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1. Introduction and summary.

In this paper the existence and uniqueness of maximum likelihood estimators in exponential families is discussed, and an example demonstrates a method of extending discrete models so that maximum likelihood estimation always is possible.

The maximization of the likelihood function $L(\cdot,t_0)$ is equivalent to the minimization of $-\log L(\cdot,t_0)$ which is convex. Therefore a result about minimization of l.s.c. quasi-convex functions is presented in section 2, using some elementary results from the theory of convex sets. In section 3 concepts as polar cone and the support of a measure are presented. Section 4 contains the main result: a necessary and sufficient condition for t_0 so that the maximum likelihood estimator $\hat{\theta}(t_0)$ exists. - Barndorff-Nielsen (1970) has given a comprehensive discussion of estimation in exponential families using convex duality theory.

In section 5 the logistic dose-response model is considered as an example, and we deduce how to extend the model so that estimation always is possible. - Barndorff-Nielsen (1970) discusses the same example (and the problem in general), and explains the extension in a different way.

M Davis (1970) has dealt with the estimation problems in the logistic model in a way that has given some of the inspiration to this paper.

2. Convex sets. Recession cone. Quasi-convex functions.

In this section E denotes a finite dimensional real Banach space.

2.1 Definition: For any subset $M \subseteq E$,

$$\mathrm{aff}M$$

denotes the smallest affine subspace in E containing M, i.e. the affine hull of M.

2.2 Definition: For any convex subset $A \subseteq E$ we define the relative interior of A,

$$\mathrm{ri}A,$$

as the interior of A considered as a subset of affA, which should be endowed with the subspace topology. (Since affA is a closed subset of E, the closure $\bar{A}$ of A in E coincides with the closure of A in the subspace topology in affA).

The convex subsets of E have the following important property.

2.3 Proposition: Let A be a convex subset of E. If $x \in \mathrm{ri}A$ and $y \in \bar{A}$, then

$$\{x + \lambda(y-x) \mid \lambda \in [0,1[\} \subseteq \mathrm{ri}A.$$

The proof will not be given here; see e.g. Bourbaki (1966), ch. II, Rockafellar (1970), Stoer and Witzgall (1970).

2.4 Definition: Let $x,y \in E$. The ray from the point x in direction y is the set

$$\mathrm{ray}(x,y) := \{x + \lambda y \mid \lambda \in [0, +\infty[\}.$$

2.5 Definition: Let A be a convex subset of E. The recession cone of A is the set

$$0^+A := \{y \in E \mid \forall x \in A : \mathrm{ray}(x,y) \subseteq A\}.$$

2.6 Proposition: Let A be a convex subset of E. Then the following properties hold:

(i). 0^+A is a convex cone.
If A is closed then 0^+A is closed.

(ii). For any $x \in A$ we have $0^+A \subseteq \{y \in E \mid ray(x,y) \subseteq A\}$. Furthermore, if $x \in riA$ then

$$\{y \in E \mid ray(x,y) \subseteq A\} = 0^+\bar{A} = 0^+riA.$$

(iii). Suppose also B is a convex subset of E.

If $\bar{A} \subseteq \bar{B}$ then $0^+\bar{A} \subseteq 0^+\bar{B}$.

If $riA \subseteq riB$ then $0^+riA \subseteq 0^+riB$.

Proof: It is easy to verify (i), and the first statement of (ii) follows from 2.5. Since (iii) follows from (ii) choosing an x from $ri\bar{A} \subseteq ri\bar{B}$ or from $riA \subseteq riB$, it therefore remains to show that

$$\{y \in E \mid ray(x,y) \subseteq A\} = 0^+\bar{A} = 0^+riA$$

for any convex subset $A \subseteq E$ and any $x \in riA$. First we shall show that

$$(*) \qquad \{y \in E \mid ray(x,y) \subseteq \bar{A}\} \subseteq 0^+riA.$$

Let $y \in \{y \in E \mid ray(x,y) \subseteq \bar{A}\}$, $z \in riA$; since $\bar{A}$ is convex and $ray(x,y) \subseteq \bar{A}$,

$$z + \frac{1}{n}(x-z) + \lambda y = (1 - \frac{1}{n})z + \frac{1}{n}(x + n\lambda y) \in \bar{A}$$

for every $n \in \mathbb{N}$ and $\lambda \in [0,+\infty[$. Letting $n \to \infty$ we see that $z + \lambda y \in \bar{A}$ for every $\lambda \in [0,+\infty[$, and hence $ray(z,y) \subseteq \bar{A}$. As $z \in riA$, 2.3 shows that $ray(z,y) \subseteq riA$, and (*) is thus established.

Next we show that

$$(**) \qquad 0^+riA \subseteq 0^+\bar{A}.$$

To this end, we consider $y \in 0^+riA$ and $w \in \bar{A}$. Choosing $x \in riA$ and putting $x_n = x + \frac{n-1}{n}(w-x)$, $(n \in \mathbb{N})$, $(x_n)_{n \in \mathbb{N}}$ is a sequence on riA (prop. 2.3) converging to w. Therefore $ray(x_n,y) \subseteq riA \subseteq A$ and hence $x_n + \lambda y \in A$ for every $n \in \mathbb{N}$ and $\lambda \in [0,+\infty[$. Letting $n \to \infty$ we see that $w + \lambda y \in \bar{A}$ for every $\lambda \in [0,+\infty[$, so that $ray(w,y) \subseteq \bar{A}$. Since this holds for every $w \in \bar{A}$, (**) is proved.

Using (**), the first statement of (ii), and (*), we obtain for any $x \in riA$

$$0^+riA \subseteq 0^+\bar{A}$$
$$\subseteq \{y \in E \mid ray(x,y) \subseteq \bar{A}\},$$

and

$$0^+\mathrm{ri}A \subseteq \{y \in E \mid \mathrm{ray}(x,y) \subseteq \mathrm{ri}A\}$$
$$\subseteq \{y \in E \mid \mathrm{ray}(x,y) \subseteq A\}$$
$$\subseteq \{y \in E \mid \mathrm{ray}(x,y) \subseteq \bar{A}\}$$
$$\subseteq 0^+\mathrm{ri}A,$$

which gives the desired results.

The following two propositions show how some topological properties of convex sets can be described by means of rays.

2.7 Proposition: Let A be a convex subset of E, and let $x \in \mathrm{ri}A$. Then A is closed, if (and only if) all the sets

$$A \cap \mathrm{ray}(x,y), \quad y \in \mathrm{aff}A - \mathrm{aff}A,$$

are closed.

Proof (of "if"): Applying 2.3 we have for $z \in \bar{A}$:

$$z \in \overline{\{x + \lambda(z-x) \mid \lambda \in [0,1[\}}$$
$$\subseteq \overline{\mathrm{ri}A \cap \mathrm{ray}(x,z-x)}$$
$$\subseteq \overline{A \cap \mathrm{ray}(x,z-x)}$$
$$= A \cap \mathrm{ray}(x,z-x) \subseteq A.$$

2.8 Proposition: Let A be a convex subset of E, and let $x \in \mathrm{ri}A$. Then the following three statements are equivalent:

(i). A is bounded (i.e. $A \subseteq \{w \in E \mid ||w|| \leq \lambda\}$ for some $\lambda \in \mathbb{R}_+$).

(ii). $0^+\bar{A} = \{\underline{0}\}$.

(iii). All the sets

$$A \cap \mathrm{ray}(x,y), \quad y \in \mathrm{aff}A - \mathrm{aff}A,$$

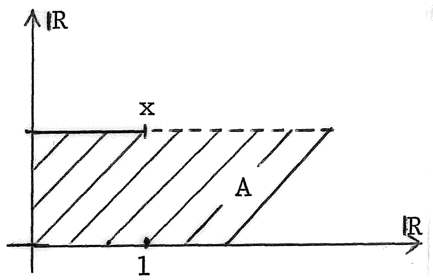
are bounded.

Proof: The equivalence (ii) $\Leftrightarrow$ (iii) is a consequence of 2.6 (ii). Since (i) $\Rightarrow$ (iii) is obvious, it remains to show that (iii) $\Rightarrow$ (i).

Suppose that A is unbounded. Then there exists a sequence $(y_n)_{n \in \mathbb{N}}$ of unit vectors with $x + n\, y_n \in A$, $\forall n \in \mathbb{N}$. As the unit ball (in affA - affA) is compact it contains a clusterpoint y for (y_n). It is easily seen that $\mathrm{ray}(x,y) \subseteqq \bar{A}$ and, by 2.3, that $\mathrm{ray}(x,y) \subseteqq \mathrm{ri}A \subseteqq A$. Thus the set $A \cap \mathrm{ray}(x,y)$ is unbounded.

<u>2.9 Example</u>, demonstrating the importance in 2.7 and 2.8 for x to be a point from $\mathrm{ri}A$.

Suppose that $E = \mathbb{R}^2$, $A = ([0,+\infty[\times [0,1[) \cup ([0,1] \times \{1\})$:



Choosing

$$x = (0,1) \in A \setminus \mathrm{ri}A$$

we have that all the sets

$$A \cap \mathrm{ray}(x,y) \quad , \quad y \in \mathbb{R}^2$$

are closed and bounded, although A is neither closed nor bounded. It is seen that

$$0^+A = \{\underline{0}\},$$

$$0^+\bar{A} = [0,+\infty[\times \{0\}.$$

If $B = [0,+\infty[\times [0,1[$, we have $B \subset A$,

$$0^+B = 0^+\bar{B} = [0,+\infty[\times \{0\},$$

that is $0^+A \subset 0^+B$.

