FALSE VARIABLE SELECTION RATES IN REGRESSION

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There has been recent interest in extending the ideas of False Discovery Rates (FDR) to variable selection in regression settings. Traditionally the FDR in these settings has been defined in terms of the coefficients of the full regression model. Recent papers have struggled with controlling this quantity when the predictors are correlated. This paper shows that this full model definition of FDR suffers from unintuitive and potentially undesirable behavior in the presence of correlated predictors. We propose a new false selection error criterion, the False Variable Rate (FVR), that avoids these problems and behaves in a more intuitive manner. We discuss the behavior of this criterion and how it compares with the traditional FDR, as well as presenting guidelines for determining which is appropriate in a particular setting. Finally, we present a simple estimation procedure for FVR in stepwise variable selection. We analyze the performance of this estimator and draw connections to recent estimators in the literature.

1. Introduction. Since the introduction of False Discovery Rates (FDR) (Benjamini and Hochberg, 1995), the idea has had a large impact on error control for many statistical problems and has inspired many further statistical developments (e.g. Tusher, Tibshirani and Chu, 2001; Efron, 2010; Dudoit and Van Der Laan, 2007). More recently, there has been an interest in generalizing the ideas from FDR to variable selection in the regression setting.

Abramovich et al. (2006) introduce the idea of FDR in the regression setting as a criterion for variable selection, and gives results about the asymptotic minimaxity of this method. The results focus on the case where the variables being considered are orthogonal. Since then, there has been work extending the idea of FDR in regression to the correlated variable setting. These works include Benjamini and Gavrilov (2009), which proposes a generalized FDR-based penalty to guide variables selection; Lin, Foster and Ungar (2011), which proposes a procedure for variable screening in regression that controls an FDR-related quantity under certain conditions; Meinshausen and Bühlmann (2010) and Shah and Samworth (2012) on stability selection; and others (e.g. Meinshausen, Meier and Bühlmann, 2009; Wu, Boos and Stefanski, 2007).

In this paper we consider linear models of the form

\[ y_i = \beta_0 + x_i^T \beta + \varepsilon_i, \quad i = 1, \ldots, n, \]

with \( x_i \in \mathbb{R}^p \), \( y_i \in \mathbb{R}^n \), \( \beta \in \mathbb{R}^p \), and \( \varepsilon_i \) independent and identically distributed.

For variable selection, we denote the selected set of variables as a subset \( \mathcal{A} \subseteq \{1, \ldots, p\} \) of the potential variables. The number of false selections, denoted by \( V \) (to be defined carefully in Section

*Supported by NSF GRFP Fellowship
†Supported by NSF Grant DMS-1007719
‡Supported by NIH Grant RO1-EB001988-15
§Supported by NSF Grant DMS-9971405
¶Supported by NIH Contract N01-HV-28183

Keywords and phrases: False discovery rate, false variable rate, variable selection
2), is then a property of the set $\mathcal{A}$. Similarly, the proportion of false selections, $V/|\mathcal{A}|$, is also a property of the set $\mathcal{A}$.

The rate of false selections is the expected value of that proportion of false selections, $E(V/|\mathcal{A}|)$, where the expectation is taken over realizations of data and conditional on the variable selection procedure. As a result, false discovery rates are not a property of a particular selected set $\mathcal{A}$, but of the variable selection procedure and the structure of the model. In the following sections, we refer to proportions and rates of false selections in this way.

In the literature, a false selection in the regression setting is usually defined as a selected variable that has a zero coefficient in the full model (e.g. Lin, Foster, and Ungar, 2011; Meinshausen and Bühlmann, 2010; Meinshausen, Meier, and Bühlmann, 2009; Wu, Boos, and Stefanski, 2007). That is, for a set of selected variables $\mathcal{A} \subseteq \{1, \ldots , p\}$ and full model 1.1, the proportion of falsely selected variables is defined as

$$FDP = \frac{\{j \in \mathcal{A} : \beta_j = 0\}}{|\mathcal{A}|}.$$ 

The FDR is the expectation of this quantity for the given procedure. For this paper, we refer to this as the full model definition of a false selection and FDR. In contrast to this definition, in Section 2.2.3 we introduce new quantities, the False Variable Proportion (FVP) and its expectation, the False Variable Rate (FVR), which are defined in terms of the projection of the full model onto the selected variables $\mathcal{A}$.

The FVR quantity we introduce is motivated by practical issues that arise when applying FDR to large screening problem such as gene expression studies. In these settings, the presence of correlated predictors can lead univariate FDR methods to select variables that are all capturing the same underlying signal. The desire to select unique variables and to detect multivariate effects has led to the use of regression variable selection techniques (Broman and Speed, 2002). When the full model definition of FDR is applied in these settings, it is difficult to distinguish the significance of the correlated predictors, which can inflate their FDR. This has led to an exploration of other approaches to defining false selections in the correlated variable setting (Frommlet et al., 2012).

In this paper we demonstrate shortcomings of existing definitions of false selection rates in regression, and propose a new error criterion, called the False Variable Rate (FVR), which we show exhibits more desirable behavior. In Section 2, we discuss what constitutes a falsely select variable, introduce our new criterion and examine the differences in these definitions when the predictors are correlated. In Section 3, we present intuition for the differences in behavior of the error criteria, and provide more concrete examples where our new criteria behaves desirably. Finally, in Section 4, we present a simple estimation algorithm for FVR in stepwise regression. We provide motivation for this estimator and examine the regimes in which it breaks down, making connections to broader issues in FVR estimation.

2. Defining a false selection. We are interested in examining the population definition of a falsely selected variable in our regression model. We begin with a toy example of our problem setting, and then move on to a discussion of different definitions of a false selection

2.1. Toy Example. This toy example may be helpful for gaining an intuition of the alternative false selection definitions, and for understanding the general purpose of these criteria.

