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Comparison of Model Selection for Regression

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Abstract.

We discuss empirical comparison of analytical methods for model selection. Currently, there is no consensus on the 'best' method for finite-sample estimation problems, even for the simple case of linear estimators. This paper presents empirical comparisons between classical statistical methods (AIC, BIC) and the SRM method (based on VC-theory) for regression problems. Our study is motivated by empirical comparisons in (Hastie et al, 2001) who claim that SRM method performs poorly for model selection. Hence, we present empirical comparisons for various data sets and different types of estimators (linear, subset selection and k-nearest neighbor regression). Our results demonstrate practical advantages of VC-based model selection, as it consistently outperforms AIC and BIC for most data sets (including those used in (Hastie et al, 2001)). This discrepancy (between empirical results obtained using the same data) is caused by methodological drawbacks in (Hastie et al, 2001)) especially in their loose interpretation and application of the SRM method. Hence we discuss methodological issues important for meaningful

comparisons and practical application of SRM method. We also point out the importance of accurate estimation of model complexity (VC-dimension) for empirical comparisons, and propose a new practical estimate of model complexity for k-nearest neighbor regression.

Key Words: Complexity control; Empirical comparisons; Model complexity; Model selection; Structural risk minimization (SRM); Vapnik-Chervonenkis (VC) theory

1 Introduction and Background

We consider standard regression formulation under general setting for predictive learning (Vapnik, 1995; Cherkassky and Mulier, 1998; Hastie et al, 2001). The goal is to estimate unknown real-valued function in the relationship:

$$y = g(\mathbf{x}) + \varepsilon \tag{1}$$

where ε is i.i.d. zero mean random error (noise), $\mathbf{x}$ is a multidimensional input and y is a scalar output. The estimation is made based on a finite number (n) of samples (training data): $(\mathbf{x}_i, y_i), (i = 1,..., n)$. The training data are independent and identically distributed (i.i.d.) generated according to some (unknown) joint probability density function (pdf),

$$p(\mathbf{x}, y) = p(\mathbf{x})\, p(y \mid \mathbf{x}) \tag{2}$$

The unknown function in (1) is the mean of the output conditional probability (aka regression function) $g(\mathbf{x}) = \int y p(y \mid \mathbf{x}) dy$.

A learning method (or estimation procedure) selects the 'best' model $f(\mathbf{x}, \omega_0)$ from a set of approximating functions (or possible models) $f(\mathbf{x}, \omega)$ parameterized by a set of parameters $\omega \in \Omega$.

The quality of an approximation is measured by the loss or discrepancy measure $L(y, f(\mathbf{x}, \omega))$. An appropriate loss function for regression is the squared error

$$L(y, f(\mathbf{x}, \omega)) = (y - f(\mathbf{x}, \omega))^2 \tag{3}$$

The squared-error loss (3) is commonly used for model selection comparisons. The set of functions $f(\mathbf{x}, \omega)$, $\omega \in \Omega$ supported by a learning method may or may not contain the regression function $g(\mathbf{x})$. Thus learning is the problem of finding the function $f(\mathbf{x}, \omega_0)$ (regressor) that minimizes the prediction risk functional

$$R(\omega) = \int (y - f(\mathbf{x}, \omega))^2 \, p(\mathbf{x}, y) d\mathbf{x} dy \tag{4}$$

using only the training data. This risk functional measures the accuracy of the learning method's *predictions* of unknown target function $g(\mathbf{x})$.

For a given parametric model (with fixed number of parameters) the model parameters are estimated by minimizing the empirical risk:

$$R_{emp}(\omega) = \frac{1}{n} \sum_{i=1}^{n} (y_i - f(\mathbf{x}_i, \omega))^2 \tag{5}$$

The problem of model selection (complexity control) arises when a set of possible models $f(\mathbf{x}, \omega)$ consists of (parametric) models of varying complexity. Then the problem of regression estimation requires optimal selection of model complexity (i.e., the number of parameters) in addition to parameter estimation via minimization of empirical risk (5).

Analytic model selection criteria attempt to estimate (unknown) prediction risk (4) as a function of (known) empirical risk (5) penalized by some measure of model complexity. Then one selects model complexity model corresponding to smallest (estimated) risk. It is important to point out that for finite-sample problems the goal of model selection is distinctly different from the goal of accurate estimation of prediction risk.

Since all analytic model selection criteria are based on certain assumptions (notably, asymptotic analysis, linearity) it is important to perform empirical comparisons in order to understand their practical usefulness in settings when these assumptions may not hold. Recently, (Cherkassky and Mulier, 1998; Cherkassky et al, 1999; Shao et al, 2000) showed such empirical comparisons for several analytic model selection methods for linear and penalized linear estimators, and concluded that SRM-based model selection is superior (to other methods). Later, (Cherkassky and Shao, 2001; Cherkassky and Kilts, 2001) successfully applied SRM-based model selection to wavelet signal denoising. Similarly, Chapelle et al (2001) suggest analytic model selection approach for small-sample problems based on VC-theory and claim superiority of the VC approach using empirical comparisons. These findings contradict a widely held opinion that VC-theory generalization bounds are too conservative for practical model selection (Bishop, 1995; Ripley, 1996; Duda et al, 2001). Recently, Hastie et al (2001) present empirical comparisons for model selection and conclude that 'SRM performs poorly overall'.

This paper is intended to clarify the current state of affairs regarding practical usefulness of SRM model selection. In addition, we address important methodological issues related to empirical comparisons in general and meaningful application of SRM model selection, in particular. The paper is organized as follows. Section 2 describes classical model selection criteria (AIC and BIC) and VC-based approach used for empirical comparisons. Section 3 describes empirical comparison for low-dimensional data sets using linear estimators and *k*-nearest neighbors method. Section 4 describes empirical comparisons for high-dimensional data sets taken from Hastie et al (2001) using k-nearest neighbor and linear subset selection regression. Conclusions are presented in Section 5.

2 Analytical Model Selection Criteria

In general, analytical estimates of (unknown) prediction risk R_{est} as a function of (known) empirical risk R_{emp} take one of the following forms

$$R_{est}(d) = R_{emp}(d) \cdot r(d,n) \tag{6}$$

or $$R_{est}(d) = R_{emp}(d) + r(d/n, \sigma^2) \tag{7}$$

where $r(d,n)$ is often called the penalization factor, which is a monotonically increasing function of the ratio of model complexity (degrees of freedom) d to the number of samples n.

In this paper, we discuss three model selection methods. The first two are representative statistical methods:

- Akaike Information Criterion (AIC) (Akaike, 1974)

$$AIC(d) = R_{emp}(d) + \frac{2d}{n}\hat{\sigma}^2 \tag{8}$$

- Bayesian Information Criterion (BIC)

$$BIC(d) = R_{emp}(d) + (\ln n)\frac{d}{n}\hat{\sigma}^2 \tag{9}$$

In AIC and BIC, d is the number of free parameters (of a linear estimator) and σ denotes the standard deviation of additive noise in (1). Both AIC and BIC are derived using asymptotic analysis (i.e. large sample size). In addition, AIC assumes that correct model belongs to the set of possible models. In practice, however, AIC and BIC are often used when these assumptions do not hold. When using AIC or BIC for practical model selection, one is faced with two issues:

- *Estimation and meaning of (unknown) noise variance*. When using a linear estimator with d parameters, the noise variance can be estimated from the training data as

$$\hat{\sigma}^2 = \frac{n}{n-d} \cdot \frac{1}{n} \sum_{i=1}^{n} (y_i - \hat{y}_i)^2 \tag{10}$$

