Satisfying positivity requirement in Complex Langevin

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Plan of the presentation

Statement of the problem

The aim of the beyond Complex Langevin approach is to obtain a positive and normalizable probability distribution $P(x, y)$ such that:

$$\int f(x)\rho(x)\ dx = \int\int f(x+iy)P(x,y)\ dxdy \quad (1)$$

for a given complex $\rho(x)$ and every $f(x)$.

Writing for the moments:

$$\int x^r\rho(x)\ dx \equiv M_r = \int\int (x+iy)^r P(x,y)\ dxdy \quad (2)$$

Satisfying positivity

Consider $\psi(x, y)$ such that $P(x, y) = |\psi(x, y)|^2$, then:

$$M_r = \int \int \psi(x, y)^* (x + iy)^r \psi(x, y) \; dxdy = \langle \psi | (x + iy)^r | \psi \rangle \tag{3}$$

and expand $|\psi\rangle$ into a basis (e.g. of two non-interacting harmonic oscillators)

$$\psi(x, y) = \sum_{mn} c_{mn} \psi_m(x) \psi_n(y), \tag{4}$$

where $c_{mn} \in \mathbb{R}$ is assumed for simplicity.

$$M_r = \sum_{m'n'mn} c_{m'n'} c_{mn} \langle \psi_{m'n'} | (x + iy)^r | \psi_{mn} \rangle \tag{5}$$

Matching conditions – exact form

$$1 = \sum_{mn} c_{mn}^2, \quad \text{Re } M_1 = \sqrt{2}\sum_{mn}\sqrt{m+1}c_{m+1,n}c_{mn}, \quad \text{Im } M_1 = \sqrt{2}\sum_{mn}\sqrt{n+1}c_{m,n+1}c_{mn} \tag{6}$$

$$\text{Re } M_2 = \sum_{mn}\left[(m-n)c_{mn} + \sqrt{(m+1)(m+2)}c_{m+2,n} - \sqrt{(n+1)(n+2)}c_{m,n+2}\right]c_{mn} \quad \text{, etc.}$$

Approximate solution

Include only a finite number of variables c_{mn} (e.g. such that $m+n \leq N$) and an equal number of equations.

Example (for $m+n \leq 4$)

$$\begin{aligned}\text{Re } M_2 = &-4c_{04}^2 - 2c_{13}^2 - \sqrt{2}c_{00}c_{02} + \sqrt{2}c_{00}c_{20} - 2c_{02}^2 - 2\sqrt{3}c_{02}c_{04} + \\ &+\sqrt{2}c_{02}c_{22} + 2c_{31}^2 - \sqrt{6}c_{11}c_{13} + \sqrt{6}c_{11}c_{31} + 4c_{40}^2 + 2c_{20}^2 - \sqrt{2}c_{20}c_{22} \\ &+ 2\sqrt{3}c_{20}c_{40}\end{aligned} \tag{7}$$

Gröbner bases method

- Extension of **Euclid's algorithm** for calculating GCDs and **Gaussian elimination** for linear systems to non-linear cases.

Buchberger's Algorithm

Input: $F = (f_1, ..., f_s)$
Output: a Gröbner basis $G = (g_1, ..., g_t)$, $F \subset G$

$G := F$
REPEAT
  $G' := G$
  FOR each pair $\{p, q\}$, $p \neq q$ in G' DO
    $S := \overline{S(p,q)}^{G'}$
    IF $S \neq 0$ THEN $G := G \cup S$
UNTIL $G = G'$

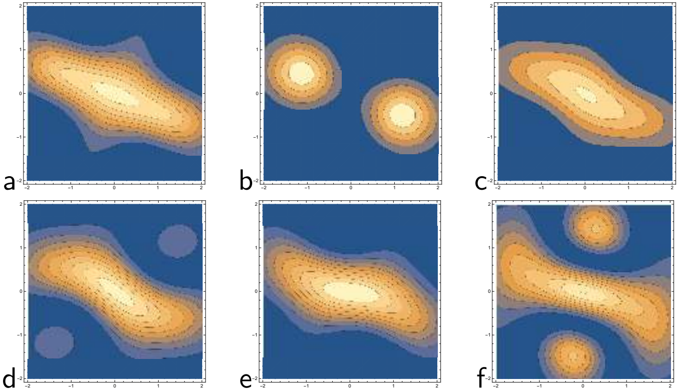
Gröbner bases method for Gaussian case

$$\rho(z) = \sqrt{\frac{\sigma}{2\pi}} e^{-\sigma x^2/2}, \qquad \sigma = (1+i)/\sqrt{2} \tag{8}$$