<u>2.10 Lemma</u>: Let $\grave{F}$ be a filterbase of closed path-connected subsets of E, and let M be the set of clusterpoints of $\grave{F}$:

$$M = \bigcap_{F \in \grave{F}} F.$$

Then M is bounded and $\neq \emptyset$, if and only if $\grave{F}$ contains a bounded set F_0.

<u>Proof</u>: If $F_0 \in \grave{F}$ is bounded, $\{F_0 \cap F \mid F \in \grave{F}\}$ is a filterbase on the compact set F_0 and hence

$$\emptyset \neq \bigcap_{F \in \grave{F}} (F_0 \cap F) \subseteqq M \subseteqq F_0,$$

that is, M is bounded and $\neq \emptyset$.

Suppose next that M is bounded and $\neq \emptyset$:

$$\emptyset \neq M \subseteq \{x \in E \mid ||x|| < \lambda\}.$$

The set $K := \{x \in E \mid ||x|| = \lambda\}$ is compact, and to each $x \in K$ we can find $F_x \in \grave{F}$ so that $x \in F_x^c$. Since $(F_x^c, x \in K)$ constitutes an open covering of K, there exists a finite subset K_0 of K with

$$\bigcap_{x \in K_0} F_x \subseteq K^c,$$

and the filterbase axioms give the existence of $F_0 \in \grave{F}$ so that

$$F_0 \subseteq \bigcap_{x \in K_0} F_x \subseteq K^c;$$

the set F_0 being path-connected, this implies that

$$F_0 \subseteq \{x \in E \mid ||x|| < \lambda\},$$

so F_0 is bounded.

We shall now introduce the quasi-convex functions, and using the preceeding results it is possible to prove a result concerning minimization of quasi-convex lower semicontinuos functions.

<u>2.11 Definition</u>: A function $f : E \to \mathbb{R} \cup \{+\infty\}$ is called <u>quasi-convex</u> if all the sets

$$f^{-1}(]-\infty, a]) = \{x \in E \mid f(x) \leq a\}, \; a \in \mathbb{R},$$

are convex.

A function $f : D \to \mathbb{R}$, $D \subseteq E$, is called quasi-convex if the function $\tilde{f} : E \to \mathbb{R} \cup \{+\infty\}$ defined by

$$\tilde{f}(x) = \begin{cases} f(x) & \text{if} \quad x \in D \\ +\infty & \text{if} \quad x \notin D \end{cases}$$

is quasi-convex.

<u>2.12 Examples</u>: Every convex function $f : D \to \mathbb{R}$, where $D \subseteq E$ is convex, is quasi-convex on E.

For any quasi-convex function $f : \mathbb{R} \to \mathbb{R}$ there exists $a, b \in \mathbb{R} \cup \{-\infty, +\infty\}$, $a \leq b$, so that f is decreasing on $\{x \in \mathbb{R} \mid x \leq b\}$ and increasing on

$\{x \in \mathbb{R} \mid a \leq x\}$. Furthermore, if $f : \mathbb{R} \to \mathbb{R}$ satisfies the latter conditions, f is quasi-convex.

Recall that a function $f : E \to \mathbb{R} \cup \{-\infty,+\infty\}$ is called <u>lower semi-continuous</u> (l.s.c.) if and only if all the sets

$$f^{-1}(]-\infty,a]) = \{x \in E \mid f(x) \leq a\},\quad a \in \mathbb{R},$$

are closed.

<u>2.13 Proposition</u>: Sufficient for a quasi-convex function $f : E \to \mathbb{R} \cup \{+\infty\}$ to be l.s.c. is that for every $a \in \mathbb{R}$ and every pair $(x,y) \in E^2$ the following holds:

$$\text{if } f(x + \lambda y) \leq a \text{ for every } \lambda \in [0,1[,$$

$$\text{then } f(x+y) \leq a.$$

<u>Proof</u>: This is an immediate consequence of proposition 2.7 with $A := f^{-1}(]-\infty,a])$.

<u>2.14 Proposition</u>: For a quasi-convex l.s.c. function $f : E \to \mathbb{R} \cup \{+\infty\}$ the following three statements are equivalent:

(i): The minimum set

$$M := \{x \in E \mid f(x) = \inf_{y\in E} f(y)\}$$

is compact and $\neq \emptyset$.

(ii): There exists an $a \in \mathbb{R}$ so that to every $y \in E\setminus\{\underline{0}\}$ there exists an $x \in f^{-1}(]-\infty,a])$ with $\lim_{\rho\to+\infty} f(x + \rho y) > a$,

$\Leftrightarrow$:

$$\exists a \in \mathbb{R}\ \forall y \in E\setminus\{\underline{0}\}\ \exists x \in f^{-1}(]-\infty,a]): \lim_{\rho\to+\infty} f(x + \rho y) > a.$$

(iii): There exists an $a \in \mathbb{R}$ so that for some (and then for any) $x \in \operatorname{ri} f^{-1}(]-\infty,a])$ $\lim_{\rho\to+\infty} f(x + \rho y) > a$ for every $y \in E\setminus\{\underline{0}\}$, $\Leftrightarrow$:

$$\exists a \in \mathbb{R}\ \exists(\forall)x \in \operatorname{ri} f^{-1}(]-\infty,a])\ \forall y \in E\setminus\{\underline{0}\}: \lim_{\rho\to+\infty} f(x + \rho y) > a.$$

<u>Proof</u>: We shall apply lemma 2.10 to the filterbase

$$\grave{F} := \{f^{-1}(]-\infty,a]) \mid a \in f(E)\setminus\{+\infty\}\},$$

which consists of closed convex sets, and it is seen that (i) is equivalent to the existence of an $a \in \mathbb{R}$ so that $f^{-1}(]-\infty,a])$ is bounded and $\neq \emptyset$. According to 2.8 ((i) $\Leftrightarrow$ (ii)), this can be expressed by saying that $f^{-1}(]-\infty,a])$ $\neq \emptyset$ and $0^+f^{-1}(]-\infty,a]) = \{\underline{0}\}$, i.e. (cfr. 2.5)

$$\exists a \in \mathbb{R}\ \forall y \in E\setminus\{\underline{0}\}\ \exists x \in f^{-1}(]-\infty,a]) : \mathrm{ray}(x,y) \nsubseteq f^{-1}(]-\infty,a])$$

The equivalence (i) $\Leftrightarrow$ (ii) is thus established by remarking, that if $f(x) \leqq a$ and $f(x + ry) > a$ $(r > 0)$ then $f(x + \rho y) > a$ for $\rho \geqq r$ since $f^{-1}(]-\infty,a])$ is convex.

In a completely analogous way (i) $\Leftrightarrow$ (iii) is proved, using 2.8 ((i) $\Leftrightarrow$ (iii)).

3. Dual space. Polar cone. The support of a measure.

We are still considering a finite dimensional real Banach space E. The totality of all (continuous) linear forms on E is E^*, the dual space of E, and constitutes a Banach space itself with the norm

$$x^* \mapsto ||x^*|| := \sup\{||x^*(x)|| \mid ||x|| \leq 1\},\ x^* \in E^*.$$

Furthermore E and E^* have the same dimension. Now, consider the natural embedding $\psi : E \to E^{**} = (E^*)^*$, where

$$\psi x : x^* \mapsto (\psi x)(x^*) = x^*(x),\ (x^* \in E^*,\ x \in E).$$

In our case ψ is an isometric isomorphism of E onto E^{**}.

In the sequel we shall use some well known results*):

3.1 The Hahn-Banach Theorem in its geometric formulation: Let A be an open convex subset of E and let M be an affine subspace of E, $M \cap A = \emptyset$. Then there exists a closed hyperplane H in E so that $M \subseteq H$ and $H \cap A = \emptyset$.

3.2 Separation Theorem: Let A be a closed convex subset of E and let B be a compact convex subset of E, $A \cap B = \emptyset$. Then there exists a closed hyperplane $H = (x^*)^{-1}(\gamma)$ in E ($x^* \in E^*$, $\gamma \in \mathbb{R}$) which separates A and B strictly, i.e. $x^*(A) \subseteq]-\infty,\gamma[$ and $x^*(B) \subseteq]\gamma,+\infty[$.

3.3 Corollary: Let C be a convex cone with vertex $\underline{0}$, $C \subset E$. Then $\bar{C}$ is the intersection of all closed halfspaces containing C whose boundary hyperplane contains $\underline{0}$.

3.4 Definition: Let A be a convex subset of F, F = E or E^*. The polar cone of A is the set

$$A^o := \{y^* \in F^* \mid \forall y \in A : y^*(y) \leq 0\}.$$

In the case $F = E^*$ we shall use the notation

$$A^p := \psi^{-1}(A^o) = \{x \in E \mid \forall x^* \in A : x^*(x) \leq 0\}.$$

If M is a subset of E then cone M denotes the smallest cone with vertex $\underline{0}$ containing M: cone $M = \{\lambda x \mid x \in M,\ \lambda \in \mathbb{R}_+\}$. If M is convex, then cone M is convex.

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*) see e.g. Bourbaki (1966).

<u>3.5 Proposition</u>: Let A be a convex subset of $F = E$ or E^*. If $F = E$, then $A^o = (\text{cone } A)^o$ is a closed convex cone, and $\overline{\text{cone } A} = \psi^{-1}(A^{oo}) = A^{op}$. If $F = E^{**}$, then $A^o = (\text{cone } A)^o$ and $A^p = (\text{cone } A)^p$ are closed convex cones, and $\overline{\text{cone } A} = [\psi^{-1}(A^o)]^o = A^{po}$.

