Linear and Kernel Classification: When to Use Which?

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Abstract

Kernel methods are known to be a state-of-the-art classification technique. Nevertheless, the training and prediction cost is expensive for large data. On the other hand, linear classifiers can easily scale up, but are inferior to kernel classifiers in terms of predictability. Recent research has shown that for some data sets (e.g., document data), linear is as good as kernel classifiers. In such cases, the training of a kernel classifier is a waste of both time and memory. In this work, we investigate the important issue of efficiently and automatically deciding whether kernel classifiers perform strictly better than linear for a given data set. Our proposed method is based on cheaply constructing a classifier that exhibits nonlinearity and can be automatically trained. Then we make a decision by comparing the performance of our constructed classifier with the linear classifier. We propose two methods: the first one trains the degree-2 feature expansion by a linear-classification method, while the second dissects the feature space into several regions and trains a linear classifier for each region. The design considerations of our methods are very different from past works for speeding up the kernel training. They still aim at obtaining accuracy close to the kernel classifier, but ours would like to give a quick and accurate decision without worrying about accuracy. Empirically our methods can efficiently make correct indications for a wide variety of data sets. Our proposed process can thus be a useful component for automatic machine learning.

1 Introduction

Machine learning is now widely applied in many areas, but its practical use remains challenging for non-experts. To make machine learning an easy-to-use technique, recently automatic machine learning (autoML) has become an important research topic. What makes autoML a challenging task is that there are too many considerations, and different components often intertwined with each other. In this work we consider the issue of automatically choosing between linear and kernel classifiers. This issue is useful in an autoML process because very often we start with using a linear classifier and move to a nonlinear one if the performance is not satisfactory.

In machine learning, kernel classifiers such as support vector machines (SVM) [4] or kernel logistic regression (LR) are known to achieve state-of-the art performances for many classification problems; see detailed comparisons in, for example, [18, 6]. However, training and prediction are slow because kernel methods nonlinearly map data to a high dimensional space and employ the kernel trick. In contrast, linear classifiers of working in the original feature space are much more scalable. Although classifiers employing certain kernels are theoretically known to be at least as good as linear [12],[1] for many problems (e.g., document classification) linear classifiers are known to be competitive (e.g., the survey in [25]). For such data, the training of kernel classifiers is a total waste because fast and simple linear classifiers are enough.

From the above discussion, a possible component in an autoML workflow can be as follows.

```
If linear is as good as kernel, then
      use a linear classifier,
else
      use a kernel classifier.
```

Note that by kernel classification we mean that highly nonlinear kernels are used. In fact, the most commonly used Gaussian (RBF) kernel will be the focus in this paper. While the above workflow is simple, the following challenging issues must be solved first.

1. The method to check if linear classifiers are as good as nonlinear ones must be fast, automatic, and effective. First, the procedure must be much faster than training kernel classifiers and, if possible, as efficient as training linear classifiers; otherwise, the workflow becomes useless. Second, it should not involve the tuning of many parameters, so the use is convenient. Third, the procedure should accurately reveal if there is a clear performance gap between linear and kernel classifiers.
2. Before employing a method to predict if linear is as good as kernel, we should ensure that the linear classifier

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[1] Specifically, [12] proves that if the Gaussian kernel is used with suitable kernel/regularization parameters, then the performance is at least as good as using linear.

is "under the best settings" including suitable data preprocessing and parameter selection. Although recent works such as [3] have made progress on this aspect, some issues remain to be addressed.

The difficulty in differentiating linear and kernel can also be seen from our development of two popular packages LIBSVM [1] and LIBLINEAR [5] for kernel and linear classification, respectively. Many users have asked why the two packages are not combined together. However, the merge is not possible unless we have resolved the above-mentioned issues.

In this paper, we focus on the issue of checking if for the same data a linear classifier is as good as a kernel one. Currently some rough guidelines are used in practice. For example, it is mentioned in [11] that "If the number of features is large, one may not need to map data to a higher dimensional space." To the best of our knowledge, we are the first to systematically investigate this kernel-check problem.

A well-studied topic related to our work is kernel approximation. To reduce the lengthy running time of training a classifier, many works [23, 26] have attempted to approximate the kernel matrix or the kernel function. Their goal is to make the performance close to that of the original one, but require less time. Therefore, both training time and performances are concerns. Ours differs from them because accuracy is not important. It is sufficient if our method can effectively tell if kernel and linear yield different accuracy values. More discussion is in Section 3.

This paper is organised as follows. Section 2 briefly introduces linear and kernel classifiers, and their relations. In Section 3, we propose some effective methods to check if kernels should be used. Section 4 addresses the second challenge mentioned above. We mainly investigate some data scaling issues so that a good setting for linear classification can be automatically found. Detailed experiments are in Section 5, while conclusions are in Section 6. Supplementary materials are at `http://www.csie.ntu.edu.tw/~cjlin/papers/kernel-check/supplement.pdf`.

2 Linear and Kernel Classifiers

Before proposing methods to check if kernels are needed, we check how linear and kernel classifiers are practically used. We focus on two-class problems with training data $(y_i, \boldsymbol{x}_i), i = 1, \ldots, l$, where label $y_i = \pm 1$ and $\boldsymbol{x}_i \in \mathbb{R}^n$.

