# Lecture 3: Some Theory for Estimation with Shape Constraints

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- Talks at YES-I Conference on Shape Restricted Inference Eurandom, The Netherlands, October 8-10, 2007
- Email: jaw@stat.washington.edu http: //www.stat.washington.edu/jaw/jaw.research.html
- Based on joint work with Piet Groeneboom, Geurt Jongbloed; former Ph.D. Students Jian Huang, Moulinath Banerjee, Fadoua Balabdaoui, Marloes Maathuis, and Shuguang Song; current Ph.D. student Marios Pavlides, current post-doc Hanna Jankowski;
  - and the work of many others.

## Outline, Lecture 3

- 1. Illustration of the pointwise limit theory pattern: convex hazards
- 2. Illustration of the pointwise limit theory pattern: log-concave densities
- 3. A functional of interest: estimation of the mode
- 4. Illustration of the pointwise limit theory pattern: competing risks with current status data
- 5. Partial illustration of the pointwise limit theory pattern: k-monotone densities
- 6. Partial illustration of the pointwise limit theory pattern: distribution functions and monotone densities on  $\mathbb{R}^2$
- 7. Summary: problems and directions

### 1. Convex hazards

Nonparametric methods for hazard rate functions.

- Grenander ('56): decreasing case
- Bray, Crawford and Proschan (1967): MLE for U-shaped hazard functions
- Prakasa Rao (1970); Groeneboom (1985); Banerjee (2007): asymptotics
- step-functions
- $n^{-1/3}$  local convergence rates

Here we assume that

$$h(t) \equiv \frac{f(t)}{1 - F(t)}$$
 is convex.

Let 
$$H(t) = \int_0^t h(s) ds$$
.

Then

$$\mathsf{L}_n(h) = \prod_{i=1}^n \left\{ h(X_i) \exp\left[-H(X_i)\right] \right\},\,$$

and hence the MLE is found by

$$\widehat{h}_n = \operatorname{argmin}_{h \ge 0, \operatorname{convex}} \left\{ \int_0^\infty (H - \log h) d\mathbb{F}_n \right\}.$$

Define Empirical CDF and Hazard:

$$\mathbb{F}_n(t) = \frac{1}{n} \sum_{i=1}^n \mathbb{1}_{[0,t]}(X_i), \quad \mathbb{H}_n(t) = \int_0^t \frac{1}{1 - \mathbb{F}_n(s-)} d\mathbb{F}_n(s).$$

Next, fix a T > 0. Then the LSE  $\tilde{h}_n$  is defined on [0, T] as

$$\widetilde{h}_n = \operatorname{argmin}_{h \ge 0, \operatorname{CONVex}} \left\{ \frac{1}{2} \int_0^T h^2(t) dt - \int_0^T h(t) d\mathbb{H}_n(t) \right\}$$

Let  $\widetilde{H}_n(t) = \int_0^t \widetilde{h}_n(s) ds$ , and  $\widetilde{\mathcal{H}}_n(t) = \int_0^t \widetilde{H}_n(s) ds$ . Also, let  $\mathbb{Y}_n(t) = \int_0^t \mathbb{H}_n(s) ds$ . The LSE must satisfy:

- $\widetilde{H}(T) = \mathbb{H}_n(T) \& \widetilde{\mathcal{H}}_n(T) = \mathbb{Y}_n(T)$
- $\widetilde{\mathcal{H}}_n(t) \ge \mathbb{Y}_n(t)$  for all  $t \in [0,T]$

• 
$$\int_0^T (\widetilde{\mathcal{H}}_n - \mathbb{Y}_n)(t) d\left[\widetilde{h}_n\right]'(t) = 0.$$

Theorem. Suppose that  $h \in \mathcal{K}$  is the true hazard function. Suppose that  $h(x_0) > 0$ ,  $h''(x_0) > 0$ , and h'' is continuous in a neighborhood of  $x_0$ . Then for  $\overline{h}_n = \widetilde{h}_n$  or  $\overline{h}_n = \widehat{h}_n$ 

$$\left(\begin{array}{c} n^{2/5}\{\overline{h}_n(x_0) - h(x_0)\}\\ n^{1/5}\{\overline{h}'_n(x_0) - h'(x_0)\}\end{array}\right) \to_d \left(\begin{array}{c} c_1 \mathcal{I}^{(2)}(0)\\ c_2 \mathcal{I}^{(3)}(0)\end{array}\right)$$

where

$$c_1 = \left(\frac{h^2(x_0)h''(x_0)}{24S^2(x_0)}\right)^{1/5} \quad \text{and} \quad c_2 = \left(\frac{h(x_0)h''(x_0)^3}{24^3S(x_0)}\right)^{1/5},$$

for both  $\overline{h} = \widetilde{h}_n$  and  $\overline{h}_n = \widehat{h}_n$ , where  $\mathcal{I}$  is the *invelope function* of  $\mathbb{Y}(t) \equiv \int_0^t W(s) ds + t^4$ : i.e.

