Cross-Validation Methods for Risk Adjustment Models

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Abstract: This paper takes a fresh look at cross-validation techniques for assessing the predictive validity of risk adjustment models within the classical linear framework. We show that a K-Fold cross-validation is more efficient than 50-50 split sample technique and illustrate that overfitting with rich risk adjustment models remains meaningful in samples of up to 500,000 observations. A new estimation algorithm is described that calculates K-Fold cross-validated R-squared efficiently, so that it can be applied easily on sample sizes in the millions without sorting or relying on split-sample techniques. The density functions obtained in repeated samples using this technique are statistically similar to those using conventional split sample methods.

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1 Introduction

In recent years interest has grown enormously in estimating and validating the use of risk adjustment models, which are useful for health plan payment, patient management, severity adjustment, and many other uses (Ellis, 2008). It is often the case that a researcher may wish to evaluate alternative sets of predictors on some new dataset, which may differ in the demographics, year, country, or even choice of the dependent variable to be predicted. (e.g., Winkelman and Mehmud, 2007, Stefos et al, 2009) A commonly used approach is split sample validation, in which a fraction of the data (usually 50 percent) is used for estimation, and the remaining sample is used for validation. We argue in this chapter that while split sample validation is a useful approach when developing and selecting explanatory variables and the model structure, it is an inefficient approach when the goal is to simply validate existing risk adjustment models and structures. Instead we demonstrate that K-fold cross validation, which sequentially uses all of the data for both estimation and validation, is meaningfully more efficient, computationally feasible (particularly for linear models), and easy to explain.

The use of split sample validation is widespread and well-illustrated by the influential 2007 Society of Actuaries report (Winkelman and Mehmud, 2007) which evaluates 12 distinct claims-based risk assessment models, using alternatively diagnoses, procedures, pharmacy information, and lagged spending, and evaluates several dozen alternative specifications of these models using a single 50-50 split sample validation on a standardized sample of 617,683 individuals. Manning et al. (2005) uses split sample methods on 200,000 observations (out of several million individuals potentially available) to evaluate linear and nonlinear predictive models using the same set of regressors. Many other important methodological papers evaluate alternative models of annual health spending (without attempting to develop new sets of explanatory variables) using split sample methods (Mullahy, 1998; and Manning and Mullahy, 2001; Basu et al (2004), Manning et al. (2005); and Fishman et al., 2006). None of these papers recognize that by using only a single split of their full sample, their results are sensitive to the particular split samples created. The lone exception is Buntin and Zaslavsky (2004) who evaluate eight linear and nonlinear models using the Medicare Current Beneficiary Survey data on 10,134 individuals, a very modest sample size. Their validation uses 100 different replications of 50/50 splits of their sample for validation.

It is well known that estimating models of health care costs is problematic due to the heavily right-skewed nature of the distribution of non-zero annual costs (Less commonly emphasized is that the explanatory variables are also often highly skewed.) Estimation of predictive models using OLS produces biased

measures and can lead to 'overfitting'. While many early studies advocated strongly for nonlinear models to reduce the overfitting problem (Duan et al 1983) this preference was driven heavily by the limited sample sizes used for estimation. Several more recent studies (Fishman et al, 2006; Ellis and McGuire, 2007, Jiang, Ellis and Kuo, 2008) have demonstrated that the overfitting problems of OLS models largely disappear when very large samples sizes (over a million individuals) are used, an issue we also revisit here. Because of their ability to accommodate enormous numbers of covariates (in the hundreds), computational speed for estimation, simplicity to use for prediction and ease of explanation, OLS models have reemerged to be even more widely used than nonlinear techniques. Although nonlinear models remain popular among academic researchers, and may be essential for hypotheses testing in small to moderate size samples, none of the commercially available predictive models evaluated by the Society of Actuaries (Winkelman and Mehmud, 2007) use nonlinear models for prediction.

We would like to highlight at this point that we are interested in validation of existing models, not validation done in the process of developing new models. This paper is written from the point of view of model implementers, not model developers. The validation methods we consider are appropriate when the researcher is comparing alternative non-nested specifications that have been previously developed using other data, not when developing new models and specifications on the same data. If data is to be used to define explanatory variables, choose exclusions and interactions, or evaluate diverse possible nonlinear structures, then K-fold cross validation techniques described here can be misleading. K-fold cross validation can help identify overfitting that results from estimation, but it cannot easily be used to understand overfitting due to model design and selection. For model development, split sample validation, or relying on validation by new samples will be a preferred method.

In this paper we show that overfitting problem can be substantial even with sample sizes as large as 200,000, but that overfitting has largely disappeared in samples in the millions. The magnitude of the overfitting problem even in samples over 100,000 has perhaps been underappreciated in studies using small to moderate size samples, and such small samples cannot themselves be relied upon to validate the extent of the overfitting problem. Moving on, we describe an efficient algorithm for implementing K-fold cross validation in linear models. This efficient algorithm is applied to large empirical samples of several million records, taking only approximately three to five times the clock time of running a single OLS regression model. The algorithm uses the K-Fold cross validation technique developed in statistics literature. Although we develop the algorithm using health expenditure data predicted using a linear risk adjustment framework, the method is general and could be applied to any data.

Some readers may be disappointed that in this paper we focus solely on R-square measure of predictive ability, which is itself a transformation of the mean squared error, normalized by the total variance of the dependent variable. We do this both because the R-square is a unit-free measure that is relatively easily interpreted across models and samples, and because the methods we present can also be applied in a straightforward way to alternative measures such as the root mean square error, mean absolute deviation, predictive ratios, and grouped R-square. See Ash et al. (1989) and Ash and Byrne (1998) for discussion of the merits of these alternative measures.

The rest of the paper is organized as follows. In section 3.2 we provide some background on risk adjustment models and estimation problems. In section 3.3 we examine more carefully the split sample and K-fold cross validation methodologies, highlighting that both are a form of cross validation. In section 3.4 we describe an efficient way to manipulate data in such a way that the K-fold cross validation can be performed much faster, making it superior to bootstrapping. We describe the data used for this exercise in section 3.5 and present the results in section 3.6.

