Optimal prior-free probabilistic variable selection in Gaussian linear regression

Ryan Martin,∗ Huiping Xu,† Zuoyi Zhang,‡ and Chuanhai Liu§

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Abstract

Model selection is fundamental to scientific discovery, but a general framework that gives valid prior-free probabilistic assessments of the quality of individual models remains to be worked out. In this paper, we propose an inferential model (IM) approach to accomplish this for the special case of variable selection in a full-rank Gaussian linear regression model. This proposal is based on the notion of simultaneously valid inference for a collection of assertions of interest, and we develop some general results and characterizations of the corresponding optimal predictive random sets. An interesting and important by-product of our IM approach is that the resulting validity holds when the IM is projected down to a sub-model, even if that sub-model is selected by the data. In other words, the proposed IM approach automatically gives valid post-selection inference. An IM-driven variable selection procedure is proposed, and are shown to compare favorably to existing methods based on real- and simulated-data examples.

Keywords and phrases: Belief; inferential model; plausibility; post-selection inference; predictive random set; validity.

1 Introduction

Linear regression is arguably one of the most widely used statistical tools in scientific applications. It is standard practice to include as many variables as possible in the planning stages, though likely only a small subset of these variables will be useful in explaining variation in the response variable. Since the inclusion of unimportant explanatory variables in the model generally increases prediction error and makes interpretation of the results more difficult, the variable selection problem—selecting a good subset of explanatory variables—is of fundamental importance. [Kadane and Lazar (2004)] go so far as to say that variable selection is “central to the pursuit of science in general.”

∗Department of Mathematics, Statistics, and Computer Science, University of Illinois at Chicago, email: rgmartin@uic.edu
†Department of Biostatistics, The Richard M. Fairbanks School of Public Health and School of Medicine, Indiana University, email: huipxu@iu.edu
‡Regenstrief Institute, Inc., email: zyizhang@indiana.edu
§Department of Statistics, Purdue University, email: chuanhai@purdue.edu
Given the importance of the variable selection problem, it is no surprise that there are many proposed methods to solve it. In general, difficulty arises because comparison of models, or subsets of variables, based on likelihood alone will always suggest selection of all the variables. To overcome this limitation, it is now standard to adjust the likelihood by adding some kind of penalty term that depends on the number of variables included in the model. The most well-known of these methods are the Akaike information criterion (AIC, Akaike 1973) and the Bayesian information criterion (BIC, Schwarz 1978), with the latter imposing a more severe penalty on the number of variables. These methods allow for a ranking of candidate models and, if a single model is required, one can naturally choose the one with highest rank based on AIC, BIC, etc. Despite the certain large-sample variable selection consistency properties of these methods, a shortcoming remains in finite-samples, namely, that the rankings these criteria provide have no inferential meaning. For example, if Model 1 has higher AIC or BIC ranking than Model 2, then we cannot conclude that Model 1 being the correct model is any more plausible than Model 2 being the correct model. In other words, these selection criteria provide no inferentially meaningful measure of the uncertainty that the selected model is correct. Lasso (Tibshirani 1996, 2011) and its variants, including adaptive lasso (Zou 2006) and elastic net (Zou and Hastie 2005), all nicely summarized in Hastie et al. (2009), are useful tools for variable selection, but they too provide no inferentially meaningful measure of uncertainty. And significance tests based on the lasso estimator (e.g., Lockhart et al. 2014) do not resolve the problem.

Bayesian methods, on the other hand, are able to produce measures of uncertainty concerning the candidate models; see, for example, Clyde and George (2004). With the introduction of a prior distribution for the set of possible models and a conditional prior distribution of the model parameters, Markov Chain Monte Carlo methods are available to search the model space for those with high posterior probability. Unfortunately, prior specification and posterior computation remain a challenging problem, especially when the model space is large. Furthermore, the posterior model probability estimates may become less reliable for large $p$ (Heaton and Scott 2010), in which case, it is not clear if the most probable model has been identified.

In this paper, we consider a new perspective. There is now a trend to look beyond the classical frequentist and Bayesian schools for new solutions to challenging problems. See, for example, recent work on generalized fiducial inference (Hannig 2009, 2013; Hannig and Lee 2009; Lai et al. 2013), confidence distributions (Xie and Singh 2013; Xie et al. 2011), Dempster–Shafer theory (Dempster 2008; Shafer 2011), and objective Bayes with default, reference, and data-dependent priors (Berger 2006; Berger et al. 2009; Fraser 2011; Fraser et al. 2010; Martin et al. 2014). Our focus is on the new inferential model (IM) framework of Martin and Liu (2013b). The key feature of this approach is that, for any assertion/hypothesis about the unknown parameter, it produces a meaningful prior-free, probabilistic summary of the evidence in data for/against the assertion. These summaries are also properly calibrated for easy interpretation across users and experiments. Consequently, one can easily develop procedures based on these summaries, known as the plausibilities, with guaranteed frequentist error rates. What distinguishes IMs is the use of suitable random sets to predict the unobservable auxiliary variable associated with observed data and unknown parameter. These statements will be made precise in Section 2, where we review IMs in the regression setting.
Some preliminary work on IMs for inference in the regression problem is presented in Zhang et al. (2011). The main contributions here are two-fold: first we provide a theoretical development of optimal IMs for the case of multiple simultaneous assertions, and apply that theory to the problem of variable selection in regression. The starting point is the classification of a particular assertion as simple or complex. For simple assertions, an optimal IM is readily available; see Section 3.2. For complex assertions, however, more work is needed. In Section 3.3, we identify the general shape of the optimal predictive random sets for complex assertions. The variable selection problem is particularly challenging because it involves simultaneous consideration of a collection of complex assertions. In Section 3.4, we extend the general shape result from one complex assertion to several simultaneous complex assertions. Balance conditions discussed in Section 3.5 are needed to distinguish the particular shape of the optimal predictive random sets. These general results are applied to the variable selection problem in Section 4.1, where we find that a hyper-cube predictive random set is optimal. An interesting and important by-product of this result, discussed in Section 4.2, is that one can naively project the IM for the full model down to a sub-model and retain validity, even if the choice of sub-model depends on data. That is, the proposed IM approach automatically handles the problem of post-selection inference and, in fact, it reproduces the “POSI” methods proposed recently in Berk et al. (2013). Section 4.3 presents an IM-driven variable selection procedure, based on thresholding the IM’s plausibilities, that is shown to control family-wise error rate. Real and simulated data examples are presented in Section 5, and there it is shown that the IM procedure actually outperforms several standard methods, which suggests that by insisting we work with inferentially meaningful summaries does not mean we must sacrifice on efficiency. The paper concludes with a short discussion in Section 6; some technical details, including proofs, are deferred to Appendices A–B.

2 Inferential models for regression

2.1 Overview of IMs

The IM developments were motivated by the idea that statistical inference is more than just designing procedures with good properties. Instead, statistical inference should be about providing meaningful summaries of the evidence available in data about the truthfulness of various assertions of interest. Because the summaries are required to be meaningful, it is then possible, if desired, to derive procedures with good properties. In other words, having a procedure with good properties is a necessary but not sufficient condition for good statistical inference. The IM approach, described below, provides such valid probabilistic summaries for any assertion/hypothesis under minimal conditions. Our focus here is on how to specify the ingredients for constructing the IM, in particular, the random sets, so that the summaries are also efficient. From these valid and efficient summaries, it will be easy to derive procedures with good properties. For more on IM foundations, see Martin and Liu (2014a) and Liu and Martin (2015).
2.2 Setup and a baseline association

To set notation, consider the following specification of the linear regression model:

\[ Y = X\beta + \sigma Z, \]  

(1)

where \( Y = (Y_1, \ldots, Y_n)^\top \) is an \( n \)-vector of response variables, \( X \) is an \( n \times p \) matrix of predictor variables, \( \beta = (\beta_1, \ldots, \beta_p)^\top \) is a \( p \)-vector of regression coefficients, \( \sigma^2 \) is the residual variance, and \( Z = (Z_1, \ldots, Z_n)^\top \) is an \( n \)-vector of standard Gaussian errors, i.e., \( Z \sim N_n(0, I_n) \), a \( n \)-dimensional Gaussian distribution with mean zero and identity covariance matrix. We assume that \( p < n \) and that \( X \) is fixed with non-singular \( X^\top X \).

Without loss of generality, we will assume that \( Y \) and the columns of \( X \) have been centered, so that we can ignore the intercept term.

In the IM framework, we refer to (1) as a baseline association between observable data \( Y \) (and \( X \)), unknown parameters \( \lambda = (\beta, \sigma) \), and unobservable auxiliary variables \( Z \). The importance of such an association can be seen as follows: if \( Z \) could be observed, then we could exactly solve (1) for \( \lambda \), leading to the “best possible inference.” Since \( Z \) cannot be observed, the next best thing would be to accurately predict the unobservable \( Z \); see Section 2.4. It is intuitively clear that accurately predicting a high-dimensional quantity is more difficult than predicting a lower-dimensional quantity. Therefore, it is advantageous to reduce the dimension of the auxiliary variable as much as possible before carrying out the prediction step.