2.1 Standard Settings for Linear Classifiers

A linear classifier involves an optimization problem.

$$\min_{\boldsymbol{w}} \frac{1}{2}\boldsymbol{w}^T\boldsymbol{w} + C\sum_{i=1}^{l} \xi(\boldsymbol{w}; y_i, \boldsymbol{x}_i), \tag{2.1}$$

where C is the regularization parameter and $\xi(\boldsymbol{w}; y, \boldsymbol{x})$ is the loss function. Commonly used losses include

$$\xi(\boldsymbol{w}; y, \boldsymbol{x}) = \begin{cases} \max(0, 1 - y\boldsymbol{w}^T\boldsymbol{x}), & \text{L1 hinge loss} \\ \max(0, 1 - y\boldsymbol{w}^T\boldsymbol{x})^2, & \text{L2 hinge loss} \\ \log(1 + e^{-y\boldsymbol{w}^T\boldsymbol{x}}), & \text{LR loss.} \end{cases} \tag{2.2}$$

From the appendix in [5], a common setting for training a linear classifier includes the following steps.

1. Instance-wisely normalize each $\boldsymbol{x}_i$ to a unit vector.
2. Choose C that gives the highest cross validation (CV) accuracy.[2]
3. Obtain the model $\boldsymbol{w}$ using the selected C.

2.2 Standard Settings for Kernel Classifiers

The main difference between a linear and a kernel classifier is that each feature vector $\boldsymbol{x}$ is mapped to $\phi(\boldsymbol{x})$ in a different dimensional space. For example, the L1 hinge loss becomes

$$\max(0, 1 - y_i(\boldsymbol{w}^T\phi(\boldsymbol{x}_i) + b)).$$

Note that a bias term b is included because of historical reasons.[3] Usually $\phi(\boldsymbol{x})$ is very high dimensional, so kernel tricks are applied [4]. Specifically, $\boldsymbol{w}$ is shown to be a linear combination of $\phi(\boldsymbol{x}_i), \forall i$:

$$\boldsymbol{w} = \sum_{i=1}^{l} y_i\alpha_i\phi(\boldsymbol{x}_i),$$

where $\alpha_i, \forall i$ are solutions of the following dual optimization problem (assuming L1 hinge loss is used).

$$\begin{array}{ll} \min_{\boldsymbol{\alpha}} & \frac{1}{2}\boldsymbol{\alpha}^T Q\boldsymbol{\alpha} - \boldsymbol{e}^T\boldsymbol{\alpha} \\ \text{subject to} & 0 \le \alpha_i \le C, \forall i \text{ and } \boldsymbol{y}^T\boldsymbol{\alpha} = 0 \end{array} \tag{2.3}$$

where $Q_{ij} = y_i y_j K(\boldsymbol{x}_i, \boldsymbol{x}_j)$, $K(\boldsymbol{x}_i, \boldsymbol{x}_j)$ is the kernel function, and $\boldsymbol{e}$ is the vector of ones. For the other two losses in (2.2), their dual problems can be seen in, for example, [24, 22]. Commonly used kernels include

- polynomial: $K(\boldsymbol{x}_i, \boldsymbol{x}_j) = \phi(\boldsymbol{x}_i)^T\phi(\boldsymbol{x}_j)$,
- Gaussian: $K(\boldsymbol{x}_i, \boldsymbol{x}_j) = \exp(-\gamma\|\boldsymbol{x}_i - \boldsymbol{x}_j\|^2)$,

where $\gamma, r > 0$, and $d \ge 1$ are kernel parameters to be decided by the users.

The popular SVM guide [11] suggests the following setting to train a kernel classifier.

1. Scale each feature to an interval like $[-1, +1]$.
2. Use Gaussian kernel. Choose C, γ that give the highest CV accuracy.
3. Obtain the model $\boldsymbol{w}$ using the selected C, γ.

[2] The selection of the loss function can be incorporated in the CV process, though practically it is directly decided by users because using these three loss functions gives similar performances.

[3] For linear classification, the bias term is often omitted because for document data with many features the performance with/without the bias term is usually similar.

2.3 Relations between Linear and Kernel Classifiers Although a linear classifier is a special kernel classifier with $K(\boldsymbol{x}_i, \boldsymbol{x}_j) = \boldsymbol{x}_i^T \boldsymbol{x}_j$, many differences occur between linear and (non-linear) kernel classifiers. We briefly discuss them in this section.

Training a linear classifier can be much more efficient because of not conducting kernel operations. For some iterative algorithms to train a model, the cost of one iteration when using a non-linear kernel can be up to l times slower. See the discussion in, for example, Section 3.2 of [2]. However, as expected, a highly non-linear kernel such as the Gaussian often gives a better model. A justification is in the following theorem.

THEOREM 2.1. (THEORM 2 IN [12]) *Given C_L. Let $(\boldsymbol{w}_K(\gamma), b_K(\gamma))$ and $(\boldsymbol{w}_L, b_L)$ denote the optimal solution for the primal form of problem* (2.3) *using Gaussian kernel (with $C = \gamma C_L$ and γ) and linear kernel (with $C = C_L$) respectively. Then $\forall \boldsymbol{x}$,*

$$\lim_{\gamma \to 0} [\boldsymbol{w}_K(\gamma)^T \phi(\boldsymbol{x}) + b_K(\gamma)] = \boldsymbol{w}_L^T \boldsymbol{x} + b_L.$$

Thus if C and γ for Gaussian kernel L1-loss SVM have been chosen properly, it can mimic the behaviour of linear L1-loss SVM. This explains why kernel classifiers perform better than linear classifiers in practice.