2 Literature on Risk Adjustment

Risk adjustment has been used in the literature to embrace many different things, but for this chapter we use the Ellis (2008) definition which is that it means "the use of patient level information to explain variation in health care spending, resource utilization, and health outcomes over a fixed interval of time, such as a year" (p. 178). Many different sets of explanatory variables have been developed for use in risk adjustment, commonly known as risk adjusters. The minimal set would include information on a person's age and gender, while more elaborate models may use socioeconomic or demographic information (e.g., income, education, race and ethnicity), diagnoses, pharmacy information, self-reported health status, provider information, or other variables. Van de Ven and Ellis (2000) highlight that the best choice of information to use depends on the intended uses of the risk adjustment model. Hence the best model to use may depend on how the predictive model will be used, which may include not only the classic use for health plan capitation payment (Ash et al, 1989; van de Ven and Ellis, 2000), but also for provider profiling (Thomas, et al, 2004a, 2004b), case management, plan rating and underwriting (Cumming and Cameron, 2002), or quality assessment and improvement (Iezzoni, 2003).

For this paper, we examine only three types of models: a simplified model that uses only age and gender, a prospective model that use diagnostic information to predict subsequent year health spending, and a

concurrent model that uses the same diagnostic information to predict health spending in the same year. Taking advantage of the fact that Ellis is one of the developers of the Diagnostic Cost Group (DCG) Hierarchical Condition Category (HCC) model, we evaluate our validation techniques using only the explanatory variables generated by that classification framework (Ash et al, 2000). Winkelman and Mehmud (2007) provide a useful overview of the various risk adjustment models used in the US, while Rice and Smith (2001) provide useful overviews of risk adjustment techniques outside of the US.

Despite its many critics, the simple approach of ordinary least squares in which the dependent variable is untransformed spending, remains popular. This approach has the great advantage of being fast and simple to estimate, interpret, and explain to non-econometricians. It is the approach used by the US Medicare program (Pope et al., 2000, 2004). Ash et al. (1989) established the concept that to get unbiased estimates for consumers where some have partial year eligibility, then the correct thing to do in an OLS setting is to annualize costs by deflating by the fraction of the year eligible, and then to weight the observation by this same fraction. This weighted annualized regression can be shown to generate unbiased means in rate cells, and corresponding linear regression models. Following Winkelman and Mehmud 2007, for the model validation exercises conducted below, we restricted our sample to include only people eligible for insurance for a full 24 months, and hence we do not have any partial year eligibles in our data. The estimation algorithms we develop work when the estimation approach is weighted least squares instead of OLS, however all of the results we present here use OLS.

3 Model Prediction and Cross-Validation

A common approach for choosing among competing alternative model specifications is based on their *validated* rather than within sample predictive power. This has attracted the attention of many researchers, not only in health care modeling but in all of social sciences. One of the most well-known methods—the ordinary cross-validation was developed as early as 1974 by statisticians. Noted seminal papers include Stone (1974, 1977). It is an old idea (predating the bootstrap) that has enjoyed a comeback in recent years with the increase in available computing power and speed. The main theme is to split the data according to some rule, estimate on one part of the data and predict using the other part. The two most common approaches are data splitting and K-Fold cross-validation. We discuss each of these techniques below.

3.1 Data Splitting or Split Sample Technique

In its most primitive but nevertheless useful form, cross-validation is done through data-splitting. In fact, cross-validation has almost become synonymous with data-splitting. In this approach, the researcher

selects (usually randomly) from the total set of observations available a subsample called the "training" or "estimation" sample to estimate the model and subsequently uses the model to predict the dependent variable for the remaining holdout or validation sample. Predictive validity then is assessed by using some measure of correlation between the values from the holdout sample and the values predicted by the model. This approach to cross-validation, sometimes with minor modifications, is generally accepted practice (Cooil et al, 1987).

In the split sample technique, the sample is split into two parts, the training sample and the validation sample. The training sample is used to estimate the coefficients while the validation sample is used to test those results. As an example, let's take the most common validation routine where 50% data is used for estimation and the rest 50% is used for validation (called the 50-50 split sample technique). The algorithm we executed on health care data was as follows.

1. Randomly divide half of the data into the training or calibration sample and half into the validation sample.

2. Run the OLS regression $Y = \sum_i \beta_i X_i + \varepsilon$ on the calibration sample to estimate the vector {β}.

3. Use these estimated vector $\widehat{\beta}$ from the calibration sample applied to the validation sample to predict Y, called $\widehat{Y}$.

4. Calculate the prediction error for each observation in the validation sample,

PE = $\left(Y - \widehat{Y}\right)$

5. Calculate various measures such as Mean Squared error, R-square, MAPE and the Copas test.

Traditionally, data splitting is done only once rather than several times. This makes the results dependent on which data points end up in the training set and which end up in the test set. Sometimes it can lead to unexpected results, such as when the validated R-square is larger than the estimation sample R-square. A more recent practice has been to perform this exercise repeatedly and then take the mean of the estimates for forecasting, as in Buntin and Zaslavsky (2004). With a large number of draws this is guaranteed to overcome the monotonicity issue, but is still using less than all of the data for calibration.

A weakness of the split sample method is that no matter how many times you perform a split sample validation; the estimates are always based on half the sample and thus will not be as efficient as if the

entire sample were being used. Even though medical claims data are large, people often fail to realize the large sample sizes needed to produce precise statistical measures in both the training and the validation samples. In many cases datasets are not large enough to eliminate overfitting. Splitting the sample in any fashion (be it a 50-50 or a 70-30 or some other combination) exacerbates the overfitting problem and increases the divergence between R-squares from the training sample and the validated sample.

3.2 K-Fold Cross Validation

In order to avoid the randomness emanating from estimates produced by splitting the data only once, "K-fold" cross-validation makes more efficient use of the available information. The algorithm for this technique can be described in the following steps:

1. Randomly split the sample into K equal parts
2. For the k^{th} part, fit the model to the other K-1 parts of the data, and use this model to calculate the prediction errors in the k^{th} part of the data.
3. Repeat the above step for k=1, 2….K and combine the K estimates of prediction errors to create a full sample of prediction errors.

If K equals the sample size (N), this is called N-fold or "leave-one-out" cross-validation. "Leave-v-out" is a more elaborate and computationally time consuming version of cross-validation that involves leaving out all possible subsets of v cases. Note that all of these forms of cross-validation are different from the "split sample" method. In the split-sample method, only a single subset (the validation set) is used to estimate the prediction error, instead of k different subsets; i.e., there is no "crossing".