2.3 Auxiliary variable dimension reduction

Martin and Liu (2015a,b) discuss two distinct approaches for reducing the dimension of the auxiliary variable. The first is an approach based on conditioning, which is particularly useful in cases where the auxiliary variable is of higher dimension than the parameter. For example, in our regression problem, \( Z \) is \( n \)-dimensional while \( \lambda \) is \((p + 1)\)-dimensional, and \( p + 1 \leq n \). Since the regression problem admits a \((p + 1)\)-dimensional minimal sufficient statistic, the IM dimension reduction is straightforward. Let \( \hat{\beta} \) be the least-squares estimator of \( \beta \), and \( \hat{\sigma} \) the corresponding estimator of \( \sigma \) based on the residual sum of squares. Then \((\hat{\beta}, \hat{\sigma})\) is a joint minimal sufficient statistic for \((\beta, \sigma)\), and we can identify a lower-dimensional (conditional) association:

\[ \hat{\beta} = \beta + \sigma V_1 \quad \text{and} \quad \hat{\sigma} = \sigma V_2 \]  

(2)

where \( V = (V_1, V_2) \) satisfies \( V_1 \sim N_p(0, M) \) and \( (n - p - 1)V_2^2 \sim \text{ChiSq}(n - p - 1) \), independent, where \( M = (X^\top X)^{-1} \). The key point is that we have replaced the \( n \)-dimensional auxiliary variable \( Z \) with a \((p + 1)\)-dimensional auxiliary variable \( V \). This reduction in dimension will help to simply the task of accurate prediction of the auxiliary variable.

Here, as is typical in regression applications, interest is in the regression coefficients, \( \beta \), and not in the error variance, \( \sigma^2 \). For such cases, it is possible to further reduce the dimension of the auxiliary variable via marginalization. Note that the (conditional) association (2) can be rewritten as

\[ \hat{\beta} = \beta + \hat{\sigma}(V_1/V_2) \quad \text{and} \quad \hat{\sigma} = \sigma V_2. \]
The general theory in Martin and Liu (2015b) says that the second equation above—the one that is free of \( \beta \)—can be ignored. This leaves a marginal association involving a \( p \)-dimensional auxiliary variable \( W = V_1/V_2 \). That is,
\[
\hat{\beta} = \beta + \hat{\sigma}W, \quad W \sim t_p(0, M; n - p - 1), \tag{3}
\]
where the auxiliary variable distribution is a \( p \)-dimensional Student-t, with \( n - p - 1 \) degrees of freedom, centered at the origin, with scale matrix \( M = (X^T X)^{-1} \). Again, the important point is that the \((p+1)\)-dimensional auxiliary variable in (2) has been replaced by a \( p \)-dimensional auxiliary variable \( W \). No further dimension reduction is possible, and we take (3) as our starting point for constructing an IM for inference on \( \beta \).

### 2.4 IM construction

It will be convenient to rewrite the (marginal) association (3) once more. Let \( D \) be a diagonal \( p \times p \) matrix with the same diagonal as \( M \). Then consider the association
\[
\hat{\theta} = \theta + \hat{\sigma}U, \tag{4}
\]
where \( \theta = D^{-1/2} \beta \), \( \hat{\theta} = D^{-1/2} \hat{\beta} \), and \( U = D^{-1/2}W \). After this transformation, the new auxiliary variable \( U \) has a \( t_p(0, L; n - p - 1) \) distribution, where \( L = D^{-1/2} MD^{-1/2} \). Note, in particular, that \( \theta_j = 0 \) if and only if \( \beta_j = 0 \), so the variable selection problem has not been changed; furthermore, the matrix \( L \) has all ones on the diagonal. For the dimension-reduced model in (4), the IM construction is as follows.

**A-step.** Associate data \( Y = y \) [or, equivalently, sufficient statistics \((\hat{\theta}, \hat{\sigma})\)] with unknown parameters \( \theta \) and auxiliary variable \( U \) as in (4). This defines a set—in this case, a singleton set—of parameter values indexed by particular values of \( U \), i.e.,
\[
\Theta_y(u) = \{ \theta : \hat{\theta} = \theta + \hat{\sigma}u \}, \quad u \in \mathbb{R}^p. \tag{5}
\]

**P-step.** Predict the unobservable auxiliary variable \( U \) with an admissible predictive random set \( \mathcal{S} \) with distribution \( P_{\mathcal{S}} \); see Section 2.5 below. This use of a random set is the chief novelty of the IM approach, and the focus of this paper is on choosing good predictive random sets for assertions relevant to variable selection.

**C-step.** Combine the results of the A- and P-steps to get
\[
\Theta_y(\mathcal{S}) = \bigcup_{u \in \mathcal{S}} \Theta_y(u).
\]

Since \( \mathcal{S} \) is a random set, so is \( \Theta_y(\mathcal{S}) \). Probabilities associated with this random set are then used to summarize uncertainty about the unknown parameter. Assume \( \mathcal{S} \) is such that \( \Theta_y(\mathcal{S}) \neq \emptyset \) with \( P_{\mathcal{S}} \)-probability 1 for all \( y \). Then, for a given assertion/hypothesis \( A \) about the unknown parameter \( \theta \), we calculate the belief function
\[
\text{bel}_y(A; \mathcal{S}) = P_{\mathcal{S}}\{\Theta_y(\mathcal{S}) \subset A\}, \tag{6}
\]
the \( P_{\mathcal{S}} \)-probability that \( \Theta_y(\mathcal{S}) \) completely agrees with the assertion \( A \). If \( \Theta_y(\mathcal{S}) = \emptyset \) with positive \( P_{\mathcal{S}} \)-probability, then an adjustment to the formula (6) is needed.
and Liu (2012); we will not need such adjustments here. The other important quantity is the plausibility function

\[ \text{pl}_y(A; S) = 1 - \text{bel}_y(A^c; S) = P_S(\Theta_y(S) \not\subset A^c), \]  

the \( P_S \)-probability that \( \Theta_y(S) \) at least partially agrees with \( A \). For given \( Y = y \), the output of the IM construction is the pair of functions \( (\text{bel}, \text{pl})_y \).

### 2.5 IM validity

The key to the success of the IM approach is an appropriate choice of the predictive random set \( S \) for \( U \) in the P-step. Validity is a first desirable property.

**Definition 1.** An IM is called **valid** if, for any assertion \( A \) about \( \theta \), the corresponding belief function satisfies

\[ \sup_{\theta \notin A} P_{Y|\theta, \sigma}(\text{bel}_Y(A; S) \geq 1 - \alpha) \leq \alpha, \quad \forall \alpha \in (0, 1). \]  

(8)

In other words, the IM is valid if, for any assertion \( A \), \( \text{bel}_Y(A; S) \) is stochastically no larger than \( \text{Unif}(0, 1) \) as a function of \( Y \) when \( A \) is false. In light of (7), validity can also be defined in terms of the plausibility function (Martin and Liu 2013b, Sec. 3.3).

Martin and Liu (2013b) showed that validity can be achieved under essentially no conditions on the model itself, provided the predictive random set \( S \) is admissible. To define this, let \( S \) be a collection of subsets of \( \mathbb{R}^p \), to be the support of the predictive random set \( S \); the individual sets in \( S \) are called focal elements.

**Definition 2.** A predictive random set \( S \), with distribution \( P_S \), is called **admissible** if the following two conditions hold:

(i) the support \( S \), which is assumed to contain \( \emptyset \) and \( \mathbb{R}^p \), is nested, that is, for any two focal elements \( S \) and \( S' \) in \( S \), either \( S \subseteq S' \) or \( S' \subseteq S \), and

(ii) the distribution \( P_S \) of \( S \) satisfies

\[ P_S(S \subset K) = \sup_{S \in S : S \subset K} P_U(S), \quad K \subseteq U. \]  

(9)

Molchanov (2005) is an excellent technical reference on random sets. In Appendix A below, we provide some general details about random sets, measurability of set-valued functions, and existence of a random set with distribution that satisfies (9).

Martin and Liu (2013b) showed that admissibility of \( S \) is sufficient for validity of the corresponding IM; see, also, Martin (2014). In general, there are many predictive random sets that give valid IMs. In that case, it is natural to look for a “best” one. These optimality considerations were first taken up in Martin and Liu (2013a, b). Our main contributions here is the development of optimal IMs for simultaneous inference on multiple assertions (Section 3) with an application to the important and challenging variable selection problem (Section 4).
3 Optimal IMs: some general theory

3.1 Preliminaries

Consider a general setup with association $X = a(\theta, U)$, where $X \in \mathbb{X}$ is the observable data, $\theta \in \Theta$ is the unknown parameter of interest, and $U$ is an unobservable auxiliary variable, with distribution $P_U$ defined on a space $\mathcal{U}$; see Appendix A.1. The corresponding sampling model is denoted by $P_{X|\theta}$. Fix an association, consisting of a relation $X = a(\theta, U)$ and a distribution $U \sim P_U$. Then, for a given assertion $A$ about $\theta$, an optimal predictive random set $S$, if it exists, makes the belief function $\text{bel}_X(A; S)$ stochastically as large as possible as a function of $X \sim P_{X|\theta}$, for all $\theta \in A$ (Martin and Liu 2013b). The following definition makes this formal.

