Multi-level discretization of phase reconstruction problems

Dirk Langemann
Technische Universität Braunschweig
Institute Computational Mathematics

d.langemann@tu-bs.de

DMV Jahrestagung München
March 9, 2010
Outline

1. 1d phase reconstruction problem
   - ambiguities and redundancy
   - multilevel approach in the numerical solution
   - first convergence results

2. 2d phase problem, frequency resolved optical gating

3. cristallographic phase problem

   typical features of the ill-posed phase reconstruction problem
1. Phase reconstruction problem

Search \( f : \mathbb{R} \rightarrow \mathbb{C} \), well-localized, sufficiently smooth with phase \( \varphi : \mathbb{R} \rightarrow \mathbb{C}/[0, 2\pi) = \mathbb{T} \), i.e. \( f(x) = |f(x)|e^{i\varphi(x)} \).

Given \( |f(x_n)|, |\hat{f}(v_k)|, \ x_k, v_n \in \mathbb{R} \) for finitely many \( n, k \in \mathbb{Z} \) with Fourier transform

\[
\hat{f}(v) = \int_{-\infty}^{\infty} f(x) e^{-ixv} \, dx
\]

Applications: electron microscopy, wave front sensing, laser optics. Only intensities are measurable due to short time intervals.

Continuous formulation:
Search well-localized, smooth \( f : \mathbb{R} \rightarrow \mathbb{C} \) for given \( |f(x)| \) and \( |\hat{f}(v)| \).

Dirk Langemann, TU Braunschweig
Relation to the autocorrelation problem

For $f \in L^2(\mathbb{R})$ is $|\hat{f}(v)|^2 = \ldots$

\[
\int_{-\infty}^{\infty} \int_{-\infty}^{\infty} f(x)\overline{f(y)}e^{-i(x-y)v} \, dx \, dy = \int_{-\infty}^{\infty} \left( \int_{-\infty}^{\infty} f(x)\overline{f(x-u)} \, dx \right) e^{-iuv} \, du
\]

and hence the autocorrelation fulfills

\[
A(u) = \int_{-\infty}^{\infty} f(x)\overline{f(x-u)} \, dx = \frac{1}{2\pi} \int_{-\infty}^{\infty} |\hat{f}(v)|^2 e^{iuv} \, dv.
\]

Autocorrelation problem: Reconstruct a function from its autocorrelation.
Ambiguities in the phase reconstruction problem

Regular: \( g(x) = f(x)e^{i\alpha}, \alpha \in \mathbb{R} \Rightarrow \)

\[ |g(x)| = |f(x)| \quad \text{and} \quad |\hat{g}(v)| = |\hat{f}(v)|. \]

Singular (example): If \( |\hat{f}(v)| = |\hat{f}(\alpha - v)| \) for some \( \alpha \in \mathbb{R} \),
then \( g(x) = f(x)e^{i\alpha x} \) fulfills \( |g(x)| = |f(x)| \) and

\[ |\hat{g}(v)| = \left| \int_{-\infty}^{\infty} f(x)e^{i\alpha x}e^{-ixv} \, dx \right| = \left| \int_{-\infty}^{\infty} f(x)e^{ix(v-\alpha)} \, dx \right| = |\hat{f}(v)|. \]

Uniqueness conditions are unknown.

Conditions for the existence of a solution are unknown.
Traditional approach: Gerchberg-Saxton algorithm

1. Fourier transform $f^{(\ell)}(x) \rightarrow \hat{f}^{(\ell)}(v)$

2. Normalization $\hat{f}^{(\ell+1/2)}(v) = \frac{\hat{f}^{(\ell)}(v)}{|\hat{f}^{(\ell)}(v)|} \cdot |\hat{f}(v)|$

3. Inverse Fourier $f^{(\ell+1/2)}(x) = \frac{1}{2\pi} \int_{-\infty}^{\infty} \hat{f}^{(\ell+1/2)}(v) e^{ixv} \, dv$

4. Normalization $f^{(\ell+1)}(x) = \frac{f^{(\ell+1/2)}(x)}{|f^{(\ell+1/2)}(x)|} \cdot |f(x)|$

- non-expansive iterative algorithm, no convergence proof
- stagnations, restarts, various initial functions $f^{(0)}(x)$, smoothing

Dirk Langemann, TU Braunschweig
Interpolation by translates of a well-localized $\lambda \in L^2(\mathbb{R})$ with $a_s \in \mathbb{C}$

$$f(x) = \sum_{s=0}^{N-1} a_s \lambda(x - x_s) \quad \text{and} \quad \hat{f}(v) = \left( \sum_{s=0}^{N-1} a_s e^{-ixsv} \right) \hat{\lambda}(v).$$

