

Nonparametric Free-Knot Spline Density & Distribution Estimation for Heavy-Tailed Data

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DDFS (Density & Distribution Func. variable-knot Spline estimation)

Novel non-parametric method for *simultaneous* variable knot spline estimation of both the pdf and the cdf of a random variable.

- ① In the literature, non-parametric density estimation methods address the estimation of *solely the pdf*. However, pdf and cdf are closely connected.
- ② Model structure under which, both the pdf and cdf spline models share the *same set of knots* + their *coefficients are connected*.
- ③ Iterative approach combining:
 - **Constrained maximum likelihood estimation** of the spline coefficients.
 - **Sequential minimum bias driven estimation** of the underlying spline knots, following the Geometrically Designed Spline (GeDS) methodology (Kaishev et al., 2016, Dimitrova et al., 2023, Dimitrova et al., 2025).
- ④ Competitive alternative to state of the art methods, e.g., kernel, logsplines (Kooperberg and Stone, 1991), and recent spline-based methods (Cui et al., 2020, Kirkby et al., 2021) + *Large sample properties*.

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✱ The **pdf**, $f(x)$, is approximated by a spline function, from the space of all n -th order spline functions, $S_{t_{k,n}}$,

$$f(x; t_{k,n}, \theta) = \theta^T \mathbf{N}_n(x) = \sum_{j=1}^p \theta_j N_{j,n}(x), \quad (1)$$

where $\theta = (\theta_1, \dots, \theta_p)^T$ is a vector of *non-negative coefficients* and $\mathbf{N}_n(x) = (N_{1,n}(x), \dots, N_{p,n}(x))^T$, $p = n + k$, are normalized B-splines of order n , defined on the set of non-decreasing knots,

$$t_{k,n} = \{t_1 = \dots = t_n < t_{n+1} < \dots < t_{n+k} < t_{n+k+1} = \dots = t_{2n+k}\}. \quad (2)$$

In order for $f(x; t_{k,n}, \theta)$, to *integrate to one* and be a valid pdf, then

$$\sum_{j=1}^p \theta_j \frac{(t_{j+n} - t_j)}{n} = 1, \text{ must hold.} \quad (3)$$

✱ For the **cdf**, $F(x)$, it is natural to take

$$F(x; \mathbf{t}_{k,n+1}, \boldsymbol{\theta}') = \int_{\underline{x}}^x f(u; \mathbf{t}_{k,n}; \boldsymbol{\theta}) du = \sum_{j=1}^p \theta'_j N_{j,n+1}(x), \quad \underline{x} \leq x \leq \bar{x}, \quad (4)$$

where

$$\boldsymbol{\theta}' = (\theta'_1, \dots, \theta'_p)^T, \quad \theta'_j = \sum_{i=1}^j \theta_i \frac{t_{i+n} - t_i}{n}, \quad (5)$$

and $N_{j,n+1}(x)$, $j = 1, \dots, p$, are B-splines of order $n + 1$, on the set of non-decreasing knots

$$\begin{aligned} \mathbf{t}_{k,n+1} = \{ & t_0 = t_1 = \dots = t_n < t_{n+1} < \dots \\ & \dots < t_{n+k} < t_{n+k+1} = \dots = t_{2n+k} = t_{2n+k+1}, \} \end{aligned} \quad (6)$$

with $N_{j,n+1}(x)$ supported on $[t_j, t_{j+n+1}]$, $j = 1, \dots, p$.

Univariate pdf/cdf estimation

1. Given a set of knots $\{t_{n+1}, \dots, t_{n+k}\} \subset \mathbf{t}_{k,n} \subset \mathbf{t}_{k,n+1}$, we find the ML estimates of the parameters, $\boldsymbol{\theta}$, by solving the optimization problem

$$\hat{\boldsymbol{\theta}} = \arg \max_{\boldsymbol{\theta}} \sum_{i=1}^N \log f(X_i; \mathbf{t}_{k,n}, \boldsymbol{\theta}), \quad (7)$$

subject to the constraints

$$\theta_j \geq 0, \quad j = 1, \dots, p, \quad \text{and} \quad \sum_{j=1}^p \theta_j \frac{t_{j+n} - t_j}{n} = 1. \quad (8)$$

2. For a ML estimate $\hat{\theta}$, obtained from (7), and estimates $\hat{\theta}'$, obtained from (5), find an updated set of knots, $\hat{t}_{k,n+1}$, such that it minimizes the L_2 -distance between $F_N(x)$ and $F(x; t_{k,n+1}, \hat{\theta}')$:

$$\hat{t}_{k,n+1} = \arg \min_{t_{k,n+1}} \sum_{i=1}^N \left\{ F_N(X_i) - F(X_i; t_{k,n+1}, \hat{\theta}') \right\}^2 \quad (9)$$

subject to the constraints $\{t_{n+1} < \dots < t_{n+k}\} \subset t_{k,n} \subset t_{k,n+1}$.