Definition 3. For a given association and assertion $A$, if $S$ and $S'$ are two valid predictive random sets, then we say that $S$ is at least as efficient as $S'$ (with respect to $A$) if

$$\text{bel}_X(A; S) \geq \text{bel}_X(A; S'),$$

as a function of $X \sim P_{X|\theta}$, $\theta \in A$. (10)

A predictive random set $S$ is called optimal (with respect to $A$) if (10) holds for all valid predictive random sets $S'$.

The name “admissible” in Definition 2 actually comes from the admissibility result in Martin and Liu (2013b, Theorem 3): given any predictive random set $S'$, there exists an $S$ that satisfies the conditions in Definition 2 and is at least as efficient as $S'$.

3.2 Simple assertions

When the assertion $A$ is simple, in a sense to be described, it is possible to find an optimal predictive random set as in Definition 3. Define the $a$-event:

$$U_A(x) = \{u \in \mathcal{U} : \Theta_x(u) \subseteq A\}.$$ (11)

Some technical measurability conditions imposed on the $a$-events are discussed in Appendix A.2. An assertion $A$ is simple if the collection of $a$-events $U_A \equiv \{U_A(x) : x \in \mathbb{X}\}$ is nested; otherwise, the assertion is called complex (Section 3.3). The following proposition shows that, if $A$ is simple, then the optimal predictive random set (relative to $A$) obtains by taking the support $S = U_A$ and the distribution $P_S$ to satisfy (9).

Theorem 1. For a simple assertion $A$, the optimal predictive random set $S$ with respect to $A$ is supported on the nested collection $U_A$ with distribution satisfying (9).

Proof. See Appendix B.1.

As an example, consider $X \sim \mathcal{N}(\theta, 1)$, with association $X = \theta + U$, $U \sim \mathcal{N}(0, 1)$. The assertion $A = \{\theta > 0\}$ is simple. To see this, write the $a$-event:

$$U_A(x) = \{u : x = \theta + u \text{ for some } \theta > 0\} = (-\infty, x).$$

Then, clearly, if $x < x'$, then $U_A(x) \subseteq U_A(x')$; so, the $a$-events are nested. The belief function based on the optimal predictive random set $S$ in Theorem 1 is

$$\text{bel}_x(A; S) = P_S\{S \subseteq U_x(A)\} = P_U\{U_A(x)\} = \Phi(x),$$
where $\Phi$ is the standard normal distribution function. Given the optimality result, it is not a coincidence that $p_l(A; \mathcal{S}) = 1 - \Phi(x)$ is the p-value for the uniformly most powerful test of $H_0 : \theta \leq 0$ versus $H_1 : \theta > 0$; see Martin and Liu (2014b).

Unfortunately, simple assertions are insufficient for practical applications. For example, in the normal mean example above, we might be interested in the assertion $A = \{\theta \neq 0\}$ or, more generally, we might be interested in several assertions simultaneously, each of which might be simple or not. The regression problem features all of these cases. (More generally, even if there is only one assertion $A$, IM efficiency considerations require that one think about $A$ and $A^c$ simultaneously, so an understanding of how to handle multiple assertions is fundamental.) The next two sections discuss how to extend the basic optimality results to these important more general cases.

### 3.3 Complex assertions

To motivate our developments, reconsider the normal mean example above. This time, suppose we are interested in the assertion $A = \{\theta \neq 0\}$. This is a union of two disjoint simple assertions, namely, $A_1 = \{\theta < 0\}$ and $A_2 = \{\theta > 0\}$. The optimal predictive random set with respect to $A_1$ is efficient for $A_1$ but very inefficient for $A_2$; likewise, for the optimal predictive random set with respect to $A_2$. Since we are interested in $A_1 \cup A_2$ we require a predictive random set that is as efficient as possible for both $A_1$ and $A_2$. For the general case of a complex assertion written as a union of two simple assertions, an intuitively reasonable strategy is to consider a predictive random set whose focal elements are intersections of the focal elements of the optimal predictive random sets with respect to the two individual simple assertions. The following result says that the optimal predictive random set for the complex assertion must be of this form. (The results below extend to more than two simple component assertions, but two-component assertions are general enough for our purposes here.)

**Theorem 2.** Let $A = A_1 \cup A_2$ be a complex assertion, where $A_1$ and $A_2$ are simple assertions. Let $\mathcal{S}_1$ and $\mathcal{S}_2$ be the optimal predictive random sets for $A_1$ and $A_2$, respectively, as in Theorem 1. For any predictive random set $\mathcal{T}$, there exists an $\mathcal{S}$, whose focal elements are intersections of the focal elements of $\mathcal{S}_1$ and $\mathcal{S}_2$, such that $\mathcal{S}$ is at least as efficient as $\mathcal{T}$ with respect to $A$.

**Proof.** See Appendix B.2

This result simplifies the search for optimal predictive random sets with respect to a complex assertion. It does not completely resolve the problem, however, since there are many choices of predictive random sets with intersection focal elements. In the normal mean problem, for example, the focal elements for the optimal predictive random sets with respect to $A_1$ and $A_2$ are one-sided intervals. Therefore, the focal elements of the optimal predictive random set for $A = A_1 \cup A_2$ must be nested intervals, but it is not clear if the intervals should be symmetric or asymmetric. See Section 3.5.

### 3.4 Multiple complex assertions

Suppose there are multiple assertions, $\{A_j : j \in J\}$, to be considered simultaneously, where $A_j = A_{j1} \cup A_{j2}, j \in J$, decomposes as a union of two disjoint simple assertions.
Each simple component has an optimal predictive random set according to Theorem 1, and the corresponding optimal predictive random set, $S_j$, for the union $A_j$ has intersection focal elements according to Theorem 2. As before, intuition suggests that the optimal predictive random set for $\{A_j : j \in J\}$ would be supported on intersections of the focal elements for the individually optimal $S_j$, $j \in J$. To justify this intuition, we need a way to measure the efficiency of a predictive random set in this multiple-assertion context.

**Definition 4.** An assertion $A$ is generated by $\{A_j : j \in J\}$ if $A$ can be written as a union of some or all of the $A_j$s. Then a predictive random set $S$ is at least as efficient as $S'$ with respect to $\{A_j : j \in J\}$ if (10) holds for all $A$ generated by $\{A_j : j \in J\}$.

The following result, a generalization of Theorem 2, shows that a restriction to predictive random sets supported on intersection focal elements is without loss of efficiency.

**Theorem 3.** Let $\{A_j : j \in J\}$ be a collection of assertions, where $A_j = A_{j1} \cup A_{j2}$ partitions as a union of disjoint simple assertions. Let $S_j$ be the optimal predictive random set for $A_j$, $j \in J$. Then, for any predictive random set $T$, there exists an $S$, whose focal elements are intersections of the focal elements of the $S_j$s, such that $S$ is at least as efficient as $T$ with respect to $\{A_j : j \in J\}$.

**Proof.** See Appendix B.3.

As in the previous section, this result simplifies the search for an optimal predictive random set but does not completely resolve the problem. More on optimality for the multiple-assertion case is given in Section 3.5, and some specific details are given for the variable selection application in Section 4.

### 3.5 Balance and optimality

To resolve the ambiguity about the shape of the optimal focal elements, here we will make use of some special structure in the problem. Suppose that there exists transformations of $X$ that do not fundamentally change the inference problem. As a simple example, if $X \sim N(\theta, 1)$ and the association of interest is $A = \{\theta \neq 0\}$, then it is clear that changing the sign of $X$ should not have an impact on how much support there is for $A$. In other words, this normal mean problem is invariant to sign changes. More generally, let $G$ be a group of bijections $g$ from $X$ to itself; as is customary, we shall write $gx$ for the image of $x$ under $g$, rather than $g(x)$. Practically, the transformations in $G$ represent symmetries of the inference problem, i.e., nothing fundamental about the problem changes if $gX$ is observed instead of $X$. The key technical assumption here is that each $g$ commutes with the association mapping $a$, i.e.,

$$g a(\theta, u) = a(g\theta, gu), \quad \forall (\theta, u), \quad \forall g \in G.$$  

(12)

Here we are implicitly assuming that $G$ also acts upon the parameter space $\Theta$ and the auxiliary variable space $U$. This can be relaxed by introducing groups acting on $\Theta$ and $U$, respectively, different from (but homomorphic to) $G$, but for our variable selection application, where the “signed permutation group” acts on both $\Theta$ and $U$ directly, we will not need this extra notational complexity. The above condition is different from that
which defines the usual group transformation models in that, in the right-hand side, $g$ also acts on $u$. In fact, our variable selection application will not fit the usual group transformation structure, unless the design is orthogonal.

