

# OPTIMIZATION TECHNOLOGY IN STATISTICAL ESTIMATION: FUSION OF HARD AND SOFT INFORMATION

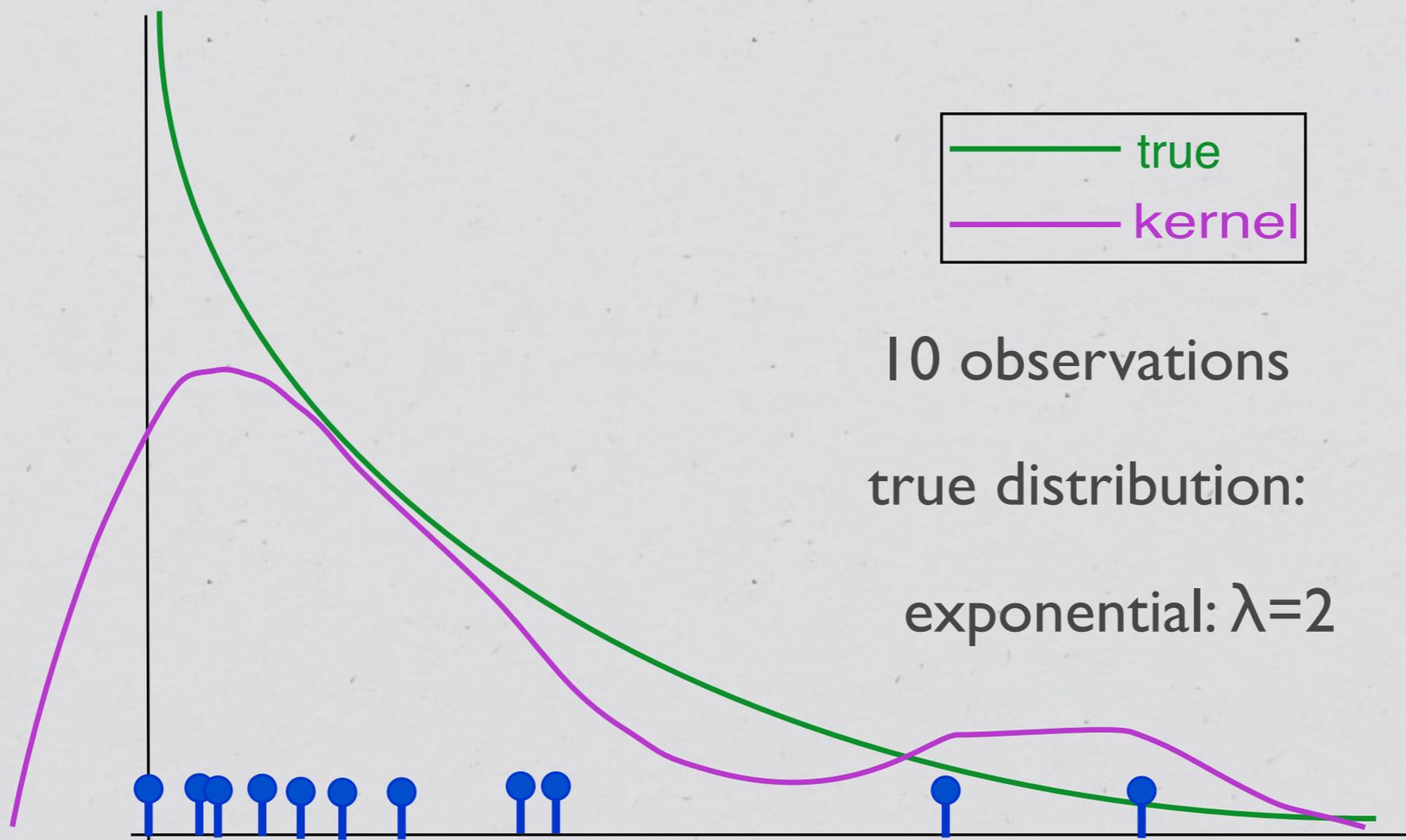
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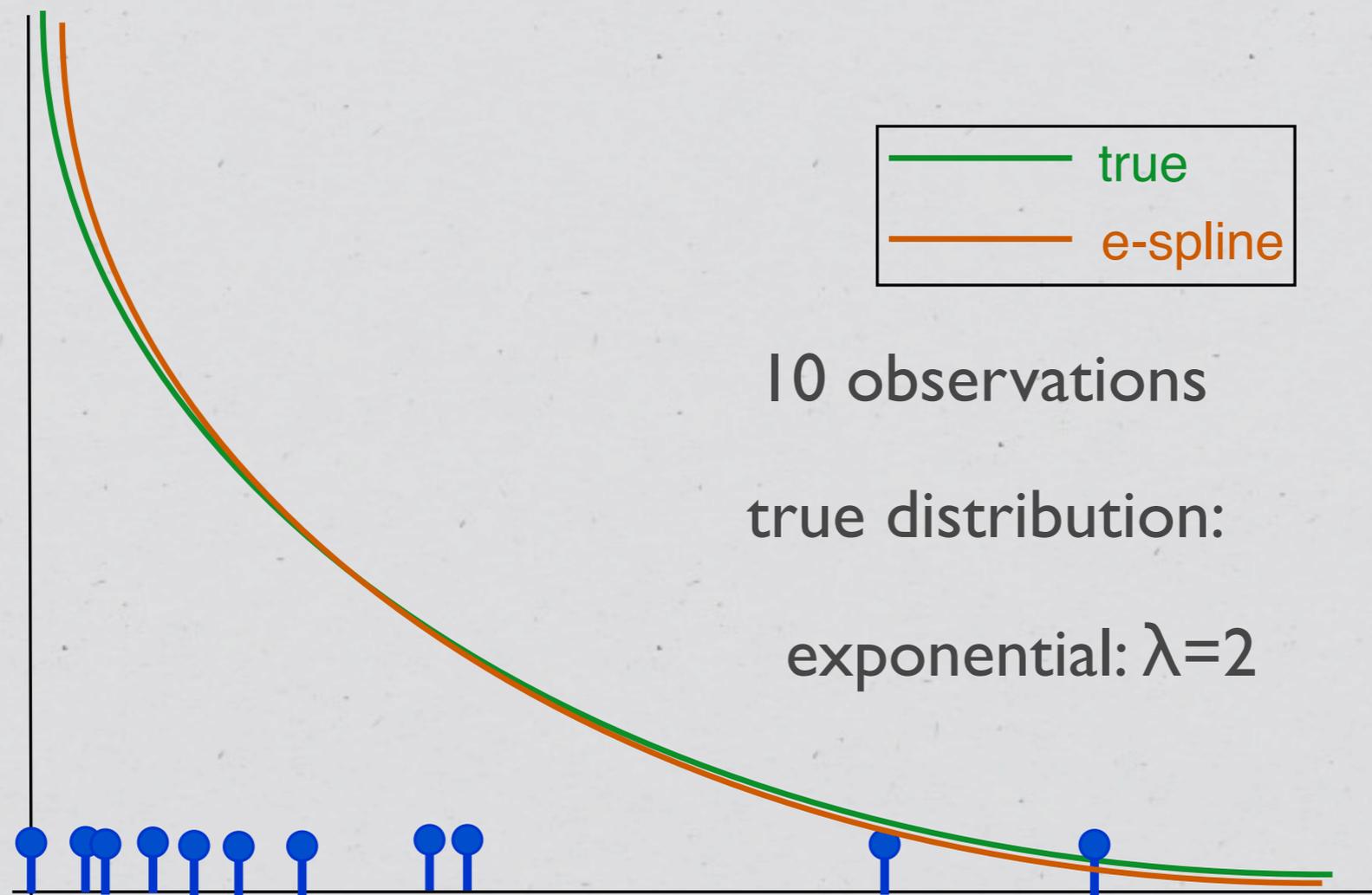
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**Partial support: Army Research Office W911NF-10-1-0246**  
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Georg Pflug (Universität Wien)  
Praha, Summer 2011

# R-STAT: Kernel Estimate



Information used: “continuous distribution” + ...

# “our” Estimate



exploiting **hard and soft** information

density + support & decreasing

# “all” information

- Observations (hard data):  $\xi^1, \xi^2, \dots, \xi^v$
- Non-data facts (soft information)
  - Support: (un)bounded, density or discrete distribution,
  - bounds on expectation, moments,
  - heavy tails
  - shape: unimodal, decreasing, parametric class
- still ‘softer’ information (modeling assumptions):
  - see above + ... level of smoothness, ‘Bayesian’ neighborhood, ..

# An optimization viewpoint

- Find  $h$  in  $H = \text{fcns-class}(\mathbb{R}^n)$  & density ( $\geq 0$ ,  $\int = 1$ )
- that maximizes the probability of observing  $\xi^1, \xi^2, \dots, \xi^v$

$$\max \frac{1}{v} \sum_{l=1}^v \ln h(\xi^l) \quad (\text{likelihood})$$

- $\max E^v \{ \ln h(\xi) \} = \max \int \ln h(\xi) P^v(d\xi)$

# “soft” information

support:  $S = [\alpha, \beta]$ ,  $S = [\alpha, \infty), \dots$

bounds on moments:  $a \leq \int \xi h(\xi) d\xi \leq b$

unimodal:  $h(x) = e^{-Q(x)}$ ,  $Q$  convex (Hessian SDP)

decreasing:  $h'(x) \leq 0$ ,  $\forall x \in S$

'smoothness':  $h \in H_0^1$ ,  $\int \frac{h'(\xi)^2}{h(\xi)} d\xi \leq \kappa$  (Fisher info.)

'Bayesian':  $\|h - h^0\| \leq \beta$ , objective:  $\alpha \cdot \text{bayes}(h, h^0)$

# Estimation: “Opt”-version

$$\max E^v \{ \ln h(x) \} = \frac{1}{v} \sum_{l=1}^v \ln h(x_l)$$

such that  $\int h(x) dx = 1,$

$$h(x) \geq 0, \quad \forall x \in \mathbb{R}$$

$$h \in A^v \subset H$$

$A^v$ : soft (non-data) information constraints

$$H = C^2(S), L^p(S), H^1(S), \dots \quad S \text{ subset } \mathbb{R}$$

# Estimation: “Opt”-version

$$\max E^{\nu} \{ \ln h(x) \} = \frac{1}{\nu} \sum_{l=1}^{\nu} \ln h(x_l)$$

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$$H = C^2(S), L^p(S), H^1(S), \dots \quad S \text{ subset } \mathbb{R}$$

$$H = (\text{lsc-fcns}(S), \text{aw-(epi)-topo}), \text{ Polish space}$$

# Consistency Theorem

Suppose  $v \rightarrow \infty$  (more data is acquired) and  $A^v \rightarrow A$  (valid information is acquired) then estimates  $h^v \rightarrow h^{true}$  *a.s.* (with probability 1).

1949 A. Wald: consistency of parametric estimates (MLH-SAA)

1982-1983 Klonias & Prakasa Rao: consistency of nonparametric estimates

1971 Good & Gaskins: nonparametric roughness penalties (proposed)

1982 B. Silverman & 1990 J. Thompson/R.Tapia: consistency with penalization

1985 P. Groeneboom: Estimating a monotone density

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1979 R. Wets: statistical approach to solution of stochastic program (Tech. Note)

1988 (with J. Dupacova): asymptotics of constrained estimators (parametric)

1991 (with H. Attouch): Law of Large Numbers for random lsc functions

2000 (with X. Dong): consistency of constrained estimators (non-parametric)

2006-10 (with M. Casey): rates of convergence (RKHS, space of lsc-functions)

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# RATES OF CONVERGENCE

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# via Consistency proof

Estimation problem: solution  $h^v$

$$\max F^v(h) = E^v \{ f(\xi, h) \}, h \in \text{lsc-fcns}(\mathbb{R}^n)$$

$$f(\xi, h) = \ln h(\xi) \text{ when } \int h = 1, h \geq 0, h \in A^v$$

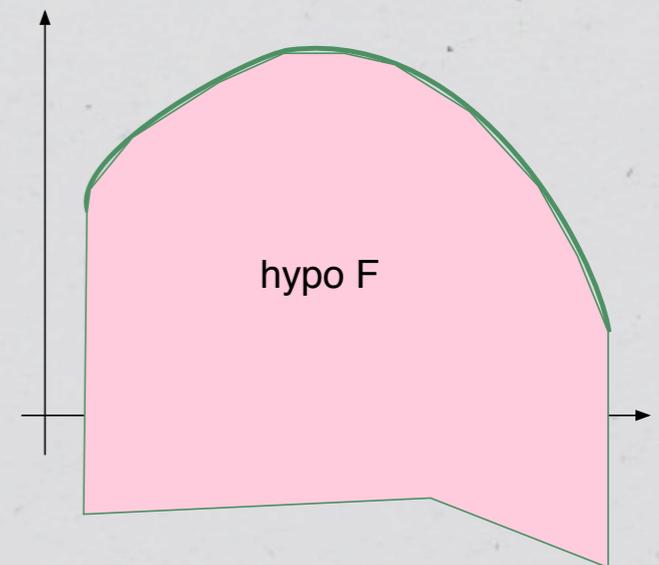
Limit problem: solution  $h^{true}$

$$\max F^\infty(h) = E \{ f(\xi, h) \}, h \in \text{lsc-fcns}(\mathbb{R}^n)$$

hypo  $F^v \rightarrow_{a.s.}$  hypo  $F^\infty$  (LLN for random usc-fcns)

with respect to the aw-distance =hypo-topology

$$\Rightarrow \text{dist}(h^v, h^{true}) \leq \kappa \text{ hypo-dist}(F^v, F^\infty) \rightarrow 0$$



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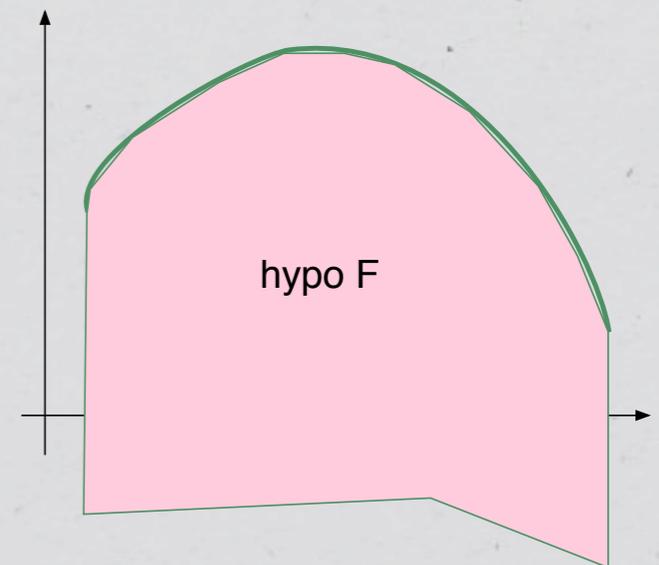
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$$\text{hypo-dist}(F^v, F^\infty) \leq \kappa_1 \mu\text{-dist}(P^v, P)$$

$\Rightarrow$  convergence rate of empirical processes (van der Vaart & Wellner)



# Under investigation (large Deviations)

- \* Hoeffding's inequalities
- \* Nemirovski's inequalities
- \* & Nemirovski's inequalities revisited
  - \* (L. Dümbgen, S. van de Geer, M. Veraar & J. Wellner)
- \* Sanov's Theorem
- \* CLT for (unbounded) random sets (A. Pichler & Co.)

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# NUMERICAL STRATEGIES

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# from infinite to finite dimensional Optimization

$$h \approx \sum_{k=1}^q u_k \phi_k(\cdot)$$

Fourier coefficients, wavelets, kernel-dictionary, ...

$h = \exp(s(\cdot))$  exponential epi-spline

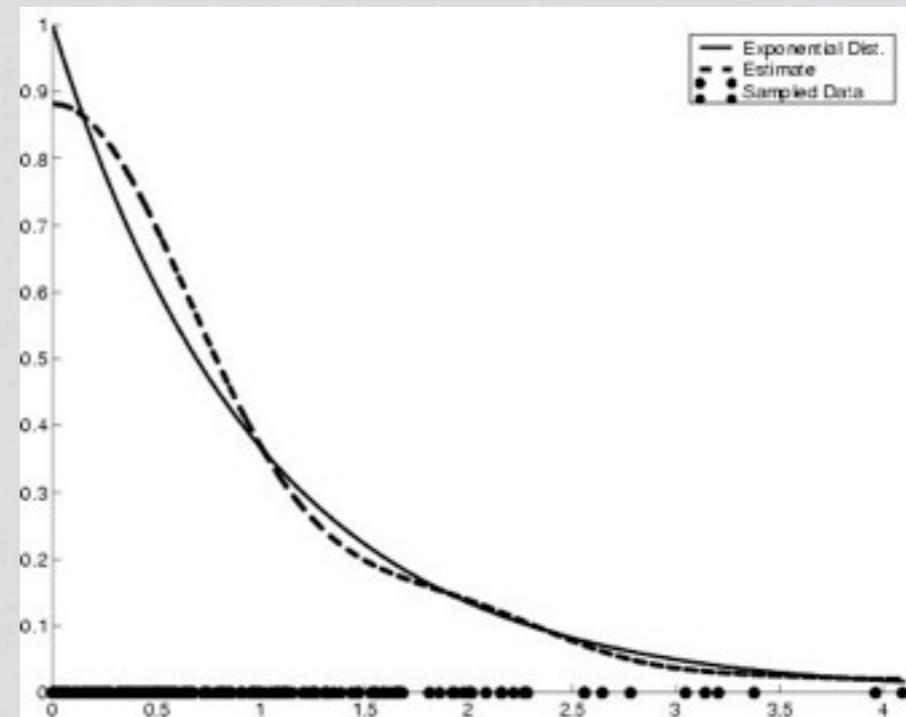
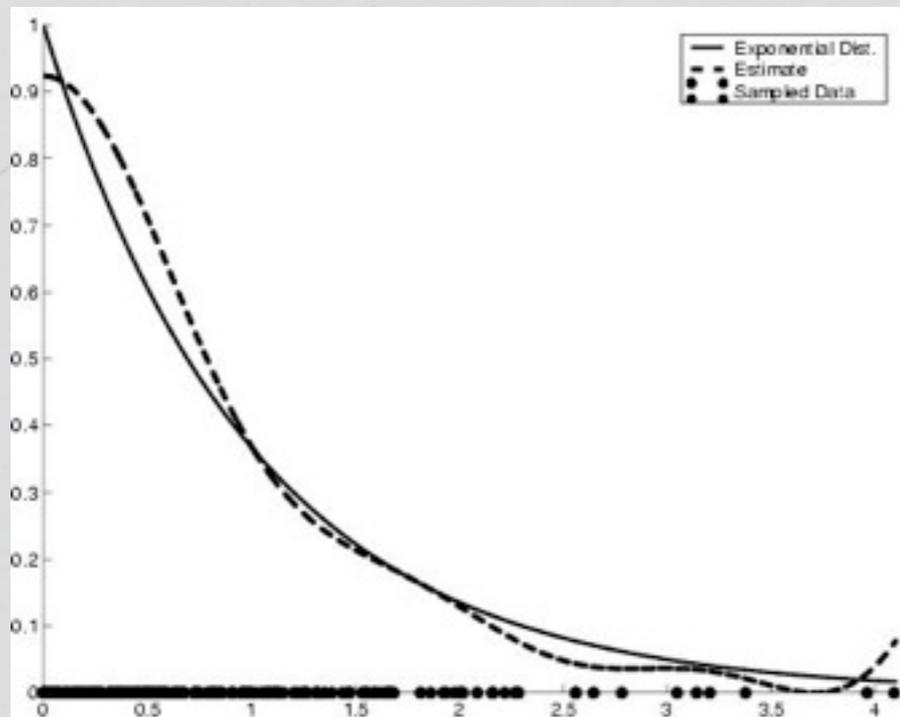
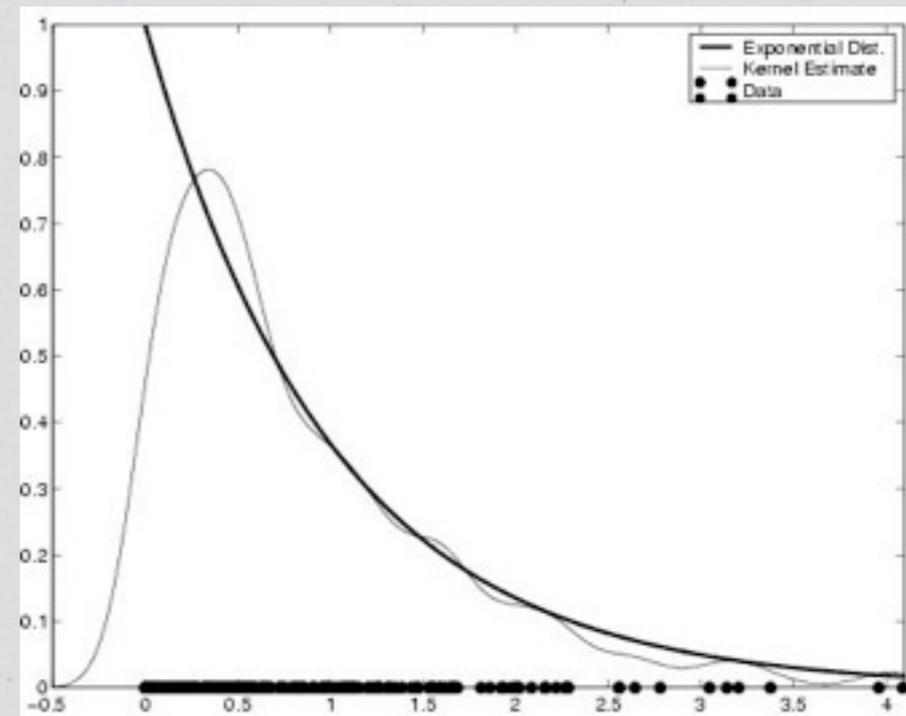
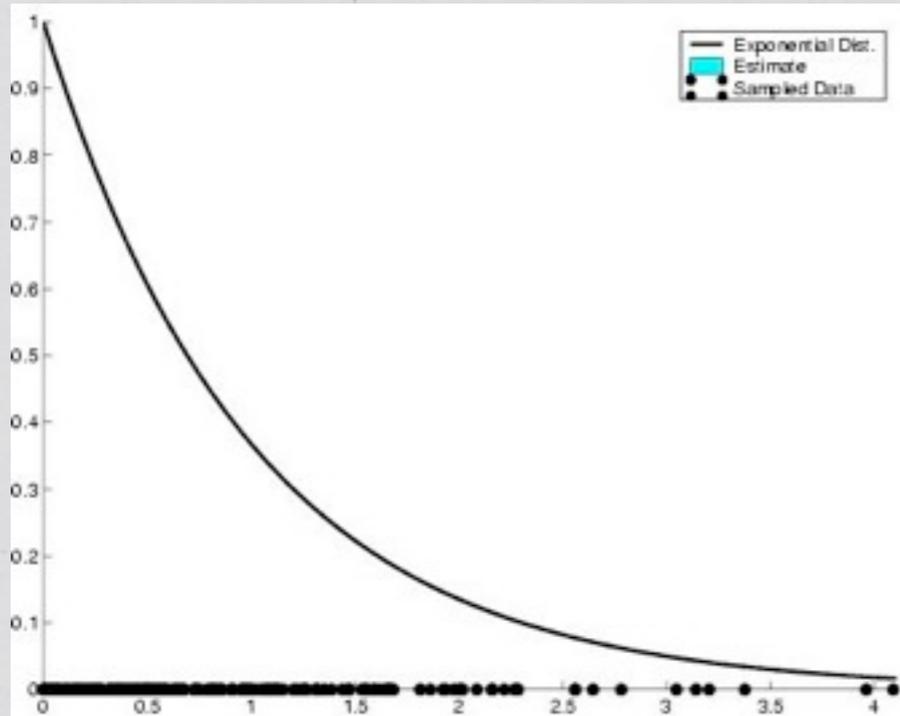
$s(\cdot)$  cubic (or quadratic) epi-spline, spline-like