- Since, k may be large, (9) is in general a *highly multivariate* optimization problem, *non-linear* in $t_{n+1}, \dots, t_{n+k}$, that is virtually impossible to solve (see, e.g., De Boor, 1978 and Lindstrom, 1999).

Instead of (9), we sequentially estimate the knots, $t_{n+1}, \dots, t_{n+k}$, applying the procedure underpinning Stage A of the **Geometrically Designed Splines (GeDS)** (Kaishev et al., 2016 and Dimitrova et al., 2023):

- At each iteration we place a knot, δ^* , within the cluster that maximizes the following-bias dominated measure:

$$w_j = \beta m'_j + (1 - \beta) \eta'_j, j = 1, \dots, u \quad (10)$$

where m'_j, η'_j denote the normalized mean and range values of the j -th cluster of residuals.

Iterative estimation process

Step 1. Given $\mathbf{t}_{k,n}$, find the ML estimates, $\hat{\boldsymbol{\theta}}$, of $f(x; \mathbf{t}_{k,n}, \boldsymbol{\theta})$.

Step 2. Use $\hat{\boldsymbol{\theta}}$ and $\mathbf{t}_{k,n}$ to compute $\hat{\boldsymbol{\theta}}'$, and then compute $F(x; \mathbf{t}_{k,n+1}, \hat{\boldsymbol{\theta}}')$, recalling that, $\mathbf{t}_{k,n+1}$ is obtained from $\mathbf{t}_{k,n}$, by adding the additional end knots, $t_0 = t_1$, and $t_{2n+k+1} = t_{2n+k}$.

Step 3. Compute the residuals

$$\rho_i = F_N(X_i) - F(X_i; \mathbf{t}_{k,n+1}, \hat{\boldsymbol{\theta}}'), \quad i = 1, \dots, N, \quad (11)$$

that provide information for the discrepancy between the ecdf, $F_N(x)$, and the estimate, $F(X_i; \mathbf{t}_{k,n+1}, \hat{\boldsymbol{\theta}}')$, of the cdf F .

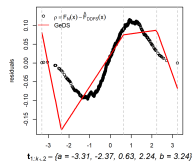
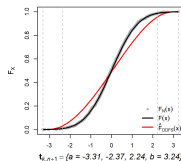
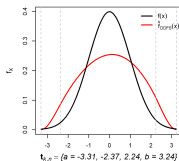
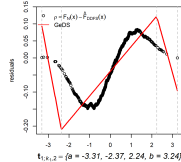
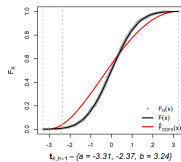
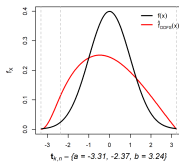
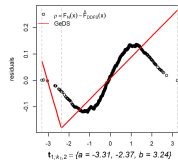
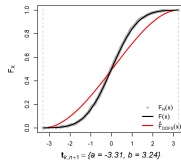
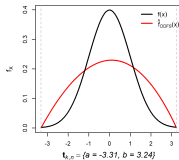
On the k -th iteration, if $k \leq q$, go to Step 4. Otherwise, use the residuals, ρ_i , $i = 1, \dots, N$, to compute the ratio

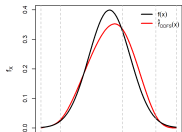
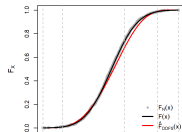
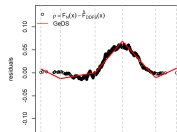
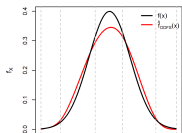
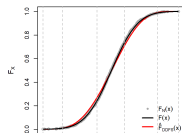
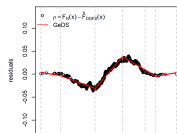
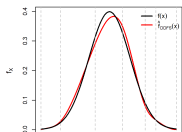
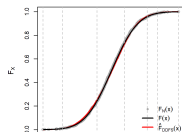
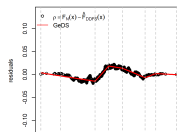
$$\phi = \frac{\sum_{i=1}^N \left\{ F_N(X_i) - F(X_i; \mathbf{t}_{k,n+1}, \hat{\boldsymbol{\theta}}') \right\}^2}{\sum_{i=1}^N \left\{ F_N(X_i) - F(X_i; \mathbf{t}_{k-q,n+1}, \hat{\boldsymbol{\theta}}') \right\}^2}. \quad (12)$$