Then one can use (10) in conjunction with AIC or BIC in one of two possible ways. Under the *first approach*, one estimates noise via (10) for each (fixed) model complexity (Cherkassky et al, 1999; Chapelle et al, 2001). Thus different noise estimates are used in AIC or BIC expression for each (chosen) model complexity. This leads to the following form of AIC known as Final Prediction Error (FPE) (Akaike, 1970):

$$AIC(d) = \frac{1 + d/n}{1 - d/n} R_{emp}(d) \tag{11}$$

Under the *second approach* one first estimates noise via (10) using a high-variance/low bias estimator, and then this noise estimate is plugged into AIC or BIC expressions (8) or (9) to select optimal model complexity. In this paper we use the latter approach since it has been used in empirical comparisons by (Hastie et al, 2001); however there seems to be no consensus on which approach is 'best' for practical model selection. Further, even though one can obtain an estimate of noise variance (as outlined above), the very interpretation of noise becomes difficult for practical problems when the set of possible models does not contain the true target function. In this case, it is not clear whether the notion of 'noise' refers to discrepancy between admissible models and training data, or reflects the difference between the true target function and the training data as in formulation (1). In particular, noise estimation becomes impossible when there is significant mismatch between an unknown target function and an estimator. Unfortunately, all data sets used in (Hastie et al, 2001) are of such kind. For example, they use k-nearest neighbor regression to estimate discontinuous target functions, even though it is well known that kernel estimators are intended for smooth target functions (Hardle, 1995). Hence, all empirical comparisons presented in this paper assume that for AIC and BIC methods the variance of additive noise in (1) is *known*. This helps to

avoid ambiguity with respect to using different strategies for noise estimation and gives an additional competitive advantage to AIC/BIC vs. SRM.

- *Estimation of model complexity.* AIC and BIC use the number of free parameters (for linear estimators) but it is not clear what is a good measure of complexity for other types of estimators (i.e., penalized linear, subset selection, k-nearest neighbors etc.). There have been several suitable generalizations of model complexity (known as 'effective' degrees-of-freedom) (Bishop, 1995; Cherkassky and Mulier, 1998; Hastie et al, 2001).

The third model selection method used in this paper is based on Structural Risk Minimization (SRM), which provides a very general and powerful framework for model complexity control. Under SRM, a set of possible models forms a nested structure, so that each element (of this structure) represents a set of models of fixed complexity. Hence a structure provides natural ordering of possible models according to their complexity. Model selection amounts choosing an optimal element of a structure using VC generalization bounds. For regression problems, we use the following VC-bound (Vapnik, 1998; Cherkassky and Mulier, 1998; Cherkassky et al, 1999):

$$R(h) \le R_{emp}(h)\left(1-\sqrt{p-p\ln p+\frac{\ln n}{2n}}\right)_{+}^{-1} \qquad (12)$$

where $p = h/n$ and h is a measure of model complexity (called the VC-dimension). The practical form of the VC-bound (12) is a special case of the general analytical bound (Vapnik, 1995) with appropriately chosen 'practical' values of theoretical constants. See (Cherkassky et al, 1999) for detailed 'derivation' of (12) from the general bounds developed in VC-theory.

According to SRM method, model selection amounts to choosing the model minimizing the upper bound on prediction risk (12). Note that under SRM approach we do not need to estimate noise variance. The bound (12) has been derived under very general assumptions (i.e., finite-sample setting, nonlinear estimation etc.). However, it requires an accurate estimation of the VC-dimension. Here we are faced

with the same problem as estimating 'effective degrees of freedom' in AIC or BIC method. Namely, the VC-dimension coincides with the number of free parameters for linear estimators, but is (usually) hard to obtain for other types of estimators.

The above discussion suggests the following common sense methodology for empirical comparisons between AIC, BIC and SRM. First perform comparisons for linear estimators, for which the model complexity can be accurately estimated for all methods. Then perform comparisons for other types of estimators either using advanced methods for estimating model complexity (Vapnik et al, 1994; Shao et al, 2000) or using crude heuristic estimates of model complexity. The latter approach is pursued in this paper for k-nearest neighbor regression (where accurate estimates of model complexity are not known).

3. Empirical Comparisons for Linear Estimators and *k*-Nearest Neighbors

We describe first experimental comparisons between AIC, BIC and SRM for *linear estimators* using comparison methodology and data sets from (Cherkassky et al, 1999). It is important to obtain meaningful comparisons for model selection with linear estimators first, since in this case the model complexity (DOF in AIC/BIC and VC-dimension in SRM) can be analytically estimated. Later (in Section 4) we show comparisons using data sets from (Hastie et al, 2001) for (nonlinear) estimators with crude estimates of the model complexity used for model selection criteria.

First we describe experimental set up and comparison metrics and then show empirical comparison results.

Target functions used:

Sine-squared function:

$$g_1(x) = \sin^2(2\pi x) \quad x \in [0,1] \ . \tag{13}$$

Discontinuous piecewise polynomial function

$$g_2(x) = \begin{cases} 4x^2(3-4x) & x \in [0,0.5] \\ (4/3)x(4x^2-10x+7)-3/2 & x \in (0.5,0.75] \\ (16/3)x(x-1)^2 & x \in (0.75,1] \end{cases} \quad (14)$$

Two dimension *sinc* function as target function.

$$g_3(\mathbf{x}) = \sin\sqrt{x_1^2 + x_2^2} \,/\, \sqrt{x_1^2 + x_2^2} \quad \text{defined on [-5,5]*[-5,5]} \quad (15)$$

Training and test samples are uniformly distributed in the input domain.

Estimators used:

(a) *Linear estimators* include polynomial and trigonometric estimators, that is

$$\text{Algebraic polynomials: } f_m(x,\omega) = \sum_{i=0}^{m-1} \omega_i x^i + \omega_0 \quad (16)$$

$$\text{Trigonometric expansion: } f_m(x,\omega) = \sum_{i=0}^{m-1} \omega_i \cos(ix) + \omega_0 \quad (17)$$

For linear estimators, the number of parameters (DOF) is used as a measure of model complexity (VC-dimension) for all model selection methods.

(b) *k-nearest neighbor*s regression where unknown function is estimated by taking a local average of *k* training samples nearest to the estimation point. In this case an estimate of effective DOF or VC-dimension is not known, even though sometimes the ratio *n/k* is used to estimate model complexity (Hastie et al, 2001). However, this estimate appears too crude, and can be criticized using both common-sense and theoretical arguments, as discussed next. With *k*-nearest neighbor method, the training data can be divided into n/k neighborhoods. If the neighborhoods were non-overlapping, then one can fit one parameter in each neighborhood (leading to an estimate $d = n/k$). However, the neighborhoods are, in fact, overlapping, so that a sample point from one neighborhood affects regression estimates in an adjacent neighborhood. This suggests that a better estimate of DoF has the form $d = n/(c*k)$ where $c > 1$. The value of (unknown) parameter c

is unknown but (hopefully) can be determined empirically or using additional theoretical arguments. Using the ratio *n/k* to estimate model complexity is inconsistent with the main result in VC-theory (that the VC-dimension of any estimator should be finite). Indeed, asymptotically (for large *n*) the ratio *n/k* grows without bound. On the other hand, asymptotic theory for k -nearest neighbor estimators [Hardle, 1995] provides asymptotically optimal k -values (when n is large), namely $k \sim n^{4/5}$. This suggests the following (asymptotic) dependency for DoF: $d \sim \frac{n}{k} * \frac{1}{n^{1/5}}$. This (asymptotic) formula is clearly consistent with 'common-sense' expression $d = n/(c * k)$ with $c > 1$. We found that a good practical estimate of DoF can be found empirically by assuming the dependency

$$d = const * n^{4/5} / k \tag{18}$$

and then empirically 'tuning' the value of *const=1* using a number of data sets. This leads to the following empirical estimate for DoF:

$$d = \frac{n}{k} * \frac{1}{n^{1/5}} \tag{19}$$

Prescription (19) is used as an estimate of DoF and VC-dimension for all model selection comparisons presented later in this paper. We point out that (19) is a crude 'practical' measure of model complexity. However, it is certainly better than an estimate $d = n / k$ used in (Hastie et al, 2001) because:

- using expression (18) instead of $d = n / k$ actually improves the prediction accuracy of all model selection methods (AIC, BIC and SRM) for all data sets used in our comparisons (including those used in (Hastie et al, 2001));
- proposed estimate (19) is consistent with DoF estimates provided by asymptotic theory and common-sense arguments.