$\Rightarrow$   $n$ -dimensional theory of epi-splines

# Test Case: exponential

- $h^{true}(x) = \lambda e^{-\lambda x}$  if  $x \geq 0$ ;  $= 0$  if  $x < 0$  ( $\lambda = 1$ )
- “empirical” estimate
- kernel estimate from **R-stat**
- unconstrained with support (non-negative)
- constrained ( $h$  decreasing)
- parametric, i.e.,  $h \in \text{exp-class}$

# 200-observations



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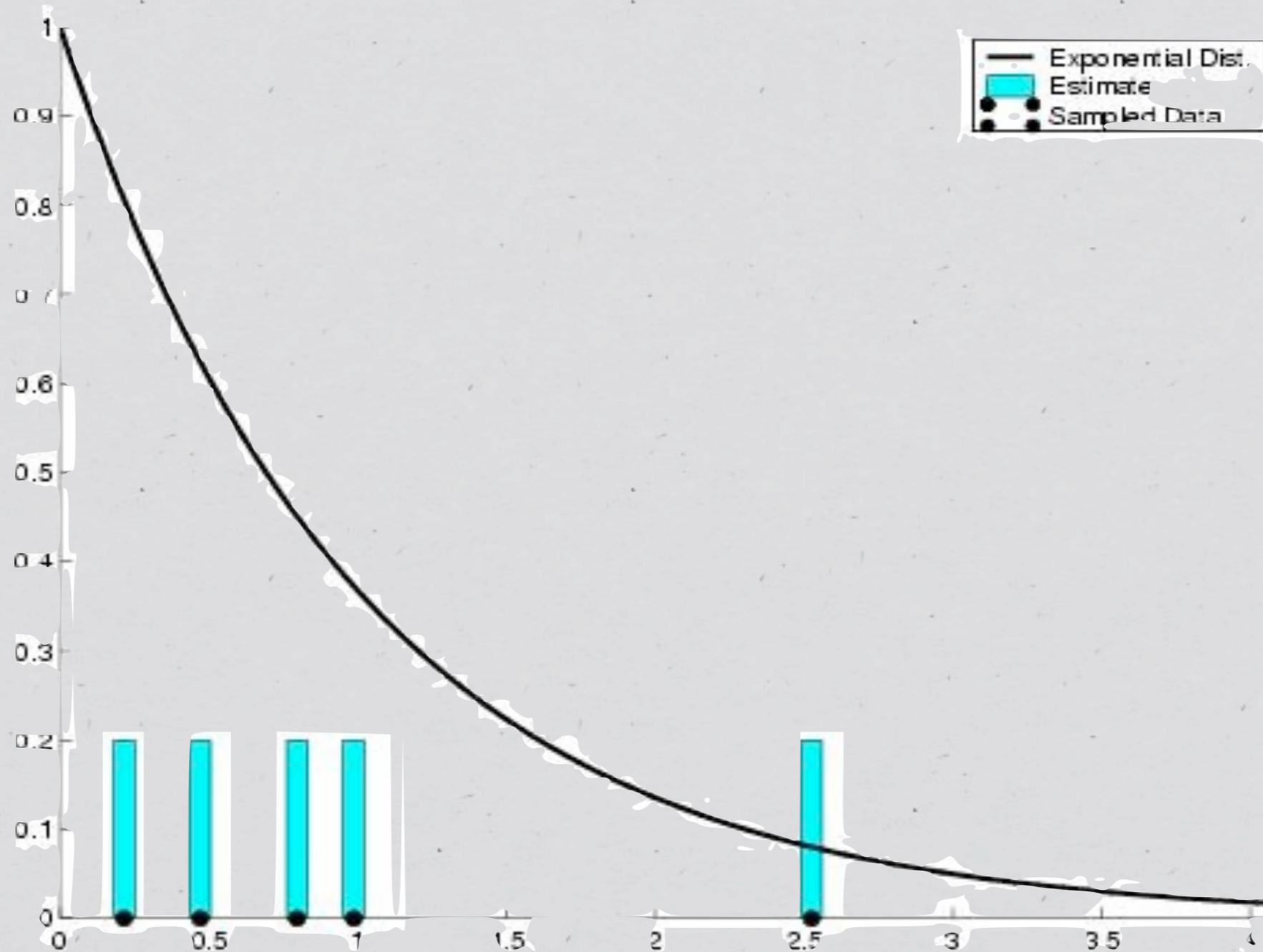
**BUT WHAT ABOUT  
5 SAMPLE POINTS?**

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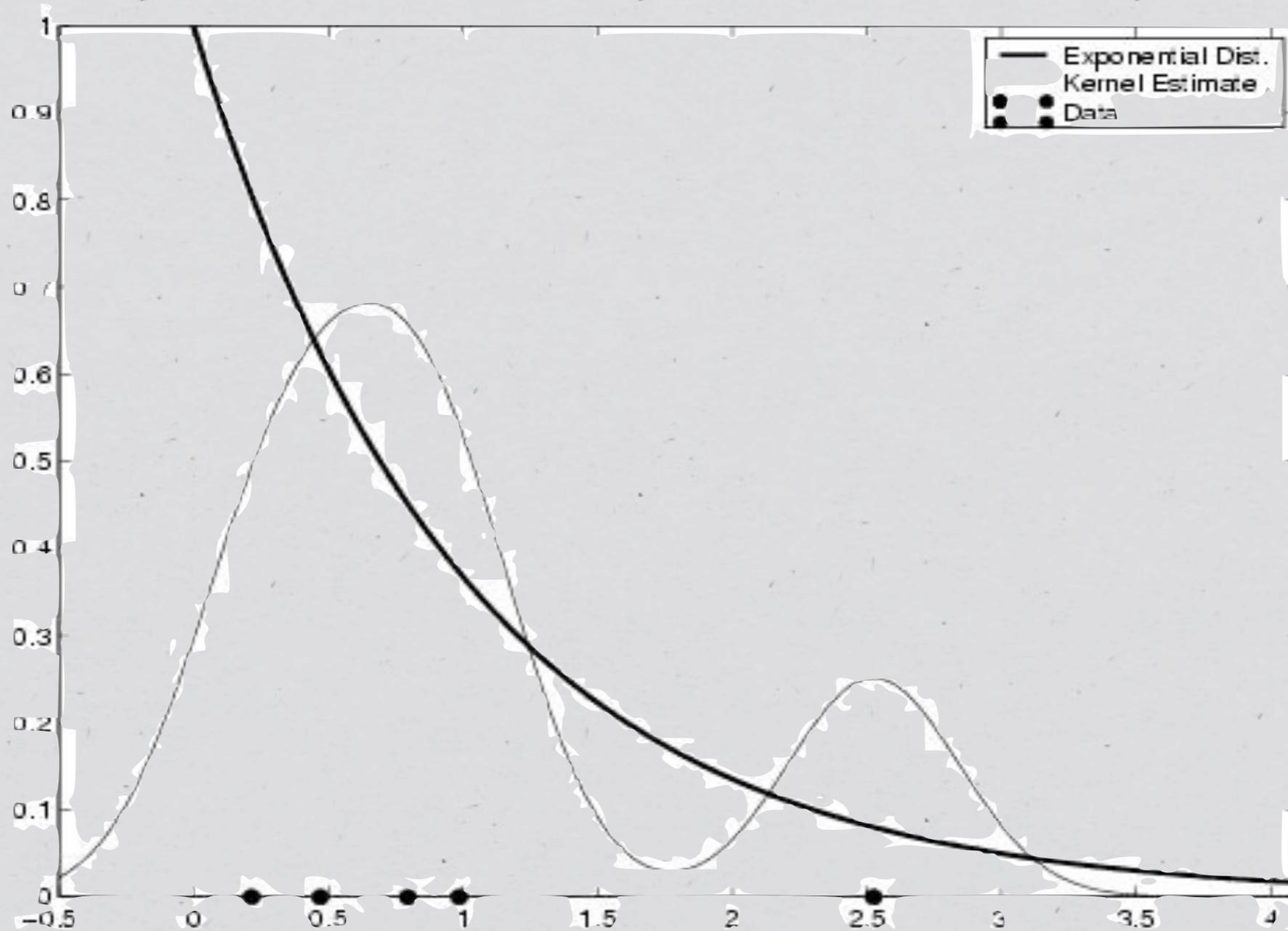
$h^{est}$

: empirical estimate



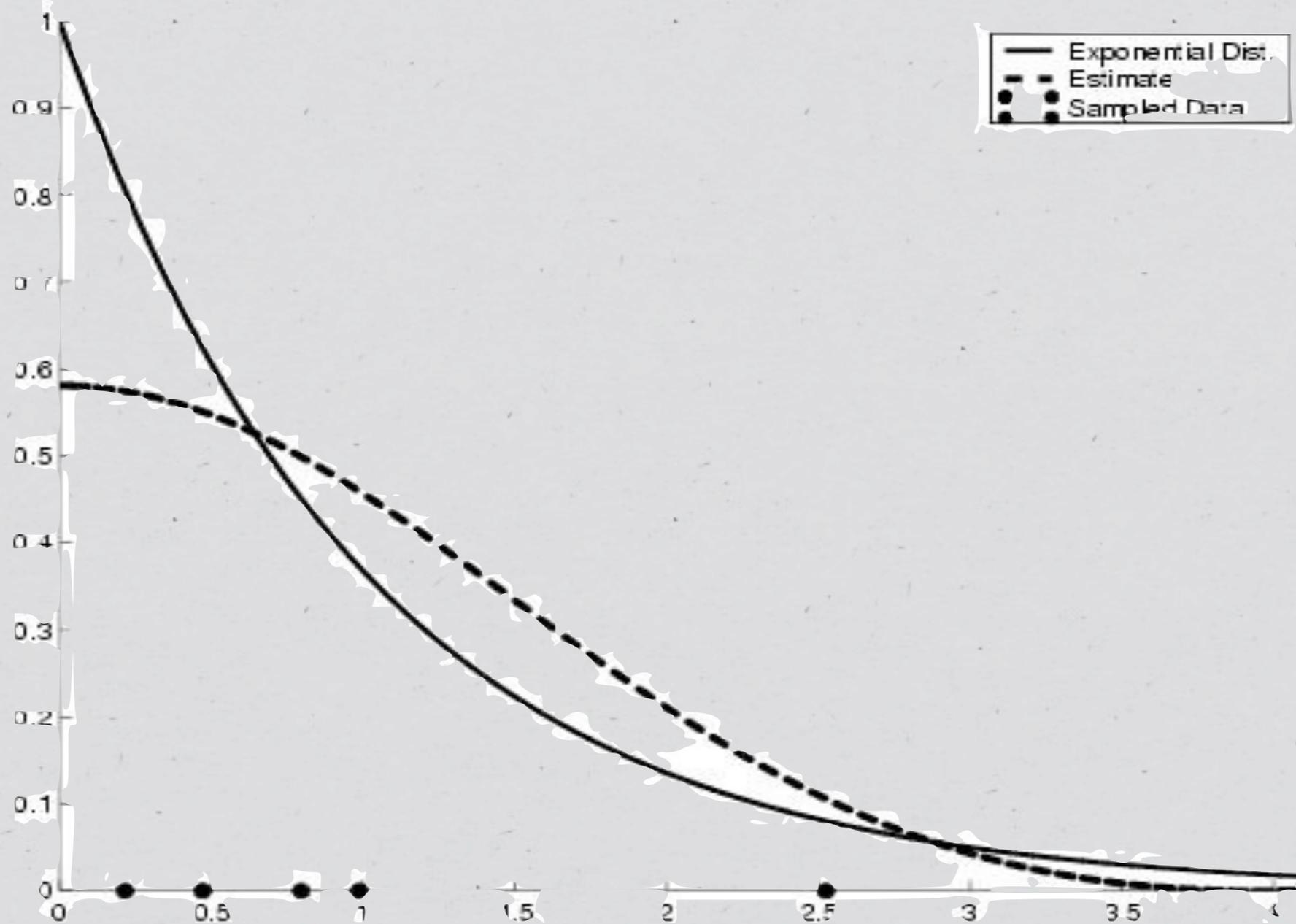
$h^{est}$

: kernel estimate (R-stat)



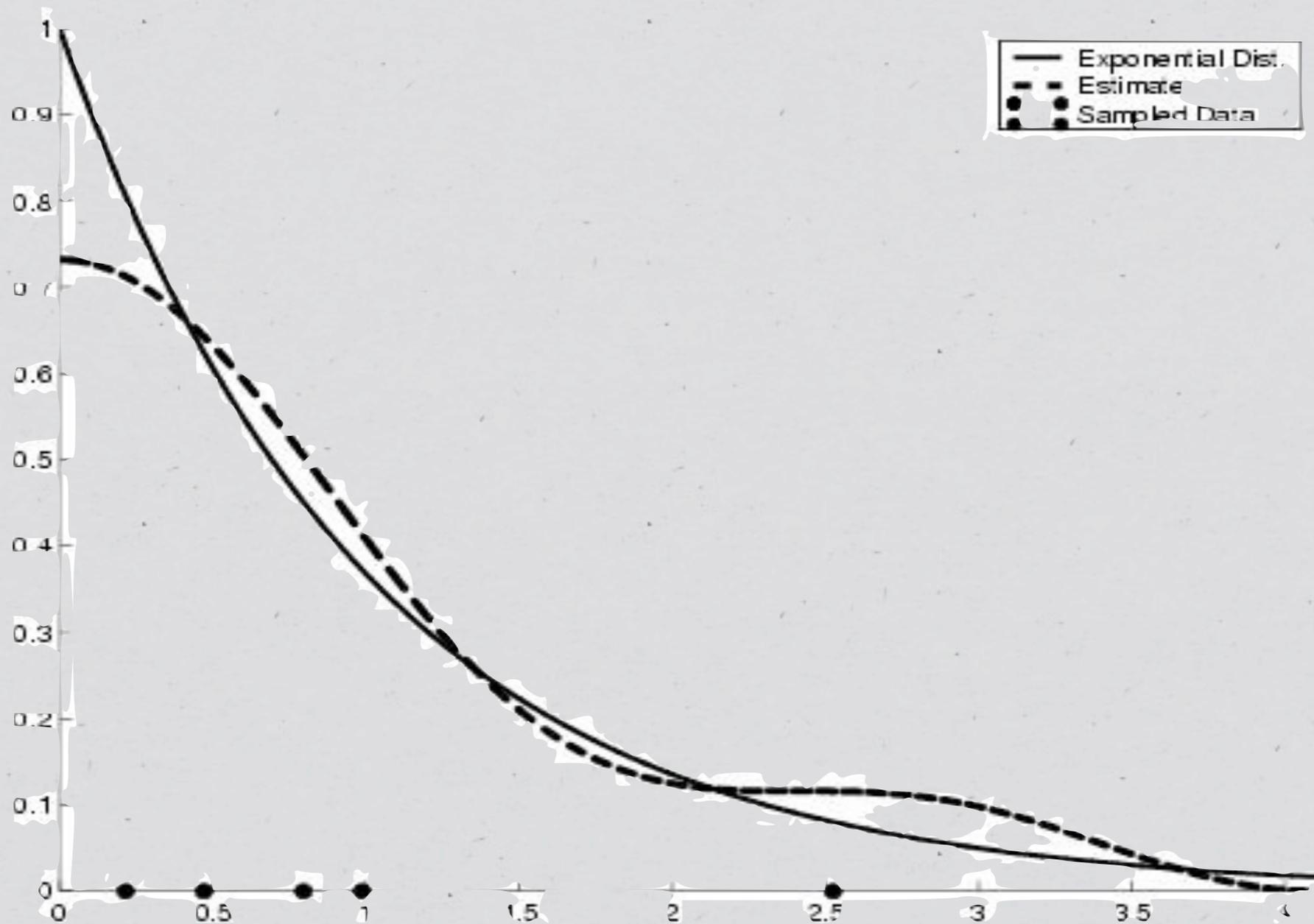
$h^{est}$

: ..with known support



$h^{est}$

: decreasing density



# ERROR 'ANALYSIS'

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## NUMERICAL EXPERIMENTATION

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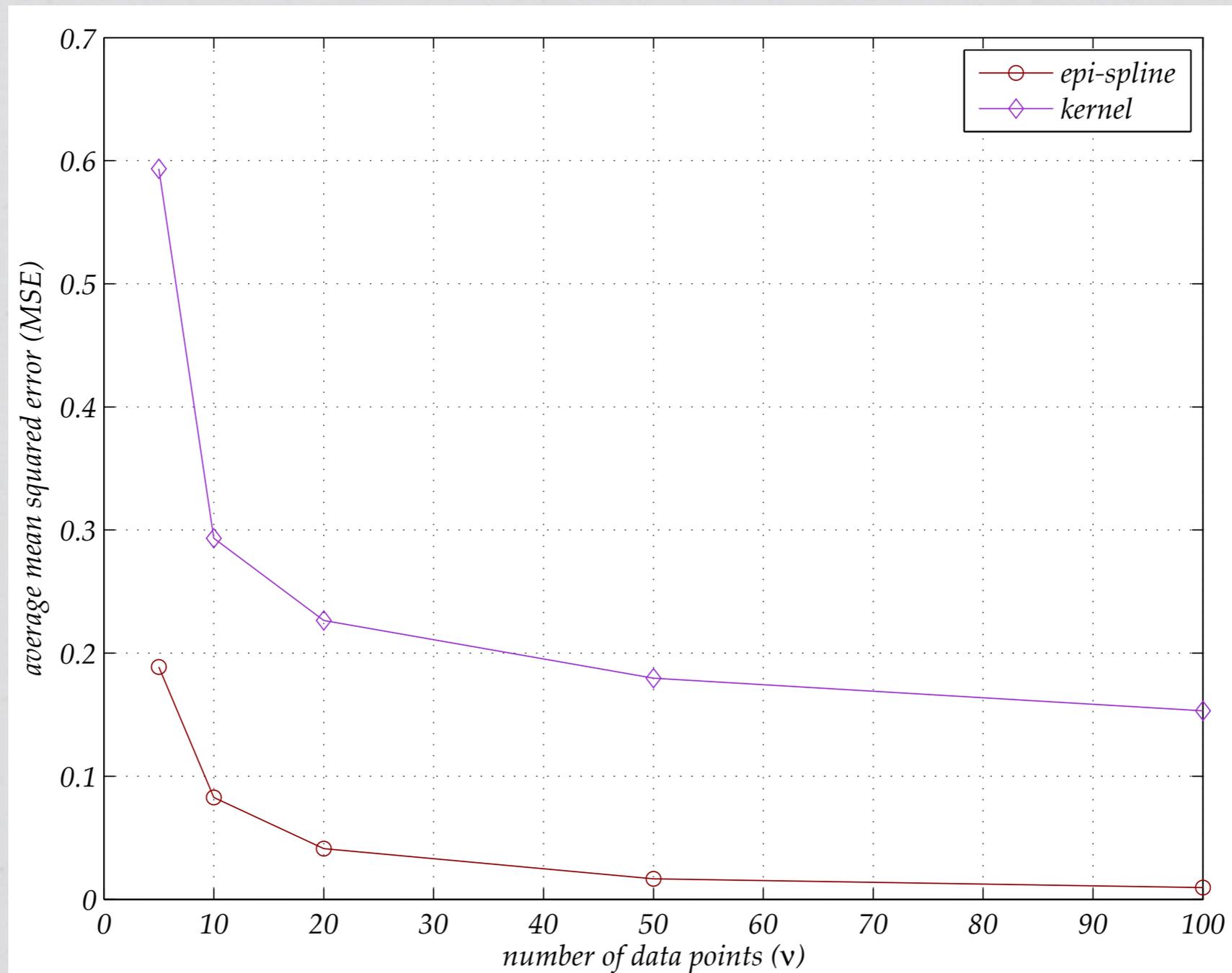
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#runs: 10,000

