Confidence Bands for Distribution Functions: The Law of the Iterated Logarithm and Shape Constraints

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I. The LIL for Brownian Motion and Bridge

Standard Brownian motion $\mathbb{W} = (\mathbb{W}(t))_{t \geq 0}$

LIL for BM:

$$\limsup_{t \downarrow 0} \frac{\pm \mathbb{W}(t)}{\sqrt{2t \log \log(t^{-1})}} = 1 \quad \text{a.s.}$$

$$\limsup_{t \uparrow \infty} \frac{\pm \mathbb{W}(t)}{\sqrt{2t \log \log(t)}} = 1 \quad \text{a.s.}$$

Refined half of LIL for BM:

For any constant $\nu > 3/2$,

$$\lim_{t \to \{0,\infty\}} \Big(\frac{\mathbb{W}(t)^2}{2t} - \log\log(t + t^{-1}) - \nu \log\log\log(t + t^{-1}) \Big) = -\infty \quad \text{a.s.}$$

Reformulation for standard Brownian bridge $\mathbb{U} = (\mathbb{U}(t))_{t\in(0,1)}$:

$$(0,1) \ni t \mapsto \operatorname{logit}(t) := \log\Big(\frac{t}{1-t}\Big) \in \mathbb{R},$$
$$\mathbb{R} \ni x \mapsto \ell(x) := \frac{e^x}{1+e^x} \in (0,1).$$

Refined half of LIL for BB:

For arbitrary constants $\nu > 3/2$,

$$\sup_{t\in(0,1)} \Big(\frac{\mathbb{U}(t)^2}{2t(1-t)} - C(t) - \nu D(t) \Big) \ < \ \infty \quad \text{a.s.}$$

where

$$C(t) \ := \ \log\sqrt{1+\text{logit}(t)^2/2} \qquad \approx \ \log\log\Big(\frac{1}{t(1-t)}\Big)$$

$$D(t) \ := \ \log\sqrt{1+C(t)^2/2} \qquad \approx \ \log\log\log\Big(\frac{1}{t(1-t)}\Big)$$

as $t \to \{0,1\}$.

II. A General LIL for Sub-Exponential Processes

Nonnegative stochastic process

$$X = (X(t))_{t \in \mathcal{T}} \quad \text{on} \quad \mathcal{T} \subset (0,1).$$

Locally uniform sub-exponentiality:

LUSE$_0$: For arbitrary $a \in \mathbb{R}$, $c \geq 0$ and $\eta \geq 0$,

$$\mathbb{P}\Big(\sup_{t \in [\ell(a), \ell(a+c)]} X(t) \geq \eta \Big) \leq M \exp(-L(c)\,\eta),$$

where $M \geq 1$ and $L : [0, \infty) \to [0,1]$ satisfies

$$L(c) = 1 - O(c) \quad \text{as } c \downarrow 0$$

Refinement for $\zeta \in [0, 1]$:

LUSE$_\zeta$: For arbitrary $a \in \mathbb{R}$, $c \geq 0$ and $\eta \geq 0$,

$$\mathbb{P}\Big(\sup_{t \in [\ell(a), \ell(a+c)]} X(t) \geq \eta \Big) \ \leq \ \frac{M \exp(-L(c)\,\eta)}{\max(1, L(c)\,\eta)^{\zeta}},$$

with M and $L(\cdot)$ as in LUSE$_0$.

Example:

$$X(t) \ := \ \frac{\mathbb{U}(t)^2}{2t(1-t)}$$

satisfies LUSE$_{1/2}$ with

$$M \ = \ 2 \quad \text{and} \quad L(c) \ = \ e^{-c}.$$

Proposition. Suppose that X satisfies LUSE_ζ.

For any $L_o \in (0,1)$ and $\nu > 2-\zeta$ there exists a constant $M_o = M_o(M, L(\cdot), \zeta, L_o, \nu) \geq 1$ such that

$$\mathbb{P}\Big(\sup_{\mathcal{T}} (X - C - \nu D) \geq \eta\Big) \;\leq\; M_o \exp(-L_o\, \eta)$$

for arbitary $\eta \geq 0$.

III. Implications for the Uniform Empirical Process

Let $U_1, U_2, \ldots, U_n$ be i.i.d. $\sim \mathrm{Unif}[0,1]$.

Auxiliary function $K : [0,1] \times (0,1) \to [0,\infty]$,

$$K(x,p) \; := \; x \log\Bigl(\frac{x}{p}\Bigr) + (1-x) \log\Bigl(\frac{1-x}{1-p}\Bigr)$$

i.e. Kullback-Leibler divergence between $\mathrm{Bin}(1,x)$ and $\mathrm{Bin}(1,p)$.

Two key properties:

$$K(x,p) \; = \; \frac{(x-p)^2}{2p(1-p)}\bigl(1+o(1)\bigr) \quad \text{as } x \to p.$$

$$K(x,p) \le c \quad \Longrightarrow \quad |x-p| \le \begin{cases} \sqrt{2c\,p(1-p)} + c \\ \sqrt{2c\,x(1-x)} + c \end{cases}$$

Implication 1: Uniform empirical distribution function

$$\widehat{G}_n(t) \;:=\; \frac{1}{n}\sum_{i=1}^{n} 1_{[U_i \le t]}$$

Lemma 1. The process $X_n = (X_n(t))_{t\in(0,1)}$ with

$$X_n(t) \;:=\; n\,K(\widehat{G}_n(t), t)$$

satisfies LUSE_0 with $M = 2$ and $L(c) = e^{-c}$.