Imagine analyzing gene expression data and trying to understand some biological outcome as a function of that expression. In our simplified example, illustrated in Figure 1, we observe the expression of eight genes, $A, B_1, B_2, B_3, C_1, C_2, C_3, D$. Of these, genes $A$ and $B_1$ are biologically
In these sections, we describe three natural definitions of a false selection, two of which are common in the literature and the last which is newly proposed in this paper.

Note: Because this section is focusing on the population definition of a false selection for a set of variables, rather than for a particular procedure, we focus on numbers (V) and proportions (FDP) of false selections, rather than rates (FDR).

2.2.1. Marginal Correlations. The simplest definition of a false selection in our model is similar to the usual univariate approach to screening using marginal correlations. It defines the $j^{th}$ variable to be falsely selected if $\text{Cov}(y^T x_j) = 0$. For a selected set of variables $\mathcal{A}$, the number of false selections $V$ and the false discovery proportion FDP are given by

$$ V = |\{j \in \mathcal{A} : \text{Cov}(y, x_j) = 0\}|, $$

$$ \text{FDP} = \frac{|\{j \in \mathcal{A} : \text{Cov}(y, x_j) = 0\}|}{|\mathcal{A}|}. $$

This definition considers a selected variable interesting if that variable captures information about the signal on its own, irrespective of any of the other variables in the data set or in the selected model. In our gene expression example, any pathway with a gene that is important to the outcome will have all of the genes in that pathway considered correct selections, since they will all have marginal correlation with the outcome (Figure 2).

This definition of a false selection is equivalent to the one used in many variable selection screening procedures, for example Tusher, Tibshirani and Chu (2001) and Efron (2010). We will not focus
Here we illustrate the marginal definition of a false selection in the context of our earlier example (Figure 1). We see that any variable that is marginally correlated with the outcome is considered correct. This includes $B_2$ in both sets, since it is correlated with $B_1$ which is in turn correlated with the outcome of interest.

This definition has been used in several papers, among them Meinshausen and Bühlmann (2010); Meinshausen, Meier and Bühlmann (2009); Wu, Boos and Stefanski (2007). A modified version of the FDR appears in Lin, Foster and Ungar (2011), using this definition of the number of false discoveries $V$.

This definition of a false discovery is natural, particularly in the setting with uncorrelated $x_j$. In that setting, it actually agrees with the definition in Equations (2.1, 2.2). When the $x_j$ are correlated, the meanings of these two definitions differ. The definition in terms of marginal correlations, as we mentioned, asks if each selected variable captures information about the signal on its own.

In contrast, the coefficient corresponding to a variable in the full model is only nonzero if that variable captures information about the signal that is not captured by any other variables in the full model. The proportion of false selections in this setting therefore corresponds to the fraction of selected model variables that fail to uniquely capture signal among all the variables in the considered data set. In our gene expression example, only the gene from an important pathway that has nonzero coefficient in the full model will be considered important (in our case $A$ or $B_1$,
This can be counterintuitive, since any one of the genes from these pathways could be strongly predictive of the outcome of interest.

Furthermore, in practice it would likely be impossible to determine which of the highly correlated variables in an important pathway actually carried the nonzero coefficient in the full model, which would lead to all the variables appearing as false selections according to this criterion.

This is a reasonable choice for some statistical problems and some scientific settings. It has a strong connection to the full model p-values in regression, where significance of a coefficient shows that a particular variable is significantly correlated with the response after the effects of all the other variables have been removed. However, as we discuss further in Section 3, this criterion has unintuitive behavior for many of the scientific problems in which variable selection is being applied. In the next section, we introduce a new criterion which is more appropriate for those settings.

2.2.3. A new approach: False Variable Rate. In this section, we propose a new approach for defining false selections which lies between these two extremes. Rather than requiring that an interesting variable be correlated with the signal in a way that is not explained by any other variables in the data set, we instead consider a variable to be an interesting selection if it captures signal that has not been explained by any other variable in the selected model.

For many of the situations where variable selection is applied, this is a more natural view. Common variable selection approaches like stepwise or $L_1$ regression attempt to include variables that capture part of the signal that the other selected variables miss. However, neither of these methods check that a variable being included captures signal that excluded variables do not also capture. For applications like the screening of predictors in biology, where predictors may be strongly correlated and the data matrix may not be carefully structured with meaningfully chosen columns, this is a more interpretable criterion. We come back to this idea when we contrast the methods more carefully in Section 3.

We now define a criterion with the desired behavior. Rather than looking at the coefficients of the full model as in Section 2.2.2, we instead look at the coefficients of the model formed by projecting the true model onto the selected variables. This resembles some ideas from Berk et al. (2012), where inference is conducted with respect to the selected model even if there may be some larger true model.

For a selected set $\mathcal{A} \subseteq \{1, \ldots, p\}$, we have a restricted data matrix $X_{\mathcal{A}}$, formed by the columns with indices in $\mathcal{A}$. We can project the mean $X\beta$ from the full linear model onto this subset of predictors $X_{\mathcal{A}}$. This gives a projected mean $X_{\mathcal{A}}\beta^{(\mathcal{A})}$, for some $\beta \in \mathbb{R}^{\mid \mathcal{A} \mid}$. In the event that $\beta^{(\mathcal{A})}$ of this form is not unique, meaning that $X_{\mathcal{A}}$ is not full rank, we choose $\beta^{(\mathcal{A})}$ to be any of the sparsest vectors satisfying the projection requirement.

We now define a selected variable to be a false selection if it has a zero coefficient in this vector. This means that the number of false selections is just the number of zeros in this vector of coefficients for the projected mean, giving

$$V = \left| \{ j \in \mathcal{A} : \beta_j^{(\mathcal{A})} = 0 \} \right| \quad (2.5)$$
$$\text{FVP} = \frac{\left| \{ j \in \mathcal{A} : \beta_j^{(\mathcal{A})} = 0 \} \right|}{|\mathcal{A}|} \quad (2.6)$$

where we refer to the proportion of falsely selected variables by this definition as the false variable proportion (FVP) to differentiate it from the usual regression definition (FDP) in Section 2.2.2. Similarly, the expectation of this proportion is referred to as the False Variable Rate, or FVR.