Leave-one-out cross-validation is also easily confused with jackknifing. Both involve omitting each training case in turn and retraining the network on the remaining subset. But cross-validation is used to estimate generalization error, while the jackknife is used to estimate the bias of a statistic. In the jackknife, you compute some statistic of interest in each subset of the data. The average of these subset statistics is compared with the corresponding statistic computed from the entire sample in order to estimate the bias of the latter. You can also get a jackknife estimate of the standard error of a statistic. Jackknifing can be used to estimate the bias of the training error and hence to estimate the generalization error (Efron, 1982)

However, one difficulty with K-fold cross-validation is that it can be computationally slow in with nonlinear models (including L' regression, tree structured methods for classification and nonlinear

regression) and even for OLS cross validation can be slow when millions of observations and hundreds of explanatory variables are used.(Breiman et al., 1984). We describe a computationally efficient algorithm for conducting the K-fold cross validation below.

3.3 COPAS Test

The COPAS test is a formal test of overfitting using split sample or K-fold cross validation. The following algorithm is used to perform this test.

1. Randomly split sample into two groups. The selection of groups can be 50-50 or 70-30 or (K-1, k). Call the first group A or the training sample and the other group B, or the validation sample

2. Estimate model on sample A and retain its coefficients $\hat{\beta}_A$

3. Forecast to sample B

$$\hat{Y}_B = \hat{\beta}_A X_B$$

4. Now regress the dependent variable from the validation sample i.e., Y_B on the predicted $\hat{Y}_B$ and test whether the slope is one. Hence estimate

$$Y_B = \delta_0 + \delta_1 \hat{Y}_B + \varepsilon \quad \text{and test } \delta_1 = 1$$

5. If reject the null hypothesis, then overfitting may be a problem— and you should prune the model and check for outliers.

If a split-sample validation is used, one can repeatedly use different splits of the sample, conducting a COPAS test for a large number of different splits, such as 100 or 1000, and then look at the percentage of times the null hypothesis was rejected. For K-fold cross validation, repeated calculations of the COPAS test on the same sample will differ little, and instead we draw different samples from our large samples and calculate both goodness of fit measures and COPAS tests on each new draw. To make the calculations and interpretation as simple as possible, we draw our samples each time without replacement.

4 A computationally efficient method for K-fold validation

As just discussed, both bootstrap methods and straightforward application of K-fold cross validation generally require multiple passes through the dataset, which can be computationally very time consuming when very large sample sizes and very large numbers of explanatory variables are involved. Part of the contribution of this paper is in verifying the usefulness of a computationally fast algorithm for conducting k-fold cross validation.

Our approach is most easily explained with a certain new notation. We use the matrix notation A_{-k} to denote a matrix A generated while excluding the proper subset A_k of observations in set k. If Y is the Nx1 array of the dependent variable and X is the NxM matrix of explanatory variables, let Z = {X Y}. It is well known that the cross product matrix Z^TZ contains all of the information needed to generate all conventional regression statistics, including betas, RSE and R-square. The algorithm we implement for a sample size of N is as follows.

1. Randomly sort the observations so that there is no significance to the initial original order.
2. Estimate the OLS model using the full data set Z, retaining $Q = Z^TZ$.
3. For each of k subsamples of size N/K, created without replacement, generate $Q_k = Z_k^TZ_k$ and take matrix differences to generate $Q_{-k} = Q - Q_k = Z^TZ - Z_k^TZ_k$
4. Use Q_{-k} to calculate the array of OLS regression coefficients $\beta_{-k}(Q_{-k})$, and then generate predicted values $\hat{Y}_k$, which were not used in $\beta_{-k}(Q_{-k})$. Save these fitted values of $\hat{Y}_k$ in an $\{\hat{Y}_{K-Fold}\}$
5. After repeating steps 3 and 4 for all of the k samples, generate validated RSE and R-square measures for the full set of size N using the original Y and $\{\hat{Y}_{K-Fold}\}$.
6. Run the COPAS regression of Y on $\{\hat{Y}_{K-Fold}\}$.

Reflecting the increased precision from larger samples, we repeated steps 1 through 6 for 1000 replications for small sample sizes of 1000, 2000, and 5000 observations; 100 replications for sample size of 10,000, 20,000, 50,000, 100,000, 200,000 and 500,000; 50 replications for the sample sizes of 1,000,000; and once for the entire sample (N = 4,688,092). We also explored the sensitivity of our results to various values of K=10, 100, and 1000.

5 Data Description

Data for this study come from the Medstat MarketScan Research Databases. These databases are a convenience sample reflecting the combined healthcare service use of individuals covered by Medstat employer clients nationwide. Personally identifiable health information is sent to Medstat to help its clients manage the cost and quality of healthcare they purchase on behalf of their employees. MarketScan is the pooled and de-identified data from these client databases. In this study we use the Commercial Claims and Encounters (CC&E) Database for 2003 and 2004. This data was not used to calibrate or

revise the DCG/HCC risk adjustment classification system used for validation, and hence this is an appropriate sample for model validation.

The Commercial Claims and Encounters Database contains the healthcare experience of approximately 10 million employees and their dependents in 2003 and 2004. These individuals' healthcare is provided under a variety of fee-for-service (FFS), fully capitated, and partially capitated health plans, including preferred provider organizations, point of service plans, indemnity plans, and health maintenance organizations. The database consists of inpatient admissions, inpatient services, outpatient services (including physician, laboratory, and all other covered services delivered to patients outside of hospitals and other settings where the patient would spend the (night), and outpatient pharmaceutical claims (prescription drugs delivered in inpatient settings are unfortunately not separately tracked in the databases). We have information on diagnoses for 2003 and covered charges ("health spending") for 2003 and 2004, enabling us estimate prospective models predicting 2004 health spending and concurrent models predicting 2003 health spending.

We excluded people who were not continuously eligible for coverage for all of 2003 and 2004, everyone Medicare eligible at any time (and hence everyone over age 63 at the start of our sample), one person with implausibly high health spending in 2003, and people not in traditional indemnity, a preferred provider organization, a point of service plan, or a health maintenance organization. Altogether this left 4,688,092 individuals in our full sample.

Using this data, we evaluate three different model specifications.