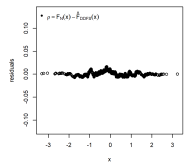
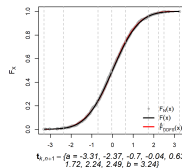
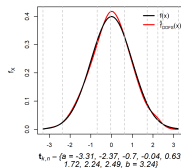
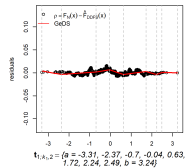
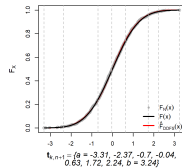
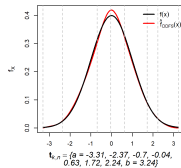
If $\phi \geq \phi_{exit}$, then exit the iterations with final estimates, $f(x; \mathbf{t}_{k-q,n}, \hat{\boldsymbol{\theta}})$ and $F(x; \mathbf{t}_{k-q,n+1}, \hat{\boldsymbol{\theta}}')$. If $\phi < \phi_{exit}$, then go to Step 4.

Step 4. Find a new knot δ^* , applying the *locally adaptive bias minimizing knot insertion scheme* of Stage A of GeDS, viewing ρ_i , from (11), as the observations y_i , $i = 1, \dots, N$.

Update the current set of knots as, $\mathbf{t}_{k+1,n+1} = \mathbf{t}_{k,n+1} \cup \delta^*$. Set, $\mathbf{t}_{k,n} \leftarrow \mathbf{t}_{k+1,n+1}$ and go back to Step 1.



 $t_{k,n} = (a = -3.31, -2.37, 0.63, 2.24, b = 3.24)$  $t_{k,n+1} = (a = -3.31, -2.37, 0.63, 2.24, b = 3.24)$  $t_{1,k;2} = (a = -3.31, -2.37, -0.7, 0.63, 2.24, b = 3.24)$  $t_{k,n} = (a = -3.31, -2.37, -0.7, 0.63, 2.24, b = 3.24)$  $t_{k,n+1} = (a = -3.31, -2.37, -0.7, 0.63, 2.24, b = 3.24)$  $t_{1,k;2} = (a = -3.31, -2.37, -0.7, 0.63, 1.72, 2.24, b = 3)$  $t_{k,n} = (a = -3.31, -2.37, -0.7, 0.63, 1.72, 2.24, b = 3.24)$  $t_{k,n+1} = (a = -3.31, -2.37, -0.7, 0.63, 1.72, 2.24, b = 3.24)$  $t_{1,k;2} = (a = -3.31, -2.37, -0.7, 0.63, 1.72, 2.24, b = 3.24)$



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Asymptotic properties of DDFS

Lemma. The spline density estimator, $f(x; \mathbf{t}_{k,n}, \boldsymbol{\theta})$ can be expressed as the following mixture

$$f(x; \mathbf{t}_{k,n}, \boldsymbol{\theta}) = \alpha_1 f_{L_1}(x; \boldsymbol{\tau}_1) + \dots + \alpha_p f_{L_p}(x; \boldsymbol{\tau}_p), \quad (13)$$

where $\alpha_j = \theta_j \frac{t_{j+n} - t_j}{n} \geq 0$, $\sum_{j=1}^p \alpha_j = 1$, and where $f_{L_j}(x; \boldsymbol{\tau}_j)$, $j = 1, \dots, p$, are densities, with respect to the Lebesgue measure, of the linear combinations, L_j , $j = 1, \dots, p$ of Dirichlet random variables (follows from (1), (3) and a result due to Ignatov and Kaishev, 1989).

Theorem. For a fixed set of knots, $\mathbf{t}_{k,n}$, the ML estimates $\hat{\boldsymbol{\theta}}$ are *strongly consistent* and *asymptotically normal* as $N \rightarrow \infty$ (the result of the theorem follows from the Lemma above and a result due to Redner and Walker, 1984).