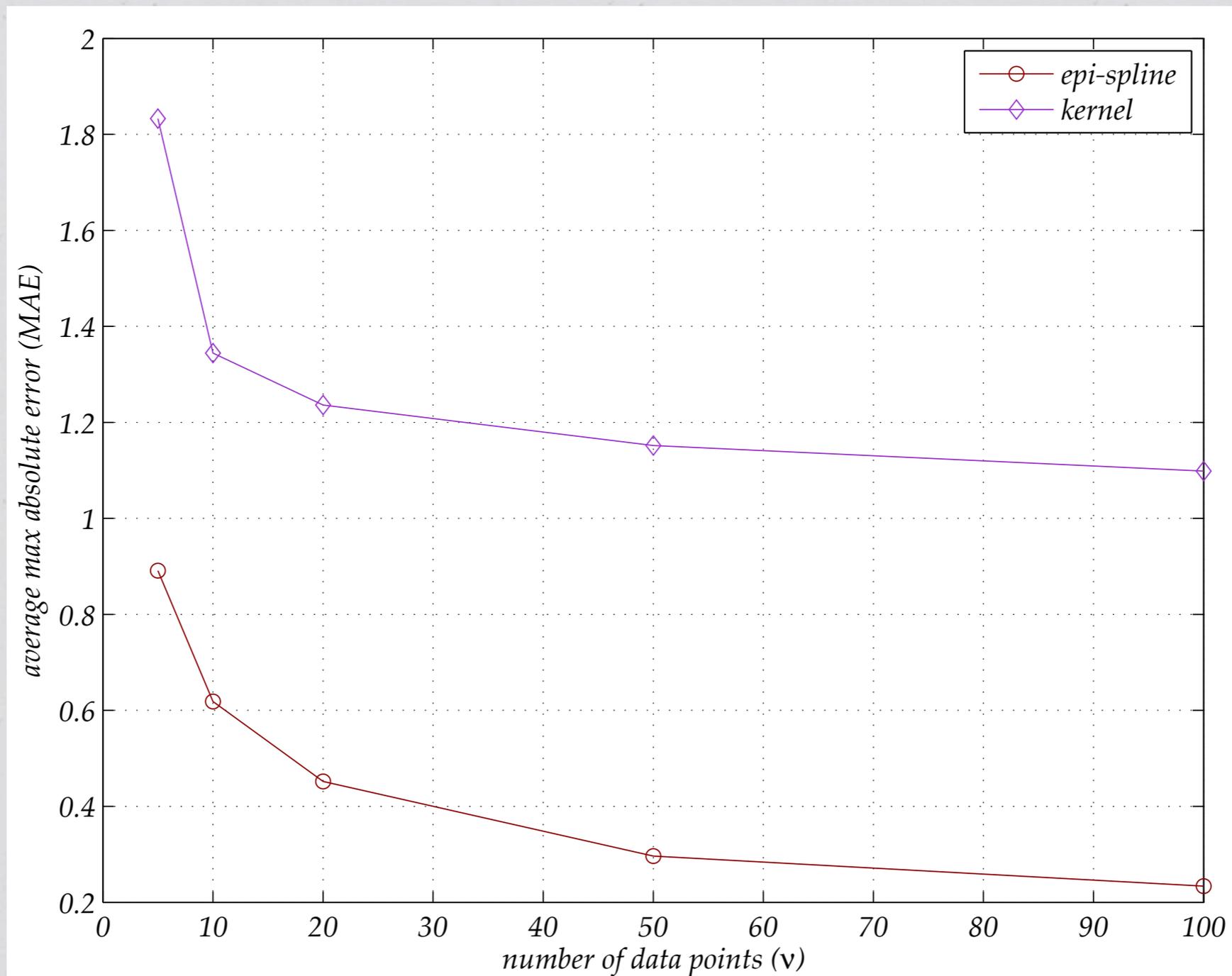
mean square error

mean absolute error

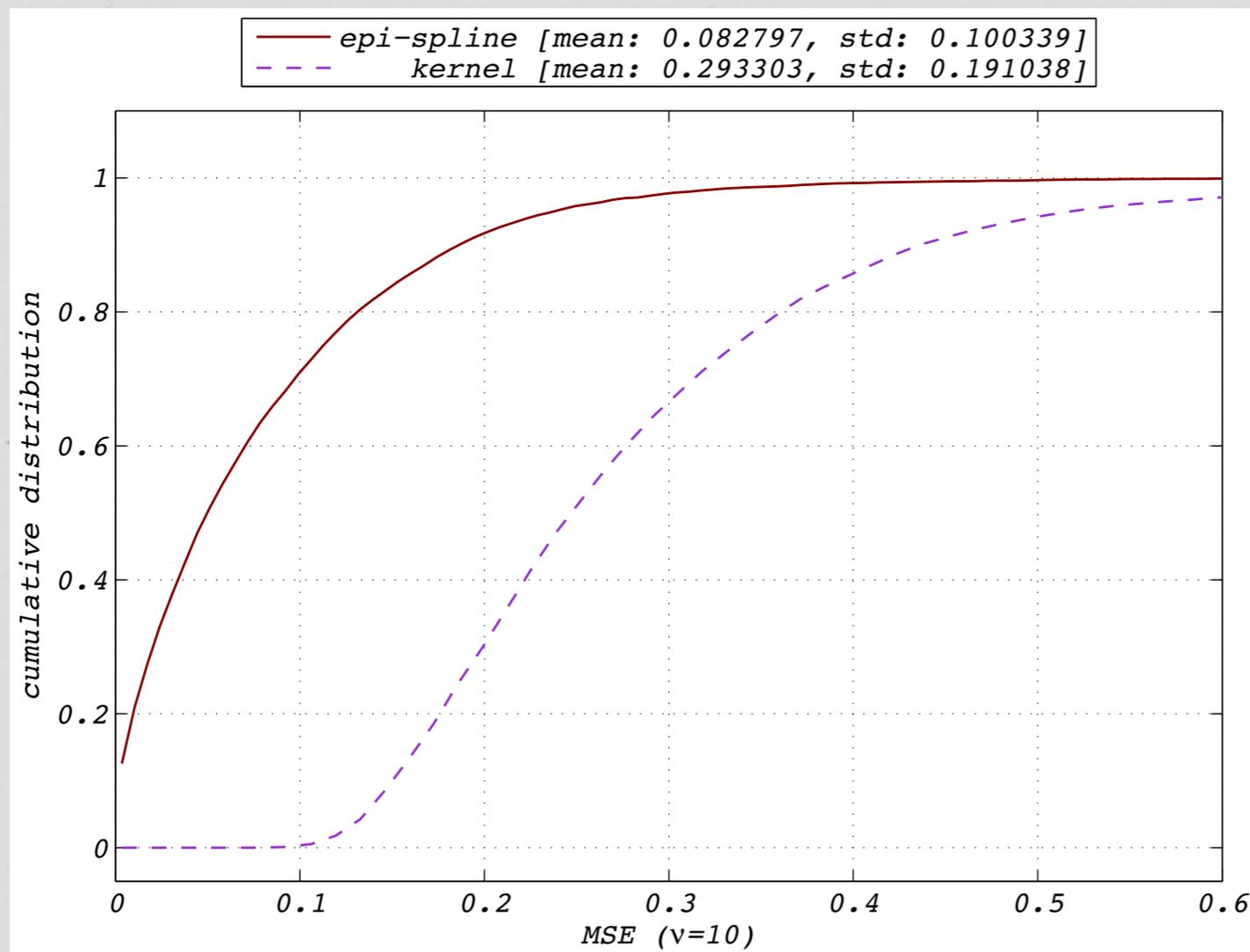
# Exponential Distribution



# Exponential Distribution



# Does it pay off? Error Analysis



Mean square error

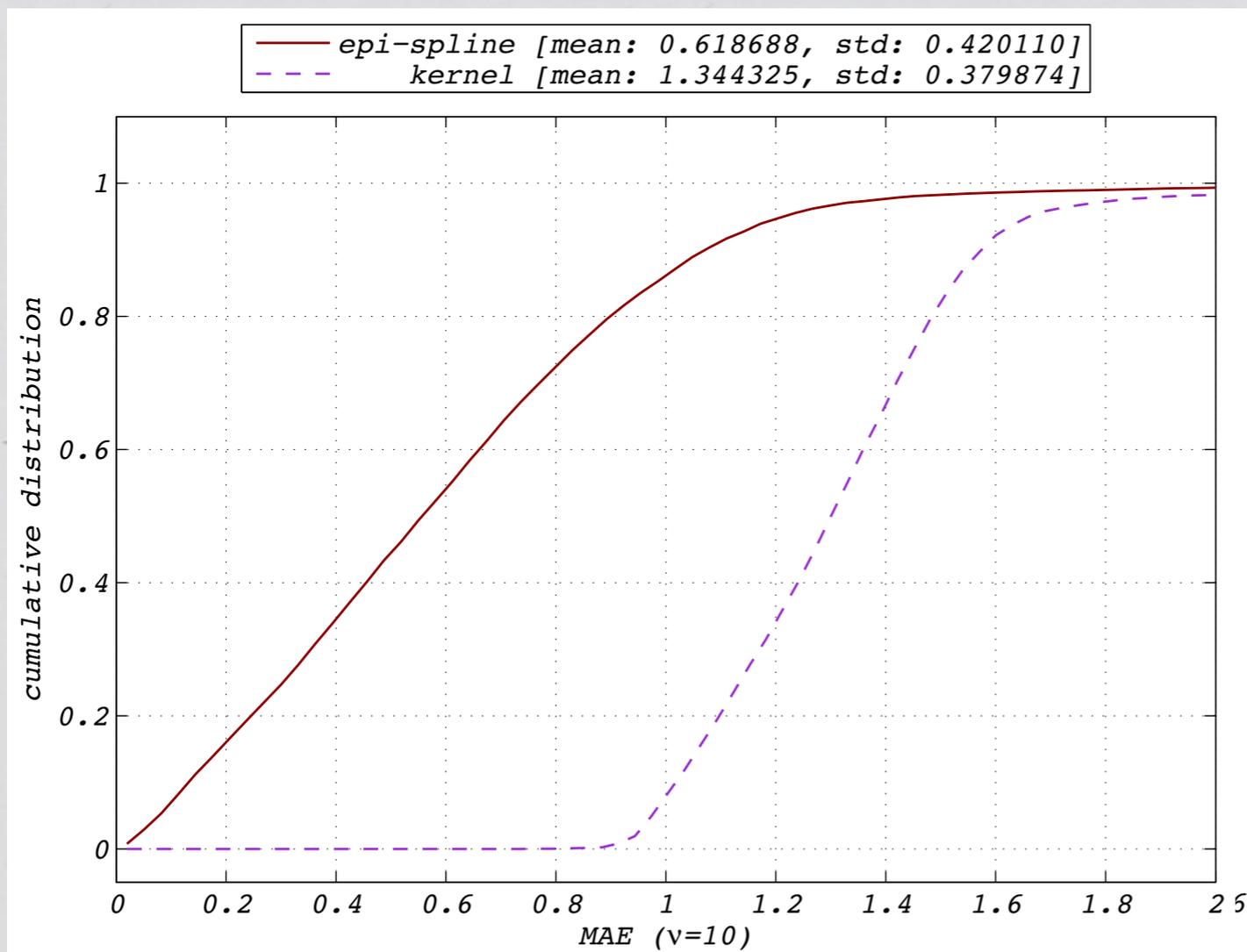
# samples: 10

# runs: 10,000

kernel estim: 0.293

epi-spline est.: 0.083

# Does it pay off? Error Analysis



Max. absolute error

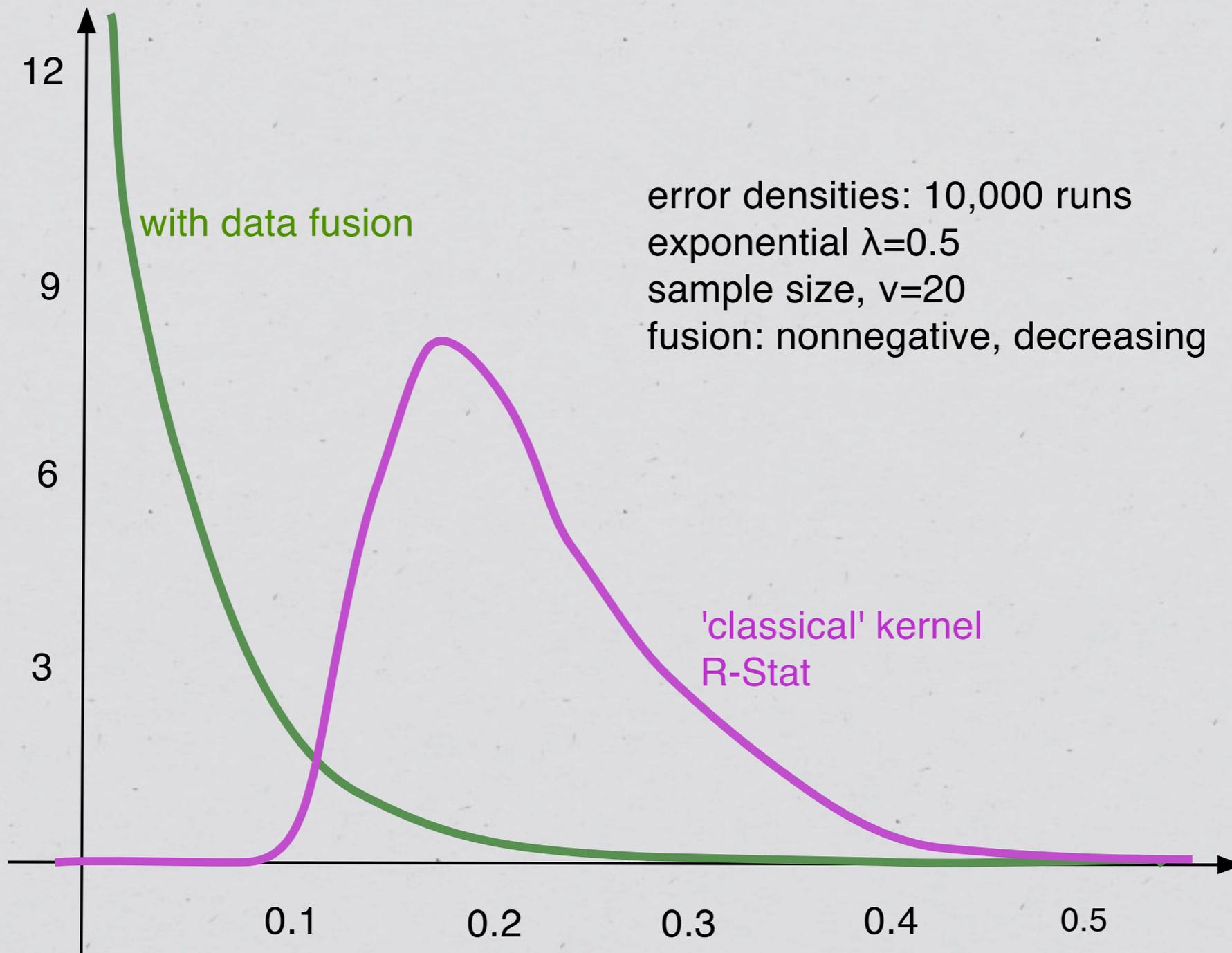
# samples: 10

# runs: 10,000

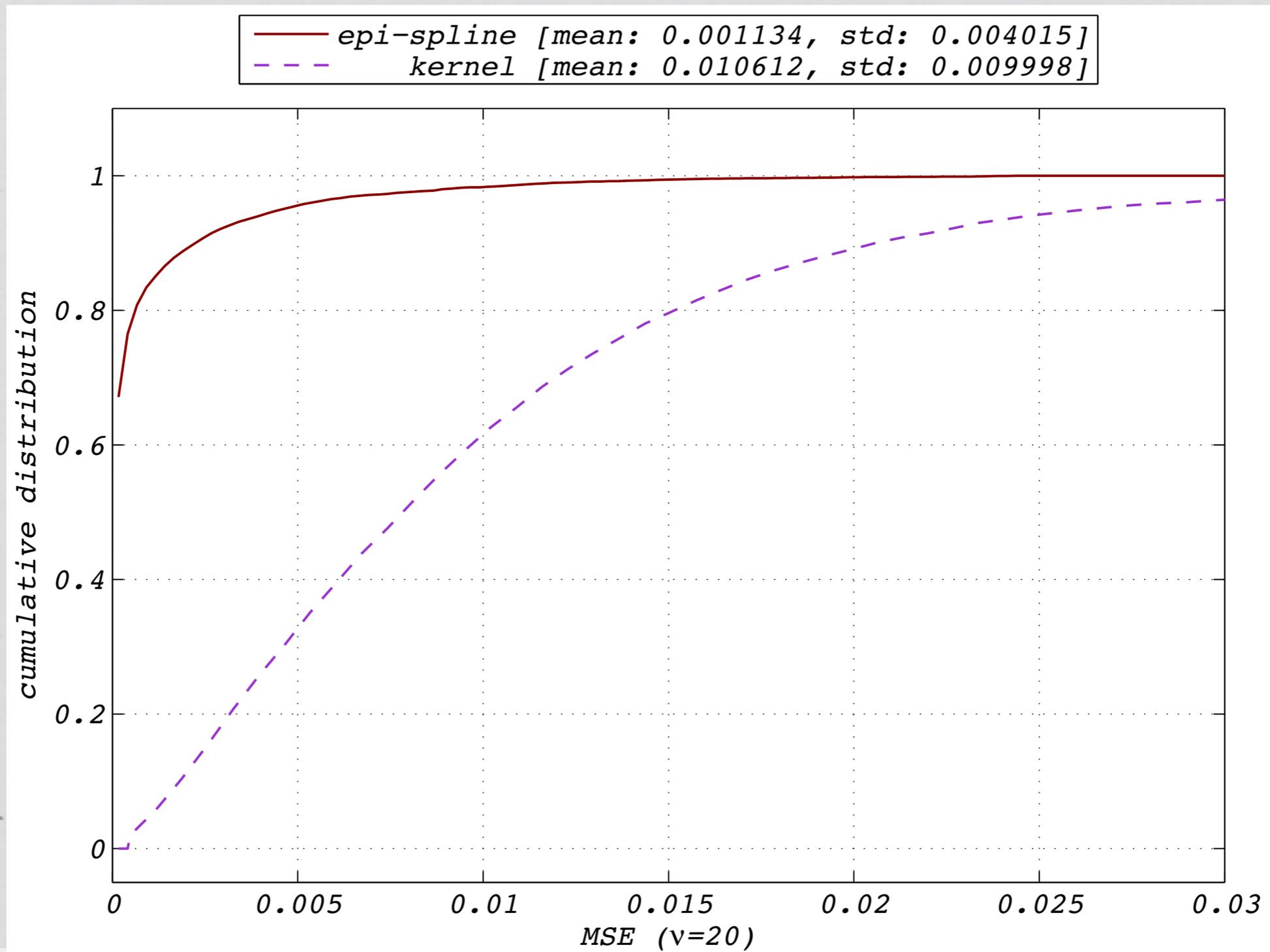
kernel estim: 1.344

epi-spline est.: 0.619

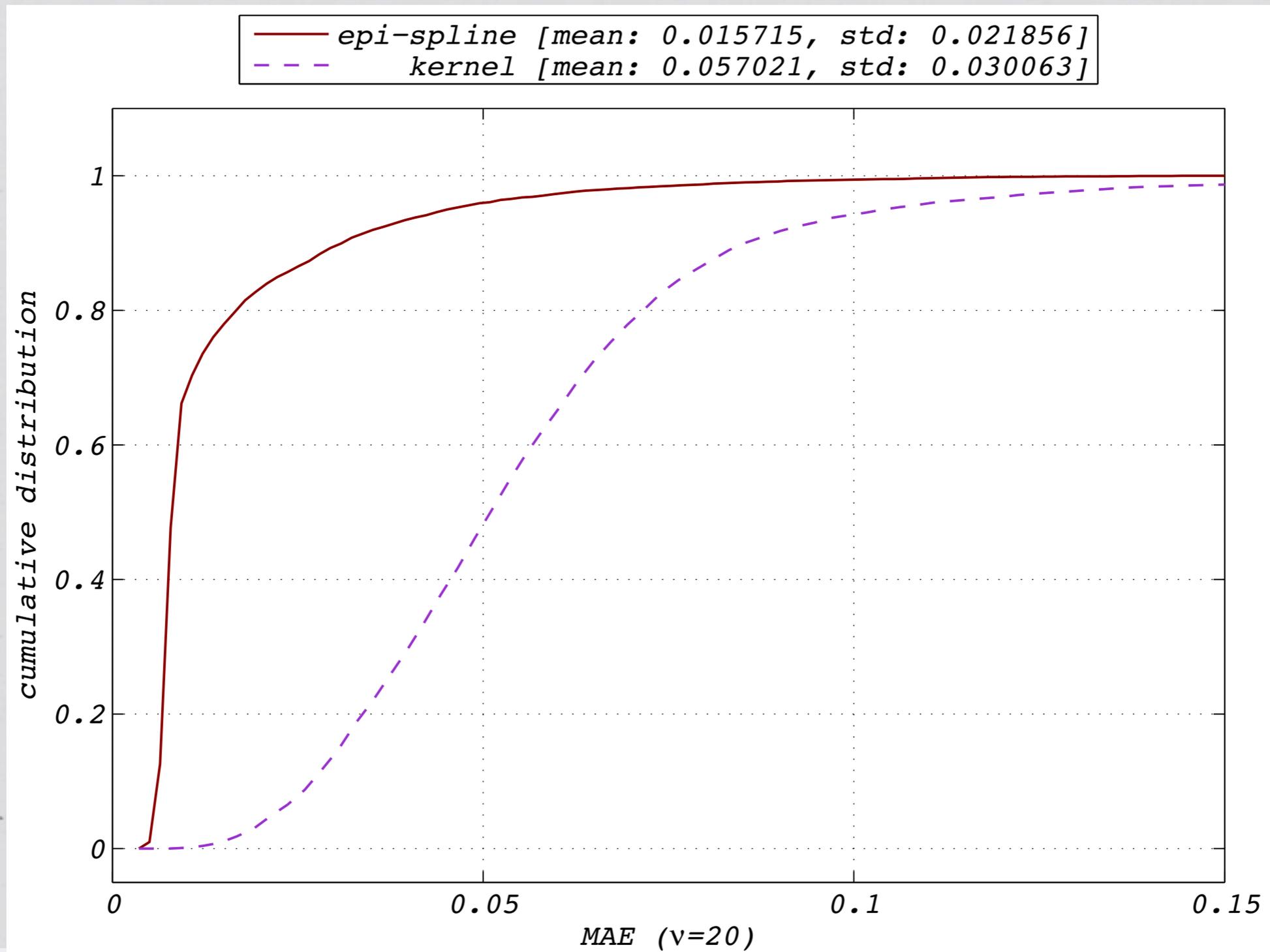
# Densities: Error distributions exponential case



