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REGRESSION WITH GIVEN MARGINALS

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ABSTRACT

We consider the class of regression functions \( m(F, G) = \{ m(x) = E[Y | X = x], (X, Y) \in \Pi(F, G) \} \) where \( \Pi(F, G) \) denotes the set of random vectors with marginal distributions \( F \) and \( G \). A characterization of \( m(F, G) \) is given together with a representation for the projection operator it induces in an appropriate Hilbert space. Applications are indicated.

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1. Introduction

Let $\Pi(F, G)$ denote the class of random vectors $(X, Y)$ with marginal distributions $F$ and $G$ ($X \sim F$, $Y \sim G$). We will consider the associated class of regression functions

$$\mathcal{M}(F, G) = \{ m(x) = E[Y | X = x], (X, Y) \in \Pi(F, G) \}.$$  

The motivation for looking at this class is similar in spirit to that of isotonic regression (from which we will in fact borrow a result): the extent to which auxiliary information be incorporated into the regression process. Knowledge of marginal distributions, in particular, is natural in certain types of problems. We may consider a census in which bivariate observations are collected, the marginal distributions are assumed given (as from a previous survey), and regression is desired. Alternatively, there is the problem of optimal, non-linear prediction in a time series $\{X_t\}$. If $F$ is the equilibrium distribution of the $X_t$, then the optimal one-step predictor (squared error loss) is $E[X_{t+1} | X_t = x] \in \mathcal{M}(F, F)$ (see [3], [5], [6] for related discussions of this problem).

In section 2, we present a characterization of $\mathcal{M}(F, G)$ for a large class of $F$ and $G$. The proof follows directly
from methods in [10]. Characterizations of the type indicated have
been investigated from a variety of points of view and we refer the reader
to [7], [9] for other discussions and references. It can be fairly stated
that the common ancestor of all such approaches is the fertile theorem
of Hardy, Littlewood and Polya [4, p. 49] on the averaging properties
of doubly stochastic matrices. In section 3, we investigate further the
structure of \( \mathcal{M}(F, G) \) by considering it as a convex subset of an
appropriate Hilbert space and examining the induced projection operator.
The discussion is motivated by a statistical estimation problem.
2. Characterization of $\mathcal{m}(F, G)$

In what follows we shall regard $F$ and $G$ as fixed and satisfying

(A1) $F$ and $G$ are each supported on all of $\mathbb{R}^1$ and are invertible.

(A2) $\int_{-\infty}^{+\infty} y^2 G(dy) < \infty$.

The first assumption can be weakened considerably, but we present it to avoid side-issues. The second insures that $\mathcal{m}(F, G)$ is a subset of $L_2[(-\infty, +\infty); F]$, the Hilbert space of real-valued functions on $\mathbb{R}^1$ square integrable with respect to the measure determined by $F$ (this can be seen directly by noting $\int_{-\infty}^{+\infty} x(E[y|x])^2$).

Turning to the characterization of $\mathcal{m}(F, G)$, we note that if $m(x) = E[Y|X = x] \in \mathcal{m}(F, G)$, then with the application of marginal probability transformations $U = F(X), V = G(Y)$, we have $m(x) = E[G^{-1}(V)|U = F(x)]$, where $U$ and $V$ are each uniformly distributed on $[0, 1]$. This is essentially the object of study of [10] and with only minor modifications, the methods employed there yield the following result.

Theorem 1. The following statements are equivalent.

(i) $m \in \mathcal{m}(F, G)$.

(ii) $m$ lies in the closed convex hull $(L_2[(-\infty, +\infty); F])$ of functions of the form $G^{-1} \circ T \circ F$.

(iii) $\int_0^x m(F^{-1}(T(u)))du \geq \int_0^x G^{-1}(u)du$

for all $x \in [0, 1]$ (with equality at $x = 1$) and all $T \in \mathcal{J}$. 

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Here $\mathcal{J} = \{T : [0, 1] \to [0, 1] \text{ one-one, Borel-measurable, measure-preserving}\}$.

We note that if $m \circ F^{-1}$ is non-decreasing, then the strongest inequality in (iii) occurs upon taking $T(u) = u$, i.e.,

$$\int_0^x m(F^{-1}(u))du \geq \int_0^x G^{-1}(u)du.$$

The equality condition in (iii) amounts to

$$\int_{-\infty}^{+\infty} m(x)F(dx) = \int_{-\infty}^{+\infty} yG(dy)$$

or $E m(X) = EY$. Finally, for the projection problem it will be useful to note that the mapping $h \in L_2[(-\infty, +\infty); F] \to h \circ F^{-1} \in L_2[[0, 1]; \mu = \text{Lebesgue measure}]$ induces an isomorphism between the two spaces. The image $m_0$ of $m(F, G)$ under the mapping can be described as follows.

