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A New Discriminative Kernel From Probabilistic Models

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February 2, 2002

None of the materials has been published or is under consideration for other journals.

Abstract

Recently, Jaakkola and Haussler proposed a method for constructing kernel functions from probabilistic models. Their so called "Fisher kernel" has been combined with discriminative classifiers such as SVM and applied successfully in e.g. DNA and protein analysis. Whereas the Fisher kernel (FK) is calculated from the marginal log-likelihood, we propose the TOP kernel derived from Tangent vectors Of Posterior log-odds. Furthermore, we develop a theoretical framework on feature extractors from probabilistic models and use it for analyzing the TOP kernel. In experiments our new discriminative TOP kernel compares favorably to the Fisher kernel.

1 Introduction

In classification tasks, the purpose of learning is to predict the output $y \in \{-1, +1\}$ of some unknown system given the input $\boldsymbol{x} \in \mathcal{X}$ based on the training samples $\{\boldsymbol{x}_i, y_i\}_{i=1}^n$. A feature extractor is a vector-valued function $\boldsymbol{f} : \mathcal{X} \to \mathbb{R}^D$ designed for converting the representation of data without losing the information necessary for discrimination.

When $\mathcal{X}$ is a vector space like $\mathbb{R}^d$, many feature extraction methods have been proposed (e.g. [Fukunaga, 1990, Chapter 10]). However, they are typically not applicable when $\mathcal{X}$ is a set of sequences of symbols and does not have the structure of a vector space as in DNA or protein analysis (e.g. [Durbin et al., 1998]). In such cases, the similarity (or proximity) between two samples plays an important role (e.g. [Cox & Ferry, 1993, Graepel et al., 1999, Hofmann & Buhmann, 1997]). The simplest method is to prepare several prototype samples and to compose a feature vector from the similarities to these samples [Graepel et al., 1999]. Alternatively in multidimensional scaling (MDS) [Cox & Ferry, 1993] the samples are mapped such that the given dissimilarity is approximated by the Euclidean distance in feature space. However, similarities are often not available, and to define a "good" similarity measure in terms of the

classification task in feature space is therefore difficult and requires a fair amount of prior knowledge.

Recently, the Fisher kernel (FK) [Jaakkola & Haussler, 1999] was proposed that allows to measure distances between symbols by computing features from probabilistic models $p(\boldsymbol{x}|\boldsymbol{\theta})$. At first, a parameter estimate $\hat{\boldsymbol{\theta}}$ is obtained from the training examples. Then, the tangent vector of the log marginal likelihood $\log p(\boldsymbol{x}|\hat{\boldsymbol{\theta}})$ is used as a feature vector. The *Fisher kernel* refers to the inner product in this feature space, but the method is effectively a feature extractor (also since the features are computed explicitly). The Fisher kernel can be combined with discriminative classifiers such as SVM and it has achieved excellent classification results in several fields, for example in DNA and protein analysis [Jaakkola & Haussler, 1999, Jaakkola et al., 2000]. Empirically, it is reported that the FK-SVM system often outperforms the classification performance of a *plug-in estimate*,[1] i.e. the pure probabilistic approach. Note that the Fisher kernel is only one possible member in the family of feature extractors $\boldsymbol{f}_{\hat{\boldsymbol{\theta}}}(\boldsymbol{x}) : \mathcal{X} \to \mathbb{R}^D$ that can be derived from a probabilistic model. We call this family *model-dependent feature extractors*, because different probabilistic models lead to different feature vectors. Exploring this family is a very important and interesting subject.

Since model-dependent feature extractors have been newly developed, the performance measures for them are not yet established. In this paper we therefore first propose two performance measures. Then, we define a new kernel (or equivalently a feature extractor) derived from the Tangent vector Of Posterior log-odds – that we denote as TOP kernel. We will analyze the performance of the TOP kernel in terms of our performance measures. Finally the TOP kernel is compared – favorably – to the Fisher kernel in experiments with artificial data and protein data.

[1] In classification by plug-in estimate, $\boldsymbol{x}$ is classified by thresholding the posterior probability $\hat{y} = \text{sign}(P(y = +1|\boldsymbol{x}, \hat{\boldsymbol{\theta}}) - \frac{1}{2})$ [Devroye et al., 1996].