We shall also require that the assertions respect these symmetries. Let $A$ be an assertion generated the collection $\{A_j : j \in J\}$ of complex assertions. Consider the subgroup of $\mathcal{G}$ to which $A$ is invariant, and write $\mathcal{G}_A = \{g \in \mathcal{G} : gA = A\}$. The intuition is that the inference problem for $\theta$, at least as it concerns the assertion $A$, is unchanged if the problem is transformed by $g \in \mathcal{G}_A$.

Before proceeding, it may help to see a simple example. Consider, again, the normal mean problem, with $X = \theta + U$, $U \sim N(0, 1)$, and assertion $A = \{\theta \neq 0\}$. Then changing the sign of $X$ will not affect the problem. So, we can take $\mathcal{G}$ to consist of the identity mapping and $x \mapsto -x$, and clearly (12) holds; also, $\mathcal{G}_A = \mathcal{G}$.

Moving on, recall the a-event $\mathcal{U}_A(x) = \{u : x = a(\theta, u)$ for some $\theta \in A\}$. In this case, an equivariance property follows immediately from the commutativity property (12):

$$\mathcal{U}_A(gx) = g\mathcal{U}_A(x), \quad \forall g \in \mathcal{G}_A.$$ 

That is, given $A$, transforming $x \to gx$, for $g \in \mathcal{G}_A$, and then solving for $u$ is equivalent to solving for $u$ with the given $x$ and then transforming $u \to gu$.

We now have the necessary structure to help specify an optimal predictive random set. It suffices to focus on predictive random sets which are admissible. So, let $\mathcal{S}$ be admissible and, for simplicity, suppose we can write the collection of closed nested focal elements as $\mathcal{S} = \{S_r : r \in [0, 1]\}$, where $r$ corresponds to the set’s $P_U$-probability; in particular, $P_U(S_r) = 1 - r$. Then we have the following useful representation.

**Lemma 1.** $P_{X|\theta}\{\text{bel}_X(A; \mathcal{S}) > 1 - r\} = P_{X|\theta}\{\mathcal{U}_A(X) \supset S_r\}$.

**Proof.** See Appendix A.4

From Lemma 1 and the equivariance property above, if $g \in \mathcal{G}_A$, then

$$P_{X|\theta}\{\text{bel}_{gX}(A; \mathcal{S}) > 1 - r\} = P_{X|\theta}\{\mathcal{U}_A(gX) \supset S_r\} = P_{X|\theta}\{\mathcal{U}_A(X) \supset g^{-1}S_r\}.$$

Since the understanding is that the inference problem, at least as it concerns the assertion $A$, is unchanged by transformations $X \to gX$ for $g \in \mathcal{G}_A$, it is reasonable to require that the distribution of $\text{bel}_X(A; \mathcal{S})$ be invariant to $\mathcal{G}_A$. The previous display reveals that the way to achieve belief function invariance is to require the focal elements of the predictive random set to be invariant to $\mathcal{G}$. This leads to the following notion of balance.

**Definition 5.** The predictive random set $\mathcal{S}$ is said to be balanced with respect to $A$ if each focal element $S \in \mathcal{S}$ satisfies $gS = S$ for all $g \in \mathcal{G}_A$. Moreover, $\mathcal{S}$ is said to be balanced if the aforementioned invariance holds for all $g \in \mathcal{G}$.

Balance itself is a reasonable property, given that the transformations are, by definition, irrelevant to the inference problem. It is also interesting and practically beneficial that balance can be checked without doing any probability calculations; however, the focal elements $\mathcal{S}$ and the transformations $\mathcal{G}$ depend on the model.

Beyond the intuitive appeal of balance, we claim that balance leads to a particular form of optimality. Recall that, for IM efficiency, the general goal is to choose the predictive random set to make the belief function stochastically large when the assertion is true. With this in mind, we propose the following notion of maximin optimality.
Definition 6. A predictive random set $S^*$, with focal elements $\{S^*_r : r \in [0,1]\}$, is maximin optimal if it maximizes

$$\min_{g \in \mathcal{F}_A} P_{X|\theta}\{\text{bel}_{gX}(A; S) > 1 - r\} \equiv \min_{g \in \mathcal{F}_A} P_{X|\theta}\{U_A(X) \supset g^{-1}S_r\}$$

over all admissible $S$ with focal elements $\{S_r : r \in [0,1]\}$, uniformly for all $A$ generated by $\{A_j : j \in J\}$, for all $\theta \in A$, and for all $r \in [0,1]$.

Theorem 4. If a predictive random set $S$ is balanced in the sense of Definition 3, then it is maximin optimal in the sense of Definition 6.

The main idea in the proof, presented in Appendix B.5, is the notion of the “core” $S^*$ of a given focal element $S$. In particular, $S^* = \bigcap_{\theta \in \mathcal{F}_A} gS$, and the proof relies on the fact that it is both balanced and contained in each $gS$.

4 Optimal IMs for variable selection

4.1 Variable selection assertions

Recall the dimension-reduced association $\hat{\theta} = \theta + \tilde{\sigma}U$ in (1), where $U$ is a $p$-vector distributed as $t_p(0,L,n-p-1)$, and $L$ is a matrix with ones on the diagonal. Recall that we have centered $Y$ and the columns of $X$ so there is no intercept term, i.e., all variables are subject to selection. That is, the goal is identify which of $\theta_1, \ldots, \theta_p$ are non-zero.

Consider the collection of complex assertions $A_j = \{\theta : \theta_j \neq 0\}$, $j = 1, \ldots, p$. Consider first a particular $A_j$. This can be written as $A_j = A_{j1} \cup A_{j2}$, where $A_{j1} = \{\theta : \theta_j < 0\}$ and $A_{j2} = \{\theta : \theta_j > 0\}$. We claim that these sub-assertions are both simple in the sense of Section 3.2. Take $A_{j1}$, for example. Then the corresponding $a$-event is

$$U_{A_{j1}}(y) = \{u : \hat{\theta} - \tilde{\sigma}u \in A_{j1}\} = \{u : u_j > T_j\},$$

where $T_j = \hat{\theta}_j/\tilde{\sigma}$. This $a$-event is nested because it shrinks and expands monotonically as a function of $T_j$. The same is true for $A_{j2}$ and for all the other $j = 1, \ldots, p$. Therefore, by Theorem 1, the optimal predictive random sets for the individual sub-assertions $A_{j1}$ and $A_{j2}$ are each supported on collections of half hyper-planes. Next, it follows from Theorem 2 that the optimal predictive random set $S_j$ for the complex assertion $A_j$ is supported on intersections of half hyper-planes, i.e., cylinders $\{u : a_j \leq u_j \leq b_j\}$. If we are considering $\{A_j : j = 1, \ldots, p\}$ simultaneously, then it follows from Theorem 3 that the optimal predictive random set is supported on boxes—intersections of $p$ marginal cylinders—in $\mathbb{R}^p$. The remaining question is what shape should the boxes be.

Towards optimality, we need to consider what transformations leave the variable selection problem invariant in the sense of Section 3.5. As in the simple normal mean example discussed previously, sign changes to coordinates of $\hat{\theta}$ are irrelevant. In addition, the labeling of the variables $j = 1, \ldots, p$ is arbitrary, so permutations of the variable labels are also irrelevant. This suggests we consider the group $\mathcal{G}$ of signed permutations; that is, each $g \in \mathcal{G}$ acts on a $p$-vector $x$ by matrix multiplication (on the left), where the matrix factors as a product of a diagonal matrix with $\pm 1$ on the diagonal and a permutation matrix. It is clear that the association commutes with $\mathcal{G}$ in the sense of
To be precise, one should first take the group as an action on the model for \((\hat{\theta}, \hat{\sigma})\), and then do the marginalization steps as discussed in Section 2.3 above. With the group \(\mathcal{G}\) specified, it is also clear what shape of boxes the optimal predictive random set should be supported on. According to Definition 5, a balanced predictive random set should have focal elements—in this case, shaped like boxes in \(\mathbb{R}^p\)—that are invariant to the transformations in \(\mathcal{G}\). The only such boxes are hyper-cubes centered at the origin.

Corollary 1. The admissible hyper-cube predictive random set \(\mathcal{S}\), given by

\[
\mathcal{S} = \{ u \in \mathbb{R}^p : \| u \|_\infty \leq \| U \|_\infty \}, \quad U \sim \mathcal{P}_{U} = \mathcal{t}_p(0, L; n - p - 1),
\]

is balanced in the sense of Definition 5 and maximin optimal for \(\{ A_j : j = 1, \ldots, p \}\) in the sense of Definition 6.

Besides the optimality properties, there are some computational advantages to the use of a hyper-cube predictive random set. Specifically, since the sides are parallel to the coordinate axes, it is straightforward to compute the belief function for various assertions related to variable selection. For example,

\[
\text{bel}_Y(A_j; \mathcal{S}) = P(U \{ \| U \|_\infty < |T_j| \}) = F(|T_j|),
\]

where \(F\) is the distribution function of \(\| U \|_\infty\), with \(U \sim \mathcal{t}_p(0, L; n - p - 1)\).