- Age and sex model with 18 independent variables, (age gender dummies)
- Prospective model with 18 independent age gender dummies and 182 hierarchical condition categories[3]
- Concurrent model with 18 independent age gender dummies and 182 hierarchical condition categories

[3] The DxCG HCC classification system contains 184 HCCs, however two of them never occurred in our data and hence are omitted. These two were HCC 129 End stage Renal Disease (Medicare program participant), and HCC 173 Major Organ Transplant Status (e.g., heart, lung, etc.) which in the first case is impossible in our data by construction, and in the second case is sufficiently rare among non-Medicare eligibles to have not occurred in our sample. Table B.3 in appendix B gives details on all HCC variables.

6 Results

6.1 Descriptive statistics

We start by examining some of the characteristics of our data, which are summarized in Table 1. We see that both health spending in 2003 and 2004 have coefficients of variation (standard deviation divided by the sample mean) over 300, large skewness measures in the (30's) and enormous kurtosis (over 2000). Note that all of these measures (the CV, skewness and kurtosis) are invariant to rescaling or normalization of the variable of interest. Also relevant are the moments of some of the explanatory variables. Age, gender, and dummy variables reflecting their interaction all have relatively low CV (less than 500), and have low skewness and kurtosis. In contrast, a relatively rare HCC such as HIV/AIDS, with a prevalence rate of .00075 has a CV that exceeds that of annual spending (CV = 3651), a skewness of 36 rivaling that of health spending, and a kurtosis of 1329. Hence despite having an acceptable sample size of over 3400 cases with HCC001 in the full sample, in modest samples this variable will be subject to overfitting in modest size samples. Congestive heart failure, a binary variable with a nearly tenfold higher prevalence (mean = .00654) still has meaningful skewness and kurtosis.

6.2 Full sample results

Table 2 presents the results of estimating our three base models using the full sample sizes of N = 4,688,092. Our base model is a prospective model, predicting 2004 total health care spending at the individual level using age, gender, and diagnostic information from 2003, the previous year to the health spending. This base "prospective model" has 200 parameters: a constant term plus 182 hierarchical condition categories and 17 of 18 mutually exclusive age-gender categories. All of these explanatory variables are binary variables. We also estimate results for an "Age-sex model" using only the age-gender dummies and finally a "concurrent model", predicting 2003 spending in the same year as the diagnostic information (2003). Since more researchers are interested in prospective than concurrent models, we concentrate on the prospective model.

Table 2 reveals that the fitted and validated R-square measures for the prospective split sample model differ by only .005. The COPAS test on overfitting has a t ratio of -15.024 indicating that with only 2 million records there is still some evidence of overfitting. In contrast the K-fold validation results differ at most by .001 when the full sample is used, and hence results are not overstated by overfitting. The age-sex model, with only its 18 parameters, does not explain much of the variation in spending, but also shows no evidence of overfitting. The COPAS test statistic on the slope for the prospective HCC model is of borderline significance with a t ratio of 1.807 (p = .07 on two-tail test).

6.3 K-Fold versus split sample results

We next present results from K-Fold cross validation and compare them with split sample technique results. Table 3 presents these results for the prospective model. First consider the split sample results. For samples under 10,000, the R-square in the fitted models is grossly overstated, with highly negative validated R2. For a more respectable sample size of 10,000 the fitted R-square has a mean of .359, while the validated R2 mean remains negative. We see that the fitted and validated R-squares diverge markedly for smaller samples—validating the well-known results that significant overfitting remains a concern even with sample sizes of 100,000 in richly predictive models using highly skewed explanatory variables. As the sample size increases, this divergence gradually disappears, and the overfitting problem seems to mitigate for large samples over 500,000 observations.

The superiority of the K-fold cross validation over split sample validation is revealed in figure 1, which highlights that the K-fold R-square means are significantly closer to the true values than the split sample methods. These also reveal that the simple average of the fitted and validated R-square is a better estimate of the asymptotic predictive power of the model then just the validated R-square. Another feature to note in this figure is that for K=100, the fitted mean R-square from split sample techniques using a sample of N observations is statistically indistinguishable from the fitted mean R-square from K-Fold cross validation technique using a sample of N/2 observations. Hence the split sample validation results on 20,000 records gives nearly identical results to the K-fold validation results on 10,000 observations. This makes sense since splitting a 20,000 observation dataset into two parts and estimating the model using one part is almost identical to taking a 10,000 observation dataset and using 99% of it to estimate the model.

Figure 2 plots not only the means but also the 90 percent confidence intervals for the fitted and validated R-squares using K-fold validation on the prospective HCC model. The 90 percent confidence intervals for the split sample model are even wider. This figure reveals that the 90 percent confidence intervals for the validated and fitted values overlap considerably, so it is not unusual for the validated and fitted R-s values to be reversed for the split sample techniques, simply due to chance. In contrast, with K-fold validation the validated measure is guaranteed to be strictly less than the fitted value, since one can never do better using an out of sample model than using within sample methods. (See Efron and Tibshirani, 1998 for a demonstration.)

In Table 4 we repeat this exercise using only 18 age sex dummies as our right hand side variable. The first four columns of table 4 show that the fitted and validated R-square estimates are very close to each other for the age-sex model even with as few as 10,000 observations. However, the 90% confidence intervals shown in figure 3 reveal that there is still a meaningful amount of variation in estimates of the R-square even with this simply parameterized model.

Figure 4 and the second set of columns in Table 4 present the concurrent model to show that K-Fold cross validation is useful for concurrent models as well. Overfitting is more significant in concurrent models with the mean R-squares differing by .005 even with a million individuals.

Table 5 evaluates the impact of different choices of how many folds should be used in the K-Fold cross validation exercise. Each cell was generated by taking the mean and standard deviation of the validated R2 from 100 replications for the given sample size for K = 10, 100 and 1000, and hence each sample was used three times. Comparing across rows, we see that estimates of the validated R-square using K-fold validation is relatively stable across values of K with a slight improvement for larger K = 10 to K = 100, but no apparent improvement going from 100 to 1000. In part because of the computational savings we rely on K=100 for all of the rest of our results.