This quantity has the desired interpretation. A variable is considered interesting if it is correlated with the signal $y$ after the effects of the other selected variables have been removed. If two variables
Fig 4. Here we illustrate our new projected model definition of a false selection in the context of Figure 1. We see that variables are now correct selections if they are capturing unique signal among the selected variables. Thus $B_2$ is correctly selected in the first set. However, $B_2$ is considered a false selection in the second set because it adds no information beyond $B_1$.

are capturing the same piece of signal, including either one of them will be a good selection, but including a second one will not be adding any new information, and will thus be a false selection.

In our gene expression example, this means that one gene selected from a given influential pathway will be considered a correct selection and any further selections from that pathway will be incorrect. This is illustrated in Figure 4, where we see that the selection of $B_2$ in the first set is considered correct, because it is adding information to the selected set. In the second set, $B_2$ is considered incorrect, because $B_1$ is already contributing the same information about the outcome. This seems like a natural definition in this setting. In Section 3, we elaborate on the differences between the criteria in detail.

*Note:* Some care needs to be taken for models with random $X$, where we want to rule out spurious correlations between the random predictors. The number of correct selections in $\mathcal{A}$ is generalized to be the size of the smallest subset $\mathcal{B} \subseteq \mathcal{A}$ such that, when conditioning on $\mathcal{B}$, $y$ is conditionally uncorrelated with the rest of $\mathcal{A}\setminus\mathcal{B}$. This has a nice form for Gaussian graphical models, discussed in Section 3.2.

2.3. Summary and comparison. Before moving on to discussion of implications and behavior of the different error criteria, we briefly summarize the three definitions that we have discussed, and their simple interpretation. Their implications for the gene expression example of Section 2.1 are shown in Figure 5.

Fig 5. A summary of the implications of the marginal, full, and projected model definitions of a false selection on our example from Figure 1. We see that there are cases in which each of the definitions disagree with the others.

*Marginal view (Section 2.2.1).* A variable $x_j$ is considered a false selection if $\text{Cov}(y, x_j) = 0$. This
implies that a variable is interesting if it is correlated with the signal, without regard to any of the other variables in the data set.

**Full Model view (Section 2.2.2).** A variable \( x_j \) is considered a false selection if \( \beta_j = 0 \) in the full model. This implies that a variable is interesting if it is correlated with the signal after conditioning on all the other variables in the entire data set.

**Projected Model view (Section 2.2.3).** A variable \( x_j \) is considered a false selection if \( \beta_j^{(A)} = 0 \) in the projected model onto the selected variables \( X_A \). This implies that a variable is an interesting selection if it is correlated with the signal after conditioning on all the other variables in the set of selected variables. This definition is used for our proposed False Variable Rate (FVR) criterion.

In the next section, we will see the impact of the differences in these definitions on the behaviors of the error criteria.

### 3. Contrasting the False Selection Criteria

In this section, we will discuss the behavior of the usual full model definition and our new projected model definition of false variable selection rates. We will see that, though the full model definition is reasonable in some settings, it leads to non-intuitive behavior in common variable selection settings. We will show that our proposed approach has intuitive and desirable behavior in those cases.

#### 3.1. A simple example

To understand the differences in behavior between these definitions, we begin with the following simple example, represented in Figure 6.

![Fig 6](image_url)

**Figure 6.** Representation of four possible variables. The projection of the true (noiseless) model into the space spanned by the variables is indicated as the green circle and label \( X\beta \). Variable 3 is perfectly correlated with the signal, variables 1 and 2 are correlated with the signal, and variable 4 is orthogonal to the signal. The red arrows indicate the variables that have been selected.

|        | Marginal FDP | Full Model FDP | Proposed FVP |
|--------|--------------|----------------|--------------|
| Figure A | 0            | 0              | 0            |
| Figure B | 0            | 1              | 0            |
| Figure C | 1/2          | 1/2            | 1/2          |
| Figure D | 0            | 2/3            | 2/3          |

Table 1: Resulting false selection proportions from applying each of the three definitions of Section 2.2 to the scenarios in Figure 6. The criteria disagree on values in Figures B and D because the definitions give different value to correlated variables that explain the same part of the signal.

We consider four different simple cases here. Note that we are examining proportions of false selections for a selected set, rather than rates of false selections for a procedure, so we will describe FDP/FVP quantities, rather than FDR/FVR rates. The false selection proportions for each scenario and each definition are shown in Table 1.

All three definitions agree on scenarios A and C, since they deal only with variables that are perfectly correlated or orthogonal to the true signal. The cases B and D are more interesting. In case
B, variables 1 and 2 are correct selections according to the projected definition, since they capture information about the signal that is not included in any other selected variable. These variables are both considered false selections by the full model definition, since the data set (though not the selected set) contains variable 3, which captures all the information in variables 1 and 2.

In scenario D, the full and projected model definitions now agree, since variable 3 is included in the selected set, rendering variables 1 and 2 uninformative. The marginal definition continues to consider all three variables correct selections, since it is not concerned with uniqueness.

We see that the definitions may all disagree, depending on the structure of the data set and the selected model. In general, the full and projected model approaches differ when variables are selected that are correlated with the signal, but would have their correlation explained away by an unselected variable in the data set.

3.2. Graphical Model View. The interpretation of and differences between these false selection definitions are particularly clear in a Gaussian graphical model setting. Suppose that the variables \(X_j\) and the response \(Y\) have a joint Gaussian distribution, with distributions \(X \sim N(0, \Sigma)\) and \(Y \sim N(X^T \beta, \sigma^2)\). We represent the dependence structure of the variables by the usual dependence graph, as illustrated in Figure 7a. Two variables are connected here if they have nonzero partial correlation after conditioning on the other variables.