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Test case	Density	Test case	Density
Gaussian	$N(0, 1)$	Merton's jump diffusion	$\sigma = 0.08, \lambda = 3 \mu_J = -0.01,$ $\sigma_J = 0.4, \Delta_t = 1/4$
Student- t	$t_v, v = 6$	Kou's double exponential	$\sigma = 0.04, \lambda = 2 p_{up} = 0.4,$ $\eta_1 = 3, \eta_2 = 5, \Delta_t = 1/4$
Exponential	$\text{Exp}(\lambda), \lambda = 1, x \geq 0$	Generalized extreme value	$\frac{1}{\sigma} \exp\left(-\left(1 + k \frac{x-\mu}{\sigma}\right)^{-\frac{1}{k}}\right) \left(1 + k \frac{x-\mu}{\sigma}\right)^{-1-\frac{1}{k}}$ $k = -0.5, 0 \text{ and } 0.5, \mu = 1, \sigma = 0, x > 0$
Chi-square	$\chi_k^2, k = 4, x > 0$	MixGauss	$0.15N(-0.25, 1/3) + 0.85N(3.25, 1)$
Gamma	$x \geq 0, k = 9, \theta = 0.5$	Mix1d	$0.8\chi^2(3) + 0.2N(7, 1)$
Weibull	$x \geq 0, \lambda = 1, k = 5$	MixGauss2	$\frac{5}{6}N(3, 1) + \frac{5}{36}N(8, (1/3)^2) + \frac{1}{36}N(10, (1/9)^2)$
Log-normal	$x > 0, \mu = 0, \sigma = 1$	Bimodal	$\frac{1}{2}N\left(0, \left(\frac{1}{10}\right)^2\right) + \frac{1}{2}N(5, 1)$
Nakagami	$\frac{2\mu^\mu x^{2\mu-1}}{\Gamma(\mu)\omega^\mu} \exp\left(-\frac{\mu}{\omega}x^2\right), x > 0, \mu = \omega = 2$	Separated bimodal	$\frac{1}{2}N\left(-2, \left(\frac{1}{2}\right)^2\right) + \frac{1}{2}N\left(2, \left(\frac{1}{2}\right)^2\right)$
Kurtotic unimodal	$\frac{2}{3}N(0, 1) + \frac{1}{3}N\left(0, \left(\frac{1}{10}\right)^2\right)$	Skewed bimodal	$\frac{3}{4}N(0, 1) + \frac{1}{4}N\left(\frac{3}{2}, \left(\frac{1}{3}\right)^2\right)$
Outlier	$\frac{1}{10}N(0, 1) + \frac{9}{10}N\left(0, \left(\frac{1}{10}\right)^2\right)$	Trimodal	$\frac{1}{3} \sum_{k=0}^2 N(80k, (k+1)^4)$
Skewed unimodal	$\frac{1}{5}N(0, 1) + \frac{1}{5}N\left(\frac{1}{2}, \left(\frac{2}{3}\right)^2\right) + \frac{3}{5}N\left(\frac{13}{12}, \left(\frac{5}{9}\right)^2\right)$	Smooth comb	$\sum_{k=0}^5 \frac{2^{5-k}}{63} N\left(\frac{65-96/2^k}{21}, \left(\frac{32/63}{2^k}\right)^2\right)$
Strongly skewed	$\sum_{k=0}^7 \frac{1}{8} N\left(3\left(\left(\frac{2}{3}\right)^k - 1\right), \left(\frac{2}{3}\right)^{2k}\right)$	Claw	$\frac{1}{2}N(0, 1) + \sum_{k=0}^4 \frac{1}{10} N\left(\frac{k}{2} - 1, \left(\frac{1}{10}\right)^2\right)$

We assess the goodness-of-fit over a regular grid of K evaluation points $x_1, \dots, x_K$ with uniform spacing $\Delta x = x_{i+1} - x_i$, based on:

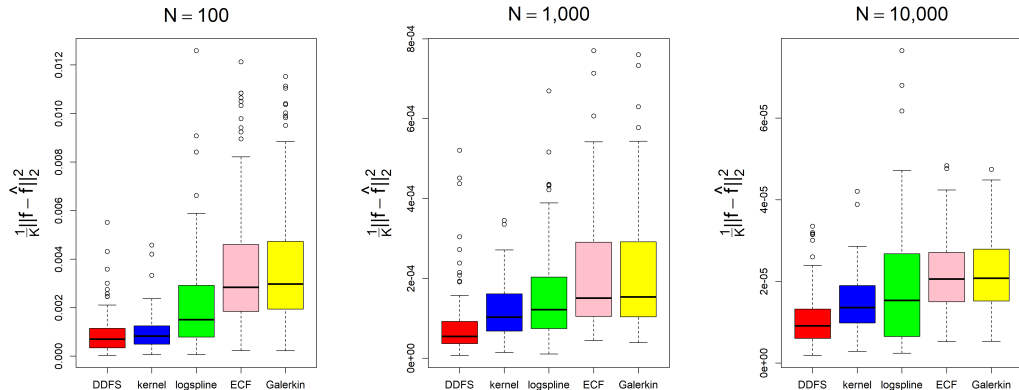
- **Mean Integrated Squared Error (MISE)**

$$\mathbb{E} \left[\int (\hat{f}(x; N) - f(x))^2 dx \right] \approx \Delta x \sum_{i=1}^K (\hat{f}(x_i; N) - f(x_i))^2$$

