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ADMISSIBLE AND OPTIMAL CONFIDENCE BANDS IN SIMPLE LINEAR REGRESSION[1]

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A framework is presented for deciding among functional forms when constructing confidence bands in simple linear regression. Using the concept of tautness, definitions of admissibility and completeness are developed. These lead to a characterization of a minimal complete class of band forms. A type of average width optimality within this class is briefly discussed.

1. Introduction. Experimental situations can involve prediction of one variable from another. A common model is the simple linear regression $Y = \beta_0 + \beta_1 x + e$. Experimenters often express the need for a confidence region, as well as point estimates, of the mean value of Y given any value of x. The result is a band around the regression line, hence the term "confidence band." The first consideration of this problem was by Working and Hotelling (1929). They derived hyperbolic bands that extended over all values of x on the real line. Later, Scheffé (1953) was able to extend his results on multiple comparisons to the problem of banding a regression line.

Perhaps the most interesting concept to be considered within this framework has been the notion that the interests of the experimenter may not extend to all x in $\mathbf{R}$. By considering a subset of $\mathbf{R}$ over which to construct the band, a narrower band with the same coverage probability will result. Bohrer (1967) first considered the case of $x > 0$. Casella and Strawderman (1980) generalized the restriction problem by deriving a general class of restricted sets. They derived exact formulae for the coverage probability of bands restricted to any set in the class. Uusipaikka (1983) specialized this concept (in the simple linear setting) by considering unions of disjoint, closed intervals as the class of restricted sets.

The most widely considered restriction has been that of constraining x to lie in some interval, $[A, B]$, where A and B define the practical limits of the experiment. Gafarian (1964) produced bands of a fixed width around the regression line for the case $A = -B$. Bowden and Graybill (1966) extended Gafarian's results to the case of any $A \le B$, and also suggested bands of increasing or decreasing width. Other papers have updated the hyperbolic bands (Halperin, et al., 1967; Halperin and Gurian, 1968; Wynn and Bloomfield, 1971) by taking the interval restriction into account.

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In one important and recent piece, Naiman (1984) extended an early work of Hoel (1951) on optimality of certain forms over $[A, B]$. This involved the notion that prior interest in the width of the band can be consolidated into mathematical form (see Definition 4.2 of Section 4 herein). An experimenter interested in making more precise statements near $\bar{x}$ might consider the hyperbolic form, since it attains its minimum width at $\bar{x}$. In fact, Bohrer (1973) noted that, for the multilinear case, the hyperbolic bands also minimize average width (with respect to Lebesgue measure) over ellipsoids when no intercept is included in the model. Naiman (1984) showed that the hyperbolic forms are optimal against a bell-shaped function when the intercept is included, and that piecewise linear bands are optimal against discrete weight functions. In a related work, Naiman (1983) examined the differences between the hyperbolic and fixed-width forms. There, he derived conditions under which the hyperbolic forms dominate (in terms of average width), and showed that these conditions depend upon the size of $[A, B]$ relative to the experimental design.

The literature concerning confidence band construction under an interval restriction on the predictor variable is obviously quite diverse. Yet, with perhaps the exception of the works by Naiman (1983, 1984), very little has appeared in the way of developing a concise statistical decision theory for the selection and use of confidence bands in the interval setting. In Section 2, the basic notation for such a theory is developed in the simple linear setting. In Section 3, the notions of admissibility and completeness are presented, and a minimal complete class is constructed. In Section 4, Hoel's average width optimality is briefly explored.