4.2 On post-selection inference

Using the balanced hyper-cube predictive random set \(\mathcal{S}\) in Corollary 1, we can construct a plausibility function for singletons \(\{\theta\}\):

\[
\text{pl}_Y(\{\theta\}; \mathcal{S}) = 1 - F(\| \hat{\sigma}^{-1}(\hat{\theta} - \theta) \|_\infty).
\]

Henceforth, we will drop the braces and write \(\text{pl}_Y(\theta; \mathcal{S})\) for \(\text{pl}_Y(\{\theta\}; \mathcal{S})\). This plausibility function satisfies \(\text{pl}_Y(\theta; \mathcal{S}) = 1\) and is decreasing in \(\theta\) away from \(\hat{\theta}\) with hyper-cube shaped contours. Consequently, by thresholding the plausibility function at level \(\alpha \in (0, 1)\), we obtain the plausibility region

\[
\{ \theta : \text{pl}_Y(\theta; \mathcal{S}) > \alpha \} = \{ \theta : F(\| \hat{\sigma}^{-1}(\hat{\theta} - \theta) \|_\infty) < 1 - \alpha \}.
\]

Since the predictive random set \(\mathcal{S}\) is admissible, it follows from the general theory in Martin and Liu (2013b) that the plausibility region above has nominal frequentist coverage \(1 - \alpha\). Moreover, the shape of these plausibility regions is a hyper-cube, with side lengths characterized by quantiles of the \(\ell_\infty\)-norm of multivariate Student-t random vectors.

A consequence of our focus on validity simultaneously across a collection of assertions is that a naive projection of these plausibility regions to any sub-model \(I \subseteq \{1, 2, \ldots, p\}\) gives a new hyper-cube plausibility region that also has nominal frequentist coverage. Since this conclusion holds for all \(I\), it also holds if \(I\) is chosen based on data. Such considerations are relevant in the context of post-selection inference. As Berk et al. (2013) argue, when data is used to select a model, then one cannot use the model-specific distribution theory for valid inference. This leads to the fundamental question of how to achieve valid inference when the model is chosen based on data. Berk et al. (2013)
propose a procedure they call “POSI” for valid post-selection inference, and it turns out that their procedure is identical to that obtained by naive projection of the above plausibility region to a sub-model selected by data. The take-away message is that, by insisting on valid probabilistic inference, IMs can automatically handle the challenging post-selection inference problem, further demonstrating their promise.

4.3 An IM-driven variable selection procedure

Section 4.1 shows how to optimally summarize the uncertainty in data concerning variable selection assertions. From this, it is possible to construct an IM-driven variable selection procedure with good properties. See Section 2.1.

To start, let $I \subseteq \{1, 2, \ldots, p\}$ be the collection of indices corresponding to the truly non-zero coefficients, i.e., $\theta_i \neq 0$ for all $i \in I$. Consider the assertion

$$B_I = \{I \subseteq I\} = \{\theta : \theta_{I^C} = 0\} = \{\theta : \theta_i = 0, \forall i \notin I\}.$$

Note that $B^c_I = \bigcup_{i \in I^C} A_i$, so this apparently new kind of assertion is still covered by the variable selection assertions $\{A_j : j = 1, \ldots, p\}$ from before. Using the optimal hyper-cube predictive random set $S$ in (13), we have

$$\operatorname{pl}_T(B_I; S) = \mathbb{P}_{U}\{\|U\|_\infty > \|T_{I^C}\|_\infty\} = 1 - F(\|T_{I^C}\|_\infty),$$

where $\|T_{I^C}\|_\infty = \max_{i \in I^C}|T_i|$. It is clear that, if $\theta_{I^C} = 0$, then $\|U\|_\infty$ is stochastically no smaller than $\|T_{I^C}\|_\infty$, which leads to the following basic calibration result.

**Lemma 2.** If $B_I$ is true, i.e., if $\theta_{I^C} = 0$, then $\operatorname{pl}_T(B_I; S)$, which depends on $T$ only through $T_{I^C}$, is stochastically no smaller than $\text{Unif}(0, 1)$.

Intuitively, a model or collection of variables $I$ has some support from data if $\operatorname{pl}_T(B_I; S)$ is not too small. In other words, good models are at least those which are “sufficiently plausible” given data, relative to the optimal IM. Following this idea, an IM-driven approach for variable selection would be to fix $\alpha \in (0, 1)$ and then pick the smallest collection $I$ such that $\operatorname{pl}_T(B_I; S) > \alpha$. That is, define

$$\hat{I}_\alpha(T) = \text{smallest set } I \text{ such that } \operatorname{pl}_T(B_I; S) > \alpha. \quad (14)$$

We claim that this IM-driven procedure controls the family-wise error rate at level $\alpha$ or, equivalently, it satisfies a certain “selection validity” property:

$$\mathbb{P}_{T|\mathcal{I}}\{\hat{I}_\alpha(T) \subseteq \mathcal{I}\} \geq 1 - \alpha, \quad \forall \mathcal{I} \subseteq \{1, 2, \ldots, p\}. \quad (15)$$

**Theorem 5.** The procedure (14) has the selection validity property (15).

**Proof.** $\operatorname{pl}_T(B_I; S) > \alpha$ implies $\hat{I}_\alpha(T) \subseteq \mathcal{I}$, so apply Lemma 2 \qed

To implement the above procedure, it is not necessary to evaluate the plausibility function at $B_I$ for each $I \subseteq \{1, 2, \ldots, p\}$. In fact, the plausibility depends on the value of $\|T_{I^C}\|_\infty$, so we only need to look at $p$ different models, based on a sorting of the t-statistics.
by their magnitude. Let \( \pi \) be a permutation that ranks the \( T \) values according to their magnitudes, i.e., \( |T_{\pi(1)}| < |T_{\pi(2)}| < \cdots < |T_{\pi(p)}| \), and then compute
\[
\eta(j) = 1 - F(|T_{\pi(j)}|), \quad j = 1, \ldots, p. \tag{16}
\]
Each \( \eta(j) \) represents a value of \( p_T(B_I; S) \), but it is important to be clear about which model \( I \) it corresponds to. To start, take \( \eta(p) \), corresponding to the largest value of \( |T| \). If \( \eta(p) \) is small, which means \( |T_{\pi(p)}| \) is rather large, then there is little evidence to support the null model with no variables. So, \( \eta(p) \) is the plausibility \( p_T(B_I; S) \) for the null model \( I = \emptyset \). In general, \( \eta(j) \) is the plausibility corresponding to the model that includes only the variables \( \pi^{-1}\{j + 1, \ldots, p\} \), \( j = 1, \ldots, p \); it is clear, both intuitively and from the formula, that the full model, with all variables included, will be assigned plausibility 1. Table 1 helps to make this clear. With this understanding, we can define the IM-based variable selection procedure as follows: set \( j^* = \max\{j : \eta(j) > \alpha\} \), and then get \( \hat{I}_\alpha(T) \) using the rule
\[
\hat{I}_\alpha(T) = \pi^{-1}\{j^* + 1, \ldots, p\}. \tag{17}
\]

Theorem 5 implies that this procedure will have the selection validity property, i.e., that it will control the family-wise error rate; see the bottom left panels in Figures 1–4.

5 Numerical results

5.1 Real data analysis

Consider the prostate cancer data analyzed previously by Tibshirani (1996) and others. This study examined the association between the prostate specific antigen (PSA) level and some clinical measures among men who were about to receive a radical prostatectomy. There were \( n = 97 \) men with \( p = 8 \) predictors, four of which, including cancer volume (lcavol), prostate weight (lweight), capsular penetration (lcp), and benign prostatic hyperplasia amount (lbph), were log transformed. The other four predictors were age, seminal vesical invasion (svi), Gleason score (gleason), and percentage Gleason scores 4 or 5 (pgg45). The response variable is the log transformed PSA level (lpsa).

Using the optimal predictive random set \( S \) in (13), we only need to compute the plausibility (16) for \( p = 8 \) models, which is shown in Table 1. Using the method described in Section 4.3 at the \( \alpha = 0.05 \) level, we see that \( j^* = 6 \) so, according to (17), variables lcavol and svi are selected; using the lasso, Tibshirani (1996) also selects the variable lweight. So, the IM selection is more conservative than lasso in this case, but lasso is known to be too aggressive in many cases, such as in Section 5.2.

5.2 Simulation studies

For further illustration, here we present the results of several simulation studies. The basic model is \( Y \sim N_n(X\beta, \sigma^2 I_n) \), where the rows of the predictor variable matrix are draws from \( N_p(0, \Omega) \) with an autoregressive correlation structure, i.e., \( \Omega_{jk} = \rho^{|j-k|} \) for all \( j, k \). We consider six different scenarios with varying \( p, \beta, \) and \( \rho \).