2 Performance Measures

To begin with, let us describe the notations. Let $\boldsymbol{x} \in \mathcal{X}$ be the input 'point' and $y \in \{-1, +1\}$ be the class label. $\mathcal{X}$ may be a finite set or an infinite set like $\mathbb{R}^d$. Let us assume that we know the parametric model of the joint probability $p(\boldsymbol{x}, y|\boldsymbol{\theta})$, where $\boldsymbol{\theta} \in \mathbb{R}^p$ is the parameter vector. Assume that the model $p(\boldsymbol{x}, y|\boldsymbol{\theta})$ is regular [Murata et al., 1994] and contains the true distribution. Then the true parameter $\boldsymbol{\theta}^*$ is uniquely determined. Let $\hat{\boldsymbol{\theta}}$ be a consistent estimator [Devroye et al., 1996] of $\boldsymbol{\theta}^*$, which is obtained by n training examples drawn i.i.d. from $p(\boldsymbol{x}, y|\boldsymbol{\theta}^*)$. Let $\partial_{\theta_i} f = \partial f / \partial \theta_i$, $\nabla_{\boldsymbol{\theta}} f = (\partial_{\theta_1} f, \ldots, \partial_{\theta_p} f)^\top$, and $\nabla^2_{\boldsymbol{\theta}} f$ denote the $p \times p$ matrix, the Hessian, whose (i, j)-th element is $\partial^2 f / (\partial \theta_i \partial \theta_j)$.

As the Fisher kernel is commonly used in combination with linear classifiers such as SVMs, one reasonable performance measure is the classification error of a linear classifier $\boldsymbol{w}^T \boldsymbol{f}_{\hat{\boldsymbol{\theta}}}(\boldsymbol{x}) + b$ in the feature space $\mathbb{R}^D$, where $\boldsymbol{w} \in \mathbb{R}^D$ and $b \in \mathbb{R}$. Usually $\boldsymbol{w}$ and b are determined by a learning algorithm, so the *optimal* feature extractor is different with regard to each learning algorithm. To cancel out this ambiguity and to make a theoretical analysis possible, we assume the optimal learning algorithm is used. When $\boldsymbol{w}$ and b are optimally chosen, the classification error is

$$R(\boldsymbol{f}_{\hat{\boldsymbol{\theta}}}) = \min_{\boldsymbol{w} \in \mathcal{S}, b \in \mathbb{R}} E_{\boldsymbol{x},y} \Phi[-y(\boldsymbol{w}^\top \boldsymbol{f}_{\hat{\boldsymbol{\theta}}}(\boldsymbol{x}) + b)], \tag{2.1}$$

where $\mathcal{S} = \{\boldsymbol{w} \mid \|\boldsymbol{w}\| = 1, \boldsymbol{w} \in \mathbb{R}^D\}$, $\Phi[a]$ is the step function, which is 1 if $a > 0$ and 0 otherwise, and $E_{\boldsymbol{x},y}$ denotes the expectation with respect to the true distribution $p(\boldsymbol{x}, y|\boldsymbol{\theta}^*)$. $R(\boldsymbol{f}_{\hat{\boldsymbol{\theta}}})$ is at least as large as the Bayes error L^* [Fukunaga, 1990] and $R(\boldsymbol{f}_{\hat{\boldsymbol{\theta}}}) = L^*$ only if the linear classifier implements the same decision rule as the Bayes optimal rule. From a geometrical point of view, $R(\boldsymbol{f}_{\hat{\boldsymbol{\theta}}}) - L^*$ describes how linear the optimal boundary is in the feature space.

Now, that we have a performance measure, it is natural to design a feature extractor that minimizes $R(\boldsymbol{f}_{\hat{\boldsymbol{\theta}}})$. However, this task is difficult because of the non-differentiable function Φ. So, we construct another measure, which upper-bounds $R(\boldsymbol{f}_{\hat{\boldsymbol{\theta}}})$: we consider

the estimation error of the posterior probability by a logistic regressor $F(\boldsymbol{w}^\top \boldsymbol{f}_{\hat{\boldsymbol{\theta}}}(\boldsymbol{x}) + b)$, with $F(t) = 1/(1+\exp(-t))$:

$$D(\boldsymbol{f}_{\hat{\boldsymbol{\theta}}}) = \min_{\boldsymbol{w}\in\mathbb{R}^D, b\in\mathbb{R}} E_{\boldsymbol{x}} |F(\boldsymbol{w}^\top \boldsymbol{f}_{\hat{\boldsymbol{\theta}}}(\boldsymbol{x}) + b) - P(y=+1|\boldsymbol{x}, \boldsymbol{\theta}^*)|. \tag{2.2}$$