Theorem 1. For any fixed $\nu > 2$,

$$\sup_{(0,1)}\bigl(X_n - C - \nu D\bigr) \;\to_{\mathcal{L}}\; \sup_{t\in(0,1)}\Bigl(\frac{\mathbb{U}(t)^2}{2t(1-t)} - C(t) - \nu D(t)\Bigr).$$

Main ingredients for proofs:

- $\left(\widehat{G}_n(t)/t\right)_{t\in(0,1]}$ is a reverse martingale.
- Exponential transform and Doob's inequality for submartingales.
- Analytical properties of $K(\cdot,\cdot)$.
- Donsker's invariance for uniform empirical process.

Implication 2: Uniform order statistics

$$0 \; < \; U_{n:1} \; < \; U_{n:2} \; < \; \cdots \; < \; U_{n:n} \; < \; 1.$$

$$\mathcal{T}_n \; := \; \{t_{n1}, t_{n2}, \ldots, t_{nn}\} \quad \text{with} \quad t_{ni} \; := \; \mathbb{E}(U_{n:i}) = \frac{i}{n+1}.$$

Lemma 2. The process $\tilde{X}_n = (\tilde{X}_n(t))_{t \in \mathcal{T}_n}$ with

$$\tilde{X}_n(t_{ni}) \; := \; (n+1) K(t_{ni}, U_{n:i})$$

satisfies LUSE_0 with $M = 2$ and $L(c) = e^{-c}$.

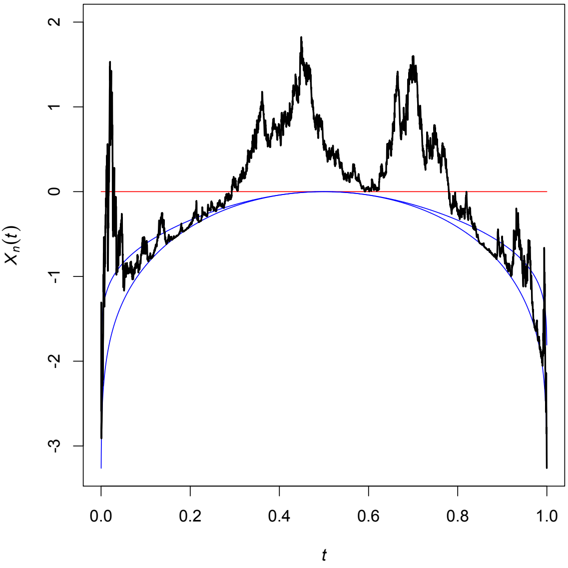
Theorem 2. For any fixed $\nu > 2$,

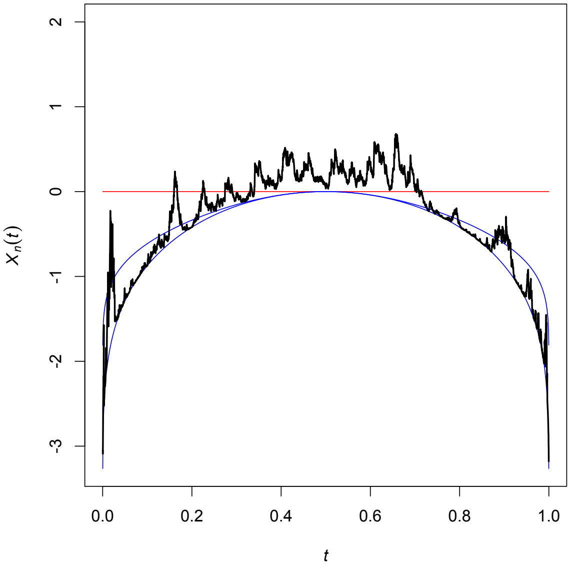
$$\sup_{\mathcal{T}_n} \bigl(\tilde{X}_n - C - \nu D \bigr) \; \to_{\mathcal{L}} \; \sup_{t \in (0,1)} \Bigl(\frac{\mathbb{U}(t)^2}{2t(1-t)} - C(t) - \nu D(t) \Bigr).$$

Main ingredients for proofs:

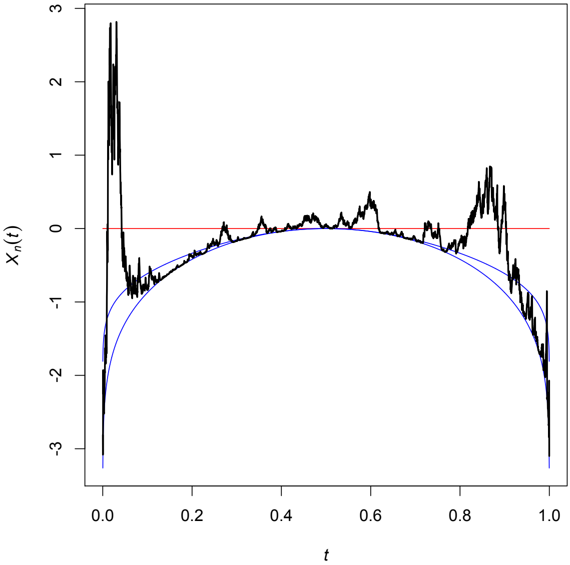
- $\left(U_{n:i}/t_{ni}\right)_{i=1}^{n}$ is a reverse martingale.
- Exponential transform and Doob's inequality for submartingales.
- Connection between Beta and Gamma distributions.
- Analytical properties of $K(\cdot,\cdot)$.
- Donsker's invariance principle for uniform quantile process.