<u>Proof</u>: It is rather trivial that $A^o = (\text{cone } A)^o$ and $A^p = (\text{cone } A)^p$ are closed convex cones. The assertions about $\overline{\text{cone } A}$ are obvious if $C := \text{cone } A = F$, and if $C \subset F$ they are simply reformulations of corollary 3.3; note however the importance in the case $F = E^*$ of ψ being surjective.

Let $\grave{X}$ be a locally compact space (e.g. $\grave{X} = E$). The <u>Borel-σ-algebra</u> on $\grave{X}$, $\grave{B}(\grave{X})$, is the σ-algebra generated by the open sets in $\grave{X}$.

<u>3.6 Definition</u>: Given a positive σ-finite measure m on $(\grave{X}, \grave{B}(\grave{X}))$. The <u>support</u> of m is the set

$$\text{supp}(m) := \{x \in \grave{X} \mid m(U) > 0 \text{ for every open neighbourhood } U \text{ of } x\}.$$

If $\grave{X} = E$ we define the <u>affine support</u> of m as the set

$$S(m) := \text{aff}(\text{supp}(m)).$$

We note that $\text{supp}(m)^c$ is open. If $\grave{X} = E$ it follows from 3.7 that $\text{supp}(m)$ is the largest set $M \subseteq \grave{X}$ so that $m(U) > 0$ for every non empty relative open subset U of M, and $\text{supp}(m)^c$ is the largest open set $N \subseteq \grave{X}$ so that $m(N) = 0$.

<u>3.7 Proposition</u>: Let m be as in 3.6 with $\grave{X} = E$. For every $B \in \grave{B}(E)$ we have

$$B \cap \text{supp}(m) = \emptyset \quad \Rightarrow \quad m(B) = 0.$$

<u>Proof</u>: Choose open sets U_x, $x \in B$, so that $x \in U_x$ and $m(U_x) = 0$. Since E is a Lindelöf space one can find a countable subset B_0 of B with

$$\bigcup_{x \in B} U_x = \bigcup_{x \in B_0} U_x \supseteq B;$$

hence
$$m(B) \leq \sum_{x \in B_0} m(U_x) = 0.$$

<u>3.8 Theorem</u>: Given a positive σ-finite measure m on $(E, \grave{B}(E))$, and a closed convex cone $K \subseteq (S(m) - S(m))^*$ with vertex $\underline{0}$. Then we have the identity

$$\text{ri}(\text{conv}(\text{supp}(m))) + K^p$$
$$= \{x \in S(m) \mid \forall x^* \in K \setminus \{\underline{0}\}: m\{y \in S(m) \mid x^*(y-x) > 0\} > 0\},$$

where K is considered as a subset of $F = (S(m) - S(m))^*$ and thus

$$K^p = \{z \in S(m) - S(m) \mid \forall x^* \in K : x^*(z) \leqq 0\}.$$

<u>Proof</u>: For shortness we put

$$A := ri(conv(supp(m))) + K^p$$

$$B := \{x \in S(m) \mid \forall x^* \in K \setminus \{\underline{0}\} : m\{y \in S(m) \mid x^*(y-x) > 0\} > 0\}.$$

First we show that $A^c \subseteqq B^c$: The set A is convex and open (relative to S(m)), so according to the Hahn-Banach theorem we can to $x \in A^c$ find $x^* \in (S(m) - S(m))^*$ with

(1) $$A \subseteqq \{y \in S(m) \mid x^*(y-x) < 0\}.$$

Using proposition 2.6, (iii), we obtain

$$\begin{aligned} K^p = 0^+(K^p) &\subseteqq 0^+A \\ &\subseteqq 0^+\{y \in S(m) \mid x^*(y-x) < 0\} \\ &= 0^+\{z \in S(m) - S(m) \mid x^*(z) < 0\} \\ &\subseteqq \{z \in S(m) - S(m) \mid x^*(z) \leqq 0\}, \end{aligned}$$

which shows that

$$x^* \in K^{po} = \bar{K} = K$$

(proposition 3.5). Inclusion (1) implies that

$$conv(supp(m)) \subseteqq \{y \in S(m) \mid x^*(y-x) \leqq 0\},$$

so

$$supp(m) \cap \{y \in S(m) \mid x^*(y-x) > 0\} = \emptyset,$$

that is,

$$m\{y \in S(m) \mid x^*(y-x) > 0\} = 0$$

(proposition 3.7), and hence $x \notin B$.

To see that $B^c \subseteqq A^c$ it sufficies to show that

$$x - z \notin ri(conv(supp(m)))$$

for all $x \in B^c$, $z \in K^p$. If $x \in B^c$ then

$$m\{y \in S(m) \mid x^*(y-x) > 0\} = 0$$

for some $x^* \in K$, and hence for $z \in K^p$

$$0 = m\{y \in S(m) \mid x^*(y-x) > 0\}$$
$$= m\{y \in S(m) \mid x^*(y-(x-z)) > x^*(z)\}$$
$$\geq m\{y \in S(m) \mid x^*(y-(x-z)) > 0\}$$

since $x^*(z) \leq 0$. It follows from 3.6 that

$$\text{supp}(m) \cap \{y \in S(m) \mid x^*(y-(x-z)) > 0\}$$

is empty, since it is a relative open subset of supp(m) with m-measure 0. This implies that

$$\text{ri}(\text{conv}(\text{supp}(m)))$$
$$\subseteq \text{ri}(\text{conv}\{y \in S(m) \mid x^*(y-(x-z)) \leq 0\})$$
$$= \{y \in S(m) \mid x^*(y-(x-z)) < 0\}$$

so

$$x-z \notin \text{ri}(\text{conv}(\text{supp}(m))).$$

Sometimes the following concept may be usefull:

<u>3.9 Definition</u>: Let A be convex subset of $F = E$ or E^*. The <u>normal cone</u> of A at $x \in A$ is

$$(A-x)^{\circ} = \{y^* \in F^* \mid \forall y \in A : \; y^*(y-x) \leq 0\}.$$

We shall use normal cones in section 5.

4. Maximum likelihood estimation in exponential families.

In this section we consider

V, a finite dimensional real Banach space with the Borel-σ-algebra $\grave{B}(V)$,

$(\grave{X},\grave{A})$, an arbitrary measurable space,

T, a measurable mapping $\grave{X} \to V$,

μ, a σ-finite positive measure on $(\grave{X},\grave{A})$,

S is the affine support of the measure $B \mapsto \mu(T^{-1}B)$, $B \in \grave{B}(V)$, and $\grave{B}(S)$ is the Borel-σ-algebra on S,

μ_T is the measure on $(S, \grave{B}(S))$ given by $\mu_T(B) = \mu(T^{-1}B)$.

$S_0 = S-S$

T_0 is an arbitrary fixed point i S.

We suppose, that the set

$$\Theta := \{\theta \in S_0^* \mid \int \exp(\theta(Tx - T_0))\ \mu(dx) < +\infty\}$$

is non empty. (Θ does not depend on the choice of T_0). In this case the measure μ_T is σ-finite.

Consider the exponential family

$$\grave{P} = \{P_\theta \mid \theta \in \Theta\}$$

of probability measures on $(\grave{X},\grave{A})$ defined by

$$\frac{dP_\theta}{d\mu}(x) = \frac{\exp(\theta(Tx - T_0))}{\int \exp(\theta(Ty - T_0))\ \mu(dy)}$$

(not depending on T_0). Corresponding to $\grave{P}$ we have the family

$$\grave{P}_T = \{P_{\theta,T} \mid \theta \in \Theta\}$$

of probability measures on $(S,\grave{B}(S))$ defined by

$$\frac{dP_{\theta,T}}{d\mu_T}(t) = \frac{\exp(\theta(t - T_0))}{\int \exp(\theta(s - T_0))\ \mu_T(ds)}.$$

(The measure $P_{\theta,T}$ is obtained from P_θ in the same way as μ_T from μ).

The likelihood function is

$$L : \Theta \times S \to [\,0,+\infty[$$

$$(\theta,t) \mapsto \frac{\exp(\theta(t - T_0))}{\int \exp(\theta(s - T_0))\, \mu_T(ds)} .$$

Now, suppose we have an observation $t_0 = Tx_0 \in S$ and that we want to estimate the parameter θ under the hypothesis $\theta \in H$, where H should be a closed convex subset of S_0^* and $H \cap \Theta \neq \emptyset$. The principle of maximum likelihood estimation then tells us to maximize $L(\theta,t_0)$ with respect to $\theta \in \Theta$, subject to the constraint $\theta \in H$, and if there exists a unique value $\hat\theta_H(t_0) \in \Theta \cap H$ with

$$L(\hat\theta_H(t_0),t_0) = \sup_{\theta \in \Theta \cap H} L(\theta,t_0)$$

then to use $\hat\theta_H(t_0)$ as an estimator for θ.

4.1 Theorem: Under the above conditions, it is necessary and sufficient for the existence of $\hat\theta_H(t_0)$ that

$$t_0 \in \operatorname{ri}(\operatorname{conv}(\operatorname{supp}(\mu_T))) + (0^+\, \overline{\Theta \cap H})^p,$$

(where the polar cone operation goes from S_0^* to S_0, cf. 3.4). In any case $L(\cdot,t_0)$ attains its supremum at at most one point in $\Theta \cap H$.