The relationship between $D(\boldsymbol{f}_{\hat{\boldsymbol{\theta}}})$ and $R(\boldsymbol{f}_{\hat{\boldsymbol{\theta}}})$ is illustrated as follows: Let $\hat{L}$ be the classification error rate of an arbitrary posterior probability estimator $\hat{P}(y=+1|\boldsymbol{x})$. The following inequality is known [Devroye et al., 1996]:

$$\hat{L} - L^* \leq 2E_{\boldsymbol{x}} |\hat{P}(y=+1|\boldsymbol{x}) - P(y=+1|\boldsymbol{x}, \boldsymbol{\theta}^*)|. \tag{2.3}$$

When we use $\hat{P}(y=+1|\boldsymbol{x}) := F(\boldsymbol{w}^\top \boldsymbol{f}_{\hat{\boldsymbol{\theta}}}(\boldsymbol{x}) + b)$, this inequality leads to the following relationship between the two measures

$$R(\boldsymbol{f}_{\hat{\boldsymbol{\theta}}}) - L^* \leq 2D(\boldsymbol{f}_{\hat{\boldsymbol{\theta}}}). \tag{2.4}$$

By this bound, it is useful to derive a new feature extractor that minimizes $D(\boldsymbol{f}_{\hat{\boldsymbol{\theta}}})$, as will be done in Sec. 4.

3 The Fisher kernel

The Fisher kernel (FK) is defined[2] as $K(\boldsymbol{x}, \boldsymbol{x}') = \boldsymbol{s}(\boldsymbol{x}, \hat{\boldsymbol{\theta}})^\top Z^{-1}(\hat{\boldsymbol{\theta}}) \boldsymbol{s}(\boldsymbol{x}', \hat{\boldsymbol{\theta}})$, where $\boldsymbol{s}$ is the Fisher score

$$\boldsymbol{s}(\boldsymbol{x}, \hat{\boldsymbol{\theta}}) = \left(\partial_{\theta_1} \log p(\boldsymbol{x}|\hat{\boldsymbol{\theta}}), \ldots, \partial_{\theta_p} \log p(\boldsymbol{x}|\hat{\boldsymbol{\theta}})\right)^\top = \nabla_{\boldsymbol{\theta}} \log p(\boldsymbol{x}, \hat{\boldsymbol{\theta}}),$$

and Z is the Fisher information matrix: $Z(\boldsymbol{\theta}) = E_{\boldsymbol{x}}\left[\boldsymbol{s}(\boldsymbol{x}, \boldsymbol{\theta}) \boldsymbol{s}(\boldsymbol{x}, \boldsymbol{\theta})^\top \middle| \boldsymbol{\theta}\right]$. The theoretical foundation of FK is described in the following theorem [Jaakkola & Haussler, 1999]: *"a*

[2] In practice, some variants of the Fisher kernel are used. For example, if the derivative of each class distribution, not marginal, is taken, the feature vector of FK is quite similar to that of our kernel. However, these variants should be deliberately discriminated from the Fisher kernel in theoretical discussions. Throughout this paper including experiments, we adopt the original definition of the Fisher kernel from [Jaakkola & Haussler, 1999].

kernel classifier employed the Fisher kernel derived from a model that contains the label as a latent variable is, asymptotically, at least as good a classifier as the MAP labeling based on the model". The theorem says that the Fisher kernel can perform at least as well as the plug-in estimate, if the parameters of linear classifier are properly determined (cf. Appendix A of [Jaakkola & Haussler, 1999]). With our performance measure, this theorem can be represented more concisely: $R(\boldsymbol{f}_{\hat{\boldsymbol{\theta}}})$ is bounded by the classification error of the plug-in estimate $R_\pi(\hat{\boldsymbol{\theta}})$

$$R(\boldsymbol{f}_{\hat{\boldsymbol{\theta}}}) \leq R_\pi(\hat{\boldsymbol{\theta}}) = E_{\boldsymbol{x},y}\Phi[-y(P(y=+1|\boldsymbol{x},\hat{\boldsymbol{\theta}}) - \tfrac{1}{2})]. \tag{3.1}$$

Note that the classification rule constructed by the plug-in estimate $P(y=+1|\boldsymbol{x},\hat{\boldsymbol{\theta}})$ can also be realized by a linear classifier in feature space. Property (3.1) is important since it guarantees that the Fisher kernel performs better when the optimal $\boldsymbol{w}$ and b are available. In the next section, we present a new kernel that also satisfies (3.1) and has a more appealing theoretical property as well.