Some realizations of $\tilde{X}_n$ for $n = 5000$ and $\nu = 3$:

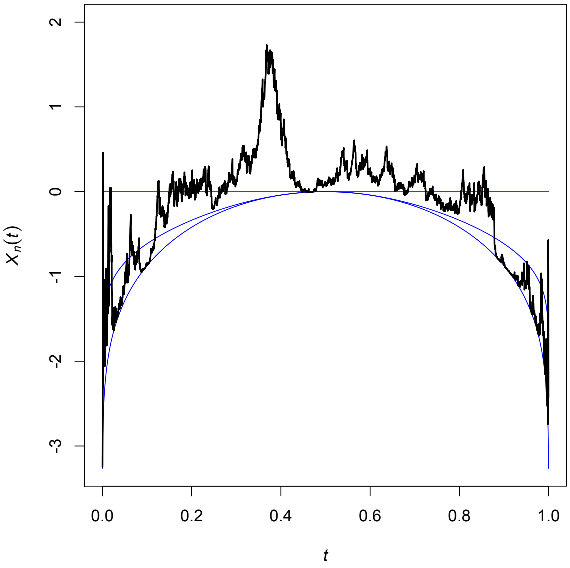




2
1
0
-1
-2
-3
$X_n(t)$
0.0
0.2
0.4
0.6
0.8
1.0
t

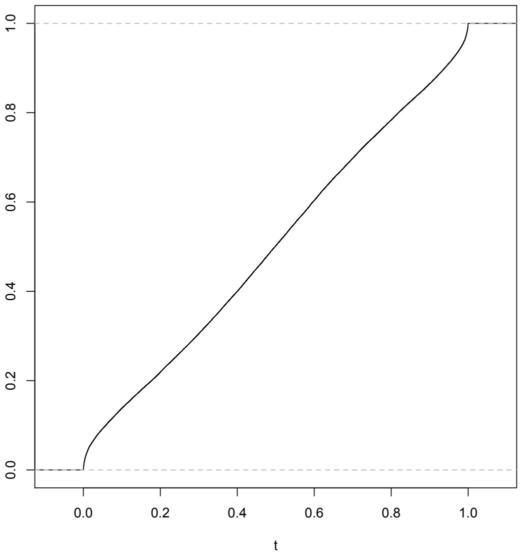


3
2
1
0
-1
-2
-3
$X_n(t)$
0.0
0.2
0.4
0.6
0.8
1.0
t



2
1
0
-1
-2
-3
$X_n(t)$
0.0
0.2
0.4
0.6
0.8
1.0
t

Distribution function of $\arg\max_t \tilde{X}_n(t)$:



III.1 Goodness-of-Fit Tests

Let $X_1, X_2, \ldots, X_n$ be i.i.d. with unknown c.d.f. F on $\mathbb{R}$.

Empirical c.d.f.

$$\widehat{F}_n(x) \ := \ \frac{1}{n}\sum_{i=1}^{n} 1_{[X_i \leq x]}.$$

Testing problem:

$$H_o \ : \ F \equiv F_o \quad \text{versus} \quad H_A \ : \ F \not\equiv F_o.$$

Berk–Jones (1979) proposed the test statistic

$$T_n(F_o) \ := \ \sup_{\mathbb{R}} \, n\, K(\widehat{F}_n, F_o)$$

with critical value

$$\kappa_{n,\alpha}^{\mathrm{BJ}} \ := (1-\alpha) - \text{quantile of } \sup_{t \in (0,1)} \, n\, K_n(\widehat{G}_n(t), t)$$

$$= \ \log\log(n) + O\big(\log\log\log(n)\big).$$

New proposal:

$$T_n(F_o) \;:=\; \sup_{\mathbb{R}}\big(n\,K(\widehat{F}_n, F_o) - C(F_o) - \nu D(F_o)\big)$$

with critical value

$$\begin{aligned}
\kappa_{n,\alpha}^{\mathrm{new}} \;&:= (1-\alpha) - \text{quantile of} \\
&\qquad\qquad \sup_{t\in(0,1)} \big(n\,K(\widehat{G}_n(t), t) - C(t) - \nu D(t)\big) \\
&\to (1-\alpha) - \text{quantile of} \\
&\qquad\qquad \sup_{t\in(0,1)} \Big(\frac{\mathbb{U}(t)^2}{2t(1-t)} - C(t) - \nu D(t)\Big).
\end{aligned}$$

Power. For any fixed $\kappa > 0$,

$$\mathbb{P}_{F_n}\big(T_n(F_o) > \kappa\big) \;\to\; 1$$

as

$$\sup_{\mathbb{R}} \frac{\sqrt{n}|F_n - F_o|}{\sqrt{(1 + C(F_o))F_o(1 - F_o)} + C(F_o)/\sqrt{n}} \;\to\; \infty.$$

Special case: Detecting heterogeneous Gaussian mixtures
(Ingster 1997, 1998; Donoho–Jin 2004)