# Gaussian Distribution



# Gaussian Distribution



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# EXTENSIVE EXPERIMENTATION

[www.math.ucdavis.edu/~prop01](http://www.math.ucdavis.edu/~prop01)

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# **EPI-SPLINES**

## **An Approximation Tool**

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# epi-spline: 2nd Order

$c : (a, b] \rightarrow \mathbb{R}$  twice differentiable (not  $C^2$ )

$c'' : (a, b] \rightarrow \mathbb{R}$  2nd derivative approximated by  $z : \mathbb{R} \rightarrow \mathbb{R}$

split  $(a, b]$ :  $\{(x_{k-1}, x_k], k = 1, \dots, N\}$ ,  $N$  relatively large

fix  $z(t) = z_k$  (constant) for  $t \in (x_{k-1}, x_k]$

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2nd order epi-spline (1-dim.) +++ mesh =  $\max_{k=1, \dots, N} |x_k - x_{k-1}| = m$

$$s_m(x) = s_0 + v_0 x + \int_0^x dr \int_0^r dt z(t), \quad z(t) \equiv z_k \text{ on } (x_k, x_{k+1}]$$

$$= s_0 + v_0 x + \sum_{j=1}^k a_{kj} z_j \quad \text{when } x \in (x_k, x_{k+1}]$$

$s_m \in C^{1, +pl}$ , linear w.r.t.  $s_0, v_0, z_1, \dots, z_N$  (finite # parameters)

as mesh  $m \searrow 0$ ,  $\max \|s_m - c\|^2 \rightarrow 0$  and  $s_m$  epi-converges to  $c$

# Epi-splines

originally (Wets, Bianchi & Yang, 2002):

derive financial curves,

later, also stochastic volatility

Epi-splines of  $k$ th order:

piece-constant  $k$ th derivative

still linear w.r.t. its parameters

and epi-convergence to  $c$

# Exponential epi-spline 1-dimensional, 2nd order

$$h(x) = e^{-s(x)}$$

$$s(x) = s_0 + v_0 x + \int_0^x dr \int_0^r dt z(t), \quad z(t) \equiv z_k \text{ on } (x_k, x_{k+1}]$$
$$= s_0 + v_0 x + \sum_{j=1}^k a_{kj} z_j \quad \text{when } x \in (x_k, x_{k+1}]$$

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$$\max E^v [\ln h(\xi)] = \frac{1}{v} \sum_{l=1}^v \ln h(\xi^l) = \min \frac{1}{v} \sum_{l=1}^v s(\xi^l)$$

$$\text{such that } \int e^{-s(\xi)} d\xi \leq 1. \quad (h \geq 0)$$

$$z_k \in [-\kappa_l, \kappa_u] \quad \text{'constrained' curvature}$$

unimodal:  $\kappa_l = 0 \Rightarrow s(\cdot)$  convex

# Higher-dimensional epi-splines

## 2-DIMENSIONAL - FIRST VERSION

$$s(x, y) = z_0 + v_1 x + v_2 y + \int_0^x d\tau \int_0^\tau d\theta a(\theta) \\ + \int_0^y d\tau \int_0^\tau d\theta b(\theta) + \int_0^x d\tau \int_0^y d\theta c(\tau, \theta)$$

on  $(x_{k-1}, x_k]$ :  $a(x) = a_k$ ,

on  $(y_{k-1}, y_k]$ :  $b(y) = b_k$ ,

on  $(x_{k-1}, x_k] \times (y_{l-1}, y_l)$ :  $c(x, y) = c_{kl}$

requires boundary continuity properties

estimation :  $a_k$  and  $b_k \Rightarrow$  marginal distributions

$c_{kl}$  correlation coefficients (locally)

# Higher-dimensional epi-splines

## 2-DIMENSIONAL - FIRST VERSION

$$\nabla^2 s(x) = \begin{pmatrix} a_{k-1,l-1} & a_{k-1,l} \\ a_{k,l-1} & a_{k,l} \end{pmatrix} \text{Hessian}$$

on open rectangle  $(x_{k-1}, x_k) \times (y_{l-1}, y_l)$

unimodal  $h(x) = e^{-s(x)} \Rightarrow s$  convex (globally)

$\nabla^2 s(x)$  positive semidefinite, symmetric

(3 parameters)

rectangle boundary values: (at a mesh)

via monotonicity of  $\nabla s(x)$

all conditions included in the optimization problem

# example: Normal density

mean = (0,0) ... data samples correlated

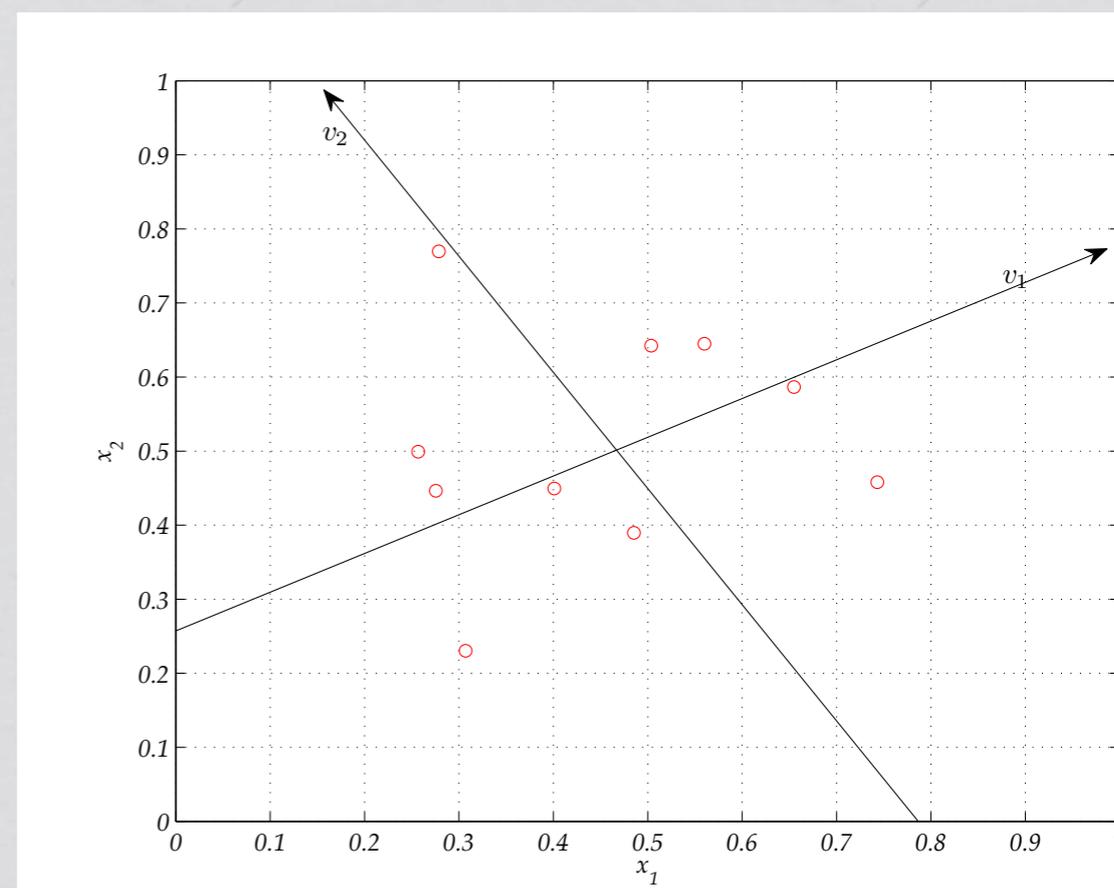
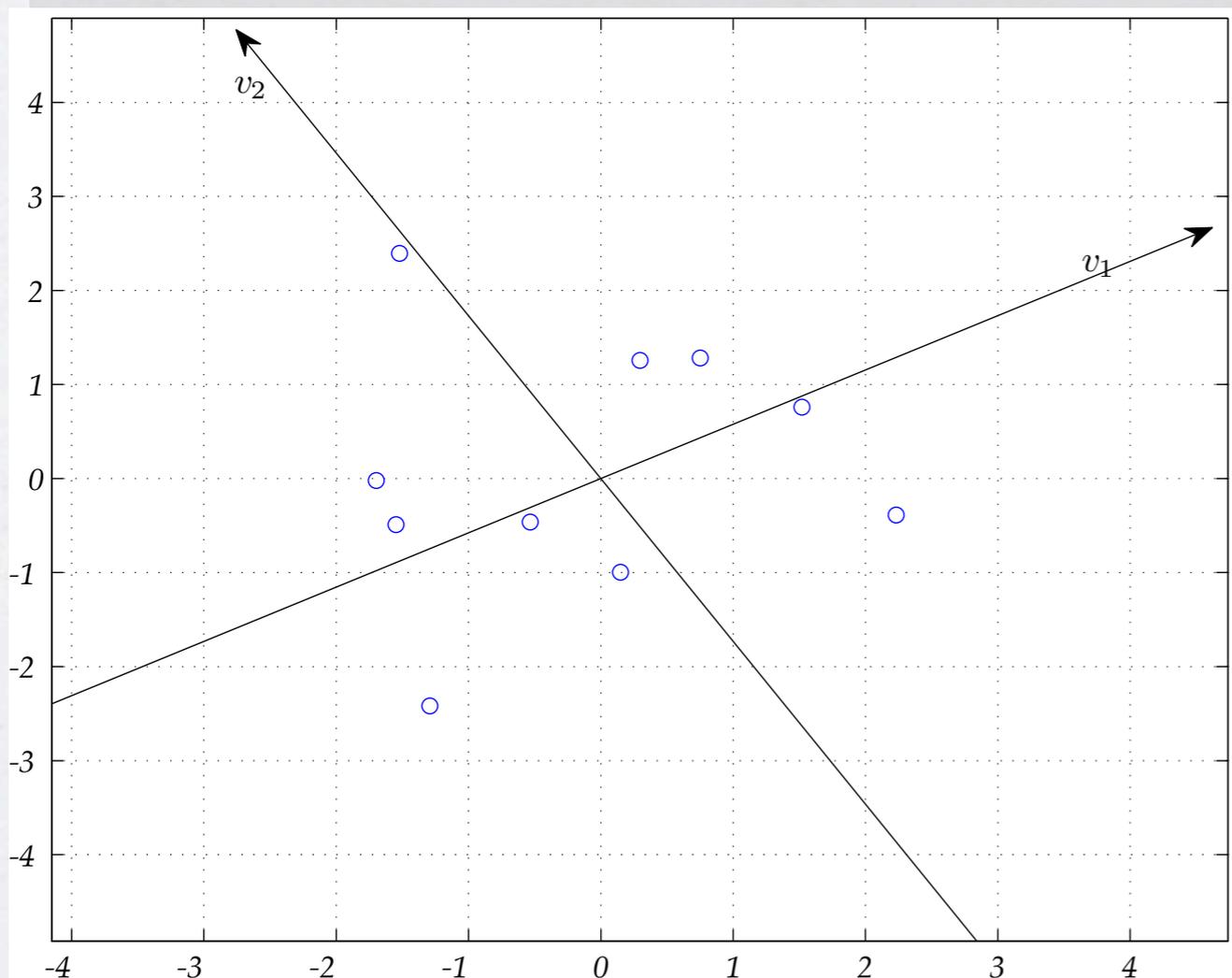
covariance:  $MDM^T$ ,  $D = \text{diag}(4,1)$ ,  $M = \begin{pmatrix} \cos(\pi / 6) & \cos(2\pi / 3) \\ \sin(\pi / 6) & \sin(2\pi / 3) \end{pmatrix}$

# samples:  $\nu = 10$ , "soft" information:  $h$  unimodal

Results:

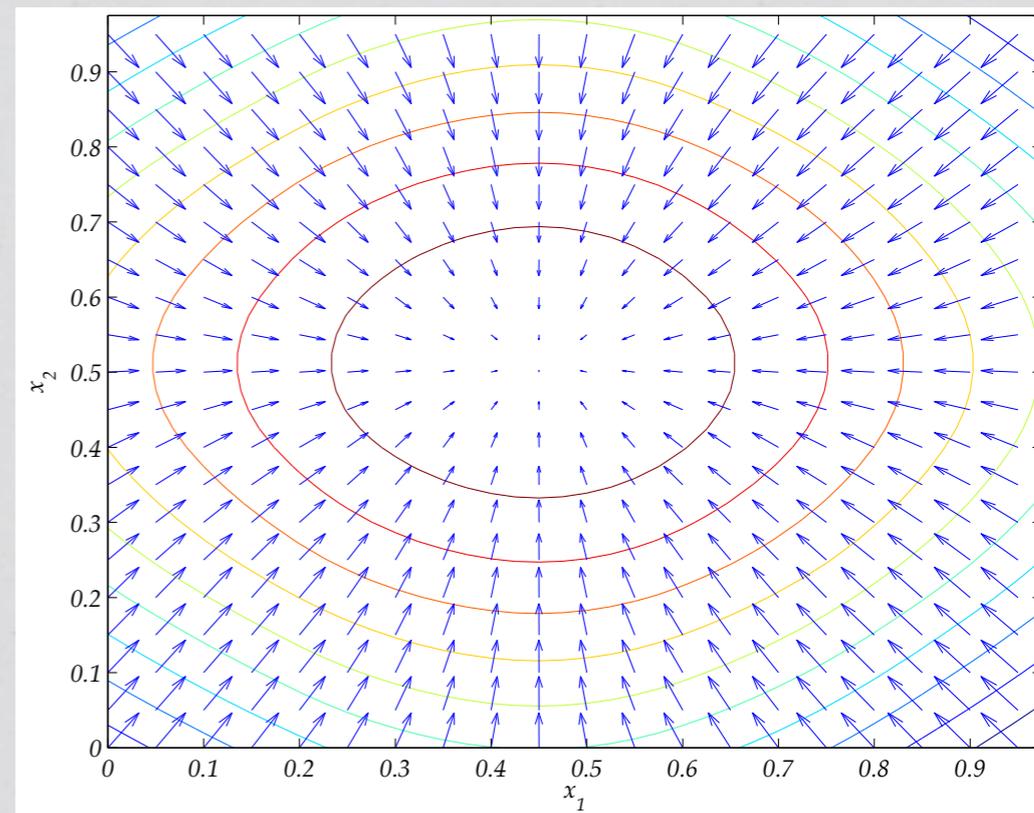
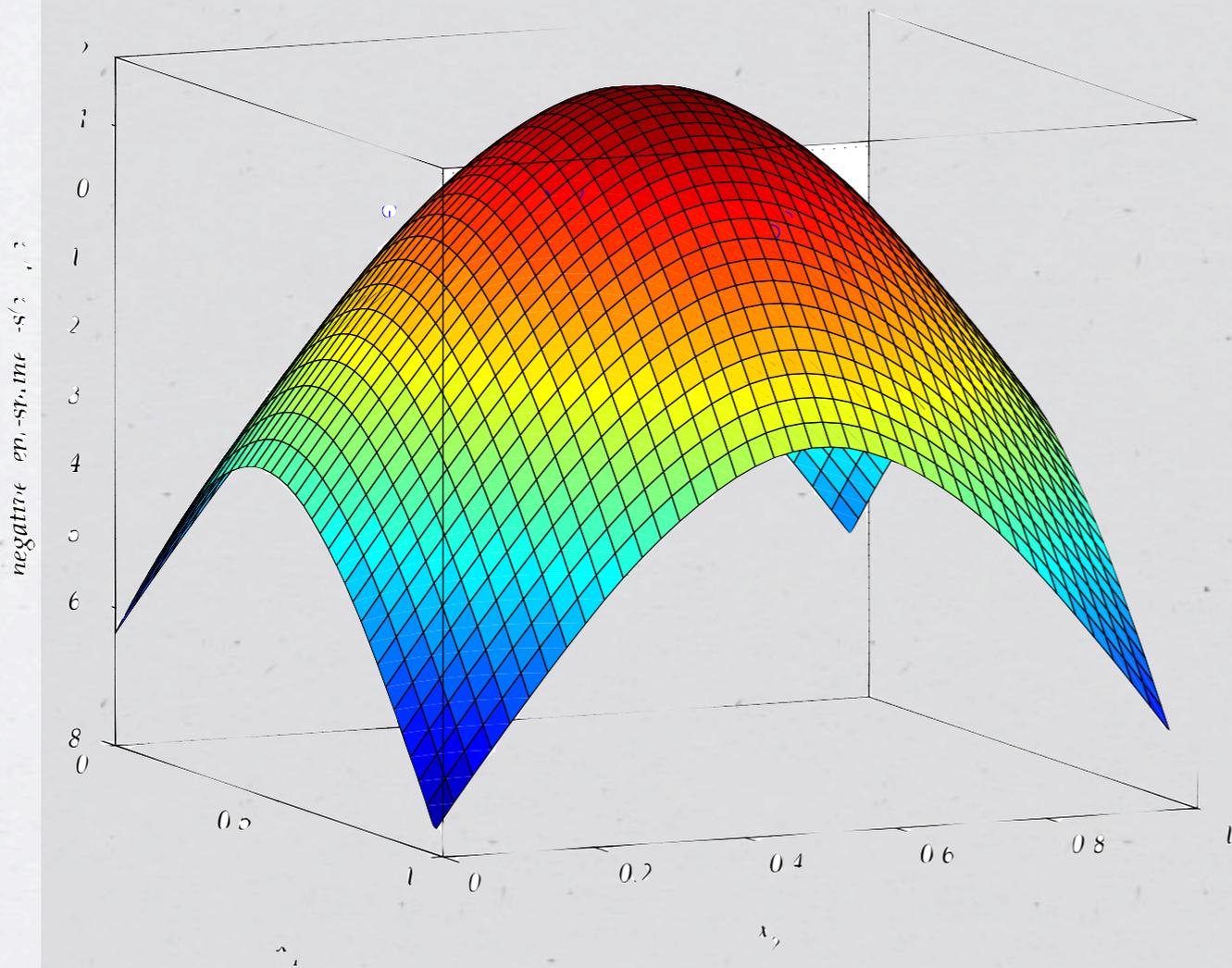
$$\|h^{true} - h^{est}\|_2^2 = 0.028, \quad \|h^{true} - h^{est}\|_\infty = 0.006$$