Noise estimation: All comparisons use the true noise variance for AIC and BIC methods. Hence, AIC and BIC have an additional competitive 'advantage' versus SRM method.

Experimental procedure: A training set of fixed size (n) is generated using standard regression formulation (1) using a target function with y-values corrupted by additive Gaussian noise. The $\mathbf{x}$-values of training data follow random uniform distribution in a [0,1] range. Then the model (of fixed complexity) is estimated using training data (i.e. via least squares fitting for linear estimators or via k-nearest neighbors regression). Model selection is performed by (least-squares) fitting of models of different complexity and selecting an optimal model corresponding to smallest prediction risk as estimated by a given model selection criterion. Prediction risk (accuracy) of the model chosen by a model selection method is then measured (experimentally). The *prediction risk* is measured as MSE between a model (estimated from training data) and the true values of target function for independently generated test inputs:

$$R_{pred}(\omega) = \frac{1}{n_{test}} \sum_{i=1}^{n_{test}} (y_{target} - f(\mathbf{x}_{test}, \omega))^2 \tag{20}$$

The above experimental procedure is repeated 100 times using 100 different random realizations of n training samples (from the same statistical distribution), and the empirical distribution of the prediction risk (observed for each model selection method) is displayed using standard box plot notation, with marks at 95%, 75%, 50%, 25% and 5% of the empirical distribution.

Experiment 1: The training data are generated using the sine-squared target function (13) corrupted by Gaussian noise. A linear estimator (using algebraic polynomials) was used. Experiments were performed using small training sample (n=30) and large sample size (n=100). Figure 1 shows comparison results between AIC, BIC and SRM for noise level σ =0.2.

Experiment 2: The training data are generated using discontinuous piecewise polynomial target function (14) corrupted by Gaussian noise. A linear estimator (using trigonometric expansion) was used.

Experiments were performed using small training sample (n=30) and different noise levels. Figure 2 shows comparison results between AIC, BIC and SRM.

Comparison results presented in Figure 1 and Figure 2 indicate that SRM method works better than AIC and BIC for small sample sizes (n=30). For large samples (see Figure 1(b)), all methods show comparable (similar) prediction accuracy, however SRM is still preferable to other methods since it selects lower model complexity (i.e., lower-order polynomials). These findings are consistent with model selection comparisons for linear estimators presented in (Cherkassky et al, 1999).

Experiment 3: Here we compare model selection methods using k-nearest neighbors regression. The training and test data is generated using the same target functions (sine-squared and piecewise polynomial) as in previous experiments. The training sample size is 30 and the noise level σ =0.2. Comparison results are shown in Figure 3. We can see that all methods provide similar prediction accuracy (with SRM and BIC having a slight edge over AIC). However, SRM is more robust since it selects models of lower complexity (larger k) than BIC and AIC. Note that all comparisons use the proposed (estimated) model complexity (19) for k-nearest neighbor method. Using (arguably incorrect) estimates of model complexity *n/k* as in Hastie et al (2001) can obscure model selection comparisons. In this case, model selection comparisons for estimating sine-squared target function using k-nearest neighbors are shown in Figure 4. According to Fig. 4, AIC provides the best model selection; however its prediction accuracy is lower than with 'more accurate' DoF estimates (19) shown in Fig. 3a. By comparing results in Figure 3a and Figure 4 we conclude that:

- The proposed model complexity estimate (19) actually improves prediction performance of all three methods (AIC, BIC and SRM) relative to using DoF= n / k ;

- Prediction performance of SRM relative to AIC and BIC degrades significantly when using estimates of DOF= n / k . This can be explained by the multiplicative form of VC-bound (12) that

is affected more significantly by incorrect estimates of the model complexity (VC-dimension) than AIC and BIC which have an additive form.

Experiment 4: Here we compare model selection using k-nearest neighbors regression to estimate two dimension *sinc* target function (15) corrupted by Gaussian noise (with σ = 0.2 and 0.4). The training size is 50, and the test size is 300. Comparison results in Figure 5 indicate that the VC-based approach yields better performance than AIC and its performance is similar to BIC.

All experiments with low-dimensional data sets indicate that SRM model selection yields better (or at least not worse) prediction accuracy than AIC/BIC. This conclusion is obtained in spite of the fact that comparisons were biased in favor of AIC/BIC since we used true noise variance for AIC and BIC. Our conclusions are in strong disagreement with conclusions presented in (Hastie et al, 2001) who used high-dimensional data sets for model selection comparisons. The reasons for such disagreement are discussed in the next section.

4. Comparisons for High Dimensional Data Sets

This section presents comparisons for higher-dimensional data sets taken from (or similar to) [Hastie et al, 2001]. These data sets are used in Hastie et al [2001] to compare model selection methods for two types of estimators: k-nearest neighbors (described in Section 3) and linear subset selection (discussed later in this section). Next we present comparisons using the same/similar data sets but our results show an overall superiority of SRM method.

Comparisons for k-nearest neighbors. Let us consider a multivariate target function of 20 variables $\mathbf{x} \in R^{20}$

$$g_4(\mathbf{x}) = \begin{cases} 1 & if \quad x_1 > 0.5 \\ 0 & if \quad x_1 \le 0.5 \end{cases} \tag{21}$$

where random $\mathbf{x}$-values are uniformly distributed in $[0,1]^{20}$.

Experiment 5: We estimate target function (21) from n=50 training samples, using k-nearest neighbor regression. The quality of estimated models is evaluated using the test set of 500 samples. We use the true noise variance for AIC and BIC methods. All methods use the proposed DOF estimate (19). Results in Figure 6a correspond to the example in Hastie et al (2001) when training samples are not corrupted by noise. Results in Fig. 6b show comparisons for noisy training samples. In both cases, SRM achieves better prediction performance than other methods. Results presented in Figure 6 are in complete disagreement with empirical results and conclusions presented in Hastie et al (2001). There are several reasons for this disagreement. First, Hastie et al (2001) use their own (incorrect) interpretation of theoretical VC-bound that is completely different from the VC-bound (12). Second, discontinuous target function (21) used by Hastie et al (2001) prevents any meaningful application of AIC/BIC model selection with k-nearest neighbors. That is, kernel estimation methods assume sufficiently smooth (or at least, continuous) target functions. When this assumption is violated (as in the case of discontinuous step function), it becomes impossible to estimate the noise variance (for AIC/BIC method) with any reasonable accuracy. For example, using 5-nearest neighbor regression to estimate noise for this data set, as recommended by (Hastie et al, p.212), gives the noise variance 0.15 that is completely wrong (since the data has no additive noise). Third, application of AIC/BIC to the data set with no additive noise (as suggested by Hastie et al, 2001) makes little sense as well, because the additive form (8) and (9) for AIC and BIC implies that with zero noise these methods should select the highest model complexity. That is why we used small noise variance 0.0001 (rather than zero) for AIC/BIC in our comparisons for this data set. Graphical illustration of overfitting by AIC/BIC for this data set can be clearly seen in Fig. 7 showing the values of AIC, BIC and VC-bound as a function of k, along with the true prediction risk. In contrast, SRM method performs very accurate model selection for this data set.

Comparisons for linear subset selection. Here the training and test data are generated using a 5-dimensional target function $\mathbf{x} \in R^5$ and $y \in R$, defined as

$$g_5(\mathbf{x}) = \begin{cases} 1 & if \quad \sum_{j=1}^{3} x_j > 1.5 \\ 0 & if \quad \sum_{j=1}^{3} x_j \le 1.5 \end{cases} \tag{22}$$

with random $\mathbf{x}$-values uniformly distributed in $[0,1]^5$.

Linear subset selection method amounts to selecting the best subset of *m* input variables for a given training sample. Here the 'best' subset of *m* variables yields the linear model with lowest empirical risk (MSE fitting error) among all linear models with *m* variables, for a given training sample. Hence, for linear subset selection, model selection corresponds to selecting an optimal value of *m* (providing minimum prediction risk). Also note that linear subset selection is a nonlinear estimator, even though it produces models linear in parameters. Hence there may be a problem of estimating its model complexity when applying AIC, BIC or SRM for model selection. In this paper we estimate the model complexity as *m* (the number of chosen input variables) for all methods, similar to Hastie et al (2001). We do not know, however, whether this estimate is correct. Implementation of subset selection used in this paper performs an exhaustive search over all possible subsets of *m* variables (out of total *d* input variables) for choosing the best subset (minimizing the empirical risk). Hence, we used moderate number of input variables (*d*=5) to avoid the combinatorial explosion of subset selection.

