ORIGINAL ARTICLE

The Power of Noise and the Art of Prediction

ZhiMin Xiao[1]* | **Steve Higgins**[2]

[1, 2]School of Education, Durham University

Correspondence
School of Education, Durham University, Durham, DH1 1TA, UK
Email: zhimin.xiao@durham.ac.uk

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Data analysis usually aims to identify a particular signal, such as an intervention effect. Conventional analyses often assume a specific data generation process, which suggests a theoretical model that best fits the data. Machine learning techniques do not make such an assumption. In fact, they encourage multiple models to compete on the same data. Applying logistic regression and machine learning algorithms to real and simulated datasets with different features of noise and signal, we demonstrate that no single model dominates others under all circumstances. By showing when different models shine or struggle, we argue it is both possible and important to conduct comparative analyses.

KEYWORDS
Cross-Validation, Evidence-Based Policy, *K*-NN, Logistic Regression, Prediction, Random Forests

1 | TWO MODELING APPROACHES

Data analysis is usually about identifying signal from noise. But data, particularly social science data, can be truly noisy, partly because the outcome is often a human construct, which can only be measured with some error. Noise can also stem from other factors, such as the collection of data on variables that are uncorrelated with the outcome of interest, or unmeasured variables that have an effect on the outcome, or simply high dimensionality as a result of interaction and/or the addition of higher order terms, which can easily fail in-sample goodness-of-fit tests (Breiman, 2001). The

noise mentioned above can be minimised in careful research designs and sound data analyses. Nevertheless, theories about best designs and views about best analysis plans can be another source of noise, because the best approach to data analysis for a given study often differs in theory from person to person, even for those who are from the same discipline. Moreover, single best models cannot be statistically compared unless some of them are nested within others (Shmueli and Koppius, 2011). Donoho called the analytical approach that relies on single best models "generative modeling" (2015), where a data generation process is assumed and a single best model, which must exist because of the assumptions made, is then deployed to analyse the data. But the choice of that model can itself be a source of variation in results because of the theoretical differences mentioned above. Consequently, the model may lead to "irrelevant theory and questionable scientific conclusions" (Breiman, 2001) because it is usually more about a data generation and selection process than about how the real world functions or the underlying problem to be solved. When published, the results may further justify the choice of the theoretically best model in subsequent studies, particularly when they are linked with research funding streams, which in turn can make the results more salient or more noticeable in the literature. This feedback loop can be pernicious (O'Neil, 2016), if policy decisions made on the evidence from a single best model produce unintentional and undesirable consequences (Merton, 1936) to those who participated in the studies and/or beyond.

Generative modeling can be theoretically best because of the asymptotic guarantee: if an intervention is to be repeated many times until all samples in a population are exhausted, the model is guaranteed to predict the correct outcome. This sounds reassuring, but in reality, we do not live in an "asymptopia" (Domingos, 2012). This implies that, if model A is better than model B given infinite data, due to bias-variance trade-off, there is no guarantee that the former will be better than the latter given finite data or a particular dataset. Therefore, we also need "predictive modeling" (Donoho, 2015; Hofman et al., 2017), which is generally agnostic about a data generating mechanism and allows multiple models to learn from and work on multiple datasets. Some of these are used to train the models, others are put aside as test sets, just as we turn a ball many times and each time we make a prediction about the patterns on the side we do not see using the information on the side we can see. The performances of the trained models are then judged against a common task, usually, predictive accuracy on test sets, which is easy-to-understand and can be compared across datasets and over time (Breiman, 2001; Donoho, 2015; Hofman et al., 2017; James et al., 2015).

Predictive modeling thus provides timely feedback for analysts to assess how successful the tools they have deployed actually are in the wild. As a result, the best performing models can be efficiently deployed for real-world applications, which can then enhance the roles evidence has to play in decision making and reduce the gap between research and practice (Shmueli, 2010). This approach overcomes one problem of single best models, where different analysts analyse the same dataset in their own manner and may produce different results and make different claims about the performance of their preferred methods (Breiman, 2001; Donoho, 2015; Hand, 2006; Xiao et al., 2016). If we do not know which, if any, of the best models actually worked because of the problems associated with in-sample strength-of-fit measures (Breiman, 2001; Shmueli and Koppius, 2011), the conclusions drawn from the results of single best models may be too dependent on error or noise making them effectively just noises themselves. This only adds to the challenge of evidence-based policy and practice by confusing decision makers with varying advice. In many social science studies, such as the educational interventions funded by the Education Endowment Foundation (EEF) in the UK, predictive modeling is yet to be widely appreciated (Shmueli and Koppius, 2011), despite the aforementioned advantages and its rapid development in other fields as well as its capability to work on large and small datasets of varying levels of complexity.

The process of randomly splitting data into training and test sets can transform the technical procedure of generative modeling into that of predictive one. This avoids denying the inferential contributions generative modeling has made and avoids dichotomising analytic approaches. To find out when different models shine and others struggle, we apply conventional logistic regression and some machine learning techniques to real and simulated datasets.