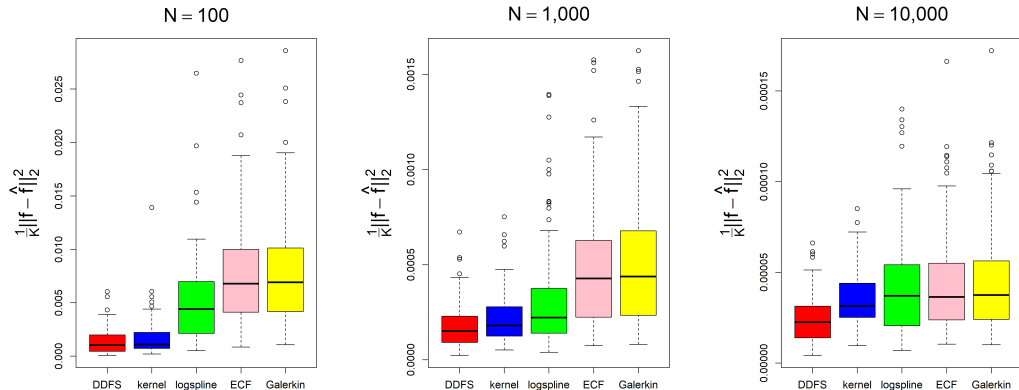
- **Roughness, $R(f)$**

$$R(f) = \int (f''(x))^2 dx \approx \Delta x \sum_{i=2}^{K-1} \left(\frac{f(x_{i+1}) - 2f(x_i) + f(x_{i-1}))}{(\Delta x)^2} \right)^2$$

MISE boxplots - Generalized Extreme Value, Type I (Gumbel)

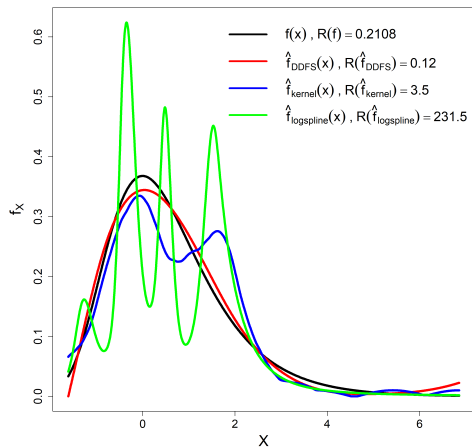


MISE boxplots - Generalized Extreme Value, Type III (Weibull)

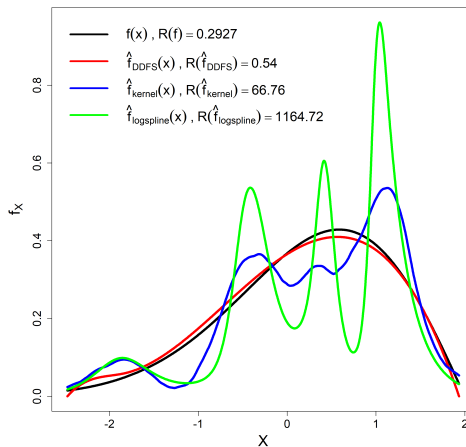


Roughness - Generalized Extreme Value, Type I and III (pdf)

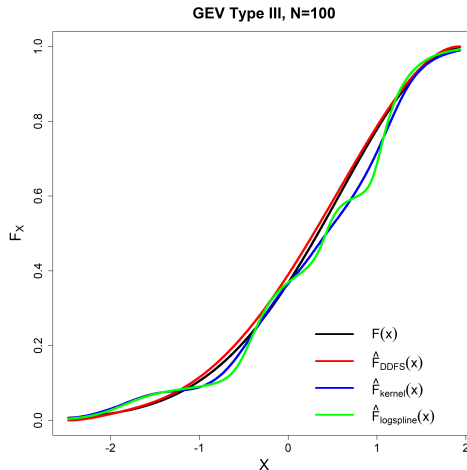
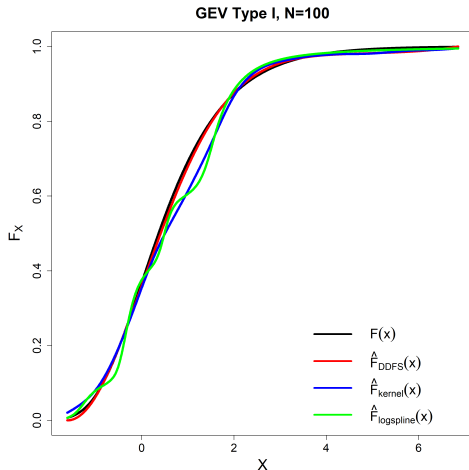
GEV Type I, N=100