- $\mathcal{I}(t) \geq \mathbb{Y}(t)$  for all  $t \in \mathbb{R}$ .
- $\int_{-\infty}^{\infty} (\mathcal{I}(t) \mathbb{Y}(t)) d\mathcal{I}^{(3)}(t) = 0.$
- $\mathcal{I}^{(2)}$  is convex.

2. Log-concave densities on  $\mathbb R$ 

Suppose that

 $f(x) = \exp(\varphi(x))$ 

where  $\varphi$  is concave. The class of all densities f on  $\mathbb{R}$  of the form is called the class of *log-concave* densities,  $\mathcal{F}_{log-concave}$ .

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- Pointwise limit theory? Yes! Balabdaoui and Rufibach (2007)

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  - $H_k^{(2)}$  is concave.

• Pointwise limit theorem for  $\widehat{f}_n(x_0)$ :

$$\left(\begin{array}{c} n^{k/(2k+1)}(\widehat{f}_n(x_0) - f(x_0))\\ n^{(k-1)/(2k+1)}(\widehat{f}'_n(x_0) - f'(x_0)) \end{array}\right) \to_d \left(\begin{array}{c} c_k H_k^{(2)}(0)\\ d_k H_k^{(3)}(0) \end{array}\right)$$

where

$$c_k \equiv \left(\frac{f(x_0)^{k+1}|\varphi^{(k)}(x_0)|}{(k+2)!}\right)^{1/(2k+1)},$$
  
$$d_k \equiv \left(\frac{f(x_0)^{k+2}|\varphi^{(k)}(x_0)|^3}{[(k+2)!]^3}\right)^{1/(2k+1)}$$

• Pointwise limit theorem for  $\widehat{\varphi}_n(x_0)$ :

$$\begin{pmatrix} n^{k/(2k+1)}(\widehat{\varphi}_n(x_0) - \varphi(x_0)) \\ n^{(k-1)/(2k+1)}(\widehat{\varphi}'_n(x_0) - \varphi'(x_0)) \end{pmatrix} \rightarrow_d \begin{pmatrix} C_k H_k^{(2)}(0) \\ D_k H_k^{(3)}(0) \end{pmatrix}$$

where

$$C_k \equiv \left(\frac{|\varphi^{(k)}(x_0)|}{f(x_0)^k(k+2)!}\right)^{1/(2k+1)},$$
  
$$D_k \equiv \left(\frac{|\varphi^{(k)}(x_0)|^3}{f(x_0)^{k+1}[(k+2)!]^3}\right)^{1/(2k+1)}$$

#### 3. Estimation of the mode

Let  $x_m$  be the *mode* of the log-concave density f, recalling that  $\mathcal{F}_{log-concave} \subset \mathcal{F}_{unimodal}$ . Lower bound calculations using G. Jongbloed's perturbation of a convex decreasing density, but now perturbing  $\varphi$  yields:

Proposition. If  $f \in \mathcal{F}_{log-concave}$  satisfies  $f(x_m) > 0$ ,  $f''(x_m) < 0$ , and f'' is continuous in a neighborhood of  $x_m$ , and  $T_n$  is any estimator of the mode  $x_m \equiv \nu(P)$ , then with  $P_n$  corresponding to  $f_{\epsilon_n} \equiv \exp(\varphi_{\epsilon_n})$  with  $\epsilon_n \equiv \nu n^{-1/5}$  and  $\nu \equiv 2f''(x_m)^2/(5f(x_m))$ ,

 $\liminf_{n \to \infty} n^{1/5} \inf_{T_n} \max \left\{ E_{n, P_n} | T_n - f_{\epsilon_n}(x_m) |, E_{n, P} | T_n - f(x_m) | \right\}$  $\geq \frac{1}{4} \left( \frac{1}{e^{10}} \right)^{1/5} \left( \frac{f(x_m)}{f''(x_m)^2} \right)^{1/5}.$ 