Scenario 1. \( p = 7, \beta = (3, 1.5, 0, 0, 2, 0, 0)^\top \), and \( \rho = 0.5 \);
Table 1: IM results for variable selection in the prostate cancer example; here $T = \hat{\theta} / \hat{\sigma}$ and “Plausibility” corresponds to the quantity $\eta(\cdot)$ in (16), ordered by $\pi$.

| Order, $\pi(j)$ | Variable | $|T|$ | Plausibility, $\eta(j)$ |
|-----------------|----------|-----|------------------------|
| 1               | gleason  | 0.288 | 1.0000                 |
| 2               | pgg45    | 1.029 | 0.9193                 |
| 3               | lcp      | 1.165 | 0.8585                 |
| 4               | age      | 1.768 | 0.4502                 |
| 5               | lbph     | 1.842 | 0.4000                 |
| 6               | lweight  | 2.688 | 0.0646                 |
| 7               | svi      | 3.154 | 0.0177                 |
| 8               | lcavol   | 6.715 | 0.0000                 |

**Scenario 2.** $p = 7$, $\beta = (3, 1.5, 0, 0, 2, 0, 0)^\top$, and $\rho = 0.8$;

**Scenario 3.** $p = 7$, $\beta = (0.85, 0.85, 0.85, 0, 0, 0, 0)^\top$, and $\rho = 0.5$;

**Scenario 4.** $p = 7$, $\beta = (0.85, 0.85, 0.85, 0, 0, 0, 0)^\top$, and $\rho = 0.8$;

**Scenario 5.** $p = 20$, $\beta = (0.85 1_{10}^\top, 0_{10}^\top)^\top$, and $\rho = 0.5$;

**Scenario 6.** $p = 20$, $\beta = (0.85 1_{10}^\top, 0_{10}^\top)^\top$, and $\rho = 0.8$.

The results of the IM-based variable selection, described in Section 4.3 with $\alpha = 0.05$, based on the hypercube predictive random set, for the four scenarios are displayed in Figures 1–6. Specifically, these figures plot the percentage of true, parsimonious, true or parsimonious, and inclusive models selected, as a function of the sample size $n$. These are compared with several standard model selection procedures, namely, those based on AIC, BIC, lasso (with ten-fold cross-validation to select the tuning parameter), and adaptive lasso; least angle regression (Efron et al. 2004) was also used, but are not displayed because the results closely match lasso’s. The comparisons are based on 1000 simulated data sets in each configuration, with sample size, $n$, ranging from 50 to 5000.

In each figure, the quantity being plotted in the “true or parsimonious” panel corresponds to the probability of including in the model no irrelevant variable. Given the theoretical results on IM validity, in particular, Theorem 5, we are not surprised to see the IM-based curves sitting at or above the 95% line. The other methods, except for BIC and adaptive lasso are generally far off the mark in this panel. That BIC and adaptive lasso can reach above 95% in the “true or parsimonious” panel is due to their asymptotic variable selection consistency property, not because they are properly calibrated at any fixed $n$. In addition to IM’s fixed-$n$ calibration, it performs as well and, in some cases, even better than the classical methods in terms of how frequently it selects the true model. This can be attributed to the optimality considerations in Section 4. So, the take-away message is that the IM’s fixed-$n$ calibration property does not come with the cost of lower efficiency.
Figure 1: Percentage of true, parsimonious, true or parsimonious, and inclusive models selected, as a function of sample size, for various methods under Scenario 1.

Figure 2: Percentage of true, parsimonious, true or parsimonious, and inclusive models selected, as a function of sample size, for various methods under Scenario 2.
Figure 3: Percentage of true, parsimonious, true or parsimonious, and inclusive models selected, as a function of sample size, for various methods under Scenario 3.

Figure 4: Percentage of true, parsimonious, true or parsimonious, and inclusive models selected, as a function of sample size, for various methods under Scenario 4.
Figure 5: Percentage of true, parsimonious, true or parsimonious, and inclusive models selected, as a function of sample size, for various methods under Scenario 5.

Figure 6: Percentage of true, parsimonious, true or parsimonious, and inclusive models selected, as a function of sample size, for various methods under Scenario 6.
6 Discussion

This paper introduces the concept of multiple simultaneous assertions in the IM framework, and develops a theory of optimal predictive random sets. These general principles are applied to the variable selection problem in regression, which leads to simultaneously valid assessments of the uncertainty across all possible models. An important consequence of the simultaneous validity is that it holds even if a model is selected based on a data-driven procedure. That is, the proposed IM leads naturally to valid post-selection inference and, in particular, a naive projection of the IM plausibility region based on the optimal hyper-cube predictive random set gives exactly the recently developed “POSI” procedure in Berk et al. (2013). In addition, a IM-driven variable selection procedure is developed which is based on the notion of picking the smallest sub-model which is sufficiently plausible given the data. And, by its connection to the valid IM, this procedure is properly calibrated in the sense that it controls the family-wise error rate. Moreover, our simulation study demonstrates that, overall, the proposed IM-based procedure performs as good or better than several standard methods, which suggests that the IM’s emphasis on inferentially meaningful probabilistic summaries does not come at the cost of decreased efficiency. Extending the developments here for application in other models, such as generalized linear models, is a focus of future research.

The IM approach has already been applied to other problems that involve multiplicity, such as large-scale multinomial inference in genome wide association studies (Liu and Xie 2014a) and multiple testing problems (Liu and Xie 2014b). We expect that the optimality considerations here, applied to those problems, would lead to some overall improvements. Perhaps the most important question is how to extend the developments in this paper to the high-dimensional $p \gg n$ context. The $p \gg n$ problem is of great practical interest, and has stimulated considerable research in the last decade; see, for example, Candes and Tao (2007), Zhang and Huang (2008), Wasserman and Roeder (2009), Huang et al. (2010), Huang et al. (2011), Johnson and Rossell (2012), Wang et al. (2013), and van de Geer et al. (2014). The basic principles of optimal predictive random sets developed here for simultaneous complex assertions are not specific to the $p < n$ case, but the initial dimension reduction steps do not carry over directly to the $p \gg n$ case. We expect that once the A-step can be completed for $p \gg n$ case, ideas similar to those presented here can be successfully applied. This is a topic of ongoing work.

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A Measure-theoretic details

A.1 Random sets and the admissibility condition

Molchanov (2005) gives a comprehensive treatment of the theory of random sets. Our goal here is present the minimal amount of technical details necessary to understand our analysis involving predictive random sets. To start, the standard theory of random sets focuses on the case of closed random sets, i.e., random sets whose values are closed sets (with probability 1). Write $S$ for the support of our random set $S$, a collection of subsets of the space $U$; we assume that $S$ contains both $\emptyset$ and $U$. Let $U$ be a separable metric space and take $\mathcal{U}$ to be a $\sigma$-algebra of subsets that contains all the closed subsets of $U$. Assume that each set, or focal element, $S \in S$ is closed, relative to the topology on $U$.

To define the random set $S$, consider a probability space $(\Omega, \mathcal{A}, P)$, and let $S$ be a mapping from $\Omega$ to $S$ which is measurable in the sense that
\[ \{ \omega : S(\omega) \cap K \neq \emptyset \} \in \mathcal{A}, \quad \text{for all compact } K \subseteq U. \]

We define the distribution $P_S$ of $S$ as the push-forward measure $P \circ S^{-1}$. Also, for compact $K$, the event $\{ S \subset K \}$ is measurable, so the probability $P_S(S \subset K)$ in (9) and also below makes sense. Moreover, since $U$ is separable and $S$ is closed, the indicator stochastic process $\{ I_S(u) : u \in U \}$ is separable and, by Proposition 4.10 in Molchanov (2005), the distribution $P_S$ is determined by probabilities assigned to the events $\{ S \subset K \}$, and can be extended to include arbitrary sets $K$.

An important class of examples are the predictive random sets described in Corollary 1 of Martin and Liu (2013b); the “default” predictive random set that has been frequently used in the IM literature, as well as the optimal predictive random set employed in this paper, are each member of this class. In particular, start by taking the probability space $(\Omega, \mathcal{A}, P)$ to be $(U, \mathcal{U}, P_U)$. Next, for a continuous function $h : U \to \mathbb{R}$, define the set-valued mapping $\psi$ on $U$ as
\[ \psi_h(u) = \{ u' \in U : h(u') \leq h(u) \}, \quad u \in U. \]

Then the focal elements $S \in S$ are closed level sets of the function $h$, and if $\mathcal{U}$ is rich enough to contain all the closed sets, then $\psi_h$ is a measurable function and, consequently, $S = \psi_h(U)$, for $U \sim P_U$, is a closed random set.

In the IM context, as a consequence of the results in Martin and Liu (2013b), we focus only on predictive random sets with nested support $S$, where nested means that, for any two focal elements, one is a subset of the other. Such supports can, and usually are, constructed as in the small example above, but requiring that the function $h$ has a unique minimizer and that it is non-decreasing (or, for simplicity, increasing) as moves further away from that minimizer. The default predictive random set, for the case $U = [0, 1]$, takes $h(u) = |u - 0.5|$, which is of the form just described. Using the terminology in Shafer (1987), we could call a predictive random set with nested support consonant and, in addition to the admissibility properties demonstrated in Martin and Liu (2013b), consonant random sets have the simplest distributional properties.