Setting 1:

$$\begin{aligned} F_o &:= \Phi, \\ F_n &:= (1 - \varepsilon_n)\,\Phi + \varepsilon_n\,\Phi(\cdot - \mu_n) \end{aligned}$$

with

$$\begin{aligned} \varepsilon_n &= n^{-\beta + o(1)}, \quad \beta \in (1/2, 1), \\ \mu_n &\to \infty. \end{aligned}$$

Theorem. For any fixed $\kappa > 0$,

$$\mathbb{P}_{F_n}\big(T_n(F_o) > \kappa\big) \ \to \ 1$$

provided that

$$\mu_n = \sqrt{2r\log(n)} \quad \text{with} \quad r > \begin{cases} \beta - 1/2 & \text{if } \beta \leq 3/4, \\ \big(1 - \sqrt{1-\beta}\big)^2 & \text{if } \beta \geq 3/4. \end{cases}$$

Setting 2 (Contiguous alternatives):

$$\begin{aligned} F_o &:= \Phi, \\ F_n &:= \Big(1 - \frac{\pi}{\sqrt{n}}\Big)\,\Phi + \frac{\pi}{\sqrt{n}}\,\Phi(\cdot - \mu), \qquad \pi, \mu > 0. \end{aligned}$$

Optimal level-α test of F_o versus F_n has asymptotic power

$$\Phi\Big(\Phi^{-1}(\alpha) + \frac{\pi^2(\exp(\mu^2) - 1)}{4}\Big).$$

Theorem. Let $\mu = \sqrt{2s \log(1/\pi)}$ for fixed $s > 0$. As $\pi \downarrow 0$,

$$\Phi\Big(\Phi^{-1}(\alpha) + \frac{\pi^2(\exp(\mu^2) - 1)}{4}\Big) \;\to\; \begin{cases} \alpha & \text{if } s < 1, \\ 1 & \text{if } s > 1, \end{cases}$$

while for any fixed $\kappa > 0$,

$$\mathbb{P}_{F_n}\big(T_n(F_o) > \kappa\big) \;\to\; \quad 1 \quad \text{if } s > 1.$$

III.2 Confidence Bands

Owen (1995) proposed $(1-\alpha)$-confidence band

$$\Big\{F : \sup_{\mathbb{R}} n\,K(\widehat{F}_n, F) \le \kappa_{n,\alpha}^{\mathrm{BJ}}\Big\}.$$

New proposal: With order statistics $X_{n:1} \le X_{n:2} \le \cdots \le X_{n:n}$,

$$\Big\{F : \max_{1\le i\le n}\big((n+1)K(t_{ni}, F(X_{n:i})) - C(t_{ni}) - \nu D(t_{ni})\big) \le \tilde{\kappa}_{n,\alpha}\Big\}$$

Resulting bounds for $F(x)$:

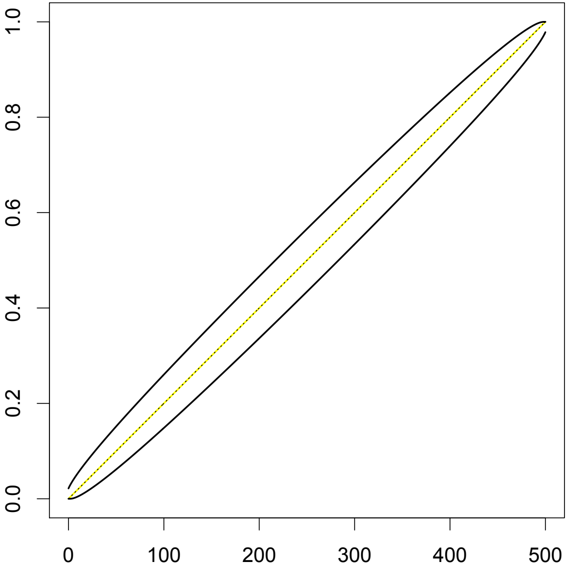
With confidence $1-\alpha$, on $[X_{n:i}, X_{n:i+1})$, $0 \le i \le n$,

$$F \in \begin{cases} [a_{ni}^{\mathrm{BJO}}, b_{ni}^{\mathrm{BJO}}] & \text{with Owen's (1995) proposal,} \\ [a_{ni}^{\mathrm{new}}, b_{ni}^{\mathrm{new}}] & \text{with new proposal,} \end{cases}$$