2. General theory. Take n pairs of observations (t_i, y_i) under the simple linear model $Y_i = \beta_0 + \beta_1 t_i + e_i$. Given some design $\mathbf{x}$, suppose that the predictor variable is standardized, $t = (x - \bar{x})/s_x$. Take $E[\mathbf{e}] = \mathbf{0}$ and $\text{var}[\mathbf{e}] = \sigma^2\mathbf{I}$. Let $\hat{\beta}_0$, $\hat{\beta}_1$, and s be the usual least squares estimators of β_0, β_1, and σ. Denote $(\beta_j - \hat{\beta}_j)/s$ by w_j, $j = 0, 1$. A confidence band is the set of solution vectors to a set of inequalities

$$C_{\ell;A,B} = \{\mathbf{w}\colon |w_0 + w_1 t| \le k\ell(t)\ \forall t \text{ in } [A, B]\}. \tag{2.1}$$

For notational and geometric simplicity, consider the case of symmetric band form functions, $\ell(t) = \ell(-t)$, (or, in general, bands symmetric around $\bar{x}$) for all t of interest. Also, consider the balanced case $A = -B$ (the former assumption is common, while the latter is not restrictive, since the theory expounded below easily extends to any $A \le B$). Thus we shall write $C_{\ell;B}$ for $C_{\ell;A,B}$. Naiman (1983) and Piegorsch (1984b) show tha $C_{\ell;B}$ is a convex set in w-space, and go into greater detail on the characteristics of this set. Notice that it is the probability content of $C_{\ell;B}$ with respect to some distribution on $\mathbf{w}$, to which a $1 - \alpha$ probability constraint corresponds.

Interest in $\ell(t)$ is, of course, restricted to $[-B, B]$, but there can be interest in defining $\ell(t)$ outside of $[-B, B]$. In this balanced, symmetric setting, the question becomes one of specifying the extension to $\ell(t)$ on (B, ∞). To find the best extension, consider the concept of tautness (Wynn and Bloomfield, 1971):

DEFINITION 2.1. A band, $\phi(t)$, is taut if for any other band, $\psi(t)$, satisfying (i) $\psi(t) \le \phi(t)\ \forall t$, and (ii) the solution sets in w-space to $|w_0 + w_1 t| \le k\psi(t)$ and $|w_0 + w_1 t| \le k\phi(t)$ are equal, then $\phi \equiv \psi\ \forall t$.

A band that is not taut is termed *slack*. Given a symmetric band over $[-B, B]$, and two different forms for the extension of $\ell(t)$ to (B, ∞), the choice should be limited to the taut form (if it exists). Indeed, one does exist when ℓ is taut and it is presented here:

DEFINITION 2.2. For any symmetric band, $\ell(t)$, on $\mathbf{B} = [-B, B]$, the straight line extension (SLE) of $\ell(t)$ is the extension to $\mathbf{B}^c$ that consists of straight line bands connecting the opposite endpoints of the restricted band.

The SLE is uniquely defined by $\ell(B)$ and B:

$$\phi_{\ell;B}(t) = k\ell(t)I_{\mathbf{B}}(t) + k\ell(B)(|t|/B)I_{\mathbf{B}^c}(t), \tag{2.2}$$

(see Figure 1). The SLE is important for the following reason:

THEOREM 2.1. *Given a taut, symmetric band over* $[-B, B]$, (2.2) *defines a taut extension to* $\mathbf{R}$.

PROOF (Sketch). Proceed by contradiction: suppose there is another extension, ψ, with the same solution set as $\phi_{\ell;B}$, but with smaller width than $\phi_{\ell;B}$