2 | THE FALLACY OF MORE DATA

In this study, we first show that measurement error in some outcome of interest can mask the relationship between covariates and the outcome. In the simulation, we suppose the outcome is an unweighted mean of two covariates, which, together with the outcome and other variables, come from a normal distribution with the same mean of zero and standard deviation one. To add measurement error into the outcome, we introduce a normal distribution with

the same mean but different standard deviations, which represent the strength of the noise in the outcome. Figure 1 visualises the effect of measurement error on the correlations between the outcome and the two signal variables, X_1 and X_2. As the noise gets louder and louder, the correlation coefficients between the outcome and the two signal variables become smaller and smaller. This change is not affected by the change in sample size, which suggests that the common focus on larger sample sizes to detect an intervention effect might be inappropriate when the outcome measure is prone to errors. For educational interventions, such as those funded by the EEF, it is therefore crucial to choose the right test as an outcome measure. Otherwise, the real effect of an intervention might never be detected, even when the sample size in a given study is large, if there is substantial measurement error in the test (see also Loken and Gelman, 2017). An example of this can be found in the Building Blocks intervention in the US, which might have suffered from some measurement error, where the large-scale pre-*K* program focused on skills such as counting that children will eventually master as they grow, even without the intervention (Mervis, 2017). To avoid this mistake, the EEF normally requires independent evaluators to pre-specify a standardised national test, which minimises the effect of the noise in measurement at either baseline or post-test.

Noise does not simply exist as measurement error. It can also exert its power through covariates, particularly when there are interactions among them. In social science research, there is usually a tendency to collect data on as many covariates as possible. This is partly due to competing theories that inform data collection. As an example, the association under the miasma theory in the mid-1800s between cholera and personal habits and characteristics, such as strong emotions like fear and immorality, specifically overindulgence in alcohol and sex, predispositions often linked at the time with the "lower classes" (Tulodziecki, 2011). But it also has something to do with the more the merrier philosophy, according to which, more information on as many variables as possible, at worst, provides no extra information about the outcome. However, one risk of the practice may be that the benefits of having more data on irrelevant covariates can be sometimes outweighed by "the curse of dimensionality" (Domingos, 2012).

Again, we use simulations to illustrate the power of noise, particularly when there are interaction terms. Suppose the outcome this time is a categorical variable with two possible values of one and zero in an educational intervention. When it takes on the value of one, it means a student gained from the intervention. Otherwise, the student made no progress from baseline to post-test. At the beginning of the intervention, we also had a number of baseline measures,

among which there might exist interactions. First, let's suppose an interaction exists between two covariates. We implement this interaction effect by randomly shifting half of the observations in the covariates up by one unit, and the other half down by one unit. We also adjust the outcomes accordingly so that observations that were randomly shifted up are more likely to take on the value of one, and those shifted down less likely to be one. Apart from the two covariates that are interacted, there are also others that are neither interacted with one another nor correlated with the outcome variable. Those null variables are in effect noises, which vary in number from dataset to dataset, as the earlier measurement errors vary in strength from one simulation to another. To illustrate the effect of interaction terms in the simulated data, we have produced some pairwise scatter plots. As shown in Figure 2, when there is no interaction, the observations in any pair of variables are randomly scattered. But, as we increase the power of an intervention by randomly shifting up or down observations in interacted covariates by more than one unit, the outcomes become increasingly separable and the interaction effect is clearer.

To analyse the simulated datasets, we introduce a number of analytical models, which are logistic regression, random forests, and k-nearest neighbours with k taking on varying number of values (James et al., 2015). To show how stable those analytical models are, we also simulate each specification three times, which results in three performance outcomes for each of the models mentioned above. As shown in Figure 3, the performance of logistic regression is no better than tossing a coin when there is just one interaction term. Random forests have higher predictive power when the sample sizes are larger. K-NN outperform others when the values of k are appropriate in a given simulation. When sample size is 100, the most appropriate k is between 5 and 10, as sample size increases to 500 or 1000, the most appropriate k is about 100. However, the results are much more stable when the sample size is 1000 across the three simulated datasets.

The scenario described above involves only one interaction term in the simulated dataset. Now let's see how the models perform when we increase the power of noise and signal by adding more interaction terms and null variables. As we can see in Figure 3, when there are two interaction terms, random forests can almost match K-NN at the most appropriate value of k. Logistic regression again crumbles, regardless of the strength of signal and noise in the simulated data. Nevertheless, when the number of interaction terms climbs up to five, the only model that can achieve acceptable predictive accuracy (or low test error) is K-NN at the right level of k, of which the choice is much narrower than when

there are only two interaction terms.