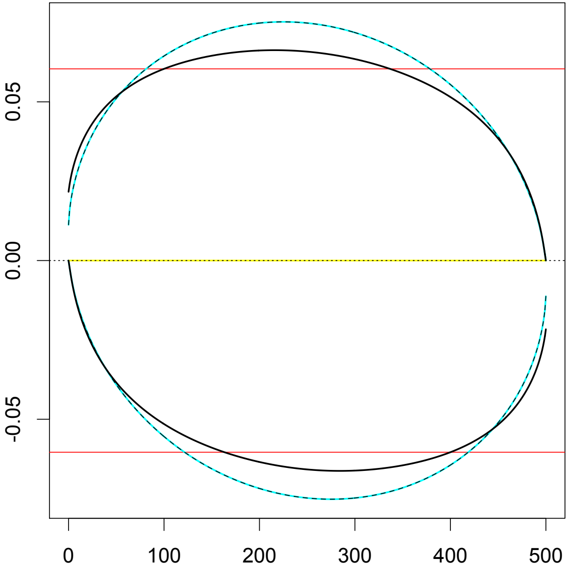
while

$$\widehat{F}_n = s_{ni} := \frac{i}{n}.$$

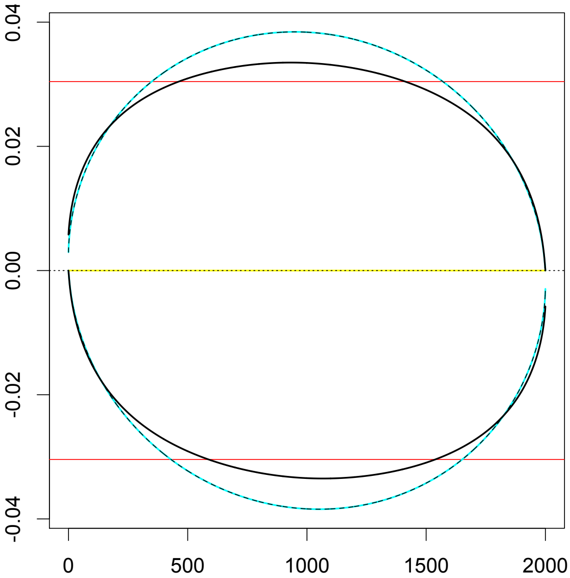
$n = 500$: $\quad i \mapsto a_{ni}^{\mathrm{new}}, s_{ni}, b_{ni}^{\mathrm{new}}$



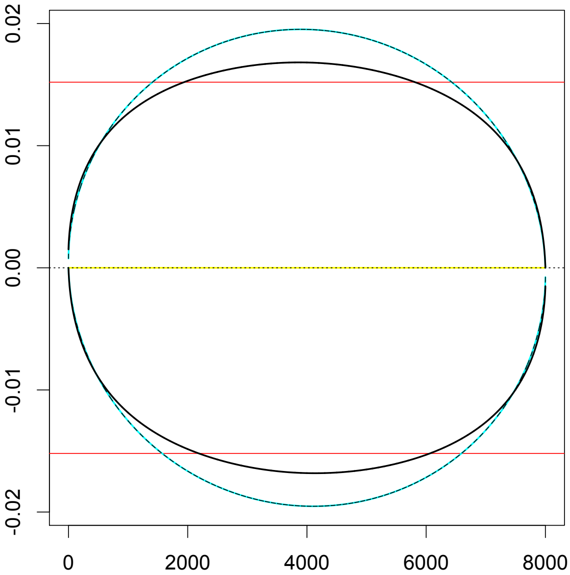
$n = 500$: $i \mapsto a^*_{ni} - s_{ni}, b^*_{ni} - s_{ni}$



$n = 2000$: $\quad i \mapsto a^*_{ni} - s_{ni}, b^*_{ni} - s_{ni}$



$n = 8000$: $\quad i \mapsto a^*_{ni} - s_{ni}, b^*_{ni} - s_{ni}$



Theorem. For any fixed $\alpha \in (0, 1)$,

$$\max_{0 \le i \le n} \frac{b_{ni}^{\mathrm{new}} - a_{ni}^{\mathrm{new}}}{b_{ni}^{\mathrm{BJO}} - a_{ni}^{\mathrm{BJO}}} \;\to\; 1,$$

while

$$\begin{aligned} \max_{0 \le i \le n} (b_{ni}^{\mathrm{BJO}} - a_{ni}^{\mathrm{BJO}}) \;&=\; (1 + o(1))\sqrt{\frac{2 \log \log n}{n}}, \\ \max_{0 \le i \le n} (b_{ni}^{\mathrm{new}} - a_{ni}^{\mathrm{new}}) \;&=\; O(n^{-1/2}). \end{aligned}$$

IV. Bi-Log-Concave Distribution Functions

Shape constraint 1: Log-concave density.

F has density $f = e^{\phi}$ with $\phi : \mathbb{R} \to [-\infty, \infty)$ concave.

Shape constraint 2: Bi-log-concave distribution function.

Both $\log(F)$ and $\log(1 - F)$ are concave.

- Log-concave density $\Longrightarrow$ bi-log-concave c.d.f.
- A bi-log-concave c.d.f. may have arbitrarily many modes!

Theorem. Let $J(F) := \{x \in \mathbb{R} : 0 < F(x) < 1\} \neq \emptyset$.
Four equivalent statements:

- F bi-log-concave.
- F has a density f. On $J(F)$,

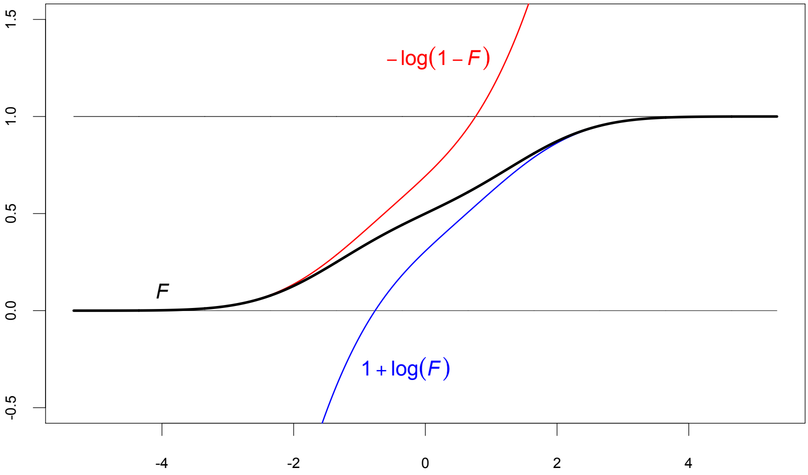
$$f = F' > 0, \quad \frac{f}{F} \searrow \quad \text{and} \quad \frac{f}{1-F} \nearrow.$$