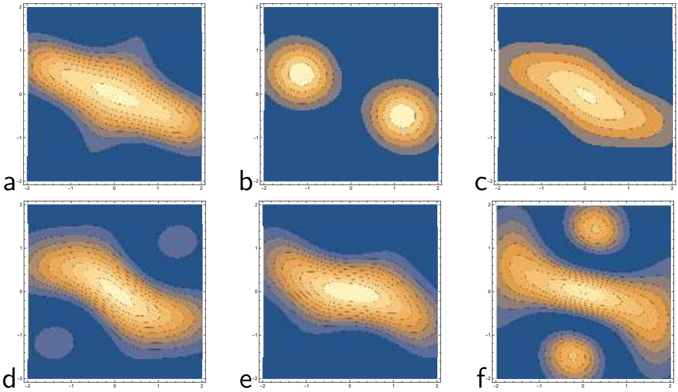
- Assumptions: $m + n \leq 4$, $c_{mn} = 0$ for odd $m + n$, symmetries $c_{02} = -c_{20}$, $c_{40} = c_{04}$ and $c_{13} = -c_{31}$ (6 variables)
  $\Rightarrow$ 12 solutions

	c_{00}	c_{02}	c_{11}	c_{04}	c_{13}	c_{22}
a	**0.827**	**-0.154**	**-0.217**	-0.00815	0.332	-0.00665
b	0.520	-0.404	-0.572	-0.129	0.126	-0.105
c	0.855	-0.101	-0.382	0.0608	0.215	-0.0627
d	0.738	-0.0817	-0.587	0.145	0.150	-0.104
e	-0.811	0.339	0.114	0.00705	-0.190	-0.166
f	-0.431	0.523	0.376	-0.145	0.0145	-0.290
exact	**0.910**	**-0.189**	**-0.267**	0.0478	0.0956	0.0390

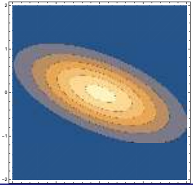
Gröbner bases method for Gaussian case



Gröbner bases method for Gaussian case



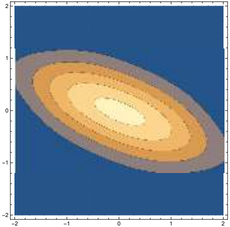
$P_g(x,y) = \frac{1}{\pi}\exp(-(x^2 + 2xy + 3y^2)/\sqrt{2})$ [Ambjorn, Yang, 1985]



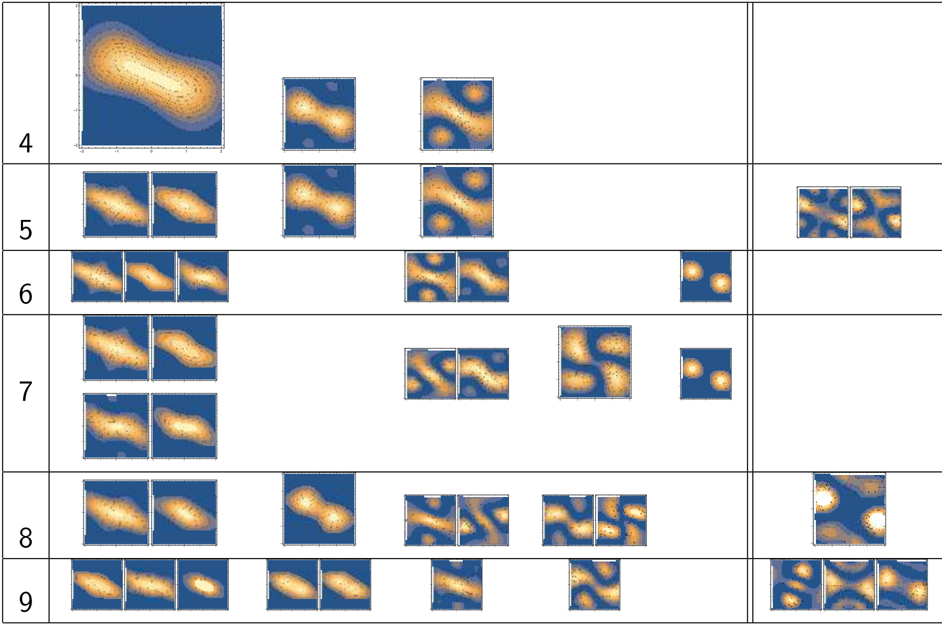
Minimization approach – Gaussian case

- numerical search for the local minima of the sum $\sum_i (\mathrm{LHS}_i - \mathrm{RHS}_i)^2$
- randomly chosen starting point