Another difference is that the training and prediction time of kernel classifiers is more sensitive to the selection of the loss function. If L1 or L2 hinge loss is used, $\alpha_i = 0$ for some i and the decision function

$$\boldsymbol{w}^T \phi(\boldsymbol{x}) + b = \sum\nolimits_{i:\alpha_i > 0} y_i \alpha_i K(\boldsymbol{x}_i, \boldsymbol{x}) + b$$

involves only kernel evaluations between the test point $\boldsymbol{x}$ and a subset of training points (called support vectors). In contrast, for the logistic loss, $\alpha_i > 0$ always holds [24], so the prediction time may be significantly longer. Similarly, in the training phase, the possibility of $\alpha_i = C$ gives L1 hinge loss some advantages over L2 loss, whose dual problem has constraints $0 \le \alpha_i$ rather than $0 \le \alpha_i \le C$. These differences disappear or become minor for linear classification. For example, regardless of the loss function, the decision function always involves a single inner product $\boldsymbol{w}^T \boldsymbol{x}$. Unfortunately, past developments separately consider the best settings for linear and kernel classifiers without worrying about linking them. For example, the kernel-based solver LIBSVM supports only the L1 hinge loss, but the linear solver LIBLINEAR has the L2 hinge loss as the default option.

There is yet one more difference on data scaling. This pre-processing step might significantly affect the performance. In Sections 2.1 and 2.2, instance-wise normalization is recommended for linear classification, but feature-wise scaling is commonly used for non-linear kernels. This inconsistency is annoying because we may need to scale data twice. When the Gaussian kernel is used, it can be proved that without data scaling, overfitting occurs for data with large feature values unless extreme parameter values are used. Additionally, features in a greater numerical range can easily dominate those in smaller ranges. In contrast, for linear classification the normalization of each data instance to a unit vector is more like a convention in practice. To have a better understanding, we detailedly investigate the issue of data scaling for linear classification in Section 4. The conclusion is that feature-wise scaling is also suitable for the linear case. Thus, we consider feature-wise scaling for both linear and kernel classifiers in this work.

3 Proposed Kernel-check Methods

In this section, we propose two kernel-check methods. The first one is based on checking the performance difference between degree-2 polynomial and linear kernels. The second one dissects the curve of the decision boundary into finite segments and checks if the difference from a linear classifier is significant.

Before getting into our methods, we briefly discuss a closely related problem: kernel approximation for reducing the training time of a kernel classifier. While we want to check whether a kernel classifier is strictly better than a linear classifier, their focus is to sacrifice unnoticeable amount of performance in order to gain speed up on training kernel classifiers. One major class of kernel approximation methods is to form a low-rank approximation to the original kernel matrix $K \approx G^T G \in \mathbb{R}^{l \times l}$, where $G \in \mathbb{R}^{d \times l}$ and $d \ll l$. Examples include [23, 7]. Similarly, one can directly approximate kernel function using low-dimensional mapping, $K(x, x') \approx z(x)^T z(x')$, where $z : \mathbb{R}^n \mapsto \mathbb{R}^d$ and n is the number of features [20, 14]. Other methods to reduce the training time of a kernel classifier include, for example, [15]. The main difference between kernel approximation methods and our task here is that they hope the performance is close to the original classifier. On the contrary, all we need is to predict if a performance gap exists between linear and kernel classifiers. Figure 1 illustrates the difference between two tasks. Each curve in Figure 1 corresponds to the result of one method. We show the prediction performance as the method's parameters change. "Method A" is suitable for kernel approximation because it eventually approaches the original kernel classifier (e.g., $d \to l$ when doing low-rank approximations of the kernel). It does not matter that the performance is even worse than the linear classifier under some parameters. However, such a method fails to quickly identify if kernel is better than linear. On the other hand, "Method B" easily fulfils the task even though it does not approach the kernel classifier under any parameter. Based on the discussion, subse-

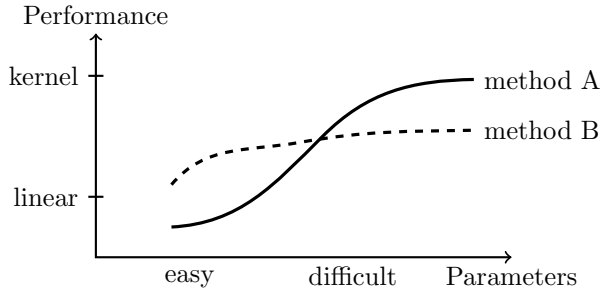


Figure 1: An illustration of the different aims of kernel approximation methods (method A) and our check between linear and kernel classifiers (method B).

quently we will design effective methods that resemble to "Method B" in Figure 1.

In Figure 1, we considered the "performance" of methods, which means the predictability on unseen data, but in practice all we have are training data with known labels. Therefore, we must estimate the prediction performance by a validation procedure of holding out some data. More details are discussed in Section 3.3, but subsequently we use Val(method) to indicate the validation accuracy of a method.