Experiment 6: Training data and test data are generated using target function (22). We used true noise variance for AIC and BIC methods. Our comparisons use 30 training samples, and 200 test samples. Regression estimates are obtained from (noisy) training data using linear subset selection. Comparison results in Figure 8 show that all methods achieve similar prediction performance when the training data has no noise. For noisy data, BIC provides superior prediction performance, and both AIC

and BIC perform better than SRM. A closer look at results in Figure 8 helps to explain the methods' performance for this data set. Namely, results in Figure 8a clearly show that over-fitting by AIC and BIC does not result in the degradation of prediction risk, whereas under-fitting (by SRM) can adversely affect the prediction performance (see Figure 8b). Also from DoF box plots in Figure 8b, SRM selects optimal model complexity (DoF=4) most of the time, unlike AIC/BIC that tend to overfit. However, this does not yield better prediction performance for SRM in terms of prediction risk. This is further explained in Figure 9 which shows the dependence of prediction risk on degrees of freedom (the number of variables +1) for one (representative) realization of training data. From Figure 9, we can clearly see that there is no overfitting. This happens due to the choice of approximating functions (i.e., linear subset selection), which results in a large bias (mismatch) for the chosen target function (22). Even using the most complex linear subset selection model, one cannot accurately fit the training data generated by this target function. In other words, there is no possibility of over-fitting for this data set; hence a more conservative model selection approach (such as SRM) tends to underperform relative to AIC and BIC.

In order to perform more meaningful comparisons for linear subset selection method, consider the data set where the target function belongs to a set of possible models (approximating functions). Namely, the training and test data are generated using 5-dimensional target function $\mathbf{x} \in R^5$ and $y \in R$, defined as

$$g_6(\mathbf{x}) = x_1 + 2x_2 + x_3 \tag{23}$$

with $\mathbf{x}$-values with uniformly distributed in $[0,1]^5$.

Experimental comparisons of model selection for this data set are shown in Figure 10. Note that experimental set up and the properties of training data (sample size, noise level σ =0.2) are identical to the setting used to produce comparisons in Figure 8b, except that we use the target function (23). Results

shown in Figure 10 indicate that SRM and BIC have similar prediction performance (both better than AIC) for this data set.

Note that all comparisons assume known noise level for AIC/BIC; hence they are biased in favor of AIC/BIC. Even with this bias, SRM performs better (or at least not worse) than AIC/BIC for linear subset selection. Our findings contradict comparisons presented by Hastie et al (2001). This can be explained by the contrived data set used in their comparisons (similar to (22)), such that no overfitting is possible with linear subset selection.

5. Discussion

Given proliferation of ad hoc empirical comparisons and heuristic learning methods, the issue of what constitutes meaningful comparisons becomes of great practical importance. Hence, in this section we discuss several methodological implications of our comparison study, and suggest future research directions. The first issue that one needs to address is what is the goal of empirical comparisons? Often the goal seems to be demonstrating that one method (learning technique, model selection criterion) is better than the other(s); and this can easily be accomplished by:

(a) Using specially chosen (contrived) data sets that favor particular method;

(b) Tuning well one method (learning algorithm), while tuning poorly other (competing) methods. This is often done unintentionally since a person performing comparisons is usually an expert in one method (being proposed).

In fact, according to Vapnik (1998), generalization from finite data is possible only when an estimator has limited capacity (i.e., complexity). Therefore, a learning method cannot solve most practical problems with finite samples, unless it uses a set of approximating functions (admissible models) appropriate for a problem at hand. Ignoring this common-sense observation leads to formal proofs that no learning method generalize better than another for all data sets (i.e., results collectively

known as 'no free lunch' theorems see Duda et al (2001)). In this sense, a clear mismatch between estimation methods and data sets used for model selection comparisons in (Hastie et al, 2001) leads to particularly confusing and misleading conclusions.

In our opinion, the goal of empirical comparisons of methods for model selection should be improved understanding of their relative performance for finite-sample problems. Since the model complexity (VC-dimension) can be accurately estimated for linear methods, it is methodologically appropriate to perform such comparisons for linear regression first, before considering other types of estimators. Recent comparison studies (Cherkassky and Mulier, 1998; Cherkassky et al, 1999; Shao et al, 2000) indicate that VC-based model selection is superior to other analytic model selection approaches for linear and penalized linear regression with finite samples. Empirical comparisons between SRM, AIC and BIC for linear estimators presented in this paper confirm practical advantages of SRM model selection. In addition, we propose a new practical estimate of model complexity for *k*-nearest neighbor regression, and use it for model selection comparisons. This paper presents the first practical application of VC-bound (12) with k-nearest neighbor methods. Our empirical results show the advantages of SRM and BIC (relative to AIC) model selection for k-nearest neighbors. Likewise, our empirical comparisons clearly show practical advantages of SRM model selection for linear subset selection regression.

Future research may be directed towards meaningful comparisons of model selection methods for other (nonlinear) estimators. Here the main challenge is:

(1) Estimating model complexity, and

(2) Avoiding potential methodological pitfalls of ad hoc comparisons.

Empirical comparisons performed by Hastie et al (2001) illustrate possible dangers of ad hoc comparisons, such as:

- *Inaccurate estimation of model complexity.* It is impossible to draw any conclusions based on empirical comparisons unless one is confident that model selection criteria use accurate estimates of model complexity. There exist experimental methods for measuring the VC-dimension of an estimator (Vapnik et al, 1994; Shao et al, 2000); however they may be difficult to apply for general practitioners. An alternative practical approach is to come up with empirical 'common-sense' estimates of model complexity to be used in model selection criteria. For example, in this paper where we successfully used a new complexity measure for *k*-nearest neighbor regression. Essentially, under this approach we combine the known analytical form of a model selection criterion, with appropriately tuned measure of model complexity taken as a function of (some) complexity parameter (i.e., the value of *k* in *k*-nearest neighbor method).
- *Using contrived data sets.* For both *k*-nearest neighbors and linear subset selection comparisons, Hastie et al (2001) used especially chosen data sets so that meaningful model selection comparisons become difficult or impossible. For example, for subset selection comparisons they use a data set such that regression estimates do not exhibit any overfitting. This (contrived) setting obviously favors model selection methods (such as AIC) that tend to overfit.
- *Using small number of data sets*. Comparisons presented in (Hastie et al, 2001) use just two data sets of fixed size with no noise (added to response variable). Such comparisons can easily be misleading, since model selection methods typically exhibit different relative performance for different noise levels, sample size etc. Reasonable comparisons (leading to meaningful conclusions) should compare model selection criteria for a broad cross-section of training data with different statistical characteristics (Cherkassky et al, 1999).
- *Using inappropriate form of VC-bounds.* The VC-theory provides an analytical form of VC-bounds, however it does not give specific (practical) values of theoretical parameters and constants. Such (practical) parameter values lead to the practical form of VC-bounds for regression problems used

in this paper. It appears that Hastie et al (2001) used the original theoretical VC-bound with poorly chosen parameter values, instead of the practical form of VC-bound (12) described in (Cherkassky and Mulier, 1998; Vapnik, 1998; Cherkassky et al, 1999).

Finally we briefly comment on empirical comparisons of model selection methods for classification, presented in Hastie et al (2001) using an experimental setting for high-dimensional data sets described in Section 4. Whereas Hastie et al (2001) acknowledge that they do not know how to set practical values of constants in VC-bounds for classification, they proceed with empirical comparisons anyway. We remain highly skeptical about scientific value of such comparisons. Selecting appropriate 'practical' values of theoretical constants in VC bounds for classification is an important and interesting research area.