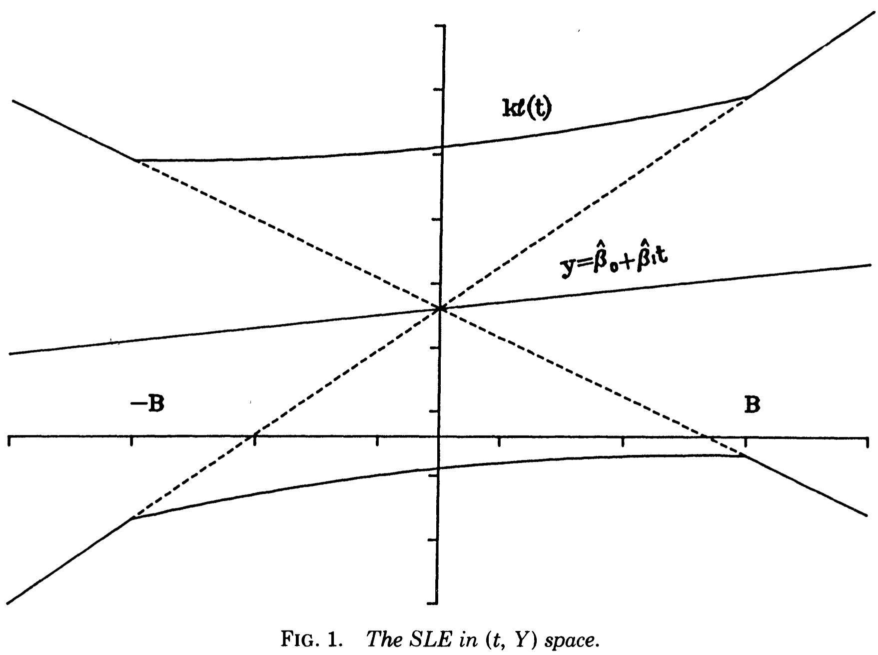

FIG. 1. *The SLE in* (t, Y) *space.*

outside of $[-B, B]$. Then, from Definition 2.1, one can show that the solution $(0, k\ell[B]/B)$ will be an element of the solution set for $\phi_{\ell;B}$, but not in the set for ψ. This is a contradiction.

3. Admissibility. Of major concern in this section will be the characterization of acceptable and unacceptable band forms. The SLE is formed by extending the diagonals of the region formed by the band (cf. Dunn, 1968, page 102). However, if $\ell(t)$ is too sharply convex, the SLE will suggest values of the parameters that will not exist in $C_{\ell;B}$. That is, one could find interior diagonals of the banded region from which to form a narrower, yet no less informative, extension. Obviously, these types of bands will not be acceptable since they will not be taut. (The interior diagonals can be used to construct a band with the same solution set, yet narrower.)

Before considering different ways to define this acceptability, a distinction among bands over varying $B > 0$ will be necessary.

DEFINITION 3.1. A band is a shape function, ℓ, defined on a fixed, given interval, $[-B, B]$.

DEFINITION 3.2. A band form is a function, ℓ, over $\mathbf{R}$.

When a band form is restricted to a particular interval, it becomes a band over that interval. As a concept, tautness is defined in terms of bands. A similar concept can be defined in terms of band forms:

DEFINITION 3.3. A symmetric band form, ℓ, is inadmissible if there is some band λ and some $B > 0$ such that (i) $C_{\ell;B} = C_{\lambda;B}$, (ii) $\lambda(t) \le \ell(t)\ \forall\, |t| \le B$, and (iii) there exists $|t'| \le B$ with $\lambda(t') < \ell(t')$.

When a band form is not inadmissible, it is *admissible*; i.e., admissibility is a uniform concept (a sort of tautness $\forall B > 0$). This leads to a number of important results regarding inadmissible band forms (notice that slackness implies inadmissibility). For some of these results the proof simply involves construction of a band that dominates the band of interest. The reader is referred to Piegorsch (1984a, Chapter II) for the details.

THEOREM 3.1. (i) *Discontinuous bands are slack.* (ii) *Any band that is not convex is slack.*

Theorem 3.1 suggests the need for the following specification of band forms:

DEFINITION 3.4. The class of all (symmetric) convex forms is

$$\Lambda_{\mathrm{CVX}} = \{\ell\colon \ell \text{ is continuous and convex on } [0, B],\ \forall B > 0\}.$$

Notice that elements of Λ_{CVX} need not be differentiable forms. Care is needed when making statements on derivatives of ℓ, since they needn't exist. To get around this, one can make limiting statements coming in from the left, i.e. $t \uparrow B$. This is used in the following subset of the convex forms:

DEFINITION 3.5. The class of restricted convex forms is

$$\Lambda^* = \{\ell \text{ in } \Lambda_{\mathrm{CVX}}\text{: } \lim_{t\uparrow B} \ell'(t) \le \ell(B)/B,\ \forall B > 0\}$$

Thus when ℓ is in Λ^*, it is rising no faster than a line (its SLE) at B, for any $B > 0$. This leads to the following, important result:

THEOREM 3.2. *A symmetric band form ℓ is admissible iff ℓ is an element of* Λ^*.