3.1 Method 1: Degree-2 Polynomial Expansion

When the Gaussian kernel is used, it is known that each input vector $\boldsymbol{x}$ is mapped to an infinite dimensional vector including all degree-d polynomial expansions of $\boldsymbol{x}$'s components. If higher dimensional mappings tend to give better performances, the following property may hold in general.

$$\begin{aligned} \text{Val(linear)} &\le \text{Val(low-degree polynomial)} \\ &\le \text{Val(Gaussian kernel)}. \end{aligned} \tag{3.4}$$

There is some theoretical support to this conceptual statement. In [16], they proved a stronger version of Theorem 2.1 by showing that for any given degree, the decision function of a polynomial kernel classifier can be approximated by the decision function of Gaussian kernel SVM under suitable C and γ.[4] The inequality in (3.4) implies that

$$\begin{aligned} &\text{Val(low-deg. poly.)} - \text{Val(linear)} \ge \epsilon \\ \Rightarrow\quad &\text{Val(Gaussian)} - \text{Val(linear)} \ge \epsilon, \end{aligned} \tag{3.5}$$

where ϵ is a given value indicating if the performance difference is significant. Of course we also hope to have the other direction ($\Leftarrow$), but this is difficult unless the method considered performs very similar to Gaussian and can be efficiently trained. Based on (3.5), we decide to consider degree-2 polynomial expansions and have the following procedure.

$$\begin{aligned} &\text{If Val(degree-2 polynomial)}-\text{Val(linear)} < \epsilon, \\ &\qquad \text{use a linear classifier,} \\ &\text{else} \\ &\qquad \text{use a Gaussian kernel classifier.} \end{aligned} \tag{3.6}$$

To make this procedure viable, we must be able to efficiently train a classifier using the degree-2 polynomial kernel $K(\boldsymbol{x}_i, \boldsymbol{x}_j) = (\gamma \boldsymbol{x}_i^T \boldsymbol{x}_j + r)^2$, where r and γ are kernel parameters. While training a data set using polynomial kernels may be equally time consuming to Gaussian, the study [2] has proposed explicitly training the degree-2 polynomial expansions without kernels. With $K(\boldsymbol{x}_i, \boldsymbol{x}_j) = \phi_{\gamma,r}(\boldsymbol{x}_i)^T \phi_{\gamma,r}(\boldsymbol{x}_j)$ and

$$\begin{aligned} \phi_{\gamma,r}(\boldsymbol{x}) = [&r, \sqrt{2r\gamma}x_1, \ldots, \sqrt{2r\gamma}x_n, \gamma x_1^2, \ldots, \\ &\gamma x_n^2, \sqrt{2}\gamma x_1 x_2, \ldots, \sqrt{2}\gamma x_{n-1} x_n]^T, \end{aligned} \tag{3.7}$$

they directly train $\phi_{\gamma,r}(\boldsymbol{x}_1), \ldots, \phi_{\gamma,r}(\boldsymbol{x}_l)$ as a linear classification problem, and show that the running time is in general significantly shorter than that via kernel operations.

Unfortunately, the above discussion shows only the efficiency of training degree-2 mappings under fixed parameters. Parameter selection is important because if we have the best setting for degree-2 expansions, the performance is closer to Gaussian and our kernel-check rule may be more accurate. Although it is often time consuming to select parameters, we will argue that using fixed values $r = \gamma = 1$ is enough. Then C is the only needed parameter, so the total cost of applying degree-2 polynomial expansions is not significantly more than linear. First, [2] has shown that γ is not necessary.[5] Second, we show that r is insensitive to the performance by the following theorem.

THEOREM 3.1. *Consider the three loss functions in Section 2 and that vectors $\boldsymbol{x}_i, \forall i$ are transformed by*

$$\boldsymbol{x}_i \to \bar{\boldsymbol{x}}_i = D\boldsymbol{x}_i, \tag{3.8}$$

where D is a diagonal matrix with $D_{jj} > 0, \forall j$. If $\boldsymbol{w}^*$ is optimal for minimizing the training loss

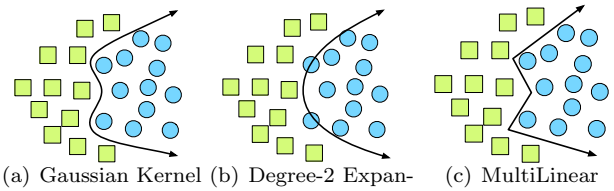
$$\min_{\boldsymbol{w}} \sum_{i=1}^{l} \xi(\boldsymbol{w}; \boldsymbol{x}_i, y_i), \tag{3.9}$$

then $D^{-1}\boldsymbol{w}^*$ is optimal for the following new problem.

$$\min_{\boldsymbol{w}} \sum_{i=1}^{l} \xi(\boldsymbol{w}; \bar{\boldsymbol{x}}_i, y_i). \tag{3.10}$$

[4] However, the polynomial kernel SVM is unregularized (or only regularised on degree-d terms for a degree-d kernel).

[5] Actually [2] proves that r is not necessary, but equivalently we can have that γ is not necessary and r is retained. They consider only L1 hinge loss, but the result holds for more general loss functions. Our proof is in Appendix I.



(a) Gaussian Kernel (b) Degree-2 Expansion (c) MultiLinear

Figure 2: An illustration of different methods to generate the decision boundary.

The proof is in Appendix II. From (3.7), we can see there exists a diagonal matrix D such that

$$\phi_{1,r}(\boldsymbol{x}) = D\phi_{1,1}(\boldsymbol{x}), \text{ with } D_{ii} = \begin{cases} r, & i = 1, \\ \sqrt{r}, & 2 \le i \le n+1, \\ 1, & \text{otherwise.} \end{cases}$$

By Theorem 3.1, if the regularization term is not considered, the optimal solutions for training $\phi_{1,1}(\boldsymbol{x}_i)$ and $\phi_{1,r}(\boldsymbol{x}_i), \forall i$ are $\boldsymbol{w}^*$ and $D^{-1}\boldsymbol{w}^*$, respectively. Thus the two decision functions are the same and we can simply set $r = 1$:

$$(D^{-1}\boldsymbol{w}^*)^T\phi_{1,r}(\boldsymbol{x}) = (\boldsymbol{w}^*)^T\phi_{1,1}(\boldsymbol{x}).$$

A serious issue of using degree-2 expansions is that when n is large, it is difficult to store $\boldsymbol{w}$, which is of size $O(n^2)$. People remedy this problem by hashing the expanded features into a smaller dimension d (e.g., [19]), but d is very hard to tune in practice. We thus present another kernel-check method in the next subsection.