# Sampled data

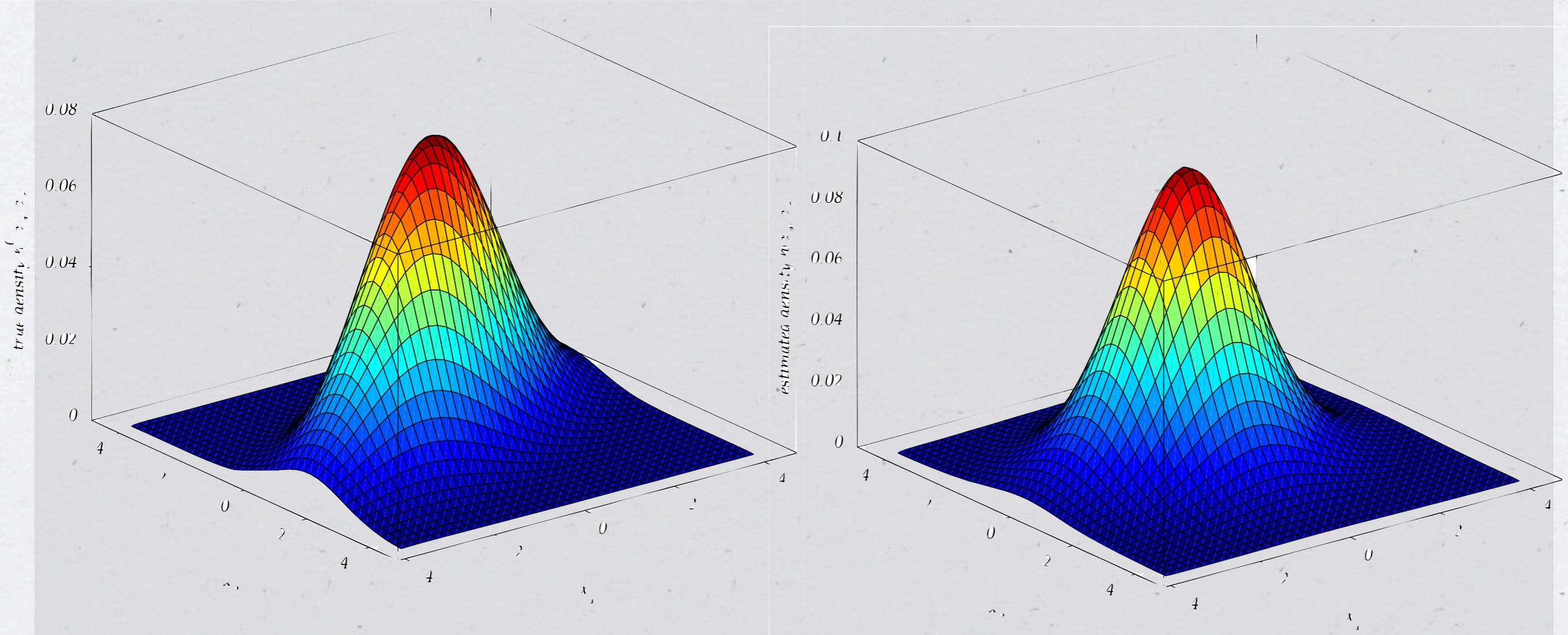


normalized

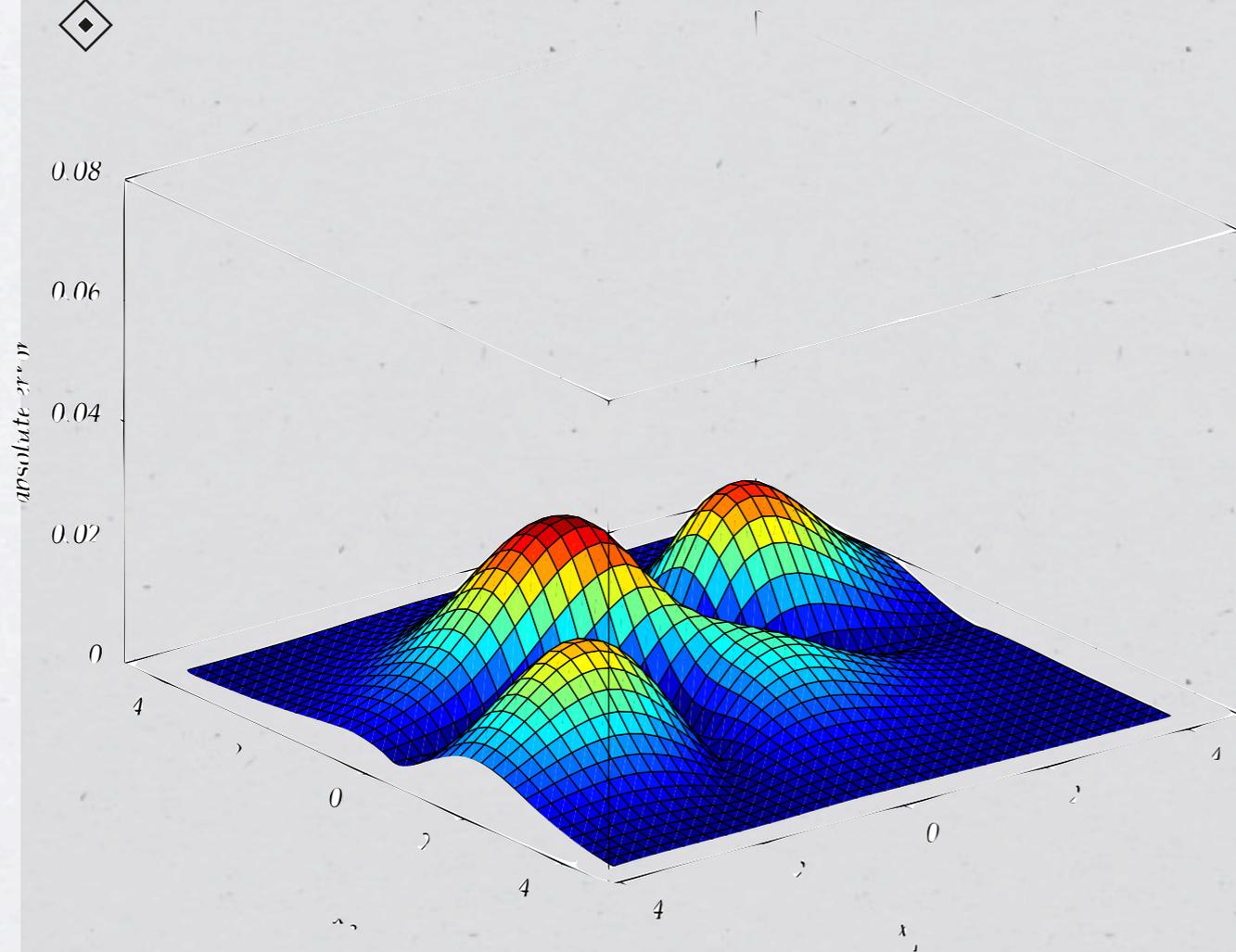
# Epi-SpLine & vector field



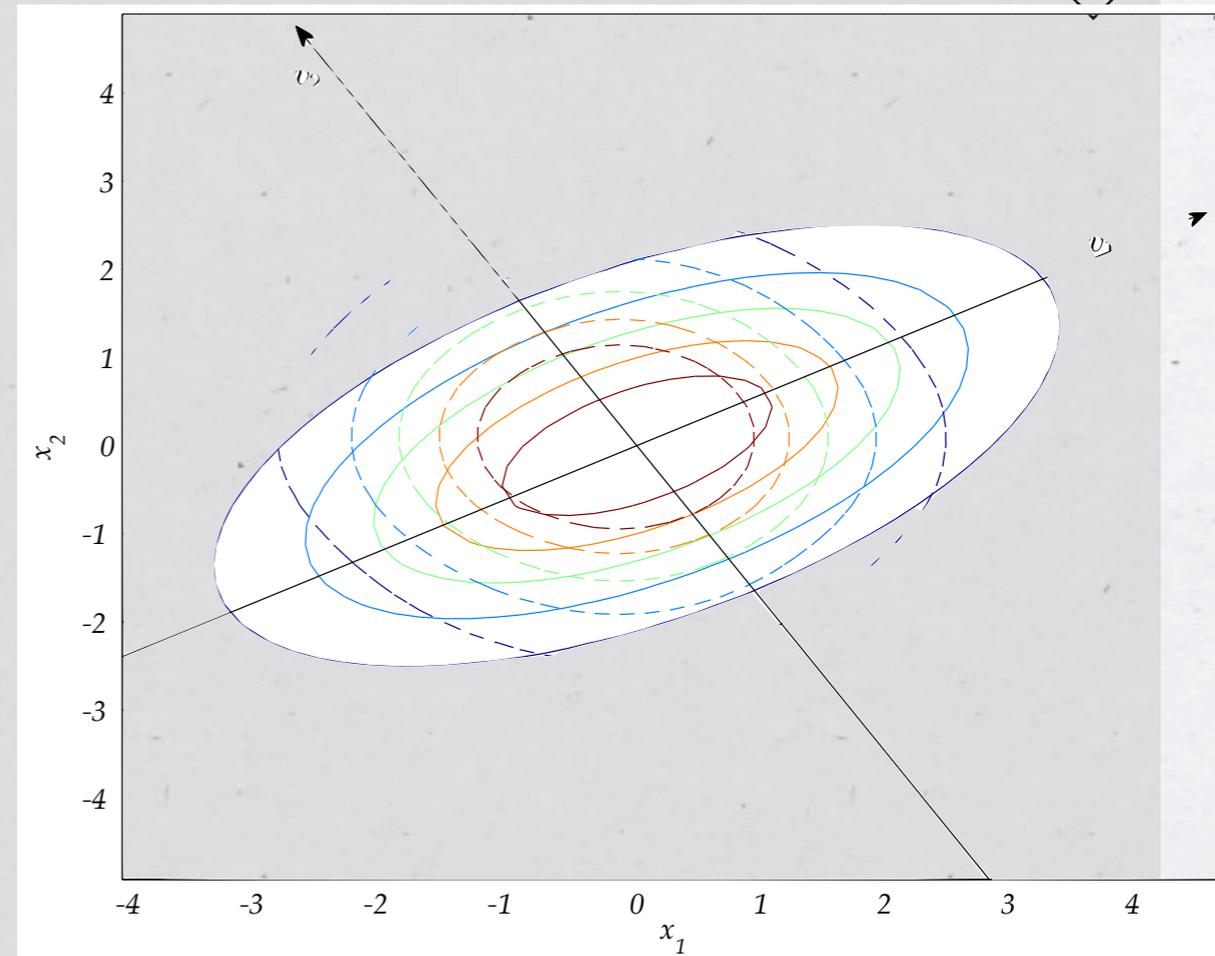
# True & Estimated density



# Measurement Errors



Absolute Error



Level curves: true & estimate

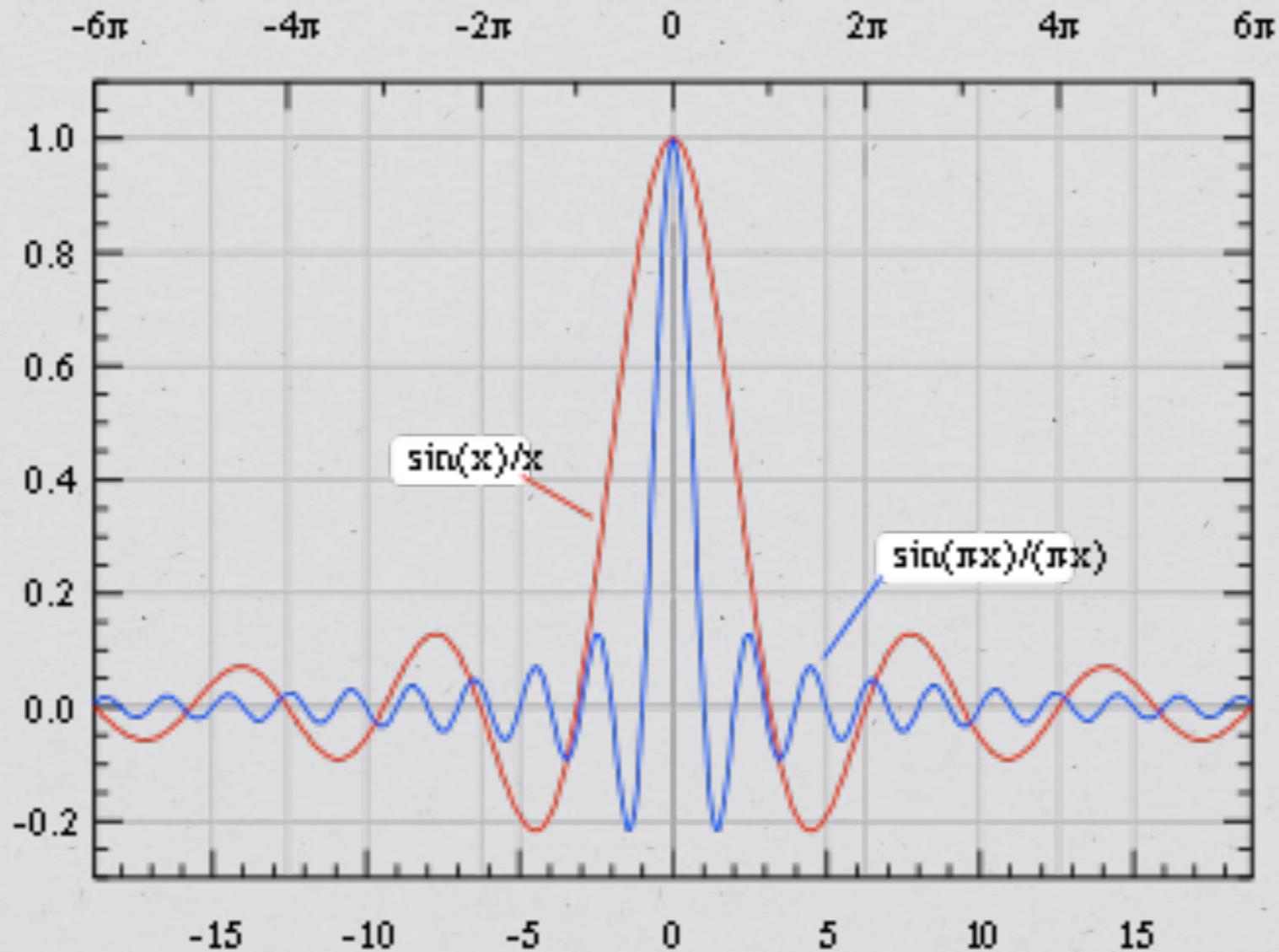
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# SPLINES & EPI-SPLINES

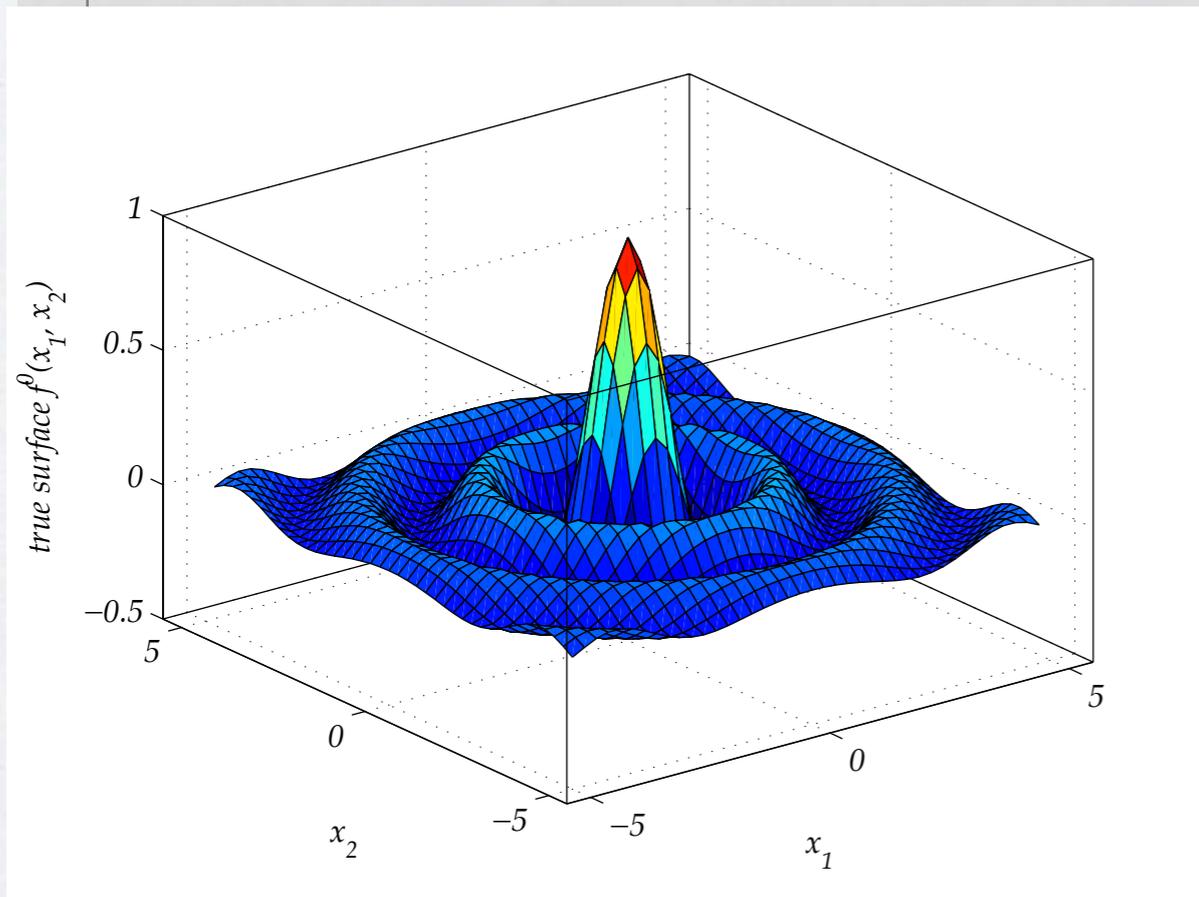


# Dirichlet (sinc-)function

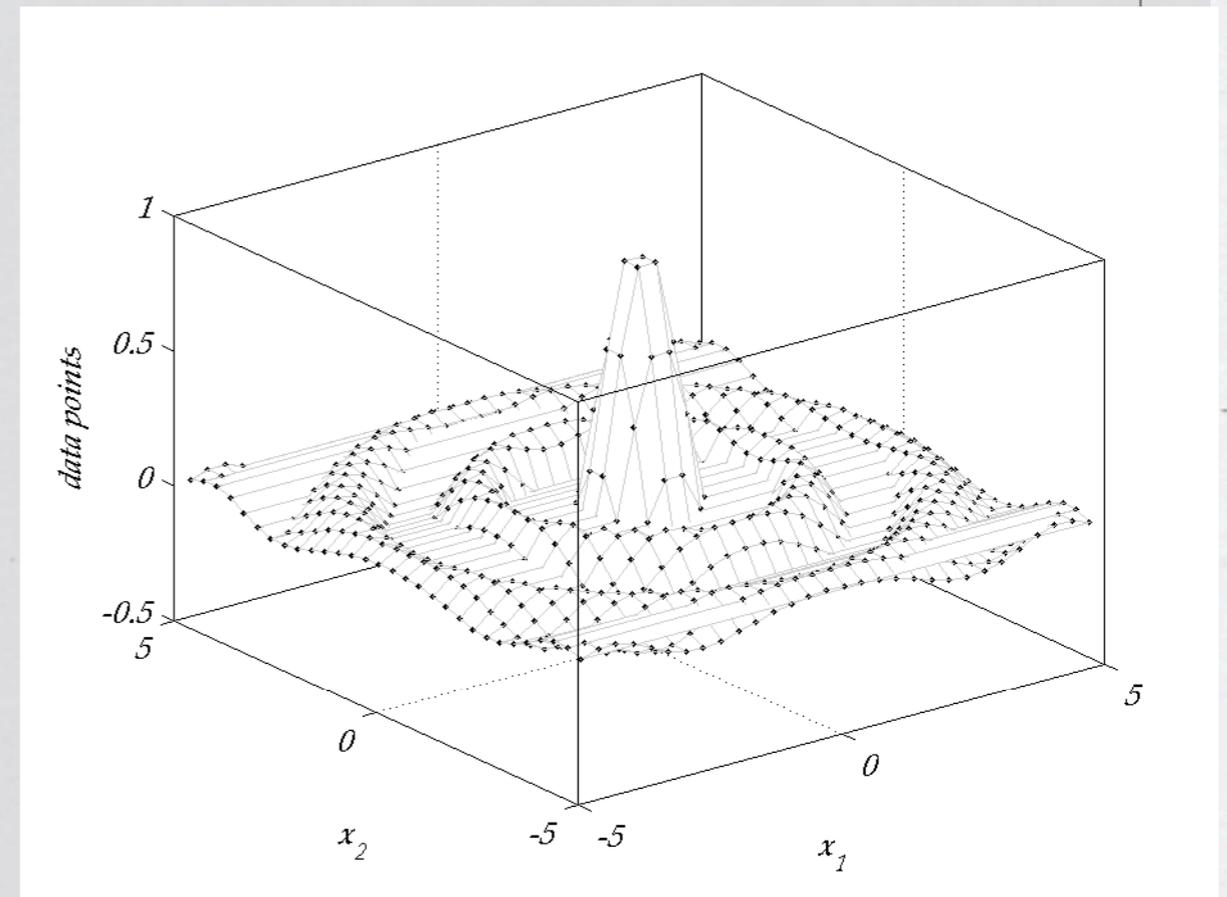
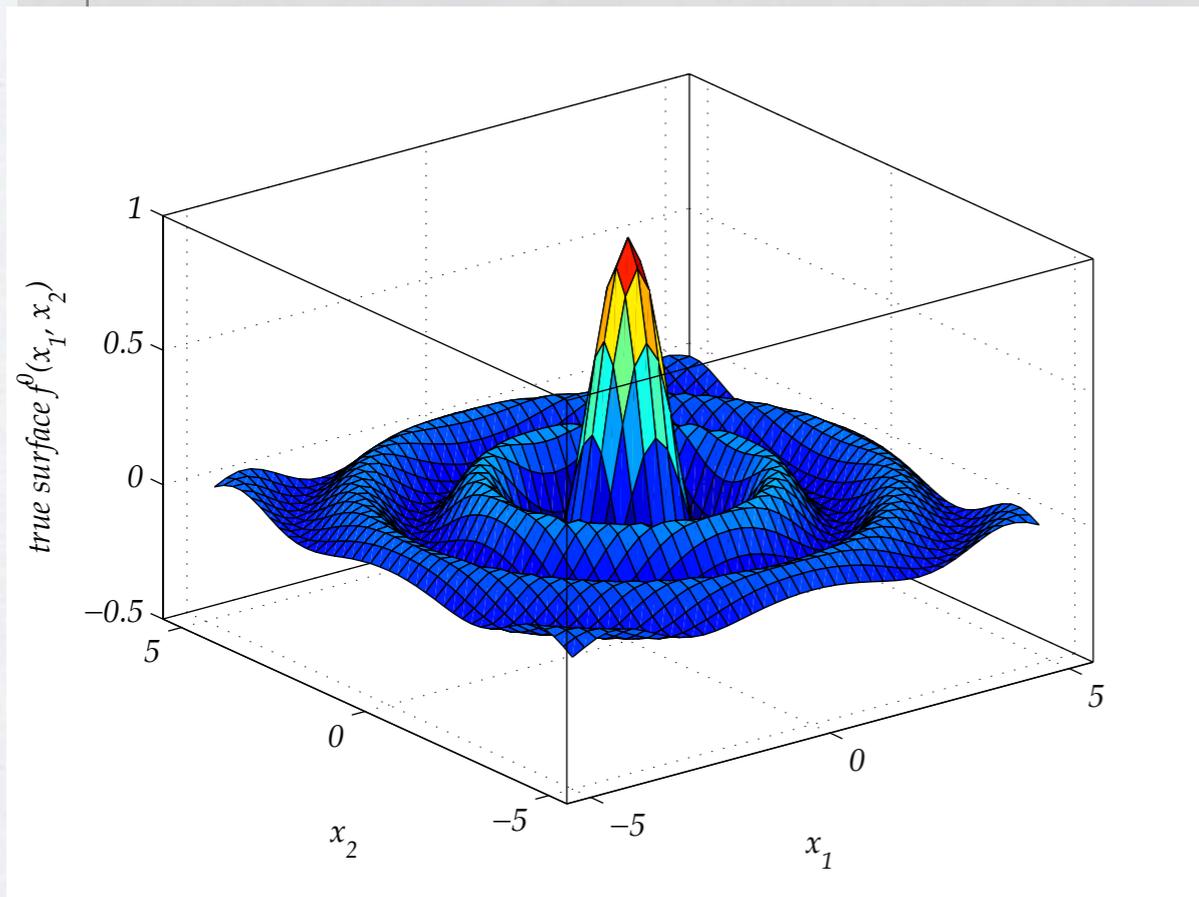


$$f(x) = \sin(\pi x / 2) / \pi x \text{ for } x \neq 0, \quad = 1 \text{ for } x = 0$$