PROOF. See the appendix.

We can go on to specify the notion of complete classes:

DEFINITION 3.6. A class of band forms, Λ, is complete if, when ℓ is admissible, ℓ is an element of Λ.

DEFINITION 3.7. A complete class of band forms, Λ, is minimal when ℓ is admissible iff ℓ is contained in Λ.

Of major concern is the construction of a minimal complete class of band forms. An experimenter considering use of a confidence band over some interval would then have a sensible class of bands from which to choose. It is clear from Theorem 3.2 that Λ^* is minimal complete within the class of symmetric forms. That is, the (symmetric) minimal complete class is made up of those band forms which rise no faster than their linear extensions at every B. Similar results can be anticipated for the polynomial or multilinear cases in terms of polynomial or planar extensions. For the parabolic case, for instance, it can be shown that the admissible convex forms rise no faster than their quadratic extensions at any endpoint (Piegorsch, 1984a, Chapter V).

Theorem 3.2 easily extends from the balanced interval case to bands over any interval $[A, B]$.

DEFINITION 3.8. Define the class of band forms Λ^{**} as those continuous forms satisfying

(1) ℓ is convex on $\mathbf{R}^+$ and $\mathbf{R}^-$,
(2) $\lim_{t\uparrow B} \ell'(t) \le M$, and
(3) $\lim_{t\downarrow A} \ell'(t) \ge -M$,

where $M = [\ell(B) + \ell(A)]/(B - A)$, $(\forall A \le 0 \le B)$ is the slope of the SLE.

A referee has pointed out that Λ^{**} can be viewed as a collection of families of classes of *bands*, each family being indexed by the center of the interval $(A + B)/2$. Then, by simply extending the concepts in Theorem 3.2, it is relatively easy to show that Λ^{**} is minimal complete.

EXAMPLE 3.1. Fixed-width bands on $[-B, B]$ (Gafarian, 1964; Knafl, et al., 1985). Take $\ell(t) = 1$. Then $\ell'(t) = 0\ \forall t$ while $\ell(B)/B = 1/B > 0$. Thus ℓ is admissible.

EXAMPLE 3.2. Bowden (1970), and later Dalal (1983), gave the following form for a confidence band:

$$\ell(t) = (1 + |t|^p)^{1/p}. \tag{3.1}$$

For $p = 2$ this is the hyperbolic form given by Halperin, et al. (1967) over $[-B, B]$. For $p = 1$ it gives a linear segment form over $[-B, B]$ (Dunn, 1968), while for $p = \infty$ it is one of the piecewise linear forms suggested by Wynn (1984). When $p < 1$, $\ell''(t) < 0\ \forall t > 0$, so (3.1) gives a concave band on any interval $[0, B]$. Hence, from Theorem 3.1, (3.1) is inadmissible if $p < 1$. Now, for $p \geq 1$ consider the condition for restricted convexity: $\lim_{t\uparrow B}\ell'(t) = B^{p-1}(1 + B^p)^{-(p-1)/p}$. However, $\ell(B)/B = B^{-1}(1 + B^p)^{1/p}$. Then, ℓ is contained in Λ^* when

$$(1/B)B^p(1 + B^p)^{-1}(1 + B^p)^{1/p} \leq (1/B)(1 + B^p)^{1/p}.$$

or $B^p \leq 1 + B^p$. This is true for any $B > 0$. Summarizing then, Bowden's form for a confidence band is admissible iff $p \geq 1$.