4 The TOP Kernel

4.1 Definition

Now we proceed to propose a new kernel: Our aim is to obtain a feature extractor that achieves small $D(\boldsymbol{f}_{\hat{\boldsymbol{\theta}}})$. When a feature extractor $\boldsymbol{f}_{\hat{\boldsymbol{\theta}}}(\boldsymbol{x})$ satisfies[3]

$$\boldsymbol{w}^\top \boldsymbol{f}_{\hat{\boldsymbol{\theta}}}(\boldsymbol{x}) + b = F^{-1}(P(y=+1|\boldsymbol{x},\boldsymbol{\theta}^*)) \text{ for all } \boldsymbol{x} \in \mathcal{X}, \tag{4.1}$$

with certain values of $\boldsymbol{w}$ and b, we have $D(\boldsymbol{f}_{\hat{\boldsymbol{\theta}}}) = 0$. However, since the true parameter $\boldsymbol{\theta}^*$ is unknown, all we can do is to construct $\boldsymbol{f}_{\hat{\boldsymbol{\theta}}}$, which approximately satisfies (4.1). Let

[3]Notice that $F^{-1}(t) = \log t - \log(1-t)$.

us define[4]

$$\begin{aligned} v(\boldsymbol{x}, \boldsymbol{\theta}) &= F^{-1}(P(y = +1|\boldsymbol{x}, \boldsymbol{\theta})) \\ &= \log(P(y = +1|\boldsymbol{x}, \boldsymbol{\theta})) - \log(P(y = -1|\boldsymbol{x}, \boldsymbol{\theta})), \end{aligned} \tag{4.2}$$

which is called the posterior log-odds of a probabilistic model [Devroye et al., 1996]. By Taylor expansion around the estimate $\hat{\boldsymbol{\theta}}$ up to the first order, we can approximate $v(\boldsymbol{x}, \boldsymbol{\theta}^*)$ as

$$v(\boldsymbol{x}, \boldsymbol{\theta}^*) \approx v(\boldsymbol{x}, \hat{\boldsymbol{\theta}}) + \sum_{i=1}^{p} \partial_{\theta_i} v(\boldsymbol{x}, \hat{\boldsymbol{\theta}})(\theta_i^* - \hat{\theta}_i). \tag{4.3}$$

Thus, by setting

$$\boldsymbol{f}_{\hat{\boldsymbol{\theta}}}(\boldsymbol{x}) := (v(\boldsymbol{x}, \hat{\boldsymbol{\theta}}), \partial_{\theta_1} v(\boldsymbol{x}, \hat{\boldsymbol{\theta}}), \ldots, \partial_{\theta_p} v(\boldsymbol{x}, \hat{\boldsymbol{\theta}}))^\top \tag{4.4}$$

and

$$\boldsymbol{w} := \boldsymbol{w}^* = (1, \theta_1^* - \hat{\theta}_1, \cdots, \theta_p^* - \hat{\theta}_p)^\top, \; b = 0, \tag{4.5}$$

equation (4.1) is approximately satisfied. Since a *Tangent vector Of the Posterior log-odds* constitutes the main part of the feature vector, we call the inner product of the two feature vectors *TOP kernel*:

$$K(\boldsymbol{x}, \boldsymbol{x}') = \boldsymbol{f}_{\hat{\boldsymbol{\theta}}}(\boldsymbol{x})^\top \boldsymbol{f}_{\hat{\boldsymbol{\theta}}}(\boldsymbol{x}'). \tag{4.6}$$

It is easy to verify that the TOP kernel satisfies (3.1), because we can construct the same decision rule as the plug-in estimate by using the first element only (i.e. $\boldsymbol{w} = (1, 0, \ldots, 0)$, $b = 0$).

4.2 A Theoretical Analysis

In this section, we compare the TOP kernel with the plug-in estimate in terms of performance measures. Later on, we assume that $0 < P(y = +1|\boldsymbol{x}, \boldsymbol{\theta}) < 1$ to prevent $|v(\boldsymbol{x}, \boldsymbol{\theta})|$

[4]One can easily derive TOP kernels from higher order Taylor expansions. However, we will only deal with the first order expansion here, because higher order expansions would induce extremely high dimensional feature vectors in practical cases.