Now $|f(x)|^2 = \sum_{s=0}^{N-1} \sum_{r=0}^{N-1} \overline{a_s}a_r \lambda(x - x_s) \lambda(x - x_r)$

and $|\hat{f}(v)|^2 = |\hat{\lambda}(v)|^2 \sum_{s=0}^{N-1} \sum_{r=0}^{N-1} \overline{a_s}a_r e^{-i(x_r-x_s)v}$ or with $a = (a_s)_{s=0}^{N-1}$

$$a^H H_n a = |f(x_n)|^2 \quad \text{and} \quad a^H J_k a = \frac{|\hat{f}(v_k)|^2}{|\hat{\lambda}(v_k)|^2}.$$ 

with $H_n \in \mathbb{R}^{N \times N}$, $J_k \in \mathbb{C}^{N \times N}$ hermitian for all $n, k$. 

Dirk Langemann, TU Braunschweig
Nature of the phase reconstruction problem

Quadratic equations, cf. Hilbert problem No. 16 (not completely solved).

Example for \( N = 2 \): Search \( a_0, a_1 \in \mathbb{C} \) for

\[
\begin{align*}
H_0 &= \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix}, & H_1 &= \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix}, & J_0 &= \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}, & J_1 &= \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}.
\end{align*}
\]

lead to

\[
\begin{align*}
|a_0|^2 + |a_1|^2 &= c_0, \\
\overline{a_0}a_1 + a_0\overline{a_1} &= c_1, \\
|a_0|^2 &= d_0^2, \\
|a_1|^2 &= d_1^2.
\end{align*}
\]

- solvable if \( c_0 = d_0^2 + d_1^2 \) and \( |c_1| \leq 2d_0d_1 \)
- solution \( a_0 = d_0e^{i\varphi_0}, \ a_1 = d_1e^{i\varphi_1}, \ \varphi_n \in \mathbb{T} \)
- perturbation of \( (c_0, c_1, d_0^2, d_1^2)^T \) may ruin the existence of a solution

We are faced to the same difficulties for larger \( N \), i.e. ambiguities, redundancy, loss of existence for disturbed measurements.

Dirk Langemann, TU Braunschweig
Linear spline approximation

equidistant \( x_s = s, \ s = 0, \ldots, N - 1, \ \nu_k = \frac{k\pi}{N}, \ k = -N, \ldots, N - 1 \)

linear spline \( \lambda(x) = M_2(x) \) with \( \hat{\lambda}(x) = \left(\text{sinc} \frac{v}{2}\right)^2 \)

Then \( J_k = \text{circ}(1, e^{ik\pi/N}, e^{2ik\pi/N}, \ldots, e^{i(N-1)k\pi/N}) \) or

\[
|a_0|^2 + |a_1|^2 + \ldots + |a_{N-1}|^2 = c_0,
\]

\[
a_0\overline{a}_1 + a_1\overline{a}_2 + \ldots + a_{N-2}\overline{a}_{N-1} = c_1,
\]

\[
a_0\overline{a}_2 + a_1\overline{a}_3 + \ldots + a_{N-3}\overline{a}_{N-1} = c_2,
\]

\[
\ldots
\]

\[
a_0\overline{a}_{N-1} = c_{N-1}
\]

and \( H_n = \text{diag}(e_n) \) or \( |a_n|^2 = d_n^2 = |f(x_n)|^2 \)

relation to the discrete autocorrelation problem

Dirk Langemann, TU Braunschweig
Further ambiguities in the discrete problem

equidistant $x_s = s$, equidistant $v_k$ and linear spline $\lambda(x) = M_2(x)$:

$$f(x) = \sum_{s=0}^{N-1} a_s \lambda(x-s) \quad \text{and} \quad \hat{f}(v) = \left( \sum_{s=0}^{N-1} a_s e^{-isv} \right) \hat{\lambda}(v) = P_f(e^{-iv}) \hat{\lambda}(v)$$

with the polynomial $P_f(z) = \sum_{s=0}^{N-1} a_s z^s$ with zeros $\zeta^f_r$, $r = 1, \ldots, N - 1$.

