers in Mathematics. Birkhäuser, Cham, 2018.

The focus of SD-SPIDER is on **phase retrieval**, where the first derivative (**group delay**) of the phase φ is of interest.

Tikhonov regul. solutions x_α^δ minimizing discretized versions of

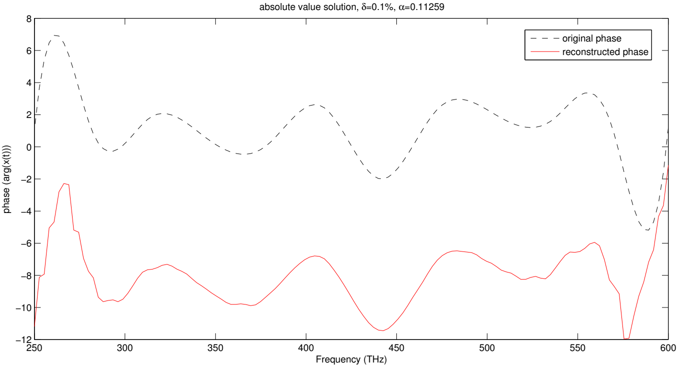
$$T_\alpha^\delta(x) := \|F(x) - y^\delta\|^2_{L^2_{\mathbb{C}}(0,2)} + \alpha\,\mathcal{R}(x)$$

can be helpful, where the penalty $\mathcal{R}(x)$, for example, approximates the L^2-norm square of the 2nd derivative of x.

Adapted a posteriori choices of $\alpha > 0$ may use data of the amplitude function $A(t)$ from independent measurements.

Typical reconstructed phase for $\delta = 0.1\%,\ \alpha = 0.11259$:

The group delay is reconstructed reasonably well. The phase has an offset of 2π. Only at the right boundary the curves do not match while the left boundary is reconstructed in an acceptable way.



Let us consider for simplicity the case of a trivial kernel $k \equiv 1$ as

$$[F(x)](s) = [x*x](s) := \int_{\max(s-1,0)}^{\min(s,1)} x(s-t)x(t)dt = y(s) \quad (0 \le s \le 2)$$

Proposition

This deautoconvolution problem solving $(*)$ is **locally ill-posed** everywhere on $L^2_{\mathbb{C}}(0,1)$.

Proof: We consider on $X = L^2_{\mathbb{C}}(0,1)$ the sequence $x_k = x^\dagger + h_k$ for $h_k(t) = r\, e^{i\,k^2 t^2}$ with $\|h_k\|_X = r$. We have $h_k \rightharpoonup 0$ in X and for $Y = L^2_{\mathbb{C}}(0,2)$ also $\|F(h_k)\|_Y \to 0$ as $k \to \infty$. The nl. operator F is **non-compact**, but its Fréchet derivative with $F'(x^\dagger)\,h = 2\,x^\dagger * h$ is **compact** for all $x^\dagger \in L^2_{\mathbb{C}}(0,1)$.
As a consequence, we obtain $\|F'(x^\dagger)h_k\|_Y \to 0$ and
$\|F(x_k) - F(x^\dagger)\|_Y = \|F(h_k) + F'(x^\dagger)h_k\|_Y \to 0$ as $k \to \infty$.
This shows the local ill-posedness everywhere.

Lemma (Titchmarsh's convolution theorem)

For functions $f, g \in L^2_{\mathbb{C}}(\mathbb{R})$ with compact supports covered by $[0,\infty)$, we have $f * g \in L^2_{\mathbb{C}}(\mathbb{R})$ with compact support in $[0,\infty)$, where $\mathrm{supp}(f*g) \subseteq \mathrm{supp}(f) + \mathrm{supp}(g)$. Notably, we conclude from

$$[f*g](s) = \int_0^\infty f(s-t)\,g(t)\,dt \;=\; 0 \quad \text{a.e. } \; s \in [0,\gamma] \quad (\gamma \ge 0)$$

that there are numbers $\gamma_1, \gamma_2 \ge 0$ with $\gamma_1 + \gamma_2 \ge \gamma$ such that

$$f(t) \;=\; 0 \quad \text{a.e. } \; t \in [0,\gamma_1] \quad \text{and} \quad g(t) \;=\; 0 \quad \text{a.e. } \; t \in [0,\gamma_2].$$

▷ E. C. TITCHMARSH: The zeros of certain integral functions. *Proc. London Math. Soc. (2)* **25** (1926), pp. 283–302.

We derive from of **Titchmarsh's convolution theorem**:

Theorem (solution twofoldness)

If for $y \in Y = L^2_{\mathbb{C}}(0,2)$ the function $x^\dagger \in X = L^2_{\mathbb{C}}(0,1)$ solves

$$\int_{\max(s-1,0)}^{\min(s,1)} x(s-t)x(t)dt = y(s) \quad (0 \le s \le 2)\,, \quad (*)$$

then $x^\dagger$ and $-x^\dagger$ are the only solutions of this operator equation.