In our restriction to admissible predictive random sets, as described in Definition 2, there is a more pressing concern, namely, does there exist a predictive random set $S$?
supported on a given nested collection $S$ of closed $P_U$-measurable subsets, such that

$$P_S\{S \subset K\} = \sup_{S \in S : S \subset K} P_U(S).$$

Specifically, while the right-hand side above is a well-defined quantity, it is not clear that there is a predictive random set $S$ with distribution $P_S$ that satisfies the above equality. However, the famous Choquet capacity theorem (Molchanov 2005, Theorem 1.13) can be applied to show existence of such an $S$, and this is relatively simple to show given the connection to the probability measure $P_U$.

A.2 Measurability assumptions

In addition to measurability of set-valued mappings, as discussed above, there are issues about some more familiar forms of measurability, pertaining to the a-events $U_A(x)$ for a given assertion $A \subseteq \Theta$. Recall that the auxiliary variable space $U$ is equipped with a $\sigma$-algebra $\mathcal{U}$ of $P_U$-measurable subsets, assumed to contain all the closed sets. Next, equip the sample space $X$ with a $\sigma$-algebra $\mathcal{X}$ and a $\sigma$-finite measure $\mu$, where $P_{X|\theta} \ll \mu$ for each $\theta$. Then the two key measurability assumptions are:

- $U_A(x) \in \mathcal{U}$ for all relevant $A$ and for $\mu$-almost all $x$, and
- $\{x : U_A(x) \supset S\} \in \mathcal{X}$ for all focal elements $S \in S$.

General sufficient conditions are can be given based properties of the association mapping $x = a(\theta, u)$ and of the assertion $A$. It is relatively easy to check the above conditions directly in a particular example and, moreover, the conditions might fail only in non-standard problems.

B Proofs

B.1 Proof of Theorem 1

Proposition 1 in Martin and Liu (2013b) shows that $bel_x(A; S) \leq P_U\{U_A(x)\}$, for any admissible $S$ and any $x$. By assumption, the collection $\{U_A(x) : x \in X\}$ is nested, so it can be taken as the support of an admissible predictive random set. In this case, since $P_S$ satisfies (9), we have that $bel_x(A; S) = P_U\{U_A(x)\}$ for all $x$. Therefore, the belief function attains its upper bound for each $x$, hence, it is optimal.

B.2 Proof of Theorem 2

Since $A_1$ and $A_2$ are simple assertions, the respective optimal predictive random sets $S_1$ and $S_2$ have focal elements given by $U_{A_1}(x)$ and $U_{A_2}(x)$, as $x$ ranges over $X$. Without loss of generality, assume that the predictive random set $T$ for $A = A_1 \cup A_2$ is admissible. That is, assume $T$ has a nested support $\mathcal{S}$ and that $P_T$ satisfies (9). Define

$$S_j(T) = \text{closure}\left\{ \bigcap_{y : U_{A_j}(y) \supset T} U_{A_j}(y) \right\} \quad j = 1, 2, \quad T \in \mathcal{T}.$$
Collect intersections of these sets, \( S = \{S_1(T) \cap S_2(T) : T \in \mathbb{T}\} \). Since \( \mathbb{T} \) is nested and the function \( T \mapsto S_1(T) \cap S_2(T) \) is monotone, the collection \( S \) is also nested. Define a new predictive random set \( \hat{S} \), supported on \( S \), with the natural measure \( P_S \) as in (9). This predictive random set satisfies the conditions stated in the theorem, i.e., admissible and has focal elements as intersections of the respective optimal predictive random set focal elements. We need to show that \( T \subset \bigcup A(x) \) if and only if \( S(T) \subset \bigcup A(x) \), where \( S(T) = S_1(T) \cap S_2(T) \). One direction is easy, since it is clear that \( T \subset S(T) \). For the other direction, we want to show that \( T \subset \bigcup A(x) \) implies \( S(T) \subset \bigcup A(x) \). Since \( \bigcup A_1(x) \) and \( \bigcup A_2(x) \) are disjoint, and the union is \( \bigcup A(x) \), \( T \subset \bigcup A(x) \) implies that either \( T \subset \bigcup A_1(x) \) or \( T \subset \bigcup A_2(x) \). By definition of \( S_1(T) \) and \( S_2(T) \), it follows that

\[
S_1(T) \subset \bigcup A_1(x) \quad \text{or} \quad S_2(T) \subset \bigcup A_2(x).
\]

In either case, \( S(T) = S_1(T) \cap S_2(T) \) is contained in \( \bigcup A(x) = \bigcup A_1(x) \cup \bigcup A_2(x) \), which completes the argument that \( \{T \subset \bigcup A(x)\} \) and \( \{S(T) \subset \bigcup A(x)\} \) are equivalent. Finally, since \( T \subset S(T) \), we get \( P_T(T) \leq P_U(S(T)) \) for all \( T \in \mathbb{T} \) and, therefore,

\[
P_T(T \subset \bigcup A(x)) = \sup_{T : T \subset \bigcup A(x)} P_U(T) \leq \sup_{T : S(T) \subset \bigcup A(x)} P_U(S(T)) = P_S(S \subset \bigcup A(x)).
\]

The left-hand side is \( \text{bel}_S(A; \mathcal{T}) \) and the right-hand side is \( \text{bel}_S(A; \mathcal{S}) \), and the inequality holds for all \( x \), completing the proof.

### B.3 Proof of Theorem 3

The proof here is similar to that of Theorem 2. Consider collection \( \{A_j : j \in J\} \) of complex assertions, where each \( A_j \) can be written as a union of disjoint simple assertions, i.e., \( A_j = A_{j_1} \cup A_{j_2} \), where \( A_{j_1} \cap A_{j_2} = \emptyset \) and the a-events \( A_{j_1} \cdot \cdot \cdot \) and \( A_{j_2} \cdot \cdot \cdot \) are nested.

By Theorem 2, we know that the optimal predictive random sets for \( A_j \), \( j \in J \), have focal elements \( S_j = \{S_j(v) : v \in V\} \), indexed by a set \( V \), which are intersections of a-events. That is, \( S_j(v) \) is (the closure of) \( \bigcup A_{j_1}(x_{j_1}(v)) \cap \bigcup A_{j_2}(x_{j_2}(v)) \) for some \( x_{j_1}(v) \) and \( x_{j_2}(v) \).

Without loss of generality, assume that the candidate predictive random set \( \mathcal{T} \) for the assertion \( A \) generated by \( \{A_j : j \in J\} \) is admissible in the sense of Definition 2. Given a focal element \( T \in \mathbb{T} \) of \( \mathcal{T} \), define

\[
\hat{S}_j(T) = \bigcap_{v \in S_j(v) \cap T} S_j(v), \quad j \in J.
\]

Next, set \( \hat{S}(T) = \bigcap_{j \in J} \hat{S}_j(T) \) and define \( \hat{S} = \{\hat{S}(T) : T \in \mathbb{T}\} \). Now take \( \mathcal{S} \) to have support \( \hat{S} \) and natural measure \( P_{\hat{S}} \) as in (9); this \( \mathcal{S} \) satisfies the conditions of the theorem. It remains to show that \( \mathcal{S} \) is more efficient than \( \mathcal{T} \).

As in the proof of Theorem 2, we need to show that \( T \subset \bigcup A(x) \) if and only if \( \hat{S}(T) \subset \bigcup A(x) \) for each \( x \) and \( T \in \mathbb{T} \). By construction, \( T \subset \hat{S}(T) \), so one direction is handled. For the other direction, assume that \( T \subset \bigcup A(x) \). Then \( T \subset \bigcup A_{j_1}(x) \) for some \( j \in J \) and, since \( A_j \) splits as a disjoint union of simple assertions, we get that \( T \subset \bigcup A_{j_1}(x) \) or \( T \subset \bigcup A_{j_2}(x) \). Then \( \hat{S}_j(T) \subset \bigcup A_{j_1} \cap \bigcup A_{j_2}(x) \) and, consequently, the no-bigger \( \hat{S}(T) \) must be a subset of \( \bigcup A(x) \). Since \( T \subset \bigcup A(x) \) if and only if \( \hat{S}(T) \subset \bigcup A(x) \), the claimed superiority of \( \mathcal{S} \) to \( \mathcal{T} \) follows just like in the last part of the proof of Theorem 2.
B.4 Proof of Lemma 1

Recall that $\text{bel}_x(A; S)$ is defined as $P_S\{S \subset \cup_A(x)\}$. Since $S$ has the natural measure $[\Theta]$, we can write, for any $b \in [0, 1],$

$$\text{bel}_x(A; S) > b \iff P_S\{S \subset \cup_A(x)\} > b \iff \sup_{r:S_r \subset \cup_A(x)} P_U(S_r) > b \iff \sup_{r:S_r \subset \cup_A(x)} (1 - r) > b \iff \cup_A(x) \supset S_{1-b}.$$  

Therefore, we have that

$$P_{X|\theta}\{\text{bel}_X(A; S) > b\} = P_{X|\theta}\{\cup_A(X) \supset S_{1-b}\}, \quad \forall \ b \in [0, 1],$$

which proves the claim, with $r = 1 - b.$

B.5 Proof of Theorem 4

Take any predictive random set $S$ as in Theorem 3 and let $S$ be a generic focal element. Take any assertion $A$ generated by $\{A_j : j \in J\}$. Define the core of $S$ as $S^o = \bigcap_{g \in \mathcal{A}} gS$; note that $S^o$ is balanced and satisfies $S^o \subset gS$ for all $g \in \mathcal{A}$. Then,

$$P_{X|\theta}\{\cup_A(X) \supset S^o\} \geq P_{X|\theta}\{\cup_A(X) \supset gS\}, \quad \forall \ g \in \mathcal{A}, \quad \forall \ \theta \in A,$$

with strict inequality in general. Maximin optimality requires that we choose the focal elements to maximize the minimum (over $g$) of the right-hand side of the above display. However, we can clearly attain the upper bound above by taking the focal element $S$ equal to its core, i.e., balanced. Therefore, balance implies maximin optimality.