If we select a subset of the variables \(\mathcal{A}\), there is an induced dependence graph for the marginal distribution of \(y \cup \mathcal{A}\). The structure follows from the usual manipulations of Gaussian covariance matrices (see Appendix A.1). This marginal graph corresponds to the dependence structure of the variables in the projected model we discussed earlier.

Each of our definitions of a false selection have an interpretation in terms of these graphical models. Suppose we select variables \(\mathcal{A} = \{2, 3, 5, 7\}\) in the example shown in Figure 7. In the marginal definition, a variable in \(\mathcal{A}\) is a false selection if it does not have a path to \(y\) in the full graph (a), since such a path would correspond to a marginal correlation with \(y\). In this case, all the variables are connected to \(y\) except variable 7, so there would be one false selection by that definition, and FDP = 1/4.

In the full model definition, a variable in \(\mathcal{A}\) is a false selection if it is not directly connected to \(y\) in the full graph (a), since such links correspond to nonzero partial correlations. By this definition, variables 2, 5, 7 would be false selections, and the FDP = 3/4 for this approach.

In our projected model definition, a variable in \(\mathcal{A}\) is a false selection if it is not directly connected to \(y\) in the graph (b) induced on the selected variables. The links in that induced graph correspond to correlations that cannot be explained by other selected variables. In the example, variables 2 and 3 are directly connected to \(y\) in the induced graph, and variables 5 and 7 are not, so the FVP = 1/2.
From these graphs, we gain an intuition for the behavior of the full and projected definitions. By switching from the full model to the projected model, represented by the induced graph, unselected variables that were important in the full model can induce importance in correlated variables. This lets selected variables that are carrying that missing information be considered correct selections when they are included.

3.3. Implications for the Choice of False Selection Criteria. So far in this section, we have described the differences between the false selection criteria we have presented. In this section, we will discuss the practical implications of these differences in statistical problems. We show that in many common settings the usual full model FDP/FDR will give misleading results, and that our proposed FVP/FVR definition will have the intuitive behavior we desire.

3.3.1. Highly correlated predictors. Suppose our dataset contains highly correlated predictors. This commonly occurs in biological data, where there might be an underlying factor driving several variables. In our gene expression example, several genes in our data set could be from the same biological pathway, leading them to be over-expressed or under-expressed together.

Now imagine that one of these pathways is biologically relevant to our outcome of interest. This could lead to several variables which are strongly correlated with the outcome, but are also highly correlated with one another. In the setup we just described, it may not be possible to distinguish which of these variables has the “true” relationship with the signal variable. In that case, what behavior do we desire from an error criterion and how do the criteria we have proposed behave?

For the usual univariate definition of a false discovery, all of these correlated variables will be considered correct detections, since they carry some information about the variable. However, this is not likely to be the behavior we are interested in, since the use of a multivariate model in the first place expresses interest in capturing “unique” signal of some kind.

In the full model definition of a false discovery, each of these variables is “interesting” only if they capture unique signal among all the variables being considered. Because of the high collinearity, it will be impossible to distinguish a unique signal that is captured by any one of the variables. As a result, they would all appear as false selections in practice.

Furthermore, if the selection procedure were guided by an attempt to control the full model FDR, it would discourage the selection of any of these variables because of the other highly correlated variables in the data set. As a result, it would be likely that such a procedure would fail to select any of these variables, even though any one of the variables could carry most of the predictive power of the data set.

Contrast these behaviors with that of the proposed FVR criterion. As we have discussed, a variable is considered interesting by FVR if it captures unique signal among all the selected variables. Consider a selected set that contains only one of the highly correlated and predictive variables. While the full model definition would consider it a false detection, the FVR definition considers it a correct selection because it is adding unique explanatory power to the selected set of variables. Furthermore, if several of these correlated explanatory variables are added, only one of them (it does not matter which) will be considered a true detection by FVR and the others will be considered false. This makes intuitive sense, as the group of correlated variables should be able to contribute “one variable” of explanatory power.

We believe that in many settings, this is the interpretation that is being sought for a false discovery rate. It is helpful to have a criterion that agrees with this interpretation, and it is convenient that defining the criteria in terms of the projected model gives this interpretation.
3.3.2. Stability to the set of considered variables. Another non-intuitive property of the full model FDR concerns its stability to changes in the data set. Suppose that our data set contains just two variables (call them 1 and 2), each of which captures some of the signal in the dependent variable. This scenario is shown in Figure 8(a). Imagine that a variable selection procedure selects both of these variables. Under the full model definition of FDR, both of these selections are considered correct. Now suppose that the data set had included another variable 3 that is very well correlated with the signal, so that variables 1 and 2 are uncorrelated with $y$ conditional on variable 3 (Figure 8(b)). Then under the full model definition of FDR, both variables 1 and 2 would now be considered false detections, even if variable 3 was not selected! The FDP of the selected set changes from 0 to 1, without any change to the variables included in that selected set.

![Figure 8](image.png)

This emphasizes that the full model FDP is not a property of a selected set, but of both a selected set and of the full data set being considered. The FDP is incredibly unstable to changes in the full set of variables being considered. The implications of this are worrisome in settings like gene screening, where the variables being measured may be a matter of convenience and the existing microarrays, rather than careful design for a particular experiment. Meaningful interpretation of the full model FDR depends very heavily on an understanding of the entire data sample that was collected and analyzed.

3.3.3. Summary. In this section we described practical examples of how the full model definition of FDR clashes with the intuitive interpretation of a false discovery rate when the predictors are correlated. We saw that when several correlated variables are capturing essentially the same signal, the FDP can be unstable and, in the presence of noise, the FDR for the selected variables can be high even if the variables are capturing a strongly predictive signal. In contrast, the FVP and FVR behave intuitively in the presence of correlated explanatory variables such as these, counting the first such variable to be selected as an interesting selection, and any of the following such variables uninformative.

In addition, we showed that the FDP and FDR are highly sensitive to all the variables included in the data set, even those variables that are not selected. As a result, the usefulness of the full model FDR depends on a careful understanding of all the variables being considered in the data set. The FVR avoids some of this trouble, since it is not affected by unselected variables in the data set.