Moreover, the equation

$$E_\theta T = t_0$$

has at most one solution $\tilde\theta \in \Theta$, and if $\hat\theta_H(t_0) \in \operatorname{ri}(\Theta \cap H)$ then $\tilde\theta = \hat\theta_H(t_0)$.

Proof: For the sake of simplification we choose $T_0 = t_0$, so that

$$L(\theta,t_0) = \Phi(\theta)^{-1},$$

$$\Phi(\theta) := \Phi(\theta,t_0) := \int \exp(\theta(t - t_0))\, \mu_T(dt) \quad , \quad \theta \in \Theta.$$

It is a convenient trick to introduce the function

$$f_H : S_0^* \to \mathbb{R} \cup \{+\infty\}$$

$$f_H(\theta) := \begin{cases} \log \Phi(\theta) & \text{for} \quad \theta \in \Theta \cap H \\ +\infty & \text{for} \quad \theta \in S_0^* \setminus (\Theta \cap H). \end{cases}$$

Obviously, every minimum point for f_H will be a maximum point for $L(\cdot, t_0)$ restricted to $\Theta \cap H$, and vice versa. It is well known (see e.g. Barndorff-Nielsen (1970) or Johansen (1970)) that Θ is convex and $\log \Phi$ is strictly convex on Θ. Hence we conclude that f_H is quasi-convex and that f_H attains its infimum at at most one point (which will be $\hat{\theta}_H(t_0)$). The idea is now to show that f_H is l.s.c. using 2.13, and then to apply 2.14. First we shall find $\lim_{\rho \uparrow r} f_H(\theta + \rho\xi)$, $\theta, \xi \in S_0^*$, $r \in \,]0, +\infty]$.

Given $\theta \in \Theta \cap H$, $\xi \in S_0^* \setminus \{\underline{0}\}$, $r \in \,]0, +\infty]$, each of the following statements is either true or false:

$$\text{(st 1)}: r = +\infty$$

$$\text{(st 2)}: \{\theta + \rho\xi \mid \rho \in [0, r[\,\} \subseteq \Theta \cap H$$

$$\text{(st 3)}: \mu_T\{\xi(t - t_0) > 0\} > 0$$

$$\text{(st 4)}: \mu_T\{\xi(t - t_0) = 0\} > 0.$$

If the logical values of the statements are known we can find the desired limit:

case	(st 1)	(st 2)	(st 3)	(st 4)	$\lim_{\rho \uparrow r} f_H(\theta + \rho\xi)$
(1)		f			$+\infty$
(2)	f	t			$f_H(\theta + r\xi)$
(3)	t	t	t		$+\infty$
(4)	t	t	f	t	$-\log L(\theta, t_0 \mid \xi(T - t_0) = 0) = \log \int_{\{\xi(t - t_0) = 0\}} \exp(\theta(t - t_0))\mu_T(dt)$
(5)	t	t	f	f	$-\infty$

(t = true, f = false)

These results are, of course, obtained by rewriting $\log \Phi(\theta)$ as

$$\log\left(\int_{\{\xi(t - t_0) > 0\}} + \int_{\{\xi(t - t_0) \leq 0\}} \exp(\theta(t - t_0))\mu_T(dt) \right)$$

and using the monotone convergence theorem. Case (2) needs a little more attention: The limit is

$$\log \int \exp((\theta + r\xi)(t - t_0))\mu_T(dt) = \log \Phi(\theta + r\xi)$$

if the expression under the integral sign is integrable, and $+\infty$ otherwise. In the non-integrable case $\theta + r\xi \notin \Theta$ and hence $f_H(\theta + r\xi) = +\infty$. If the expression in fact is integrable, $\theta + r\xi \in \Theta$, and since $\{\theta + \rho\xi | \rho \in [0,r[\} \subseteq H$ and H is closed, $\theta + r\xi \in H$, and so $f_H(\theta + r\xi) = \log \Phi(\theta + r\xi)$.

In case (4) $L(\cdot,\cdot|\xi(T - t_0) = 0)$ is the likelihood function in the distribution of T conditional on $\xi(T - t_0) = 0$,

$$L(\omega,t_1|\xi(T - t_0) = 0) := \frac{\exp(\omega(t_1 - T_0))}{\int_{\{\xi(t - t_0) = 0\}} \exp(\omega(t - T_0))\ \mu_T(dt)}$$

for $t_1 \in \{t|\xi(t - t_0) = 0\}$, $\omega \in \Theta$.

For every $\theta \in \Theta \cap H$ and $\xi \in S_0^*$ we have

$$f_H(\theta + \xi) = \lim_{\lambda \uparrow 1} f_H(\theta + \lambda\xi)$$

(case (1) or case (2)), so proposition 2.13 gives that f_H is l.s.c.

We can now examine for which t_0's the condition 2.14 (iii) is fulfilled. Choose $a \in \mathbb{R}$, $\theta \in \text{ri} f_H^{-1}(]-\infty,a])$, $\xi \in S_0^* \setminus \{\underline{0}\}$. Then

$$\lim_{\rho \uparrow +\infty} f(\theta + \rho\xi) > a,$$

if and only if we are in case (1) or case (3) (in case (4)

$$\log \int_{\{\xi(t - t_0) = 0\}} \exp(\theta(t - t_0))\mu_T(dt) \leq \log \Phi(\theta) \leq a).$$

The following bi-implications hold (since $r = +\infty$):

[we are in case (1) or case (3)]

$\Leftrightarrow$ [((st 1) $\wedge$ (st 2) $\wedge$ (st 3)) $\vee$ non (st 2)]

$\Leftrightarrow$ [(st 2) $\Rightarrow$ (st 3)]

$\Leftrightarrow$ [$\text{ray}(\theta,\xi) \subseteq \Theta \cap H \Rightarrow \mu_T\{\xi(t - t_0) > 0\} > 0$]

$\Leftrightarrow$ [$\xi \in 0^+ \overline{\Theta \cap H} \Rightarrow \mu_T\{\xi(t - t_0) > 0\} > 0$]

according to 2.6 (ii). (Note the independence on a!)

We have thus found that condition 2.14 (iii) is fullfilled if and only if

$$\forall \xi \in S_0^* \setminus \{\underline{0}\} : [\xi \in 0^+ \overline{\Theta \cap H} \Rightarrow \mu_T\{\xi(t - t_0) > 0\} > 0].$$

Applying 3.8 it is seen to be equivalent to

$$t_0 \in \mathrm{ri}(\mathrm{conv}(\mathrm{supp}(\mu_T))) + (0^+ \overline{\Theta \cap H})^p.$$

This finishes the deduction of the criterion for existence of maximum likelihood estimators.

It is known (see e.g. Barndorff-Nielsen (1970) or Johansen (1970)) that the mapping $\theta \mapsto E_\theta T$ is injective and that

$$E_\theta T = t_0 + D \log \Phi(\theta)$$

for $\theta \in \mathrm{ri}\Theta$. If $\hat{\theta}_H(t_0) \in \mathrm{ri}(\Theta \cap H)$, it is a stationary point, i.e. $D \log \Phi(\hat{\theta}_H(t_0)) = \underline{0}$, and therefore solution to

$$E_\theta T = t_0.$$

This completes the proof of 4.1.

4.2 <u>Corollary</u>: The functions Φ and $\log\Phi$ $S_0^* \to \mathbb{R} \cup \{+\infty\}$ defined by

$$\Phi(\theta) = \begin{cases} \int \exp(\theta(t - T_0))\mu_T(dt) & , \quad \theta \in \Theta \\ + \infty & , \quad \theta \in S_0^* \setminus \Theta, \end{cases}$$

are l.s.c.

<u>Proof</u>: $\Phi = f_H$, $H = S_0^*$, with f_H as in the proof of 4.1.

4.3 <u>Corollary</u>: The level sets

$$\{\theta \in S_0^* \mid -\log L(\theta, t_0) \leqq a\} \quad , \quad a > \inf(-\log L(\cdot, t_0)),$$

are all bounded or all unbounded.

<u>Proof</u>: In the proof of 4.1 we found a criterion for $\lim_{\rho \uparrow +\infty} f(\theta + \rho\xi)$ to be $>a$ for every $\xi \in S_0^* \setminus \{\underline{0}\}$, and this criterion did not depend on a. The result then follows from 2.8 (i, iii).

4.4 Corollary: Suppose $\grave{X}$ is a locally compact vector space and $\grave{A}$ the Borel-σ-algebra on $\grave{X}$, and suppose μ is discrete (i.e. supp(μ) is discrete in the subspace-topologi). If $t_0 \in \mathrm{conv}(\mathrm{supp}(\mu_T))$ and $\xi \in 0^+\mathrm{ri}(\Theta \cap H)$ so that

$$\mu_T\{t \mid \xi(t - t_0) > 0\} = 0$$

$$\mu_T\{t \mid \xi(t - t_0) = 0\} > 0,$$

then for $\theta_0 \in \mathrm{ri}(\Theta \cap H)$

$$P_{\theta_0 + \rho\xi} \xrightarrow{w} P_{\theta_0}(\cdot \mid \xi(T - t_0) = 0)$$

for $\rho \to +\infty$. Since $P_{\theta_0,T}\{t_0\} \leqq P_{\theta_0,T}(\{t_0\} \mid \xi(T - t_0) = 0)$, this implies that

$$\sup_{\theta \in \Theta \cap H} P_{\theta,T}\{t_0\} = \sup_{\theta \in \Theta \cap H} P_{\theta,T}(\{t_0\} \mid \xi(T - t_0) = 0).$$

Proof: This is an immediate consequence of the examinations of $\lim f(\theta + \rho\xi)$ in the proof of 4.1, since

$$P_\theta\{x\} = \exp(-f(\theta))\,\mu\{x\}, \quad f(\theta) = \log\Phi(\theta, Tx),$$

so that it is seen that

$$\lim_{\rho\to+\infty} P_{\theta_0 + \rho\xi}\{x\} = P_{\theta_0}(\{x\} \mid \xi(T - t_0) = 0)$$

for all $x \in \mathrm{supp}(\mu)$.