Sample results for 17 variables:



	c_{00}	c_{02}	c_{11}	c_{04}	c_{13}	c_{22}
Approx.	0.907	-0.187	-0.264	-0.00341	0.102	-0.00279
Exact	0.910	-0.189	-0.267	0.0478	0.0956	0.0390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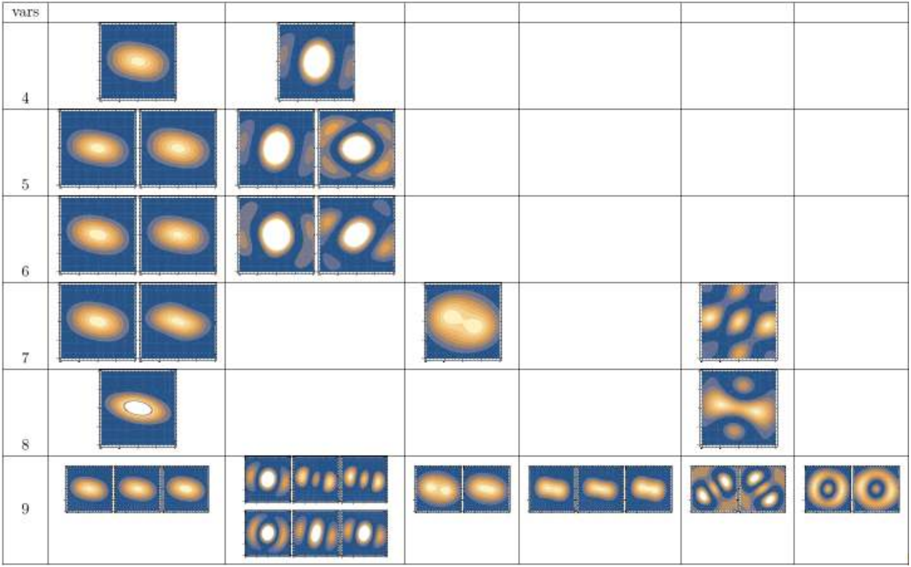
Non-uniqueness of the problem

- Gröbner method, minimization methods $\Rightarrow$ a large number of solutions
- The number of solutions increases with the number of matching conditions
- These results explicitly illustrate non-uniqueness of the problem
- Classification of the solutions

Quartic case, $\rho(z) = e^{-\lambda z^4/2}$ – classification of solutions



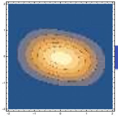
Quartic case – stability

Distance: $\| P_1 - P_2 \|_2 = \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} (P_1(x,y) - P_2(x,y))^2 \; dx \; dy$

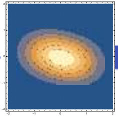
Quartic case – stability

Distance: $\parallel P_1 - P_2 \parallel_2 = \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} (P_1(x,y) - P_2(x,y))^2 \ dx \ dy$

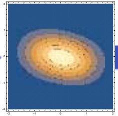
5 variables



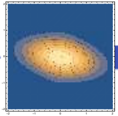
6 variables



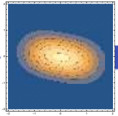
7 variables



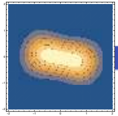
8 variables



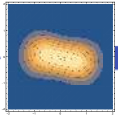
9 variables



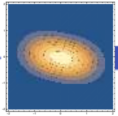
10 variables



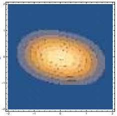
11 variables



12 variables



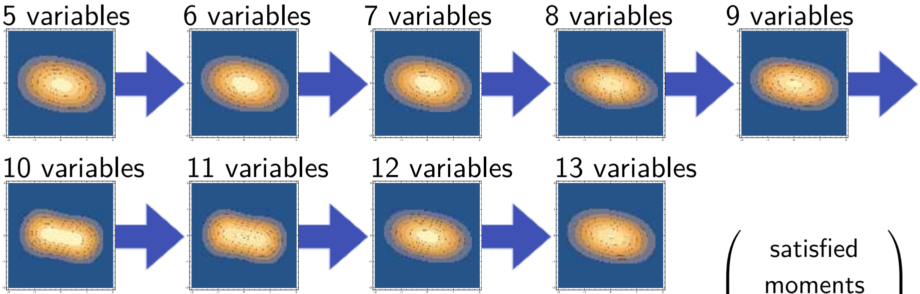
13 variables



$\left(\begin{array}{c} \text{satisfied} \\ \text{moments} \\ M_0 - M_{12} \end{array} \right)$

Quartic case – stability

Distance: $\| P_1 - P_2 \|_2 = \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} (P_1(x,y) - P_2(x,y))^2 \; dx \; dy$



(satisfied moments $M_0 - M_{12}$)

- Even though there is a lot of solutions, classification of solutions seems to appear.
- There exist stable solutions, present in all steps of the algorithm, and unstable solutions.

Summary

- Positivity: $P(x,y) \to |\psi(x,y)|^2$
- Gröbner bases method provides exact solutions of the matching conditions. With this approach all solutions are found.
- Non-uniqueness of the problem is directly observed.
- Gaussian case: the known solution is observed with the methods proposed in this talk and new solutions are present.
- Quartic case: approximate solutions.
- Classification of the solutions: proximity of solutions in subsequent steps of the algorithm, stable and unstable solutions.

Literature

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