from going to infinity. Also, it is assumed that $\nabla_{\boldsymbol{\theta}} P(y=+1|\boldsymbol{x},\boldsymbol{\theta})$ and $\nabla^2_{\boldsymbol{\theta}} P(y=+1|\boldsymbol{x},\boldsymbol{\theta})$ are bounded. Substituting the plug-in estimate (denoted by the subscript π) into $D(\boldsymbol{f}_{\hat{\boldsymbol{\theta}}})$, we have

$$D_\pi(\hat{\boldsymbol{\theta}}) = E_{\boldsymbol{x}}|P(y=+1|\boldsymbol{x},\hat{\boldsymbol{\theta}}) - P(y=+1|\boldsymbol{x},\boldsymbol{\theta}^*)|.$$

Define $\Delta\boldsymbol{\theta} = \hat{\boldsymbol{\theta}} - \boldsymbol{\theta}^*$. By Taylor expansion around $\boldsymbol{\theta}^*$, we have

$$\begin{aligned} D_\pi(\hat{\boldsymbol{\theta}}) &= E_{\boldsymbol{x}}|(\Delta\boldsymbol{\theta})^\top \nabla_{\boldsymbol{\theta}} P(y=+1|\boldsymbol{x},\boldsymbol{\theta}^*) + \frac{1}{2}(\Delta\boldsymbol{\theta})^\top \nabla^2_{\boldsymbol{\theta}} P(y=+1|\boldsymbol{x},\boldsymbol{\theta}_0)(\Delta\boldsymbol{\theta})| \\ &= O(\|\Delta\boldsymbol{\theta}\|), \end{aligned} \tag{4.7}$$

where $\boldsymbol{\theta}_0 = \boldsymbol{\theta}^* + \gamma\Delta\boldsymbol{\theta}$ $(0 \le \gamma \le 1)$. When the TOP kernel is used,

$$D(\boldsymbol{f}_{\hat{\boldsymbol{\theta}}}) \le E_{\boldsymbol{x}}|F((\boldsymbol{w}^*)^\top \boldsymbol{f}_{\hat{\boldsymbol{\theta}}}(\boldsymbol{x})) - P(\boldsymbol{y}=+1|\boldsymbol{x},\boldsymbol{\theta}^*)|, \tag{4.8}$$

where $\boldsymbol{w}^*$ is defined as in (4.5). Since F is Lipschitz-continuous, there is a finite positive constant M such that $|F(a) - F(b)| \le M|a-b|$. Thus,

$$D(\boldsymbol{f}_{\hat{\boldsymbol{\theta}}}) \le M E_{\boldsymbol{x}}|(\boldsymbol{w}^*)^\top \boldsymbol{f}_{\hat{\boldsymbol{\theta}}}(\boldsymbol{x}) - F^{-1}(P(\boldsymbol{y}=+1|\boldsymbol{x},\boldsymbol{\theta}^*))|. \tag{4.9}$$

Since $(\boldsymbol{w}^*)^\top \boldsymbol{f}_{\hat{\boldsymbol{\theta}}}(\boldsymbol{x})$ is the Taylor expansion of $F^{-1}(P(\boldsymbol{y}=+1|\boldsymbol{x},\boldsymbol{\theta}^*))$ up to the first order (4.3), the first order terms of $\Delta\boldsymbol{\theta}$ are excluded from the right side of (4.9), thus $D(\boldsymbol{f}_{\hat{\boldsymbol{\theta}}}) = O(\|\Delta\boldsymbol{\theta}\|^2)$. Since both, the plug-in and the TOP kernel, depend on the parameter estimate $\hat{\boldsymbol{\theta}}$, the errors $D_\pi(\hat{\boldsymbol{\theta}})$ and $D(\boldsymbol{f}_{\hat{\boldsymbol{\theta}}})$ become smaller as $\|\Delta\boldsymbol{\theta}\|$ decreases. However,the rate of convergence of the TOP kernel is much faster than that of the plug-in estimate, if $\boldsymbol{w}$ and b are optimally chosen.

This result is closely related to large sample performances: Assuming that $\hat{\boldsymbol{\theta}}$ is a $n^{1/2}$ consistent estimator with asymptotic normality (e.g. the maximum likelihood estimator), we have $\|\Delta\boldsymbol{\theta}\| = O_p(n^{-1/2})$ [Murata et al., 1994], where O_p denotes stochastic order [Barndorff-Nielsen & Cox, 1989]. So we can directly derive the convergence order as $D_\pi(\hat{\boldsymbol{\theta}}) = O_p(n^{-1/2})$ and $D(\boldsymbol{f}_{\hat{\boldsymbol{\theta}}}) = O_p(n^{-1})$. By using the relation (2.4), it follows that