3.2 Method 2: MultiLinear SVM For a kernel like Gaussian, the decision boundary may be highly nonlinear. Our idea is to break the boundary into finite pieces, say K pieces, of hyperplanes. The reason is that several hyperplanes can better approximate a nonlinear decision boundary than a single one; see the illustration in Figure 2. Roughly speaking, degree-2 expansions form a smoother boundary to approximate Gaussian. In contrast, the MultiLinear strategy here uses piecewise segments to form the decision boundary.

What we shall do is to dissect the feature space to K disjoint regions. Then for each region, we train a linear classifier based on only the data points lying inside it. Each classifier chooses its own C by for example a validation procedure on the region's data. For any unseen data point $\boldsymbol{x}$, we consider the region it belongs to and apply the corresponding linear classifier for predicting its label. The rule (3.6) is then applied by replacing the model of degree-2 expansions with the MultiLinear model.

An easy way for dissecting the feature space is to use k-means clustering, which aims to minimize the intra-cluster variance,

$$\sum_{k=1}^{K} \sum_{\boldsymbol{x}_i \in C_k} d(\boldsymbol{x}_i, \boldsymbol{c}_k), \tag{3.11}$$

where data are assigned to clusters C_k, $k = 1, \ldots, K$ with centers $\boldsymbol{c}_1, \ldots, \boldsymbol{c}_K$ by the distance measure $d(\boldsymbol{x}_i, \boldsymbol{c}_k)$. It is difficult to find the optimal cluster centers, so heuristics such as Lloyd's algorithm [17] are used. At each iteration of the algorithm, K clusters are formed by minimising (3.11) with centres fixed, and the K centres are recalculated in order to minimise (3.11) with clusters fixed. Deciding the number of iterations is not too difficult because usually a small value is used. Our focus here is to partition data rather than obtain the best clustering, so a simple choice (15 in our experiments) should be sufficient. Regarding the distance measure $d(\boldsymbol{x}_i, \boldsymbol{c}_k)$, we consider the Euclidean distance $\|\boldsymbol{x}_i - \boldsymbol{c}_k\|^2$ and the cosine distance $1 - \boldsymbol{x}_i^T\boldsymbol{c}_k/(\|\boldsymbol{x}_i\|\|\boldsymbol{c}_k\|)$, corresponding to (standard) k-means and spherical k-means clustering. Even though (standard) k-means is widely used, it may perform poorly when applying on high dimensional sparse documents [21]. For such data, spherical k-means is often used, so we consider both distances in our experiments.

A strong point of MultiLinear SVM is its efficiency. The cost of a training algorithm is at least linear to the number of data. By training several disjoint subsets, the total cost may be smaller than that of training the whole set. We will observe this advantage in the experiments.

The idea of using local linear classifiers through clustering is not new. However, similar to how kernel approximation methods differ from ours, these past studies such as [13, 8] try to get as high accuracy as possible. For example, [8] tried to ensure that their setting gives better accuracy than a single linear classifier. Therefore, their methods are more complicated by for example introducing a new and large optimization problem to link the K classifiers. For ours, accuracy is not an important concern. Indeed, as we will see in experiments, our method often gives slightly worse accuracy than linear when kernel is not needed, but better accuracy when kernel should be used. Such properties are more useful in deciding if kernel is needed or not.

3.3 Unbiased Validation Accuracy for Kernel-check Methods As mentioned in the beginning of this section, we must estimate the prediction performance on unseen data. With only training data at hand, we hold out a subset for validation. Conventionally, when we are choosing the best method among several (here is two), each with its own untuned parameters, we evaluate all the settings (including different parameters) on the validation set and choose the one with the highest validation accuracy. Such a validation procedure effectively identifies a reasonable setting, but the resulting validation accuracy is known to be biased. Because validation accuracy is what to be used in our kernel-check, it is important to have a more unbiased estimator. To

this end, we consider a two-stage validation process. The training set is split to two parts T and V. Each method did its own parameter selection on the set T, and is then evaluated on the set V. Therefore, the set V is dedicated only to get an accuracy estimation for the kernel-checker. In our experiments we use a 3 to 1 split to generate the sets T and V.

4 Data Scaling for Linear Classification

We mentioned in Section 2.3 the different data scaling methods used in linear and kernel classification. To see if the same method can be applied, in this section we investigate various scaling methods for linear classification. In fact, we are not aware of any past study that comprehensively addresses this issue. Our conclusion is that the commonly used feature-wise scaling for kernel is also suitable for linear.

4.1 Instance-wise Scaling Past studies did not clearly explain why all instances need to be normalized to unit vectors. For document data sets, a possible reason is to make short and long documents equally important. In fact, a more compelling reason may be related to the optimization method and the regularization parameter C. Past developments (e.g., [10]) have shown that for linear classification, low-order optimization methods (e.g., coordinate descent methods) are efficient under small C, but may have slow convergence under large C. One explanation is that when C is small, we do not overfit the training data and the optimization problem becomes easier. Interestingly, we show in the following theorem that instance-wise normalization is a mechanism to avoid using a large C.