In Table 6 we show the average time it took for us to validate our model using split sample and K-fold technique. It matters critically in this analysis whether the time taken generating the sample splits themselves are included in the estimates. Because split sample validation only estimates the model on half as much data, and forecasting the remaining half is very fast, split sample validation when efficiently programmed can take even less time than OLS. However, the more interesting thing to note is that the K-fold Cross validation only took at most 5 times longer than the OLS, despite running 100 regression models. Even for the full sample of 4.7 million records, K-fold validation took only 4:02 versus :43 for OLS, a 5.6 fold multiple. Straightforward bootstrap techniques with 100 repetitions will have taken on the order of 100 times as much time as OLS to generate similar results. All of the times shown here were generated on a basic Dell Pentium IV desktop that had only 2.8 GHZ of processor speed and 2.0 GB of RAM and many research settings would typically have access to much faster machines. As a comparison, researchers at DxCG inc. estimated and validated a concurrent regression model using this K-Fold algorithm with 13.65 million records and 835 explanatory variables. Our algorithm took only 3.3 times as much clock time (115 minutes) as doing OLS (35 minutes), despite doing 100 regressions with 835 betas, each on over 13 million records. The overfitting problem was also trivial, with only a .002 overstatement

in the R-square. Bootstrap methods on this large sample could have taken multiple days to generate comparable statistics.

7 Conclusions

In this paper we have illustrated the value of using K-fold cross validation instead of split sample validation for validating linear models on large datasets. This technique is relevant in settings where the researcher is interested in comparing alternative sets of explanatory variables in a risk adjustment setting without exploring model specification, as in Winkelman and Mehmud (2007) and Manning et al (2008). If model selection tasks such as identifying which variables to include, searching among highly nonlinear models, or evaluating interactions and constraints are being considered, then split sample techniques will isolate the validation sample from contamination in ways that K-fold validation cannot.

This paper documents the magnitude of overstatement of the R-square using three specification of common risk adjustment – age-gender, prospective and concurrent models. We have used DCG risk adjustment framework for all of our estimates, but the techniques should be relevant for any setting in which overfitting is of concern. K-Fold cross validation is superior to split sample techniques, even when multiple splits are considered, since it achieves the same level of precision with half the amount of data. We have used the K-fold validation to calculate only one measure of goodness of fit – the R-square, but the individual level out-of-sample predictions can be used for any number of other measures – including mean absolute deviations, predictive ratios and grouped R-squares – with a simple modification.

Our demonstration that K-fold validation is relatively robust to relatively small values of K, such as ten, suggests that for nonlinear models, where computation time is a critical issue, K-fold cross validation using only K=10, and hence requiring only ten replications of estimation of the nonlinear model, may be attractive as an alternative to split sample techniques. Often the very large sample sizes available to researchers imply that the relevant choice of models is between using all of the data for simple linear model versus a fraction of it for nonlinear estimation. We have not validated the relative attractiveness of these two competing approaches to model estimation.

Part of the contribution of this chapter is that we develop a computationally efficient method of calculating K-fold validation which requires only on the order of five times as long as the amount of time running a simple OLS in large samples. Given that bootstrap techniques require a much larger multiple of

time to generate comparable measures of out of sample predictive power, our hope is that this technique, long known in the statistical literature, will see increased use in empirical studies of large datasets.

Table 1 Summary statistics

MEDSTAT Marketscan Data, 2003-2004, N = 4,688,092						
Variable	Mean	Std. Dev	CV*100	Skewness	Kurtosis	Maximum
Covered total charges, 2003	2905	10859	374	32	2,405	1,909,854
Covered total charges, 2004	3463	11675	337	27	2,174	2,222,606
Age (years)	34.953	18.406	53	-0.323	-1.207	63
Male = if male	0.528	0.499	94	-1.110	-1.990	1
Agesex1=1 if male and age = 0-5	0.048	0.213	447	4.25	16.03	1
HCC001 HIV/AIDS	0.00075	0.027	3651	36	1,329	1
HCC080 Congestive Heart Failure	0.00654	0.081	1233	12	148	1

Table 2 Full Sample Results

MEDSTAT Marketscan Data, 2003-2004, N = 4,688,092				
	Parameters	Fitted R-Square	Validated R-Square	COPAS T-Ratio
Prospective HCC	200	0.175	0.174	1.807
Prospective AgeSex	18	0.030	0.030	0.045
Concurrent HCC	200	0.398	0.397	2.028
Prospective HCC Split Sample Technique	200	0.177	0.172	-15.024

Table 3: R Squares generated for Prospective Model with 218 parameters, HCC+ AGE + SEX, 100-Fold, Cross Validation Vs. 50-50 Split

	K-Fold, K=100				50-50 Split Sample			
	Fitted R2		Validated R2		Fitted R2		Validated R2	
Sample	Mean	Std Dev	Mean	Std Dev	Mean	Std Dev	Mean	Std Dev
500	0.638	0.180	-0.539	0.791	0.743	0.172	-1.864	4.267
1000	0.547	0.175	-0.362	0.562	0.637	0.189	-1.221	2.988
2000	0.467	0.152	-0.219	0.408	0.554	0.172	-0.707	2.057
5000	0.355	0.099	-0.045	0.173	0.444	0.134	-0.319	1.405
10,000	0.287	0.072	0.062	0.089	0.359	0.103	-0.091	0.359
20,000	0.236	0.050	0.112	0.053	0.282	0.078	0.026	0.183
50,000	0.201	0.029	0.146	0.035	0.225	0.048	0.114	0.070
100,000	0.189	0.022	0.160	0.024	0.203	0.028	0.148	0.031
200,000	0.182	0.016	0.167	0.016	0.188	0.022	0.162	0.020
500,000	0.177	0.010	0.171	0.010	0.180	0.013	0.169	0.014
1,000,000	0.176	0.007	0.173	0.007	0.178	0.010	0.172	0.011

Table 4: R Squares generated for Age-Sex model and Concurrent Model using K-Fold Cross Validation

	Age-Sex Model				Concurrent Model			
	Fitted R2		Validated R2		Fitted R2		Validated R2	
Sample	Mean	Std Dev	Mean	Std Dev	Mean	Std Dev	Mean	Std Dev
500	0.072	0.036	0.004	0.044	0.893	0.069	-0.121	0.569
1000	0.055	0.023	0.020	0.022	0.832	0.096	-0.085	0.622
2000	0.043	0.016	0.026	0.016	0.780	0.097	0.059	0.449
5000	0.037	0.011	0.031	0.011	0.659	0.107	0.181	0.287
10,000	0.033	0.008	0.029	0.008	0.603	0.103	0.314	0.178
20,000	0.032	0.008	0.030	0.008	0.543	0.110	0.371	0.135
50,000	0.029	0.006	0.029	0.006	0.489	0.101	0.406	0.116
100,000	0.031	0.004	0.030	0.004	0.437	0.073	0.391	0.078
200,000	0.030	0.003	0.030	0.003	0.419	0.058	0.395	0.061
500,000	0.030	0.002	0.030	0.002	0.404	0.028	0.393	0.028
1,000,000	0.030	0.001	0.030	0.001	0.400	0.012	0.395	0.012