In the above-simulated datasets, the conventional logistic regression is no better than guesswork even when a single interaction term exists. This does not suggest that it is no use at all. For the logistic regression to have higher predictive power, we can add into the regression an interaction term, which will substantially improve the predictive accuracy of the model. The addition of the interaction term is straightforward when we know which variables are interacted and when the number of covariates is not large so that we can explore all possible pairwise combinations of covariates in the data. But when there are many variables in a dataset, as is the case in many social science studies, it will be practically impossible to exhaust all possible combinations. Usually, analysts of social research data add interaction terms when a theory suggests them what covariates are likely to interact with one another. If serious interaction exists but analysts fail to address it accordingly, the logistic regression will produce evidence that is inadequate to inform decision making. The so-called evidence would be just another source of noise in the literature. Given that we normally do not know how many interaction terms exist in a dataset and it is prohibitive to examine all the combinations when there are as few as ten covariates, it is no surprise that machine learning techniques such as random forests and K-NN are increasingly perceived to be better models for data analysis. As it becomes easier and perhaps less expensive to collect more data, these techniques are likely to appeal to more and more social scientists in the years to come. But they also have limitations, as the above simulations show, when there are five interaction terms or more, random forests are no better than logistic regression, even when the signal is strong.

3 | THE FALLACY OF FREE LUNCHES

The simulations described above are, after all, only simulations. The performances of these models may change when they are tested on a new dataset with different features. In this section, we use a dataset that is openly available to the public and well-known to the machine learning community (LeCun et al., 1998). The dataset has 60,000 observations in the training set and 10,000 in the test set. Each observation represents a hand-written digit ranging from 0 to 9, and there are 784 columns, each of which contains values that represent degrees of grey. To see which model has

the highest level of prediction accuracy in reading the digit 8 in the test set, we use observations from the training set to train candidate models, which are then used to predict the outcome in the test set. In the training, we also alter the number of sample sizes in each re-sample, so that we can observe how the models learn from the data. The models trained are logistic regression, decision trees, bagging, and random forests (James et al., 2015; Liaw and Wiener, 2002). We exclude K-NN for this dataset because it is known to have high predictive accuracy in reading hand-written digits (Domingos, 2012) and the main purpose of using this dataset is to show the effect of input knowledge on the performances of conventional and machine learning techniques. The last three of the learners selected are related, because each decision tree is a hierarchy of cuts using either continuous or categorical variables, and bagging refers to bootstrapped aggregation, where each bootstrapped re-sample is used to grow a decision tree. Since bagging uses all features in each re-sample, and variables that are highly correlated with the outcome are likely to be selected first, the algorithm will produce very similar trees in the end. Random forests overcome this problem by randomly choosing a subset of features in each bootstrapped re-sample of the data. As a result, the trees grown in the model will be very diverse, and the average performance of the forests is usually better than that of bagging (James et al., 2015). However, the algorithm of random forests runs much faster than that of bagging. A useful metaphor is that it is like randomly opening a subset of drawers in a chest of drawers that contain different pieces of information about the outcome, rather than all the drawers each time.

Figure 4 (b) shows the performances of the four models mentioned above. As we can see, when the training sample size is 300, the accuracy level of logistic regression is slightly above 50%. However, when the sample size increases to about 1000, logistic regression can achieve about 80% accuracy, which slowly increases as more samples are used to train the model. Nevertheless, it is no match for the other three machine learning techniques, particularly when the training size is small. This dataset is unique in the sense that there are 784 covariates, when the training size is below 1000, logistic regression really struggles in pulling the accuracy level up to those of its counterparts, which have at least 90% accuracy even when sample size is as low as 300. Their performances, particularly those of random forests, increase as more and more training data are fed into them. However, it is worth mentioning that the computational costs for bagging and logistic regression are remarkably high, although they can achieve comparable accuracy levels of random forests in this case. The performance of decision trees also increases as training samples increase, but it is less

accurate than bagging and random forests. Decision trees are said to be highly sensitive to changes in the data (James et al., 2015), but in this case, its performance is acceptable and it does not take long for the algorithm to run.

As we have demonstrated, developing models with high predictive accuracy requires a lot of "black art" (Domingos, 2012), which can rarely be found in statistical textbooks. Although conventional logistic regression can eventually achieve a similar level of accuracy to that of random forests in the above case, the latter can get more from less and it runs much faster than the former. The results reported above also show that machine learning techniques cannot do magic without input knowledge. There is no such thing as a free lunch. But they can, as with a lever, turn a small amount of input into a large amount of output, but this obviously varies from model to model (Domingos, 2012).

So far, we have used simulated and real datasets to test and compare the performances of both logistic regression and machine learning techniques such as decision trees, bagging, and random forests. When there are more variables than observations in a dataset and there are very few interaction terms, the performance of random forests is truly impressive in terms of predictive accuracy. Unlike logistic regression and bagging, it is not computationally expensive to run. Moreover, it does not require analysts to fine tune many parameters, such as the values of k in K-NN. Unsurprisingly, it appeals to more and more analysts.