THEOREM 4.1. *Suppose $\boldsymbol{w}$ is the optimal solution of* (2.1) *under loss functions* (2.2). *If each instance $\boldsymbol{x}_i$ is changed to $\Delta\boldsymbol{x}_i$, then $\boldsymbol{w}/\Delta$ is optimal to the new training set under the regularization parameter C/Δ^2.*

See proof in Appendix III. We consider two scenarios: $C = 1$ with data $\boldsymbol{x}_i, \forall i$ versus $C = 1$ with $\boldsymbol{x}_i/100, \forall i$. From the theorem, the former is equivalent to $C = 10,000$ with data $\boldsymbol{x}_i/100, \forall i$. Thus, under the default C of any linear-classification package, instance-wise normalization may help to avoid the slow convergence. However, this normalization may not be needed if the software can select a suitable C according to the size of feature values. See more discussion in Section 4.3.

4.2 Feature-wise Scaling For linear classifiers, we argue that the performance with/without feature-wise scaling is about the same. Feature-wise scaling calculates $D\boldsymbol{x}_i+\boldsymbol{v}$, where D and $\boldsymbol{v}$ are constant diagonal matrix and vector, respectively. Commonly we set $\boldsymbol{v} = \mathbf{0}$ to preserve the sparsity (e.g., each feature is divided by its largest value). Then by Theorem 3.1, if the regularization term is not considered, the optimal solutions before and after scaling are $\boldsymbol{w}^*$ and $D^{-1}\boldsymbol{w}^*$, respectively. Thus the two decision functions are the same.

Table 1: Data statistics (density is calculated by using the training set)

Data set	l	l (test)	n	density
a9a	32,561	16,281	123	11.3%
cod-rna	59,535	271,617	8	100%
covtype	581,012	NA	54	22.0%
fourclass	862	NA	2	100%
german.numer	1,000	NA	24	100%
gisette	6,000	1,000	5,000	99.1%
ijcnn1	49,990	91,701	22	59.1%
madelon	2,000	600	500	100%
mnistOvE	60,000	10,000	780	19.2%
news20	15,935	3,993	62,061	0.1%
poker	25,010	1,000,000	10	100%
rcv1	20,242	677,399	47,236	0.2%
real-sim	72,309	NA	20,958	0.2%
svmguide1	3,089	4,000	4	100%
webspam	350,000	NA	254	33.5%

4.3 Summary The discussion indicates that if suitable settings (e.g., proper C is chosen) have been considered, with/without scaling does not affect the predictability much. Appendix V gives detailed experiments to confirm this result. Then we need efficient parameter selection regardless of the magnitude of feature values. Fortunately, the recent study [3] has resolved the issue for linear classification. For data in large numeric ranges but not scaled, the approach in [3] can identify a smaller C value without problem. Because feature-wise scaling gives comparable results and is what used for the Gaussian kernel, we perform this preprocessing step before running all subsequent experiments.

In [3], by an effective setting to select C, an automatic procedure for linear classification is almost there. We feel that the scaling issue is the last mile. With the investigation in this section, a fully automated process for linear classification is ready. Thus checking if kernel is needed is naturally the next frontier.

5 Experiments

We conduct experiments to support the statements discussed in Section 3, and to show the effectiveness and efficiency of our proposed kernel-check methods. Programs used for experiments are available at `http://www.csie.ntu.edu.tw/~cjlin/papers/kernel-check`, while more details of experimental settings are in Appendix IV.

5.1 Data Sets and Performance Evaluation We use 15 data sets (Available from LIBSVM

Table 2: Validation accuracy of training degree-2 expansions under different r values.

Data set\r	0.01	0.1	1	10	100
a9a	85.30	85.29	85.31	85.33	85.39
cod-rna	94.81	94.83	94.85	94.73	94.60
covtype	79.88	79.89	79.89	79.84	79.85
fourclass	77.12	79.24	77.54	77.54	77.97
german.numer	76.35	76.35	75.93	76.76	76.76
ijcnn1	97.53	97.55	97.53	97.54	97.49
madelon	56.56	56.56	56.56	58.40	58.20
mnistOvE	98.18	98.18	98.21	98.37	98.35
poker	59.67	59.52	59.54	59.37	59.08
svmguide1	95.67	95.67	95.41	95.67	94.88
webspam	98.51	98.56	98.58	98.40	97.66

data sets `https://www.csie.ntu.edu.tw/~cjlin/libsvmtools/datasets/`) as shown in Table 1. We do not focus on small data sets that can be trained by kernel classifiers within several minutes, so most data sets considered are rather large. We only consider binary problems, so news20, mnistOvE and poker are transformed from their original multi-class sets.

Our kernel-check methods and the reference linear/Gaussian classifiers all need parameter selection. When linear classifiers are used, we have mentioned in Section 4 that effective selection schemes are available. Similar techniques have not been fully developed for Gaussian, so we do five-fold CV on a grid of points: $C = [2^{-5}, 2^{-4}, \ldots, 2^{15}]$, $\gamma = [2^{-15}, 2^{-14}, \ldots, 2^{3}]$.[6]

For most experimental results we present validation accuracy because, as discussed in Section 3.3, it is what a kernel-check method relies on. On the other hand, to have the final answer of whether linear is as good as kernel, a test set completely independent of the kernel-check process should be considered. Among data sets listed in Table 1, some come with a separate test set, so we use them to rigorously evaluate if the prediction on using kernel or not is correct; see Table 3. To predict if Gaussian is better than linear, we apply the rule (3.6) with the performance gap $\epsilon = 2\%$.

