A Spline-based approach to Uncertainty Quantification and Density Estimation

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- Adi Ditkowski
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Motivation

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Control of multiple filamentation in air

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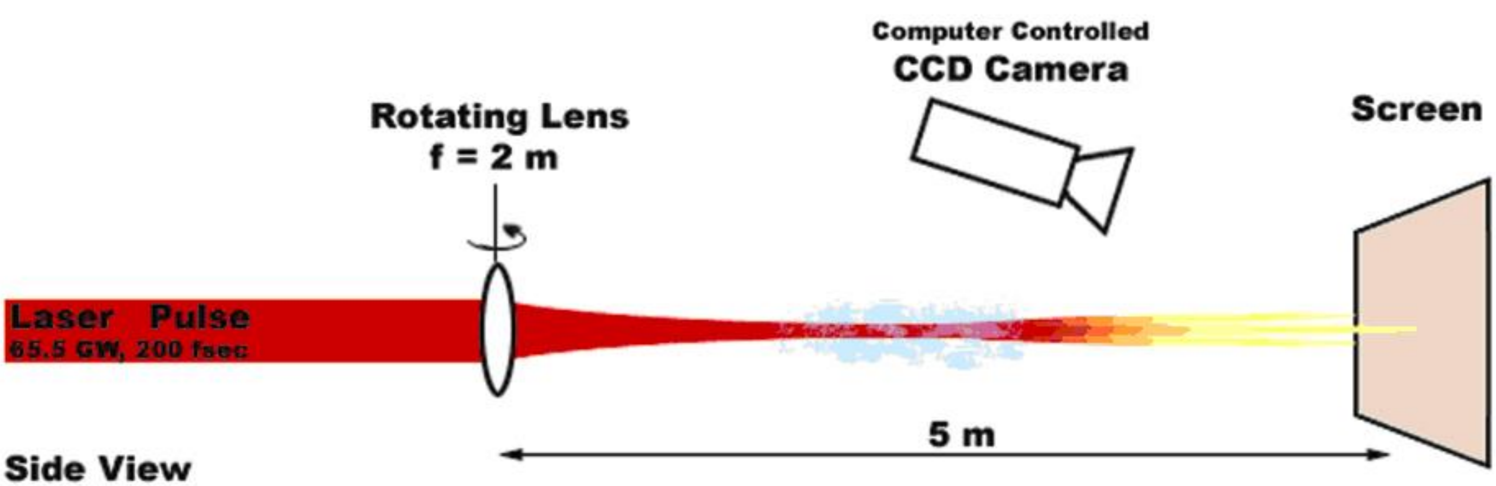
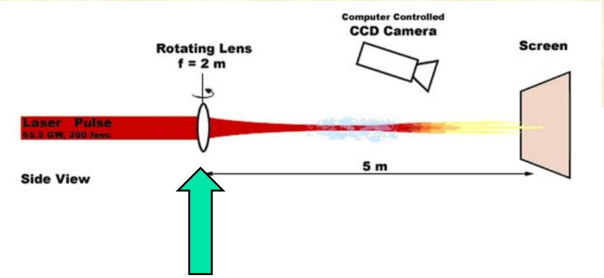
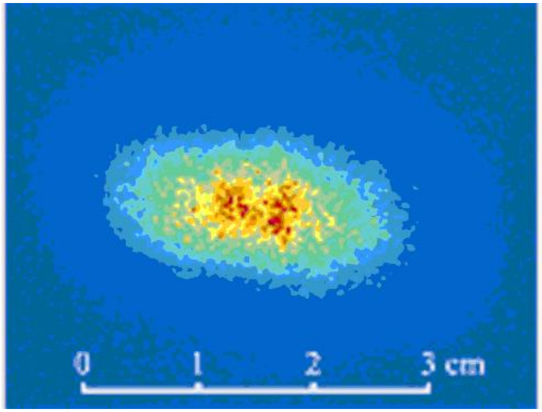


Input pulse characteristics



- Elliptic



typical shot

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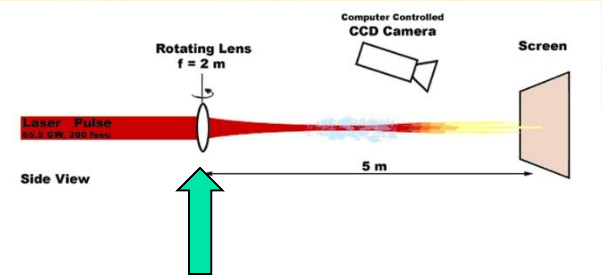

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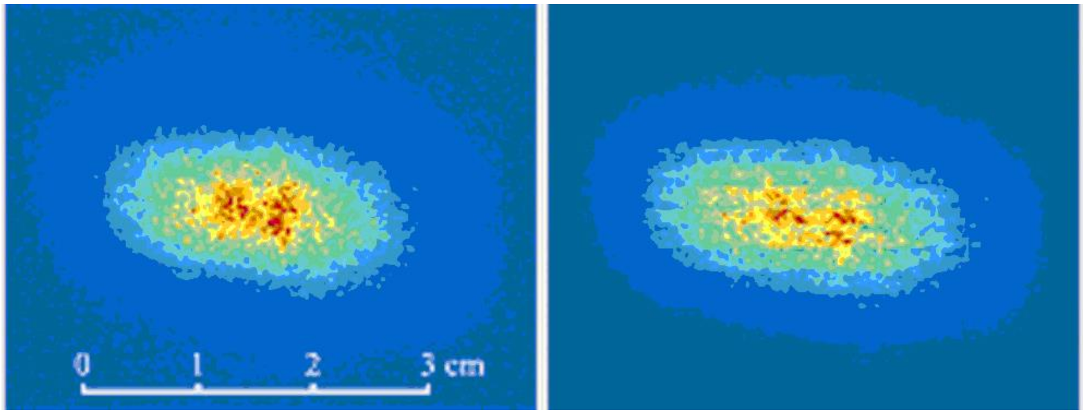
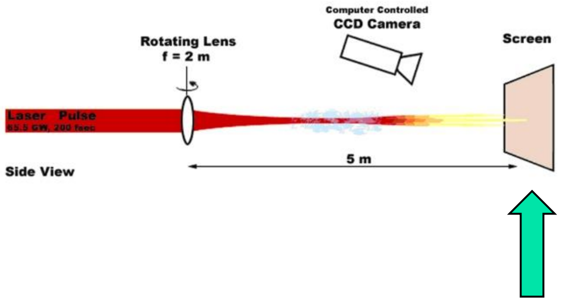


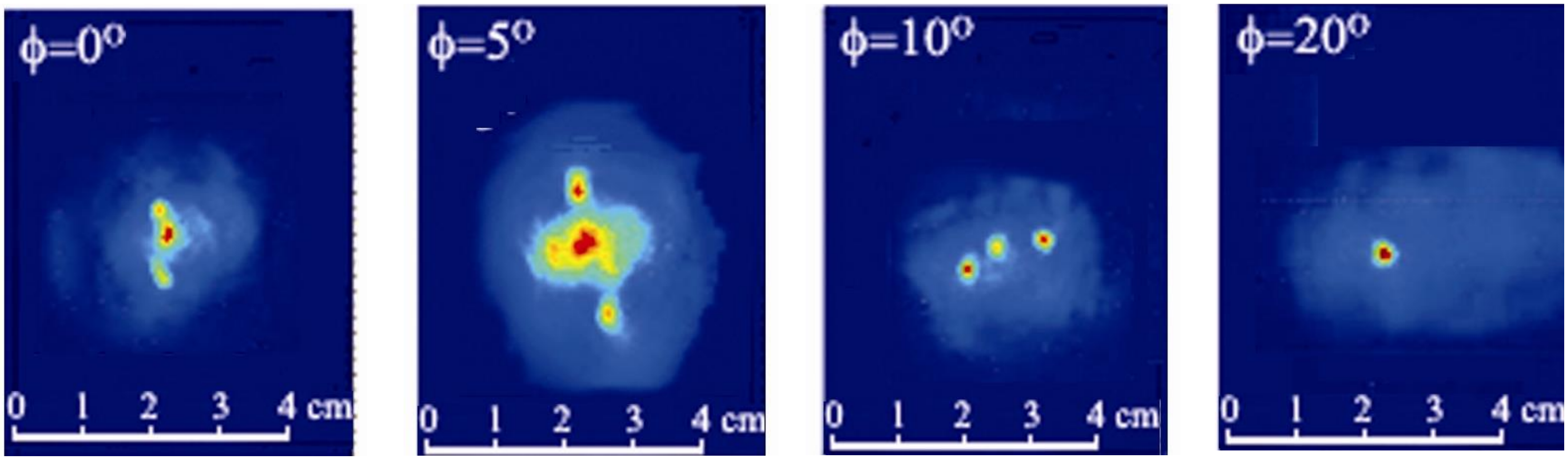
typical shot | average over 1000 shots

- Varies from shot to shot
  - Always the case

After 5 meters in air



typical



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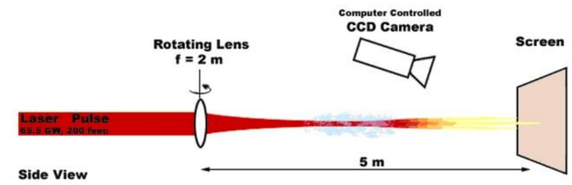
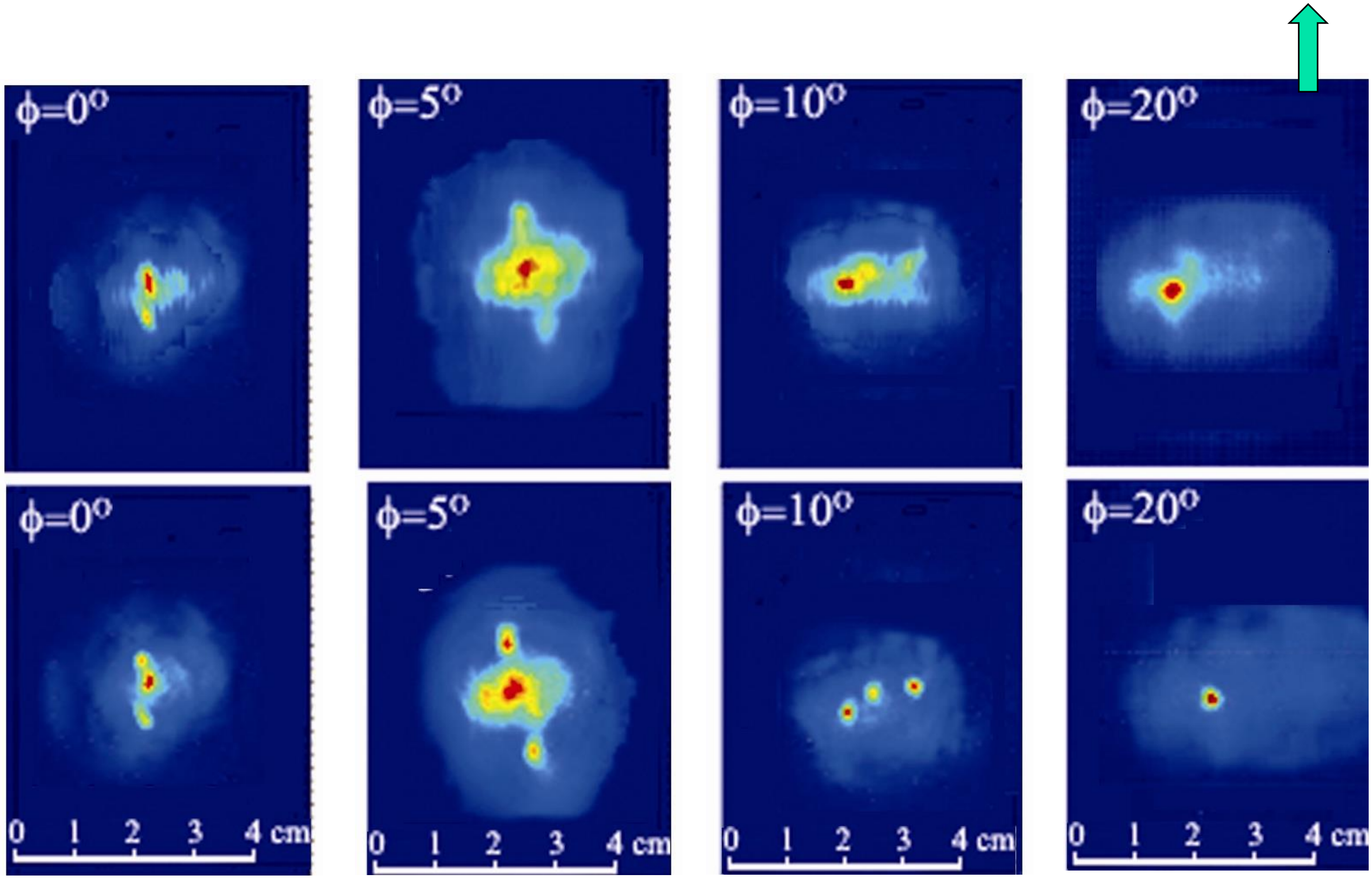


Average over 1000 shots

typical



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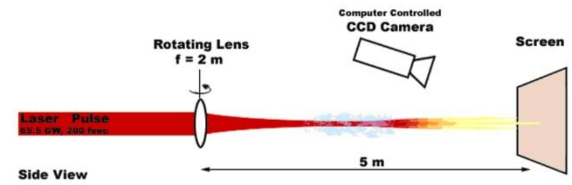
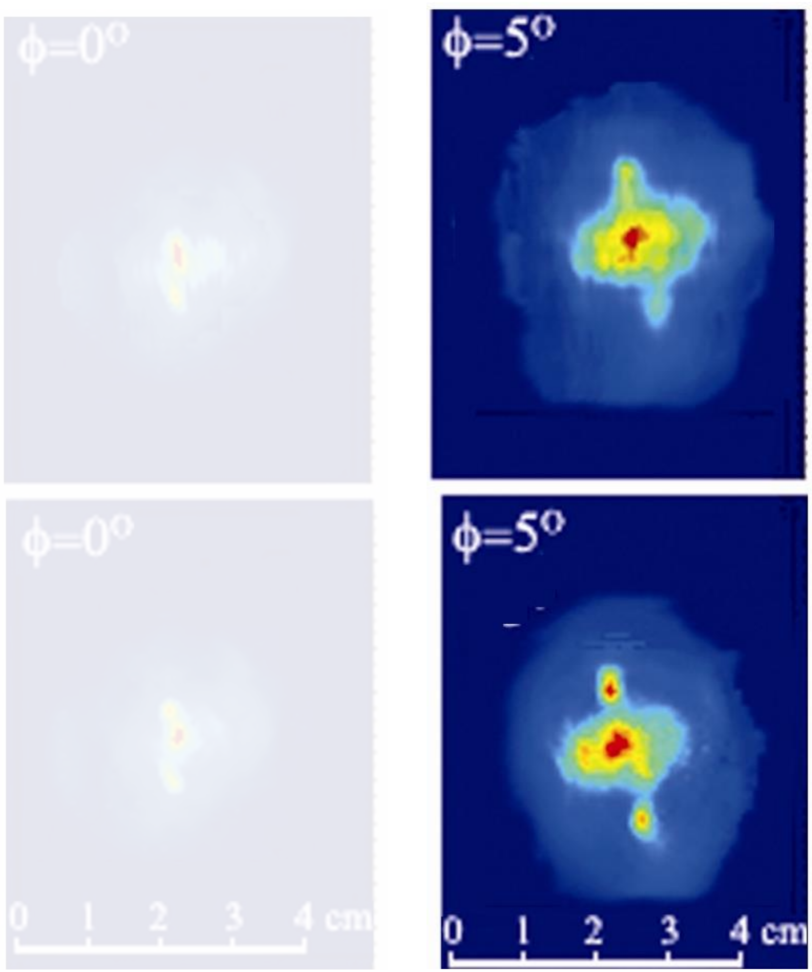


Average over 1000 shots

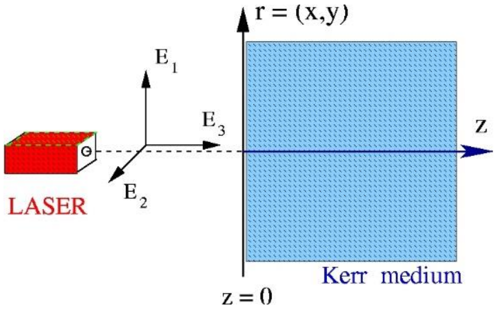
typical



Want to predict

- Average intensity after 5m
- Probability for 0,1,2, or 3 filaments

Mathematical model



initial condition

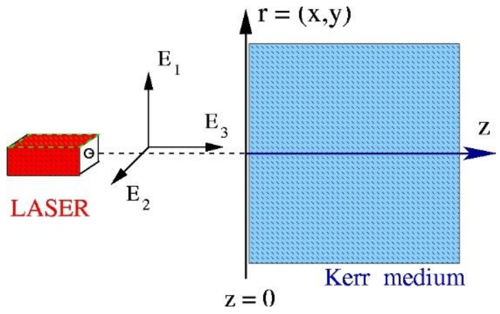
$$\psi_0(x, y)$$

NLS

output

$$\psi(z, x, y)$$

Shot to shot variation



random initial condition

$$\psi_0(x, y; \alpha)$$

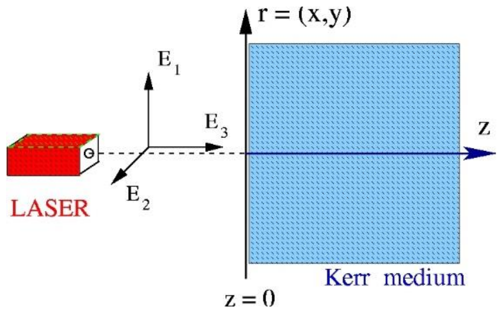
α - noise parameter

NLS

random output

$$\psi(z, x, y; \alpha)$$

Shot to shot variation



random initial condition **NLS** **random output**

$$\psi_0(x, y; \alpha) \Rightarrow \psi(z, x, y; \alpha)$$

α - noise parameter

Computational goals

Moment estimation
e.g., average intensity $\mathbf{E}_\alpha(|\psi|^2)$

Density estimation
e.g., probability for 2 filaments

General setting

Nonlinear initial value problem

$$\begin{cases} u_t(t, \boldsymbol{x}) = Q(\boldsymbol{x}, u)u \\ u(t = 0, \boldsymbol{x}) = u_0(\boldsymbol{x}) \end{cases}$$

- "Quantity of interest" (model output) $f = f[u]$
  - e.g., $f = \arg(u(t_i, x_i))$, $\mathrm{f} = \int |\mathrm{u}|^2 dx, \ldots$
  - $u, f[u]$ not given explicitly, but can be evaluated numerically

General setting with randomness

Add randomness (in u_0 and/or Q)

$$\begin{cases} u_t(t,\boldsymbol{x};\boldsymbol{\alpha}) = Q(\boldsymbol{x},u;\boldsymbol{\alpha})u \\ u(t=0,\boldsymbol{x};\boldsymbol{\alpha}) = u_0(\boldsymbol{x};\boldsymbol{\alpha}) \end{cases}$$

- $\boldsymbol{\alpha}$ distributed according to a known measure
- "Quantity of interest" (model output) $f(\boldsymbol{\alpha}) \coloneqq f[u(t,\boldsymbol{x};\boldsymbol{\alpha})]$
- $f(\boldsymbol{\alpha})$ is a random variable

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Computational goals:

- Moment estimation $\mathbf{E}_{\boldsymbol{\alpha}}[f]$
- Density estimation Probability Density Function (PDF) of $f(\boldsymbol{\alpha})$

Standard statistical methods

Step I – draw samples $\{\alpha_1, \dots, \alpha_N\}$
Step II – compute $\{f_1, \dots, f_N\}$, $f_n := f(\alpha_n)$

Moment estimation

- Monte-Carlo $\mathbf{E}_\alpha[f] \approx \frac{1}{N}\sum_{n=1}^{N} f_n$
- …

Density (PDF) estimation

- Histogram method
- Kernel density estimators (KDE)
- …

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Constraint:

- Computation of $f(\boldsymbol{\alpha_j})$ is expensive (e.g., solving the (3+1)D NLS)
  - Can only use a small samples $\{f(\alpha_1), \dots, f(\alpha_N)\}$

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  - Poor approximations for small N

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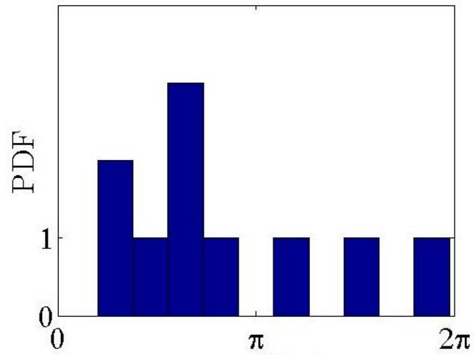
e.g. Histogram method with N=10 samples



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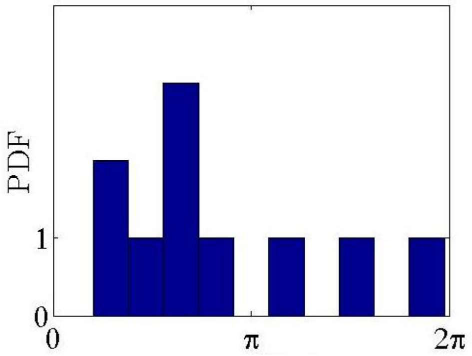
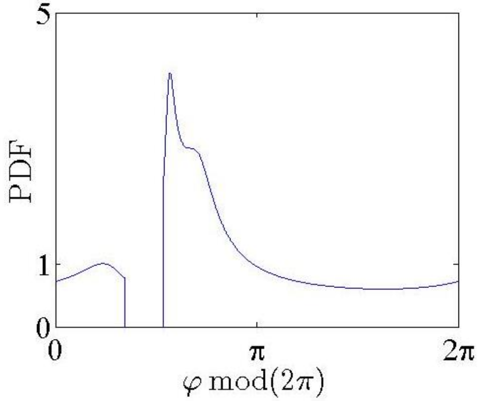


Exact PDF



Standard statistical methods

Given a sample $\{f_1, \ldots, f_N\}$ of $f(\alpha)$

Moment estimation

- Monte-Carlo $\mathbf{E}_{\alpha}[f] \approx \frac{1}{N}\sum_{n=1}^{N} f_n$
- …

Density (PDF) estimation

- Histogram method
- Kernel density estimators (KDE)
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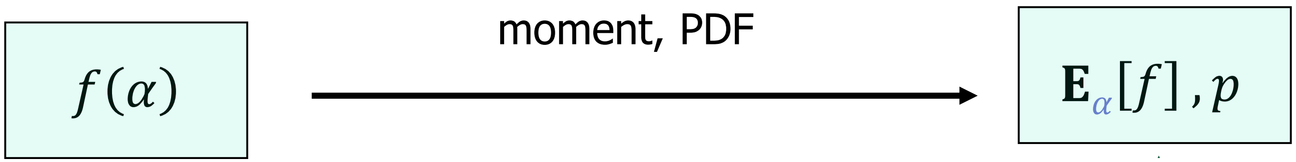
How to improve?

- Above methods only use $\{f_1, \ldots, f_N\}$
- **Uncertainty Quantification** (UQ) approach: Utilize
  1. The relation $f(\alpha)$
  2. Smoothness of $f(\alpha)$

Approximation-based estimation

- p is the PDF of f



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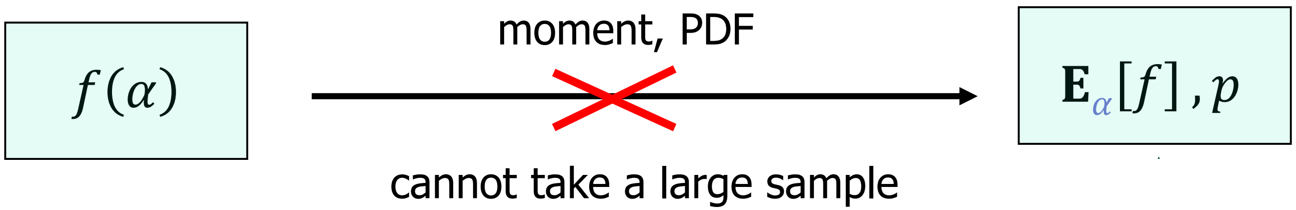

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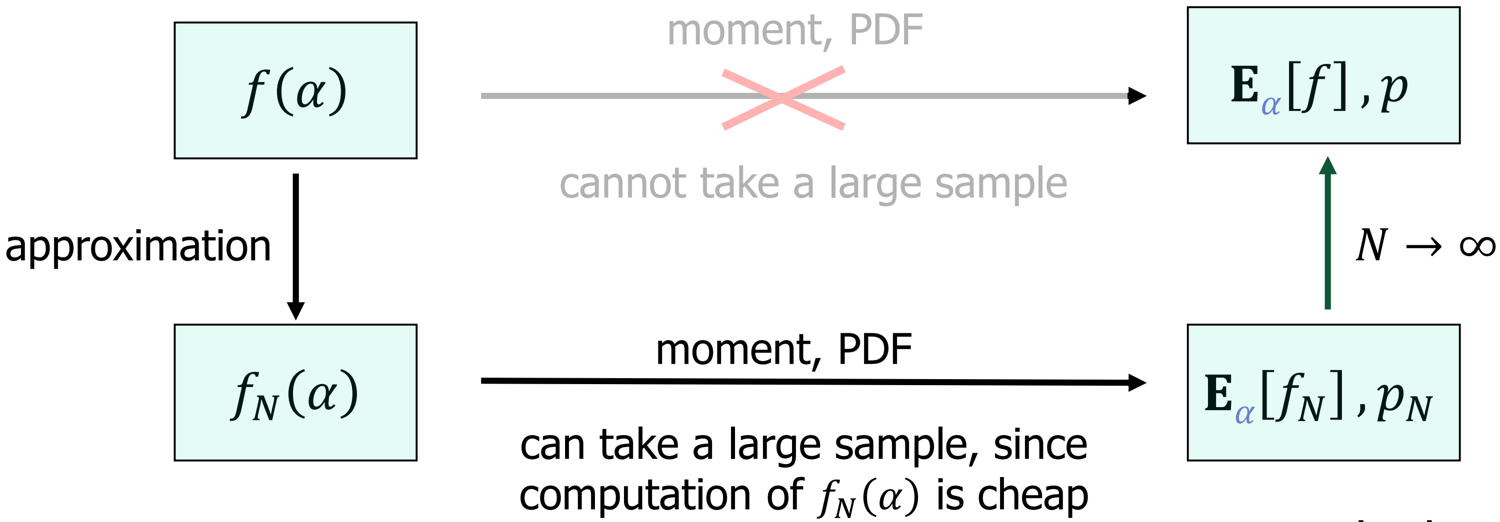

- p_N is the PDF of f_N

Questions

- Which approximation should be used?
- How small are $\mathrm{E}_\alpha[f] - \mathrm{E}_\alpha[f_N]$ and $||p - p_N||$?

Noise dimension

- **One-dimensional** noise $\alpha \in R$
  - Random input power $\psi_0 = (1 + \alpha)e^{-r^2}$
  - Random temperature
  - …
- **Multi-dimensional** noise $\alpha \in R^d$
  - Random input power and incidence angle
  - …

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Generalized Polynomial Chaos (gPC)

Standard uncertainty quantification approach:

- Approximate f using orthogonal polynomials $\{q_n(\alpha)\}$

$$f_N(\alpha) = \sum_{n=0}^{N-1} \langle q_n\,, f\rangle\, q_n(\alpha)$$

- Spectral accuracy for moments

$$\mathbf{E}_\alpha[f] - \mathbf{E}_\alpha[f_N] = O(e^{-\gamma N}), \qquad N \gg 1 \quad \text{if f is analytic}$$

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- Problem solved

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- ~~Problem solved~~

But,

<u>Moment estimation</u>
Spectral accuracy reached only for large N

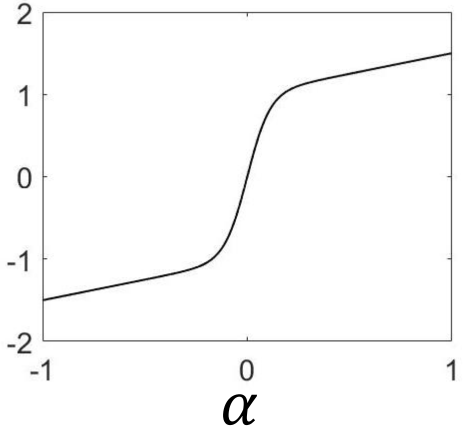
How to achieve ``good'' accuracy with e.g. $N = 10$ samples?

<u>Density estimation</u>
No theory for $\|p - p_N\|$

Will it work in practice?

Example: Density estimation with gPC

$f = \tanh(9\alpha) + \frac{\alpha}{2}, \quad \alpha \sim \text{Uniform}\,[-1, 1]$



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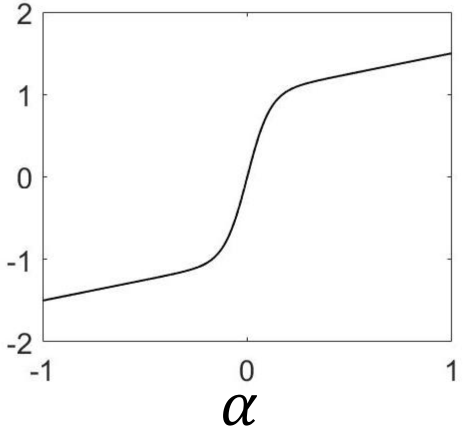
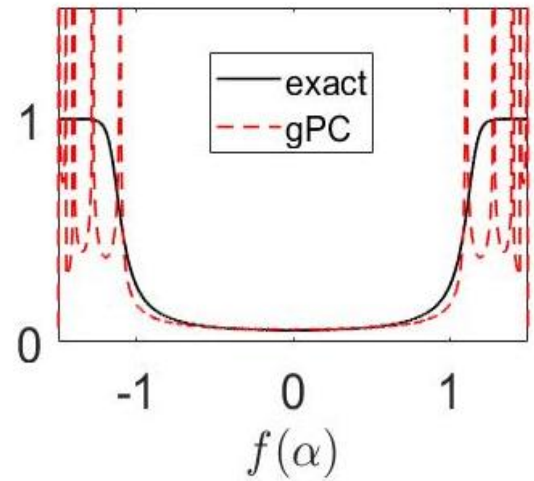


PDF approximation, $N = 12$



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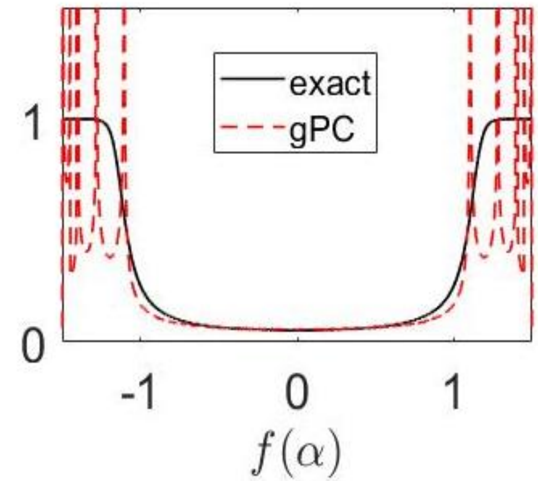

Lemma

$$p(y) = \sum_{f(\alpha)=y} \frac{1}{|f'(\alpha)|}$$

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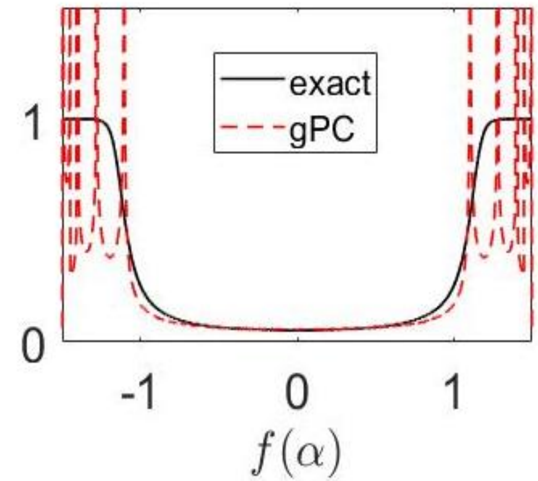

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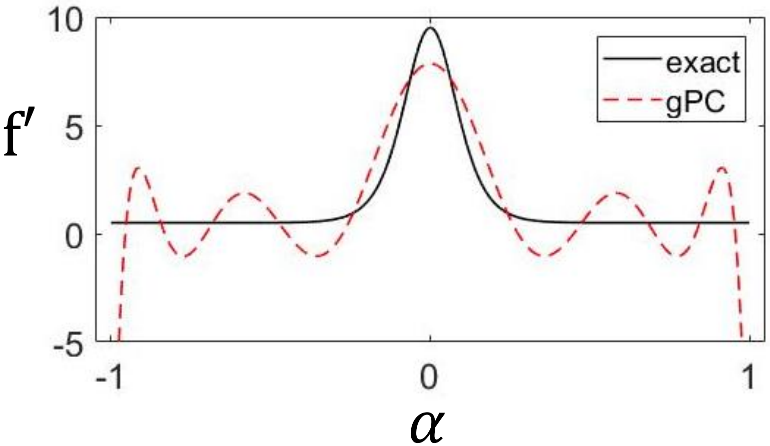

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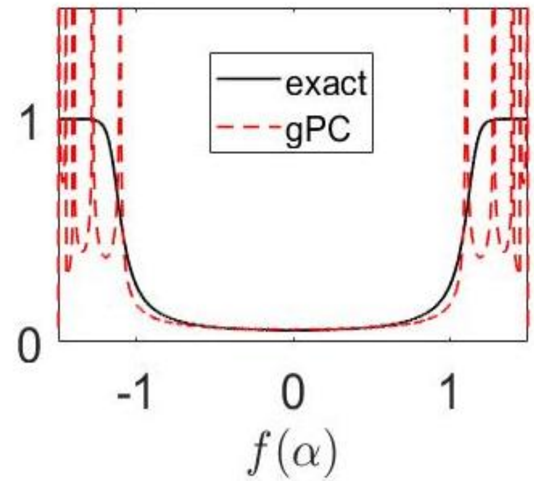

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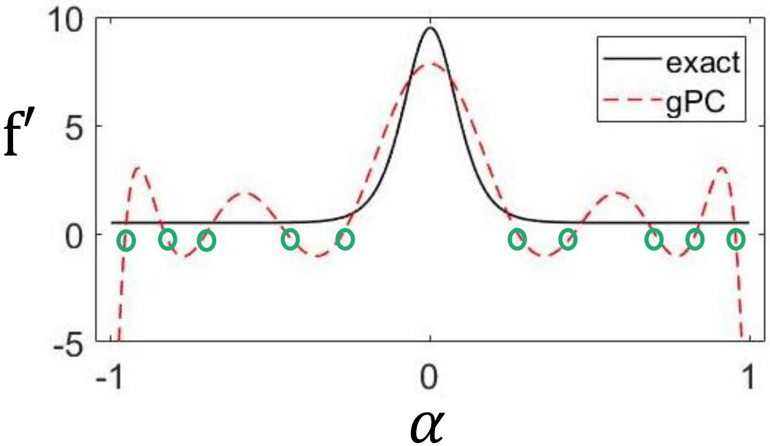

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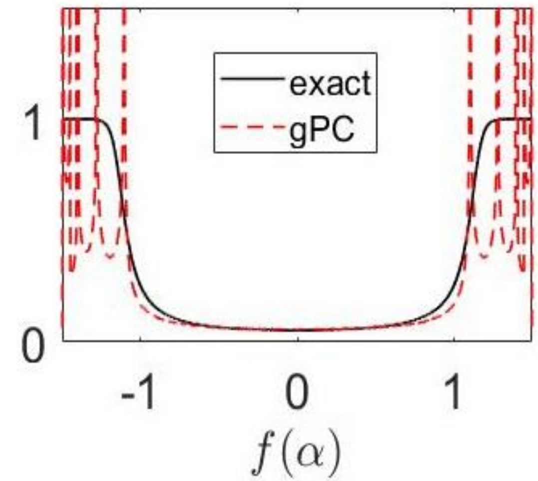

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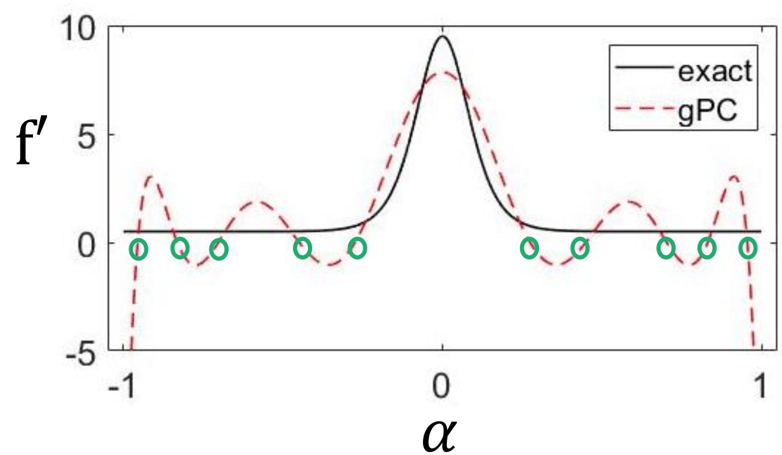
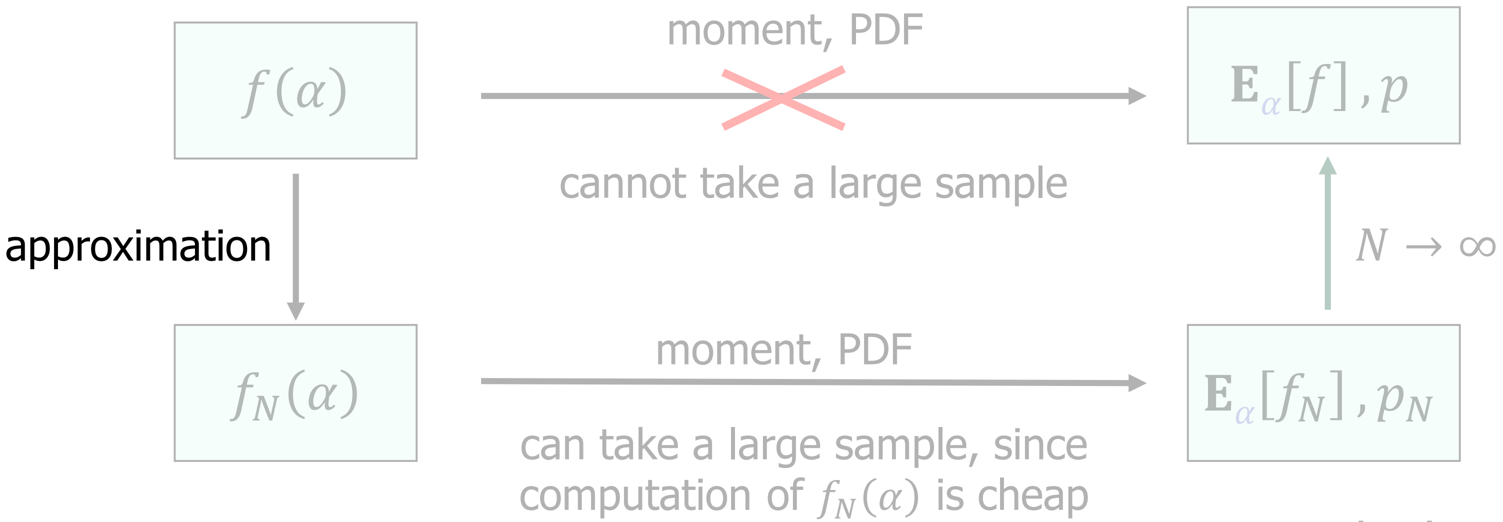


Conclusion
Although gPC is spectrally accurate in L^2, it produces "artificial" zero derivatives which ``contaminate" the PDF

Approximation-based estimation

- p is the PDF of f



- p_N is the PDF of f_N

Question: Which approximation should be used?

Answer

- For density approximation, require that $f_N' = 0 \;\Leftrightarrow\; f' = 0$
- "Monotonicity-preserving" approximation

Adopt a spline-based approach

Ditkowski, Fibich, Sagiv, 18: Approximate *f* using a cubic spline over N grid points

Thm (Ditkowski, Fibich, Sagiv, 18) : Let p and p_N denote the PDFs of $f(\alpha)$ and its cubic spline interpolant over N points. Then

$$\|p - p_N\|_1 \leq CN^{-3}, \qquad C = O(1)$$

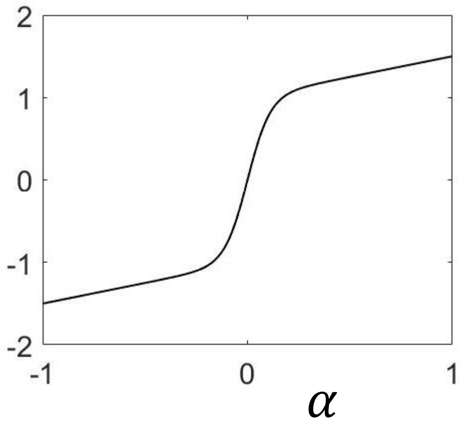
- No equivalent thm for gPC

Thm: $\mathbf{E}_\alpha[f] - \mathbf{E}_\alpha[f_N] \leq CN^{-4}, \quad C = O(1)$

- Worse than gPC for large *N*
- But, usually better than gPC for small *N*

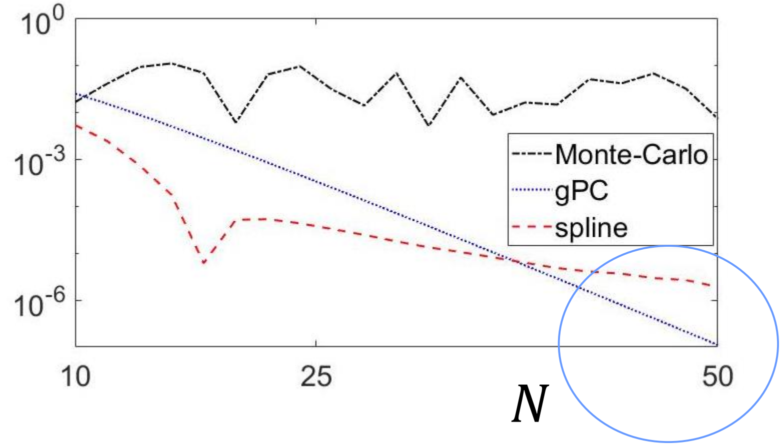
Example – moment estimation

$f = \tanh(9\alpha) + \frac{\alpha}{2}, \quad \alpha \sim \text{Uniform}\,[-1, 1]$



Moment estimation

$\sigma(f) - \sigma(f_N)$



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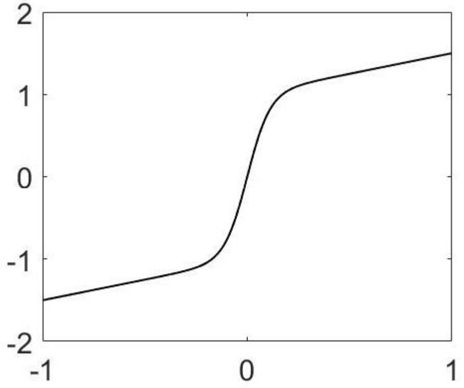

α

Moment estimation

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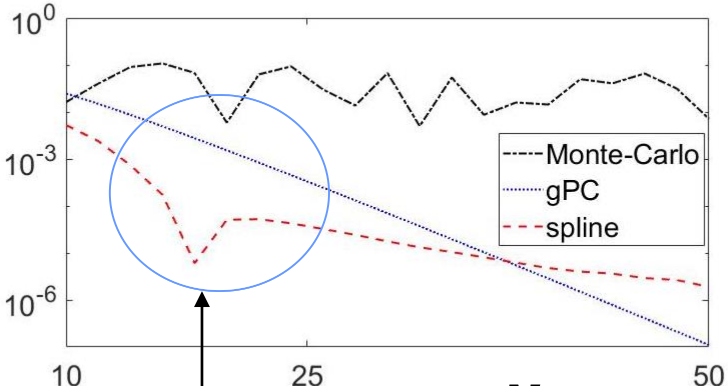

N

Spline better than gPC for small *N*

PDF estimation

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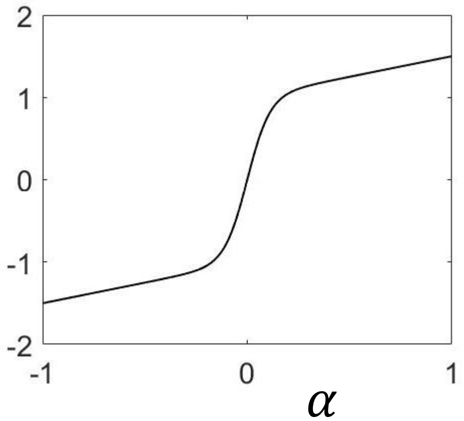
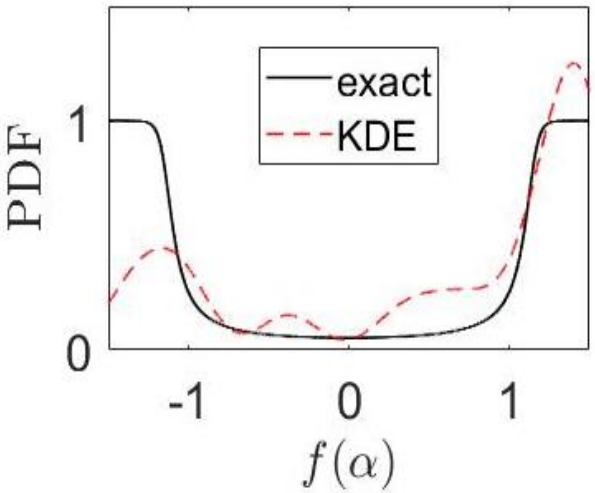
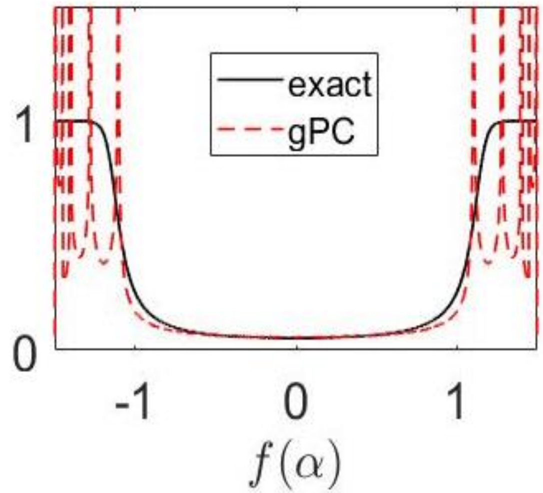


PDF approximation, $N = 12$

Statistically optimal





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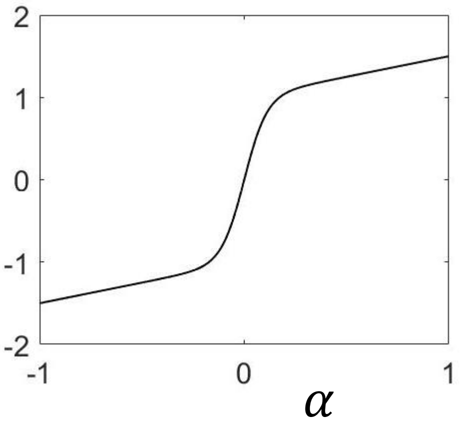

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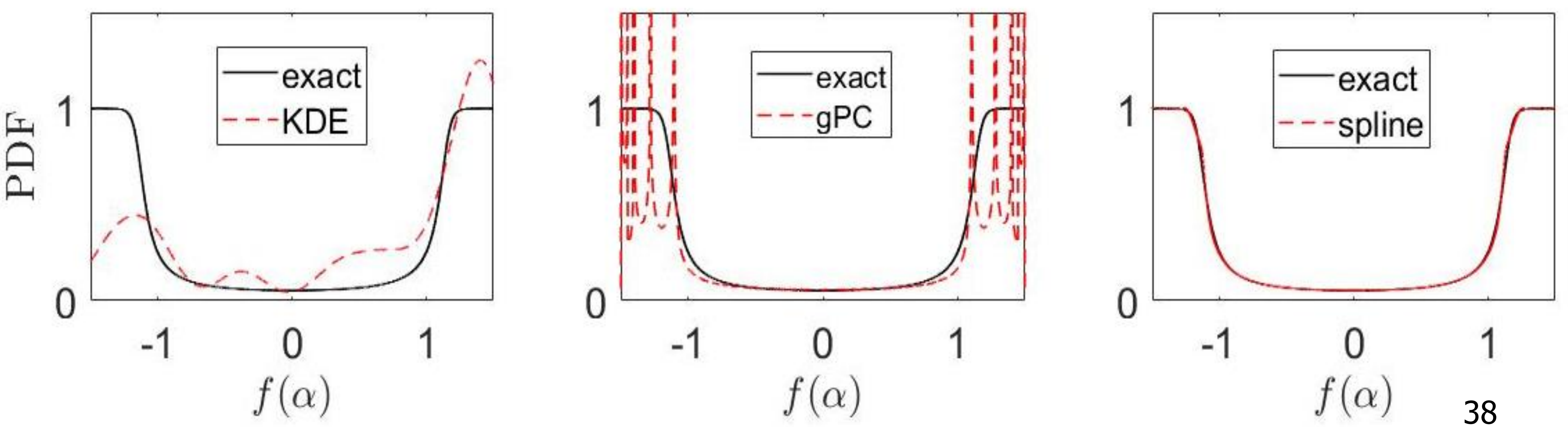
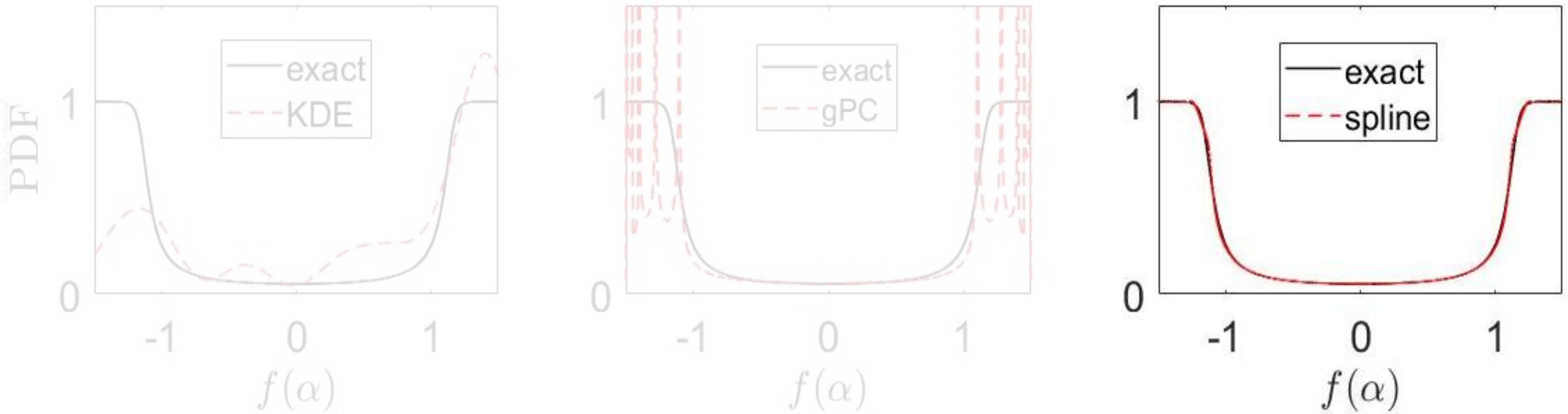
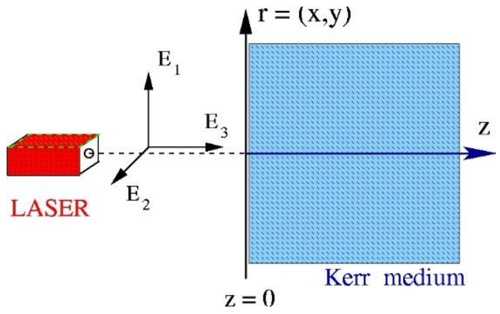


Matlab code for PDF estimation

```
alpha_min = −1; alpha_max = 1 ; N = 18;
f = @(x) tanh (9∗x) + x/2;
samplingGrid = linspace(alpha_min, alpha_max, N) ;
sample_s = f (samplingGrid); M = 2e6 ;
denseGrid = linspace (alpha_min, alpha_max ,M) ;
fNspline = spline ( samplingG rid, samples, denseGrid)
Cf = 1 . 6 9 ; L =Cf∗Mˆ (1/3 ) ;
[histogram, binsEdges ] = hist( fNspline ,L) ;
binWidth = (max( binsEdges)−min (binsEdges)) /L;
pdf = histogram / (sum(histogram) ∗binWidth ) ;
plot(binsEdges, pdf )
```



Shot to shot variation



random initial condition **NLS** **random output**

$$\psi_0(x, y; \alpha) \quad \Rightarrow \quad \psi(z, x, y; \alpha)$$

α - noise parameter

Loss of Phase Lemma (Sagiv, Ditkowski, Fibich, 2017)

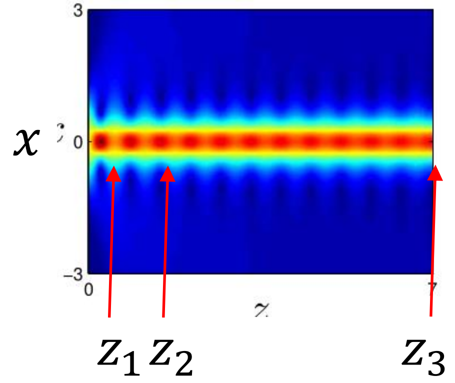
Let $f(z; \alpha) \coloneqq \arg \psi(z, x = 0, y = 0; \alpha) mod(2\pi)$. Then

$$\lim_{z\to\infty} f(z; \alpha) \sim U(0,2\pi)$$

Example: PDF of on-axis phase

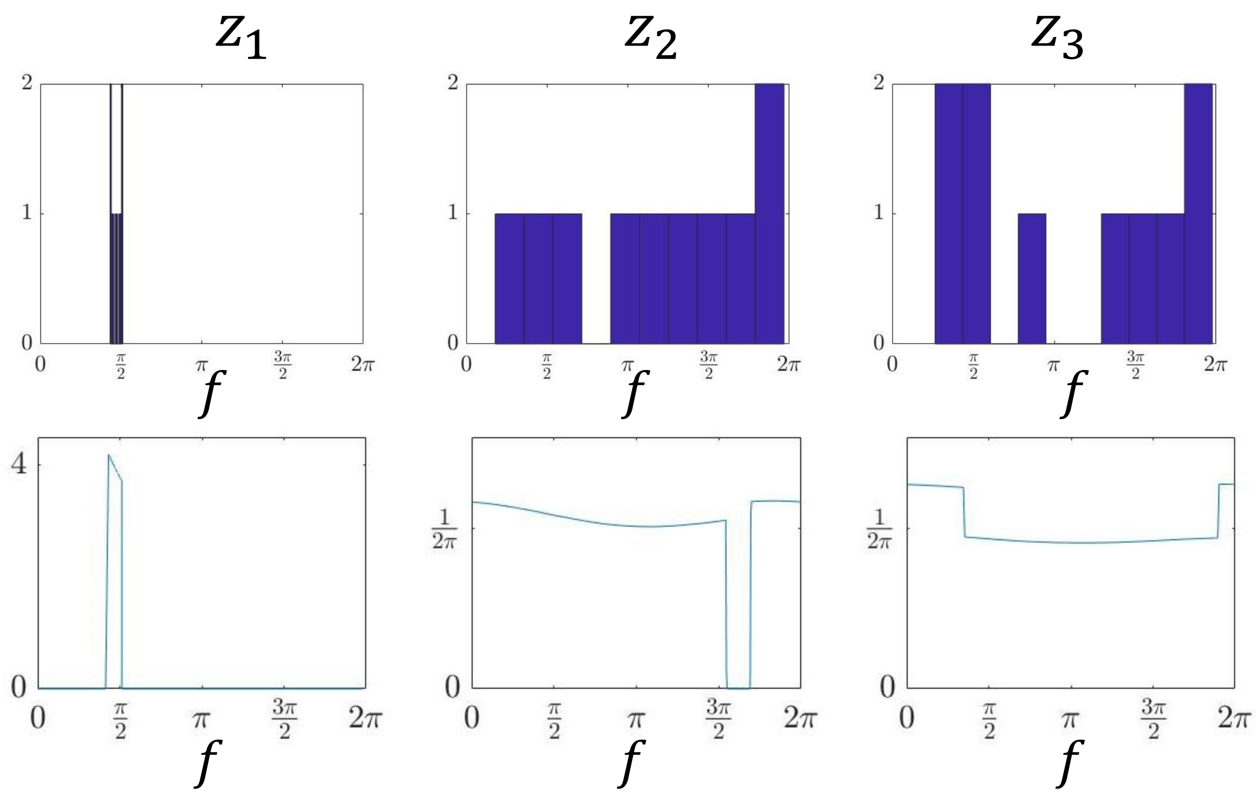
$$f(\alpha) = \arg\big(\psi(z,0;\alpha)\big) \bmod 2\pi$$

Use N=10 NLS simulations



Histogram PDF

Spline PDF



Coupled NLS – loss of polarization angle

$$i\frac{\partial}{\partial t}A_{\pm}(t,x)+\frac{\partial^2}{\partial x^2}A_{\pm}+\frac{2}{3}\left(|A_{\pm}|^2+2|A_{\mp}|^2\right)A_{\pm}=0$$

Patwardhan et al., 2018

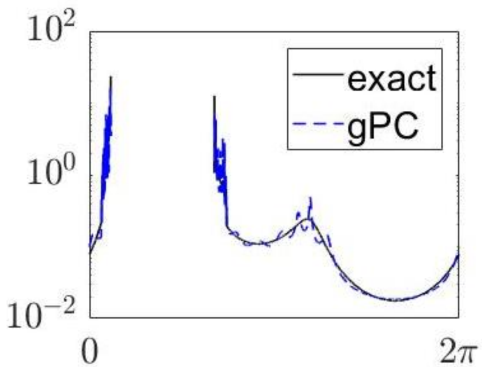
phase: $\varphi_{\pm}(t)=\arg\left(A_{\pm}(t,x=0)\right)\ mod\ (2\pi)$

polarization $\theta(t)=\varphi_{+}(t)-\varphi_{-}(t)$

Random elliptical beam –

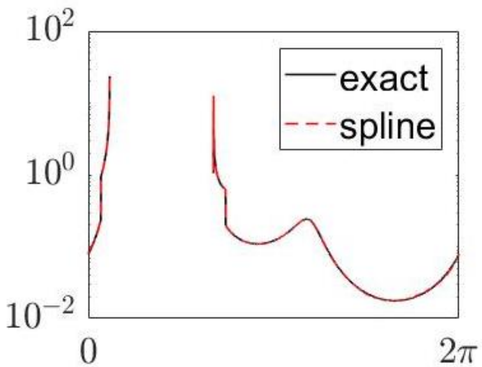
$$A_{\pm}(t=0)=(1+\alpha)C_{\pm}e^{-x^2},\qquad \alpha\sim U(-0.1,0.1)$$

PDF, N=64



θ

PDF, N=64



θ

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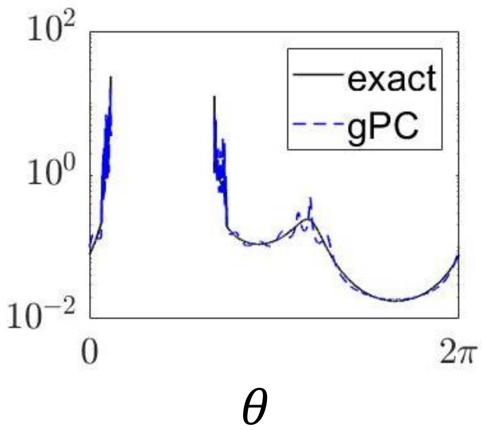
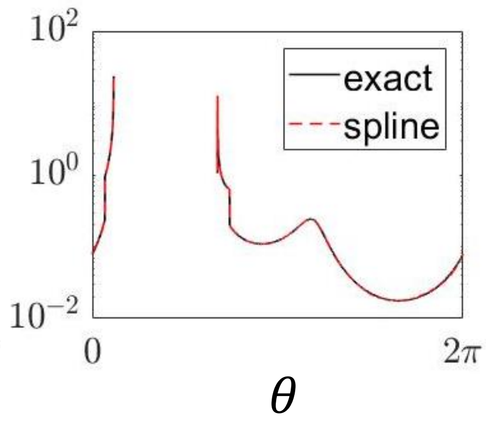
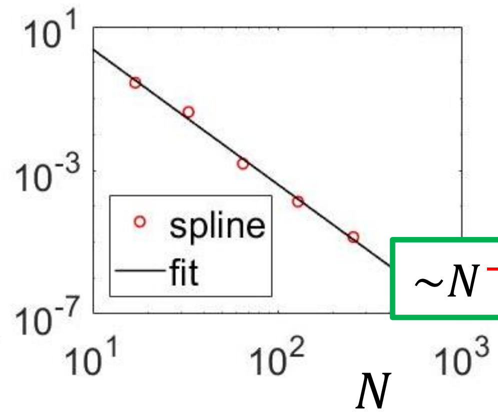


PDF, N=64



$\|p-p_N\|_1$



$\sim N^{-3.7}$

$(theory:\ N^{-3})$

Burgers equation – shock location

$$u_t(t,x) + \frac{1}{2}\left(u^2\right)_x = \frac{1}{2}\left(sin\,(x)\right)_x$$

Chen, Gottlieb, Hesthaven, JCP 2005

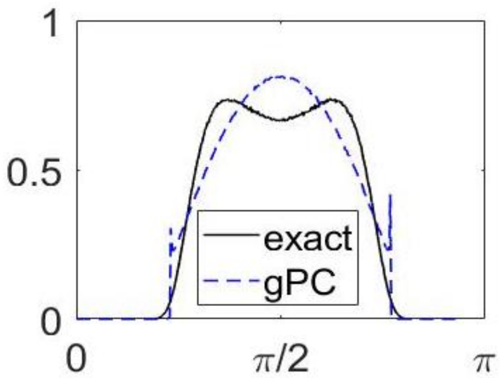
Initial condition: $u_0(x) = \alpha \sin(x)$

Shock location at $t \to \infty$ $\alpha = -cos(X_s)$

Distribution of random initial amplitude –

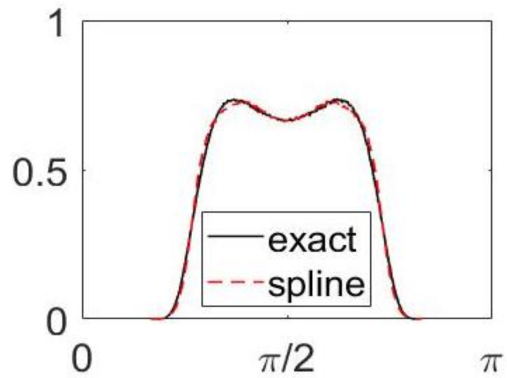
$$\alpha(\nu) = \begin{cases} \frac{-1+\sqrt{1+4\nu^2}}{2\nu} & \nu \neq 0 \\ 0 & \nu = 0 \end{cases} \qquad \nu \sim N(0,\sigma)$$