Table 5: Comparison of Validated R-Square Mean and Standard Deviation for various Choices of K and sample sizes, K-Fold Cross Validation on Prospective HCC + Age + Sex Model, and 218 parameters

	Validated R2 Mean			Validated R2 Std Dev		
Sample Size	K=10	K=100	K=1000	K=10	K=100	K=1000
2000	-0.154	-0.219	-0.127	0.220	0.408	0.203
5000	-0.047	-0.045	-0.032	0.139	0.173	0.134
10,000	0.050	0.062	0.067	0.095	0.089	0.084
20,000	0.099	0.112	0.108	0.057	0.053	0.056
50,000	0.142	0.146	0.146	0.035	0.035	0.034
100,000	0.157	0.160	0.158	0.023	0.024	0.023
200,000	0.165	0.167	0.165	0.015	0.016	0.015
500,000	0.170	0.171	0.171	0.010	0.010	0.010

Table 6: Comparison of Average Computer Time Utilized in validating in 100 samples of different sizes, Prospective Model, 218 parameters HCC + AGE +SEX

	OLS	50-50 Split Design	K-Fold, K=100
Sample Size	Time in Seconds	Time in Seconds	Time in Seconds
1000	0.246	0.047	20.640
2000	0.341	0.046	21.219
5000	0.276	0.078	21.984
10,000	0.288	0.109	22.796
20,000	0.411	0.187	23.063
50,000	0.737	0.391	24.640
100,000	1.588	0.750	27.266
200,000	2.463	1.609	34.407
500,000	7.382	3.375	45.297
1,000,000	17.593	8.547	69.234

Table 7: Average T-Ratio on Copas Test, Various Sample Sizes, 50-50 Split vs. K-Fold Cross Validation

	K-Fold, K=100	50-50 Split Design
Sample Size	Mean	Mean
500	15.672	16.711
1000	18.649	19.194
2000	22.007	21.078
5000	24.572	24.910
10,000	22.338	24.755
20,000	19.527	24.279
50,000	14.920	20.220
100,000	11.318	14.956
200,000	8.681	11.812
500,000	5.517	8.885
1,000,000	3.950	3.716

Figure 1: Fitted and Validated R^2 means by sample size, 200 parameters HCC + Age + Sex model, 50-50 Split Technique Vs. K-Fold Cross Validation

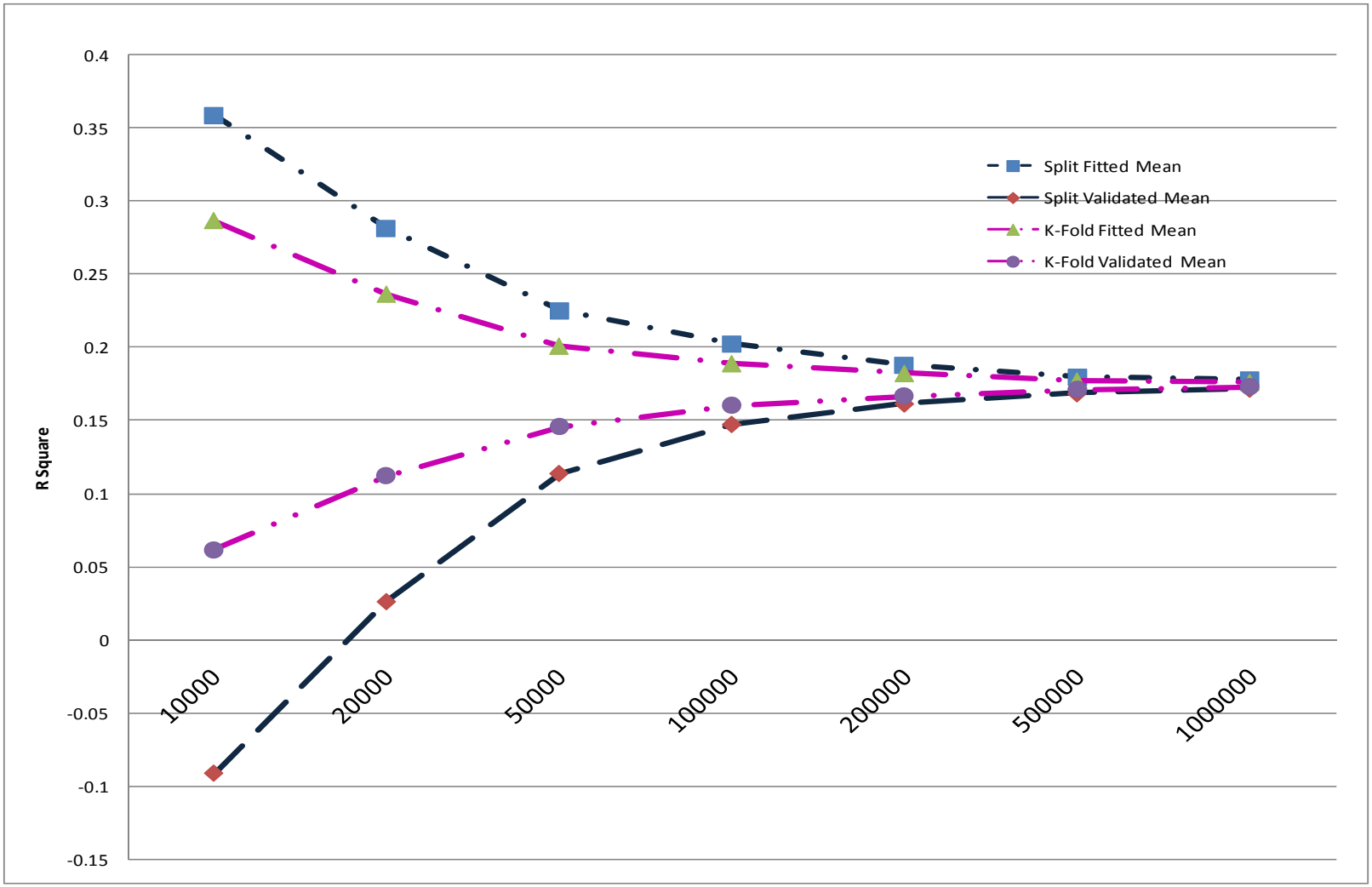


Figure 2: Fitted and Validated R2 by sample size, 200 parameter Prospective HCC + Age + Sex model, means and 90% confidence intervals, K-Fold Cross Validation Method