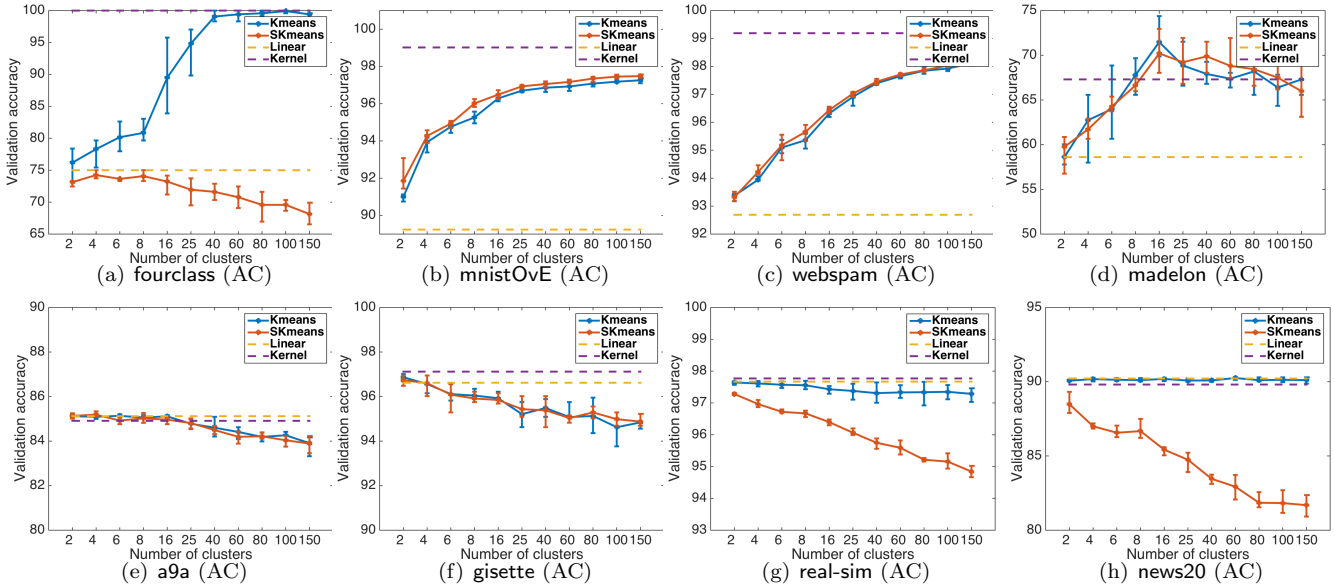
5.2 Degree-2 Expansions under Different r Values A result in Section 3.1 on the training process of degree-2 expansions is that the performance for different r does not vary much. We confirm this result by showing in Table 2 validation accuracy (proper C is chosen using a training subset different from the validation set) of changing r from 0.01 to 100. Results of some data sets are not shown because their numbers of features are too large. Then the high dimensionality of $\boldsymbol{w}$ after degree-2 expansions causes difficulties. From Table 2, all data sets except fourclass and madelon have performance differences within 1%. The slightly higher variance of fourclass and madelon may be because they are relatively smaller than others. Overall our results verify the statement made in Section 3.1.

5.3 MultiLinear SVM using Different Settings In Figures 3 and 4, we compare the performance when using k-means and spherical k-means clustering under several different numbers of clusters (results for all data sets are in Appendix VI). The cluster numbers used are $\{2, 4, 6, 8, 16, 25, 40, 60, 80, 100, 150\}$. We run five times for each setting because of the initial random selection of cluster centers. The circles in the figure are the mean validation accuracy, with the error bar denoting the maximum and minimum accuracy among the five runs.[7] Several observations can be made.

1. When the linear is as good as the Gaussian kernel, e.g. a9a, gisette and german.numer, MultiLinear SVM may be worse than linear starting from some small K. In this situation, linear may have reached the best performance under the given feature information. If we divide the data into smaller sub-groups and train them independently, their combination may not be able to reach similar performances. Alternatively, when Gaussian is better than linear, MultiLinear SVM is always better than linear for a wide range of K. Therefore, although MultiLinear SVM may not be always a competitive classifier, it possesses advantages as a useful kernel-check method.
2. We consider spherical k-means because of its good clustering of document sets. However, in Figure 3, for data such as news20 and real-sim, the accuracy of using spherical k-means is worse than k-means. This result is implicitly from the first observation. When applying k-means on document data sets, a bad clustering is obtained; there are a few huge clusters but many small ones. On the other hand, spherical k-means partition a data set into balanced clusters. For document data, it is known that linear is often as good as Gaussian. Thus from the previous observation, those huge clusters from k-means can retain better performances. Besides, for the data set fourclass that is very low dimensional ($n = 2$), spherical k-means gives a wrong decision because of much worse validation accuracy. The reason might be some information loss after projecting data to a sphere. Based on the various observations, we conclude that using the standard k-means may be more suitable.
3. When Gaussian is significantly better than linear, for

[6] While we can consider a loose grid of fewer points to save the running time, with a parallel cluster the total running time is still huge. This situation indicates the importance of pre-identifying if the Gaussian kernel should be used or not.