**Zero flipping:** $f, g$ linear splines with $|f(s)| = |g(s)|$, $|\hat{f}(v_k)| = |\hat{g}(v_k)|$

$$\Leftrightarrow \begin{cases} \zeta^f_r, (\bar{\zeta}^f_r)^{-1} \end{cases} = \begin{cases} \zeta^g_r, (\bar{\zeta}^g_r)^{-1} \end{cases} \quad \text{and} \quad \exists |z_0| = 1 : |P(z_0)| = |Q(z_0)| \neq 0$$

Discretization produces further ambiguities.

Dirk Langemann, TU Braunschweig
Multilevel approach

Idea:
- discretize on coarse grid, e.g. \( \{x_s\} = \{0, N/2^j, 2 \cdot N/2^j, \ldots \} \)
- solve the nonlinear system,
- interpolate solution to refined grid for \( j + 1 \),
- use interpolation as initial value on refined grid

Difficulty:
Given values \( \hat{f}(v_k) \) for original function \( f \), not for the linear spline.
Discretization error behaves like measurement error in the original data.

Remark: Other interpolations (e.g. cardinal splines) with same difficulty.
Numerics of the nonlinear system

set $a_s = |f(s)| e^{i\varphi_s}$, phase vector $\varphi = (\varphi_{2^j s})_{s=0}^{N/2^j-1} \in \mathbb{R}^{N/2^j}$

combine the quadratic equations (including one fixed $\varphi_{N/2} = 0$) in

$$G(\varphi) = g \approx g^\delta$$

only approximation $\|g - g^\delta\| \leq \delta$ due to discretization, measurement

• minimization problem $\|G(\varphi) - g^\delta\|^2 \rightarrow \min$ highly non-convex

minimization of the Tykhonov functional

$$J_\alpha(\varphi) := \|G(\varphi) - g^\delta\|^2 + \alpha \|\varphi - \varphi_{j,0}\|^2 \rightarrow \min$$

with initial guess $\varphi_{j,0}$ on level $j$ and regularizer $\alpha > 0$

e. g. by iterative regularized Gauss-Newton (IRGN) algorithm
**Illustration (real parts)**

![Graphs showing real parts at different levels](image)

- **Level j=3**
  - Minimizer
  - Regularization
  - True value

- **Level j=4**
  - Minimizer
  - Regularization
  - True value

- **Level j=5**
  - Minimizer
  - Regularization
  - True value

- **Level j=6**
  - Minimizer
  - Regularization
  - True value

The multilevel approach goes together with Tykhonov regularization. The minimizer on the coarse level serves as an initial guess $\varphi_j$ on the finer level.

Dirk Langemann, TU Braunschweig
A discrepancy principle from Bakushinsky

1. the exact nonlinear system $G(\varphi) = g$ has a solution $\varphi = \varphi^\dagger$,
2. $G$ differentiable, $\|G'(\varphi)\| \leq M$, $\|G'(\varphi) - G'(\psi)\| \leq L \|\varphi - \psi\|$,
3. $g$ is approximately known with $g^\delta$,
4. $\{\alpha_n\}_{n=0}^\infty$ satisfies $\alpha_n > 0$, $\lim_{n \to \infty} \alpha_n = 0$, $\alpha_n \leq r \alpha_{n+1}$ with $r > 1$,
5. source condition $\varphi^\dagger - \varphi_0 = G'(\varphi^\dagger)^T v$ with $\|v\| \leq \varepsilon$,
6. for some $\tau > 1$, constants exist with

$$\sqrt{r} \left( L \varepsilon + \sqrt{\frac{L\varepsilon}{2}} + \frac{M^2 \varepsilon}{(\sqrt{\tau} - 1)^2} \right) \leq 1, \quad \frac{\|\varphi^\dagger - \varphi_0\|}{\sqrt{\alpha_0}} \leq \ell = \frac{\sqrt{r} \varepsilon}{1 - L \varepsilon \sqrt{r}}.$$

Then $\|\varphi^\dagger - \varphi_n\| \leq \ell \sqrt{\alpha_n}$ for $n = 0, \ldots, N(\delta)$ and $\lim_{\delta \to +0} \varphi_{N(\delta)} = \varphi^\dagger$ and $\|G(\varphi_{N(\delta)}) - g^\delta\|^2 \leq \tau \delta < \|G'(\varphi_n) - g^\delta\|^2$ for $n = 0, \ldots, N(\delta) - 1$.

green: fulfilled, red: not sure, not feasible, constants for $2L\varepsilon < 1$

Our $M, L \Rightarrow \varepsilon$ very small $\Rightarrow \varphi_0 \approx \varphi^\dagger$ very accurate, still large $\tau$ 😞
First convergence results

$L$ increases with level $j$, i.e. better initial values at finer levels required.