4 | THE FALLACY OF SINGLE BEST MODELS

Next, we use a few further datasets from large scale educational interventions funded by the EEF in England. Unlike the datasets we have seen so far, EEF datasets are highly curated and structured. In three of the four cases that follow, participants were randomly assigned to intervention or control groups, and the tests used in the trials were standardised national tests in England, suggesting that the measurement error is likely to be low. As in earlier datasets, observations are randomly split into training and test sets, the models are first trained in the training set, and then tested for their predictive accuracy, test error, sensitivity, and specificity. Four out-of-sample performance metrics are used this time because the costs associated with different misclassification errors can be different (Hand, 2006). Since there are many ways to split the data into training and test sets, we report the results from two splitting methods, the first rows use 68%

of the observed samples in the interventions to train the models and the rest as test sets. The second rows result from bootstrapped training and test sets, meaning sample sizes in the training sets are equal to the observed sample sizes of the interventions. However, some observations will be selected more than once for the training sets while others will not be selected at all, which are then used as test sets. As expected, the two rows in Figure 5 (a–d) have almost identical results across all the metrics. This is ideal because we do not want the results to be sensitive to different cross-validation methods. The four datasets also vary in sample and effect sizes. Using zero gain as the cut-off, the outcome takes on either one or zero, meaning either progress or no progress in the tests at the end of the interventions.

Before we look at the results, we will provide some background information about the trials. The metacognition intervention, called ReflectED, aimed to improve pupils' ability to think about and manage their own learning (Motteram et al., 2016). It is a school-based randomised controlled trial with randomisation at class level. In the final analysis, the study involved 1507 pupils from 30 schools, and the primary outcome was age standardised mathematics score. Chess in Schools is an intervention that randomly allocated 100 schools (4009 pupils) to either intervention or control. Intervention schools taught children how to play chess over a year, whereas control schools were business-as-usual. The primary outcome was Key Stage 2 mathematics score one year after the intervention (Jerrim et al., 2016). Improving Writing Quality is a smaller intervention with a large effect size. It involved 261 pupils from 23 primary schools, which were randomly allocated to receive training on writing or to continue with business-as-usual (Torgerson et al., 2014). Unlike the first three, Tutor Trust Secondary is a quasi-experimental design, which matched 781 participating pupils with 100,991 others in a comparison group who did not participate in the small group or one-to-one tutoring intervention but had similar demographic and socio-economic characteristics (Buchanan et al., 2015). The outcome chosen for this study is performance on GCSE mathematics.

Figure 5 shows the performances of three models, which are logistic regression, random forests, and K-NN with varying number of neighbours in the training set used for prediction on the test set. As for predictive accuracy in (a), random forests have the most impressive performance, which is followed by logistic regression. K-NN, across all values of k, do not perform as well as expected. However, when k is 100, it has the highest level of specificity, meaning when the outcome is zero, the model accurately predicts zero with the highest level of accuracy. This model is therefore less likely to produce false positives than others for this intervention. In terms of sensitivity, logistic regression and random

forests are about equal. When k is 100, K-NN has the lowest level of sensitivity, which means it has the lowest level of predictive accuracy when the outcome is one and it accurately predicts one. This model is thus more likely to produce false negatives. In sub-figure (b), logistic regression and random forests perform about equally well in terms of accuracy and test error. However, the former has the highest level of specificity and the latter the highest level of sensitivity. K-NN, again, is far behind the first two across all metrics of performance. In (c), the performance of logistic regression is better than any other model considered across all the metrics. Random forests closely follow that of logistic regression. Given the large sample size and imbalanced structure of the data in (d), random forests and K-NN truly shine in all aspects.

As we can see, across the four trial datasets, higher levels of accuracy always correlate with lower levels of test error, but higher levels of sensitivity do not always imply lower levels of specificity. The patterns thus suggest that it is important to compare model performances across multiple metrics. Besides, random forests, while impressive when sample size is relatively large, are not necessarily better than conventional logistic regression. When the sample size is relatively small and the data is clean and well structured, the widely perceived superior machine learning technique cannot outperform its conventional counterpart. However, this does not imply that more experienced users of random forests cannot fine tune its parameters to "squeeze" the best performance out of it (Domingos, 2012; Hand, 2006).

5 | CONCLUSION

Taken together, we have demonstrated that no single model dominates others under all circumstances. Most studies using single best models explain why their models are the best, but say little or nothing about how or why their predictions or inferences might be wrong (Subrahmanian and Kumar, 2017). To demonstrate the risks of taking this approach, we have shown both. For instance, logistic regression is no better than tossing a coin when sample sizes are small, and when there are more covariates than observations, not to mention the roles interaction terms may play. Random forests are no better than logistic regression when there are many interaction terms and when the noise swamps the signal. K-NN at the appropriate value of K can achieve the lowest level of test error, even when there are

many interaction terms and null variables. However, they are far behind logistic regression and random forests when the data are "overly clean" (Shmueli, 2010) and the observations are very similar across intervention and control groups, in which case, *K*-NN at all levels of *K* simply make random predictions. The findings from all the datasets used in the study thus present a compelling case that single best models cannot be known *a priori* and it is crucial to cross-validate results and compare model performances using multiple metrics.