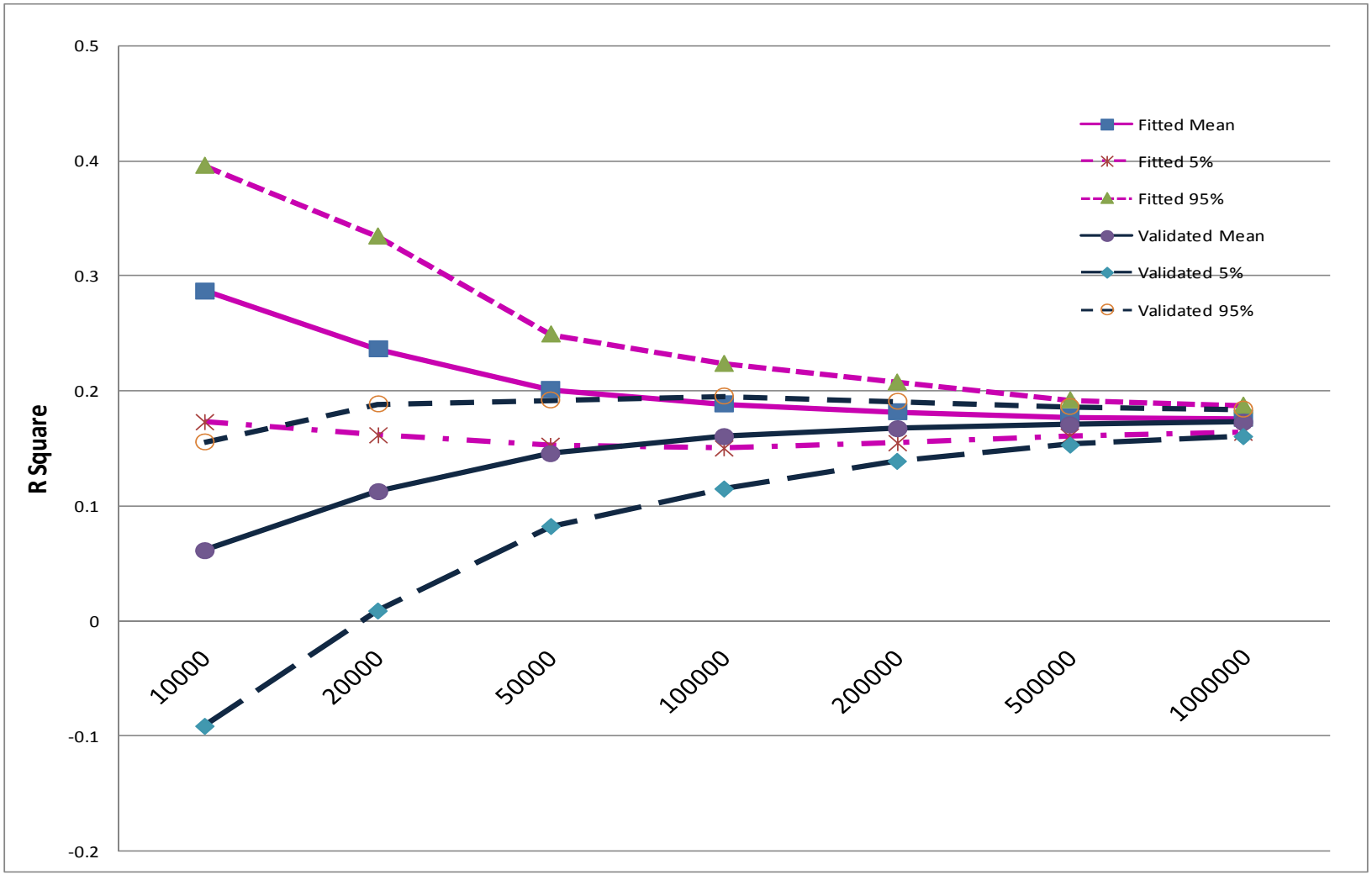


Figure 3: Fitted and Validated R^2 by sample size, 18 parameter Age + Sex model, means and 90% confidence intervals, K-Fold Cross Validation