On the other hand, the limit theory of Balabdaoui and Rufibach (2007) noted in the previous section implies that the mode estimator derived from the MLE of  $\hat{f}_n$ , namely  $\hat{x}_m \equiv \min\{u : \hat{f}_n(u) = \sup_t \hat{f}_n(t)\} \equiv M(\hat{f}_n)$ , satisfies

$$n^{1/(2k+1)}(\widehat{x}_m - x_m) \to_d \left(\frac{(4!)^2 f(x_m)}{f''(x_m)^2}\right)^{1/(2k+1)} M(H_k^{(2)})$$

where  $M(H_k^{(2)}) = \operatorname{argmax}(H_k^{(2)})$ . Note that when k = 2 this agrees with the lower bound calculation, at least up to absolute constants. 4. Competing risks with current status data

See two papers by Groeneboom, Maathuis, and Wellner (2007), *Ann. Statist.* to appear:

http://www.stat.washington.edu/jaw/jaw\_papers.html

http://stat.ethz.ch/ maathuis/papers/

5. k-monotone densities

See paper by Balabdaoui and Wellner (2007), Ann. Statist., to appear:

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6. Distribution functions & monotone densities on  $\mathbb{R}^2$ 

Monotone densities on  $\mathbb{R}^d$ : two types

• Block decreasing:  $\mathcal{F}_{BD}$ 

Consider step 8 in the case of mixtures of uniform monotone densities first first:

6. Distribution functions & monotone densities on  $\mathbb{R}^2$ 

Monotone densities on  $\mathbb{R}^d$ : two types

- Block decreasing:  $\mathcal{F}_{BD}$
- Mixtures of uniform densities (on rectangular densities anchored at 0):  $\mathcal{F}_{SMU}$

$$f(\underline{x}) = \int_{(0,\infty)^d} \frac{1}{|\underline{y}|} \mathbf{1}_{(\underline{0},\underline{y}]}(x) dG(\underline{y})$$

for some distribution function G on  $(0,\infty)^d$ .

Consider step 8 in the case of mixtures of uniform monotone densities first first:

**Proposition 1.** (Pavlides, 2007). Suppose that  $f \in \mathcal{F}_{SMU}$  where  $\underline{x}_0 \in (0, \infty)^d$  satisfies  $f(\underline{x}_0) > 0$ ,  $\partial f(\underline{x}_0) / \partial x_j < 0$  for  $j = 1, \dots, d$ ,

$$(-1)^d \frac{\partial^d f(\underline{x})}{\partial x_1 \cdots \partial x_d}\Big|_{\underline{x} = \underline{x}_0} > 0,$$

and the mixed derivative in the last display is continuous on some neighborhood of  $\underline{x}_0$ . Then there is a sequence  $\{f_n\}_{n\geq 1} \subset \mathcal{F}_{SMU}$  such that

$$\liminf_{n \to \infty} \inf_{T_n} \max \left\{ E_{f_n} n^{1/3} |T_n - f_n(\underline{x}_0)|, E_f n^{1/3} |T_n - f(\underline{x}_0)| \right\}$$
$$\geq \left( \frac{e^{-1} 3^{d-1}}{2^{3d}} \right)^{1/3} \left\{ (-1)^d \frac{\partial^d f(\underline{x})}{\partial x_1 \cdots \partial x_d} \Big|_{\underline{x} = \underline{x}_0} \cdot f(\underline{x}_0) \right\}^{1/3}.$$

- Rate of convergence is  $n^{1/3}$  for all d.
- Constant reduces to the familiar constant when d = 1.
- Shuguang Song (2001): estimation of a distribution function *F* with rectangular "current status" censoring.

**Proposition 2.** (Pavlides, 2007). Suppose that  $f \in \mathcal{F}_{BD}$  where  $\underline{x}_0 \in (0, \infty)^d$  satisfies  $f(\underline{x}_0) > 0$ ,

$$\frac{\partial f(\underline{x}_0)}{\partial x_j} < 0 \qquad j = 1, \dots, d,$$

and all the derivatives in the last display are continuous on some neighborhood of  $\underline{x}_0$ . Then there is a sequence  $\{f_n\}_{n\geq 1} \subset \mathcal{F}_{BD}$  such that

$$\liminf_{n \to \infty} \inf_{T_n} \max \left\{ E_{f_n} n^{1/(d+2)} |T_n - f_n(\underline{x}_0)|, E_f n^{1/(d+2)} |T_n - f(\underline{x}_0)| \right\}$$
$$\geq \frac{e^{-1/(d(d+2))}}{4} \left\{ \frac{12f(\underline{x}_0)d^{d+1}}{2^d(d+2)} \cdot \prod_{j=1}^d \left\{ \left| \frac{\partial f(\underline{x})}{\partial x_j} \right|_{\underline{x} = \underline{x}_0} \right| \right\} \right\}^{1/(d+2)}.$$