References

Akaike, H. (1973). Information theory and an extension of the maximum likelihood principle. In Second International Symposium on Information Theory (Tsahkadsor, 1971), pages 267–281. Akadémiai Kiadó, Budapest.

Berger, J. (2006). The case for objective Bayesian analysis. Bayesian Anal., 1(3):385–402.

Berger, J. O., Bernardo, J. M., and Sun, D. (2009). The formal definition of reference priors. Ann. Statist., 37(2):905–938.

Berk, R., Brown, L., Buja, A., Zhang, K., and Zhao, L. (2013). Valid post-selection inference. Ann. Statist., 41(2):802–837.

Candes, E. and Tao, T. (2007). The Dantzig selector: statistical estimation when $p$ is much larger than $n$. Ann. Statist., 35(6):2313–2351.

Clyde, M. and George, E. I. (2004). Model uncertainty. Statist. Sci., 19(1):81–94.
Dempster, A. P. (2008). The Dempster–Shafer calculus for statisticians. *Internat. J. Approx. Reason.*, 48(2):365–377.

Efron, B., Hastie, T., Johnstone, I., and Tibshirani, R. (2004). Least angle regression. *Ann. Statist.*, 32(2):407–499. With discussion, and a rejoinder by the authors.

Ermini Leaf, D. and Liu, C. (2012). Inference about constrained parameters using the elastic belief method. *Internat. J. Approx. Reason.*, 53(5):709–727.

Fraser, D. A. S. (2011). Is Bayes posterior just quick and dirty confidence? *Statist. Sci.*, 26(3):299–316.

Fraser, D. A. S., Reid, N., Marras, E., and Yi, G. Y. (2010). Default priors for Bayesian and frequentist inference. *J. R. Stat. Soc. Ser. B Stat. Methodol.*, 72(5):631–654.

Hannig, J. (2009). On generalized fiducial inference. *Statist. Sinica*, 19(2):491–544.

Hannig, J. (2013). Generalized fiducial inference via discretization. *Statist. Sinica*, 23(2):489–514.

Hannig, J. and Lee, T. C. M. (2009). Generalized fiducial inference for wavelet regression. *Biometrika*, 96(4):847–860.

Hastie, T., Tibshirani, R., and Friedman, J. (2009). *The elements of statistical learning*. Springer-Verlag, New York, 2nd edition.

Heaton, M. J. and Scott, J. G. (2010). Bayesian computation and the linear model. In Cheh, M.-H., Dey, D., Müller, P., Sun, D., and Ye, K., editors, *Frontiers of Statistical Decision Making and Bayesian Analysis*, pages 527–545. Springer.

Huang, J., Horowitz, J. L., and Wei, F. (2010). Variable selection in nonparametric additive models. *Ann. Statist.*, 38(4):2282–2313.

Huang, J., Ma, S., Li, H., and Zhang, C.-H. (2011). The sparse Laplacian shrinkage estimator for high-dimensional regression. *Ann. Statist.*, 39(4):2021–2046.

Johnson, V. E. and Rossell, D. (2012). Bayesian model selection in high-dimensional settings. *J. Amer. Statist. Assoc.*, 107(498):649–660.

Kadane, J. B. and Lazar, N. A. (2004). Methods and criteria for model selection. *J. Amer. Statist. Assoc.*, 99(465):279–290.

Lai, R. C. S., Hannig, J., and Lee, T. C. M. (2013). Generalized fiducial inference for ultrahigh dimensional regression. *J. Amer. Statist. Assoc.*, to appear, *arXiv:1304.7847*.

Liu, C. and Martin, R. (2015). Frameworks for prior-free posterior probabilistic inference. *WIREs Comp. Stat.*, to appear.

Liu, C. and Xie, J. (2014a). Large scale two sample multinomial inferences and its applications in genome-wide association studies. *Internat. J. Approx. Reason.*, 55(1, part 3):330–340.
Liu, C. and Xie, J. (2014b). Probabilistic inference for multiple testing. *Internat. J. Approx. Reason.*, 55(2):654–665.

Lockhart, R., Taylor, J., Tibshirani, R. J., and Tibshirani, R. (2014). A significance test for the lasso. *Ann. Statist.*, 42(2):413–468.

Martin, R. (2014). Random sets and exact confidence regions. *Sankhyā A*, 76:288–304.

Martin, R. and Liu, C. (2013a). Correction: ‘Inferential models: A framework for prior-free posterior-posterior probabilistic inference’. *J. Amer. Statist. Assoc.*, 108(502):1138–1139.

Martin, R. and Liu, C. (2013b). Inferential models: A framework for prior-free posterior probabilistic inference. *J. Amer. Statist. Assoc.*, 108(501):301–313.

Martin, R. and Liu, C. (2014a). Discussion: Foundations of statistical inference, revisited. *Statist. Sci.*, 29:247–251.

Martin, R. and Liu, C. (2014b). A note on p-values interpreted as plausibilities. *Statist. Sinica*, 24:1703–1716.

Martin, R. and Liu, C. (2015a). Conditional inferential models: combining information for prior-free probabilistic inference. *J. R. Stat. Soc. Ser. B. Stat. Methodol.*, to appear; arXiv:1211.1530.

Martin, R. and Liu, C. (2015b). Marginal inferential models: prior-free probabilistic inference on interest parameters. *J. Amer. Statist. Assoc.*, to appear; arXiv:1306.3092.

Martin, R., Mess, R., and Walker, S. G. (2014). Empirical Bayes posterior concentration in sparse high-dimensional linear models. Unpublished manuscript, arXiv:1406.7718.

Molchanov, I. (2005). *Theory of Random Sets*. Probability and its Applications (New York). Springer-Verlag London Ltd., London.

Schwarz, G. (1978). Estimating the dimension of a model. *Ann. Statist.*, 6(2):461–464.

Shafer, G. (1987). Belief functions and possibility measures. In Bezdek, J. C., editor, *The Analysis of Fuzzy Information, Vol. 1: Mathematics and Logic*, pages 51–84. CRC.

Shafer, G. (2011). A betting interpretation for probabilities and Dempster–Shafer degrees of belief. *Internat. J. Approx. Reason.*, 52(2):127–136.

Tibshirani, R. (1996). Regression shrinkage and selection via the lasso. *J. Roy. Statist. Soc. Ser. B*, 58(1):267–288.

Tibshirani, R. (2011). Regression shrinkage and selection via the lasso: a retrospective. *J. R. Stat. Soc. Ser. B Stat. Methodol.*, 73(3):273–282.

van de Geer, S., Bühlmann, P., Ritov, Y., and Dezeure, R. (2014). On asymptotically optimal confidence regions and tests for high-dimensional models. *Ann. Statist.*, 42(3):1166–1202.
Wang, L., Kim, Y., and Li, R. (2013). Calibrating nonconvex penalized regression in ultra-high dimension. *Ann. Statist.*, 41(5):2505–2536.

Wasserman, L. and Roeder, K. (2009). High-dimensional variable selection. *Ann. Statist.*, 37(5A):2178–2201.

Xie, M. and Singh, K. (2013). Confidence distribution, the frequentist distribution of a parameter – a review. *Int. Statist. Rev.*, 81(1):3–39.

Xie, M., Singh, K., and Strawderman, W. E. (2011). Confidence distributions and a unifying framework for meta-analysis. *J. Amer. Statist. Assoc.*, 106(493):320–333.

Zhang, C.-H. and Huang, J. (2008). The sparsity and bias of the LASSO selection in high-dimensional linear regression. *Ann. Statist.*, 36(4):1567–1594.

Zhang, Z., Xu, H., Martin, R., and Liu, C. (2011). Inferential models for linear regression. *Pak. J. Statist. Oper. Res.*, 7:413–432.

Zou, H. (2006). The adaptive lasso and its oracle properties. *J. Amer. Statist. Assoc.*, 101(476):1418–1429.

Zou, H. and Hastie, T. (2005). Regularization and variable selection via the elastic net. *J. R. Stat. Soc. Ser. B Stat. Methodol.*, 67(2):301–320.