This is a troubling time for evidence-based policy, partly because we do not always agree on what constitutes as the best evidence, but it also stems from the fact that the path from knowledge to power is not always linear. Evidence is just one ingredient that goes into the policy mix (Malakoff, 2017). In order to present the best possible evidence, the conclusions made above are ever more important. As we do not live in an asymptopia and sometimes decisions have to be made in a timely fashion, we can no longer safely say at the end of an intervention that the findings are mixed, therefore more studies are needed. When an answer straddles both sides of "maybe", it precludes accountability (Tetlock et al., 2017). So, we suggest that one way forward is to concede our exclusive reliance on generative modeling, which risks producing research results that may have little relevance to practice. Although the theoretical approach can have high in-sample explanatory power or breadth, it does not necessarily follow that its out-of-sample predictive power will be precise (Trafimow and Uhalt, 2015). Therefore, it is important to make sure that research findings from social science research such as the educational interventions in this study can explain the causal mechanism well, but also have sufficient predictive quality (Shmueli, 2010), or give us some idea, in advance, of what impact an intervention will have, for whom and where (Clauset et al., 2017). Otherwise, the gap between methodological advance and practical application will be widened and the path of evidence to impact becomes even more winding.

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CONFLICT OF INTEREST

We have no conflicts of interest to disclose.

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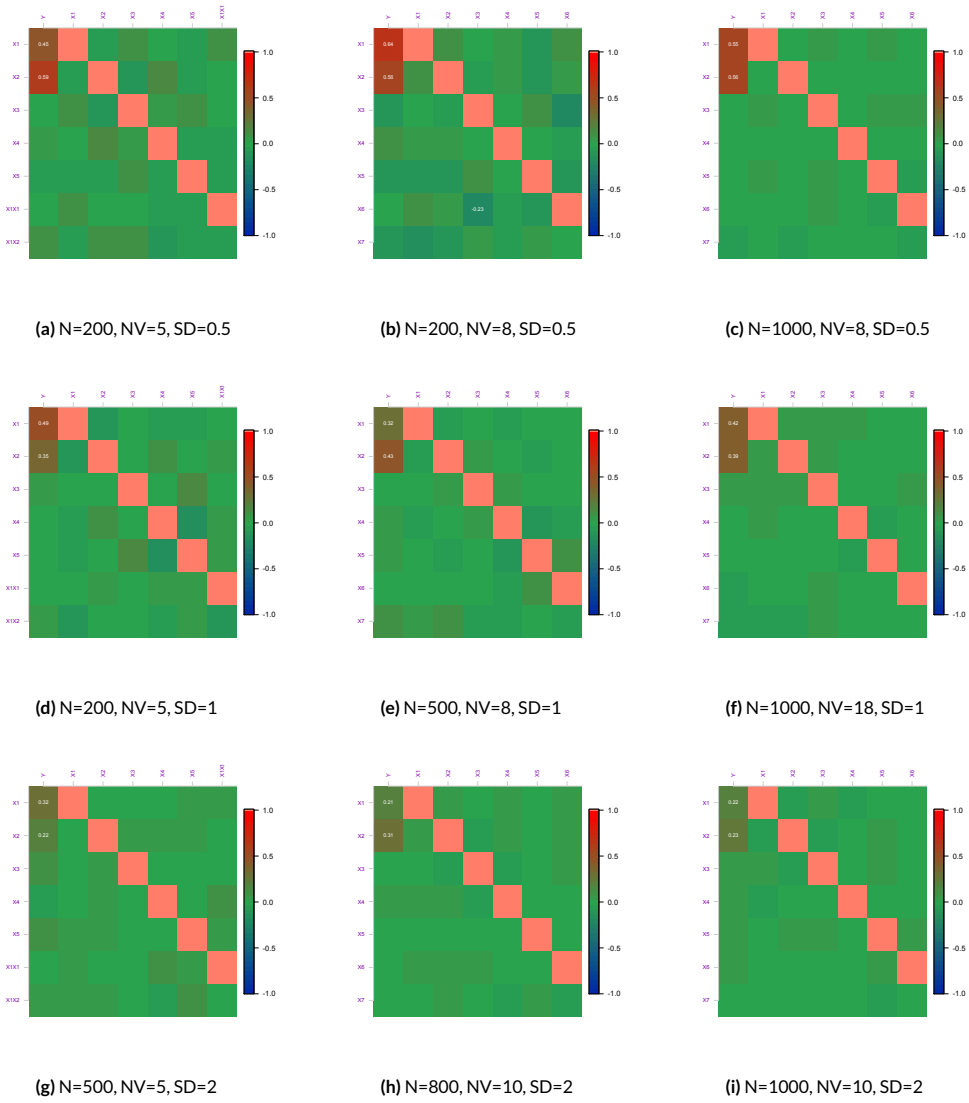
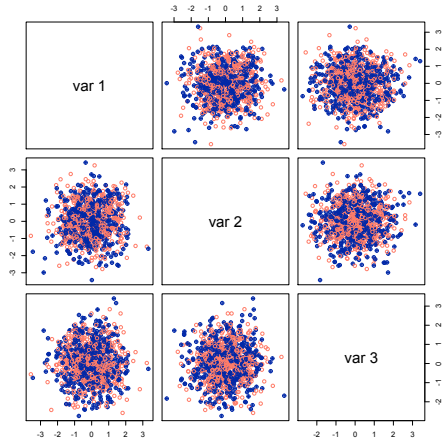