**Corollary.** The following are equivalent.

(i) $m_0 \in m_0$.

(ii) $m_0$ lies in the closed convex hull $(L_2[[0, 1]; \mu])$ of functions of the form $G^{-1} \circ T$.

(iii) $\int_0^x m_0(T(u))du \geq \int_0^x G^{-1}(u)du$

for all $x \in [0, 1]$ (with equality at $x = 1$) and all $T \in \mathcal{J}$.

**Proof.** Change of variables.

**Remark.** From (ii), it is evident that for each $T \in \mathcal{J}$, $m_0 \preceq m_0 \iff m_0 \circ T \in m_0$. 
3. **Projection**

Under the assumption \((X, Y) \sim \Pi(F, G)\), a natural criterion for judging an estimate \(\hat{m}(x)\) of the unknown regression function \(m(x)\) is the squared error loss

\[
E[ m(x) - \hat{m}(x) ]^2 = \int_{-\infty}^{+\infty} [ m(x) - \hat{m}(x) ]^2 F(dx) .
\]

It is evident that this loss can be reduced (or at least made no larger) by constructing a new estimate \(\tilde{m}(x)\) which is the projection of \(\hat{m}\) onto the convex \(\mathcal{M}(F, G)\). For this reason, it is of interest to investigate the projection operator associated with \(\mathcal{M}(F, G)\) in \(L^2_{\mathbb{R}}((-\infty, +\infty); F)\):

that is, for \(h \in L^2_{\mathbb{R}}((-\infty, +\infty); F)\), we seek the (unique) element \(\tilde{h} \in \mathcal{M}(F, G)\) which yields

\[
\int_{-\infty}^{+\infty} [ h(x) - \tilde{h}(x) ]^2 F(dx) = \inf_{m \in \mathcal{M}(F, G)} \int_{-\infty}^{+\infty} [ h(x) - m(x) ]^2 F(dx)
\]

(\(\tilde{\cdot}\) throughout will denote projection in the appropriate space). A feature of this projection is that if a constant is added to \(h\), then \(\tilde{h}\) remains the same: this can be seen by expanding

\[
\int_{-\infty}^{+\infty} [ h(x) + c - m(x) ]^2 F(dx) = \int_{-\infty}^{+\infty} [ h(x) - m(x) ]^2 F(dx) + c^2 + 2c \int_{-\infty}^{+\infty} h(x) F(dx) - 2c \int_{-\infty}^{+\infty} m(x) F(dx)
\]
and noting that the first term alone depends on \( m \) since, as we have noted, 
\[
\int_{-\infty}^{+\infty} m(x)F(dx) = \int_{-\infty}^{+\infty} yG(dy)
\]
for \( m \in \mathcal{M}(F, G) \). This being the case, we shall have occasion to invoke the normalization
\[
(A3) \quad \int_{-\infty}^{+\infty} h(x)F(dx) = \int_{-\infty}^{+\infty} yG(dy)
\]
and, equivalently, for \( t = h \circ F^{-1} \)
\[
(A3)' \quad \int_{0}^{1} t(u)du = \int_{0}^{1} G^{-1}(u)du.
\]

We now investigate the projection operator, isolating the main aspects of the argument in two lemmas. Some notation will prove to be convenient: let \( I(x) = \int_{0}^{x} G^{-1}(u)du \) and let capitalization generally indicate integration, e.g. \( L(x) = \int_{0}^{x} t(u)du \). If \( A(x) \in \mathcal{C}[0, 1] \), then denote by \( A^*(x) \) the convex minorant of \( A \) (i.e. the greatest convex function less than or equal to \( A \)).

**Lemma.** Let \( t \in L_{2}([0, 1]; \mu) \) be non-decreasing (a.e.) and satisfy \((A3)'\).

The projection \( \tilde{t} \) of \( t \) onto \( \mathcal{M}_0 \) satisfies
\[
\tilde{L}(x) = \int_{0}^{x} \tilde{t}(u)du = L(x) - (L - 1)^*(x).
\]

**Proof.** The proof will be given first for step functions and then extended.

(I) For a fixed integer \( N \geq 1 \), suppose that \( t \) is of the form
\[
t(u) = \sum_{j=0}^{N-1} t(j \langle x_j, x_{j+1} \rangle(u), \quad x_j = \frac{j}{N}, \quad \ell \leq \ell_{j+1}.
\]
We argue first that it is enough to restrict attention to candidates for projection which are similarly non-decreasing step functions: given \( n \in \mathcal{M}_0 \), we apply the Cauchy-Schwarz inequality to get

\[
\frac{1}{N} \sum_{j=0}^{N-1} \int_{x_j}^{x_{j+1}} \left( t(u) - n(u) \right)^2 \, du \geq \frac{1}{N} \int_{0}^{1} \left( t(u) - n_i(u) \right)^2 \, du
\]

where \( n_j = \frac{1}{N} \int_{x_j}^{x_{j+1}} n(u) \, du \). The lower bound is attained for \( n(u) \) identically constant on sub-intervals. Moreover, it can further be reduced by rearranging the \( n_j \) to be non-decreasing ([4, theorem 378]).