It is worth noting that there are cases where the full model FDR is the correct definition to use. First, if the predictors are uncorrelated, all three definitions of a false selection are equivalent.
Second, there are scientific setups where the interpretations described above are the desired ones. Suppose one has carefully selected all the variables being considered, and that a guarantee is desired that any selected variable is actually uniquely related to the signal among all the variables being considered. Then one might desire to only select a variable if its relation without outcome $y$ stands out among all the variables. If two variables cannot be distinguished, the scientist might not wish to select either until enough data can be gathered to distinguish between them. In that setting, the FDR definition will have the proper interpretation. However, we feel that in the majority of experimental setups, particularly experiments where the focus is on screening, the FVR definition is more in line with research goals and intuitive interpretations.

We conclude this section with a simple simulation. This simulation demonstrates the differences in behavior between FDR and FVR when evaluating stepwise regression on a set of correlated variables. The simulation is constructed to fit the setting of Section 3.3.1, where predictive variables are present but appear in strongly correlated groups.

3.4. Simulation Example. To see the difference in behavior between the full model definition and our projected model definition, consider the following simple setup, illustrated in Figure 9.

![Fig 9. Illustration of the simulation setup for Section 3.4. Nonzero elements of $\Sigma$ and $\beta$ are shown by the shaded rectangles, and the graph illustrates the corresponding joint dependence structure of $X$ and $y$.](image)

We create several blocks of variables, each of which is highly correlated internally. For a subset of the blocks, we select one variable within the block to have a nonzero coefficient in $\beta$. The structures of the resulting matrices are shown in 9, along with the corresponding dependence graph.

We choose this setup because we expect it to demonstrate a strong difference between the methods. The correlation within the blocks is strong enough that the selection method will be unable to distinguish the true signal variable within each correlated block, but the signal associated with the nonzero coefficients is large enough to be detected at the group level. As a result, selection methods should be able to pick those blocks that have signal, but choosing the “correct” variable within each block should be nearly random. By the usual full model definition of a false selection, these selections will be counted as false. By our new definition, it is recognized that any variable within that block carries essentially the same signal, so the first selection within each block will be considered correct.

The plots of the true population FDR and FVR are shown in Figure 10. This particular simulation has 20 blocks of two variables each. Ten of those blocks are selected to have a nonzero coefficient in $\beta$ for one of the variables. The correlation within each block is 0.95, the additional noise on $y$ is 0.8, and the total number of observations is $n = 50$.

We see that the usual FDR criterion finds a false discovery rate of about 40% for the first 10 selections, while our new criterion gives an FVR of nearly zero for the first 10 selections. These ten
selections correspond to correctly selecting the ten blocks with signal, though not necessarily the variable within those blocks with nonzero $\beta$ coefficient.

While there are situations where both criteria could make sense, we believe that in many settings, the value reported here for FVR is more in line with people's interpretation and goals in these settings. The first ten variable selections were highly predictive about $y$, and it is often reasonable to have a sense of false discovery rate that is in line with this fact.

4. Estimation of False Variable Rates. In this section, we discuss estimation of FVR. Classically, estimation of FDR in the regression setting has been quite difficult when the variables are correlated (Lin, Foster and Ungar, 2011, e.g.). We expect the FVR to be easier to control, since it is more closely related to traditional variable selection procedures. Nevertheless, more development of good estimation and control procedures is needed.

In this section, we will construct a very simple, illustrative estimate of FVR for stepwise regression. This is not intended to be the ideal estimator of FVR, it should instead be viewed as an illustration of FVR and how one might approach its estimation. Through simulation, we will demonstrate that this simple estimator works reasonably well, even with correlated predictors, providing further evidence that FVR may be an easier target for control.

We will also examine the assumptions behind this estimation scheme and the regimes in which this simple estimation procedure breaks down. These weaknesses are instructive, as our procedure shares those limitations with several recent methods for controlling false selections in regression. We hope that a better understanding of this simple estimator can inform the construction of future estimators.
4.1. **Motivation for the Estimator.** The motivation for this algorithm comes from the idea that at each step of stepwise regression, the procedure admits the variable that appears to capture the most signal *once the effects of the other currently selected variables have been removed*. This approach is in the same spirit as the FVR criterion we have been discussing.

At each step, we can imagine the hypothesis that the new model is a true improvement over the old. This is the usual statistical hypothesis comparing two nested models, where we test whether the coefficient of the new variable is zero in the larger of the two models. We will neglect for a moment that the selection of the variable would make the usual tests for this hypothesis invalid.

If we look at the number of these incremental hypotheses that are “null,” this seems similar to the number of false selections as defined in the FVR. While this statement is not necessarily true in reality, there is a relationship between these two quantities. We will make this relationship more explicit later in this section and justify it more carefully. Using this relationship, our simple algorithm will amount to estimating the number of null incremental hypotheses that were traversed in arriving at our selected model.

4.2. **Algorithm.** Before delving into a more careful justification of our algorithm, we present it in its complete form here.

To avoid issues with inference after selection, this algorithm relies on random splits of the data to separate the selection and inference stages. The following algorithm describes the action for one random split of the data.

1. Split the data randomly into two pieces, call them $X^{(1)}$ and $X^{(2)}$. For convenience we use even splits, though this is not necessary.
2. On $X^{(1)}$, fit a stepwise selection path. This gives an ordering $P$ to all $p$ of our variables, by the order in which they are selected. Notationally, we define $P_j$ to be the set of the first $j$ variables in the ordering.
3. Define the incremental hypotheses $H_j^{(P)}$ as follows. Let $\ell_j$ be the variable added at the $j^{th}$ step in $P$. Let $\beta^{(P)}$ be the coefficients of the model projected on $X_{P_j}$, the $j$ variables selected by step $j$. Then
   \[ H_j^{(P)} : \beta^{(P)}_{\ell_j} = 0, \]
   which is just the hypothesis that the $j^{th}$ addition was not a useful one (at the point that it was added).