(a) N=200, NV=5, SD=0.5 **(b)** N=200, NV=8, SD=0.5 **(c)** N=1000, NV=8, SD=0.5

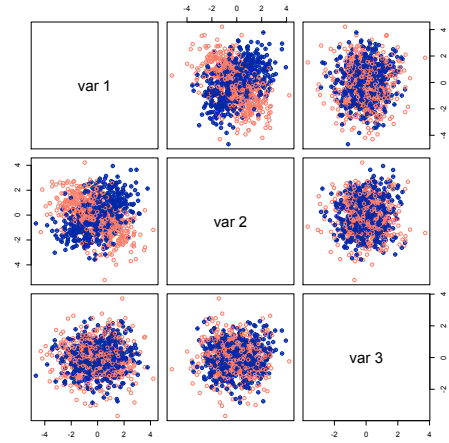
(d) N=200, NV=5, SD=1 **(e)** N=500, NV=8, SD=1 **(f)** N=1000, NV=18, SD=1

(g) N=500, NV=5, SD=2 **(h)** N=800, NV=10, SD=2 **(i)** N=1000, NV=10, SD=2

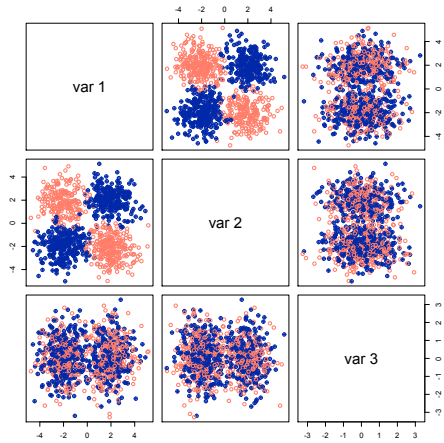
FIGURE 1 Simulated impact of measurement error. Correlation matrices between outcome Y, signal variables X_1, X_2, and other null variables, which are weakly correlated with the outcome. The greener the cells, the weaker the correlations. In the first row, the standard deviation of the noise in outcome is 0.5, which increases to 1 in the middle row and 2 in the bottom row. Note the first two cells of the Y column become greener and greener as the noise gets louder and louder. N represents simulated sample size. NV is the number of variables, and SD is the standard deviation of the noise. For a better visualisation effect, each matrix plots the correlations between the first eight variables of the corresponding simulation only.