It may be worthwhile to point out that Hastie et al (2001) use identical data sets for regression and classification comparisons; the only difference is in the choice of the loss function. Likewise, classical model selection criteria (AIC and BIC) have an identical form (for regression and classification). This observation underscores an important distinction between classical statistics and VC-based approach to learning/ estimating dependencies from data. Namely, the classical approach to learning (estimation) problems is to apply maximum likelihood method (ML) for estimating parameters of a density function. Hence, the same approach (density estimation via ML) can be used for both classification and regression, and AIC/BIC prescriptions have an identical form for both types of learning problems. In contrast, the VC approach clearly differentiates between regression and classification settings, since the goal of learning is not density estimation, but rather estimation of certain properties of unknown densities via empirical risk minimization or structural risk minimization. This results in completely different forms of VC-bounds for classification (additive form) and for regression (multiplicative form). Based on the above discussion, it becomes clear that Hastie et al (2001) use identical data sets for both classification and regression comparisons following classical statistical approach. In contrast, under

VC-based methodology, it makes little sense to use the same data sets for classification and regression comparisons, since we are faced with two completely different learning problems.

Acknowledgements

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FIGURE CAPTIONS

Fig. 1. Comparison results for sine-squared target function estimated using polynomial regression, noise level σ =0.2 (SNR=1.77) (a) small size n=30 (b) large size n=100

Fig. 2. Comparison results for piecewise-polynomial target function estimated using trigonometric regression, sample size n=30 (a) σ =0.2, SNR=1.5 (b) σ =0.1, SNR=3

Fig. 3. Comparison results for univariate regression using *k*-nearest neighbors. Training data: n=30, noise level σ =0.2 (a) sine squared target function (b) piecewise polynomial target function

Fig. 4. Comparison results for sine-squared target function using *k*-nearest neighbors when DOF=n/k for all methods. Training data: n=30, noise level σ =0.2

Fig. 5. Comparisons results for two dimension *sinc* target function using *k*-nearest neighbors, sample size n=50 (a) σ =0.2 (b) σ =0.4

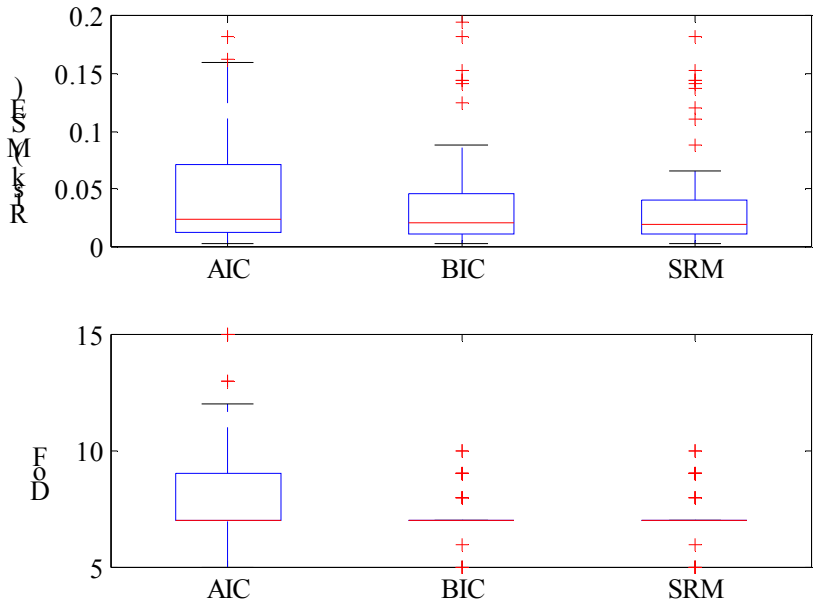
Fig. 6. Comparisons for high-dimensional target function (21) using *k*-nearest neighbors method, sample size n=50 (a) σ =0 (b) σ =0.2

Fig. 7. True prediction risk and its estimates provided by AIC/BIC and SRM (VC-bound) as a function of *k* (number of nearest neighbors) for a single realization of training data for high-dimensional target function (21) with sample size n=50 and noise σ =0. Note: risk estimates given by AIC and BIC are identical due to zero noise (assumed to be known). Minimal values of risk and estimated risk are marked with a star.

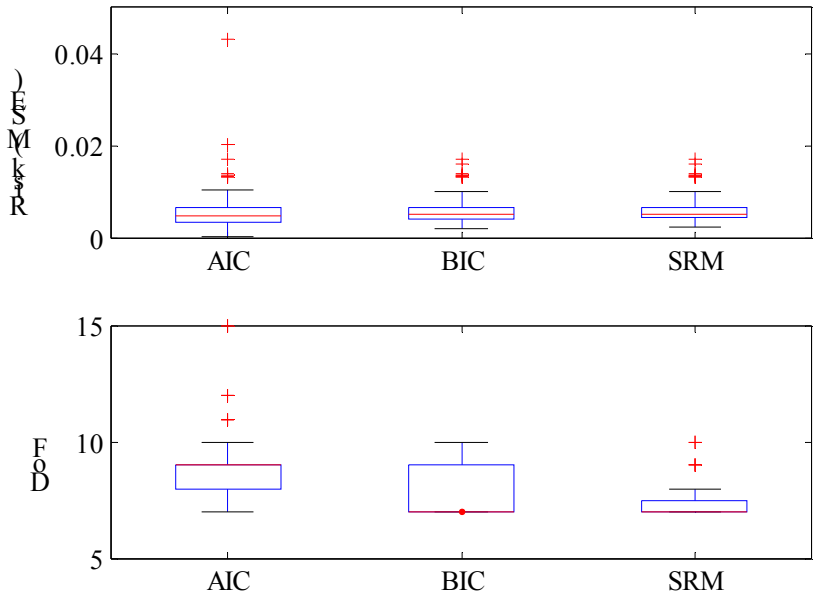
Fig. 8. Comparisons results for high-dimensional target function (22) using linear subset selection for n=30 samples (a) σ =0 (b) σ =0.2

Fig. 9. Prediction risk as a function of DoF with linear subset selection for a single realization of training data generated using high-dimensional target function (22), n=30 samples, σ =0.

Fig. 10. Comparisons results for high-dimensional target function (23) using linear subset selection for n=30 samples, noise level σ =0.2

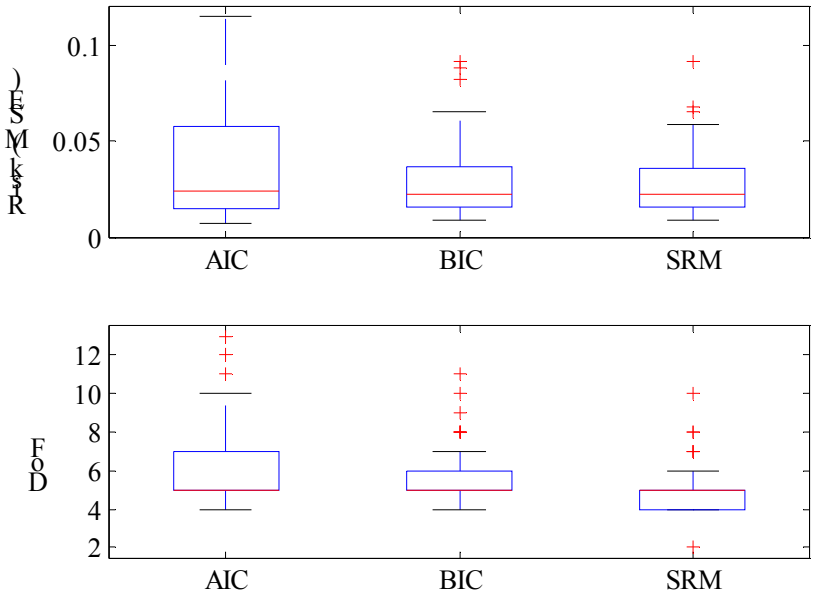


(a)