$R_\pi(\hat{\boldsymbol{\theta}}) - L^* = O_p(n^{-1/2})$ and $R(\boldsymbol{f}_{\hat{\boldsymbol{\theta}}}) - L^* = O_p(n^{-1})$.[5] Therefore, the TOP kernel has a much better convergence rate in $R(\boldsymbol{f}_{\hat{\boldsymbol{\theta}}})$. However, we must notice that this fast rate is possible only when the *optimal* linear classifier is combined with the TOP kernel. Since non-optimal linear classifiers typically have the rate $O_p(n^{-1/2})$ [Devroye et al., 1996], the overall rate is dominated by the slower rate and turns out to be $O_p(n^{-1/2})$. But this theoretical analysis is still meaningful, because it shows the existence of a very efficient linear boundary in the TOP feature space. This result encourages practical efforts to improve linear boundaries by engineering loss functions and regularization terms with e.g. cross validation, bootstrapping or other model selection criteria [Devroye et al., 1996].

4.3 Exponential Family: A Special Case

When the distributions of the two classes belong to the exponential family, the TOP kernel can achieve an even better result than shown above. Distributions of the exponential family can be written as $q(\boldsymbol{x}, \boldsymbol{\eta}) = \exp(\boldsymbol{\eta}^\top \boldsymbol{t}(\boldsymbol{x}) + \psi(\boldsymbol{\eta}))$, where $\boldsymbol{t}(\boldsymbol{x})$ is a vector-valued function called sufficient statistics and $\psi(\boldsymbol{\eta})$ is a normalization factor [Geiger & Meek, 1998]. Let α denote the parameter for class prior probability of the positive model $P(y = +1)$. Then, the probabilistic model is described as

$$p(\boldsymbol{x}, y = +1|\boldsymbol{\theta}) = \alpha q_{+1}(\boldsymbol{x}, \boldsymbol{\eta}_{+1}), \quad p(\boldsymbol{x}, y = -1|\boldsymbol{\theta}) = (1 - \alpha) q_{-1}(\boldsymbol{x}, \boldsymbol{\eta}_{-1}),$$

where $\boldsymbol{\theta} = \{\alpha, \boldsymbol{\eta}_{+1}, \boldsymbol{\eta}_{-1}\}$. The posterior log-odds reads

$$v(\boldsymbol{x}, \boldsymbol{\theta}) = \boldsymbol{\eta}_{+1}^\top \boldsymbol{t}_{+1}(\boldsymbol{x}) + \psi_{+1}(\boldsymbol{\eta}_{+1}) - \boldsymbol{\eta}_{-1}^\top \boldsymbol{t}_{-1}(\boldsymbol{x}) - \psi_{-1}(\boldsymbol{\eta}_{-1}) + \log \frac{\alpha}{1 - \alpha}. \tag{4.10}$$

The TOP feature vector is described as

$$f_{\hat{\boldsymbol{\theta}}}(\boldsymbol{x}) = (v(\boldsymbol{x}, \hat{\boldsymbol{\theta}}), \partial_\alpha v(\boldsymbol{x}, \hat{\boldsymbol{\theta}}), \nabla_{\boldsymbol{\eta}_{+1}} v(\boldsymbol{x}, \hat{\boldsymbol{\theta}})^\top, \nabla_{\boldsymbol{\eta}_{-1}} v(\boldsymbol{x}, \hat{\boldsymbol{\theta}})^\top)^\top,$$

[5] For detailed discussion about the convergence orders of classification error, see Chapter 6 of [Devroye et al., 1996]

where $\nabla_{\boldsymbol{\eta}_s} v(\boldsymbol{x}, \hat{\boldsymbol{\theta}}) = s(\boldsymbol{t}_s(\boldsymbol{x}) + \nabla_{\boldsymbol{\eta}_s} \psi_s(\hat{\boldsymbol{\eta}}_s))$ for $s = \{+1, -1\}$. So, when

$$\boldsymbol{w} = (1, 0, {\boldsymbol{\eta}^*_{+1}}^\top - \hat{\boldsymbol{\eta}}^\top_{+1}, {\boldsymbol{\eta}^*_{-1}}^\top - \hat{\boldsymbol{\eta}}^\top_{-1})^\top$$

and b is properly set, the true log-odds $F^{-1}(P(y = +1|\boldsymbol{x}, \boldsymbol{\theta}^*))$ can be constructed as a linear function in the feature space (4.1). Thus $D(\boldsymbol{f}_{\hat{\boldsymbol{\theta}}}) = 0$ and $R(\boldsymbol{f}_{\hat{\boldsymbol{\theta}}}) = L^*$. Furthermore, since each feature is represented as a linear function of sufficient statistics $\boldsymbol{t}_{+1}(\boldsymbol{x})$ and $\boldsymbol{t}_{-1}(\boldsymbol{x})$, one can construct an equivalent feature space as $(\boldsymbol{t}_{+1}(\boldsymbol{x})^\top, \boldsymbol{t}_{-1}(\boldsymbol{x})^\top)^\top$ without knowing $\hat{\boldsymbol{\theta}}$.[6] This result has some importance because all graphical models without hidden states can be represented as members of the exponential family, for example Markov models [Geiger & Meek, 1998].