5. The dose-response model.

In this section we shall - as an example - discuss the estimation problems in the dose-response model.

5.1

Consider mutually independent random variables $X_1,\ldots,X_k$, so that X_i is binominally distributed with known number parameter $n_i \in \mathbb{N}$ and unknown probability parameter $p^{(i)} \in [0,1]$, $i = 1,\ldots,k$. Furthermore, $z_1 < \ldots < z_k$ are given real numbers. Now the statistical problem is obtained assuming that for some $\theta = (\alpha,\beta) \in \mathbb{R}^2$

$$p^{(i)} = p_\theta(z_i) := \frac{1}{1 + \exp(-\alpha-\beta z_i)}, \quad i = 1,\ldots,k.$$

Note, that the logistic function

$$p_\theta = p_{\alpha,\beta} : z \mapsto \frac{1}{1 + \exp(-\alpha-\beta z)} = \frac{\exp(\alpha+\beta z)}{1 + \exp(\alpha+\beta z)}, \quad z \in \mathbb{R},$$

for $\beta > 0$ is increasing, for $\beta = 0$ constant, and for $\beta < 0$ decreasing. For $\beta \neq 0$ $p_{\alpha,\beta}$ is a bijection from $\mathbb{R}$ to $]0,1[$; the inverse mapping of $p_{0,1}$ is

$$\lambda : u \mapsto \log \frac{u}{1-u}, \quad u \in]0,1[.$$

($\lambda(u)$ is sometimes called the logistic transform of u). Finally, $\{p_\theta(z) | \theta \in \mathbb{R}^2\} =]0,1[$ for every $z \in \mathbb{R}$.

5.2

The distribution of $X = (X_1,\ldots,X_k)$ when $p_\theta(z_1),\ldots,p_\theta(z_k)$ are the parameters is P_θ given by

$$P_\theta\{(x_1,\ldots,x_k)\} := P\{X_1 = x_1,\ldots,X_k = x_k\}$$

$$= \begin{cases} \dfrac{\exp(\alpha \sum x_i + \beta \sum z_i x_i)}{\prod_{i=1}^{k} [1 + \exp(\alpha+\beta z_i)]^{n_i}} \prod_{i=1}^{k} \binom{n_i}{x_i}, & \text{for } (x_1,\ldots,x_k) \in \prod_{i=1}^{k} \{0,1,\ldots,n_i\} \\ 0, & \text{for } (x_1,\ldots,x_k) \notin \prod_{i=1}^{k} \{0,1,\ldots,n_i\} \end{cases}$$

so we are concerned with an exponential family of order 2. Introducing the measure μ on $(\mathbb{R}^k, \mathcal{B}^k)$ with

$$\mu(\{x\}) = \begin{cases} \prod_{i=1}^{k} \binom{n_i}{x_i} & \text{for } x = (x_1,\ldots,x_k) \in \prod_{i=1}^{k} \{0,1,\ldots,n_i\} \\ 0 & \text{else} \end{cases},$$

and the functions $T : \mathbb{R}^k \to \mathbb{R}^2$ and $\Phi : \mathbb{R}^2 \to \mathbb{R}$:

$$T : x \mapsto (T_1x, T_2x) := (\sum_i x_i, \sum_i z_i x_i) = \sum_i x_i(1,z_i),$$

$$\Phi : \theta = (\alpha,\beta) \mapsto \int \exp(\alpha T_1 x + \beta T_2 x)\, \mu(dx)$$

$$= \prod_{i=1}^{k} [1 + \exp(\alpha + \beta z_i)]^{n_i},$$

we have

$$\frac{dP_\theta}{d\mu}(x) = \frac{\exp(\theta \cdot Tx)}{\Phi(\theta)}, \quad \theta \in \mathbb{R}^2,$$

(where $\cdot$ denotes the ordinary inner product in $\mathbb{R}^2$), to be compared with the family of section 4.

The support of the transformed measure μ_T is

$$\text{supp}(\mu_T) = T(\text{supp}(\mu))$$

$$= \{\sum x_i(1,z_i) \mid x_i \in \{0,1,\ldots,n_i\},\ i=1,\ldots,k\},$$

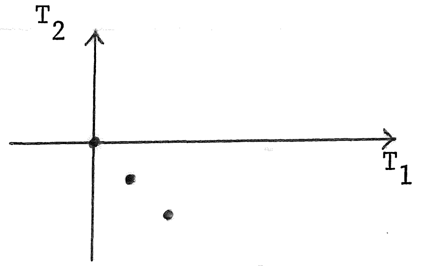
and the convex hull of $\text{supp}(\mu_T)$ is a (convex) polygon with 2k sides and the corners

$$(0,0), \quad \sum_{i=j}^{k} n_i(1,z_i), \quad \sum_{i=1}^{j} n_i(1,z_i), \quad j=1,2,\ldots,k.$$

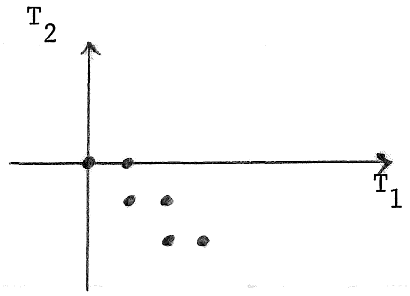
Since $(0^+ \mathbb{R}^2)^p = (\mathbb{R}^2)^p = \{(0,0)\}$, it follows from theorem 4.1 that the maksimum likelihood estimator $\hat{\theta}(t_0)$, $t_0 = Tx_0$, exists if and only if t_0 belongs to the interior of the polygon $\text{conv}(\text{supp}(\mu_T))$.

5.3

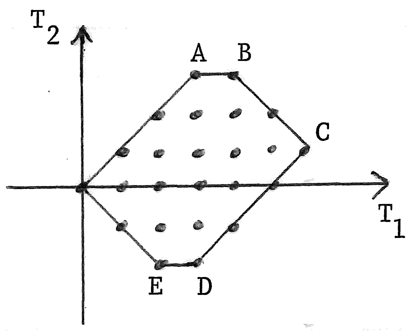
Example: The case $k = 3$; $n_1 = 2$, $n_2 = 1$, $n_3 = 3$; $z_1 = -1$, $z_2 = 0$, $z_3 = 1$.



$$\{x_1(1,-1) \mid x_1 = 0,1,2\}$$



$$\{x_1(1,-1) \mid x_1 = 0,1,2\}$$
$$+ \{x_2(1,0) \mid x_2 = 0,1\}$$



$$\{x_1(1,-1) \mid x_1 = 0,1,2\}$$
$$+ \{x_2(1,0) \mid x_2 = 0,1\}$$
$$+ \{x_3(1,1) \mid x_3 = 0,1,2,3\}$$
$$= \{ \sum_{i=1}^{3} x_i(1,z_i) \mid x_i=1,\ldots,n_i\}$$

A: $n_3(1,z_3)$

B: $n_3(1,z_3) + n_2(1,z_2)$

C: $n_3(1,z_3) + n_2(1,z_2) + n_1(1,z_1)$

D: $n_1(1,z_1) + n_2(1,z_2)$

E: $n_1(1,z_1)$.

5.4

It is possible in an explicit manner to describe the observations x_0 leading to a $t_0 = Tx_0$ on the boundary of $\mathrm{conv}(\mathrm{supp}(\mu_T))$, since the corners are known; $t_0 = Tx_0$ is a boundary point if and only if x_0 is of the form

$$(0,\ldots,0, x_{0j}, n_{j+1},\ldots,n_k)$$

or

$$(n_1,\ldots,n_{j-1}, x_{0j}, 0,\ldots,0),$$

where $x_{0j} \in \{0,1,\dots,n_j\}$, $j \in \{1,\dots,k\}$, and t_0 is a corner point if and only if also $x_{0j} \in \{0,n_j\}$.

Indeed, it is quiet an inconsistent behavior to want to estimate the parameter θ by the maximum likelihood method when it is possible to get observations x_0 with $P_\theta(\{x_0\}) > 0$, $\forall\theta \in \mathbb{R}^2$, so that no maximum likelihood estimator exists. Therefore an extension of the model is needed.

In the case of $t_0 = Tx_0 \in \mathrm{supp}(\mu_T)$ on the boundary, it turns out that for some sequences $(\theta_n)_{n\in\mathbb{N}}$ so that the likelihood function converges to its supremum (and therefore (θ_n) converges to infinity), the corresponding sequence of logistic functions (p_{θ_n}) converges to a kind of a degenerate logistic function which fits the observed x_{0i}-values perfectly; this has been discussed by Silverstone (1957). One might then use the family of degenerate and ordinary logistic functions as a parametrization of an extended model.

Passing to polar coordinates for θ and allowing the module to be $+\infty$ is another convenient method, which has been used by Davis (1970), who also notices that the t_0's giving rise to nonsolvable maximum likelihood equations are those on the boundary of $\mathrm{conv}(\mathrm{supp}(\mu_T))$.

A different approach has been made by Barndorff-Nielsen (1970), who proves a general result about extending certain types of exponential families; Barndorff uses the mean value parametrization, which makes many things very nice.