If \( n_j(T) \) are the rearranged values, then we have

\[
\frac{1}{N} \sum_{j=0}^{N-1} \int_{x_j}^{x_{j+1}} \left( t(u) - n(u) \right)^2 \, du \geq \frac{1}{N} \int_{0}^{1} \left( t(u) - n_j(T)(u) \right)^2 \, du
\]

where \( n_j(T)(u) = \sum_{j=0}^{N-1} n_j(T)(x_j, x_{j+1})(u) \). We now show that \( n_j(T)(u) \in \mathcal{M}_0 \).

Since \( n_j(T)(u) \) is non-decreasing (a.e.), by the remark after theorem 1, it is enough to show that \( N(T)(x) = \int_{0}^{x} n_{j}(T)(u) \, du \geq I(x) \) with equality at \( x = 1 \). The latter condition follows from the normalization (A3).'

Since \( I(x) \) is convex and \( N(T)(x) \) is piece-wise linear, it is enough to verify the inequality constraints at the nodes \( \{x_j\} \). We have

\[
N(T)(x_k) = \int_{0}^{x_k} n(T)(u) \, du = \frac{1}{N} \sum_{j=0}^{k-1} n_j(T), \text{ which is the integral of } n(u)
\]

over \( k \) of the sub-intervals. Equivalently, it is equal to \( \int_{0}^{x_k} n(T)(u) \, du \).
for some $T$ which appropriately permutes the sub-intervals. By (ii) of the corollary, this is bounded from below by $I(x_k)$.

We now have a discrete problem to solve:

$$\text{minimize } \sum_{j=0}^{N-1} (t_j - n_j)^2$$

subject to (a) the $n_j$ are non-decreasing,

$$\sum_{j=0}^{k-1} n_j \geq I(x_{k-1}), \quad k = 1, \ldots, N-1 \text{ with equality at } k = N.$$ 

Imposing only constraint (b), the problem is treated in [1, pp. 46-51] as a generalized isotonic regression. Letting $L$ and $\tilde{L}$ denote the partial sum vectors of $l$ and the solution vector $\tilde{l}$ respectively and setting $I = (I(x_1), I(x_2), \ldots, I(x_N))$, we have

$$\tilde{L} = L - (L - I)^*$$

where $^*$ here denotes the convex minorant of a vector. A straightforward argument shows that $\Delta_k^2 (L - I)^* \leq \Delta_k^2 (L - I)$ ($\Delta_k^2$ denoting a second difference). Hence

$$\Delta_k^2 \tilde{L} = \Delta_k^2 [L - (L - I)^*] = \Delta_k^2 L - \Delta_k^2 (L - I)^* \geq \Delta_k^2 I \geq 0 .$$

It follows that $\tilde{L}$ is convex and that $\tilde{l}$ is non-decreasing. Thus (a) is satisfied automatically.

Translating the solution of the discrete problem into step function terms, we get $\tilde{L}(x) = L(x) - (L - I)^*(x)$. 

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(II) If $f(u)$ is not a step function, then for each $N \geq 1$, approximate $f(u)$ with

$$I_N(u) = \sum_{j=0}^{N-1} \left[ N \int_{x_j}^{x_{j+1}} f(u) \, du \right] I_{[x_j, x_{j+1}]}(u).$$

By (I), we have

$$\tilde{I}_N(x) = I_N(x) - (I_N - 1) \ast (I_N - 1).$$

Now as $N \to \infty$, $I_N \to I$ and $\tilde{I}_N \to \tilde{I}$ in $L^2([0,1];\mu)$. Since

$$\int_0^x I_N(u) \, du \leq \int_0^x I_N(u) \, du + \int_0^x I_2(u) \, du,$$ the dominated convergence theorem yields $I_N(x) \to I(x)$. Similarly, $\tilde{I}_N(x) \to \tilde{I}(x)$. Further, since $L_N \to L$ uniformly and $\ast$ operates continuously in the uniform norm, $(L_N - 1) \ast (L - 1)$. Taking limits $(N \to \infty)$ in (1) yields the lemma.