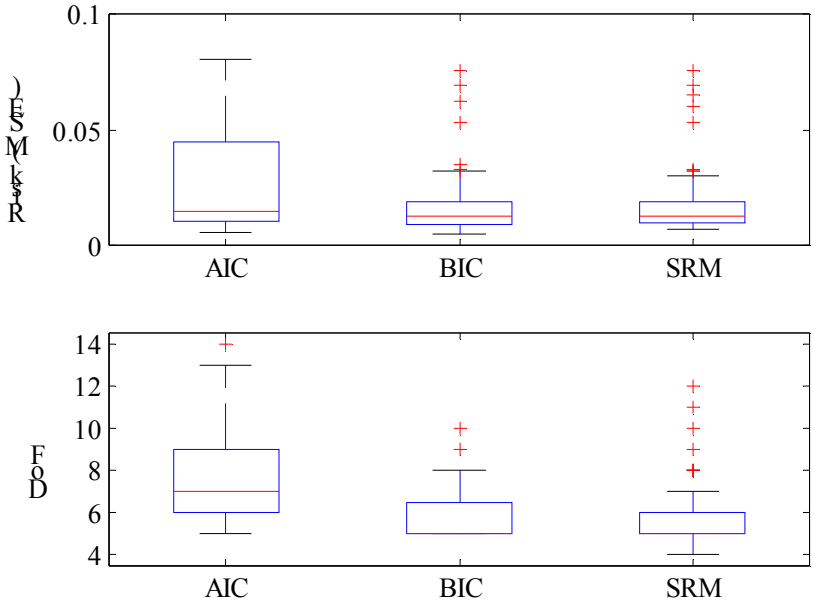


(b)

Figure 1: [Cherkassky] Comparison results for sine-squared target function estimated using polynomial regression, noise level σ =0.2 (SNR=1.77) (a) small size n=30 (b) large size n=100

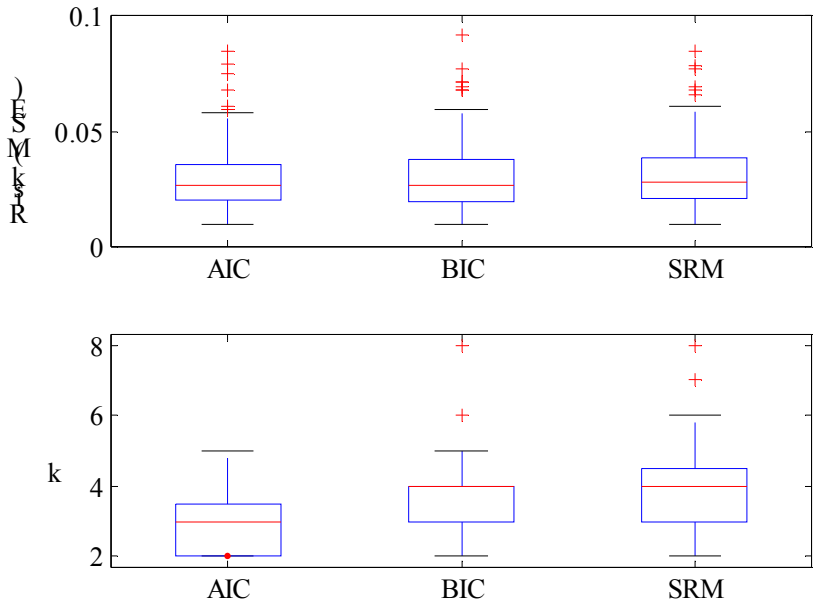


(a)

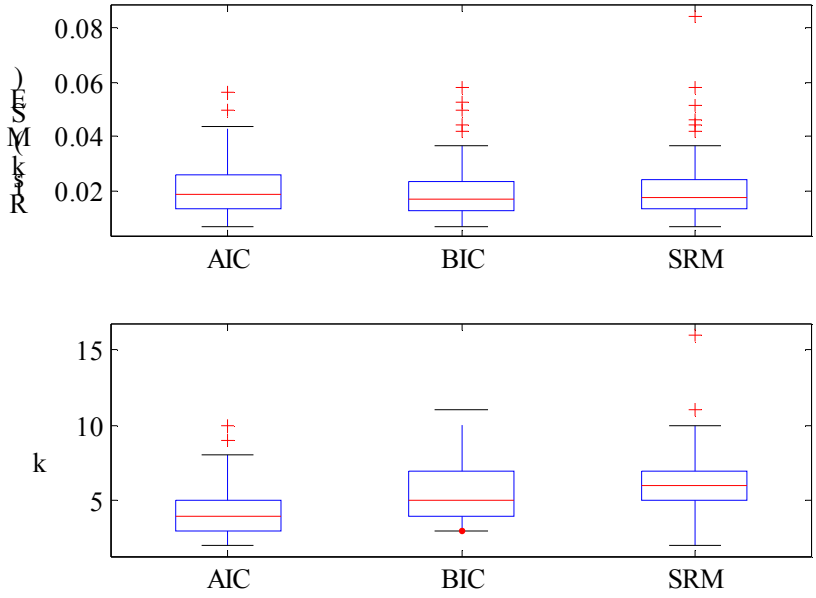


(b)

Figure 2: [Cherkassky] Comparison results for piecewise-polynomial target function estimated using trigonometric regression, sample size n=30 (a) σ =0.2, SNR=1.5 (b) σ =0.1, SNR=3



(a)



(b)

Figure 3: [Cherkassky] Comparison results for univariate regression using *k*-nearest neighbors. Training data: n=30, noise level σ =0.2 (a) sine squared target function (b) piecewise polynomial target function

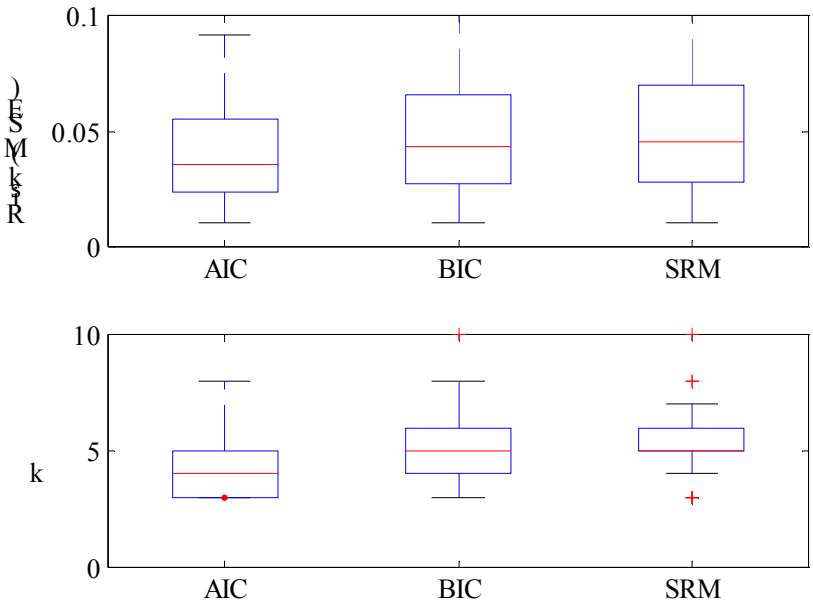


Figure 4: [Cherkassky] Comparison results for sine-squared target function using *k*-nearest neighbors when DOF=n/*k* for all methods. Training data: n=30, noise level σ =0.2