   For each hypothesis $H_j^{(P)}$, we can obtain a $p$-value $p_j$ through the usual $F$ or $t$ test of the nested models, using the data from $X^{(2)}$. This inference is valid because our variables were not selected on $X^{(2)}$. Nonparametric tests, like those based on permutations or the bootstrap, can also be used here to avoid distributional assumptions.
4. For each model size $k$, we now estimate the number of null hypotheses in our set of hypotheses $\{H_j^{(P)}; j = 1, \ldots, k\}$. We use a threshold estimator as in Storey (2002), giving the estimator
   \[ \hat{V}_k^{(\lambda)} = \frac{\# \{p_j > \lambda; j \leq k \}}{(1 - \lambda)} \]
   for any threshold $\lambda \in (0, 1)$. We will show that $E \hat{V}_k$ bounds the number of null hypotheses in $\{H_j^{(P)}; j \leq k\}$.
5. The estimate from this split for the FVR for model size $k$ is $\hat{V}_k^{(\lambda)}/k$. 

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We average these estimates, \( \hat{V}^{(\lambda)}_k / k \), over many splits of \( X \) to obtain a final estimated FVR for each selected model size.

In the remainder of this section, we will provide justification for this algorithm and present simulation results.

4.3. **Justification.** In this section we will provide justification for the estimation procedure presented in Section 4.2. Due to the length of some of these explanations, some of the details have been moved to Appendix A.3 and summaries are presented here.

There are three pieces of this algorithm that require justification.

1. That the hypotheses \( H_j^{(P)} \) resulting from the selected path \( P \) are appropriate hypotheses to be looking at, in the sense that the number of null hypotheses in \( \{H_j^{(P)}\} \) should correspond to the number of false selections appearing in the FVR definition.
2. That we are estimating the number of true null hypotheses in the set \( \{H_j^{(P)}\} \) in an appropriate way.
3. That splitting the data give reasonable estimates of the quantity of interest.

We will address each of these points in the following subsections.

4.3.1. **Appropriateness of \( H_j^{(P)} \).** Here we argue that the hypotheses \( \{H_j^{(P)}\} \) corresponding to the steps of the selected path are reasonable hypotheses to consider, in the sense that the number of true null hypotheses in \( \{H_j^{(P)}\} \) should be a good estimate of the number of variables with zero coefficients in the final projected model. In cases where the variables are correlated, there is no reason that this should be true for the incremental hypotheses corresponding to a general ordering of the variables.

The details of this argument can be found in Appendix A.3. The general idea is that there exist particular orderings of the variables for which the number of null incremental hypotheses is exactly the number of zero coefficients in the projected model. Furthermore, the ordering produced by stepwise selection is not too far from these ideal orderings, so the resulting estimate is not badly biased.

This dependence on the ordering of the variables has implications for FVR and FDR estimation. One is that the estimation method of Section 4.2 can only be extended to selection methods that provide a reasonable ordering of the variables. Similarly, one should be wary of potential bias in other methods that estimate FVR or FDR based on the incremental hypotheses along a variable ordering, particularly those that rely on random or arbitrary orderings.

4.3.2. **Justification of the threshold estimator.** The next piece of the algorithm uses a threshold estimator, as in Storey (2002), to estimate the number of true null hypotheses in \( \{H_j^{(P)}\} \) based on the \( p \)-values \( p_j \).

We can show that the expectation of the threshold estimator \( \hat{V}^{(\lambda)}_k \) is an upper bound on the number of true null hypotheses in \( \{H_j^{(P)}\}, j \leq k \):
This bound depends only on the \( p \)-values from the true null hypotheses, so the bound will be loose when there is a large contribution from the false null hypotheses. This will happen when the \( p_i \) corresponding to the false nulls have a significant probability of exceeding \( \lambda \), or when there are a large number of false null hypotheses in the selected set. This is demonstrated in the simulation in Figure 13.

This also suggests a bias-variance trade off when selecting \( \lambda \), as a large \( \lambda \) will give a smaller bias but a larger variance. Appendix A.2 mentions a bootstrap approach to calibrating \( \lambda \), like that of Storey (2002).

4.3.3. Effects of splitting. Because we split our data and use the two halves in our estimator, the quantity we are estimating actually corresponds to the FVR for a data set with half as many observations. As in cross validation, it is reasonable to wonder what effect this has on our estimate.

The sample size influences the true FVR only through differences in the resulting variable orderings from stepwise selection. As a result, we expect the true FVR values for both sample sizes to be reasonably close, and for the uncertainty in FVR estimation to dominate the difference in most cases. This is supported by the simulations of Section 4.4.

In the cases where the true FVR values do diverge, the value for the half-sized data set will be larger, leading our estimate to be conservative. We observe this for particularly noisy data in Figure 14.

4.4. Simulation. Here we present simulations of the performance of our estimation method for FVR in stepwise regression. We will see that the method performs well overall. We will also simulate under parameters specifically selected to demonstrate the potential biases discussed in Section 4.3.

For these simulations, we use blocked settings similar to those used in Section 3.4 and illustrated in Figure 9. These examples are constructed to clearly illustrate the difference between FVR and FDR, and to show how our estimates relate to those quantities. To do so, the parameters are chosen so that the blocks of variables will be reasonably significant, but the variables within the blocks are correlated enough to be difficult to distinguish in the presence of noise. For convenience, the parameters of all the simulations are laid out in Table 2. All of these simulations use \( \lambda = 0.5 \) for the threshold in the estimator. All estimates are obtained by averaging 50 splits of the data set. All curves and standard errors are the result of 100 Monte Carlo simulations.

|          | \( n \) | # blocks | # per block | # signal | \( \sigma \) | \( \rho \) |
|----------|--------|---------|-------------|--------|---------|--------|
| Figure 11| 100    | 20      | 2           | 6      | 0.8     | 0.95   |
| Figure 12| 100    | 5       | 3           | 3      | 0.5     | 0.95   |
| Figure 13| 100    | 20      | 2           | 10     | 0.5     | 0.95   |
| Figure 14| 100    | 20      | 2           | 10     | 2       | 0.95   |

**Table 2**

Parameters for the simulation settings used to make Figures 11, 12, 13 and 14. The parameters are number of observations, number of blocks of variables, number of variables per block, number of blocks where one variable is made significant, noise variance, and within block correlation. The coefficient for any significant variables is fixed at 1 across all simulations, and all estimators use \( \lambda = 0.5 \).