- $|f''(x)| \leq \mu \Rightarrow$ interpolation error of $f \sim 4^{-j}c$

- $C$ exists with $\|g_j - g^{\delta_j}_j\| \leq 2^{-j/2} C$, i.e. $\delta$ decreases in $j$, $\delta_{j+1} \approx \delta_j / \sqrt{2}$

- interpolation $\|\varphi_{j+1,0} - \varphi_{j+1}^\dagger\| \leq \sqrt{2} \|\varphi_{j,N(\delta_j)} - \varphi_j^\dagger\| + 2^{j/2-1} \mu_j^{(\varphi)}$

- $\|\varphi_{j}^\dagger - \varphi_{j,N(\delta_j)}\| \leq M_j \varepsilon_j r_j^{-N(\delta_j)/2} + E_j$ with small additional $E_j$

- update $\varepsilon_{j+1} \approx \sqrt{2} \frac{M_j}{M_{j+1}} \varepsilon_j r_j^{-N(\delta_j)/2} + 2^{j/2-1} \frac{\mu_j^{(\varphi)}}{M_{j+1}}$

Slightly curved $f$ can be well-reconstructed in general.

No proof, because discrepancy can be fulfilled by $\varphi_{j,0}$, no improve in $\varepsilon$. 

Dirk Langemann, TU Braunschweig
Results I for linear spline $f$

reconstruction von $\varphi(x)$ at levels $j = 3, \ldots, 7$ and without multilevel

Dirk Langemann, TU Braunschweig
Residual norms

L-shape residual norms $\|G_j(\varphi_n) - g_j^{\delta_j}\|$, most steps in coarse levels

Dirk Langemann, TU Braunschweig
reconstruction of $\varphi(x)$ for a less simple phase function

Dirk Langemann, TU Braunschweig
Disturbed input data

\[ f \text{ linear spline, } \pm 10\% \text{ uniformly distributed error in } |f(x_n)|, |\hat{f}(v_k)| \]

Dirk Langemann, TU Braunschweig
Alternatives

• approximation:
  linear splines, higher order splines, cardinal splines, Gaussian bells, . . .

• objective function:
  squared norm or not, other norms, smoothing, other regularization, . . .

• numerical methods:
  IRGN, Marquardt-Levenberg-algorithm, CG-reginn, genetic algorithms

⇝ comparable difficulties
Interpretation

- phase reconstruction problem analytically not completely understood
- highly nonlinear equations or strictly non-convex objective function
- multilevel technique shifts the numerical effort into the coarse levels
- ambiguities and redundancy make the phase problem ill-posed
- very sensitive to perturbations of input parameters
- discrepancy principle provides first convergence results
- theoretical results are much weaker than practical applicability
2. Frequency resolved optical gating

**Search** $f_1, f_2 : \mathbb{R} \rightarrow \mathbb{C}$ well-localized, sufficiently smooth
two phases $f_1(x) = |f_1(x)| e^{i\varphi_1(x)}$, $f_2(x) = |f_2(x)| e^{i\varphi_2(x)}$

**Given** $|f_1(x)|$, $|f_2(x)|$ and $|F(y, v)|$ with

$$F(y, v) = \int_{-\infty}^{\infty} f_1(x) f_2(y - x) e^{-ixv} dx$$

abbreviation $f(y, x) = f_1(x) f_2(y - x)$

**FROG**: ultrashort laser pulse measurement technique,
pulse splitted, interacted spectrum measured
(H. Stolz, Rostock)

Dirk Langemann, TU Braunschweig
Relation to autocorrelation

\[ F(y, v) = \int_{-\infty}^{\infty} f(y, x)e^{-ixv} dx \quad \Rightarrow \]

one-dimensional autocorrelation problem for each \( y \)

\[ A(y, u) = \int_{-\infty}^{\infty} f(y, x)f(y, x-u) dx = \frac{1}{2\pi} \int_{-\infty}^{\infty} |F(y, v)|^2 e^{iuv} dv \]

1. find \( f(y, x) = |f(y, x)|e^{i\varphi(y, x)} \) by multilevel approach for each \( y = y_k \)

2. determine \( f_1, f_2 \) with \( f(y, x) = f_1(x)f_2(y-x) \) (\( y \)-slices of \( f \) adapted) by best-approximation on the grid \( (y_k, x_n) \)

- 2. problem \( \varphi(y, x) = \varphi_1(x) + \varphi_2(y-x) \mod 2\pi \) is overdetermined again

- numerical \( f \) need not fulfill condition \( |f(y, x)| = |f_1(x)| \cdot |f_2(y-x)| \)