5 Experiment with Artificial Data

In this section, we present a classification experiment with artificial data. Here, the probabilistic model of each class is a mixture of two Gaussians:

$$q(\boldsymbol{x}, \boldsymbol{\xi}) = \beta g(\boldsymbol{x}, \boldsymbol{\eta}_1) + (1 - \beta) g(\boldsymbol{x}, \boldsymbol{\eta}_2), \tag{5.1}$$

where $\boldsymbol{\xi} = [\beta, \boldsymbol{\eta}_1, \boldsymbol{\eta}_2]$ and g is the natural parameter representation of a Gaussian distribution

$$g(\boldsymbol{x}, \boldsymbol{\eta}) = \exp\left\{ \eta_1 \|\boldsymbol{x}\|^2 + \sum_{i=1}^{d} x_i \eta_{i+1} + \sum_{i=1}^{d} \eta_{i+1}^2/(4\eta_1) - \frac{d}{2} \log(-\pi/\eta_1) \right\}. \tag{5.2}$$

Notice that the natural parameter $\boldsymbol{\eta}$ corresponds to the conventional parameters (mean $\boldsymbol{\mu}$ and standard deviation σ) as $\eta_1 = -1/(2\sigma^2), \quad \eta_i = \mu_{i-1}/\sigma^2$ $(i \geq 2)$. The true parameter of the two classes are defined as

$$\boldsymbol{\mu}_1 = \boldsymbol{\mu}_2 = (0, \ldots, 0), \sigma_1 = 1, \sigma_2 = \tfrac{1}{2}, \beta = \tfrac{1}{2} \qquad \text{(First Class)}$$

$$\boldsymbol{\mu}_1 = \boldsymbol{\mu}_2 = (\tfrac{1}{10}, \ldots, \tfrac{1}{10}), \sigma_1 = \tfrac{4}{5}, \sigma_2 = \tfrac{2}{5}, \beta = \tfrac{1}{2} \quad \text{(Second Class)}$$

[6] It is a well-known fact that the Bayes optimal boundary of exponential family distributions forms a hyperplane in the space of sufficient statistics [Devroye et al., 1996].

Also the true class prior probability is defined as $\alpha = \frac{1}{2}$. The derivatives in TOP and Fisher kernels are calculated with respect to the parameters $\boldsymbol{\xi}_{+1}$, $\boldsymbol{\xi}_{-1}$ in both classes and the class prior probability α as well.

In this experiment, the dimensionality of the input space is set to 100. The number of training samples is 30 in the first and 240 in the second experiment. The performance is measured by the error rate on a test set with 1000 samples. We compared the TOP kernel with the Fisher kernel. As subsequent classifier an SVM is chosen, which has a regularization parameter C. As candidate values of C, 10 equally spaced points in the log scale are taken from $[10^{-6}, 10^{-1}]$. The value of the parameter C is chosen from the candidate values according to the error rate on a validation set (100 samples).[7] The parameters $\boldsymbol{\xi}_{+1}$ and $\boldsymbol{\xi}_{-1}$ are estimated by the EM algorithm [Bishop, 1995] and α is estimated by the ratio of training samples of two classes.

The test errors over 30 different samplings of training, validation and test sets are shown in Figure 1. For reference, we also show the test errors of the Bayes optimal classifier and the test errors of the plug-in estimate. To illustrate the difference of FK and TOP in a detailed way, Figure 2 shows comparative plots of test errors. It is clearly observed that the TOP kernel has the smaller error rates in many cases. In order to investigate whether the differences in error rates are significant or not, two kinds of statistical tests are applied (Tab. 1): One is the t-test (i.e. T), which compares the averages of error rates under the assumption that both distributions are Gaussian. The other is the Wilcoxson signed rank test (i.e. WX), which uses the rank of differences of error rates. This is a nonparametric test, so it can be applied to any distribution. Because the distributions of error rates seem to be skewed (see. Figure 1), we favor this test more than the t-test. When $n = 30$, both tests judged that the average error rate of TOP is significantly smaller than that of FK, whereas, when $n = 240$, only the Wilcoxson signed rank test judged that the TOP is significantly better. So, it is observed that the TOP kernel is especially effective in small

[7] See [Rätsch et al., 2001] for details on how model selection is conducted in this type of experiment.

sample cases.