Ideal performance of our estimate can be seen in Figure 11. The plot shows the true FVR for both the full sample size and the half sample size (in black and red, respectively), along with the true FDR (dotted black) and our estimate (green). We show both of these true FVR values to demonstrate that splitting our sample has not dramatically altered our target quantity, as discussed in Section 4.3.3.
In the simulation shown in Figure 11, stepwise selection correctly selects the six groups with signal, but not the particular variable within each of those groups. Thus the FDR is reasonably large from the beginning, as we would expect from the construction of the example, while the FVR remains low. We see that the FVR estimate, using the method from Section 4.2, closely matches the true FVR for both sample sizes.

The simulation in Figure 12 illustrates the low bias in our estimator due to incorrect ordering of the variables, as discussed in Section 4.3.1. This simulation is constructed to have a few signal variables, along with many very strongly correlated noise variables in relatively low noise. When the noise variables enter early in the path, they temporarily appear informative due to spurious correlations. This causes a downward bias in the estimated number of false selections.

The simulation in Figure 13 illustrates the upward bias in the threshold estimator that was discussed in Section 4.3.2. Here many signal signal variables into the simulation. The FVR estimate (green) is biased upward from the true values (black/red), particularly at the start of the path. While this is worrisome, it is comforting that the dramatic bias is upward, leading to conservative estimates. The selection of $\lambda$ in this simulation was made without tuning to reduce this bias; bootstrap calibration as in Storey (2002) might help to reduce this bias.

Finally, the simulation is conducted with a much higher noise level, shown in Figure 14. This has the effect of inflating the difference between true FVR values for the full and half samples. The half sample FVR (red) is now larger than the full sample FVR (black), implying that the additional information from the larger sample is important for obtaining good selections. Our estimate (green) is estimating the higher of these curves, and is therefore very conservative.

We see from these simulations that the proposed estimator works reasonably well in simulation. The biases discussed in Section 4.3 do exist. The downward bias from relying on the stepwise selection ordering appears to be weak in practice and to occur mostly in the later part of the selection path, supporting our belief that stepwise selection is providing a reliable ordering. The upward bias from the threshold estimator of true null hypotheses appears when there are many
5. Conclusion. In this paper, we discussed the interpretations and implications of different definitions of false selection in the regression setting. We saw that these error criteria behave differently in cases where variables are correlated. In particular, we described difficulties for the standard full model definition, which lead to unintuitive or undesirable behavior in many cases.

As a solution, we introduced a new false selection error criteria, FVR, which is defined in terms of signal variables present in the data, but it skews the results in a conservative direction.
of the projected model. This error criterion focuses on guaranteeing uniqueness of the explanatory variables only among the selected variables, rather than the entire data set. In doing so, it avoids the concerning behaviors of the traditional full model definition, leading to intuitive behavior in many settings. We presented several interpretations of FVR, demonstrating its differences from FDR and where each criterion might be appropriate to use.

Finally, we presented a simple estimation method for FVR in stepwise regression. We showed that this method gave reasonable estimates of FVR over a range of simulation parameters. We also examined the regimes in which this estimator performed poorly, giving insight that could be helpful when constructing future estimators or assessing existing ones.

The idea that each of the error criteria impose a different idea of an “interesting” selected variable is a convenient view. The full model definition considers a selected variable interesting if it explains signal that is not captured by any other variable in the data set. In contrast, the projected model definition (corresponding to FVR) considers a selected variable interesting if it captures unique signal only among the other variables in the data set. Contrasting the error criteria in this way could help provide an intuition of which criterion is most suitable to a particular problem.

There is plenty of interesting work to be done in understanding this new error criterion. More work is needed to understand better estimation or control procedures. Very preliminary work suggests that other common variable selection procedures like the LASSO (Tibshirani, 1996) may control FVR well. Existing methods that seek to control FDR in the regression setting are also likely to have appealing FVR properties. In another direction, one can construct an analog to the False Negative Rate of Genovese and Wasserman (2002) which is related to FVR and might be interesting to consider. Our main goal in this paper has been to identify potential concerns with the accepted full model FDR definition when predictors are correlated, and to propose this new FVR criterion which may be more appropriate to consider in those settings.

Fig 14. Simulation of FVR estimate for forward stepwise selection on blocked data in a high-noise setting. This setting shows that, in the presence of high noise, the lack of data in the half samples cause that true FVR (red) to be larger than the true FVR for a full sample (black). This inflates our estimator, since our estimator splits the data and actually estimates the half-sample FVR.
APPENDIX A: DETAILS

A.1. Gaussian formulation of FVP in terms of the covariance matrices. It is particularly straightforward to compute the FVP in the joint multivariate Gaussian setting where the parameters are known. This is particularly useful when running simulations, so we include our approach here.