EXAMPLE 3.3. The only example of an asymmetric band currently available in the literature is the Bowden-Graybill (1966) increasing width form:

$$\ell(t) = H(t - A)/(B - A) + \ell(A). \tag{3.2}$$

This can be specified as $\ell(A) = 1$ (so $\ell(B) = 1 + H$), with H as any positive constant. For decreasing width bands, simply choose $H < 0$. The band form is clearly convex over any $[A, B]$, so examine $\lim_{t\uparrow B}\ell'(t) = H/(B - A) = \lim_{t\downarrow A}\ell'(t)$. From Definition 3.8, $M = (2 + H)/(B - A)$ is certainly larger than $\lim_{t\uparrow B}\ell'(t)$ and $-\lim_{t\downarrow A}\ell'(t)$. Thus ℓ is contained in Λ^{**}.

4. Optimality within Λ^*. Up until now, admissibility was defined with an implicit assumption that the coverage probability, $1 - \alpha$, was fixed. Comparisons were limited to bands with a fixed $C_{\ell;B}$. Probability considerations were rare, since no restrictive assumptions were made on the distribution of $\mathbf{w}$. Indeed, the admissibility formulation is *distribution-free*. [Note that we implicitly supposed that the distribution of $\mathbf{e}$ was spherically symmetric, since we constructed the band symmetrically around $w_0 + w_1 t$ in (2.1). If we relaxed this assumption, and considered the asymmetric statement $k_1\ell_1(t) \leq w_0 + w_1 t \leq k_2\ell_2(t)$, an analog to Theorem 3.2 would be easy to develop.]

Comparisons with an eye towards optimality do, however, require probabilistic specifications. Within Λ^*, considerations of varying solution sets becomes critical in deciding among bands or band forms under a certain optimality criterion. One thing that must now be true is that $P[C_{\ell;B}] = 1 - \alpha$.

DEFINITION 4.1. $\Lambda^*(B; \alpha) = \{\ell \text{ in } \Lambda^*: P[C_{\ell;B}] = 1 - \alpha\}$.

With this, attention can be turned to optimality within Λ^*. For instance, consider Hoel's (1951) average weighted width. This criterion is tantamount to specifying a weight function, $\tau(t)$, and minimizing the weighted area of the resulting band.

DEFINITION 4.2. The average weighted width of a band over $[-B, B]$ with respect to a weighting measure $\tau = dT$ is

$$r_B(\ell, \tau) = \int_{-B}^{B} k\ell(t)\, dT(t), \tag{4.1}$$

where τ is normalized to unit measure (note that k may be absorbed into ℓ).

DEFINITION 4.3 (Naiman, 1984). A symmetric band, ℓ^*, over $[-B, B]$ is τ-optimal if it satisfies

$$r_B(\ell^*, \tau) = \inf_{\ell}\{r_B(\ell, \tau)\} \quad \forall B > 0, \tag{4.2}$$

where the infimum is taken over all ℓ in Λ^*.

The following theorem is simply a consequence of the fact that the elements of Λ^* are pointwise narrower than other forms with the same solution set (hence they have the same coverage probability with narrower width under any measure):

THEOREM 4.1. *$r_B(\ell, \tau) = \min_\lambda\{r_B(\lambda, \tau)\}$ implies that ℓ is in $\Lambda^*(B; \alpha)$, or there exists an L in $\Lambda^*(B; \alpha)$ such that $r_B(L, \tau) = r_B(\ell, \tau)$.*

Then, by varying B and α one can justify restricting ℓ to Λ^* in (4.2).