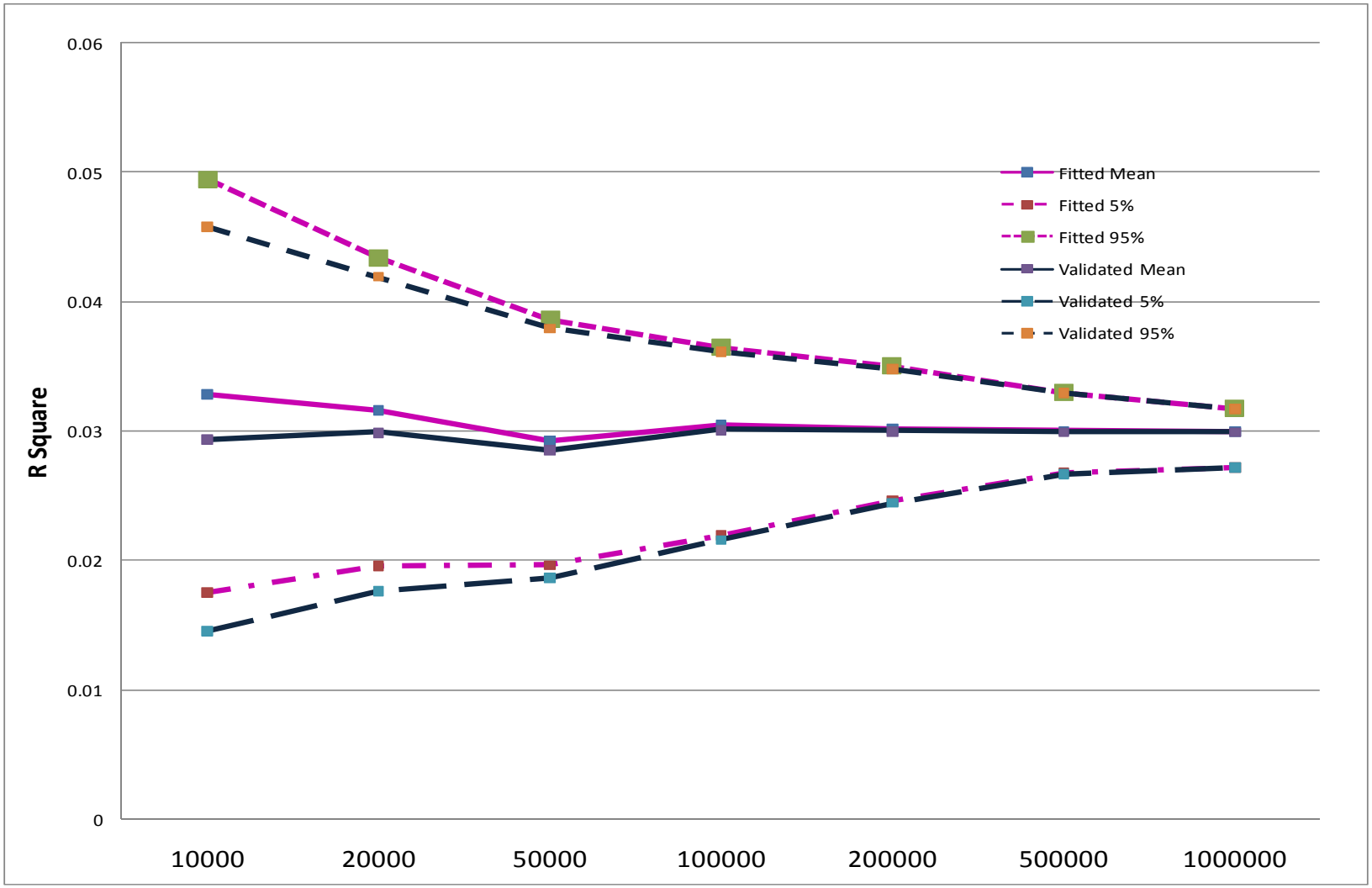
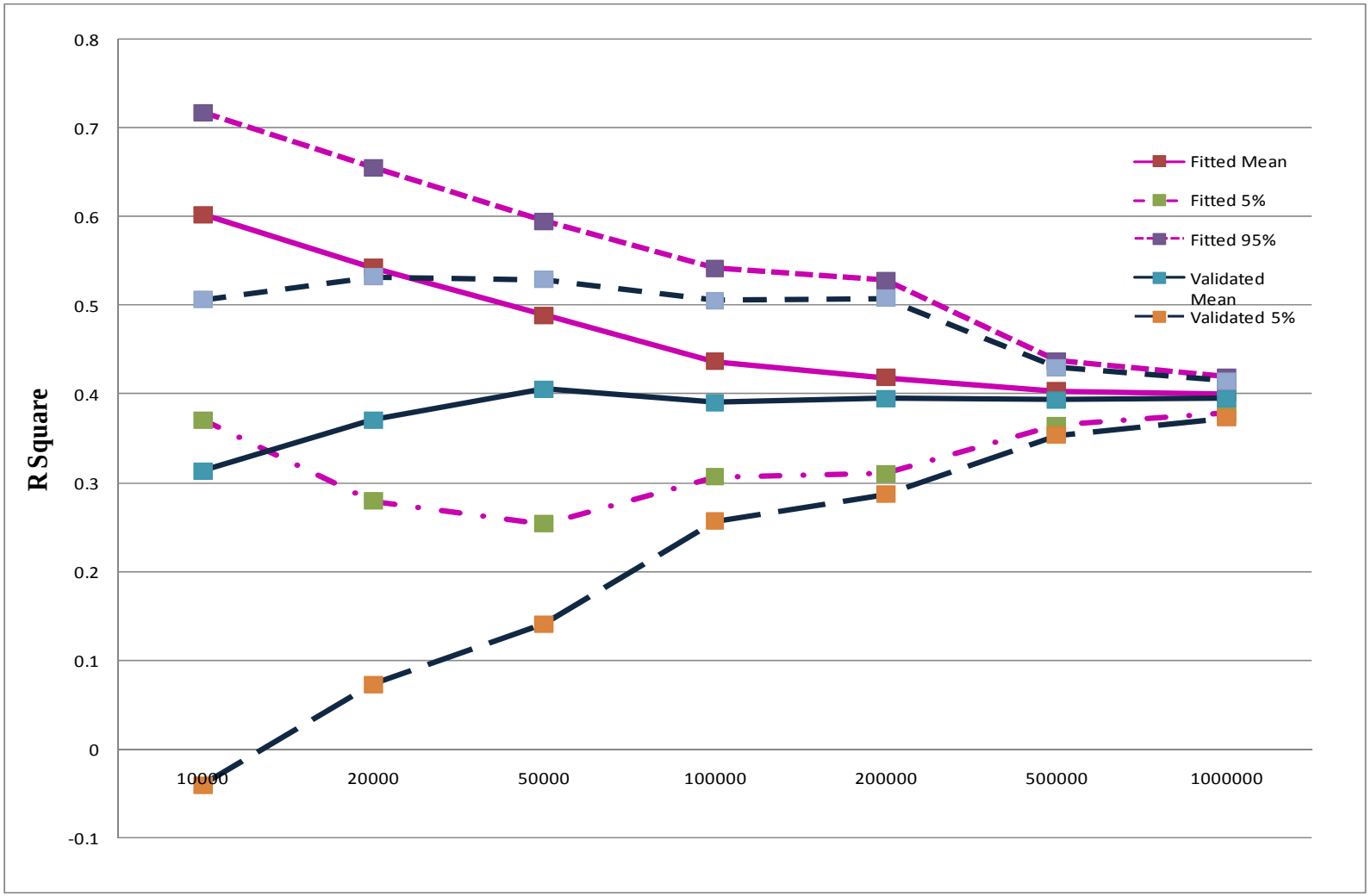


Figure 4: Fitted and Validated R^2 by sample size, 200 parameter Concurrent HCC + Age + Sex model, means and 90% confidence intervals, k-Fold Cross Validation



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