Set

$$\widetilde{F}_n(\underline{x}) \equiv \int_{[\underline{0},\underline{x}]} \widetilde{f}_n(\underline{y}) d\underline{y}.$$

Then the Fenchel conditions for the LSE  $\tilde{f}_n$  in  $\mathcal{F}_{SMU}$  are:

- $\widetilde{F}_n(\underline{x}) \ge \mathbb{F}_n(\underline{x})$  for all  $\underline{x}$
- $\int_{(0,\infty)} (\widetilde{F}_n(\underline{x}) \mathbb{F}_n(\underline{x}) d\widetilde{f}_n(\underline{x}) = 0$

Localization? Driving process? Localization of  $\mathbb{F}_n$ : write  $|\underline{t}| \equiv \prod_{j=1}^d t_j$ .

Let  $\Delta^d$  denote the *d*-dimensional difference operator:

$$(\Delta^{d}g)(\underline{u},\underline{v}) = \sum_{2^{d} \text{ corners}} (-1)^{\mathsf{par}(v_{j})} g(v_{j},v_{j+1}).$$

Then I conjecture that

$$\begin{aligned} \mathbb{Y}_{n}^{loc}(\underline{t}) &\equiv n^{2/3} \left\{ \Delta^{d} \mathbb{F}_{n}(\underline{x}_{0}, \underline{x}_{0} + \underline{t} n^{-1/(3d)}) - \Delta^{d} F(\underline{x}_{0}, \underline{x}_{0} + \underline{t} n^{-1/(3d)}) \\ &- n^{-1/3} |\underline{t}| f(x_{0}) \right\} \\ &\Rightarrow \sqrt{f(\underline{x}_{0})} W(\underline{t}) - \sigma(f_{0}) |\underline{t}|^{2} \quad \text{in } C[[-K, K]^{d}] \\ &\equiv \mathbb{Y}(\underline{t}) \end{aligned}$$

for each K > 0 where  $W(\underline{t})$  is a  $2^d$ -sided Brownian sheet and

$$\sigma(f_0) \equiv c_d(-1)^d \frac{\partial^d f(\underline{x})}{\partial x_1 \cdots \partial x_d} \Big|_{\underline{x} = \underline{x}_0} \equiv c_d(-1)^d \partial^d f(\underline{x}_0).$$

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$$n^{1/3}(\widetilde{f}_n(\underline{x}_0) - f(\underline{x}_0)) \to_d \frac{\partial^d}{\partial t_1 \cdots \partial t_d} \mathbb{H}(\underline{t})\Big|_{\underline{t}=\underline{0}}$$
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where the process  $\mathbb{H}(\underline{t})$  is determined by

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- localize  $\widetilde{F}_n$  analogously to  $\mathbb{Y}_n^{loc}$  to get  $\widetilde{H}_n^{loc}$
- verify localized Fenchel relations
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- $\circ \ \int_{\mathbb{R}^d} (\mathbb{H}(\underline{t}) \mathbb{Y}(\underline{t})) d\left\{ \partial^d \mathbb{H}(\underline{t}) \right\} = 0.$
- $^{\circ} \ \Delta^d \{ \partial^d \mathbb{H}(\underline{t}) \} (\underline{u}, \underline{v}) \geq 0 \text{ for all } \underline{u}, \underline{v} \in \mathbb{R}^d.$

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$$\sqrt{n}(\widehat{f}_n^{convex}(t) - f(t)) \to \text{Invelope of } \int_0^t \mathbb{U}(F(s))ds?$$

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 Banerjee and Wellner (2001) studied likelihood ratio tests of *H* : *f*(*t*<sub>0</sub>) = θ<sub>0</sub> versus *K* : *f*(*t*<sub>0</sub>) ≠ θ<sub>0</sub> in the case of monotone *f*. Is there a nice theory of pointwise likelihood ratio tests in other shape-constrained problems, e.g. when *f* is convex?
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- Pointwise limit theory for MLE of a completely monotone density (= scale mixture of exponential)?
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- Higher dimensional shape constraints?

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