- F has a bounded density f. On $J(F)$,

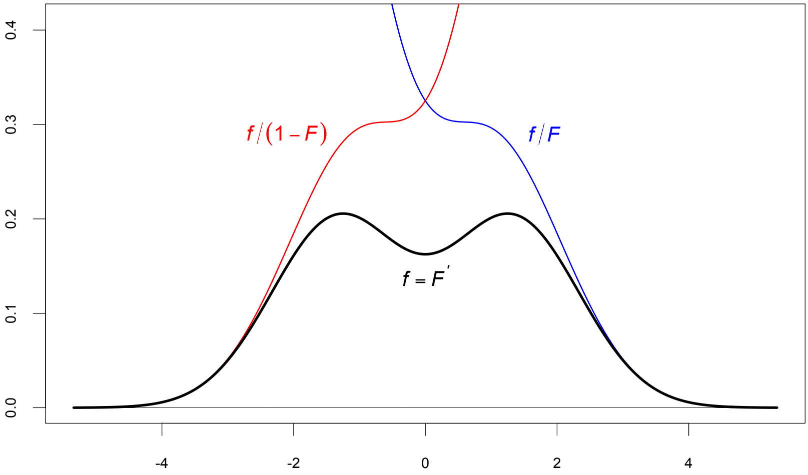
$$f = F' > 0 \quad \text{and} \quad \frac{-f^2}{1-F} \leq f' \leq \frac{f^2}{F}.$$

- F has a density f s.t. for arbitrary $x \in J(F)$ and $t \in \mathbb{R}$,

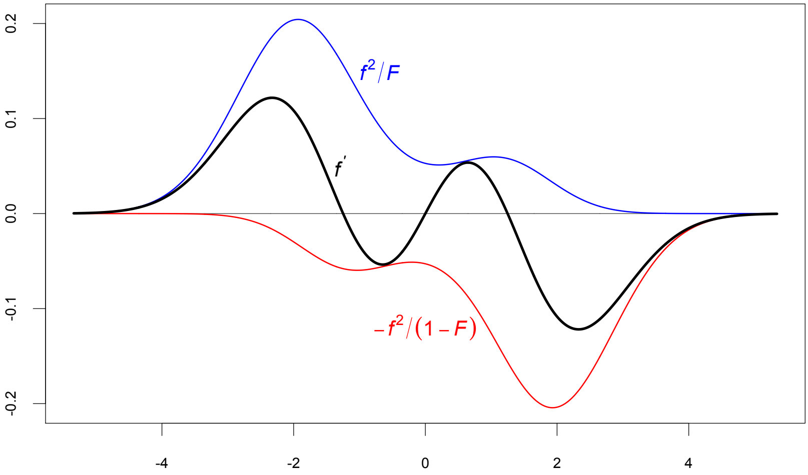
$$F(x+t) \begin{cases} \leq F(x) \exp\Big(\dfrac{f}{F}(x) \cdot t\Big), \\ \geq 1 - (1 - F(x)) \exp\Big(-\dfrac{f}{1-F}(x) \cdot t\Big). \end{cases}$$



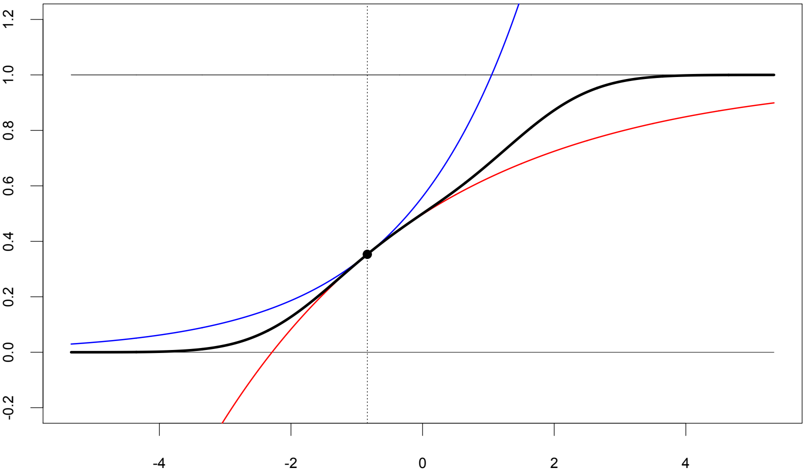
−log(1 − F)
F
1 + log(F)
1.5
1.0
0.5
0.0
-0.5
-4
-2
0
2
4