Suppose that \((x^{(1)}, \ldots, x^{(p)}, y)^\top\) is joint multivariate normal, with \(X \sim N(0, \Sigma)\) and \(y \sim N(X\beta, \sigma^2_\varepsilon)\). Note that

\[
\text{Cov}(y_i, x_i^{(j)}) = \mathbb{E}(x_i^{(j)}y_i) = \sum_{j'=1}^p \beta_{j'} \mathbb{E}(x_i^{(j')}) = \sum_{j'=1}^p \beta_{j'} \Sigma_{j'j'}
\]

\[
\text{Cov}(y_i, y_i) = \text{Cov}(X^\top \beta, x_i^\top \beta) + \sigma^2_\varepsilon = \mathbb{E}\left(\left(\sum_{j=1}^p x_i^{(j)} \beta_j\right)\left(\sum_{j'=1}^p x_i^{(j')} \beta_{j'}\right)\right) + \sigma^2_\varepsilon
\]

\[
= \sum_{j'j''} \beta_j \beta_{j'} \mathbb{E}(x_i^{(j)} x_i^{(j')}) = \beta^\top \Sigma \beta
\]

This lets us construct the augmented covariance matrix for \((x^{(1)}, \ldots, x^{(p)}, y)^\top, \hat{\Sigma}\).

\[
\hat{\Sigma} = \begin{pmatrix} \Sigma & \Sigma \beta \\ \beta^\top \Sigma & \beta^\top \Sigma \beta + \sigma^2_\varepsilon \end{pmatrix}
\]

Now suppose we select a set of variables \(A\). We want to assess the FVP of this set of variables. Let \(A^+\) be \(A \cup y\). The covariance matrix for the marginal distribution on \(A^+\) is just \(\hat{\Sigma}_{A^+,A^+}\). We can compute the inverse \(\hat{\Sigma}_{A^+,A^+}^{-1}\), and the FVP is the number of zeros in the row corresponding to \(y\).

A.2. Selecting \(\lambda\) for the threshold estimator. In Section 4.2, we introduce a threshold estimator \(\hat{V}^{(\lambda)}_k = \#\{p_j > \lambda; j \leq k\}^{(1-\lambda)}\) for estimating the number of true nulls in our set of hypotheses, and show that the expectation of this estimator provides a lower bound on the number of true nulls in \(\{H_j^{(p)}; i; j \leq k\}\).

As mentioned in Section 4.3.2, there is a bias-variance trade-off involved in selecting \(\lambda\). As \(\lambda\) increases, the probability of a false null hypothesis entering will decrease, decreasing the bias in the estimator. However, the probability that a true null hypothesis is counted will also decrease, increasing the variance of the estimator.

In Storey (2002), a bootstrap-based approach is presented for tuning \(\lambda\) in a similar threshold estimator of \(pFDR\). It can be shown that an equivalent condition, \(\mathbb{E}V^{(\lambda)}_k \geq \min_{\lambda'} \mathbb{E}V^{(\lambda')}_k \geq V_k\), holds for our estimator, so a similar tuning approach could be used to select \(\lambda\) for a particular application. This would mean choosing \(\lambda\) to minimize

\[
\frac{1}{B} \sum_{b=1}^B \left(\hat{V}^{(\lambda)^{sb}}_k - \min_{\lambda'} \hat{V}^{(\lambda')}_k\right)^2,
\]

where \(b\) indexes \(B\) bootstrap simulations, each of which contributes a bootstrap estimate \(\hat{V}^{(\lambda)^{sb}}_k\).
A.3. Effects of variable ordering. Here we present more details in our discussion of variable ordering and the estimator of Section 4.

Let $\mathcal{A}$ be the selected set of variables and $V$ be the number of variables in $\mathcal{A}$ with zero coefficients in the model projected onto $X_{(\mathcal{A})}$, making $V$ the numerator of the FVP for $\mathcal{A}$. Let $\mathcal{B} \subseteq \mathcal{A}$ be a minimal subset of the variables in $\mathcal{A}$, such that the projection of the true model $X\beta$ onto $X_{\mathcal{B}}$ is the same as the projection of that model onto $X_{\mathcal{A}}$. Note that $V = |\mathcal{A}| - |\mathcal{B}|$.

Suppose that $\hat{\mathcal{P}}$ is an ordering of the variables in $\mathcal{A}$ such that all the variables in $\mathcal{B}$ appear before any other variables. Then, except for very special cases, the incremental null hypothesis is false at each of the first $|\mathcal{B}|$ steps along $\mathcal{P}$. Furthermore, the subsequent $|\mathcal{A}| - |\mathcal{B}|$ steps are true null hypotheses, since the projected model has been obtained once the variables in $\mathcal{B}$ have been included. This means that there will be exactly $V = |\mathcal{A}| - |\mathcal{B}|$ true null incremental hypotheses in $\{H_i^{(\mathcal{P})}\}$, which is identical to the number of zero coefficients in the projected model.

The special cases above refer to the unlikely cases where some of the variables in $\mathcal{B}$ have exactly zero correlation with $y$ when a strict subset of $\mathcal{B}$ are conditioned upon. However, while the statements above will not hold in that case for all orderings where $\mathcal{B}$ appears first, there will still exist a subset of such orderings for which the statements hold. Furthermore, stepwise selection will tend not to select the invalid orderings, so the issue should not arise in practice.

In practice, an ideal path $\hat{\mathcal{P}}$ is not known. Our algorithm relies on the idea that the paths produced by stepwise selection are close to one of these perfectly-ordered paths. We can view a real path $\mathcal{P}$ as a modification of a “nearest” path $\hat{\mathcal{P}}$, where the path is modified by moving noise variables forward in the ordering, and the path $\hat{\mathcal{P}}$ is nearest if it requires the fewest such moves. If $t$ is the number of these erroneous moves, then at worst all $t$ improperly inserted variables will appear significant at the time of their selection. In that worst case, the quantity being estimated by looking at the incremental null hypotheses is actually $FVP - t/|\mathcal{A}|$.

This means that an improper ordering could bias the FVR estimate low, by as much as $t/|\mathcal{A}|$. The fact that this bias is downward is worrisome, since it could potentially lead to over-optimistic estimates of FVR. In simulation, we have found that stepwise regression produces orderings that are quite reasonable, leading to small $t$ and minimal bias. It could be interesting to investigate the settings in which $t$ can be shown to be controlled by stepwise selection or other methods.

ACKNOWLEDGEMENTS

The authors would like to thank Noah Simon, Alexandra Chouldechova, and Jacob Bien for helpful discussions.

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