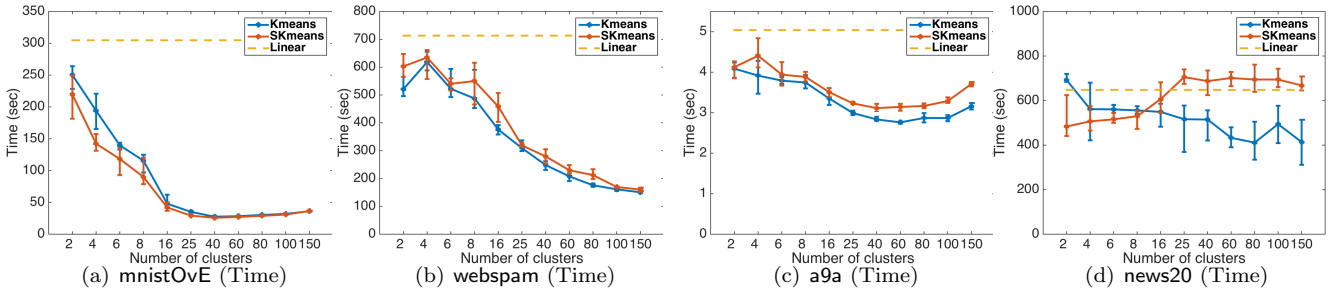
[7] We do not show standard deviation because maximum and minimum better reflect the situation in the kernel-check problem.



(a) fourclass (AC) (b) mnistOvE (AC) (c) webspam (AC) (d) madelon (AC)

(e) a9a (AC) (f) gisette (AC) (g) real-sim (AC) (h) news20 (AC)

Figure 3: Validation accuracy of MultiLinear SVM under different settings



(a) mnistOvE (Time) (b) webspam (Time) (c) a9a (Time) (d) news20 (Time)

Figure 4: Training time (including parameter search) of MultiLinear SVM under different settings

small K, MultiLinear SVM already has some improvements over linear. This makes the problem of selecting K easy. Further, training MultiLinear SVM is very efficient. For all data sets and all K values tried, the training time is in the same order of magnitude as linear. Because intuitively a larger data set should be split to more clusters, we think a setting like $K = \lfloor 5\ln(l) \rfloor$ (which is actually $\lfloor 5\ln(0.75l) \rfloor$ after taking the validation set out) might be appropriate. We will use this K value in subsequent experiments.

5.4 Performance of Proposed Methods We demonstrate the efficiency and the effectiveness of our proposed method for checking whether linear is as good as kernel. Table 3 shows the comparision results. A few entries for degree-2 expansions are not given because of the issue of high dimensionality. Although degree-2 expansions generally give correct decisions, the result is wrong for madelon. A careful check shows that this synthetic set contains 96% useless features generated for a feature selection competition [9]. The degree-2 expansion adds many more useless features, so the performance drops below linear. To illustrate this reasoning, we add another data set, madelon(s), by eliminating useless features. Then the degree-2 expansion can give a correct decision. On the other hand, the simple MultiLinear SVM correctly indicates for all 15 data sets if the Gaussian kernel should be used.

6 Conclusion

We have studied the issue of deciding whether linear or Gaussian kernel should be used. The aim is to make this decision process a useful component for autoML. Our proposed methods can efficiently identify problems for which a linear classifiers is as good as a kernel one, so the training and testing time can be significantly saved.

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Table 3: Performance of our proposed methods. Some abbreviations: val (validation accuracy in %), tme (time in seconds), dec (using Gaussian or not?), accL (testing accuracy of linear in %), accK (testing accuracy of Gaussian in %), Y (Yes), N (No), X (Not available) and U (Yes and No because the difference is neither small nor large enough). The value for MultiLinear SVM is averaged over five runs. The columns of "True answer" are by using an independent test set that is not involved in the kernel-check process.

	Linear		Degree-2			MultiLinear				Kernel		True answer		
data set	val	tme	val	tme	dec	K	val	tme	dec	val	dec	accL	accK	dec
ijcnn1	92.4	11.22	97.5	28.47	Y	52	98.3	2.54	Y	98.6	Y	91.8	98.4	Y
madelon	58.6	18.09	56.6	3,969.30	N	36	68.4	2.75	Y	67.2	Y	59.7	67.7	Y
madelon(s)	62.4	0.23	68.0	20.02	Y	36	77.4	0.34	Y	78.7	Y	59.0	78.3	Y
mnistOvE	89.2	304.79	98.2	2,635.86	Y	53	97.0	26.10	Y	99.1	Y	89.8	99.1	Y
poker	50.0	0.85	59.5	11.79	Y	49	55.1	0.96	Y	61.3	Y	50.0	61.7	Y
svmguide1	82.9	0.05	95.4	0.16	Y	38	95.4	0.06	Y	96.4	Y	78.9	96.6	Y
webspam	92.7	713.23	98.6	11,476.02	Y	62	97.7	204.79	Y	99.1	Y	NA	NA	X
fourclass	75.0	0.01	77.5	0.03	Y	32	97.3	0.02	Y	100.0	Y	NA	NA	X
covtype	75.7	615.97	79.9	9,949.78	Y	64	80.9	51.42	Y	96.1	Y	NA	NA	X
a9a	85.1	5.04	85.3	195.3	N	50	84.7	2.85	N	84.9	N	85.0	85.1	N
gisette	96.6	148.84	NA	NA	X	42	95.5	86.23	N	97.1	N	98.0	98.0	N
news20	90.2	648.02	NA	NA	X	46	90.1	497.63	N	88.6	N	90.2	87.9	N
rcv1	96.6	44.07	NA	NA	X	48	96.7	53.72	N	97.2	N	96.1	94.9	N
real-sim	97.7	100.23	NA	NA	X	54	97.4	101.84	N	97.8	N	NA	NA	X
german.numer	77.2	0.10	75.9	28.54	N	33	68.5	0.13	N	77.3	N	NA	NA	X
cod-rna	93.2	4.36	94.8	17.18	U	53	95.0	1.80	U	95.9	U	95.0	96.4	U

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