Proof: Let, for $0 \neq h \in L^2_{\mathbb{C}}(0,1)$, the perturbed element $x^\dagger + h$ also solve $(*)$. Then $[(x^\dagger + h) * (x^\dagger + h)](s) = [x^\dagger * x^\dagger](s)$ and

$$[(2x^\dagger + h) * h](s) = 0 \quad \text{a.e. } \; s \in [0,2]\,.$$

The lemma applies with $f := 2x^\dagger + h$, $g := h$ and $\gamma := 2$. For $h \neq 0$ we have $\gamma_2 < 1$. This requires $\gamma_1 \geq 1$ with $[2x^\dagger + h](t) = 0$ a.e. for $t \in [0,1]$ and yields with $h = -2x^\dagger$ the element $x^\dagger + h = -x^\dagger$ as the only second solution.

The twofoldness theorem applies to n dimensions, see in detail:

▷ B.H., F. WERNER AND Y. DENG: On uniqueness and ill-posedness for the deautoconvolution problem in the multidimensional case. In preparation, Fall 2022.

Lemma (Lions' extension of Titchmarsh's theorem)

Let the functions $f, g \in L^2(\mathbb{R}^n)$ with $n \in \mathbb{N}$ have compact supports $\mathrm{supp(f)}$ and $\mathrm{supp(g)}$. Then we have $f * g \in L^2(\mathbb{R}^n)$ for the convolution and that the inclusion

$$\mathrm{supp(f * g)} \subseteq \mathrm{supp(f)} + \mathrm{supp(g)},$$

but for the convex hulls of the supports even the equation

$$\mathrm{conv\,supp(f * g)} = \mathrm{conv\,supp(f)} + \mathrm{conv\,supp(g)}$$

hold true. In the special case that $\mathrm{supp(f * g)} = \emptyset$, i.e., the function $f * g$ vanishes a.e. on $\mathbb{R}^n$, then we have that one of the sets $\mathrm{supp(f)}$ or $\mathrm{supp(g)}$ is the empty set, which means that at least one of the underlying functions f or g vanishes a.e. on $\mathbb{R}^n$.

▷ J. L. LIONS: Supports de produits de composition I (in French). *Comptes Rendus Acad. Sci. Paris* **232** (1951), pp. 1530–1532.

Outline

Variational regularization of deautoconvolution ($n = 2$)

For $X = L^2([0,1]^2)$ and variational regularized solutions x_α^δ of

$$T_\alpha^\delta(x) := \|F(x) - y^\delta\|_Y^2 + \alpha\,\mathcal{R}(x)$$

there have been performed case studies for
full data case $Y = L^2([0,2]^2)$ and **limited data case** $Y = L^2([0,1]^2)$
with penalty functionals

$$\mathcal{R}_1(x) := \|x - \bar{x}\|_X^2 \quad \text{(classical norm square penalty)},$$

$$\mathcal{R}_2(x) := \int\limits_{t \in [0,1]^2} \|\nabla x\|_2^2 dt \quad \text{(gradient norm square penalty)},$$

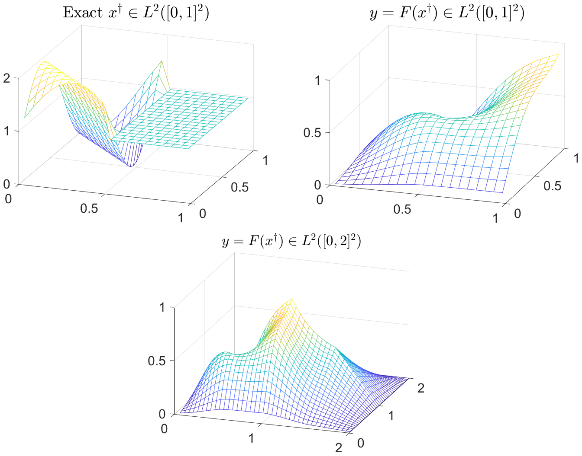
$$\mathcal{R}_3(x) := \int\limits_{t \in [0,1]^2} \|\nabla x\|_1 dt \quad \text{(total variation penalty)}.$$

We present here only one example, more material in:

▷ Y. Deng, B. Hofmann and F. Werner: Deautoconvolution in the 2D case. Paper submitted to ETNA, Oct. 2022, arXiv:2210.14093v1.

The example refers to the **non-smooth, non-factored** and **non-negative solution**

$$x^\dagger(t_1,t_2) = \begin{cases} \sin(1.5\pi(t_1+t_2))+1 & (0 \le t_1 \le 0.5,\ 0 \le t_2 \le 1) \\ 1 & (0.5 < t_1 \le 1,\ 0 \le t_2 \le 1) \end{cases}$$



Estimated Hölder exponents κ for Hölder convergence rates

$$\|x^{\delta}_{\alpha_{opt}} - x^{\dagger}\|_X \sim \delta^{\kappa} \quad \text{as} \quad \delta \to 0$$

	full data case $Y = L^2([0,2]^2)$			limited data case $Y = L^2([0,1]^2)$		
Penalty	$\mathcal{R}_1(x)$	$\mathcal{R}_2(x)$	$\mathcal{R}_3(x)$	$\mathcal{R}_1(x)$	$\mathcal{R}_2(x)$	$\mathcal{R}_3(x)$
Hölder exponent κ	0.6059	0.6320	0.5083	0.3753	0.4522	0.3787

Regularized solutions with optimal regularization parameters for different penalties in **limited data case** with noise level $\delta \sim 0.8\%$: