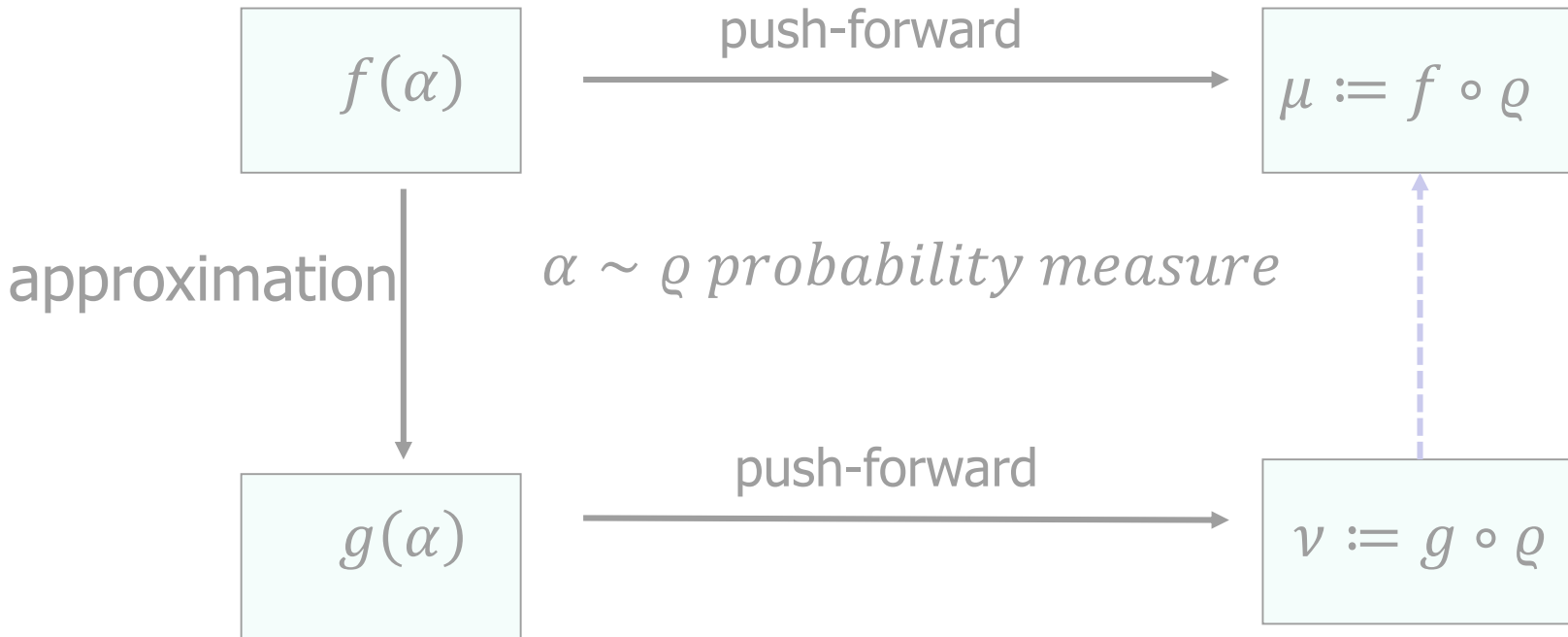


# An Optimal Transport Perspective on Uncertainty Quantification



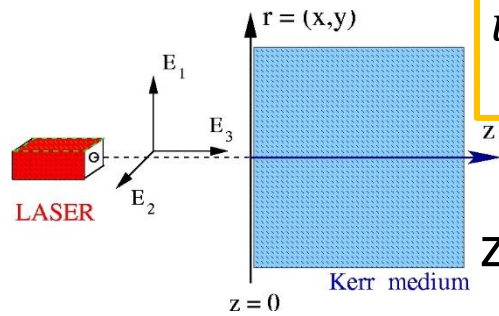
Amir Sagiv  
Columbia University

# Two motivation slides:

nonlinear laser propagation

$$i\psi_z(z, x, y) + \Delta\psi + |\psi|^2\psi - \epsilon|\psi|^4\psi = 0$$

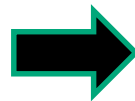
Nonlinear Schrodinger equation



**initial condition**

$$\psi_0(x, y)$$

**PDE model**



**output**

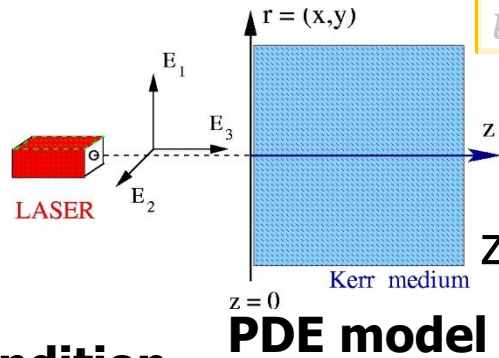
$$\psi(z, x, y)$$

# Two motivation slides:

nonlinear laser propagation

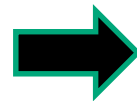
$$i\psi_z(z, x, y) + \Delta\psi + |\psi|^2\psi - \epsilon|\psi|^4\psi = 0$$

Each laser shot  
is different



random initial condition

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



random output

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

$\alpha$  - noise parameter

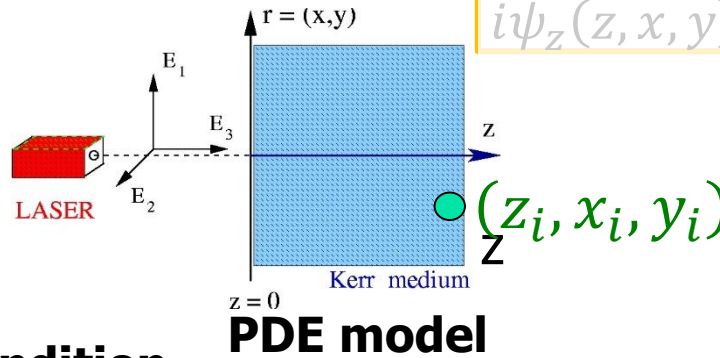
[Sagiv, Ditzkoski, Fibich, Opt. Exp. 2017]

# Two motivation slides:

nonlinear laser propagation

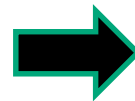
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What kind of statistics do we want to compute?

Moment estimation

e.g.,  $E(|\psi(z_i, x_i, y_i)|^2)$ ,  
over many realizations  
(repetitions)

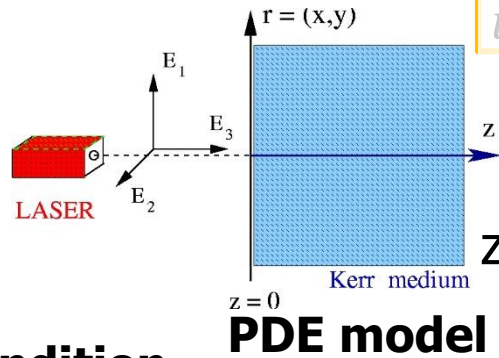
[e.g., Fibich, Eisenman, Ilan, Zigler, Opt. Lett.  
2005]

# Two motivation slides:

nonlinear laser propagation

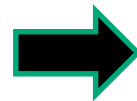
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**Moment estimation**

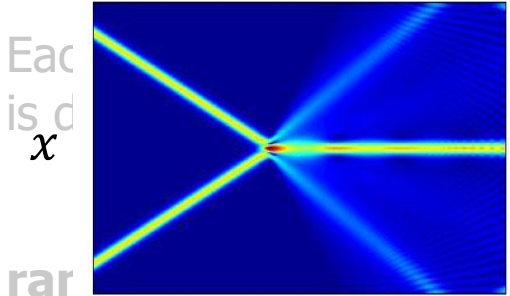
e.g.,  $E(|\psi(z_i, x_i, y_i)|^2)$ ,  
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**Density estimation**

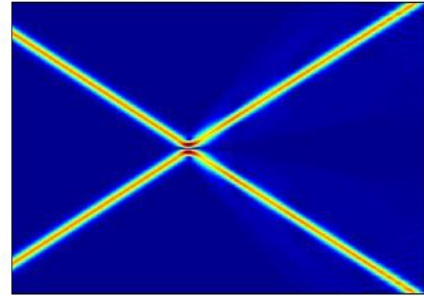
Probability Density Function  
(PDF) of some “quantity of  
interest”  $f(\psi)$

# Why study the PDF – Examples from optics

Beam fusion



Beam repulsion



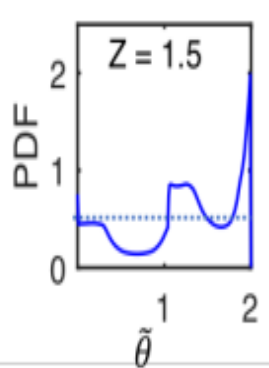
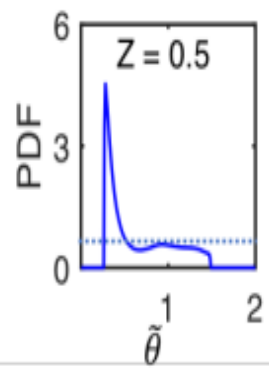
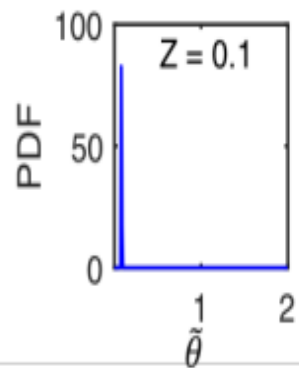
**Example I:** over many repetitions, what are the chances of fusion vs. repulsion?

$$\psi_0 = R_{\kappa_1}(x + d)e^{i\theta x} + (1 + 0.1\alpha)R_{\kappa_1}(x - d)e^{-i\theta x}$$

$\alpha$  - noise parameter

Random amplitude

[Sagiv, Ditwkoski, Fibich, Opt. Exp. 2017]



**Example II:** Distribution of *polarization* as a function of propagation distance

[w Patwardhan et al, PRA 2019]

# General standard nonlinear PDE settings

Initial value problem

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

- “quantity of interest” (model output)  $f(u(t, \mathbf{x}))$ 
  - e.g.,  $f = u(t_i, x_i)$ ,  $f = \int dx |u|^2, \dots$
  - $u$  &  $f(u)$  are evaluated numerically

# General Settings – Nonlinear PDE with randomness

Initial value problem with randomness (both i.c.  $u_0$  and operator  $Q$ )

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

- $\boldsymbol{\alpha}$  distributed according to a known measure
- “quantity of interest” (model output)  $f(\boldsymbol{\alpha}) := f(u(t, \mathbf{x}; \boldsymbol{\alpha}))$ 
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How to approximate the PDF of  $f(\boldsymbol{\alpha})$ ,  
a random variable, numerically?

# Agenda

- PDF approximation
  - Is moment-estimation sufficient?
  - An algorithm & convergence results
- Transport-theory point of view

# Agenda

- PDF approximation

- Is moment-estimation sufficient?

How does standard UQ methods perform in this task

- An algorithm & convergence results

- Transport-theory point of view

# General Settings – Nonlinear PDE with randomness

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How to approximate the PDF of  $f(\boldsymbol{\alpha})$ ,  
a random variable, numerically?

## Constraints:

- Can only compute  $f(\boldsymbol{\alpha}_j)$  for a given  $\boldsymbol{\alpha}_j$
- Computation of  $f(\boldsymbol{\alpha}_j)$  is expensive (e.g., solving the (3+1)dimensional NLS)
  - Can only use a **small sample**  $\{f(\boldsymbol{\alpha}_1), \dots, f(\boldsymbol{\alpha}_N)\}$

# Standard statistical methods

**Step I** – draw i.i.d. samples  $\alpha_1, \dots, \alpha_N$

**Step II** – compute the samples  $\{f(\alpha_1), \dots, f(\alpha_N)\}$



## 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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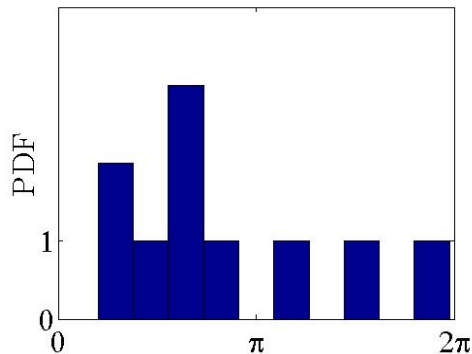
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## Density (PDF) estimation

- Histogram method
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- Poor approximations for small N ( $\frac{1}{\sqrt{N}}$  error)  
e.g. **Histogram method** with N=10 samples



# Standard statistical methods

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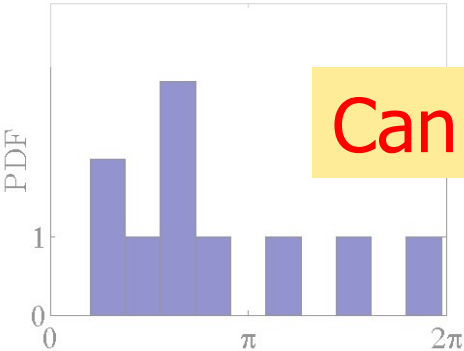
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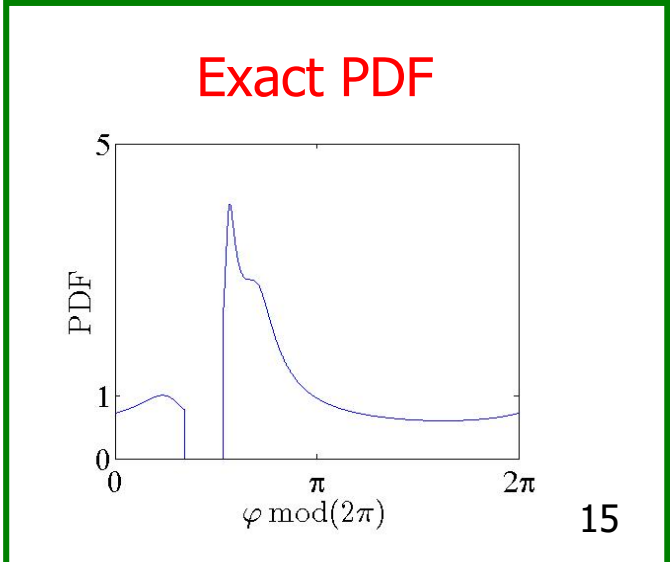
## Density (PDF) estimation

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e.g. Histogram method with **N=10 samples**



Can we improve?



# Standard statistical methods

**Step I** – draw i.i.d. samples  $\alpha_1, \dots, \alpha_N$

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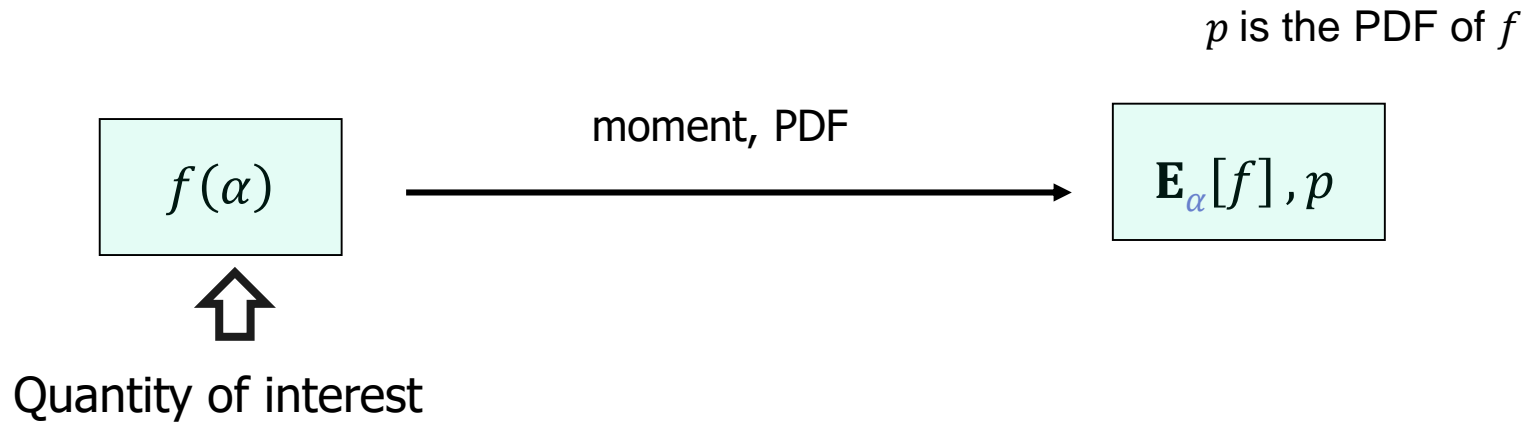
## Can we improve?

- Methods above only use  $\{f(\alpha_1), \dots, f(\alpha_N)\}$ .
- We can also use
  1. The relation  $f(\alpha) \leftrightarrow \alpha$
  2. Smoothness of  $f(\alpha)$

These assumptions underly many studies in uncertainty quantification (UQ), specifically in uncertainty propagation

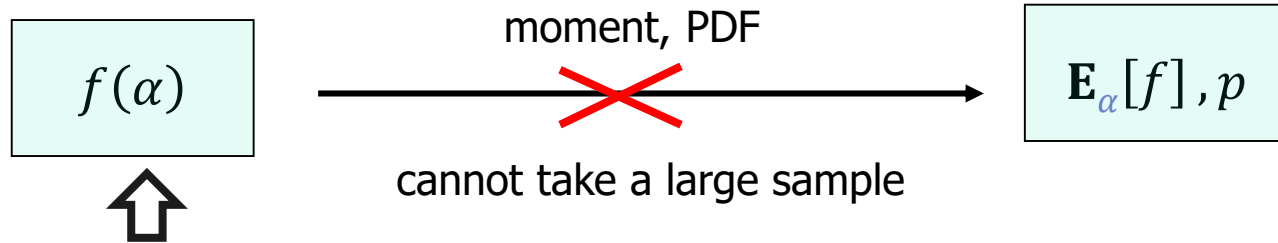


# Approximation-based estimation



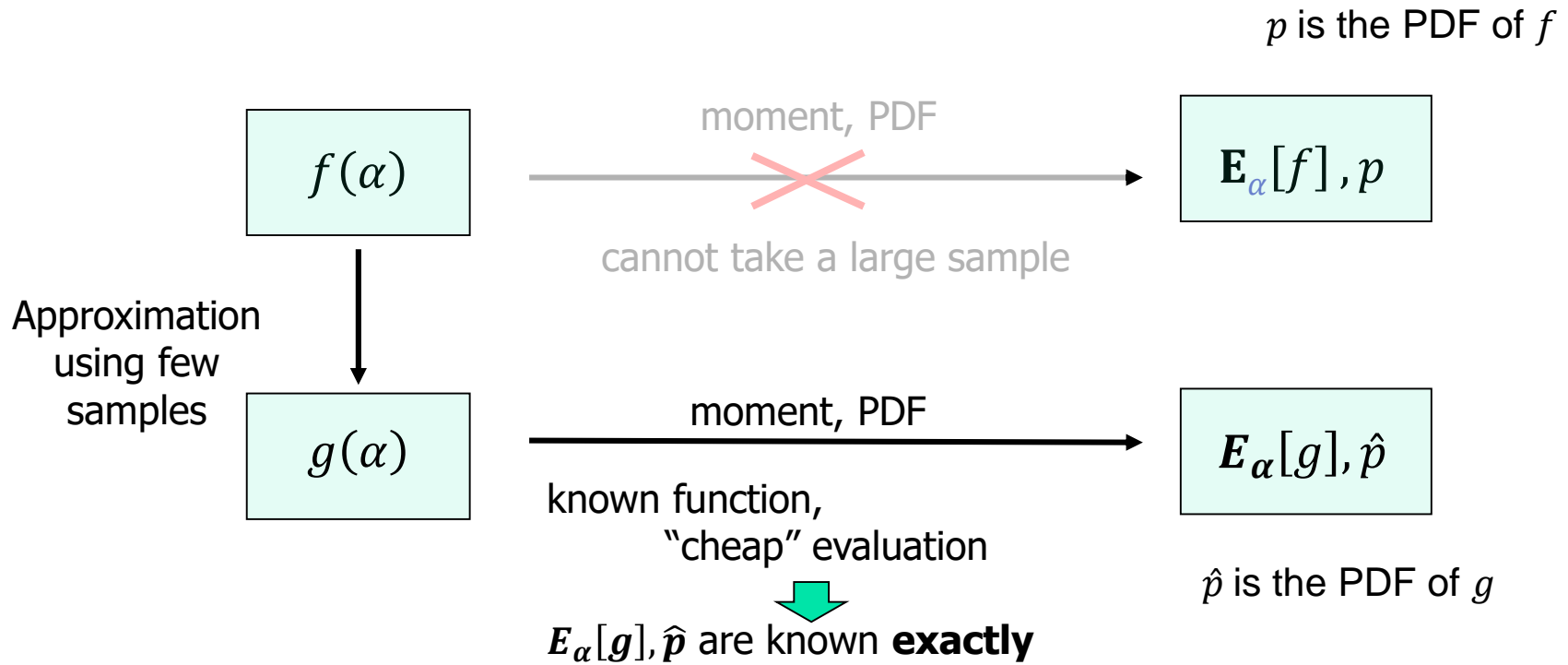
# Approximation-based estimation

$p$  is the PDF of  $f$

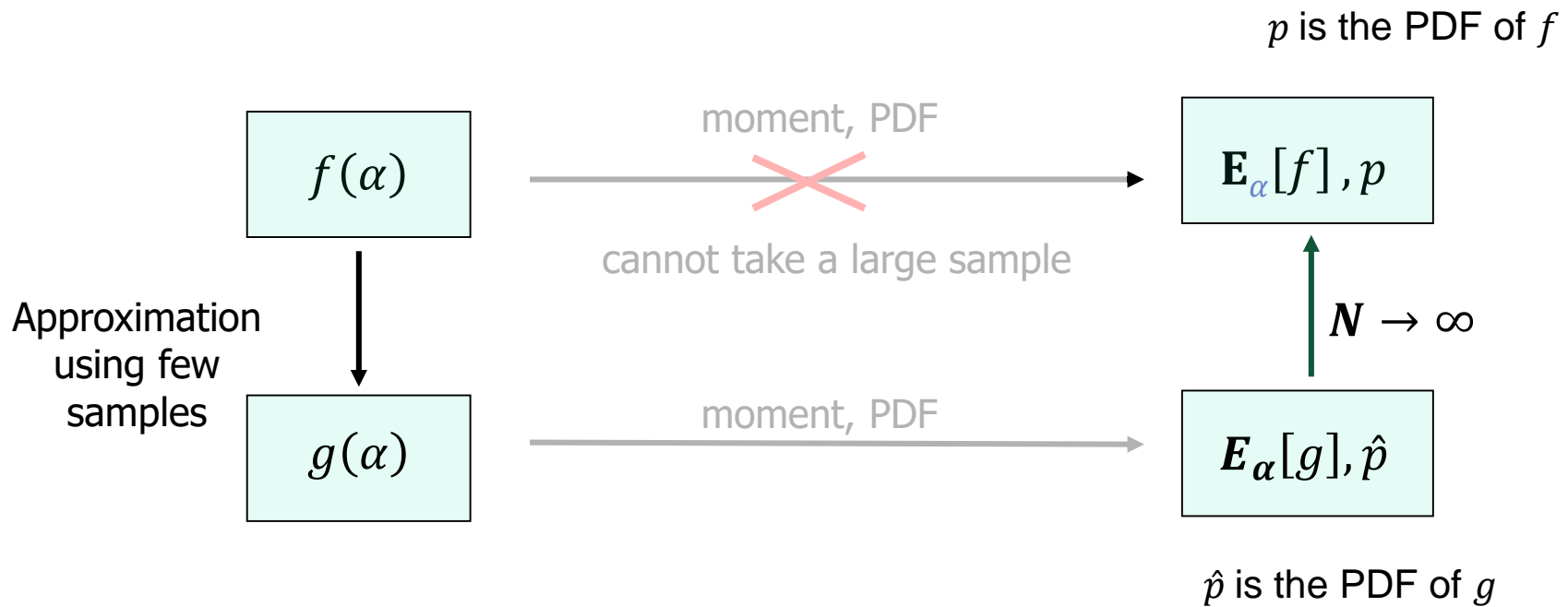


- Unknown explicitly
- Each evaluation is computationally expensive

# Approximation-based estimation



# Approximation-based estimation



## Questions

- Which approximation  $g(\alpha) \approx f(\alpha)$  should be used?
- How small are  $E_\alpha[f] - E_\alpha[g]$  and  $\|p - \hat{p}\|$  ?

# Attempt I - generalized polynomial chaos (gPC)

Standard in the field of uncertainty quantification (UQ)

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 (moments and  $L^2$ )

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

[see e.g., D. Xiu, 2010]

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But,

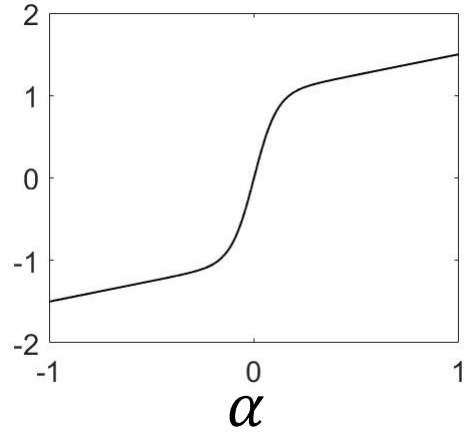
PDF estimation

**No theory** for  $\|p - p_N\|$

Will it work in practice?

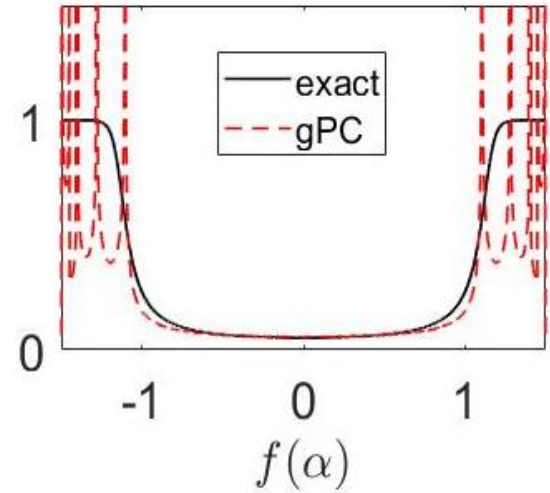
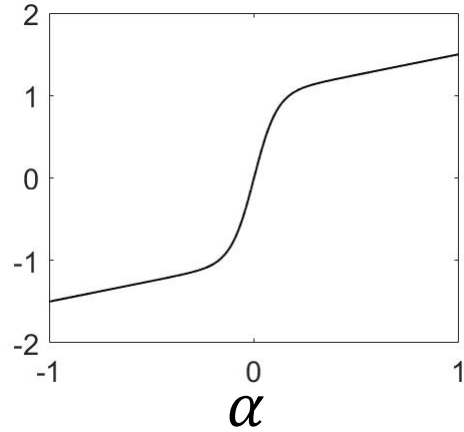
# Example – gPC fails at PDF estimation

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



# Example – gPC fails at PDF estimation

$f = \tanh(9\alpha) + \frac{\alpha}{2}$ ,  $\alpha \sim \text{Uniform}[-1, 1]$  PDF approximation,  $N = 12$  samples

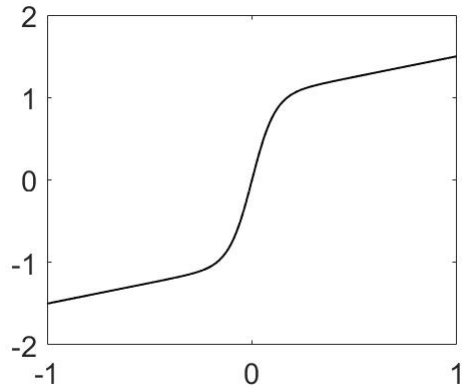


Why does it fail?



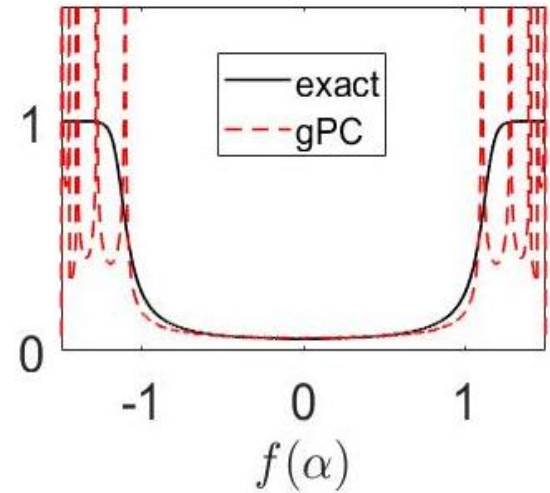
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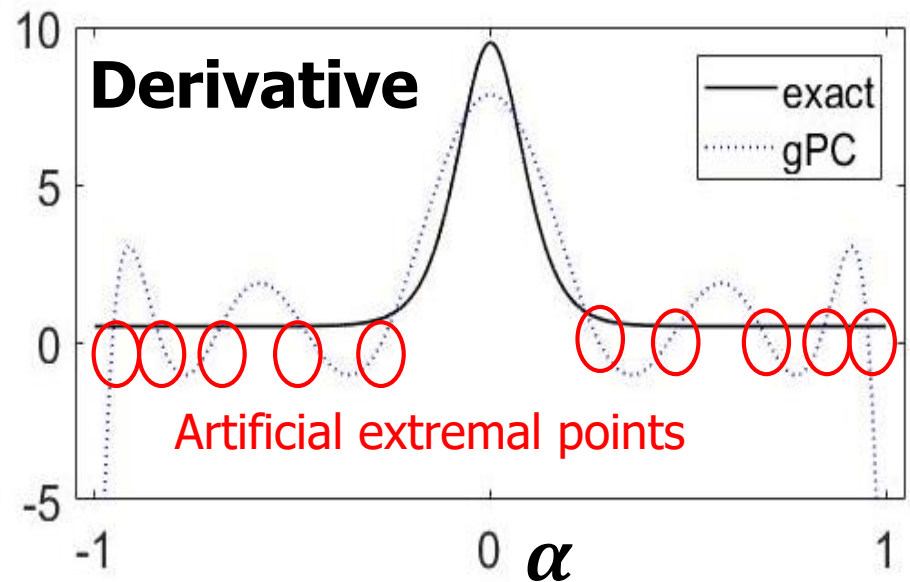
PDF approximation,  $N = 12$  samples



Lemma: Under general smoothness conditions

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

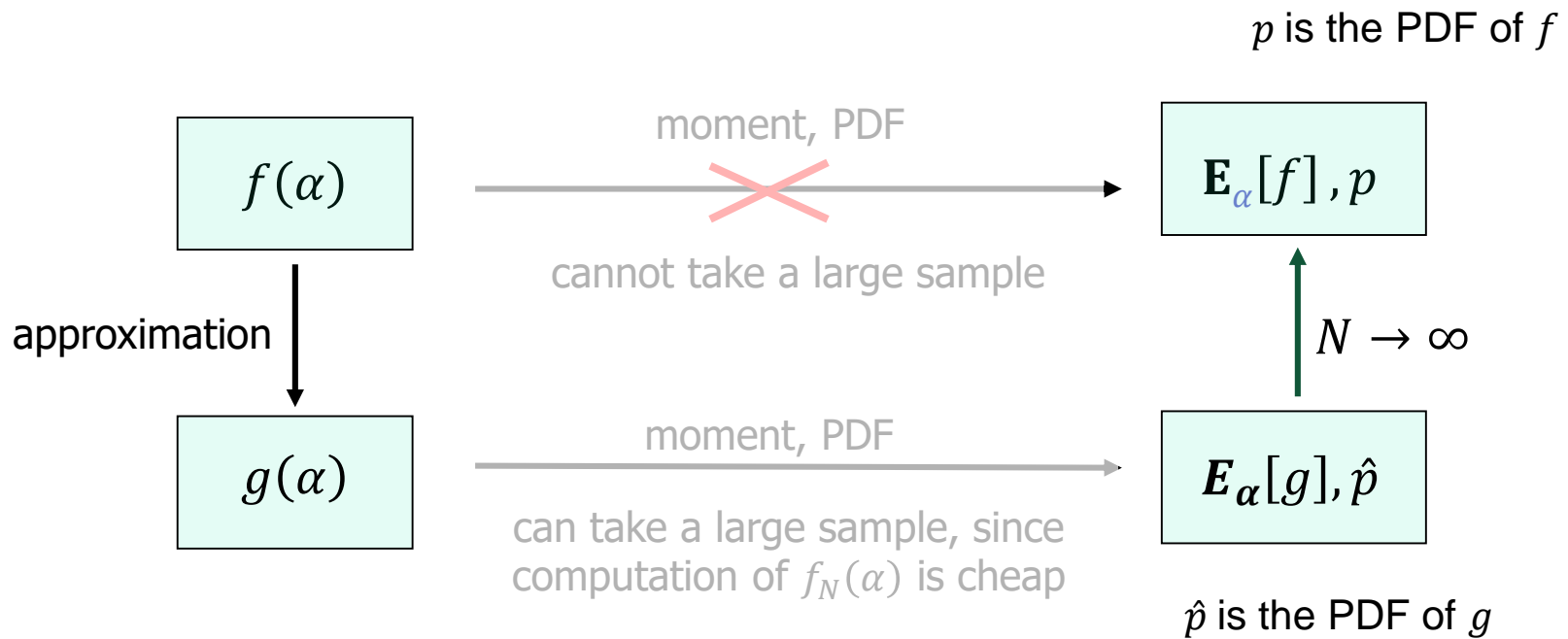
Although gPC is spectrally accurate (in  $L^2$ ), it produces "artificial" zero derivatives.



# Agenda

- PDF approximation
  - Is moment-estimation sufficient?
  - An algorithm & convergence results  
Approximating pushed-forward densities, provably
- Transport-theory point of view

# An Alternative Approximation-based estimation



## Lessons learned

- For PDF approximation, spectral moment accuracy is not sufficient.
- It is necessary that  $g' \neq 0 \leftrightarrow f' \neq 0$   
 $|g - f|, |g' - f'| \ll 1$ ,
- "Monotonicity preserving approximation"

Solution: use spline interpolation  
 (piece-wise polynomials)

# The solution - Spline-based approach (1d)

**Theorem 1 (Ditkowski, Fibich, AS '18):**

Let  $p$  and  $p_N$  be the probability density functions (**PDF**) of  $f(\alpha)$  and its **m-degree spline** interpolant on  $N$  equi-distributed points. Then

$$\|p - p_N\|_1 \leq KN^{-m},$$

# The solution - Spline-based approach (1d)

## Theorem 1 (Ditkowski, Fibich, AS '18):

Let  $f \in C_{\text{piecewise}}^{m+1}([\alpha_{\min}, \alpha_{\max}])$  with  $|f'| > a > 0$ , let  $\alpha$  be distributed by  $c(\alpha)d\alpha$  where  $c \in C^1([\alpha_{\min}, \alpha_{\max}])$ .

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For all

$$N > \sqrt[m]{\frac{2C_m \|f^{(m+1)}\|_\infty}{a}} (\alpha_{\max} - \alpha_{\min})$$

# Proof “ingredients”

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Theorem (Meyer, Hall, '76): for  $f \in C^{m+1}$ ,  
Then

$\|(f - s)^{(j)}\|_\infty \leq C_m(f)h^{m+1-j} \quad j = 0, \dots, m - 1$   
where  $h > 0$  is the maximal spacing between interpolation points



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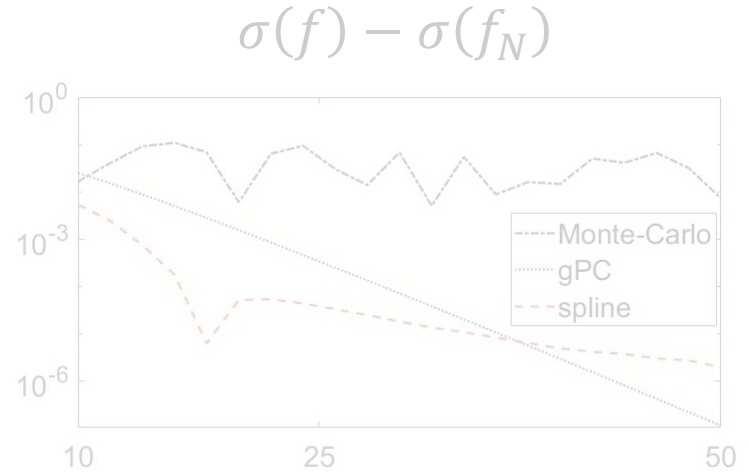
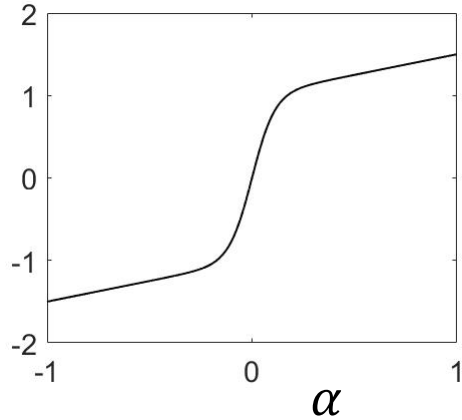
Hence, if  $f$  is monotone,  $N$  is high enough, and  $y$  in  $f$ 's image,  $\alpha \sim U(-1,1)$

$$\|p - p_N\|_1 = \int dy |p(y) - p_N(y)| = \int dy \left| \frac{1}{f'(f^{-1}(y))} - \frac{1}{s'(s^{-1}(y))} \right|$$

= ...

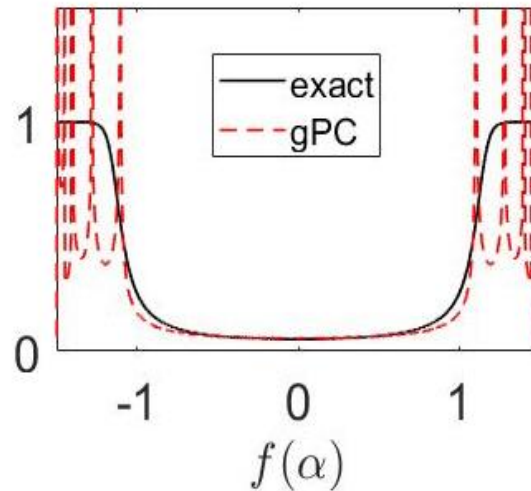
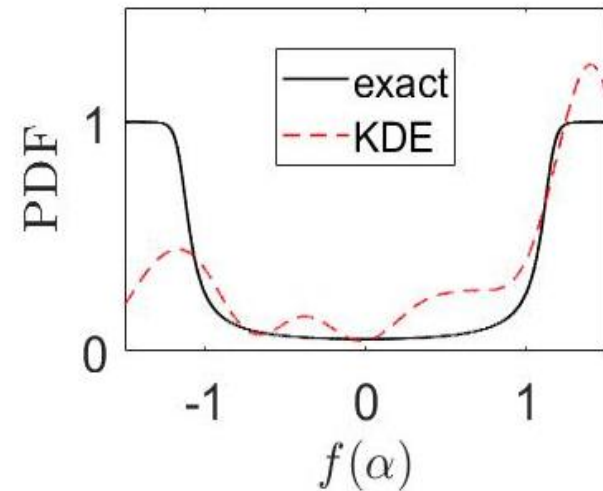
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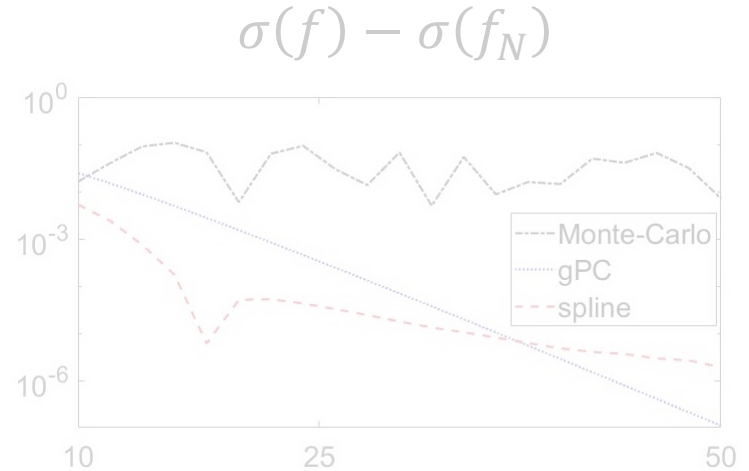
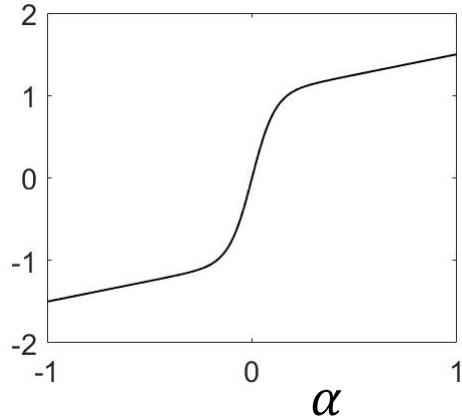
PDF approximation,  $N = 12$

Statistically optimal

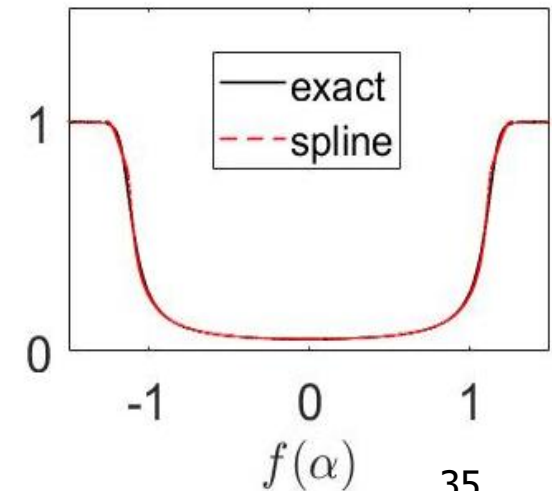
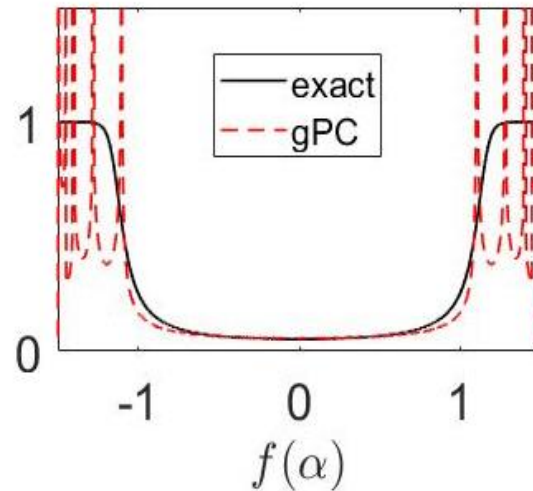
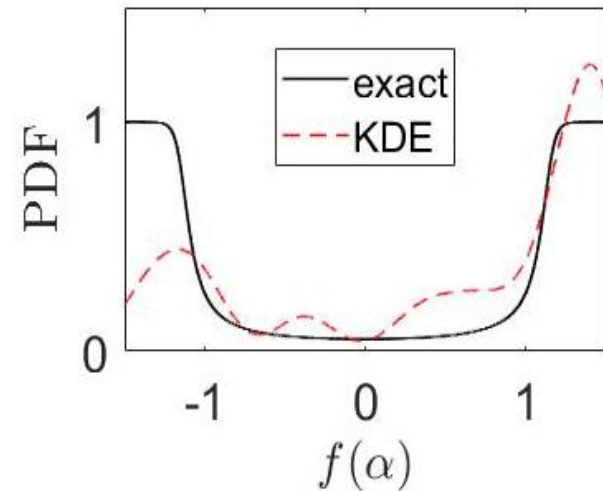


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PDF approximation,  $N = 12$



# Coupled NLS example

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

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

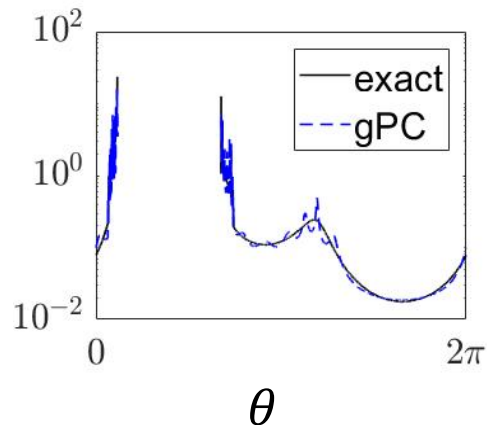
polarization  $\theta(t) = \varphi_+(t) - \varphi_-(t)$

Random elliptical beam –

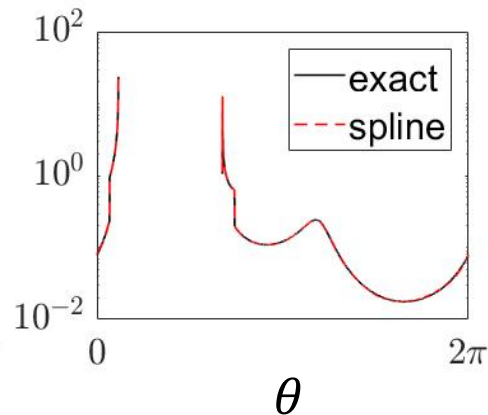
$$A_{\pm}(t = 0) = (1 + \alpha) C_{\pm} e^{-x^2}, \quad \alpha \sim U(-0.1, 0.1)$$

[with Patwardhan et al, PRA, 2019]

PDF, N=64



PDF, N=64



# Coupled NLS example

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

[with Patwardhan et al, PRA, 2019]

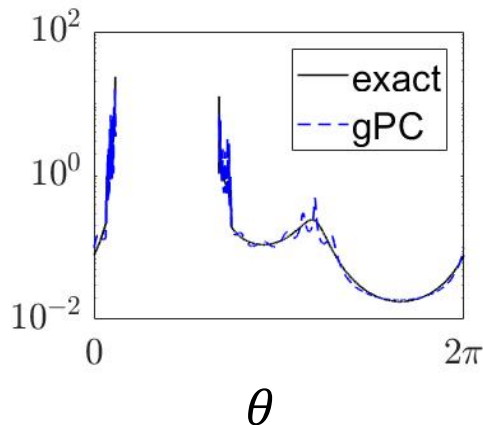
phase:  $\varphi_{\pm}(t) = \arg \left( A_{\pm}(t, x = 0) \right) \bmod (2\pi)$

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

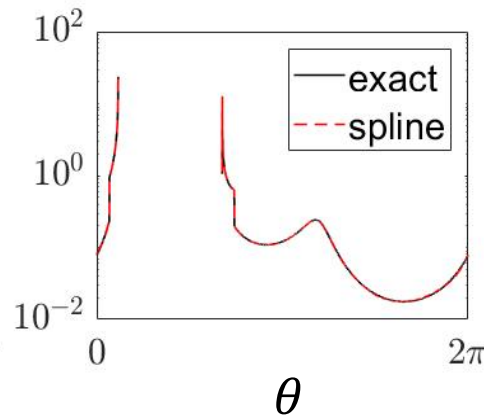
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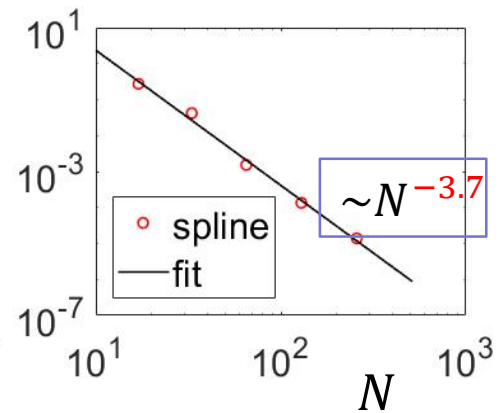
PDF, N=64



PDF, N=64



$\|p - p_N\|_1$



# Burgers equation – shock location

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

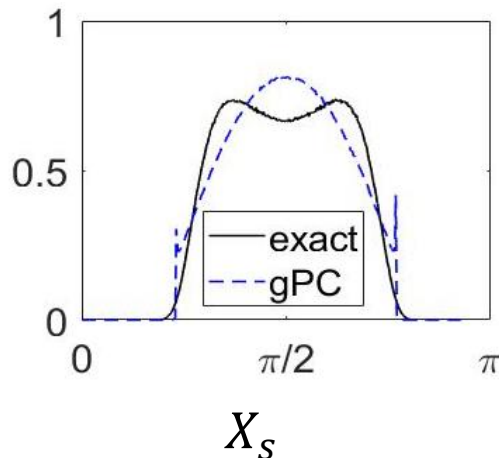
Initial condition:  $u_0(x) = \alpha \sin(x)$

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

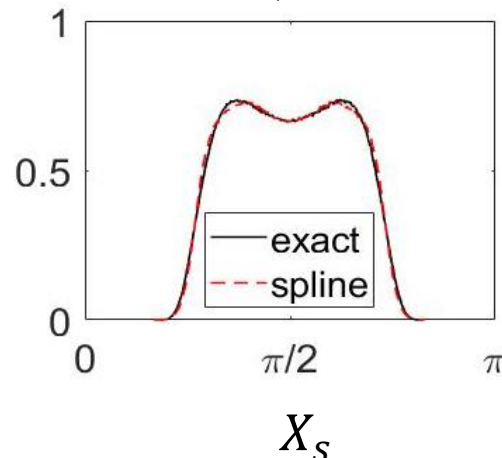
Distribution of random initial amplitude –

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

PDF, N=11



PDF, N=11



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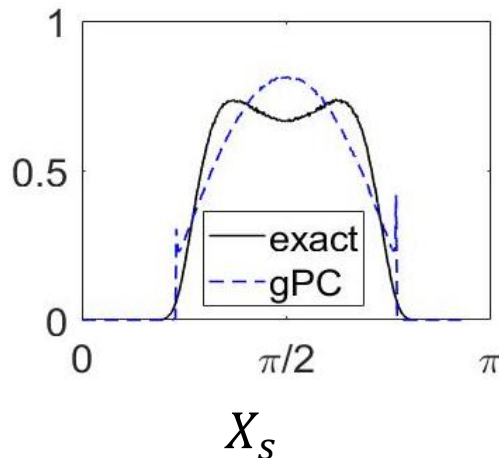
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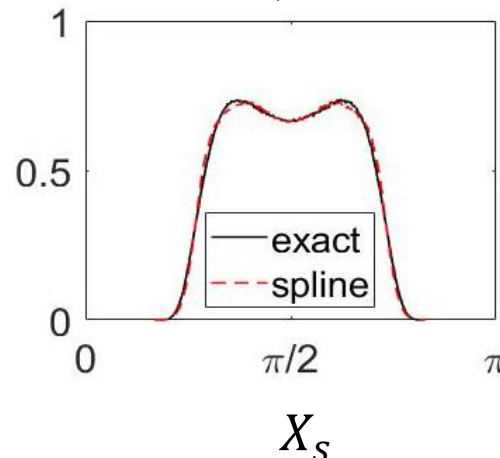
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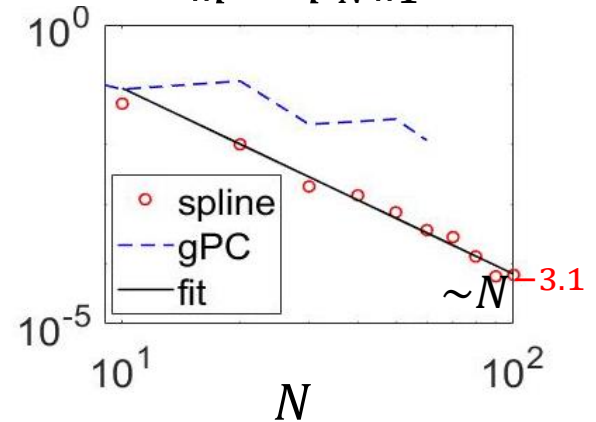
PDF, N=11



PDF, N=11



$\|p - p_N\|_1$



# Spline-based density estimation for multidimensional noise

Can this problem be solved if the input noise is multi-dimensional?

(physically – multiple uncertain or noisy terms in the system)



# Spline-based density estimation for multidimensional noise

## Theorem 2 (Ditkowski, Fibich, AS '18):

Let  $\Omega = [0,1]^d$ , let  $f \in C^{m+1}(\Omega)$  with  $|\nabla f| > a > 0$ , let  $\alpha$  be uniformly distributed in  $\Omega$ ,

and

Let  $p$  and  $p_N$  be the probability density functions (PDF) of  $f(\alpha)$  and its  $m$ -degree tensor-product spline interpolant on  $N^d$  equi-distributed points. Then

$$\|p - p_N\|_1 \leq KN^{-\frac{m}{d}},$$

# Curse of dimensionality

## Theorem 2 (Ditkowski, Fibich, AS '18):

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$$\|p - p_N\|_1 \leq K N^{-\frac{m}{d}},$$

For kernel density estimators [e.g., Devroye '84]

$$\|p - p_{kde,N}\|_1 \sim N^{-0.4}$$

Our method is preferable when  $d \leq \frac{5m}{2}$

From  $d=1$  to  $d>1$ :

“Same” result, more complicated proof

**Theorem 1 (Ditkowski, Fibich, AS '18):**

Let  $p$  and  $p_N$  be the probability density functions (PDF) of  $f(\alpha)$  and its  $m$ -degree spline interpolant on  $N$  equi-distributed points. Then

$$\|p - p_N\|_1 \leq KN^{-\frac{m}{d}}$$

Theorem (Schultz, '69): for  $f \in C^{m+1}$ ,

Then

$$\|(f - s)^{(j)}\|_\infty \leq C_m(f)h^{m+1-j} \quad j = 0, \dots, m-1$$

where  $h>0$  is the maximal spacing between interpolation points

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Lemma: Under general smoothness conditions

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

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Under some conditions

$$\|p - p_N\|_1 = \int dy |p(y) - p_N(y)| = \int dy \left| \int_{f^{-1}(y)} \frac{1}{|\nabla f|} d\sigma - \int_{g^{-1}(y)} \frac{1}{|\nabla g|} d\sigma \right| = \dots$$

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“Same” result, more complicated proof

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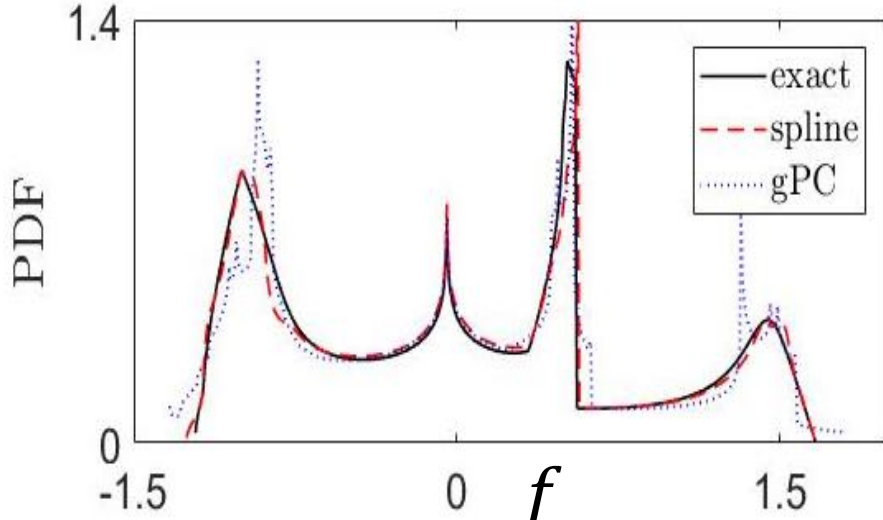
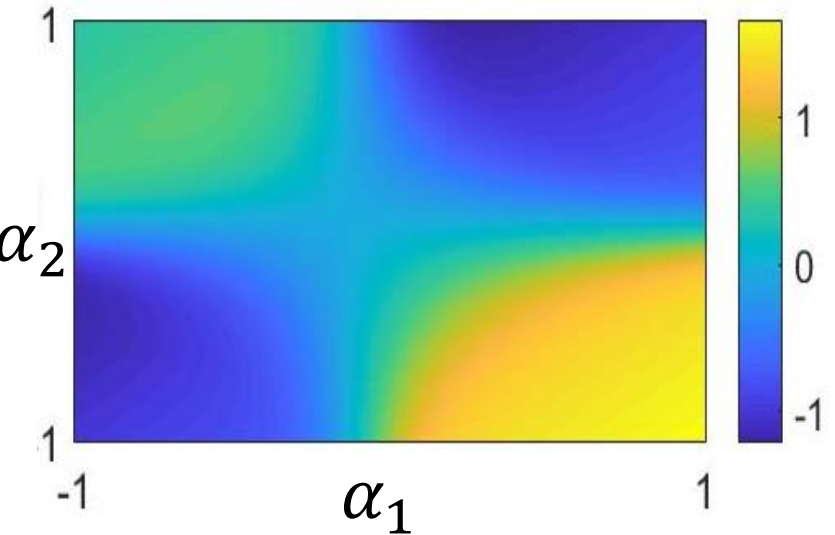
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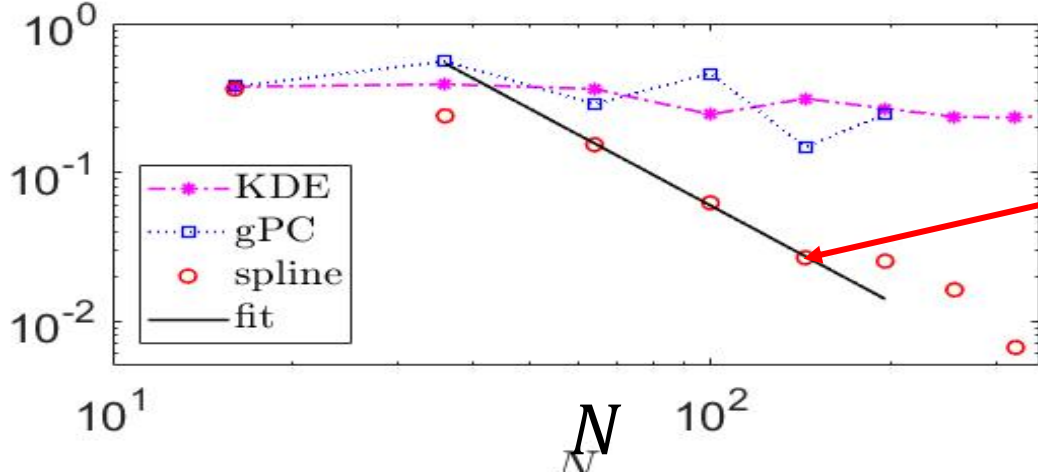
Different manifolds – more complications

# 2-dimensional example

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



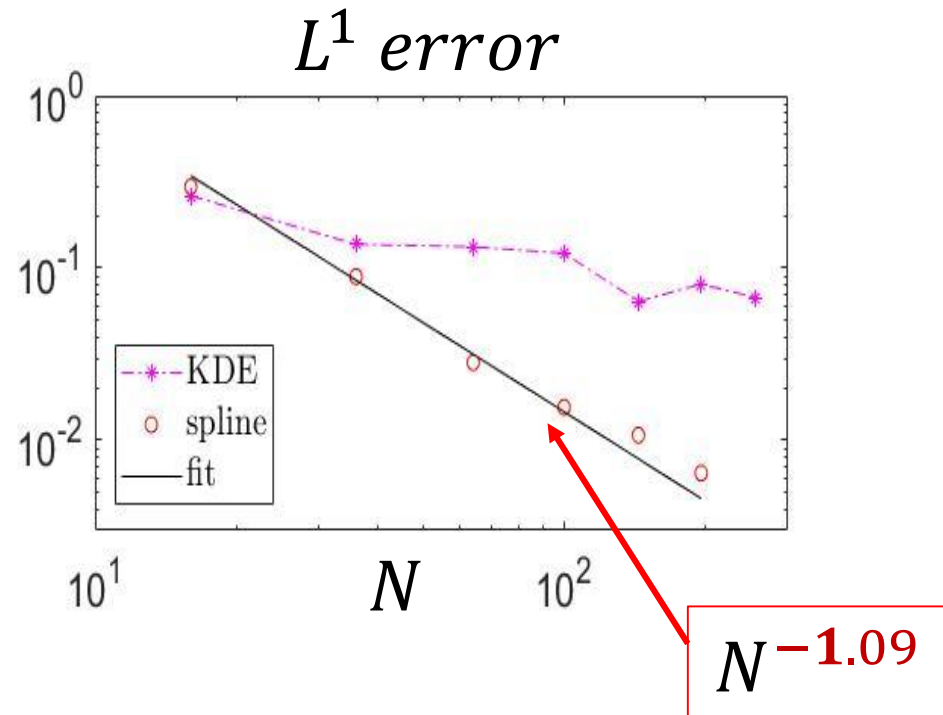
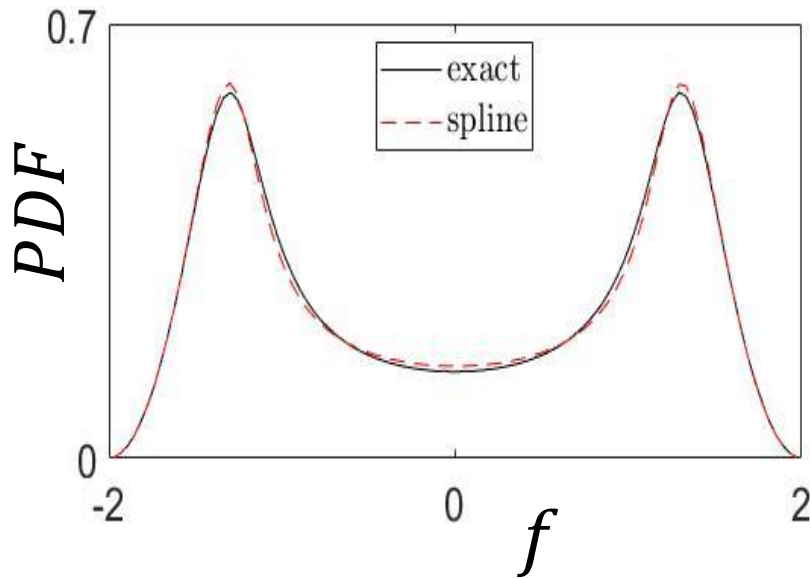
$L^1$  error



$N^{-2.1}$

# 3 dimensional example

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





# Conclusions (non-transport outlook)

- Convergence of moments and in  $L^2$  does not guarantee convergence in PDFs
- Spline perform well for PDF approximation
  - Any other “local” method might do – RBFs, other splines, GMM,...
  - With theoretical guarantees in all dimensions.
  - With explicit “maximal dimensions” of effectiveness

A. Sagiv, A. Ditkowski, G. Fibich

Density estimation in uncertainty propagation problems using a surrogate model

arXiv 1803.10991 (under review)

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Open question:  
Can the theory of push-forwarded densities be simplified?

# Agenda

- PDF approximation
  - Is moment-estimation sufficient?
  - An algorithm & convergence results

- **Transport-theory point of view**

**Simplifying the theory of measure approximation**

# Spline PDF Theory revisited

## Theorem 2 (Ditkowski, Fibich, AS '18):

Let  $\Omega = [0,1]^d$ , let  $f \in C^{m+1}(\Omega)$  with  $|\nabla f| > a > 0$ , let  $\alpha$  be uniformly distributed in  $\Omega$ ,

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$$\|p - p_N\|_1 \leq KN^{-\frac{m}{d}},$$

Problem I – “arbitrary” derivative condition from application standpoint

Problem II – spline approximate derivatives in  $L^\infty$ , other methods do not

# Spline PDF Theory revisited

**Theorem 2 (Ditkowski, Fibich, AS '18):**

Let  $\Omega = [0,1]^d$ , let  $f \in C^{m+1}(\Omega)$  with  $|\nabla f| > a > 0$ , **let  $\alpha$  be uniformly distributed in  $\Omega$ ,**

and

Let  $p$  and  $p_N$  be the probability density functions (PDF) of  $f(\alpha)$  and its  $m$ -degree tensor-product spline interpolant on  $N^d$  equi-distributed points. Then

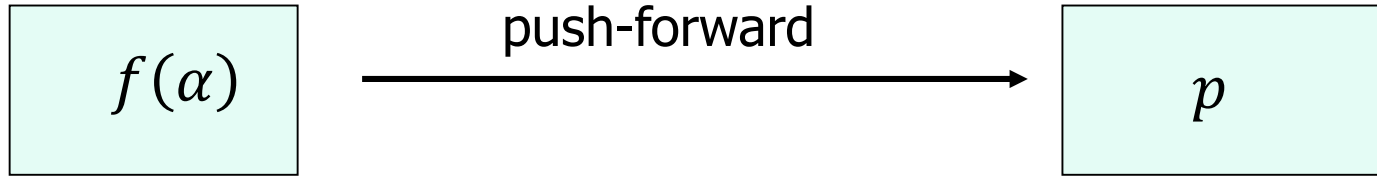
$$\|p - p_N\|_1 \leq KN^{-\frac{m}{d}},$$

Problem III – uniform measure (or absolutely continuous)

Problem IV – Omega is a box (compact)

# Approximation-based estimation

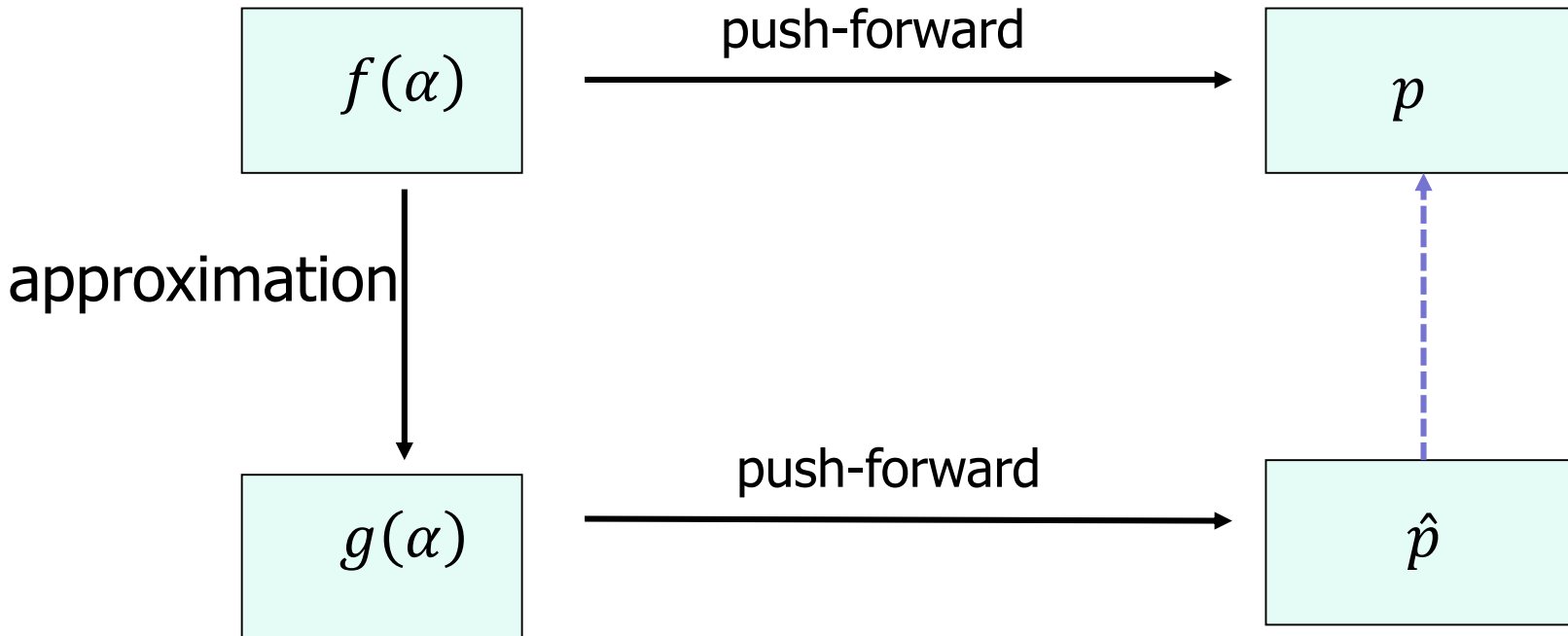
$\alpha \sim q$  probability measure



density of interest

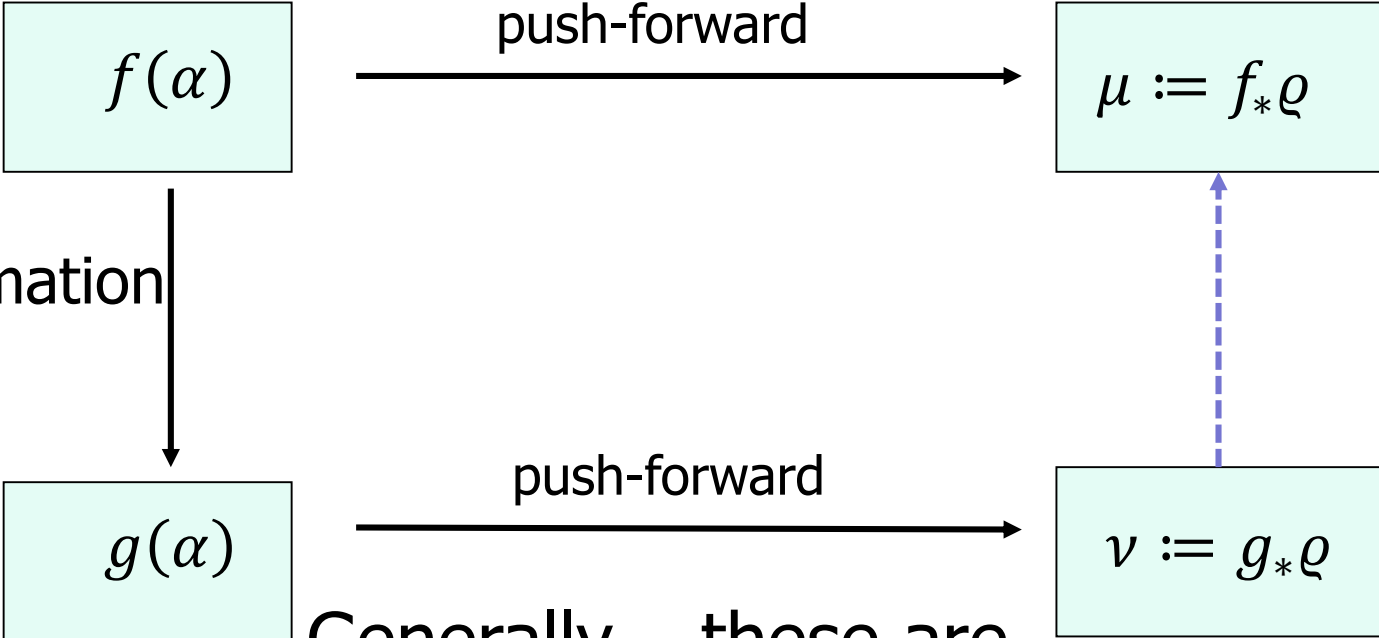
# Approximation-based estimation

$\alpha \sim \varrho$  probability measure



# Approximation-based estimation

$\alpha \sim \varrho$  probability measure



Generally – these are measures, not densities



# Approximation-based estimation

$\alpha \sim \varrho \text{ prob}$

[Gibbs and Su, Int. Stats. Rev. 2002]

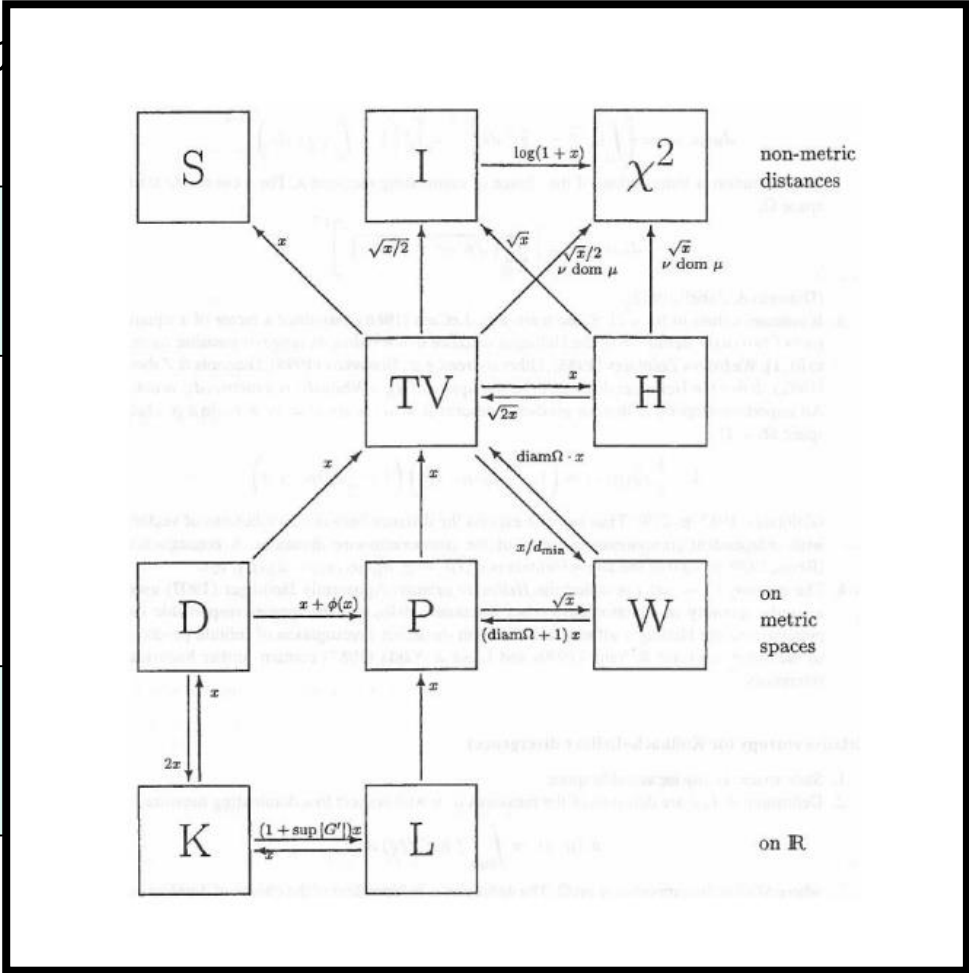
$f(\alpha)$

$f_*\varrho$

$g(\alpha)$

$g_*\varrho$

approximation

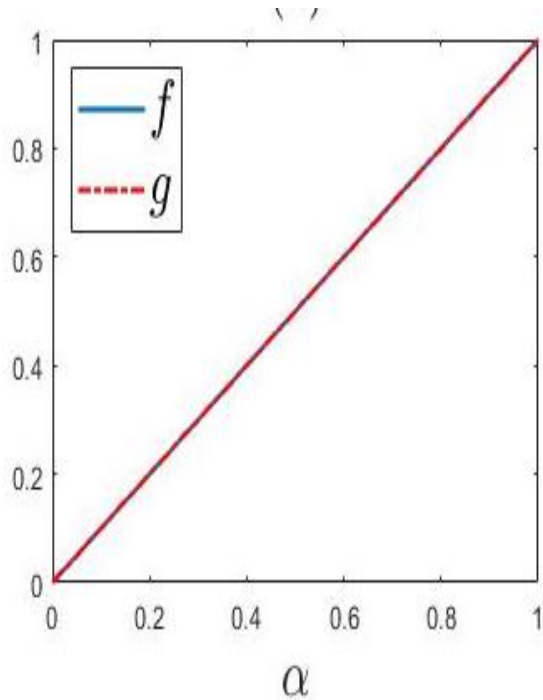


How should the difference between  $\mu$  and  $\nu$  be measured?

# Is PDF the right way to measure?

A numerical example:

$$f(\alpha) = \alpha; \quad g(\alpha) = \alpha + 10^{-3} \sin(100\alpha)$$
$$\Rightarrow \|f - g\|_{L^q} \sim 10^{-3}$$



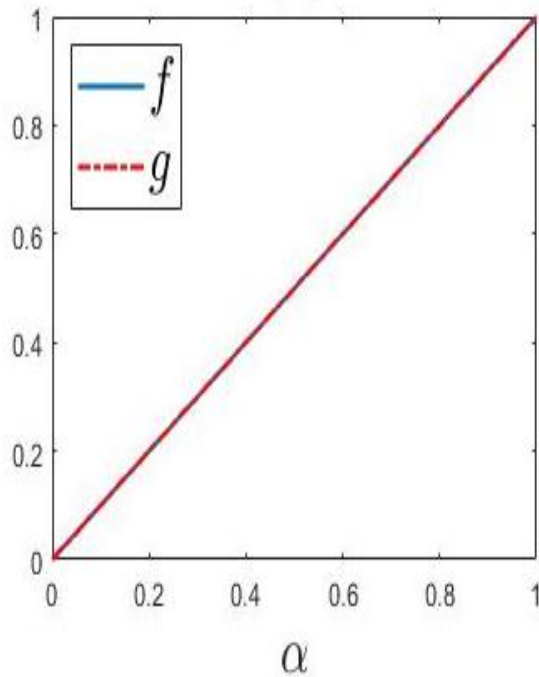
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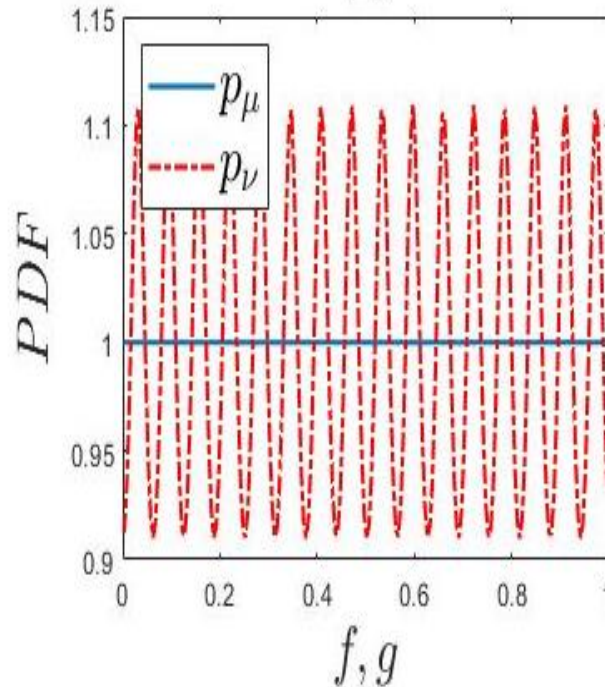
$$f(\alpha) = \alpha; \quad g(\alpha) = \alpha + 10^{-3} \sin(100\alpha)$$

$$\varrho = \text{Lebesgue}, \quad \mu := f_*\varrho; \quad \nu := g_*\varrho$$

$10^{-3}$  error



$10^{-1}$  error



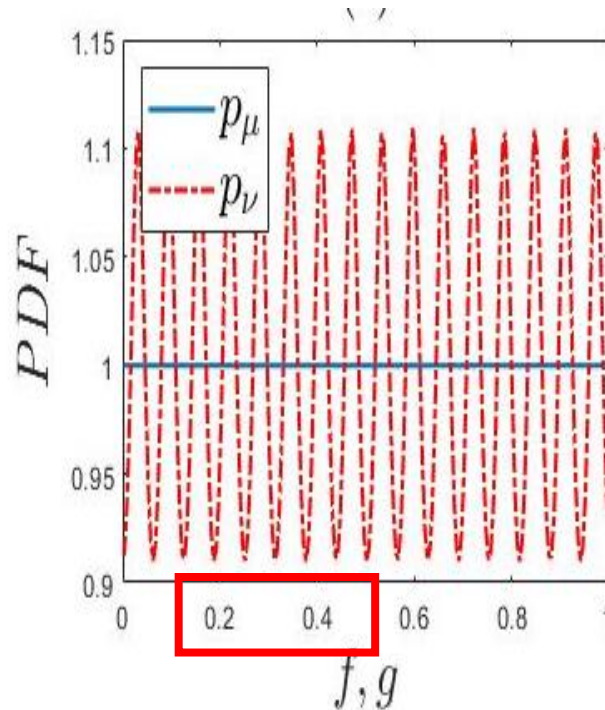
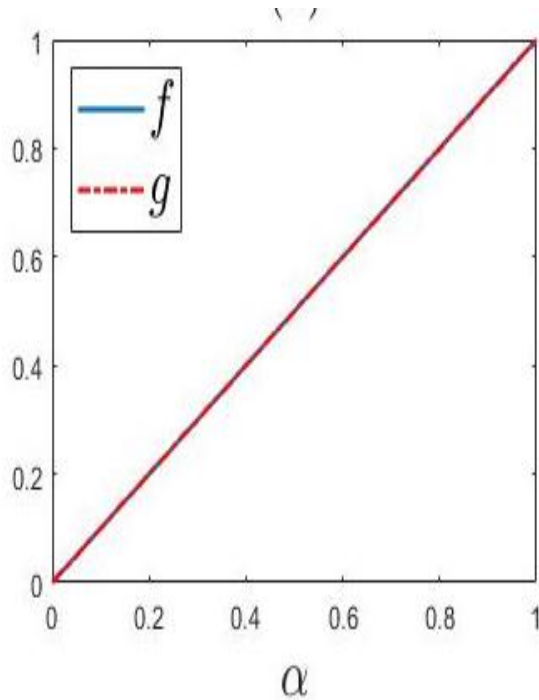
This difference can be made arbitrarily large

# Is PDF the right way to measure?

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PDFs are different, but

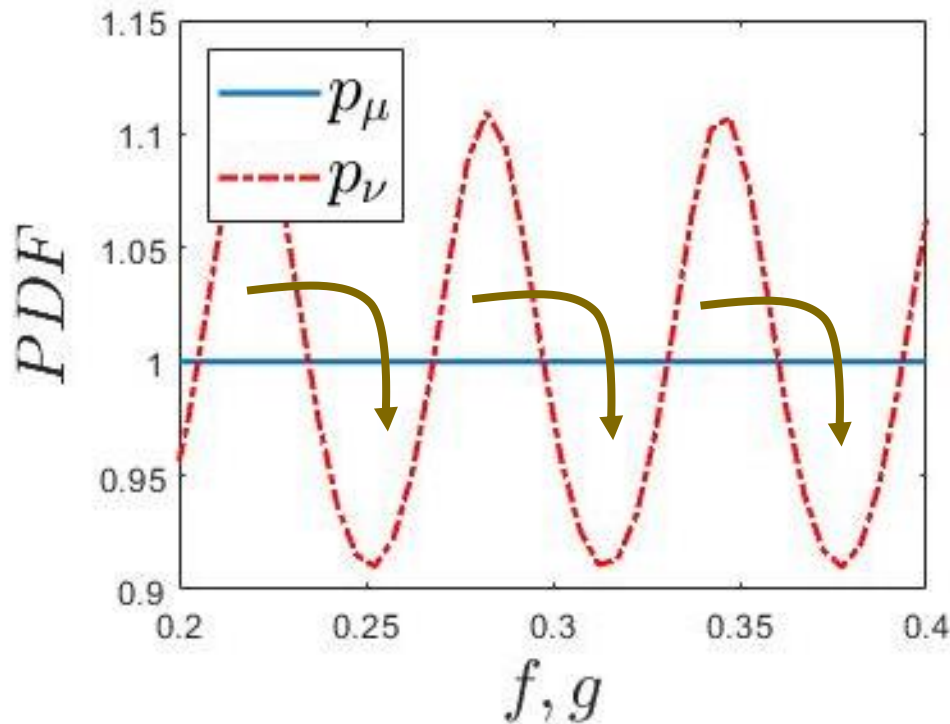
$$\mu([0.2, 0.4]) \approx \nu([0.2, 0.4])$$

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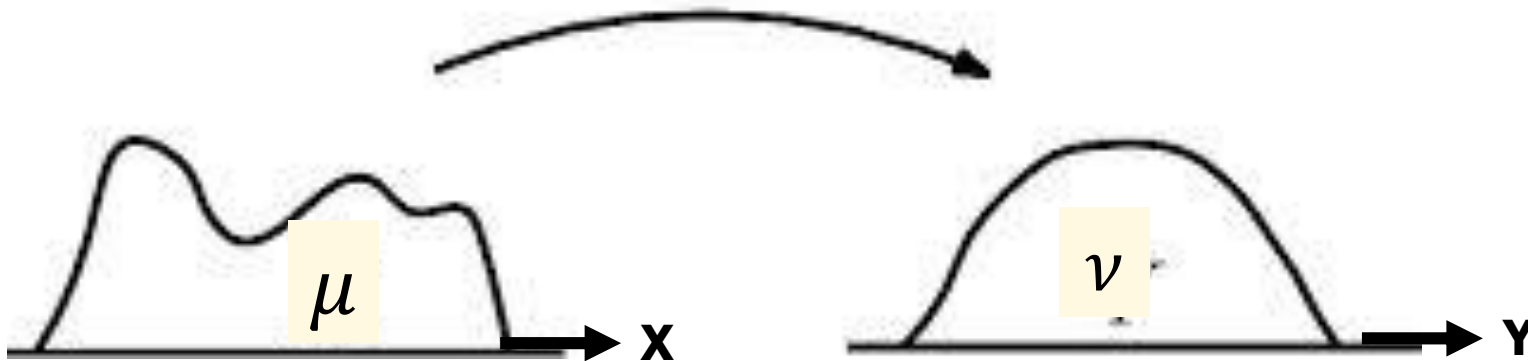
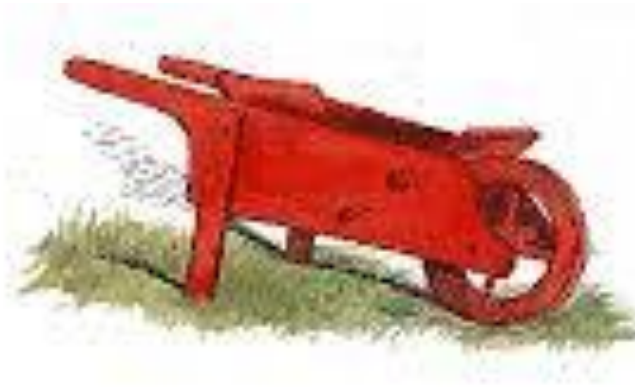
"transfer" mass on a local scale

# Underlying Theory – Wasserstein Metrics

$$W_p(\mu, \nu) = \left[ \inf \int_{R \times R} |x - y|^p d\gamma(x, y) \right]^{\frac{1}{p}}$$

Such that  $\mu, \nu$  are marginals of  $\gamma$

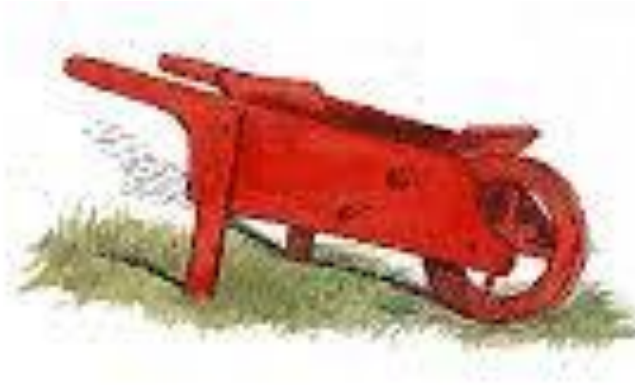
Intuitively (for  $p=1$ )  
a transport plan: move  
 $\gamma(x, y)$  mass over  
 $|x - y|$  distance



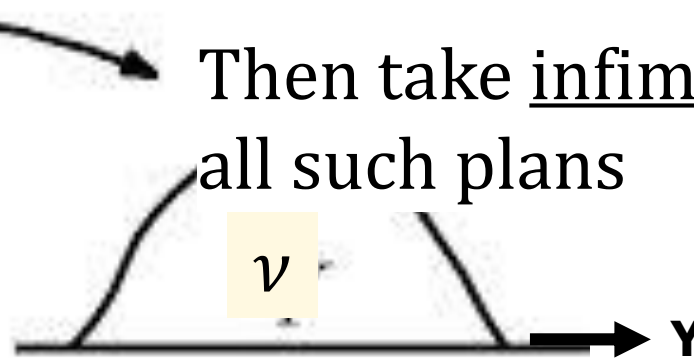
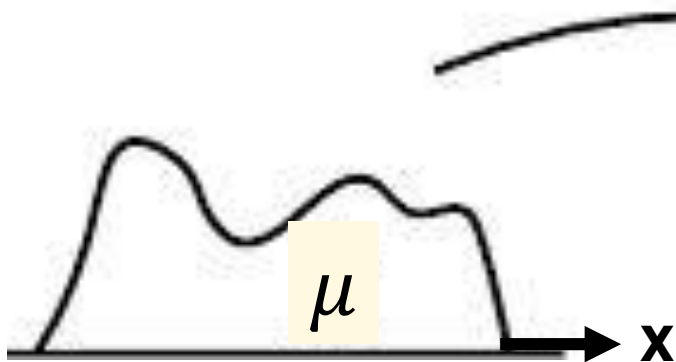
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Intuitively (for  $p=1$ )  
a transport plan: move  
 $\gamma(x, y)$  mass over  
 $|x - y|$  distance



Then take infimum over  
all such plans

# Indeed – Wasserstein theory **is** simple

## **Theorem 3 (AS '19):**

Let  $\Omega \subseteq R^d$ , let  $f, g \in C(\bar{\Omega})$ , and let  $\varrho$  be a Borel measure and  $\mu = f_*\varrho$ ,  $\nu = g_*\varrho$

1.  $W_p(\mu, \nu) \leq \|f - g\|_\infty$

**i.e., pointwise accuracy guarantees Wasserstein accuracy**



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**i.e.,  $L^p$  accuracy guarantess Wasserstein accuracy**

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3.  $W_p(\mu, \nu) \leq C(p, q) \|f - g\|_q^{\frac{p}{q+p}} \cdot \|f - g\|_\infty^{\frac{q}{q+p}}$  for all  $q \geq 1$

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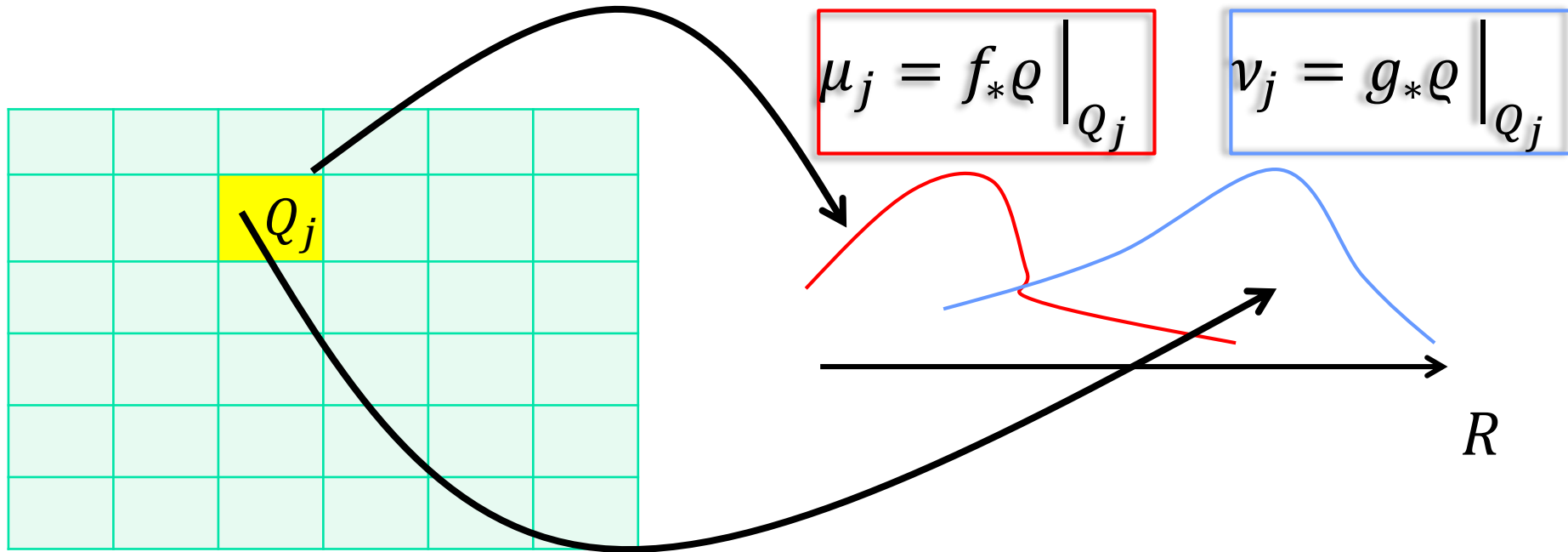
Let  $\Omega \subseteq \mathbb{R}^d$ , let  $f, g \in C(\bar{\Omega})$ , let  $\varrho$  be a Borel measure and  $\mu = f_*\varrho$ ,  $\nu = g_*\varrho$

1.  $W_p(\mu, \nu) \leq \|f - g\|_\infty$
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- No conditions on the underlying measure and domain (**=many noise models**)
- No derivative approximation conditions
- Every  $L^q$  convergence works (**=many possible approximation methods**)

# Proof sketch

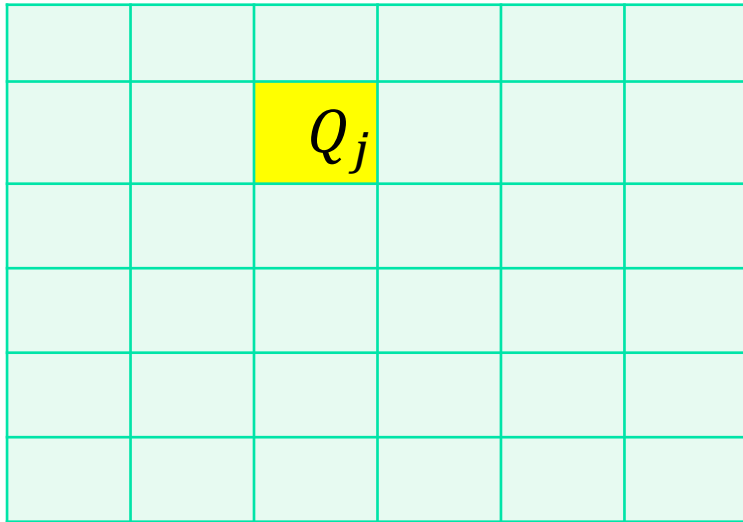
Here –  $\Omega$  is a cube,  $\varrho$  is Lebesgue



Step I – push forward a small cube  $Q_j$  to define to measures (of same mass) on  $\mathbb{R}$

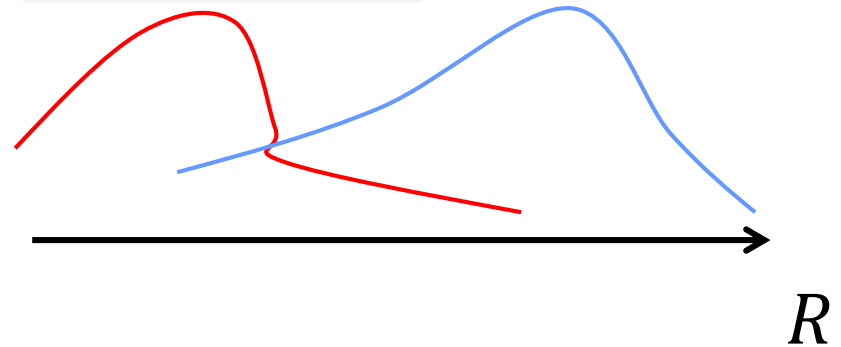
# Proof sketch

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$$\mu_j = f_* \varrho \Big|_{Q_j}$$

$$\nu_j = g_* \varrho \Big|_{Q_j}$$



Step II – for  $\varepsilon > 0$ , by continuity, if  $\text{diam}(Q_j) < \delta$

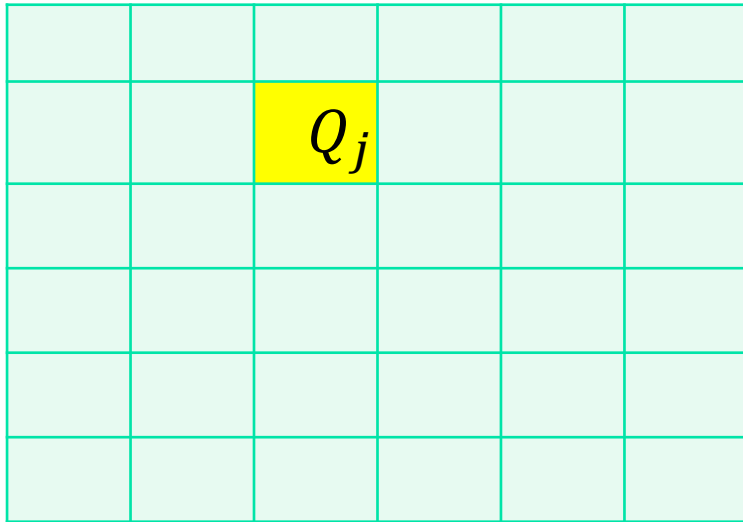
Then  $|f(x) - f(y)|, |g(x) - g(y)| \leq \varepsilon$

And so for any transport,

the mass  $\varepsilon^d$  travels a distance  $\leq \|f - g\|_{L^\infty} + o(\varepsilon)$

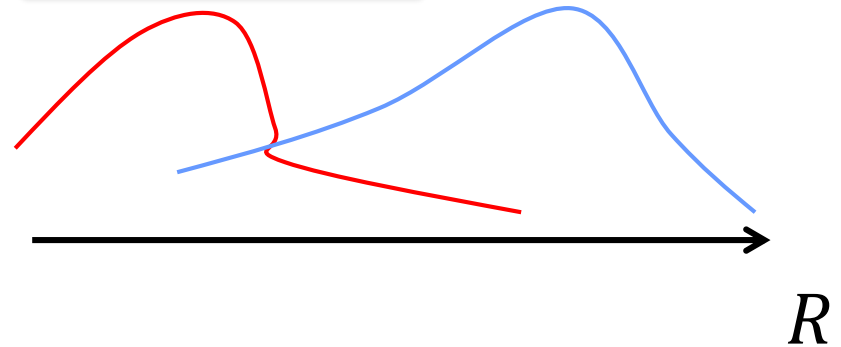
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Step III – this is true for *all cubes*, for *any*  $\varepsilon > 0$

# Agenda

- PDF approximation
  - Is moment-estimation sufficient?
  - An algorithm & convergence results
- **Transport-theory point of view**

**Back to the Uncertainty-quantification problem**

# Pause, why Wasserstein?

- The distance between PDFs is natural and intuitive to use...
  - But difficult to work with.
- Wasserstein-theory is easier to work with, better approximation results...
  - But is it useful for applications?



# Wasserstein and CDFs

The CDF bounds are a result of a wider theory for **Wasserstein Metrics**, since

$$W_1(\mu, \nu) = \|F_\mu - F_\nu\|_1$$

[Salvemini '43, Vallender '74]

Cumulative distribution function (CDF)

$$F_\mu(y) := \mu([y, \infty))$$

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## **Theorem 3 – for CDFs (AS '19):**

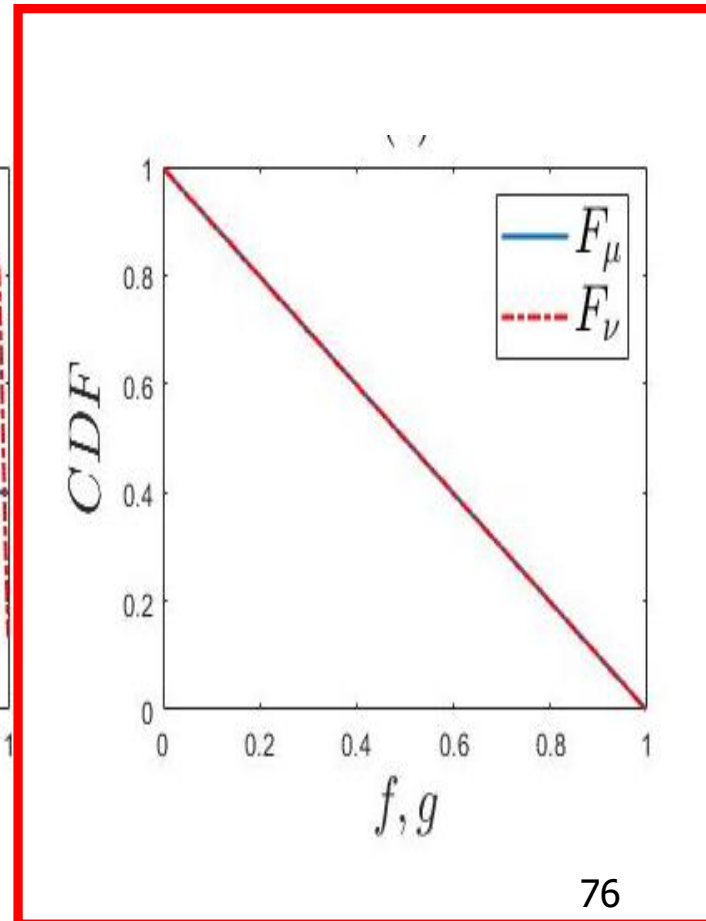
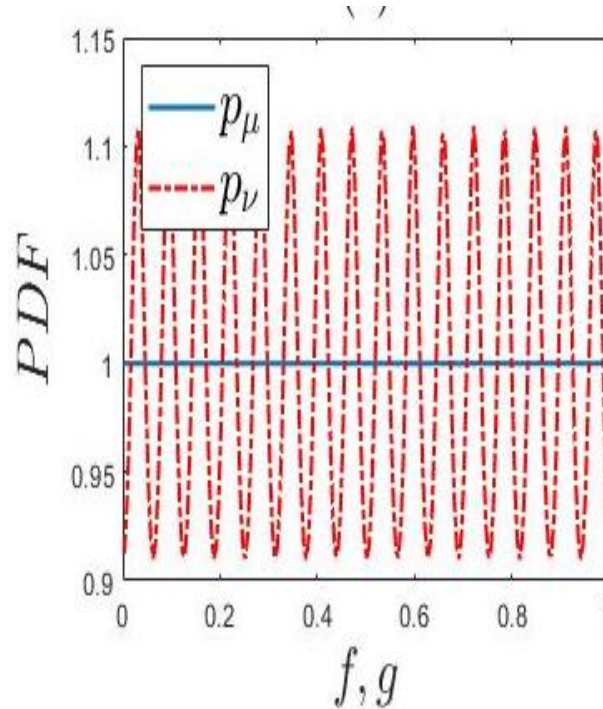
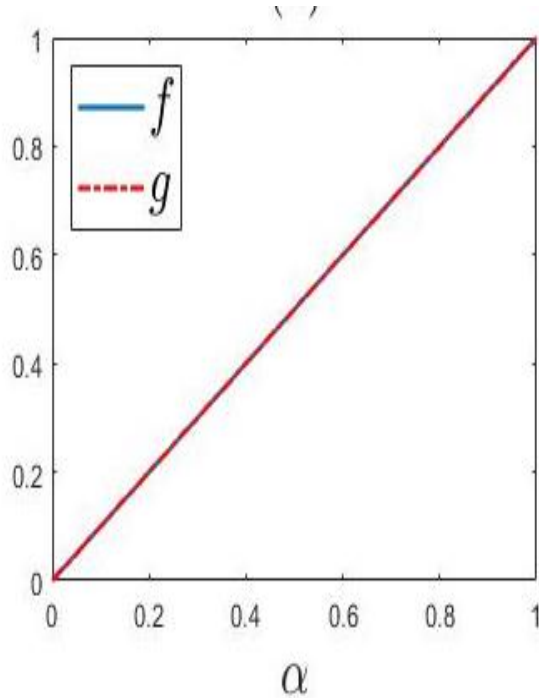
Let  $\Omega \subseteq \mathbb{R}^d$ , let  $f, g \in C(\bar{\Omega})$ , and let  $\varrho$  be a Borel measure