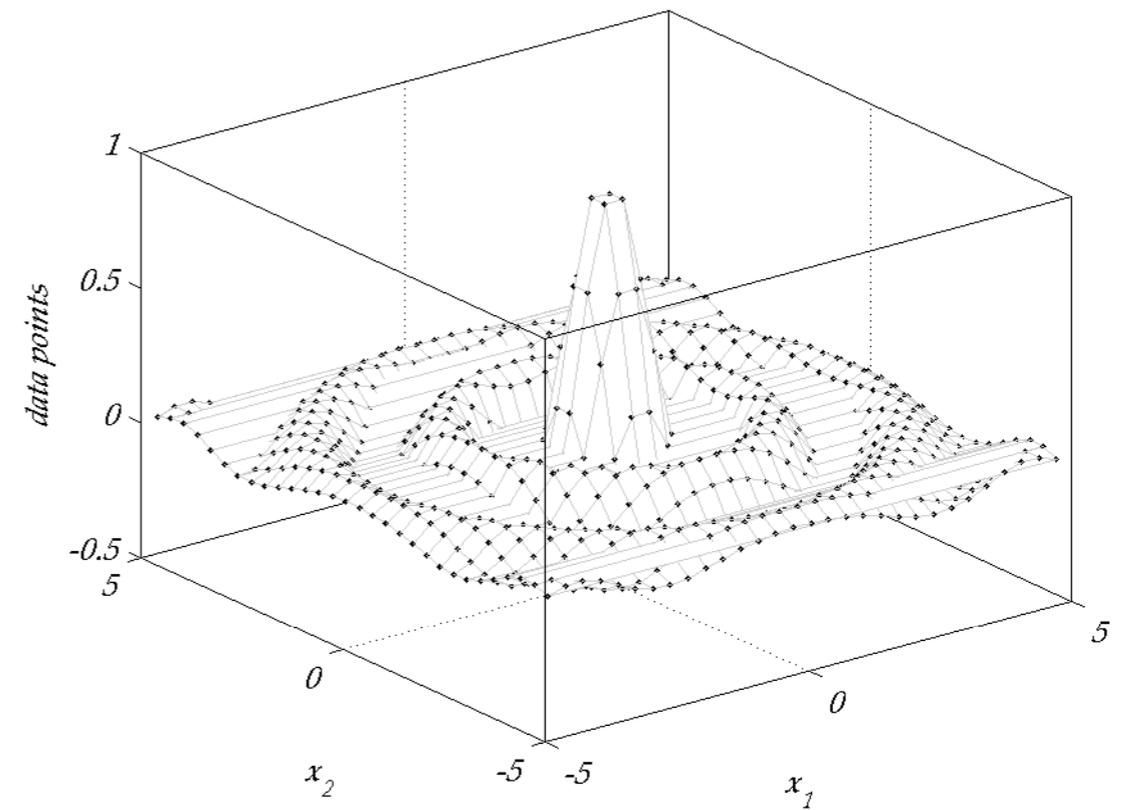
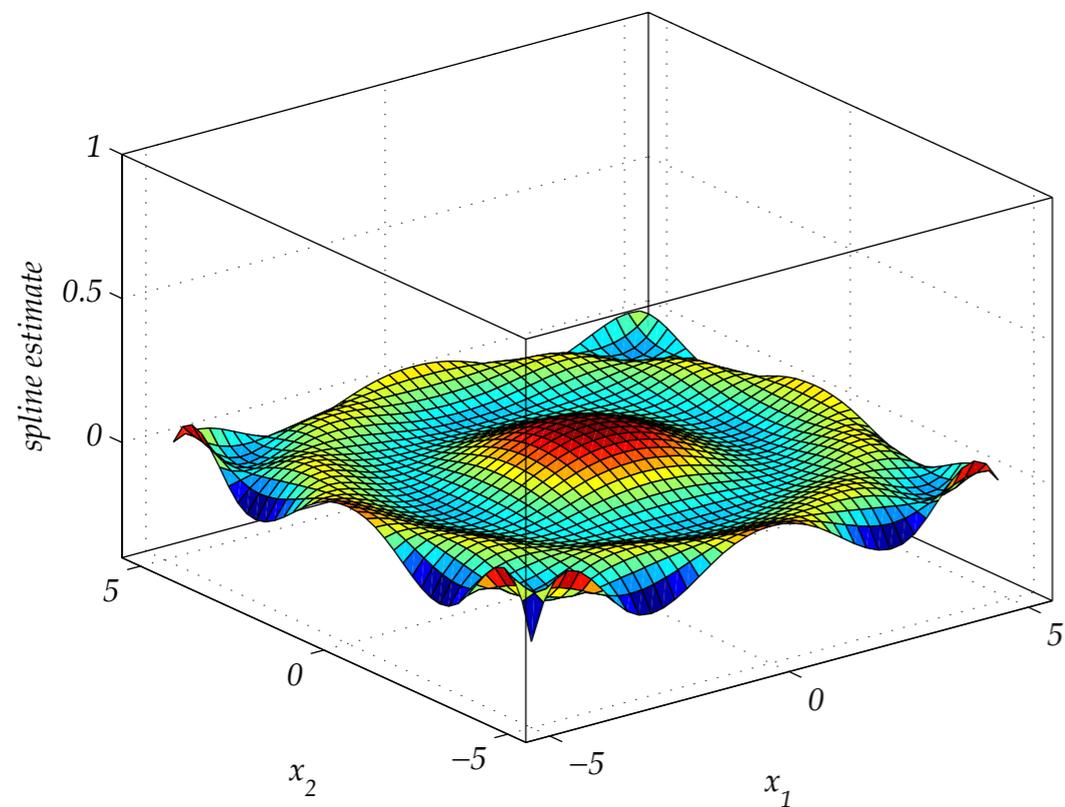
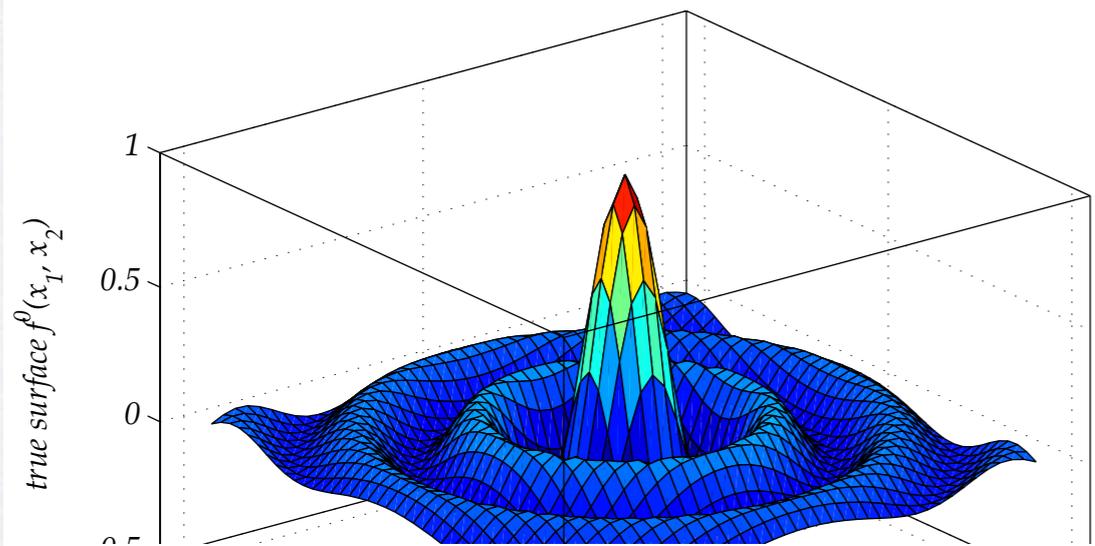
# SPLINES & EPI-splines



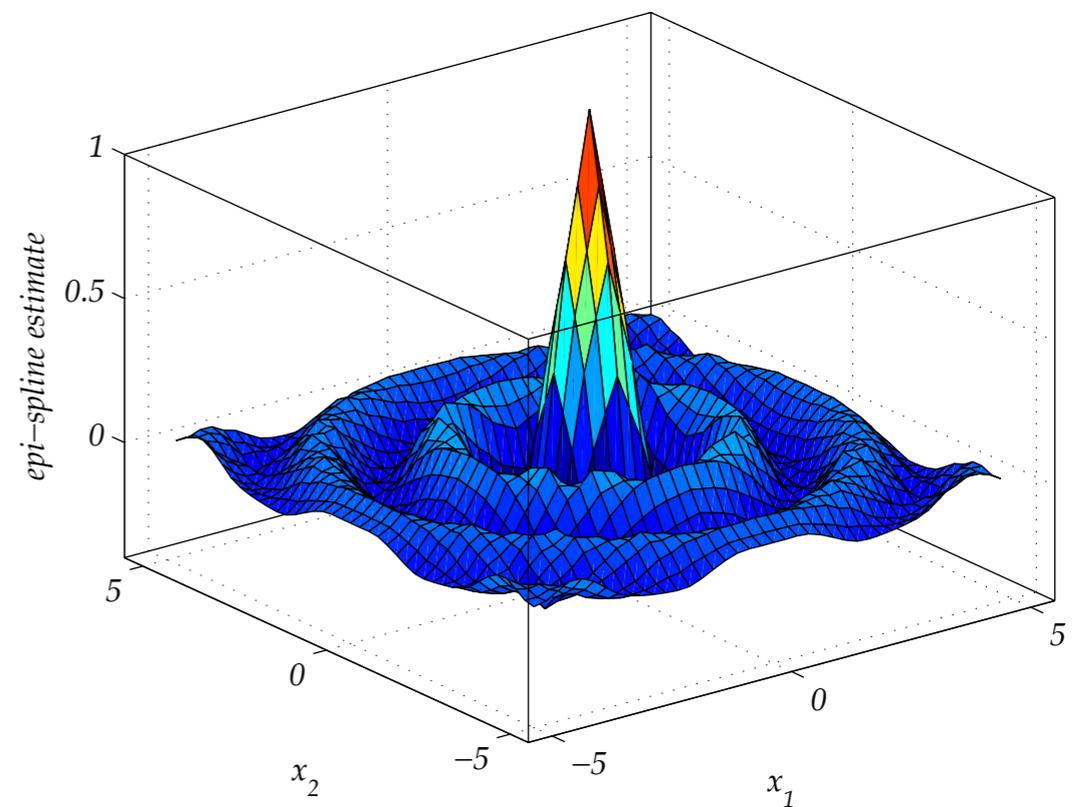
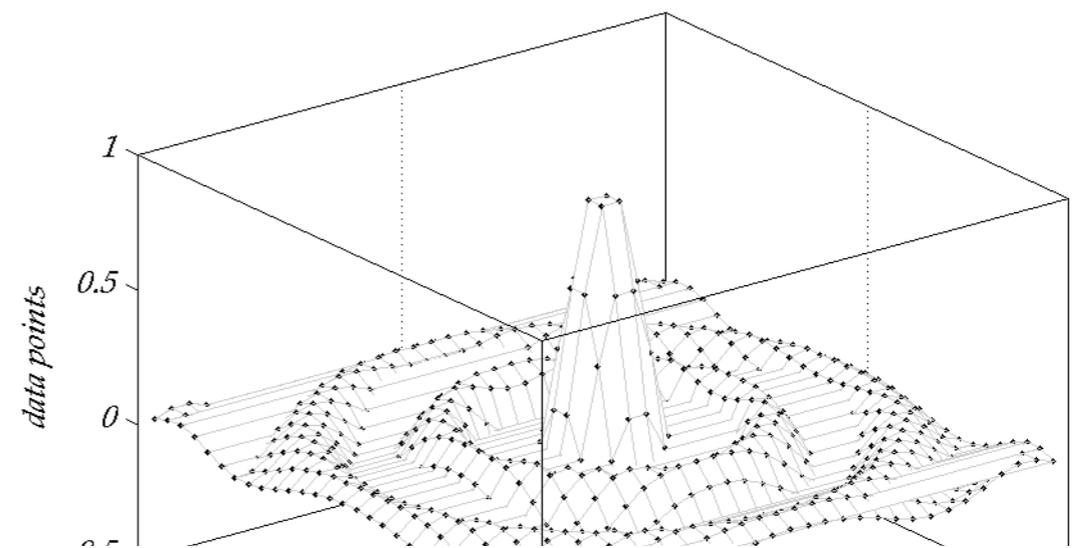
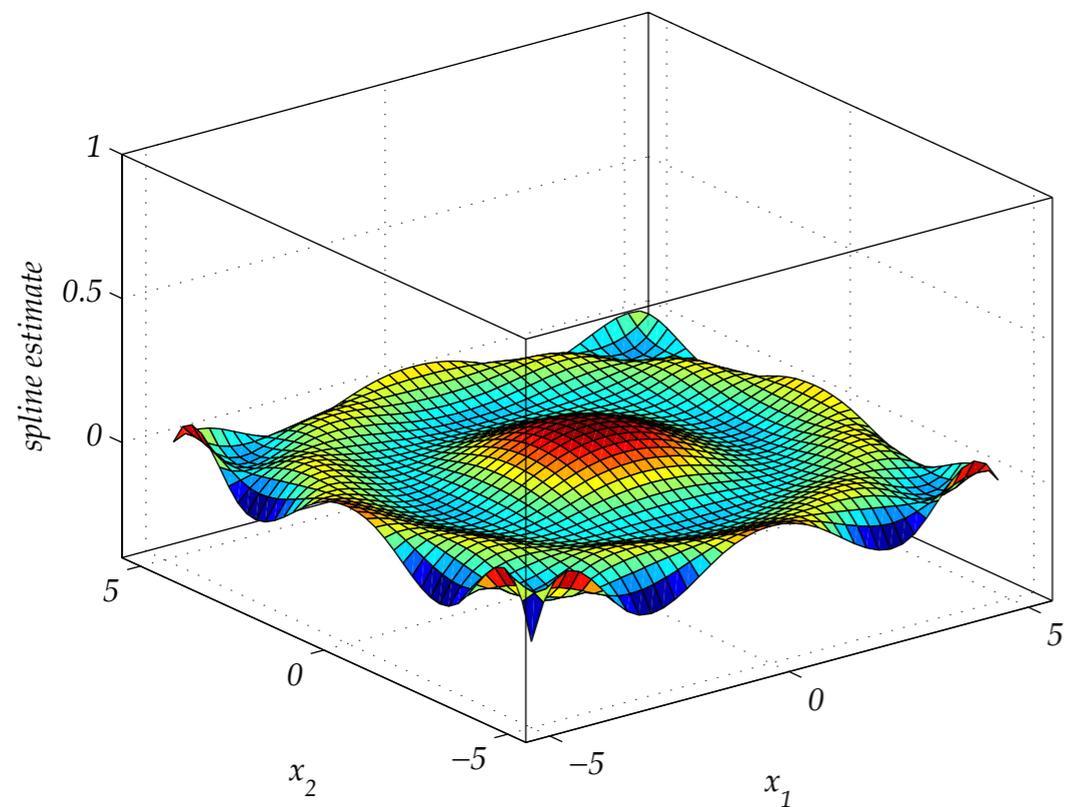
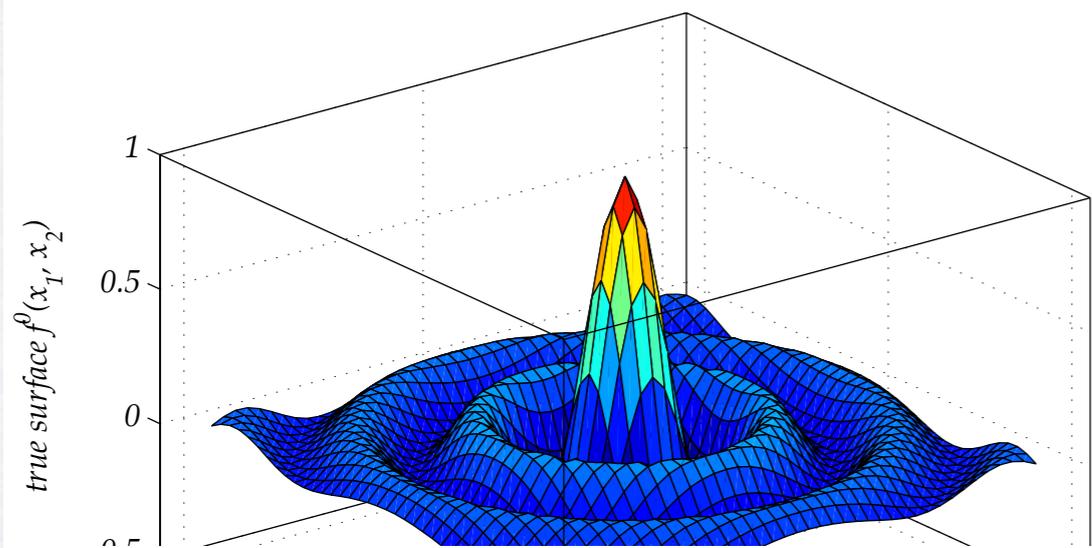
# SPLINES & EPI-splines



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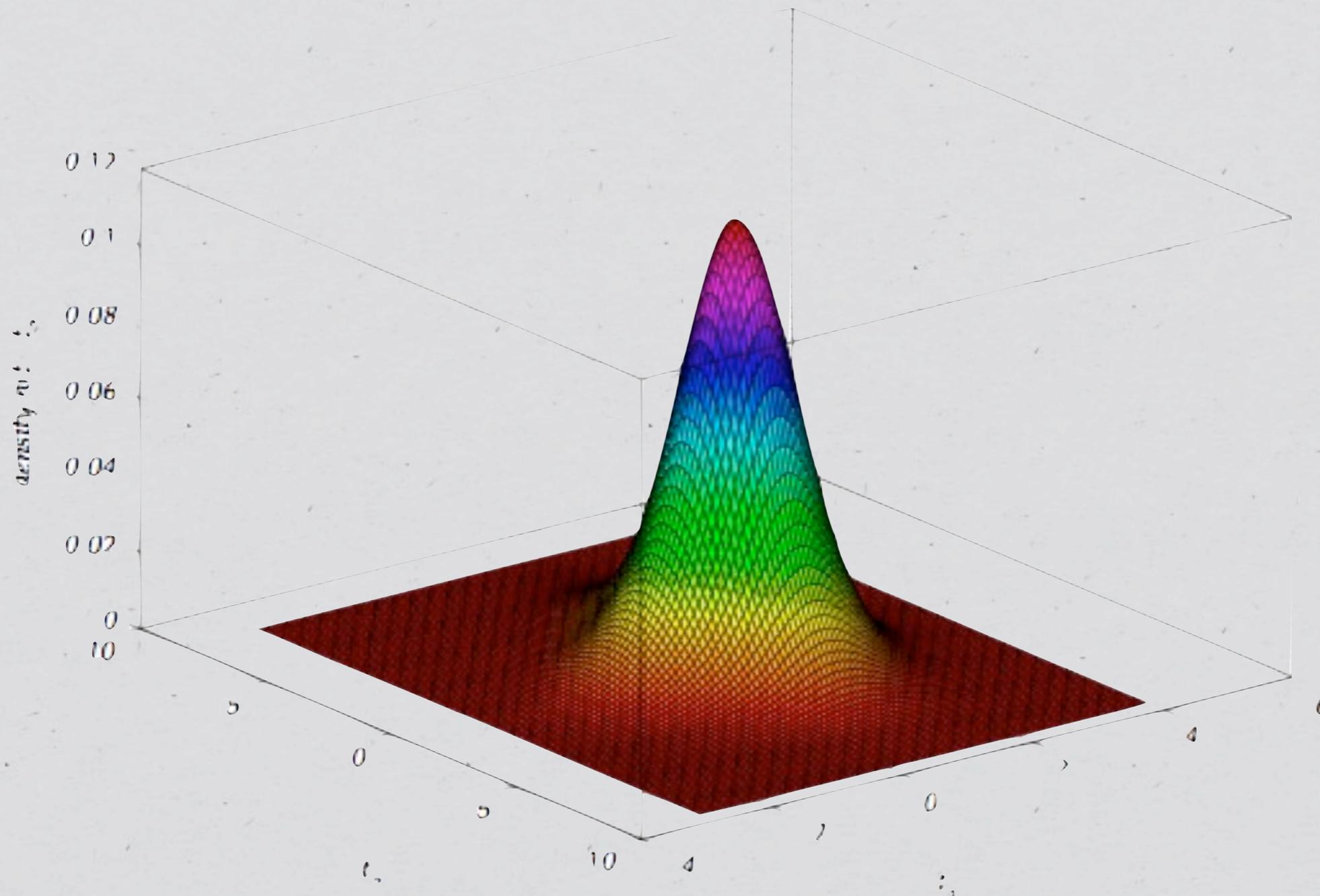