APPENDIX

PROOF OF THEOREM 3.2 (sufficiency). Proceed with a contrapositive argument: suppose ℓ is not restricted convex. Then there exists $B > 0$ such that $\lim_{t\uparrow B}\ell'(t) > \ell(B)/B$. This B is the point at which ℓ goes from acceptability to rising too quickly. See Figure 2. Now, ℓ is a convex function, thus continuous over $(0, B)$. The difference between $\ell(t)$ and the line connecting $(t, k\ell[t])$ with the origin has a left derivative at any t in $(0, B)$. As $t \to 0$, $\lim_{x\uparrow t}\ell'(x)$ approaches a finite value, $\lim_{x\uparrow 0}\ell'(x)$. However, the slope of this connecting line, $\ell(t)/t$, approaches ∞. Thus, as $t \to 0$, the left derivative (of this difference of functions), $\lim_{x\uparrow t}\ell'(x) - [\ell(t)/t]$, approaches $-\infty$. At B this difference is positive (since ℓ is not restricted convex). Thus, using Darboux's intermediate value theorem (Goldberg, 1976, Section 7.6) for (left) derivatives, there exists Γ in $(0, B)$ such that $\lim_{t\uparrow\Gamma}\ell'(t) = \ell(\Gamma)/\Gamma$. Then $y(t) = k\ell(\Gamma)t/\Gamma$ will be the interior diagonal that dominates $k\ell(t)$ on (Γ, B), but keeps $C_{\ell;B}$ intact. Thus, this is a better band with the same solution set, so ℓ is slack, hence inadmissible.

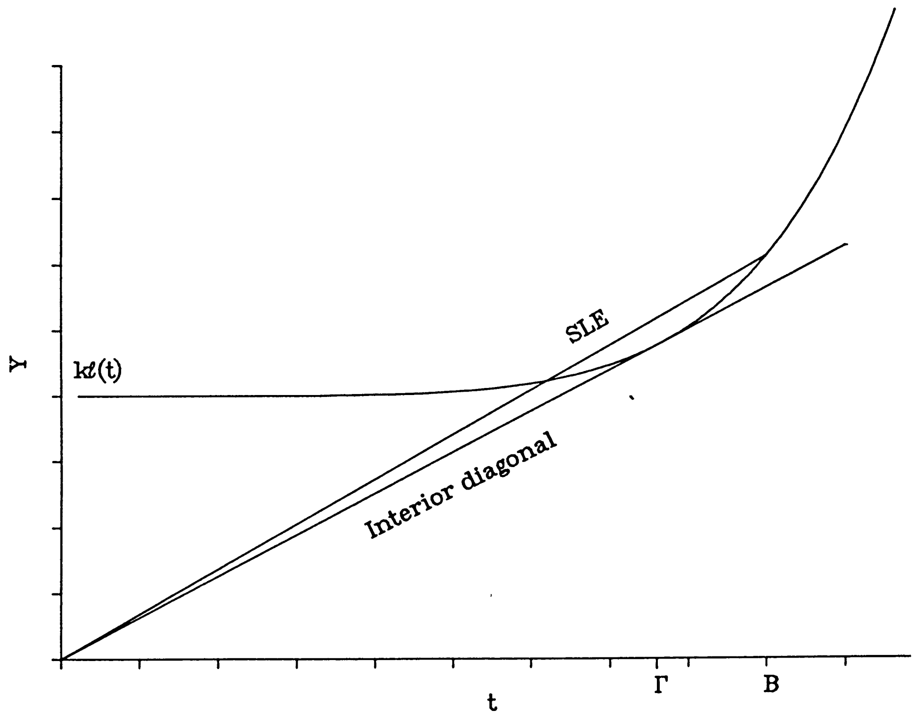

FIG. 2. *The interior diagonal and SLE for sufficiency in Theorem* 3.2.

(necessity). Again, prove the contrapositive. Let ℓ be inadmissible. Proceed by contradiction: let ℓ be restricted convex.

Since ℓ is inadmissible, there exists an admissible form λ in Λ_{CVX} such that, for some $B > 0$, (i) $C_{\ell;B} = C_{\lambda;B}$, (ii) $\lambda(t) \le \ell(t)\ \forall\, |t| \le B$, and (iii) there exists $\mathbf{H} = (h_1, h_2)$ such that $\lambda(t) < \ell(t)\ \forall t$ in (h_1, h_2) (the existence of $\mathbf{H}$ follows from the continuity of all forms in Λ_{CVX}). By symmetry of ℓ and λ, this holds on $(-h_2, -h_1)$ so suppose $h_1 > 0$.