Dirk Langemann, TU Braunschweig
Example of a FROG

rather simple case with very smooth phase functions

Dirk Langemann, TU Braunschweig
3. Phase reconstruction in crystallography

Search \( f : \mathbb{R}^3 \rightarrow \mathbb{R} \) with \( f(x) \geq 0 \), periodic, sufficiently smooth

Given finitely many modulus \( |c_k|, \ k \in \mathbb{Z}^3 \) of Fourier coefficients

Application: crystallography, electron density \( f \),
interference pattern from X-ray spectroscopy (J. Mesters, Lübeck)

One-dimensional formulation:
find \( f : [0, 2\pi) \rightarrow \mathbb{R}, \ f(x) \geq 0 \) from \( |c_k| \) with \( c_k = \frac{1}{2\pi} \int_0^{2\pi} f(x)e^{-ikx} \, dx \)

Continuous formulation: find \( f : \mathbb{R} \rightarrow \mathbb{R}, \ f(x) \geq 0 \) from \( |\hat{f}(v)| \).

Dirk Langemann, TU Braunschweig
Phase information as image information

\[ f : [−\pi, \pi]^2 \rightarrow \mathbb{R} \]
\[ f = \text{char(}, \text{A}) \]
\[ c_k = |c_k^A|e^{i\varphi(c_k^A)} \]
\[ \tilde{c}_k = |c_k^A|e^{i\varphi(c_k^B)} \]

modulus of A \(\oplus\) phase of B

Dirk Langemann, TU Braunschweig
**Constraint of real $f$**

one-dimensional $f \in \mathbb{R} \iff c_k = \overline{c_{-k}}$

- if $|c_k| = |c_{-k}|$ for all $k$ then
  any phases with $\varphi_k = -\varphi_{-k}$ in $c_k = |c_k|e^{i\varphi_k}$ give real $f$
  the constraint is trivial

- if $|c_k| \neq |c_{-k}|$ for some $k$ then
  all phases gives $f \not\in \mathbb{R}$, the constraint is not feasible

analogue for the continuous formulation

\[ g(v) = |\hat{f}(v)|, \ v \geq 0 \Rightarrow \hat{f}(v) = e^{i\varphi(v)}g(|v|) \text{ with } \varphi(-v) = -\varphi(v) \text{ and } \]

\[
f(x) = \frac{1}{\pi} \int_{0}^{\infty} \cos(xv + \varphi(v))g(v)dv \in \mathbb{R} \text{ for all } x
\]

again redundancy and ambiguities

Dirk Langemann, TU Braunschweig
Positiveness constraint

assume $|c_k|$ with $|c_k| = |c_{-k}|$, i.e. real solutions $f$ exist

$$f(x) = \sum_{k=-\infty}^{\infty} c_k e^{ikx} = c_0 + \sum_{k=0}^{\infty} |c_k| \cos(kx + \varphi_k)$$

• if $c_0 \geq \sum_{k=1}^{\infty} |c_k|$ then all arbitrary $\varphi_k$ provide positive functions $f$

• if $c_0 = 0$ (or small) then no choice of $\varphi_k$ give positive functions $f$

Cristallographic phase problem is mathematically not correctly posed.
– application: simply connected shape of the molecule
– erroneous $c_0$ from total molecular weight due to fluid support
– stepwise recognition of molecular groups

Dirk Langemann, TU Braunschweig
Optimization problem

1. penalize negative values and minimize

\[
J = \int_0^{2\pi} P(f(x)) \, dx \quad \text{with e.g. } P(z) = e^{-z/\nu}
\]

or other monotonously decreasing penalty functions.

Unfortunately \( \phi_1 = \phi_2 = \ldots \text{ e.g.} \) 0 is always a hot candidate.

2. maximize the minimum of \( f \)

- right \(|c_1| = 3, |c_2| = 2, |c_1| = 1\)
- w. l. o. g. \( \phi_1 = 0 \)
- solutions \((\phi_2, \phi_3)\) for increasing \(c_0\)

special role of smallest \(c_0\)?
Conclusion

- Multilevel techniques diminish the numerical effort of phase reconstruction. Ill-posedness of the problem enters the convergence investigation.

- A consequent analysis of a phase reconstruction problem seems to be the key to suitable and successful numerical techniques.

---


Thanks

• Manfred Tasche
• Tobias Ahnert
• Christina Brandt
• Myra Noëmi Chavez Rosas
• Sindy Laurat

Thank you.

Dirk Langemann, TU Braunschweig