Here we shall proceed in the following way. Since a parametrization of our family $\grave{P} := \{P_\theta | \theta \in \mathbb{R}^2\}$ - from a mathematical point of view - just serves to define the subset $\grave{P}$ of the set of all probability measures on $\mathbb{R}^k$, let us for a while reformulate our problem of estimating θ to a problem of estimating a probability measure from $\grave{P}$. If we want to extend $\grave{P}$ in order to make maximum likelihood estimation, it is good to have a non parametric definition of "likelihood function". Obviously we can use the function

$$Q \mapsto Q\{T = t_0\} = Q_T\{t_0\}.$$

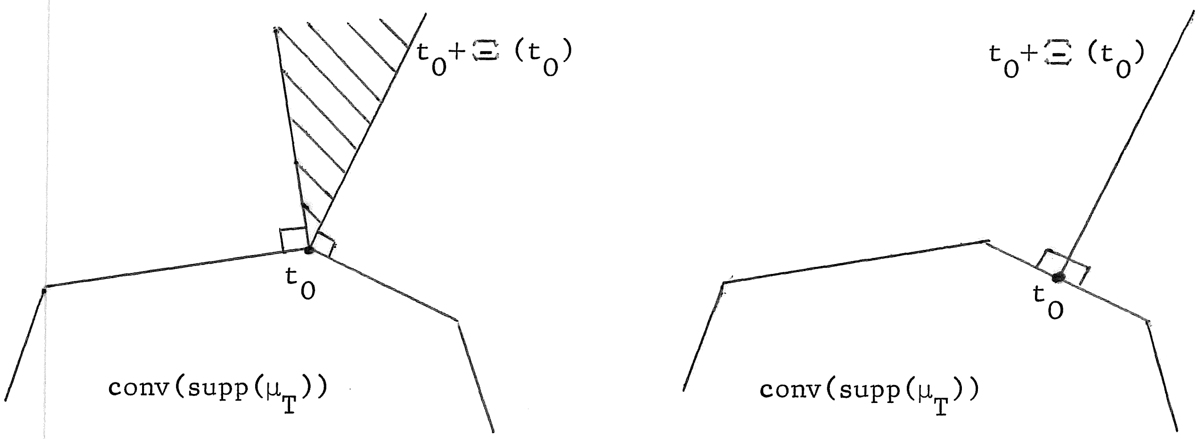
We are now able to find the smallest family of probability measures on $\mathbb{R}^k$ containing $\grave{P}$, so that maximum likelihood estimation always is possible.

5.6

If t_0 is a boundary point of $\mathrm{conv}(\mathrm{supp}(\mu_T))$ let $\Xi(t_0)$ denote the normal cone of $\mathrm{conv}(\mathrm{supp}(\mu_T))$ at t_0, i.e.

$$\Xi(t_0) := \{\xi = (\xi_1,\xi_2) \in \mathbb{R}^2 \mid \forall t \in \mathrm{supp}(\mu_T) : \xi\cdot(t-t_0) \leqq 0\}.$$

$\Xi(t_0)$ is a closed convex cone with vertex $\underline{0}$.



Let x_0 be an observed value, $t_0 = Tx_0$. If t_0 belongs to the relative interior of $\mathrm{conv}(\mathrm{supp}(\mu_T))$ we can (as already mentioned) solve the estimation problem. If t_0 is a boundary point then choose $\xi \in \Xi(t_0)\setminus\{\underline{0}\}$; from 4.4 we know that for $\theta \in \mathbb{R}^2$ the conditional distribution $P_\theta(\cdot\,|\,\xi\cdot(T - t_0) = 0)$ belongs to the closure $\bar{\grave{P}}$ of $\grave{P}$ and that

$$\sup_{Q \in \grave{P}} Q_T\{t_0\} = \sup_{Q \in \grave{P}} Q_T(\{t_0\}\,|\,\xi\cdot(T - t_0) = 0)$$

Since the family

$$\grave{P}^\xi := \{Q(\cdot\,|\,\xi\cdot(T - t_0) = 0) \mid Q \in \grave{P}\}$$

of conditional distributions can be written in the same way as in section 4, - with the same statistic T and another measure μ^ξ, $\mu^\xi\{x\} = \mu\{x\}\cdot 1_{\{\xi\cdot(Tx - t_0) = 0\}}$, - we are in a similar situation as before: given $t_0 \in \mathrm{supp}(\mu_T^\xi)$ we seek the $Q \in \grave{P}^\xi$ that maximizes the likelihood function $Q_T\{t_0\}$; and again this problem is solvable if and only if t_0 is a point of the relative interior of $\mathrm{conv}(\mathrm{supp}(\mu_T^\xi))$. If

$t_0 \notin \mathrm{ri}(\mathrm{conv}(\mathrm{supp}(\mu_T^{\xi})))$ we choose an η from the normal cone of $\mathrm{conv}(\mathrm{supp}(\mu_T^{\xi}))$ at t_0 so that ξ and η are linearly independent, and form the conditional distributions

$$\grave{P}^{\xi,\eta} := \{Q(\cdot \mid \eta\cdot(T - t_0) = 0) \mid Q \in \grave{P}^{\xi}\}.$$

From 4.4 we know that $\grave{P}^{\xi,\eta} \subseteq \overline{P}$ and that

$$\sup_{Q \in \grave{P}} Q_T\{t_0\} = \sup_{Q \in \grave{P}^{\xi}} Q_T\{t_0\} = \sup_{Q \in \grave{P}^{\xi,\eta}} Q_T\{t_0\}.$$

The sequence $(\grave{P}, \grave{P}^{\xi}, \grave{P}^{\xi,\eta})$ is a sequence of families of decreasing order, and because $\grave{P}$ is of order 2 $\grave{P}^{\xi,\eta}$ will contain only one element so that estimation is trivial. This means that it is always possible to find $\hat{Q} \in \overline{P}$ so that

$$\hat{Q}_T\{t_0\} = \sup_{Q \in \grave{P}} Q_T\{t_0\}.$$

It is a reasonable demand to $\hat{Q}$ that it does not depend on our choise of ξ's and η's, and it is seen from the following investigation that this demand indeed is fulfilled.

<u>5.7</u>

Consider an observation x_0 with $t_0 = Tx_0$ on the boundary of $\mathrm{conv}(\mathrm{supp}(\mu_T))$. We will confine ourselves to the case

$$x_0 = (0,\dots,0, x_{0,k-1}, n_k),\ x_{0,k-1} \in \{1,2,\dots,n_{k-1}\},$$

$$t_0 = n_k\cdot(1,z_k) + x_{0,k-1}\cdot(1,z_{k-1}),$$

but the results are generalized in an obvious way.

If $x_{0,k-1} \in \{1,\dots,n_{k-1} - 1\}$, t_0 is not corner point (cf. 5.4), and the normal cone is

$$\Xi(t_0) = \{\sigma\cdot(-z_{k-1},1) \mid \sigma \in [\,0,+\infty[\,\}.$$

If $x_{0,k-1} = n_{k-1}$, t_0 is a corner point, and the normal cone is

$$\Xi(t_0) = \{\sigma\cdot(-z_{k-1},1) + \tau\cdot(-z_k,1) \mid \sigma,\tau \in [\,0,+\infty[\,\}.$$

The distribution of $X = (X_1,\dots,X_k)$ conditionally on $\xi\cdot(T-t_0) = 0$, $\xi \in \Xi(t_0)\setminus\{\underline{0}\}$, is easily found; there are two cases:

A: $\text{supp}(\mu_T) \cap \{t \mid \xi\cdot(t - t_0) = 0\} = \text{supp}(\mu_T^\xi) = \{t_0\}$.

This happens if and only if t_0 is a corner point ($x_{0,k-1} = n_{k-1}$) and $\xi = \sigma\cdot(-z_{k-1},1) + \tau\cdot(-z_k,1)$ for $\sigma,\tau \in \mathbb{R}_+$. For every $\theta = (\alpha,\beta) \in \mathbb{R}^2$

$$\hat{Q} = P_\theta(\cdot \mid \xi\cdot(T - t_0) = 0) = \text{the one-point distribution on } \mathbb{R}^2 \text{ at } x_0 = (0,\dots,0, n_{k-1}, n_k).$$

B: $\text{supp}(\mu_T) \cap \{t \mid \xi\cdot(t - t_0) = 0\} = \text{supp}(\mu_T^\xi) \supset \{t_0\}$.

Here we must distinguish between two cases:

B1: $\xi = \sigma\cdot(-z_{k-1},1) \quad , \quad \sigma \in \mathbb{R}_+$.

B2: $\xi = \tau\cdot(-z_k,1) \quad , \quad \tau \in \mathbb{R}_+$.

We shall only discuss B1; B2 can be treated in a completely analogous way.