GEV Type III, N=100



Roughness - Generalized Extreme Value, Type I and III (cdf)



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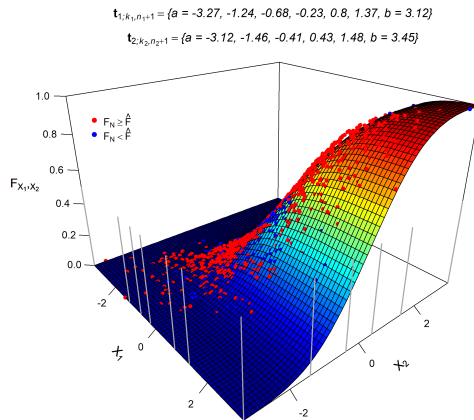
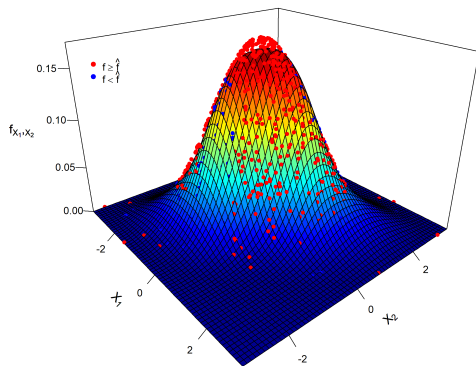
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4.1 Univariate examples

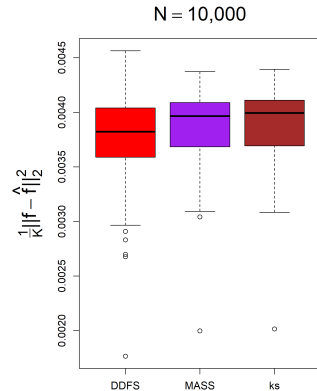
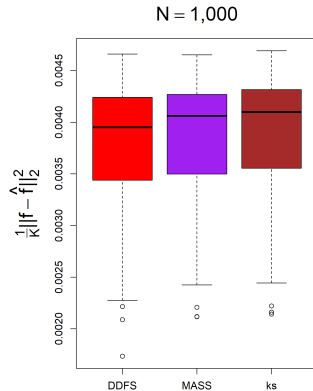
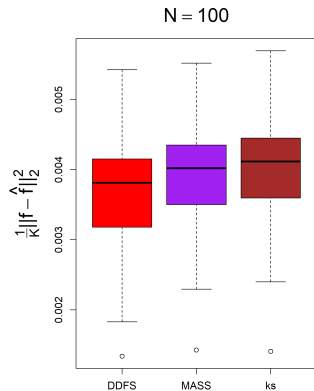
4.2 Bivariate examples

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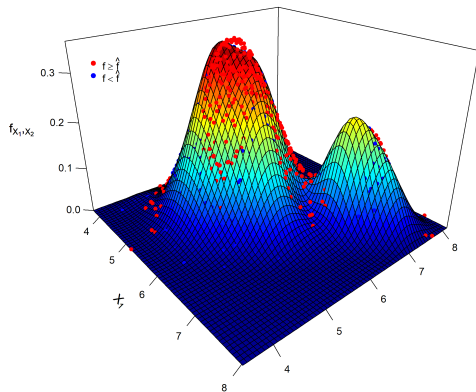
Bivariate Gaussian, $\rho = 0.5$