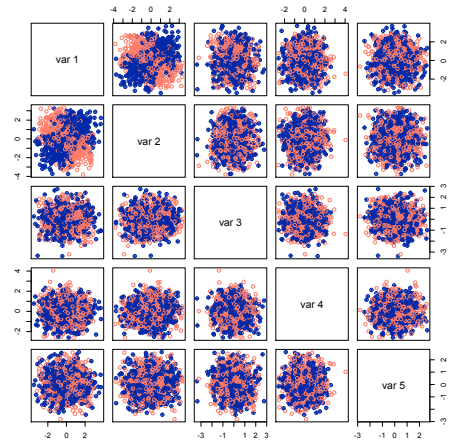
(a) N = 1000, Vs = 3, D = 0.1



(b) N = 1000, Vs = 3, D = 1

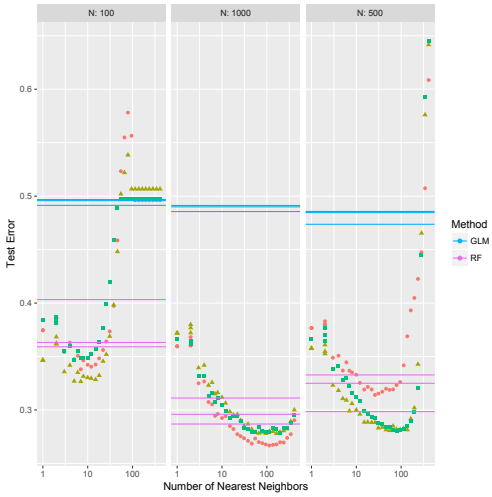


(c) N = 1000, Vs = 3, D = 2

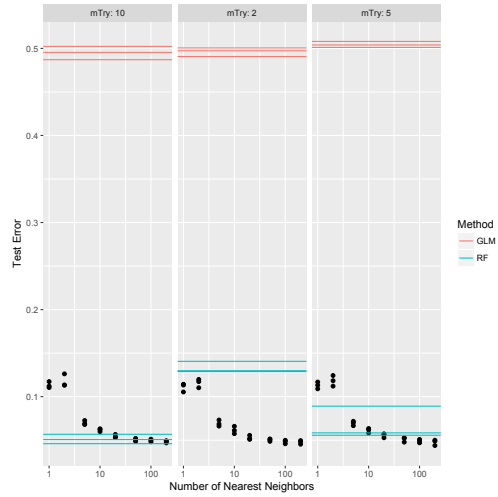


(d) N = 1000, Vs = 5, D = 1

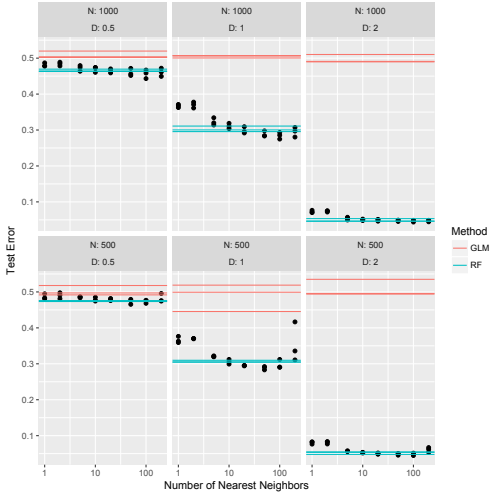
FIGURE 2 **Visualising interaction effect.** The four simulated datasets have the same sample size (N) of 1000, and in each case, only the first two variables are interacted. However, the datasets differ in the number of variables (Vs) and degree of separability in outcome (D), or intervention effect if we suppose it is trial data.



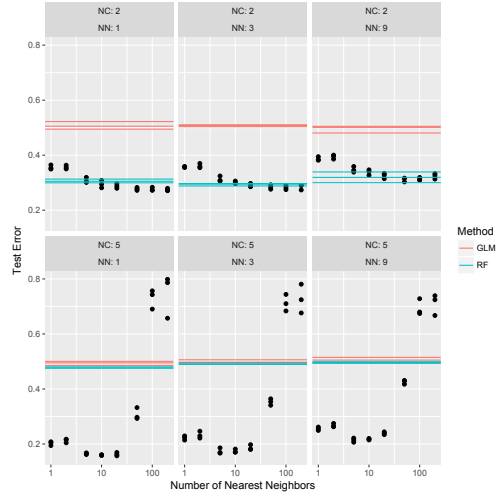
(a) N=(100, 500, 1000), NC=2, NN=3, D=1



(b) N=2500, NC=2, NN=18, D=2

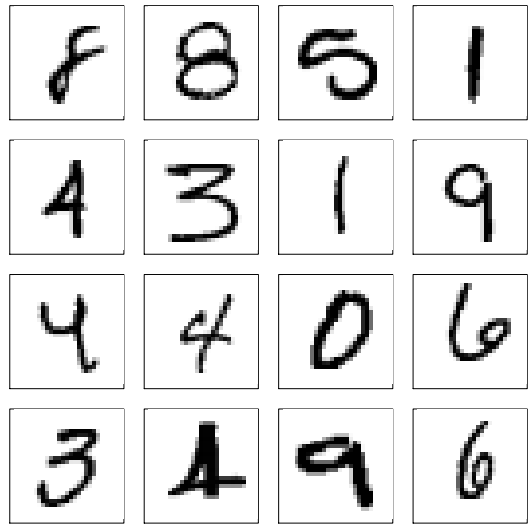


(c) N=(500, 1000), NC=2, NN=3, D=(0.5, 1, 2)

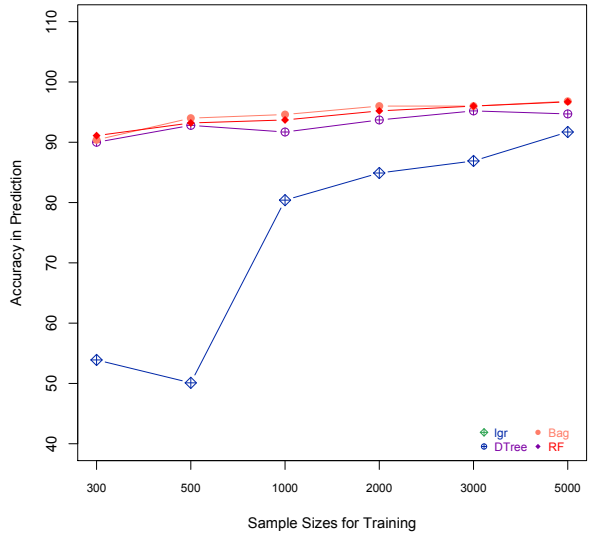


(d) N=1000, NC=(2, 5), NN=(1, 3, 9), D=(1, 2)

FIGURE 3 **Analysing simulated datasets with interactions.** Performances of different models on simulated datasets with different sample sizes (N) and intervention effects (D), varying numbers of interaction terms (NC) and null variables (NN). Sub-figure (b) shows the effect of change in the number of features (`mTry`) used in each re-sample for random forests. The simulations use only one performance metric, which is prediction error on the test set.