Take the following two cases: (a) $h_2 = B$, (b) $h_2 < B$.

(a) If $h_2 = B$, $k\ell(B) > \lambda(B)$. Since λ is admissible, it is restricted convex (from the first part of this theorem). Thus the maximum slope corresponding to a point in $C_{\lambda;B}$ is $\le \lambda(B)/B$. But this is less than $k\ell(B)/B$. Thus $C_{\lambda;B}$ does not contain points with slopes corresponding to $k\ell(B)/B$. But ℓ is also restricted convex, so a similar argument shows that some points in $C_{\ell;B}$ do correspond to slopes equal to $k\ell(B)/B$. Hence $C_{\ell;B} \ne C_{\lambda;B}$, which contradicts (i).

(b) For $h_2 < B$, there exists h in $\mathbf{H}$ such that $\lambda(h) < k\ell(h)$. Construct the line $y(t) = k\ell'(h) \cdot (t - h) + k\ell(h)$, i.e., a line through the point $(h, k\ell[h])$ with slope $k\ell'(h)$. As Figure 3 shows, this solution cannot be in $C_{\lambda;B}$, since this line is above the band λ at h. This solution is wholly within the band ℓ over $[-B, B]$, so it is an element of $C_{\ell;B}$. Hence $C_{\ell;B} \ne C_{\lambda;B}$, again contradicting (i).

Thus in either of these mutually exclusive and exhaustive cases, (i) is contradicted. Hence ℓ cannot be restricted convex.

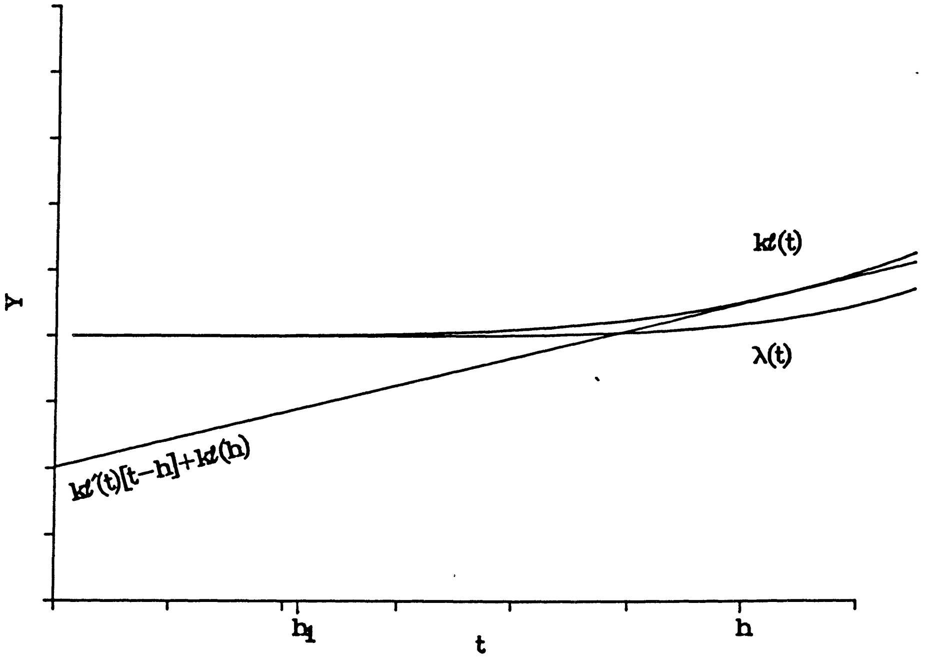

FIG. 3. *Necessity, case* (b), *in Theorem* 3.2.

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