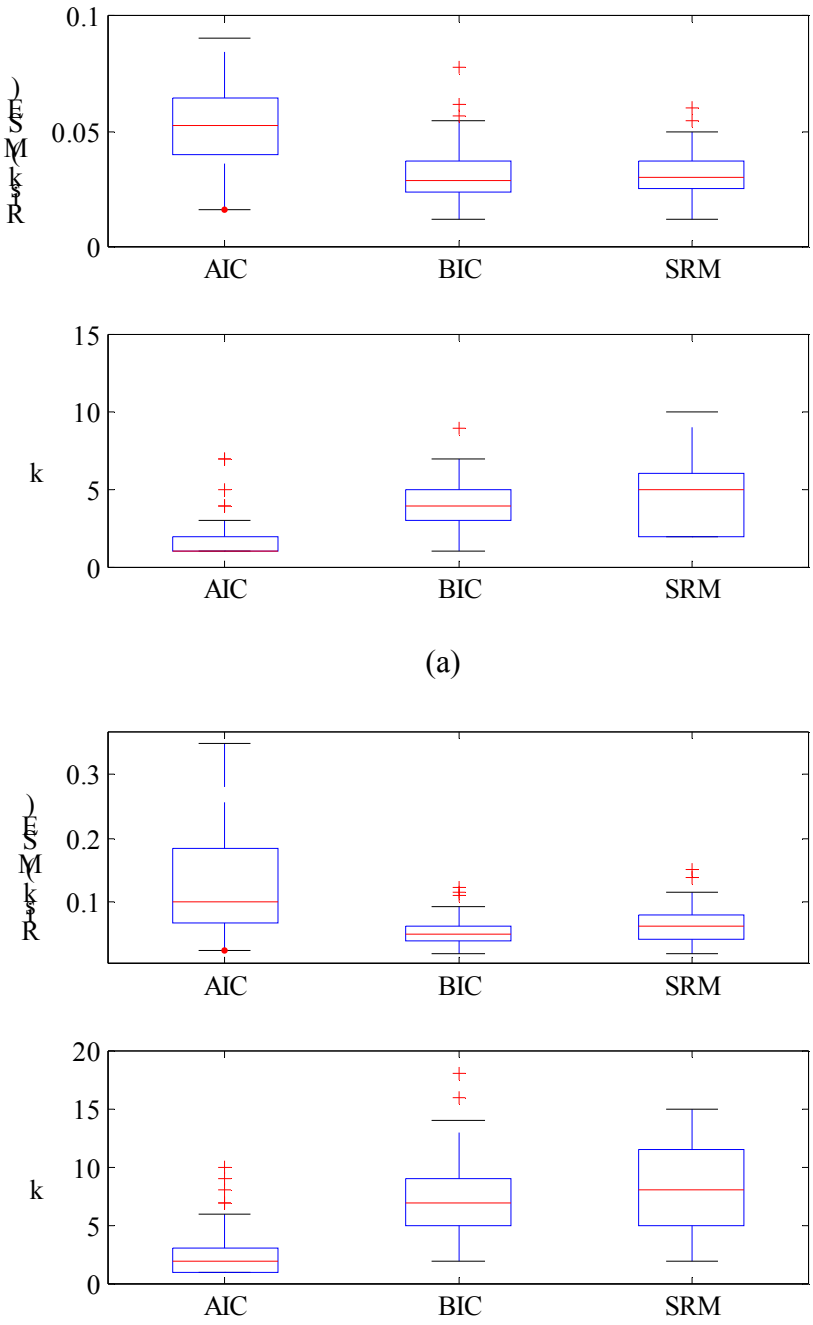
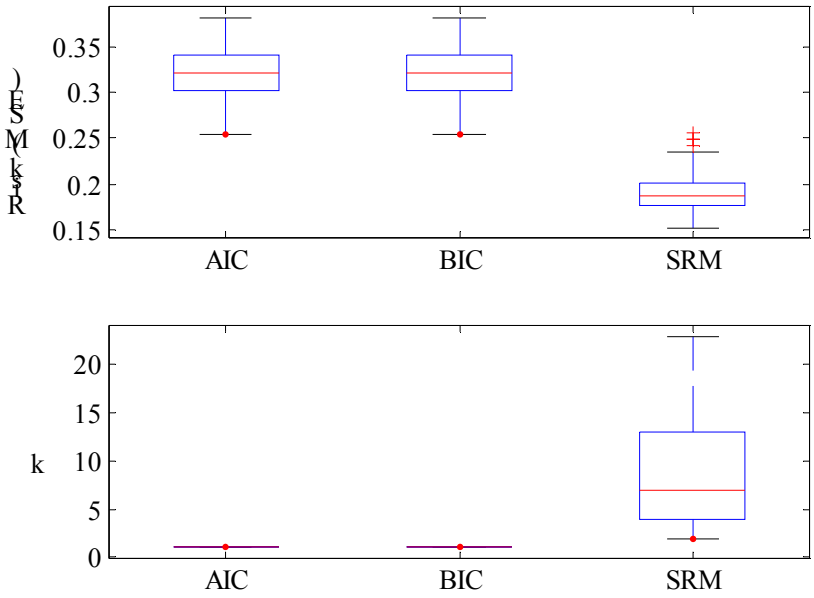
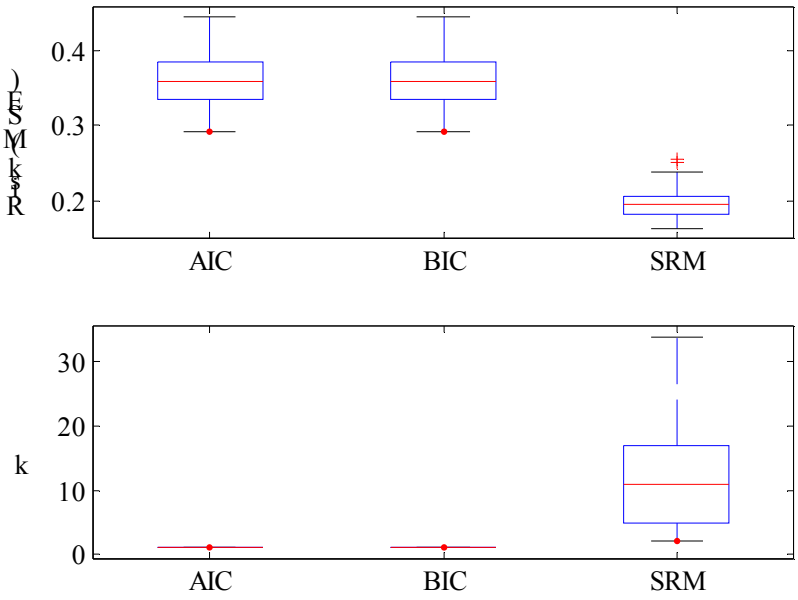


Figure 5: [Cherkassky] Comparisons results for two dimension *sinc* target function using *k*-nearest neighbors, sample size n=50 (a) σ =0.2 (b) σ =0.4



(a)



(b)

Figure 6: [Cherkassky] Comparisons for high-dimensional target function (21) using *k*-nearest neighbors method, sample size n=50 (a) σ =0 (b) σ =0.2