MISE boxplots - Bivariate Gaussian, $\rho = 0.5$

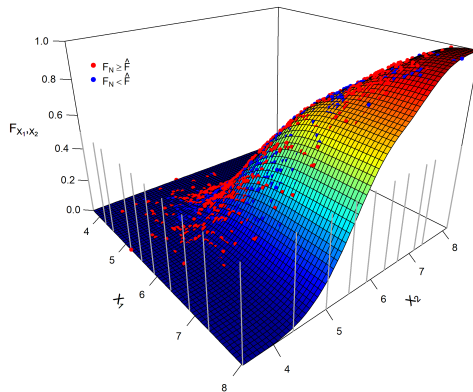


Bivariate Bimodal Mixed Gaussian

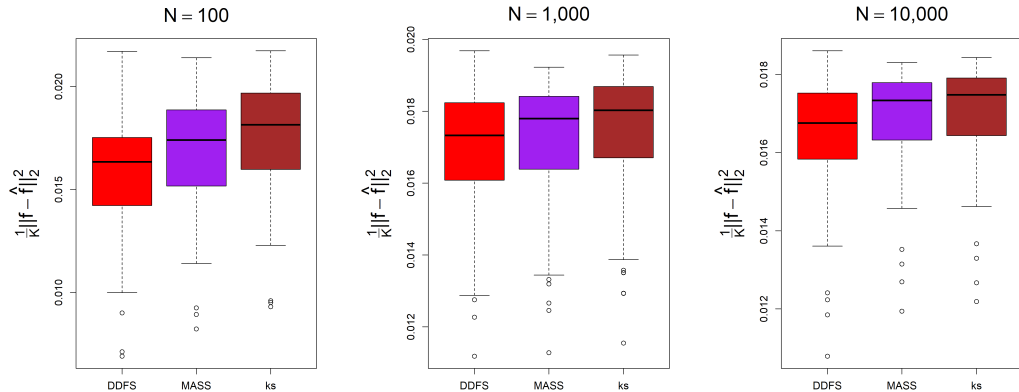


$$\mathbf{t}_{1; k_1, n_1+1} = \{a = 3.74, 4.26, 4.55, 5.18, 5.54, 5.92, 6.39, 6.87, 7.33, b = 8.02\}$$

$$\mathbf{t}_{2; k_2, n_2+1} = \{a = 3.48, 4.36, 5, 5.49, 5.9, 6.34, 6.68, 7.14, 7.38, b = 8.14\}$$



Bivariate Bimodal Mixed Gaussian



1. Introduction

2. Simultaneous pdf and cdf estimation with variable knot splines

3. Large sample properties

4. Numerical examples

4.1 Univariate examples

4.2 Bivariate examples

5. An application for risk measurement

Loss data modelling

Proliferation of composite and mixture (parametric) models proposed for the modelling of insurance loss data (Marambakuyana and Shongwe, 2024).

✱ Estimation often requires **large samples to converge** (data availability might be a problem) + **high computational burden**:
—→ many actuarial studies only fit the model once (on the whole dataset) and perform backtesting on a static forecast (see, e.g., Abu Bakar et al., 2015);

✗ *rolling-window historical simulation backtesting.*

Some frequently considered loss-datasets are:

1. *Danish Fire Insurance.*
2. *Norwegian Fire Insurance Data.*
3. *US Allocated Loss Adjustment Expenses.*

➤ Assess model reliability via **rolling window back-testing** (Basel III, EIOPA):
Proportion of Failures (Kupiec, 1995), *Conditional Coverage* (Christoffersen, 1998),
Dynamic Quantile (Engle and and, 2004).

Danish Fire Insurance

VaR Backtesting: Actual Claims vs. VaR Forecast

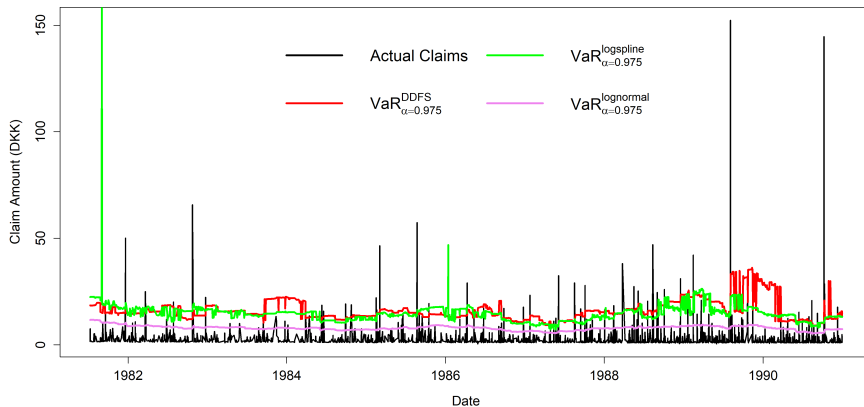


Table 1: Backtesting statistics for VaR models (data = danish).