B1: For every $\theta = (\alpha,\beta) \in \mathbb{R}^2$ and $x_{k-1} \in \{0,1,\dots,n_{k-1}\}$ we find

$$P_\theta(\{(0,\dots,0, x_{k-1}, n_k)\} \mid \xi\cdot(T - t_0) = 0)$$

$$= \binom{n_{k-1}}{x_{k-1}} p_\theta(z_{k-1})^{x_{k-1}} (1 - p_\theta(z_{k-1}))^{n_{k-1} - x_{k-1}}$$

and

$$\frac{dP_\theta(\cdot \mid \xi\cdot(T - t_0) = 0)}{d\mu^\xi}(x) = \left.\frac{\exp(\omega\cdot(Tx - T_0))}{\int \exp(\omega\cdot(Ty - T_0))\mu^\xi(dy)}\right|_{\omega = \omega_\theta} , x \in \mathbb{R}^k,$$

where

$$\mu^\xi\{x\} = \mu\{x\}\cdot 1_{\{\xi\cdot(Tx - t_0) = 0\}} \quad , x \in \mathbb{R}^k,$$

$$T_0 = n_k(1,z_k) \quad (\text{so that } Tx - T_0 = x_{k-1}\cdot(1,z_{k-1}),\ x \in \text{supp}(\mu^\xi))$$

$$\omega_\theta = \lambda(p_\theta(z_{k-1}))\cdot(1,0) = (\alpha + \beta z_{k-1})\cdot(1,0),$$

$$\omega = \gamma\cdot(1,0), \quad \gamma \in \mathbb{R} = \{\lambda(p_\theta(z_{k-1})) \mid \theta \in \mathbb{R}^2\}$$

(λ is the logistic transformation, see 5.1); thus

$$\frac{\exp(\omega\cdot(Tx - T_0))}{\int \exp(\omega\cdot(Ty - T_0))\mu^\xi(dy)}\mu^\xi\{x\} = \binom{n_{k-1}}{x_{k-1}} \frac{e^{\gamma x_{k-1}}}{(1 + e^\gamma)^{n_{k-1}}}$$

for $x \in \mathrm{supp}(\mu^{\xi})$, i.e. X_{k-1} is binomially distributed with parameters n_{k-1} and $e^{\gamma}/1+e^{\gamma}$.

Now $t_0 \in \mathrm{ri}(\mathrm{conv}(\mathrm{supp}(\mu_T^{\xi})))$ if and only if $x_{0,k-1} \in \{1,\dots,n_{k-1}-1\}$, and in this case the maximum likelihood estimator $\hat{\omega} = \hat{\gamma}\cdot(1,0)$ is of course given by

$$\hat{\gamma} = \lambda(\hat{p}), \quad \hat{p} = \frac{x_{0,k-1}}{n_{k-1}},$$

obtained from the relation

$$E_{\hat{\omega}}(T \mid \xi(T - t_0) = 0) = t_0 ,$$

that is,

$$n_k\cdot(1,z_k) + n_{k-1}\frac{e^{\hat{\gamma}}}{1+e^{\hat{\gamma}}}\cdot(1,z_{k-1}) = n_k\cdot(1,z_k) + x_{0,k-1}\cdot(1,z_{k-1});$$

consequently

$$\hat{Q}\{x\} = \frac{d\hat{Q}}{d\mu^{\xi}}(x)\mu^{\xi}\{x\} = \frac{\exp(\hat{\omega}\cdot(Tx - T_0))}{\int \exp(\hat{\omega}\cdot Ty - T_0))\mu^{\xi}(dy)}\mu^{\xi}\{x\}$$

$$= \begin{cases} \binom{n_{k-1}}{x_{k-1}}\hat{p}^{x_{k-1}}(1-\hat{p})^{n_{k-1}-x_{k-1}} & \text{if } \begin{cases} x_1 = \dots = x_{k-2} = 0, \\ x_{k-1} \in \{0,1,\dots,n_{k-1}\} \\ x_k = n_k \end{cases} \\ 0 & \text{else.} \end{cases}$$

If $x_{0,k-1} = n_{k-1}$ no $\hat{\omega}$ exists. In this case we shall choose an η from the normal cone of $\mathrm{conv}(\mathrm{supp}(\mu_T^{\xi}))$ so that ξ and η are linearly independent:

$$\eta \in \{\eta = (\eta_1,\eta_2) \in \mathbb{R}^2 \mid \eta_1 + \eta_2 z_{k-1} < 0\}$$

For any such η

$$\mathrm{supp}(\mu_T^{\xi}) \cap \{t \mid \eta\cdot(T - t_0) = 0\} = \{t_0\},$$

so we are in a situation similar to A; we find

$$\hat{Q} = P_{\theta}(\cdot \mid \xi\cdot(T - t_0) = 0,\ \eta\cdot(T - t_0) = 0)$$

$$= \text{the one-point distribution on } \mathbb{R}^k \text{ at } x_0 = (0,\dots,n_{k-1}, n_k)$$

for all $\theta \in \mathbb{R}^2$.

5.8

The distribution of $X = (X_1,\dots,X_k)$ is estimated as follows:

$X_1,\dots,X_k$ are independent binomially distributed with parameters $n_1,\dots,n_k \in \mathbb{N}^k$ (known) and $p^{(1)},\dots,p^{(k)} \in [0,1]$. The observation is x_0.
If $t_0 = Tx_0 \in ri(conv(supp(\mu_T)))$, then $p^{(i)} = p_{\hat\theta}(z_i)$, $i=1,\dots,k$; if t_0 is on the boundary of $conv(supp(\mu_T))$, then $p^{(i)} = \frac{x_{0i}}{n_i}$, $i=1,\dots,k$, (see 5.4). Thus if we put

$$P_p\{(x_1,\dots,x_k)\} := \prod_{i=1}^{k} p_i^{x_i}(1-p_i)^{n_i-x_i} \cdot \mu\{x\},\ x \in \mathbb{R}^k,$$
$$p \in [0,1]^k,$$

the smallest extension $\grave{P}_1$ of $\grave{P} = \{P_p \mid p_i = p_\theta(z_i),\ i=1,\dots,k\}$ ($\theta \in \mathbb{R}^2$) so that maximum likelihood estimation always is possible (and unique) is

$$\grave{P}_1 = \grave{P} \cup \{P_p \mid p = (0,\dots,0, \tfrac{x_i}{n_i}, 1,\dots,1),\ x_i=1,\dots,n_i;\ i=1,\dots,k\}$$

$$\cup \{P_p \mid p = (1,\dots,1, \tfrac{x_i}{n_i}, 0,\dots,0),\ x_i=1,\dots,n_i;\ i=1,\dots,k\}.$$

It seems, however, more natural to consider the extension

$$\grave{P}_2 = \grave{P} \cup \{P_p \mid p = (0,\dots,0, p_i,1,\dots,1),\ p_i \in [0,1];\ i=1,\dots,k\}$$

$$\cup \{P_p \mid p = (1,\dots,1, p_i,0,\dots,0),\ p_i \in [0,1];\ i=1,\dots,k\},$$

since

$$\{p = (p_1,\dots,p_k) \in [0,1]^k \mid P_p \in \grave{P}_2\}$$

is independent of $n_1,\dots,n_k$.
With each element P_θ, $\theta = (\alpha,\beta) \in \mathbb{R}^2$, of P we can associate the logistic function

$$\mathbb{R} \to [0,1]$$
$$z \mapsto p_\theta(z)$$

If $P_p \in \grave{P}_2 \setminus \grave{P}$ we may associate with P_p the degenerate logistic function which is the pointwise limit of $p_{\theta+\rho\xi+\rho'\eta}$ for any θ,ξ,η so that $P_{\theta+\rho\xi+\rho'\eta} \to P_p$ for $\rho,\rho' \to +\infty$. This leads to the following functions:

if $p = (0,\dots,0, p_i, 1,\dots,1)$, $p_i \in]0,1[$, $i \in \{1,\dots,k\}$:

$$\begin{aligned} \mathbb{R} &\to [0,1] \\ z &\mapsto \begin{cases} 0 & \text{for } z \in]-\infty, z_i[\\ p_i & \text{for } z = z_i \\ 1 & \text{for } z \in]z_i,+\infty[; \end{cases} \end{aligned}$$

if $p = (0,\ldots,0,\underset{\uparrow \text{i'th place}}{1},\ldots,1)$, $i \in \{2,3,\ldots,k\}$:

$$\begin{aligned} \mathbb{R}\backslash]z_{i-1},z_i[&\to [0,1] \\ z &\mapsto \begin{cases} 0 & \text{if } z \in]-\infty,z_{i-1}] \\ 1 & \text{if } z \in [z_i,+\infty[; \end{cases} \end{aligned}$$

if $p = (0,\ldots,0)$:

$$\begin{aligned} [z_1,z_k] &\to [0,1] \\ z &\mapsto 0 ; \end{aligned}$$

if $p = (1,\ldots,1)$:

$$\begin{aligned} [z_1,z_k] &\to [0,1] \\ z &\mapsto 1 \end{aligned}$$

(plus some analogous functions for the p_i-sequence decreasing).

The reason why some of the functions are undefined for some $z \in \mathbb{R}$ is that for these z $\lim_{\rho,\rho'} p_{\theta+\rho\xi+\rho'\eta}(z)$ is a non-constant function of (θ,ξ,η) on the set of all applicable (θ,ξ,η)'s. Thinking of the information contained in the observations $(x_{01},\ldots,x_{0k})$ about the graph of the logistic function, it is indeed very reasonable that the function is indetermined in some intervals.