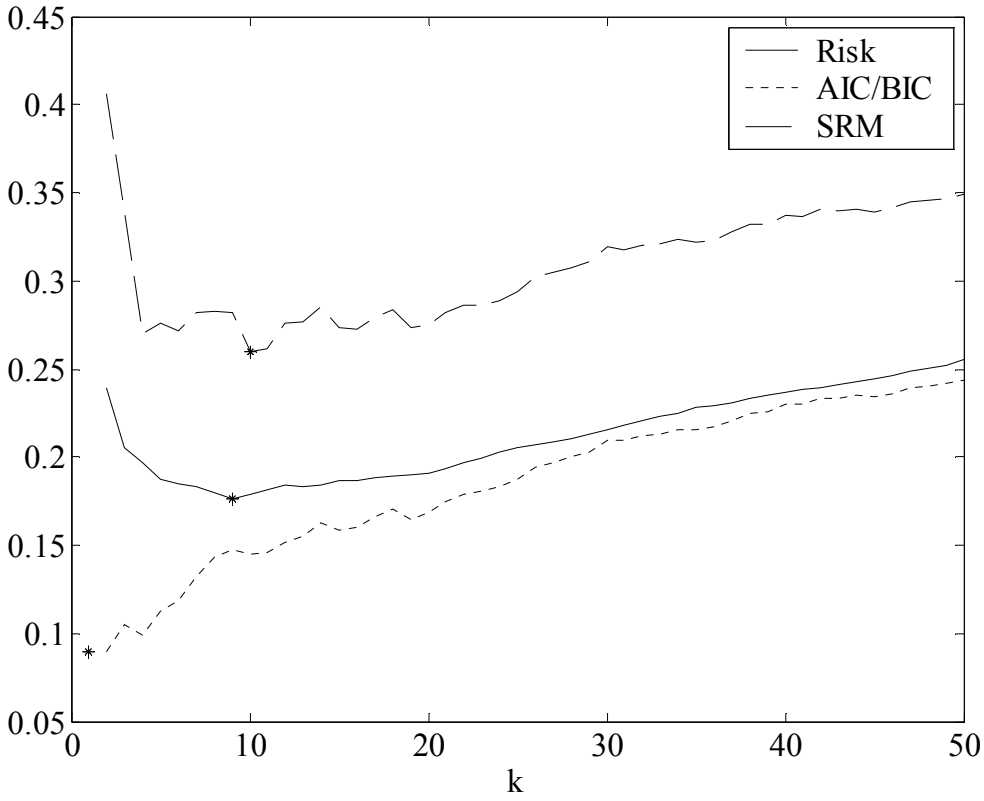
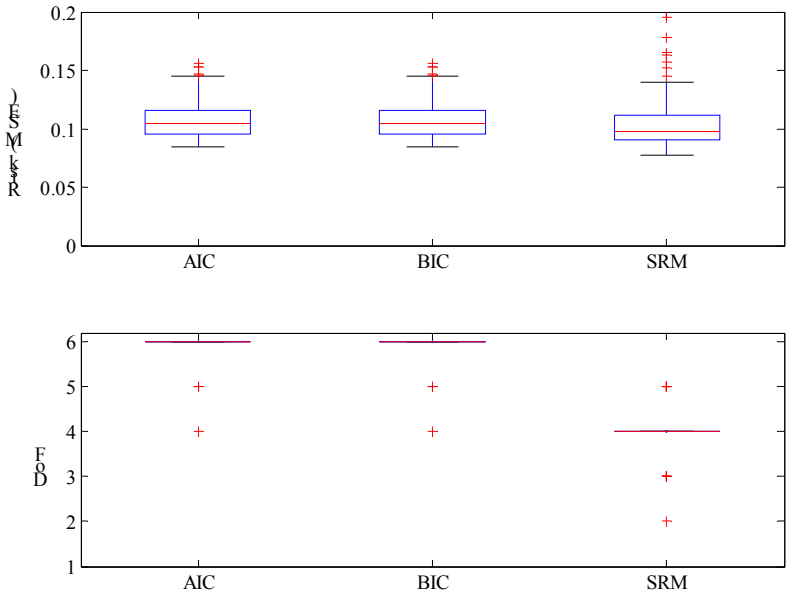


Figure 7: [Cherkassky] True prediction risk and its estimates provided by AIC/BIC and SRM (VC-bound) as a function of *k* (number of nearest neighbors) for a single realization of training data for high-dimensional target function (21) with sample size n=50 and noise σ =0. Note: risk estimates given by AIC and BIC are identical due to zero noise (assumed to be known). Minimal values of risk and estimated risk are marked with a star.



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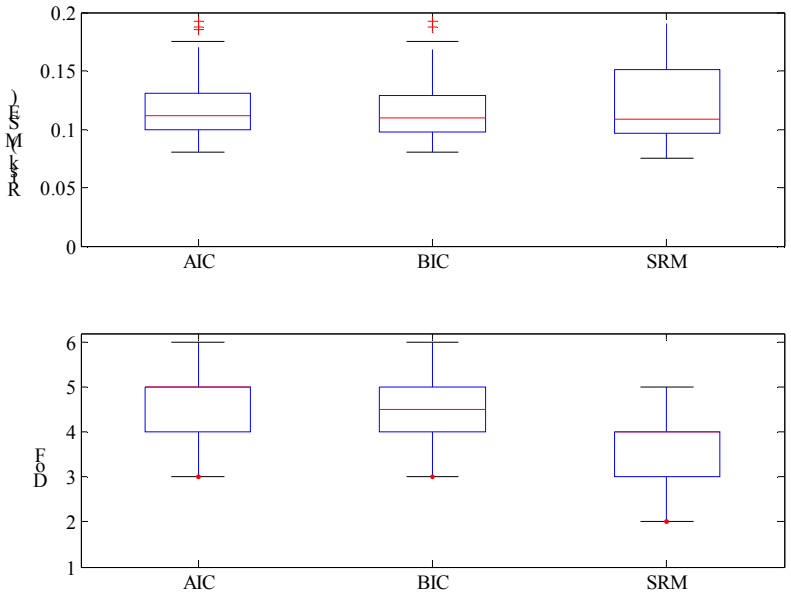

(b)

Figure 8: [Cherkassky] Comparisons results for high-dimensional target function (22) using linear subset selection for n=30 samples (a) σ =0 (b) σ =0.2

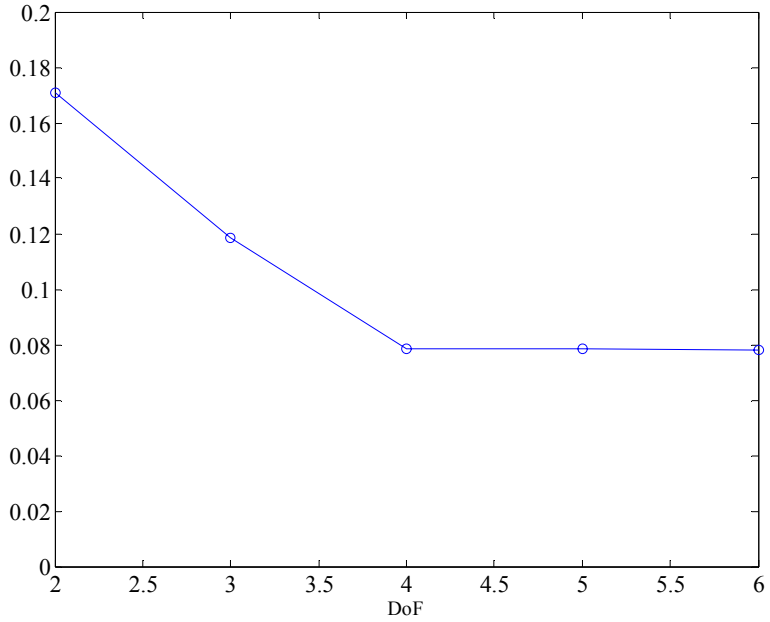

Figure 9: [Cherkassky] Prediction risk as a function of DoF with linear subset selection for a single realization of training data generated using high-dimensional target function (22), n=30 samples, σ =0

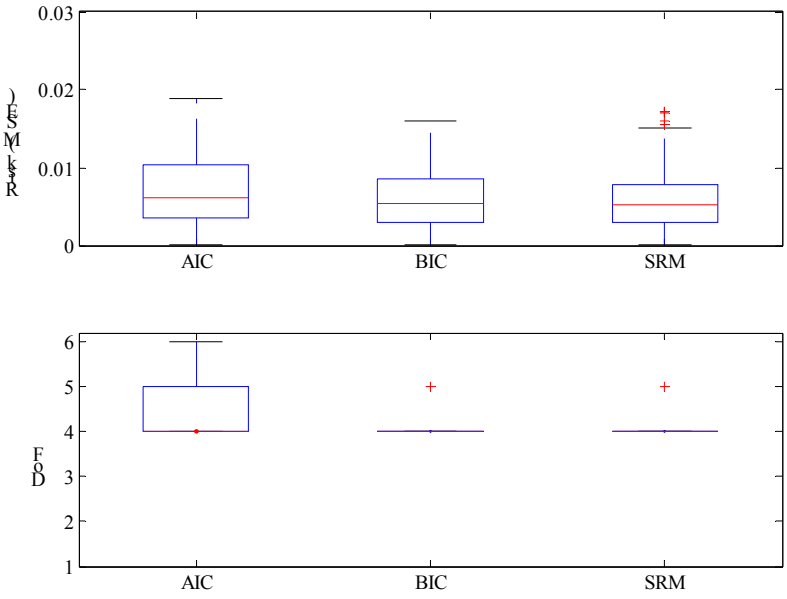

Figure 10: [Cherkassky] Comparisons results for high-dimensional target function (23) using linear subset selection for n=30 samples, noise level σ =0.2