If $f$ is not monotone, then some additional preparation is required to obtain its projection on $\mathcal{P}_0$. For $f \in L^2\left([0,1];\mu\right)$, define

$$f_\uparrow \in L^2\left([0,1];\mu\right)$$

as the increasing rearrangement of $f$. There exists a measure-preserving transformation $S_\uparrow : [0,1] \to [0,1]$, not necessarily one-one, such that $f = f_\uparrow \ast S_\uparrow$. ([8])

**Lemma.** Let $f \in L^2\left([0,1];\mu\right)$ and satisfy (A3)''. Then if $f$ and $\tilde{f}_\uparrow$ are the projections of $f$ and $f_\uparrow$, respectively onto $\mathcal{P}_0$,

$$\tilde{f} = \tilde{f}_\uparrow \ast S_\uparrow.$$

**Remark.** The construction for $\tilde{f}_\uparrow$ has been given in the previous lemma.

**Proof.** If $f \in L^2\left([0,1];\mu\right)$, then $f_\uparrow \in L^2\left([0,1];\mu\right)$. Using a change of
variables, we have

\[ \int_0^1 [I, (u) - g(u)]^2 du = \int_0^1 [I(u) - (g \circ S_t)(u)]^2 du \]

and taking infima over \( g \in \mathcal{M}_0 \)

\[ \int_0^1 [I, (u) - I_t(u)]^2 du = \inf_{g \in \mathcal{M}_0} \int_0^1 [I(u) - (g \circ S_t)(u)]^2 du \]

\[ = \int_0^1 [I(u) - (\tilde{I}_t \circ S_t)(u)]^2 du. \]

The lemma will follow if we can show

(i) \( \inf_{g \in \mathcal{M}_0} \int_0^1 [I(u) - (g \circ S_t)(u)]^2 du = \inf_{g \in \mathcal{M}_0} \int_0^1 [I(u) - g(u)]^2 du \)

and

(ii) \( \tilde{I}_t \circ S_t \in \mathcal{M}_0. \)

Each is a consequence of the identity \( \mathcal{M}_0 \circ S_t = \mathcal{M}_0, \) that is,

\( g \circ S_t \in \mathcal{M}_0 \Longleftrightarrow g \in \mathcal{M}_0. \) The point of interest is that \( S_t \) may not be one-one.

However, Brown [2, theorem 3] has shown that there exists a sequence \( \{T_n\} \subseteq \mathcal{J} \) such that \( g \circ T_n \to g \circ S_t. \) Accordingly, if \( g \in \mathcal{M}_0, \) then \( g \circ T_n \in \mathcal{M}_0 \) (see the remark after the corollary of section 1) and since \( \mathcal{M}_0 \) is closed \( \lim_{n \to \infty} g \circ T_n = g \circ S_t \in \mathcal{M}_0. \) Conversely, if \( g \circ S_t \in \mathcal{M}_0, \)

then using an approximating sequence \( \{T_n\} \)

\[ \|g \circ S_t - g \circ T_n\|_{L^2([0,1];\mu)} = \|g \circ S_t \circ T_n^{-1} - g\|_{L^2([0,1];\mu)} \to 0. \]
Since \( g \circ S_t \circ T_n^{-1} \) for each \( n \) and \( m_0 \) is closed, we have \( g \in m_0 \).

We can now state our main result.

**Theorem 2.** Let \( h \in L_2([-\infty, +\infty);F] \) and satisfy (A3). Let \((h \circ F^{-1})_+\) be the increasing rearrangement of \( h \circ F^{-1} \) with \( h \circ F^{-1} = (h \circ F^{-1})_+ \circ S \).

Then the projection \( h \) of \( h \) onto \( m(F, G) \) is given by

\[
\tilde{h} = (h \circ F^{-1})_+ \circ S \circ F
\]

where \((h \circ F^{-1})_+\) satisfies

\[
\int_0^x (h \circ F^{-1})_+(u) du = J_1(x) - J_2(x)
\]

and \( J_1(x) = \int_0^x (h \circ F^{-1})_+(u) du, \ J_2(x) = J_1(x) - \int_0^x G^{-1}(u) du \).

**Proof.** Together with the indicated isomorphism between \( L_2([0, 1];\mu] \) and \( L_2([-\infty, +\infty);F] \), the statement combines the two lemmas.
4. **Concluding Remarks**

We have investigated the structure of $\mathcal{M}(F, G)$ through a characterization result and an examination of the induced projection operator. Despite the rather formidable description of the latter, computational versions have proved to be accessible. In particular, the operations $\ast$ and $\dagger$ together with the extraction of the measure-preserving transformation $S$ are reasonably straightforward (a discussion of some relevant algorithms can be found in [1]).

As in isotonic regression, the fact that analytical resources are available to attack the problem investigated here suggests that other nonlinear regression problems may be amenable to similar treatment.
REFERENCES


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