5.9

The dose-response model is often applicated when describing experiments where a number of animals are treated with different doses of a certain drug - n_i animals are treated with the i-th dose; z_i is most commonly the logarithme of the dose - and one observes the number X_i of animals that die in group i, i=1,...,k. It is often assumed that the probability of dying is an increasing function of the dose, leading to the consideration of the family

$$\grave{P}_0 := \{P_\theta \mid \theta = (\alpha,\beta) \in \mathbb{R} \times [0,+\infty[\}.$$

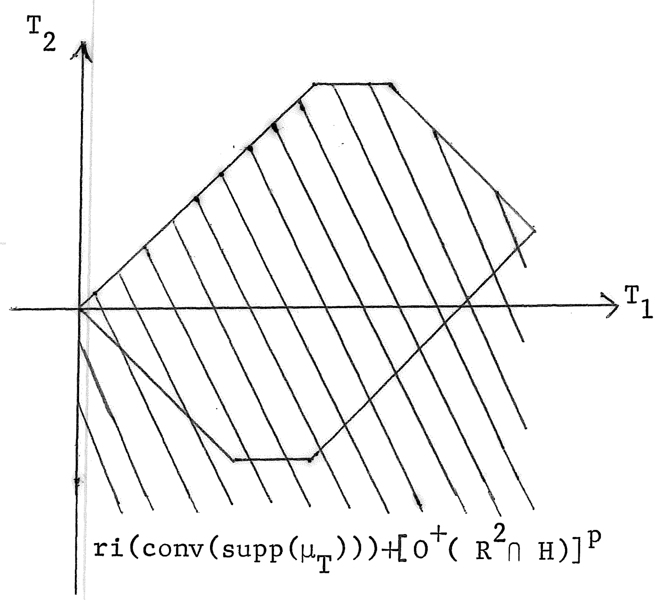
Here the parameter set thus is $\mathbb{R}^2 \cap H$, where

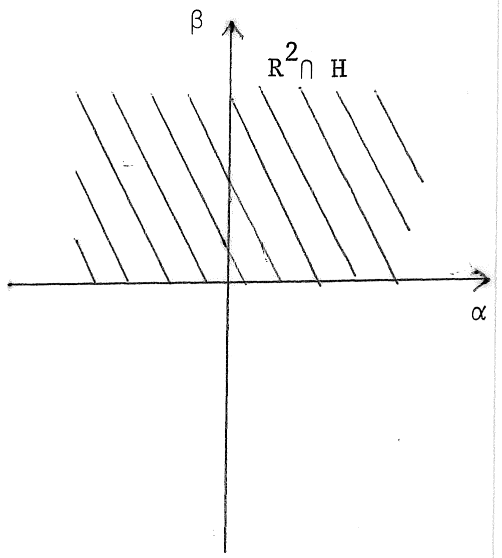
$$H = \{\theta = (\alpha,\beta) \in \mathbb{R}^2 \mid \beta \geqq 0\}$$

is closed and convex. Moreover

$$[0^+(\mathbb{R}^2 \cap H)]^p = \{(0,\delta) \mid \delta \in]-\infty,0]\}.$$

On applying Theorem 4.1 it is seen that the existence of a maximum likelihood estimator $\hat{\theta}_H(t_0) \in \mathbb{R}^2 \cap H$ is equivalent to the existence of $s_0 \in \mathrm{ri}(\mathrm{conv}(\mathrm{supp}(\mu_T)))$, $\delta \in]-\infty,0]$, so that $t_0 = s_0 + (0,\delta)$.





We shall now discuss the t_0's giving rise to a $\hat{\theta}_H(t_0) = (\hat{\alpha},\hat{\beta})$ in the interior of $\mathbb{R}^2 \cap H$, i.e. $\hat{\beta} > 0$; in this case $\hat{\theta}_H(t_0)$ is the solution $\tilde{\theta}$ to

$$E_{\tilde{\theta}}\, T = t_0.$$

According to 4.1 the mapping

$$\tau : \mathbb{R}^2 \to \mathrm{ri}(\mathrm{conv}(\mathrm{supp}(\mu_T)))$$
$$\theta \mapsto E_\theta T$$

is a bijection (as a matter of fact a homeomorphism) with the inverse mapping

$$\hat{\theta} : \text{ri}(\text{conv}(\text{supp}(\mu_T))) \to \mathbb{R}^2$$
$$t_0 \mapsto \hat{\theta}(t_0)$$

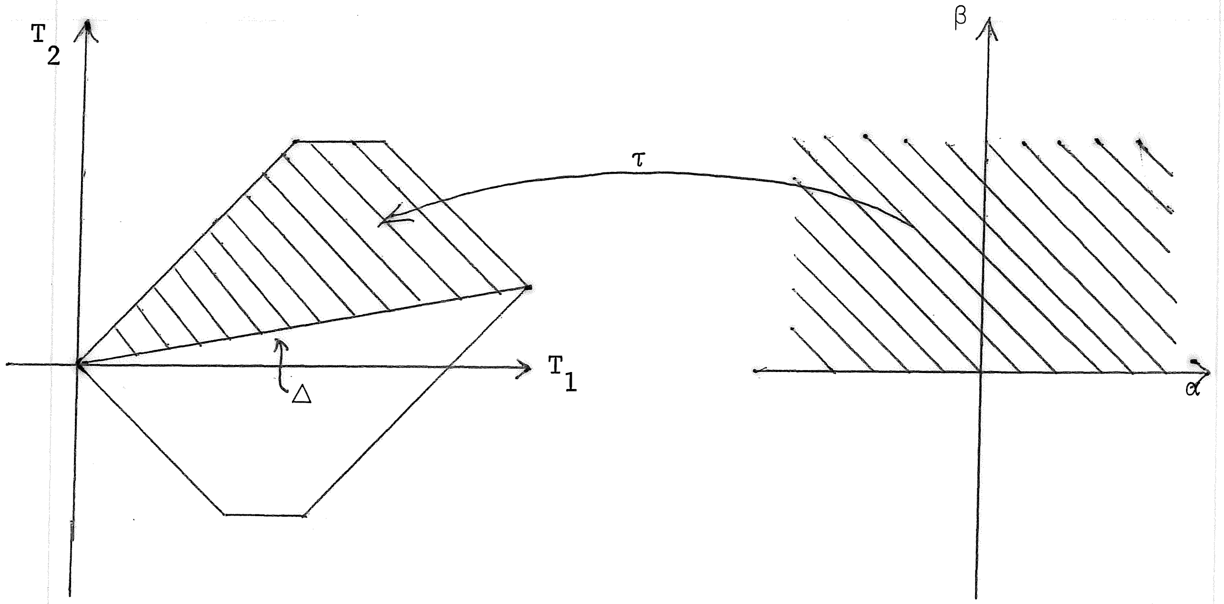
Since

$$\tau : \theta = (\alpha,\beta) \mapsto \sum_{i=1}^{k} \frac{n_i}{1 + \exp(-\alpha-\beta z_i)} (1,z_i) ,$$

the image of the α-axis is

$$\Delta : = \{\sigma \cdot \sum_{i=1}^{k} n_i(1,z_i) \mid \sigma \in]0,1[\}.$$

The set $\text{ri}(\text{conv}(\text{supp}(\mu_T)))\setminus\Delta$ consists of two path-connected components, as does $\mathbb{R}^2\setminus\{(\alpha,\beta)|\beta=0\}$, and as τ is continuous and bijective, the image by τ of $\text{ri}(\mathbb{R}^2 \cap H) = \{(\alpha,\beta) \in \mathbb{R}^2|\beta>0\}$ is one of the two components of $\text{ri}(\text{conv}(\text{supp}(\mu_T)))\setminus\Delta$; it is seen that it is the upper one:



If t_0 belongs to the interior of the upper sub-polygon we can find $\hat{\theta}_H(t_0)$ as the solution $\tilde{\theta}$ to

$$E_{\tilde{\theta}}T = t_0.$$

For any other t_0 for which $\hat{\theta}_H(t_0)$ exists, $\hat{\theta}_H(t_0)$ must be a point on the α-axis; because if $\hat{\theta}_H(t_0) \in \text{ri}(\mathbb{R}^2 \cap H)$ then $t_0 = E_{\hat{\theta}_H(t_0)}T$ was an interior point of the upper sub-polygon!

For $\theta = (\alpha,0)$, $\alpha \in \mathbb{R}$,

$$\frac{dP_\theta}{d\mu}(x) = \frac{\exp(\alpha \cdot T_1 x)}{(1+e^\alpha)^n} \quad , \quad x \in \mathbb{R}^k ,$$

where $n = \sum_{i=1}^{k} n_i$, $T_1 x = \sum_{i=1}^{k} x_i$, that is, $X_1,\ldots,X_k$ are independent, binominally distributed with the same probability parameter $e^\alpha/1+e^\alpha$. The maximum likelihood estimator $\hat{\alpha}$ thus exists if and only if

$$t_{01} = T_1 x_0 \in \mathrm{ri}(\mathrm{conv}(\mathrm{supp}(\mu_{T_1}))) =]\, 0,n[,$$

but this is implied by the assumption that $\hat{\theta}_H(t_0)$ exists, i.e. that $t_0 \in \mathrm{ri}(\mathrm{conv}(\mathrm{supp}(\mu_T))) + [0^+(\mathbb{R}^2 \cap H)]^p$.

We have, of course, that

$$\hat{\alpha} = \lambda(\frac{t_{01}}{n}).$$

In cases where $\hat{\theta}_H(t_0)$ does not exists, one should proceed in a similar way to 5.6, although for example the ξ's now should be chosen from $0^+(\mathbb{R}^2 \cap H) = H$. The results are not surprising. One should however be aware of the cases $t_0 = \underline{0}$ and $t_0 = \sum_{i=1}^{k} n_i(1,z_i)$; in the former case the degenerate logistic function is

$$\begin{aligned}]-\infty,z_k] &\to [0,1] \\ z &\mapsto 0 \end{aligned}$$

and in the latter case

$$\begin{aligned} [z_1,+\infty[&\to [0,1] \\ z &\mapsto 1. \end{aligned}$$

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