	$\alpha = 0.975$				$\alpha = 0.99$			
	Viol. rate	UC	CC	DQ	Viol. rate	UC	CC	DQ
ddfs	0.0250	0.9946	0.1776	0.0244	0.0103	0.9024	0.7819	0.0349
kernel	0.0259	0.7931	0.0623	0.0001	0.0116	0.4586	0.5600	0.0006
logspline	0.0245	0.8867	0.4458	0.1013	0.0120	0.3462	0.4617	0.0256
lognormal	0.0531	0.0000	0.0000	0.0000	0.0397	0.0000	0.0000	0.0000
gamma	0.0437	0.0000	0.0000	0.0000	0.0361	0.0000	0.0000	0.0000

Norwegian Fire Insurance Data

VaR Backtesting: Actual Claims vs. VaR Forecast

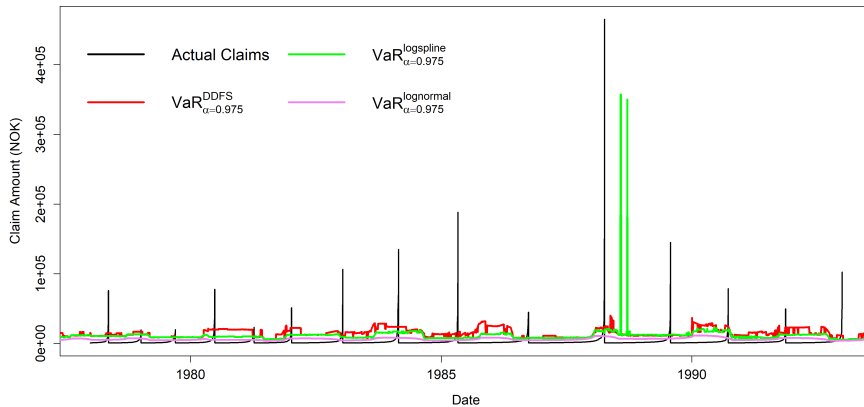


Table 2: Backtesting statistics for VaR models (data = norwegian).

	$\alpha = 0.975$				$\alpha = 0.99$			
	Viol. rate	UC	CC	DQ	Viol. rate	UC	CC	DQ
ddfs	0.0265	0.3816	0.0000	0.0206	0.0100	0.9832	0.0000	0.0001
kernel	0.0351	0.0000	0.0000	0.0078	0.0156	0.0000	0.0000	0.0000
logspline	0.0356	0.0000	0.0000	0.0074	0.0147	0.0001	0.0000	0.0000
lognormal	0.0583	0.0000	0.0000	0.0032	0.0390	0.0000	0.0000	0.0000
gamma	0.0466	0.0000	0.0000	0.0048	0.0336	0.0000	0.0000	0.0000

US Allocated Loss Adjustment Expenses

VaR Backtesting: Actual Claims vs. VaR Forecast

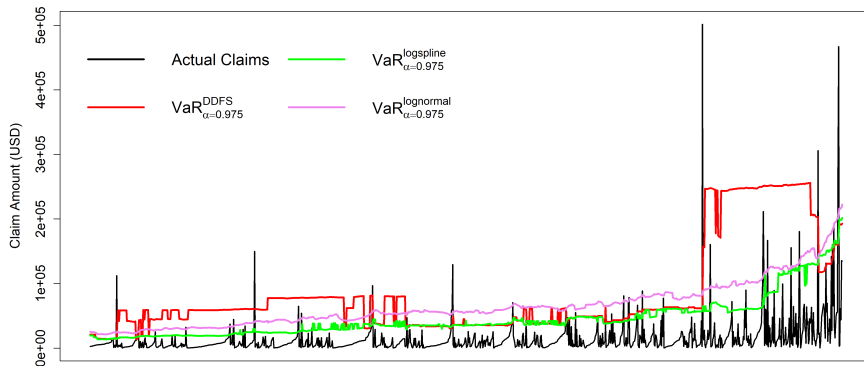


Table 3: Backtesting statistics for VaR models (data = lossalae).

	$\alpha = 0.975$				$\alpha = 0.99$			
	Viol. rate	UC	CC	DQ	Viol. rate	UC	CC	DQ
ddfs	0.0256	0.8923	0.0000	0.9663	0.0112	0.6757	0.0000	0.6161
kernel	0.0448	0.0001	0.0000	0.4172	0.0224	0.0002	0.0000	0.2674
logspline	0.0448	0.0001	0.0000	0.4292	0.0272	0.0000	0.0000	0.0133
lognormal	0.0200	0.2410	0.0218	0.9555	0.0072	0.2950	0.5413	0.6525
gamma	0.0488	0.0000	0.0000	0.4018	0.0360	0.0000	0.0000	0.0040

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