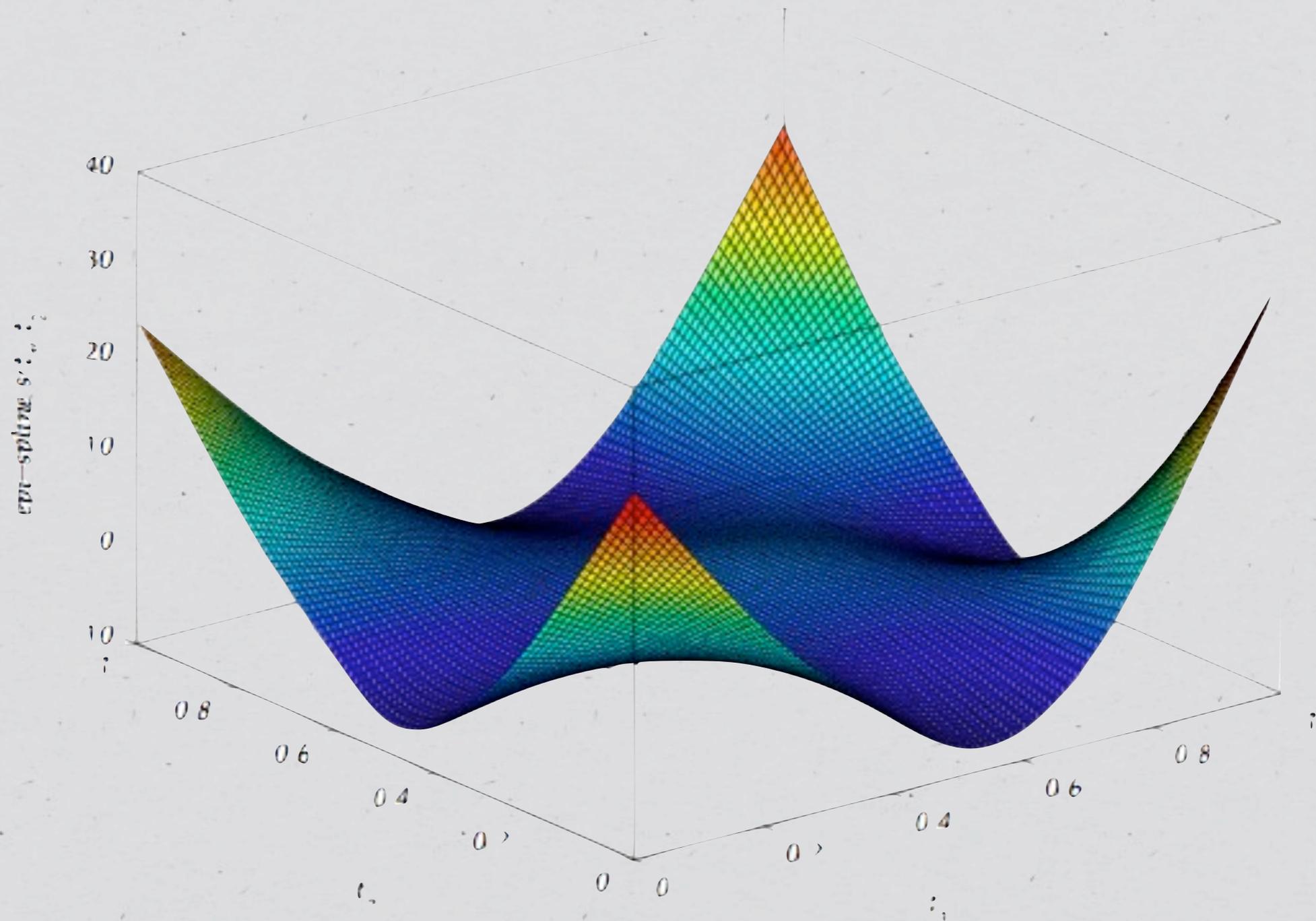
Wednesday, September 5, 2012



# Normal, 20 samples Diagonal Covariance



# ... the -(epi-spline function)



# Approximation Theory

$\min f_0(x)$  such that  $x \in X \subset H$  (for our use:  $H$  Polish space)

$\min f(x)$  on  $x \in X$  with  $f(x) = \begin{cases} f_0(x) & \text{when } x \in X \\ \infty & \text{otherwise} \end{cases}$  lsc function:  $H \rightarrow \overline{\mathbb{R}}$

$(f_0^v, X_0^v) \rightarrow (f_0, X)$  sequence of optimization problems converging(?) to,  $f$

$\arg \min f^v \rightarrow \arg \min f$  ( $\inf f^v \rightarrow \inf f$ )

$\arg \min (f^v + g) \rightarrow \arg \min (f + g)$ ,  $g$  continuous perturbation

$\Rightarrow f^v$  **epi-converges** to  $f$  ( $\text{epi } f^v \rightarrow \text{epi } f$ ): for all  $x \in H$ ,

(a)  $\forall x^v \rightarrow x, \liminf_v f^v(x^v) \geq f(x)$ ,

(b)  $\exists x^v \rightarrow x, \limsup_v f^v(x^v) \leq f(x)$ .

pointwise?, uniform?,

# LLN: Random lsc functions

$f : \Xi \times H \rightarrow \overline{\mathbb{R}}$  a random lsc function,  $\xi$  values in  $(\Xi, \mathcal{A}, P)$

(a) lsc (lower semicontinuous) in  $h$ ,  $(\forall \xi \in \Xi)$

(b)  $(\xi, h)$ -measurable  $(\mathcal{A} \times B_X)$ -measurable

recall:  $f(\xi, h) = f_0(\xi, h)$  when  $h \in X(\xi)$  -- stochastic constraints

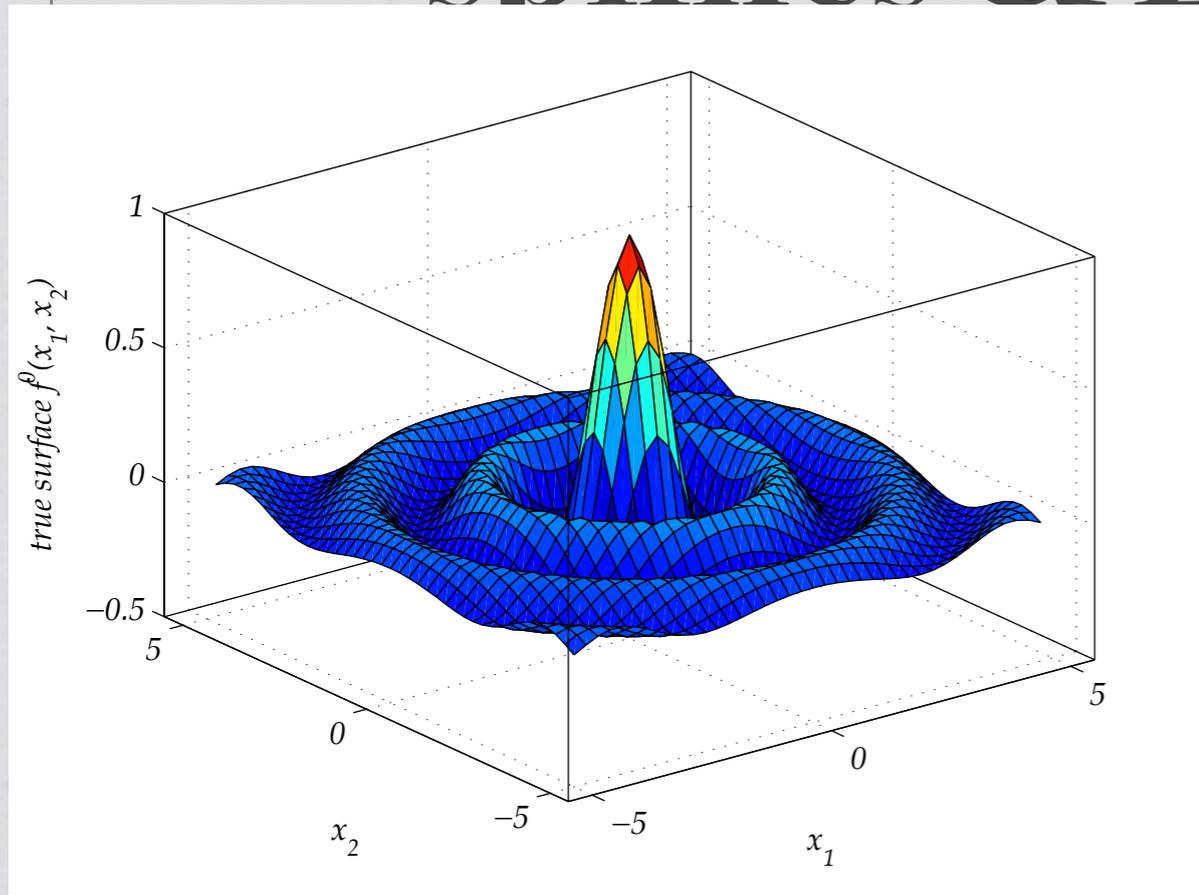
$$f^\nu(\xi, h) = \begin{cases} \frac{1}{\nu} \sum_{l=1}^{\nu} \ln h(\xi^l) & \text{if } h \geq 0, \int_{\Xi} h(\xi) d\xi = 1, h \in A^\nu \\ \infty & \text{otherwise} \quad (\sim \text{SAA of optimisation problems}) \end{cases}$$

**Question:** Do the  $f^\nu(\xi, \cdot)$  epi-converge to  $\mathbb{E}\{f(\xi, h)\}$   $P$ -a.s.?

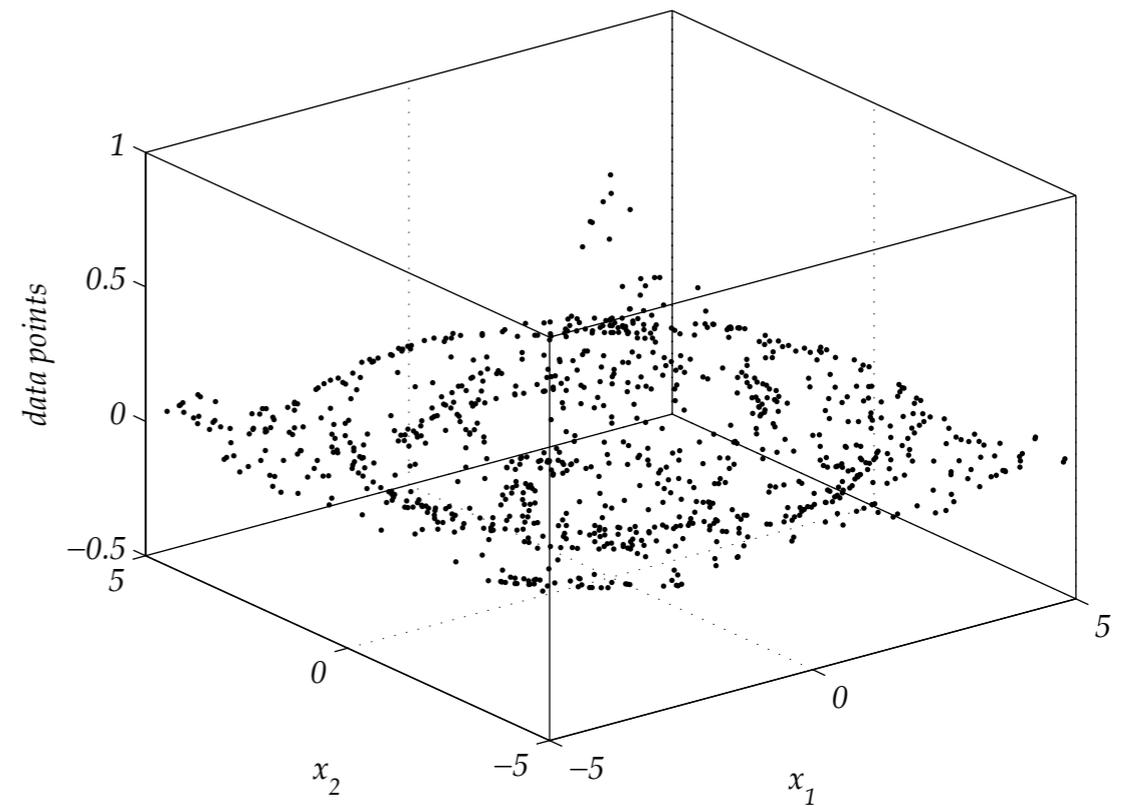
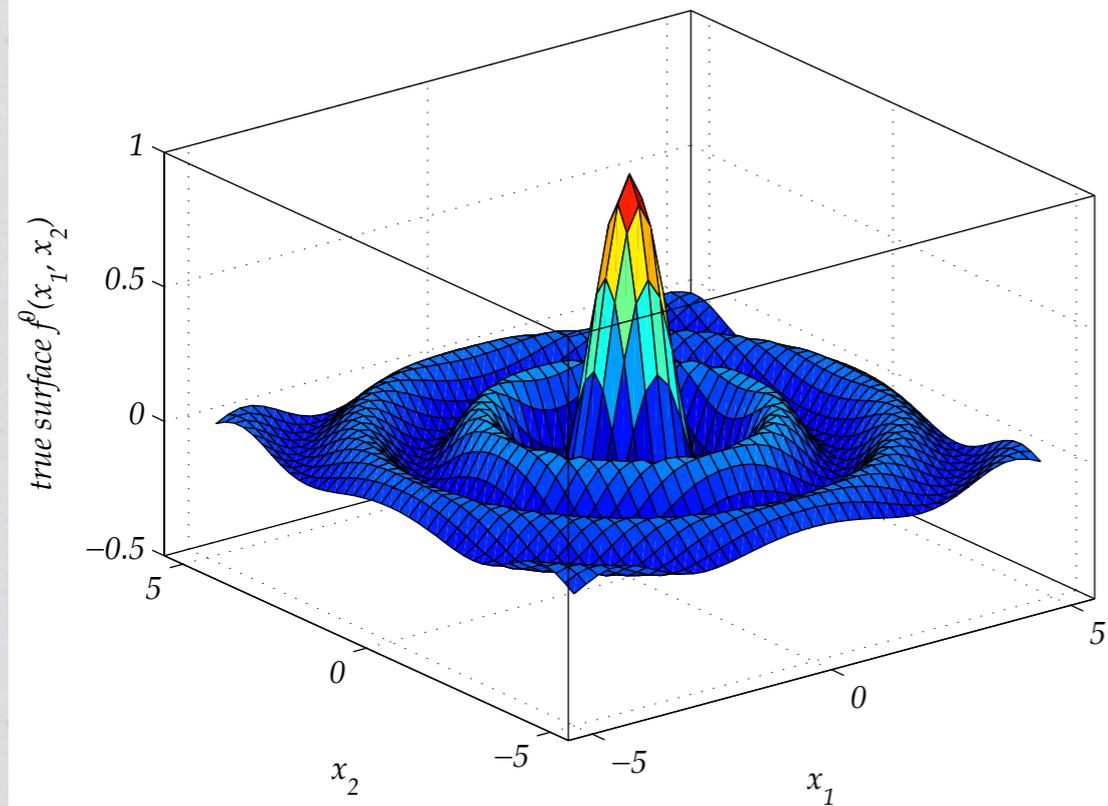
$$h^{\text{true}} \in \arg \min \mathbb{E}\{f(\xi, h)\}$$

$$\text{where } f(\xi, h) = \begin{cases} \ln h(\xi) & \text{if } h \geq 0, \int_{\Xi} h(\xi) d\xi = 1, h \in A \\ \infty & \text{otherwise} \end{cases}$$

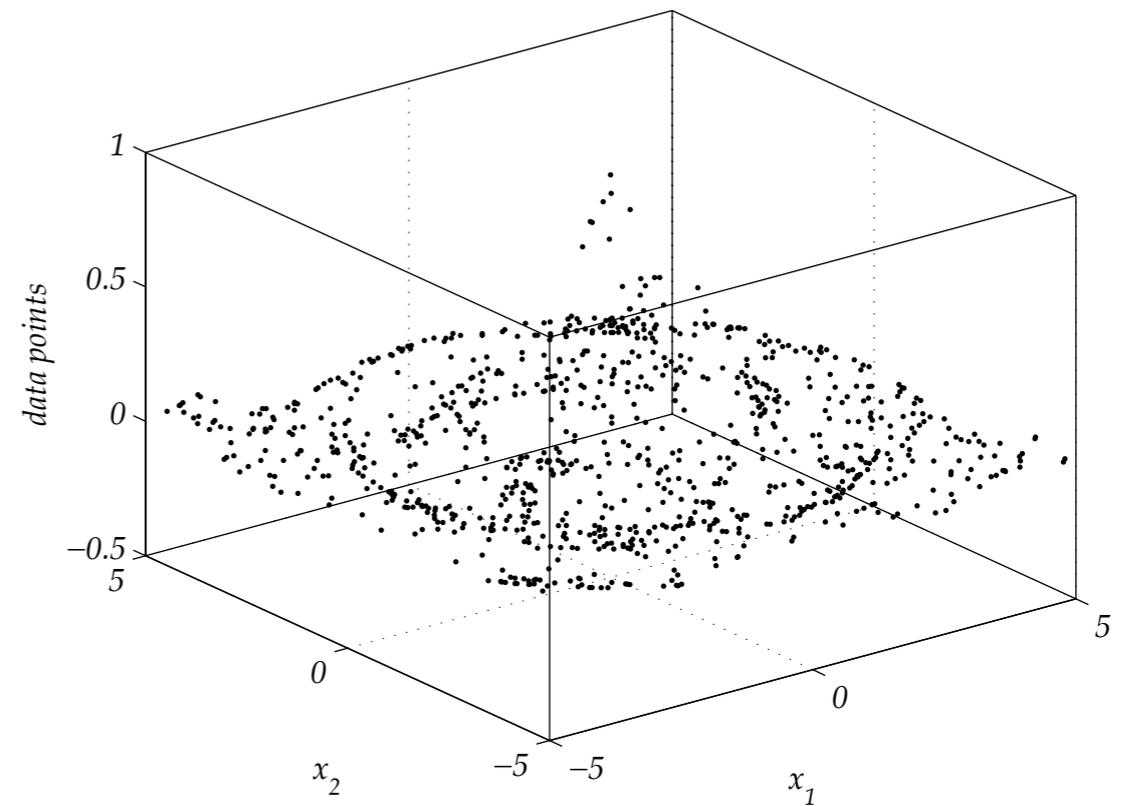
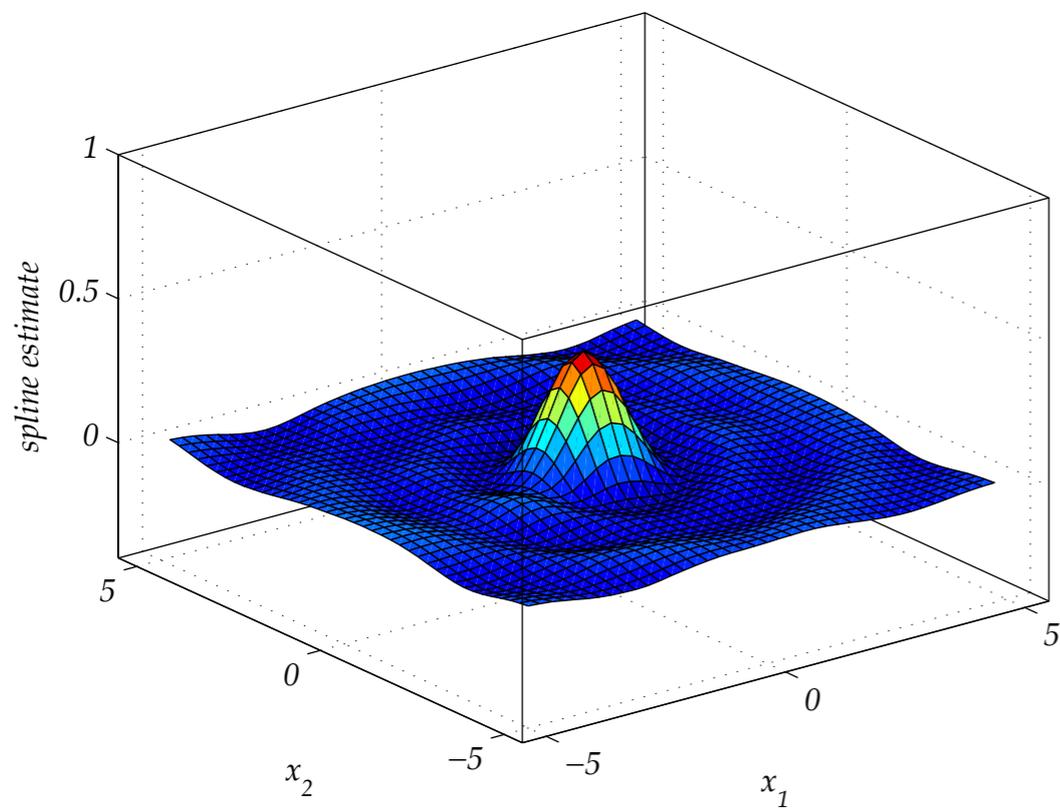
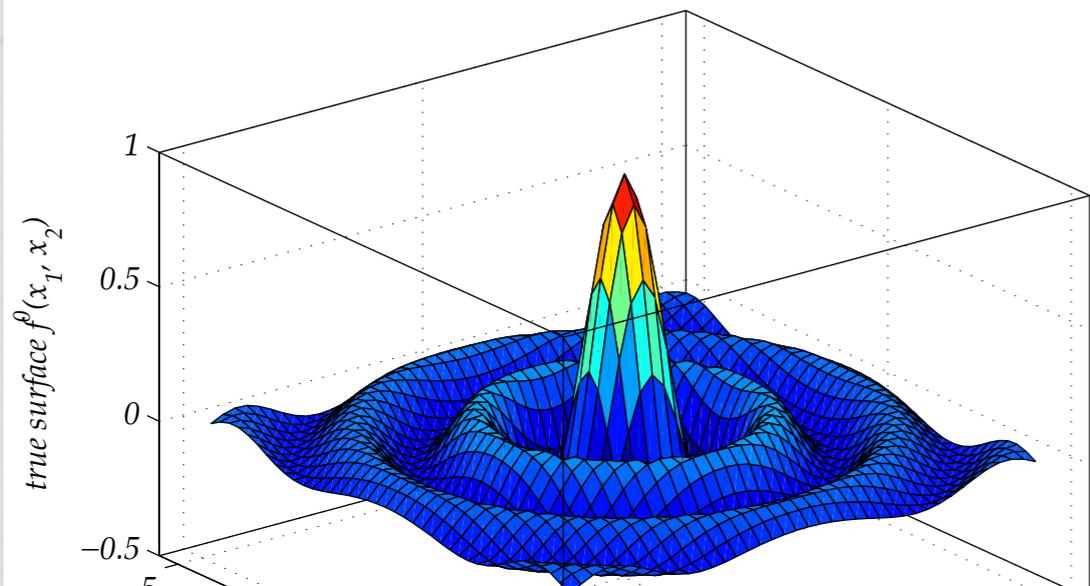
# splines & Epi-Splines 2