0.4
0.3
0.2
0.1
0.0
-4
-2
0
2
4
f/(1 − F)
f/F
f = F′



0.2
0.1
0.0
-0.1
-0.2
-4
-2
0
2
4
f^2/F
f'
$-f^2/(1-F)$



-0.2
0.0
0.2
0.4
0.6
0.8
1.0
1.2
-4
-2
0
2
4

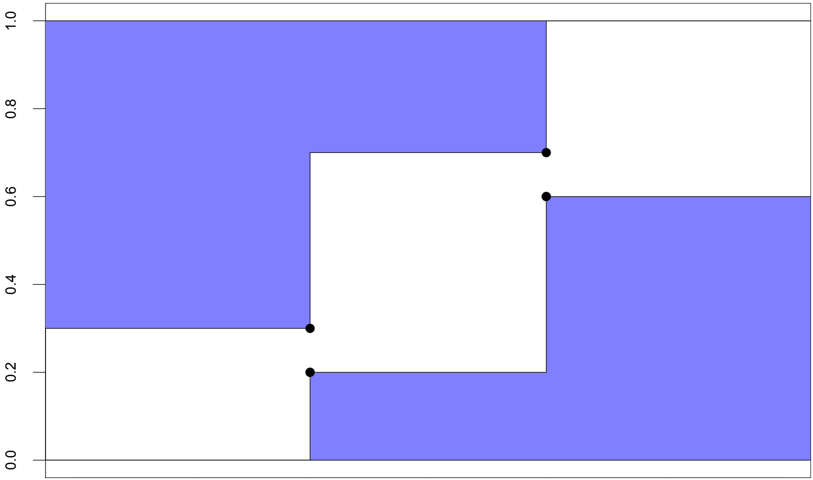
Estimation. Presumably no NPMLE of a bi-log-concave F :-(

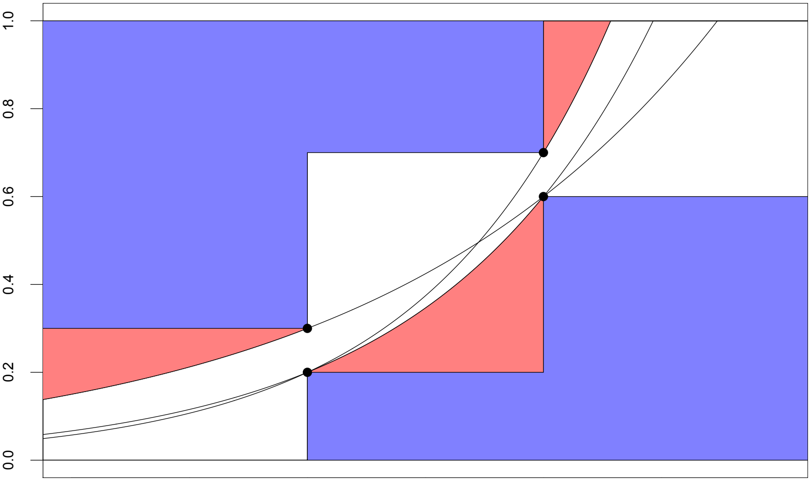
Confidence bands. Starting from a standard $(1-\alpha)$-confidence band (L_n, U_n) for F,

$$\mathbb{P}\big(L_n \le F \le U_n \text{ on } \mathbb{R}\big) \;=\; 1-\alpha,$$

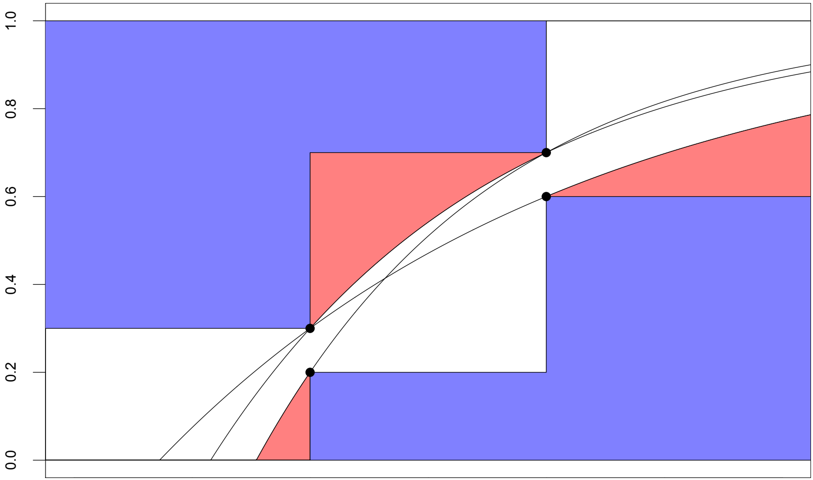
define

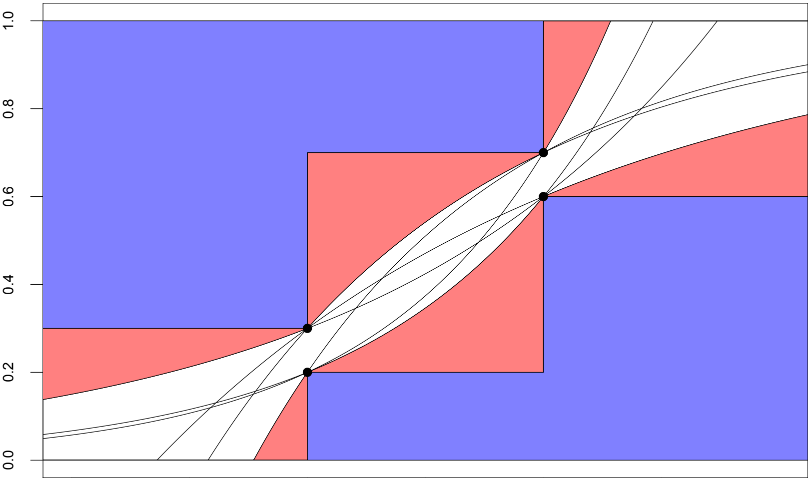
$$\begin{aligned} L_n^o(x) \;&:=\; \inf\big\{G(x) : G \text{ bi-log-concave}, L_n \le G \le U_n \text{ on } \mathbb{R}\big\}, \\ U_n^o(x) \;&:=\; \sup\big\{G(x) : G \text{ bi-log-concave}, L_n \le G \le U_n \text{ on } \mathbb{R}\big\}. \end{aligned}$$