PDF, N=7



X_s

PDF, N=7



X_s

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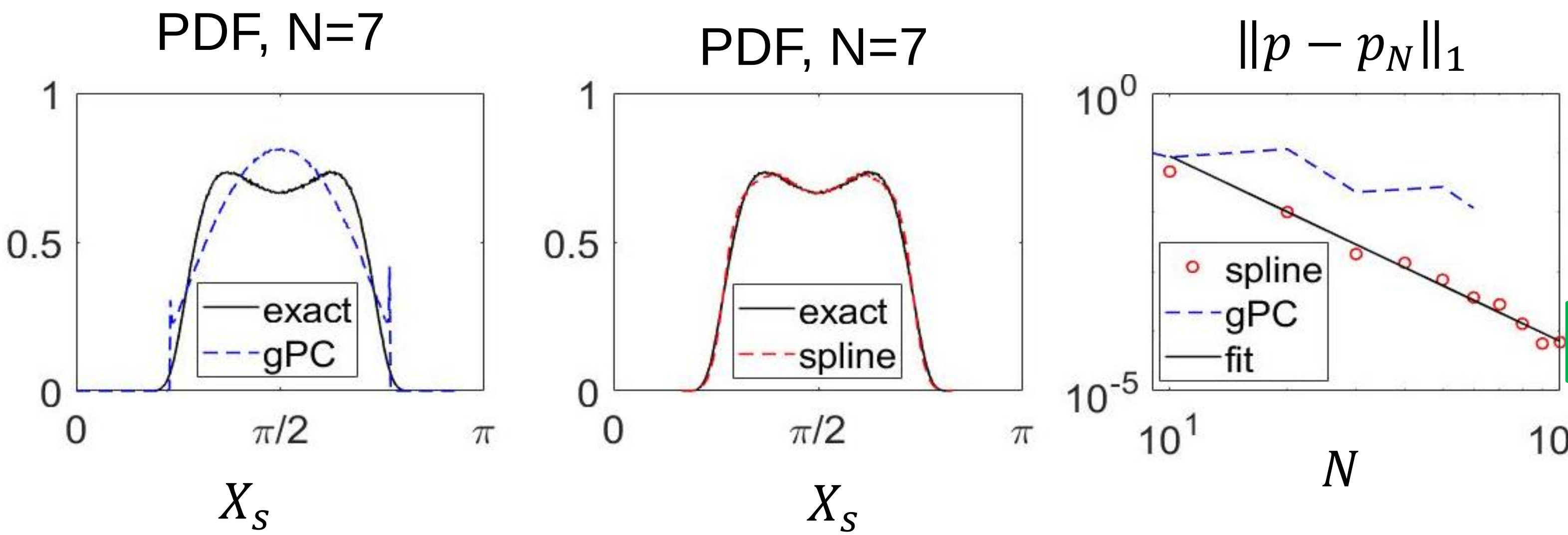


$\sim N^{-3.1}$

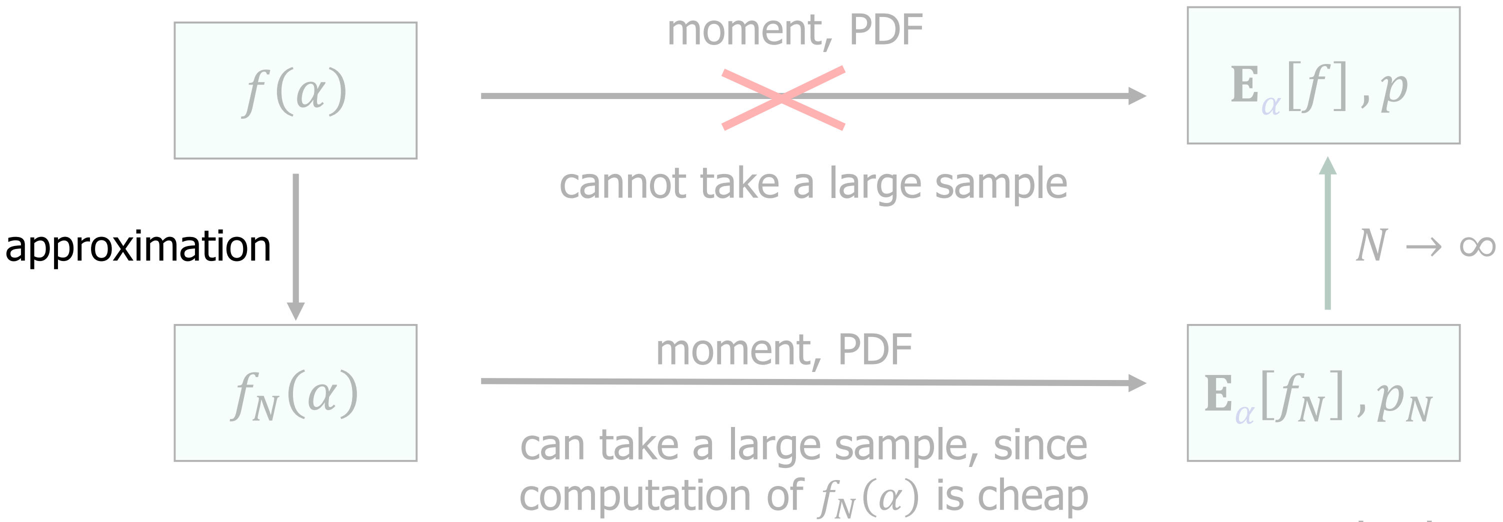
$(theory: N^{-3})$

Noise dimension

- **One-dimensional** noise $\alpha \in R$
  - Random input power $\psi_0 = (1 + \alpha)e^{-r^2}$
  - Random temperature
  - …
- **Multi-dimensional** noise $\alpha \in R^d$
  - Random input power and incidence angle
  - …

Approximation-based estimation

- p is the PDF of f



- p_N is the PDF of f_N

Questions

- Which approximation should be used?
- How small are $\mathrm{E}_{\alpha}[f] - \mathrm{E}_{\alpha}[f_N]$ and $||p - p_N||$?

Tensor product spline

Ditkowski, Fibich, Sagiv, 18: If α is **d-dimensional,** approximate f with a tensor product cubic spline over N grid points

Lemma

$$p(y) = \frac{1}{\mu(\Omega)} \int_{f^{-1}(y)} \frac{1}{|\nabla f|} d\sigma$$

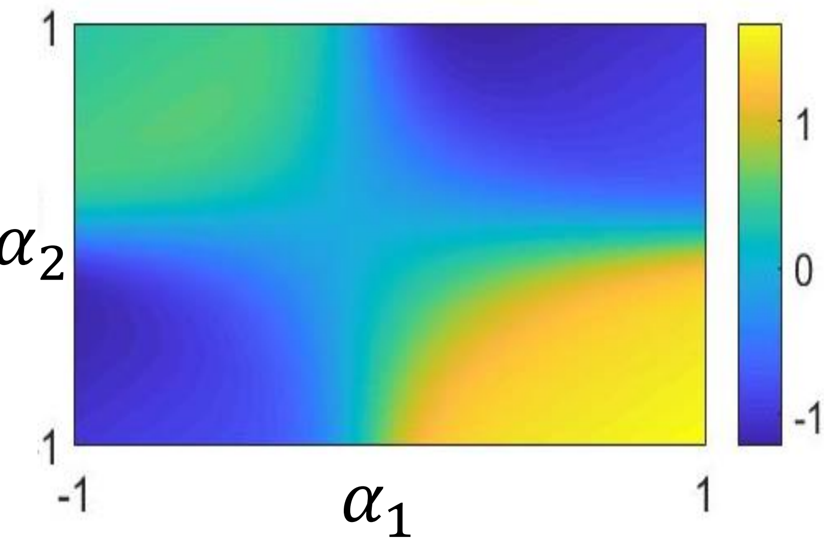
Thm (Ditkowski, Fibich, Sagiv, 18): $\|p - p_N\|_1 = O(N^{-3/\boldsymbol{d}})$

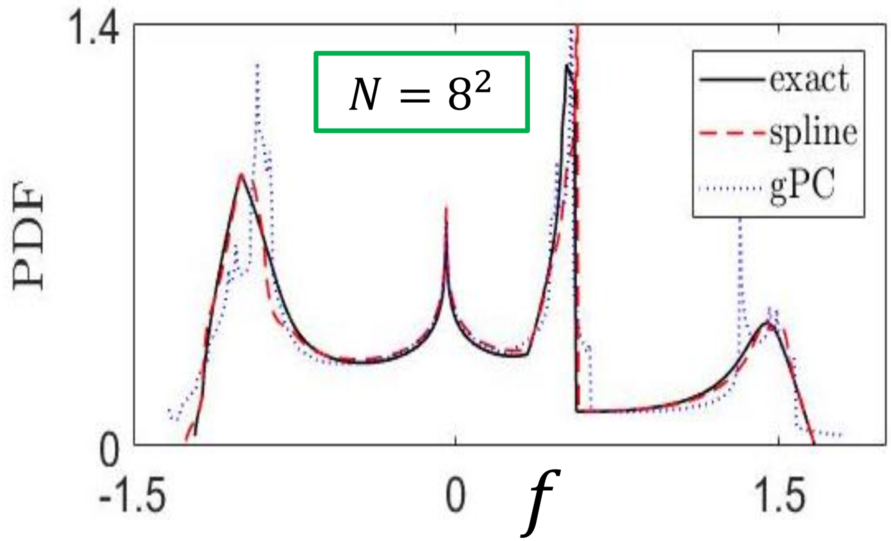
- Optimal statistical method (KDE) converges as $N^{-2/5}$
  - Hence, our method is faster for d $\leq$ 7
- For higher dimensions, can use m^{th}-order splines:

Thm (Ditkowski, Fibich, Sagiv, 18): $\|p - p_N\|_1 = O(N^{-m/\boldsymbol{d}})$

2D example

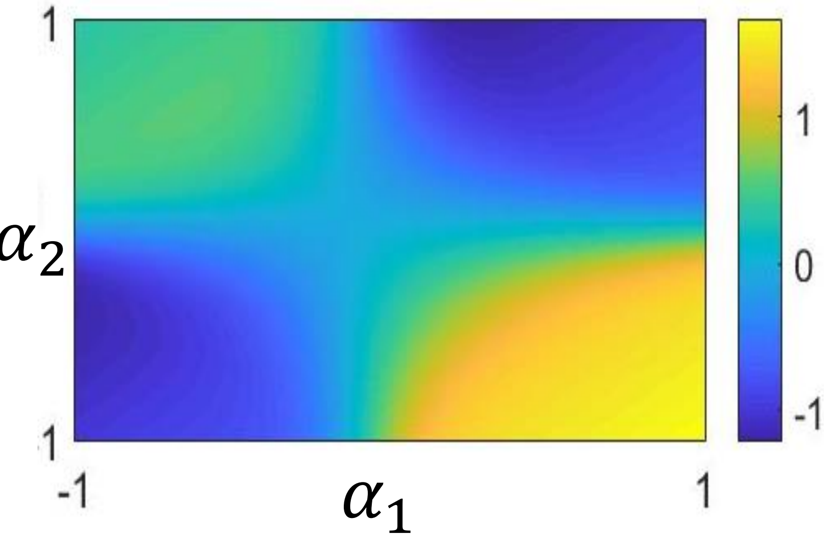
$$f(\alpha_1, \alpha_2) = \tanh\left(6\alpha_1\alpha_2 + \frac{\alpha_1}{2}\right) + \frac{\alpha_1 + \alpha_2}{2}, \qquad \alpha_1, \alpha_2 \sim \text{Uni}(-1,1), \qquad i.i.d.$$

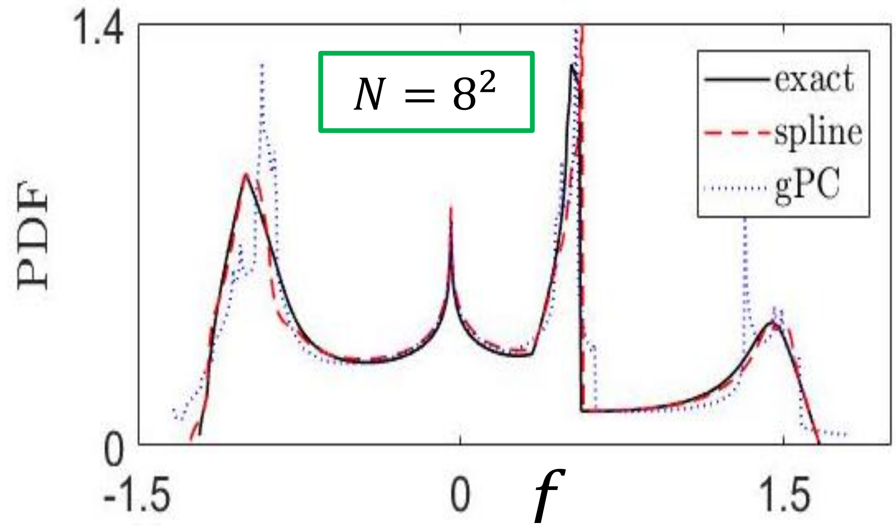


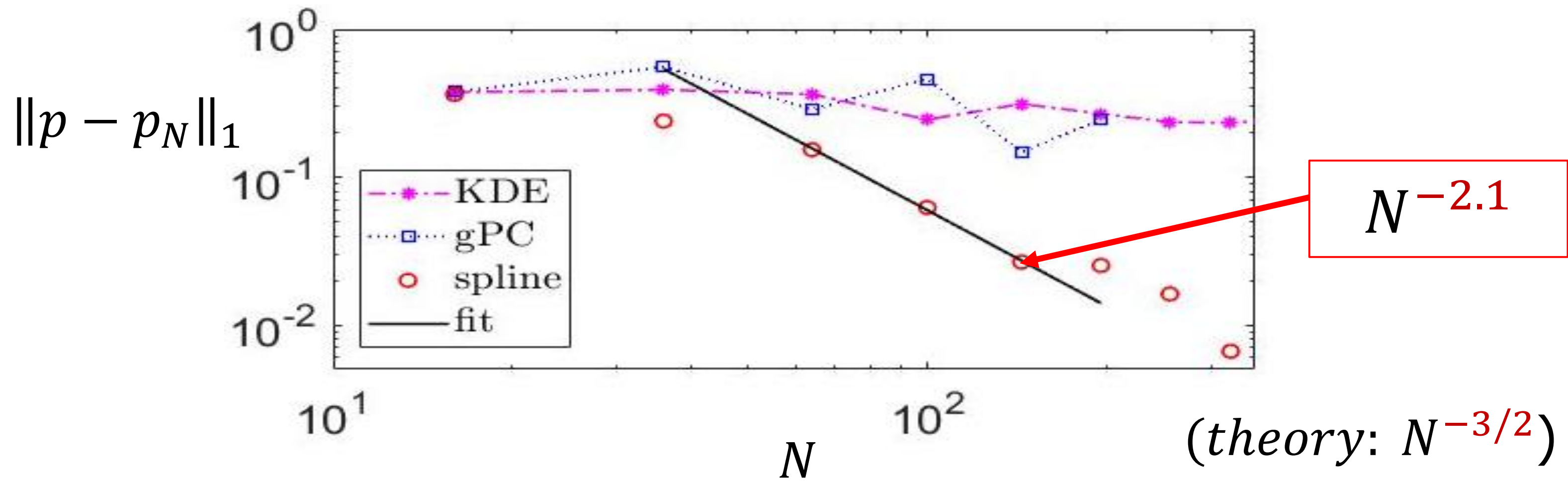


2-dimensional example

$$f(\alpha_1,\alpha_2) = \tanh\left(6\alpha_1\alpha_2 + \frac{\alpha_1}{2}\right) + \frac{\alpha_1+\alpha_2}{2}, \qquad \alpha_1,\alpha_2 \sim \text{Uni}(-1,1), \qquad i.i.d.$$







Matlab code for 2D PDF estimation

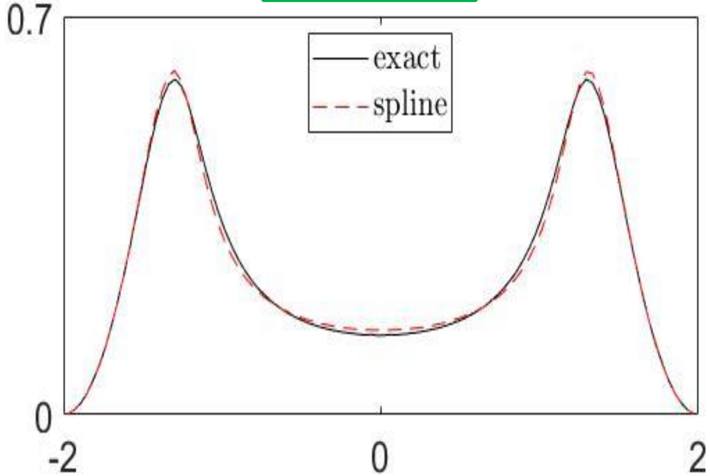
```
func = @(x,y) atan(1.3*y.^2 - .4*x.*y+1.1*x.^2)+(x+y)
MCpointsPerBlock = 2e3; MCsqrtNumBlock = 10; binsNum = 750; N=10;
[xs,ys] = ndgrid(linspace(xmin,xmax,N),linspace(xmin,xmax,N));
[pdf_spline,y_spline] = pdfSampleSquare(@(t,v) interpn(xs,ys,func(xs,ys),t,v,'cubic'),...
                                        MCsqrtNumBlock,MCpointsPerBlock,binsNum);
function [pdf,binsEdges] = pdfSampleSquare(func,sqrtNumBlocks,sqrtSamplesBlock, numBins)
xmin =-1; xmax = 1;  smallGridSize = 3e6; blockLength = (xmax-xmin)/sqrtNumBlocks; nsmall =1e3;
[x_calibrate,y_calibrate] = ndgrid(linspace(xmin,xmax,1e3),linspace(xmin,xmax,1e3));
[~,binsEdges] = hist(func(x_calibrate,y_calibrate),numBins);
binWidth = (max(binsEdges)-min(binsEdges))/numBins;
histogram = zeros(1,numBins);
for k=1:sqrtNumBlocks
        for m=1:sqrtNumBlocks
        [xg,yg] = ndgrid(linspace(xmin+(k-1)*blockLength,xmin+(k)*blockLength, sqrtSamplesBlock),...
                                      linspace(xmin+(m-1)*blockLength,xmin+(m)*blockLength,sqrtSamplesBlock));
        funcBlock =func(xg,yg);
        [hist_temp] = hist(funcBlock(:),binsEdges);
        histogram = histogram+hist_temp;
    end
end
pdf = histogram/(sum(histogram)*binWidth);
```

3 dimensional example

$$f(\alpha_1, \alpha_2, \alpha_3) = \tanh(2\alpha_1 + 3\alpha_2 + 3\alpha_3) + \frac{\alpha_1 + \alpha_2 + \alpha_3}{3},$$
$$\alpha_1, \alpha_2, \alpha_3 \sim \text{Uni}(-1,1), \qquad i.i.d.$$

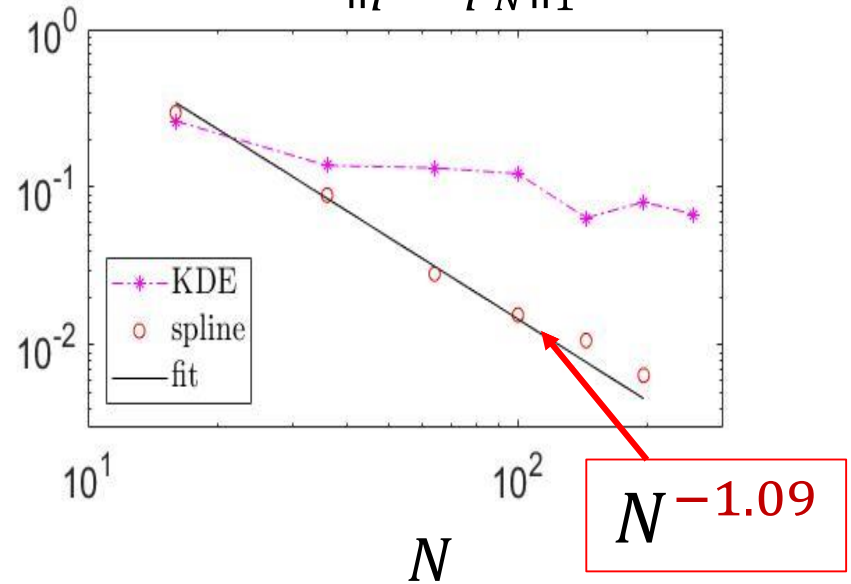
$N = 8^3$

PDF



f

$\|p - p_N\|_1$



N

$(theory: N^{-1})$

Conclusions

- New method for computing PDF and moments of nl PDEs with randomness
  - Outperforms standard statistical methods and gPC
  - Guaranteed to converge for PDF approximation
  - Non-intrusive: can use any deterministic numerical solver
  - Achieves good accuracy using small samples
  - Extends to multi-dimensional noise
  - Can also handle non-smooth ``*quantity of interest*''

References

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A spline-based approach to uncertainty quantification and density estimation
ArXiv 1803.10991

A. Sagiv, A. Ditkowski, G. Fibich
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