1.  $\|F_\mu - F_\nu\|_1 \leq \|f - g\|_\infty$
2.  $\|F_\mu - F_\nu\|_1 \leq \|f - g\|_1$  (if  $\Omega$  is bounded)
3.  $\|F_\mu - F_\nu\|_1 \leq \|f - g\|_q^{\frac{1}{q+1}} \cdot \|f - g\|_\infty^{1 - \frac{1}{q+1}}$  for all  $q \geq 1$

# Is CDF the right way to measure?

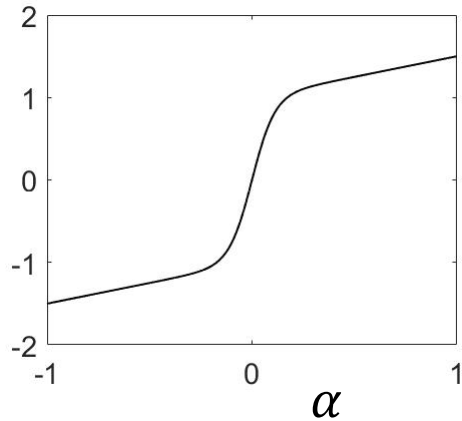
A numerical example:

$$f(\alpha) = \alpha; \quad g(\alpha) = \alpha + 10^{-3} \sin(100\alpha)$$

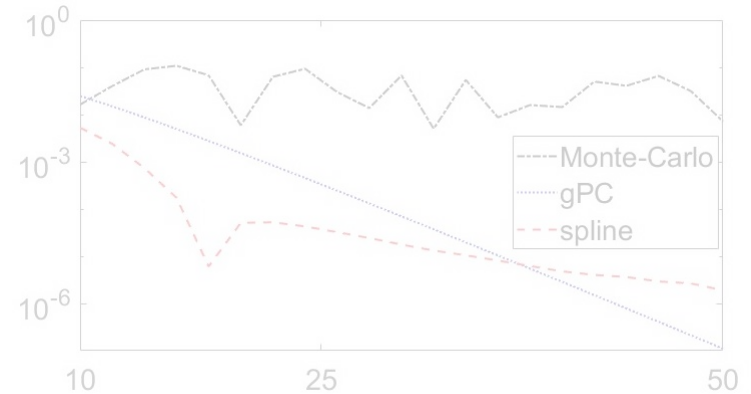


# Numerical example - revisited

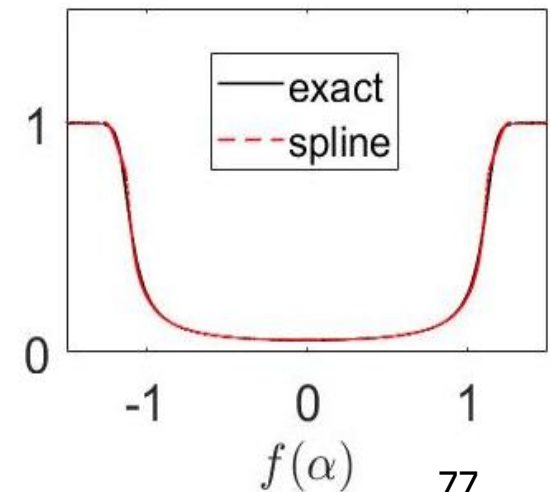
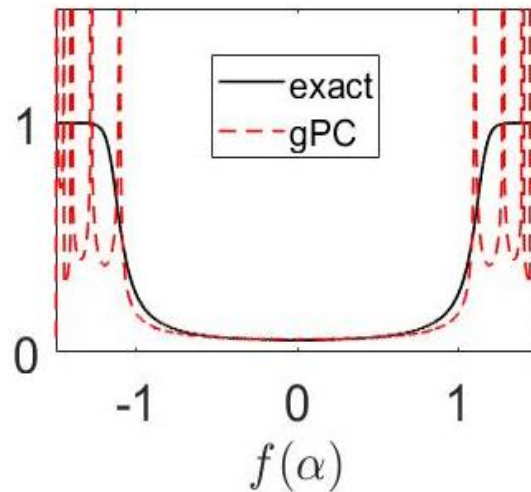
$$f = \tanh(9\alpha) + \frac{\alpha}{2}, \quad \alpha \sim \text{Uniform}[-1, 1]$$



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



PDF approximation,  $N = 12$



# Numerical methods

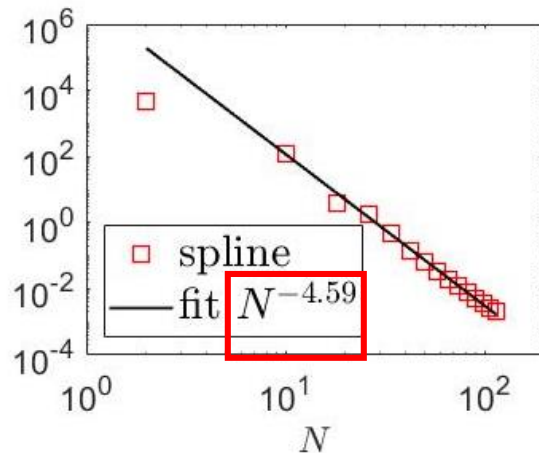
## Theorems 4-5 (AS '19):

Under general smoothness conditions

1. For  $m$  order spline with spacing  $h > 0$ , then

$$\|F_\mu - F_\nu\|_1 \leq Kh^{m+1}$$

CDF error - spline



# Numerical methods

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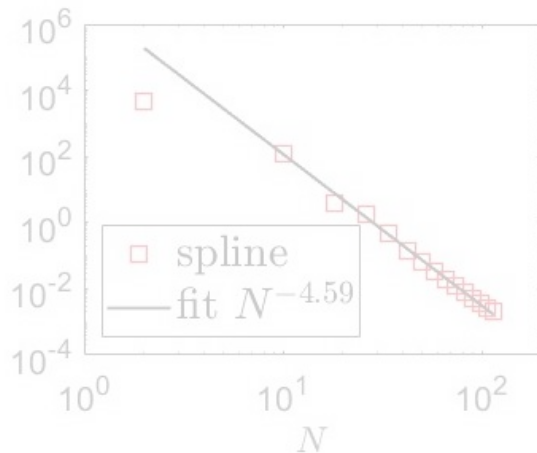
$$\|F_\mu - F_\nu\|_1 \leq Kh^{m+1}$$

2. For analytic function  $f$  and gPC of order  $N$

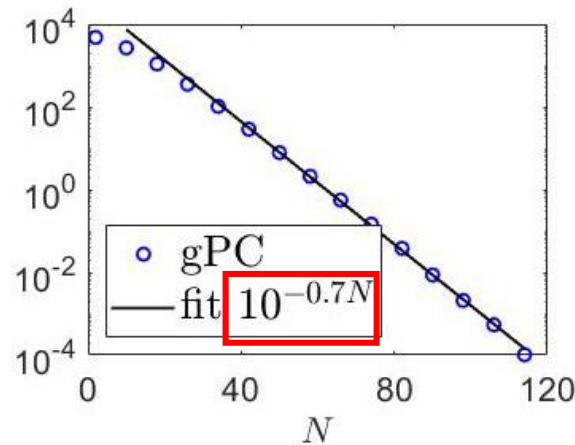
$$\|F_\mu - F_\nu\|_1 \leq C \exp(-\gamma N)$$

gPC result – in sharp contrast to PDF approximation

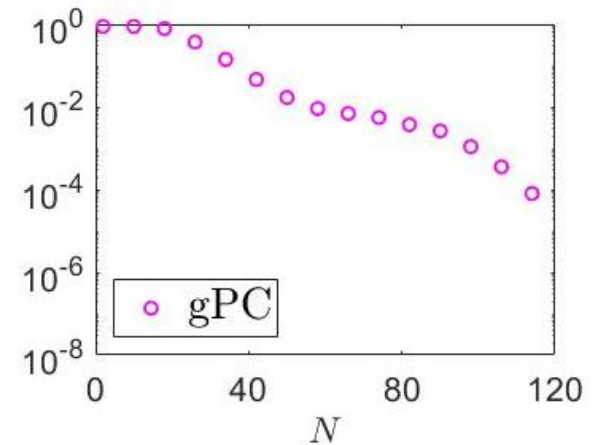
CDF error - spline



CDF error - gPC

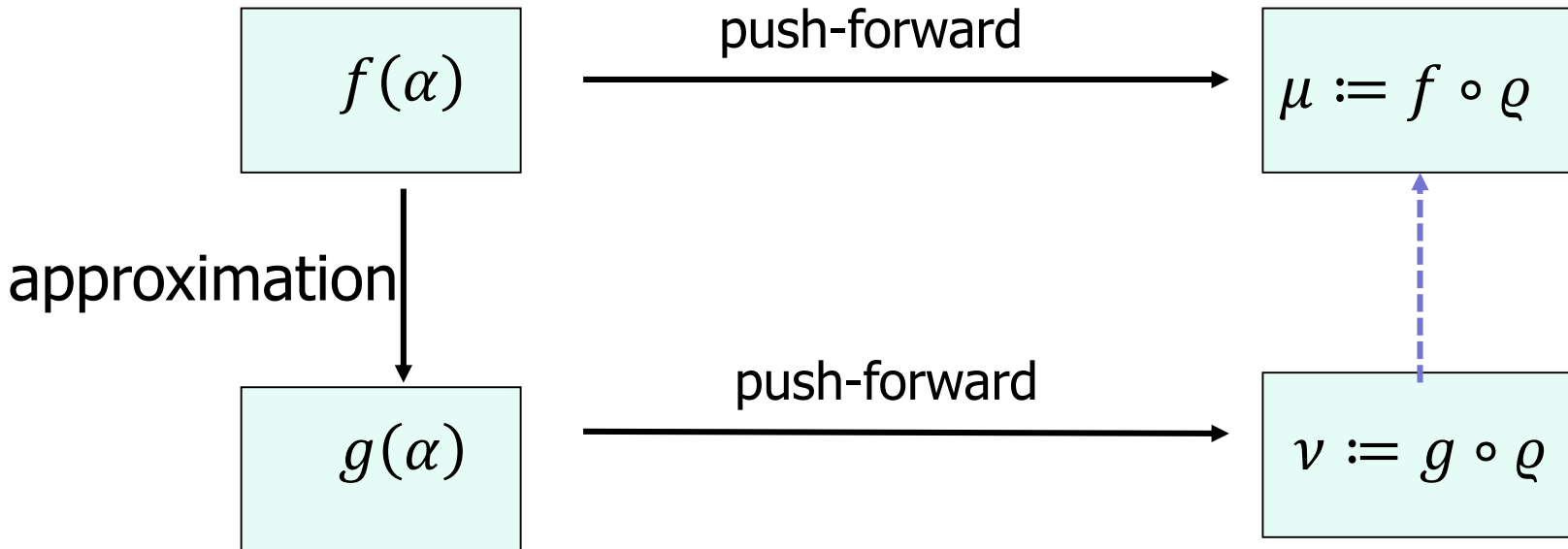


PDF error - gPC



# Lower bounds

$\alpha \sim \varrho$  probability measure



So far

We bounded  $W_p(\mu, \nu)$  by  $\|f - g\|_{L^q}$  **from above**

What about lower bounds?

# Lower bounds – key idea

Wasserstein metric is defined as an infimum, so any transport plan provides an upper bound

Can it be restated as a supremum?



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Can it be restated as a supremum?

Monge Kantorovich–

$$W_1(\mu, \nu) = \sup \left\{ \int_{\mathbb{R}} w(d\mu - d\nu) \mid \text{Lip}(w) \leq 1 \right\}$$

Loeper (2005) & Peyre (2018)

Under certain smoothness assumptions

$$W_2(\mu, \nu) \sim \|\mu - \nu\|_{\dot{H}^{-1}} \quad (\text{supremum functional on } w \in \dot{H}^1)$$

# Lower bounds – proof sketch

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## Proof sketch

choose  $w(z) = c_k y^k$  and recover moments by change of variables, e.g.,

$$\int_{\mathbb{R}} y(d\mu - d\nu) = \int_{\Omega} f(\alpha) d\rho(\alpha) - \int_{\Omega} g(\alpha) d\rho(\alpha)$$

And similarly for  $W_2(\mu, \nu) \dots$

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Under certain smoothness assumptions

$$W_2(\mu, \nu) \sim \|\mu - \nu\|_{\dot{H}^{-1}} \quad (\text{supremum functional on } w \in \dot{H}^1)$$

## Theorems 5&6 (AS '19):

Let  $\Omega \subseteq \mathbb{R}^d$  be bounded, let  $f, g \in C(\bar{\Omega})$ , let  $\varrho$  be a Borel measure

$$W_1(\mu, \nu) \geq |E_{\varrho} f - E_{\varrho} g|,$$

On an interval with Lebesgue measure-

$$W_2(\mu, \nu) \geq C(f, k) |E_{\varrho} f^k - E_{\varrho} g^k| \quad k \geq 1$$

# Conclusions

- Convergence of moments and in  $L^2$  does not guarantee convergence in PDFs
- Spline perform well for PDF approximation
  - With theoretical guarantees in all dimensions.
- Convergence in CDF is “better-behaved” than in PDFs
  - Most popular methods converge in CDF, but not always in PDF
  - Underlying theory – Wasserstein metric

# Thank you!

## References

- A. Sagiv [The Wasserstein Distances Between Pushed-Forward Measures with Applications to Uncertainty Quantification](#) arXiv 1902.05451 (under review at **Communications in Mathematical Sciences**)
- A. Sagiv, A. Ditzkowski, G. Fibich [Density estimation in uncertainty propagation problems using a surrogate model](#) arXiv 1803.10991 (under review)