0.0
0.2
0.4
0.6
0.8
1.0

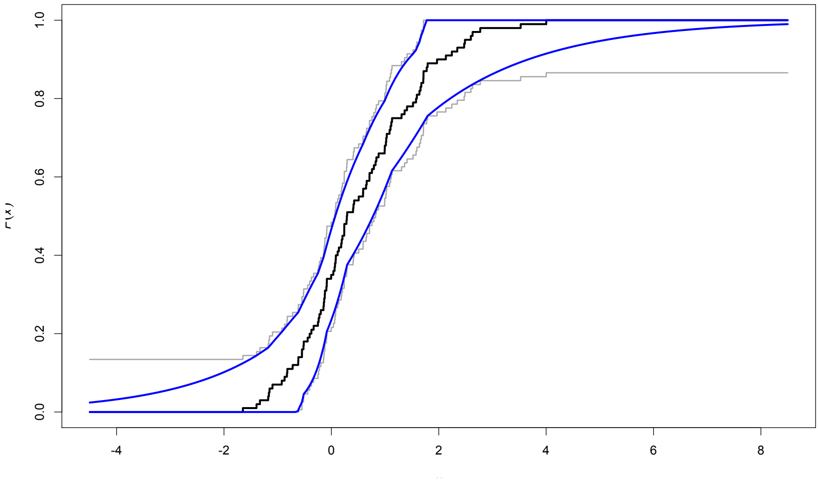


1.0
0.8
0.6
0.4
0.2
0.0

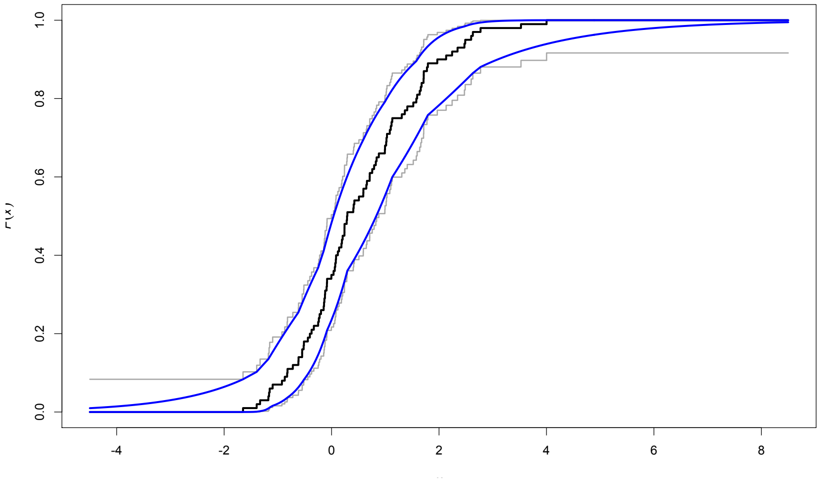

0.0
0.2
0.4
0.6
0.8
1.0



1.0
0.8
0.6
0.4
0.2
0.0



0.0
0.2
0.4
0.6
0.8
1.0
-4
-2
0
2
4
6
8



1.0
0.8
0.6
0.4
0.2
0.0
F(x)
-4
-2
0
2
4
6
8

Theorem. For any integer $k > 0$,

$$\sup_{G\,:\,L_n^o \le G \le U_n^o} \Big| \int x^k \, G(dx) - \int x^k \, F(dx) \Big| = \begin{cases} O_p\big((\log n)^k n^{-1/2}\big) & \text{with KS band,} \\ O_p\big(n^{-1/2}\big) & \text{with new band.} \end{cases}$$

Whenever $\int e^{\lambda x} \, F(dx) < \infty$,

$$\sup_{G\,:\,L_n^o \le G \le U_n^o} \Big| \int e^{\lambda x} \, G(dx) - \int e^{\lambda x} \, F(dx) \Big| \; = \; o_p(1).$$

V. Bi-Log-Concave Binary Regression

Generic observation: $(X, Y) \in \mathbb{R} \times \{0, 1\}$ (or $\mathbb{R} \times [0, 1]$).

Shape constraint:

$$\mathbb{E}(Y \mid X = x) \;=\; \mu(x)$$

with $\mu : \mathbb{R} \to [0, 1]$ bi-log-concave:

$$\log(\mu) \text{ and } \log(1 - \mu) \text{ both concave.}$$

Nonparametric extension of logistic regression, because

$$x \;\mapsto\; \ell(a + bx) \;\text{ strictly bi-log-concave}$$

for arbitrary $a, b \in \mathbb{R}$.