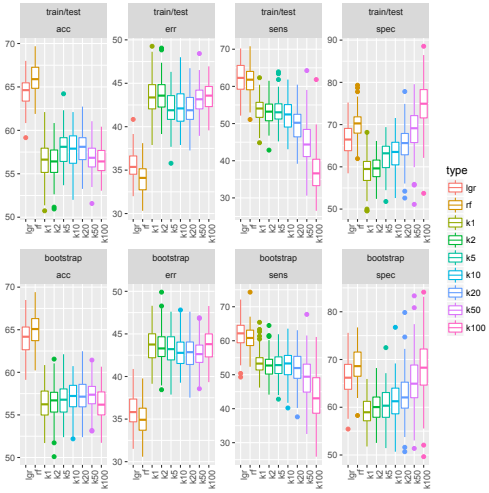


(a) 16 random digits

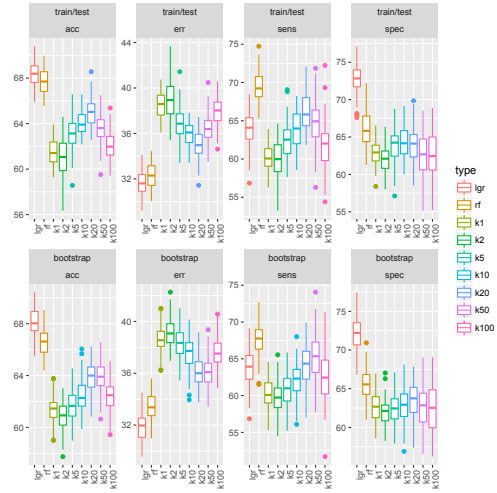


(b) Effect of input knowledge

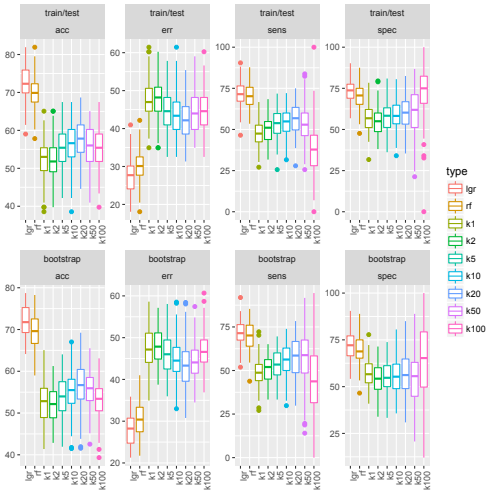
FIGURE 4 **Training models to read hand-written digits.** Sub-figure (a) is a random reading of 16 hand-written digits from the training set. Each digit is located in the center of a 28 by 28 grid, which forms a row with 784 columns if the cells in the grid are stacked up to form just one row. When there are 10,000 rows in the test set, there are 10,000 digits. Sub-figure (b) shows the effect of sample sizes in the training set on the prediction accuracy of the four models, logistic regression (`lgr`), decision trees (`DTree`), bagging (`Bag`), and random forests (`RF`).



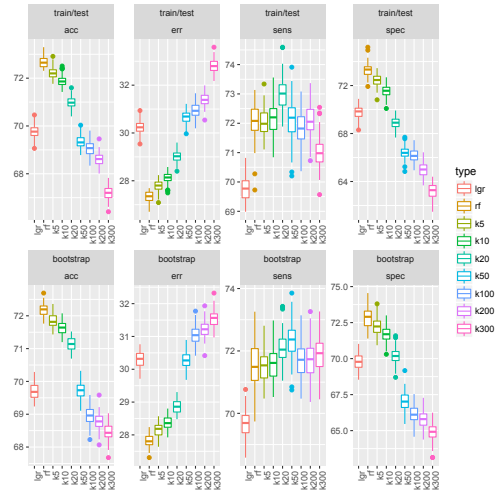
(a) ReflectED



(b) Chess in Schools



(c) Improving Writing Quality



(d) Tutor Trust Secondary

FIGURE 5 Performances of multiple models on EEF data. There are four performance metrics, prediction accuracy (`acc`), prediction error (`err`), sensitivity (`sens`), and specificity (`spec`). `train/test` and `bootstrap` represent two different data splitting methods. `lgr` and `rf` refer to logistic regression and random forests, respectively. All models with a letter `k` in the label are K-NN with different values of k.