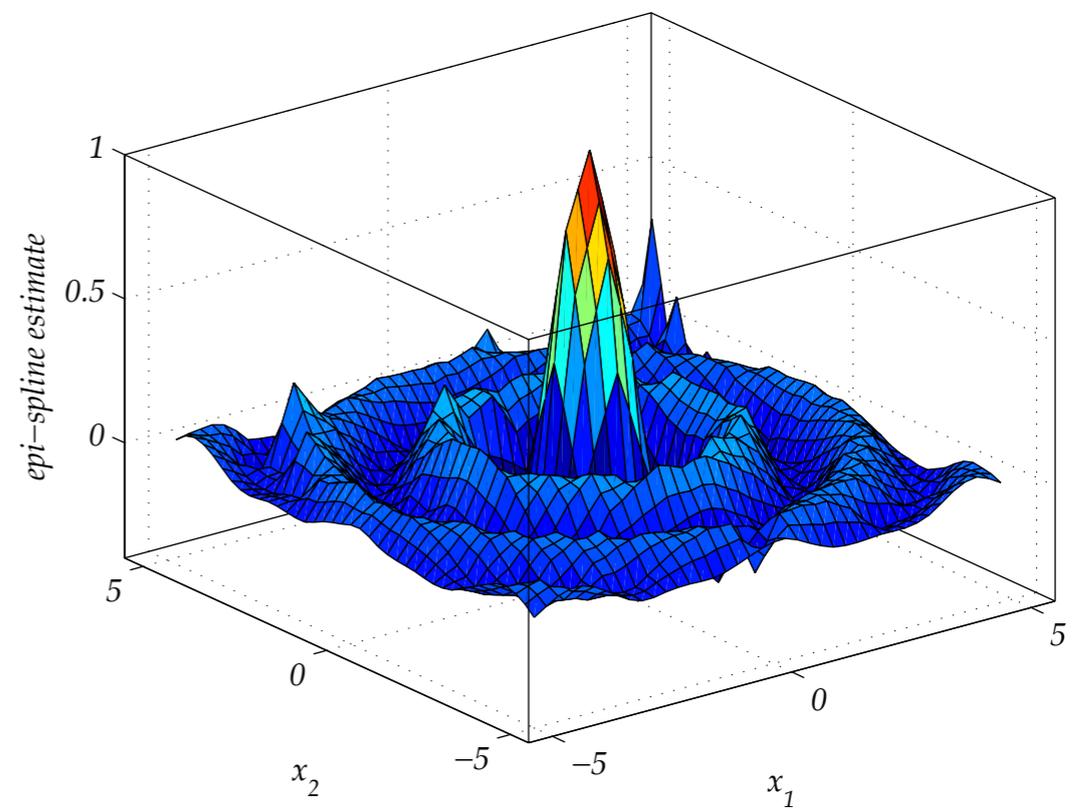
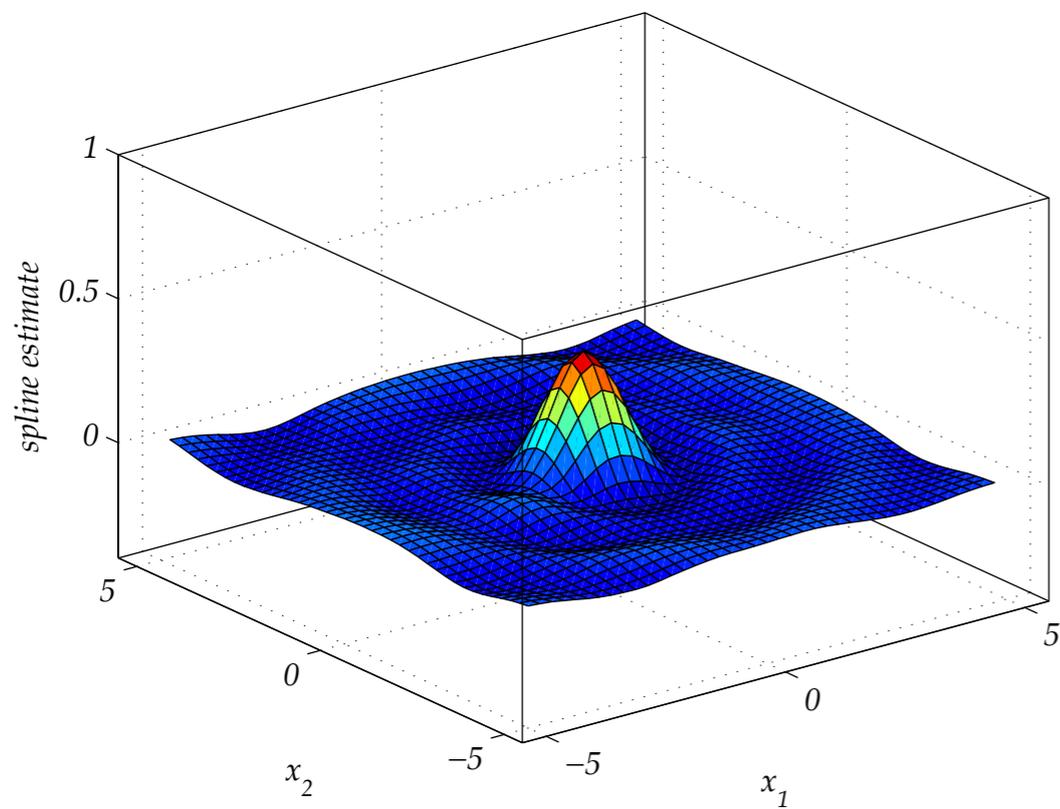
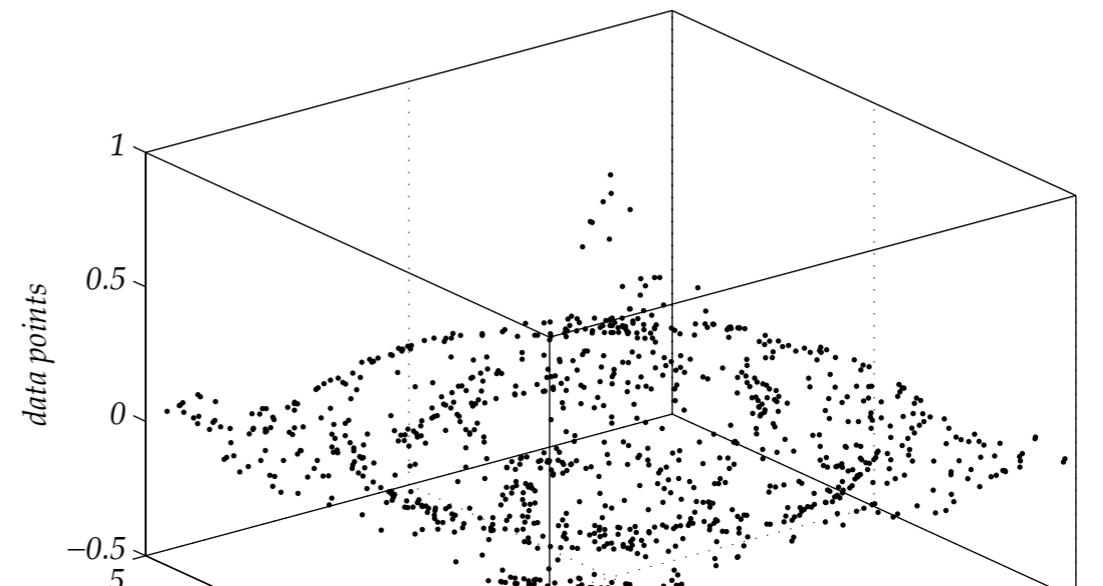
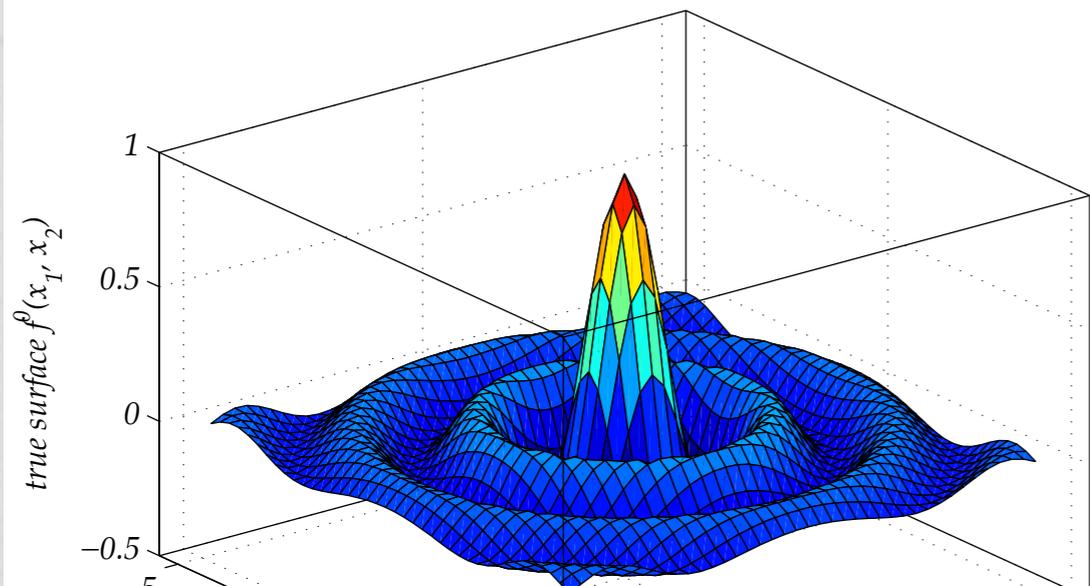
# splines & Epi-Splines 2



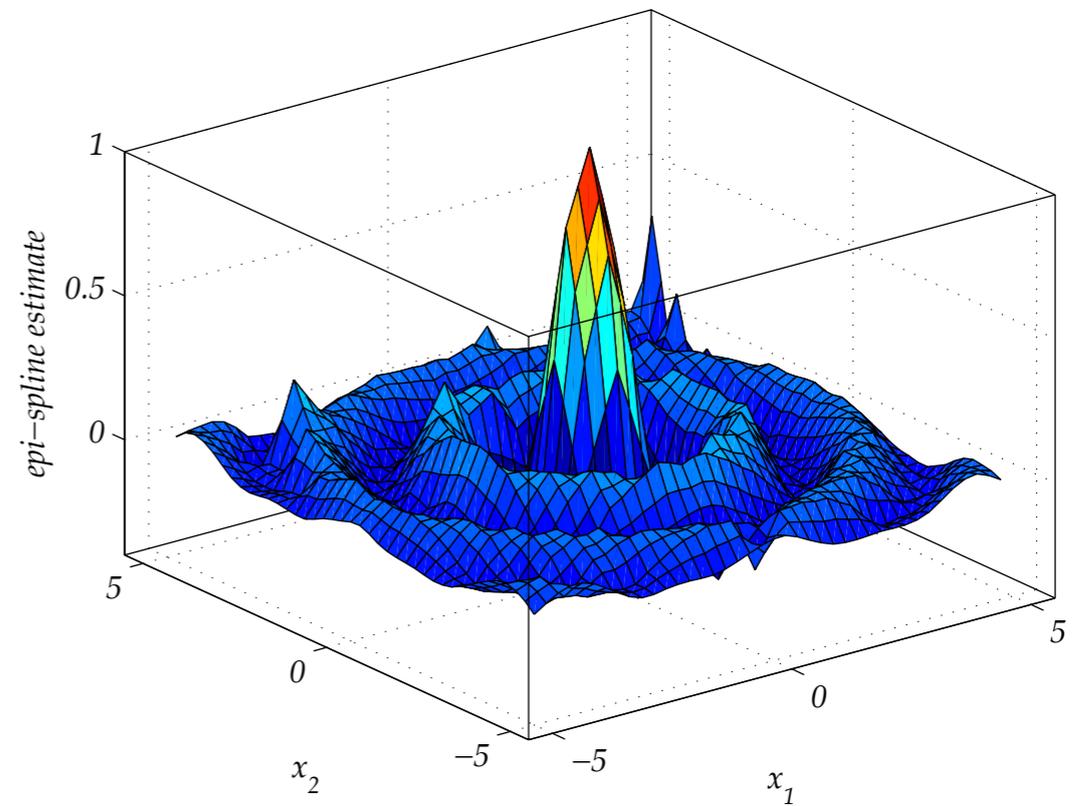
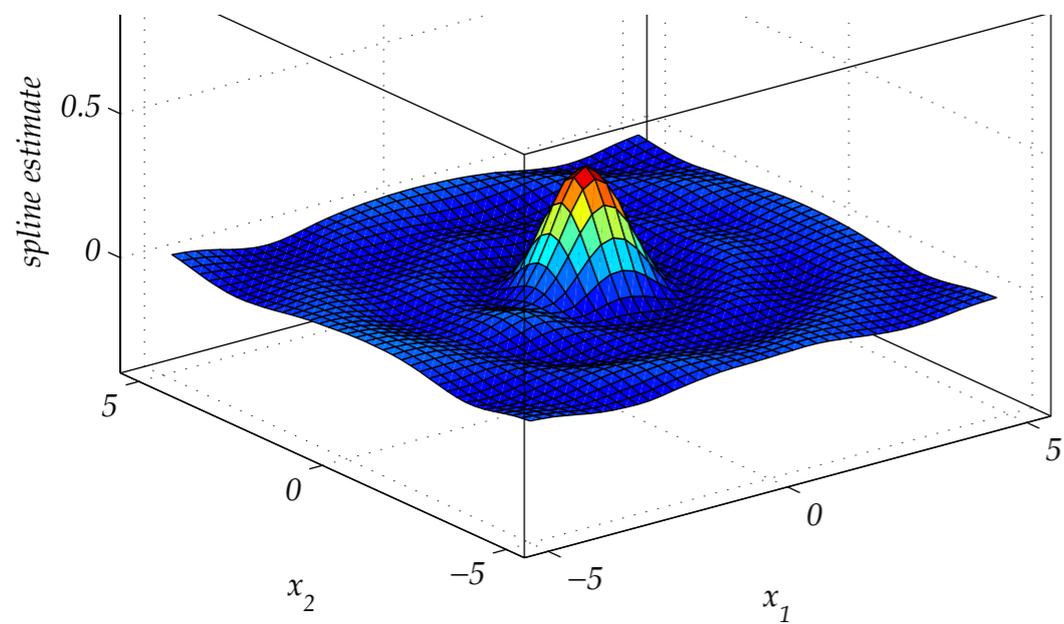
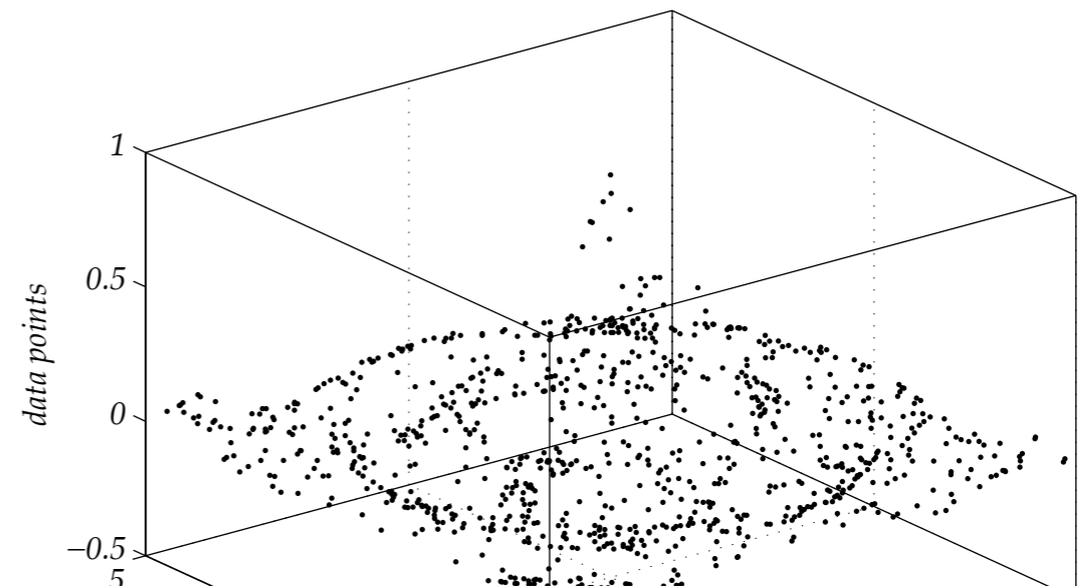
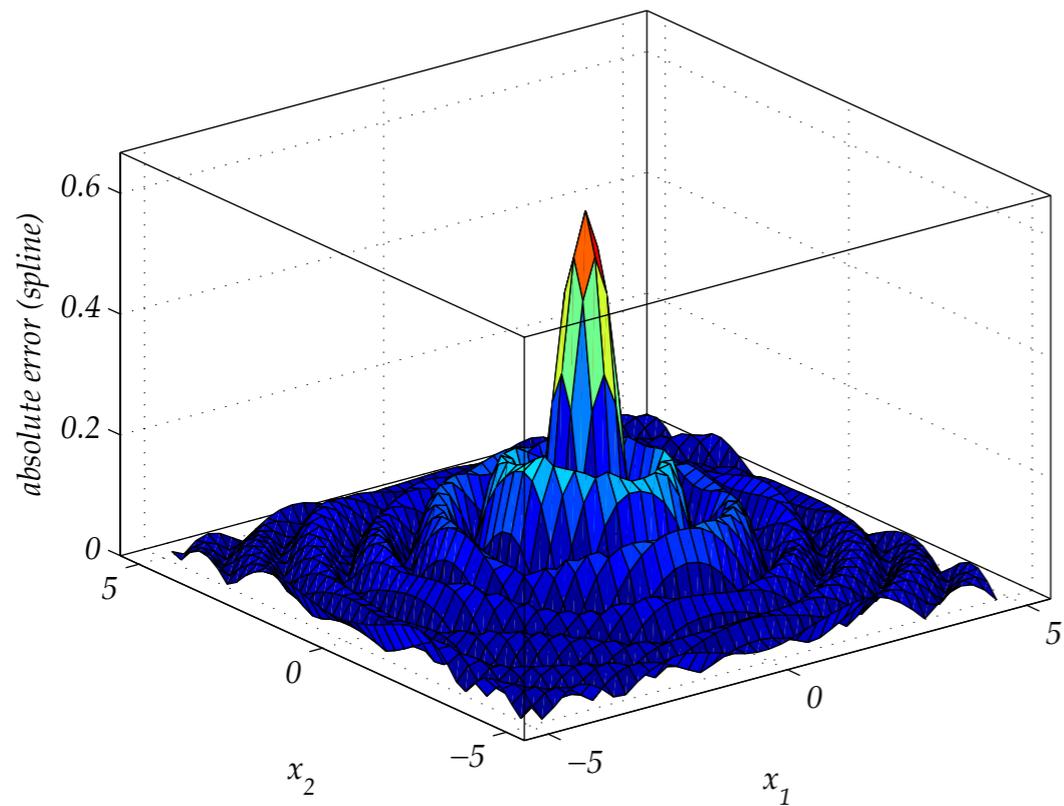
# splines & Epi-Splines 2



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