So far, we have shown the performance of the *combination* of a feature extractor (FK or TOP) and SVM. In order to focus on feature extraction performance itself, it is desirable to observe the minimum achievable error by the optimal linear boundary. However, since it is difficult to analytically derive the optimal boundaries, a nearly optimal one is constructed by means of 3000 additional training samples, which are not used in constructing features but in determining linear boundaries. As the learning algorithm in feature space, we used the linear discriminant analysis [Fukunaga, 1990] without regularization. In Figure 1 and 2, these nearly optimal results are shown as FK* and TOP*. For reference, we also show the results of TOP when the Taylor coefficient $\boldsymbol{w}^*$ (4.5) is used as the weight vector (i.e. W^* in Figure 1) [8].

As seen in the test result (Tab. 1), the TOP kernel is significantly better than FK in both cases ($n = 30$ and 240). Thus, we are lead to the conclusion that the TOP kernel extracts better discriminative features – at least in this experiment.

6 Experiments on Protein Data

In order to illustrate that the TOP kernel works also well for real-world problems, we present results on protein classification. The protein sequence data is obtained from the Superfamily web-site.[9] This site provides sequence files with different degrees of redundancy filtering; we used the one with 10% redundancy filtering. Here, 4541 sequences are hierarchically labeled into 7 classes, 558 folds, 845 superfamilies and 1343 families according to the SCOP(1.53) scheme. In our experiment, we determine the top category "classes" as the learning target. The numbers of sequences in the classes are listed as 791, 1277, 1015, 915, 84, 76, 383. We only use the first 4 classes, and 6 two-class problems

[8] When $n = 30$, the error rates of W^* are often larger than TOP* and have very large variance, because the Taylor expansion (4.3) has large higher order terms when the number of samples is small.

[9] `http://stash.mrc-lmb.cam.ac.uk/SUPERFAMILY/`

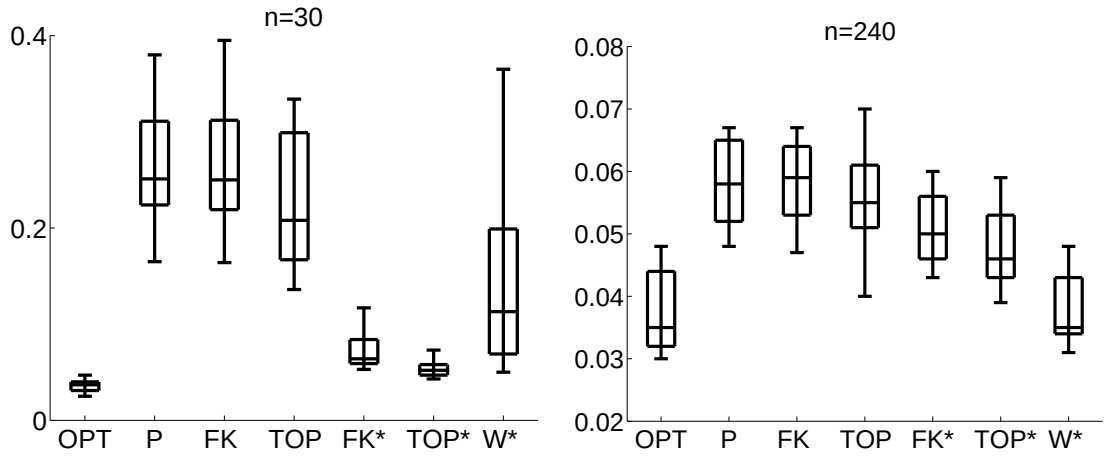

Figure 1: The error rates of various classifiers in the artificial data experiment. OPT: Test errors of the Bayes optimal classifier, P: Probabilistic models only, FK: the Fisher kernel with SVM, TOP: the TOP kernel with SVM, FK*: the Fisher kernel with the nearly optimal linear boundary constructed by a sufficient number of additional samples, TOP*: the TOP kernel with the nearly optimal linear boundary, W*: the TOP kernel with the weight vector $\boldsymbol{w}^*$.

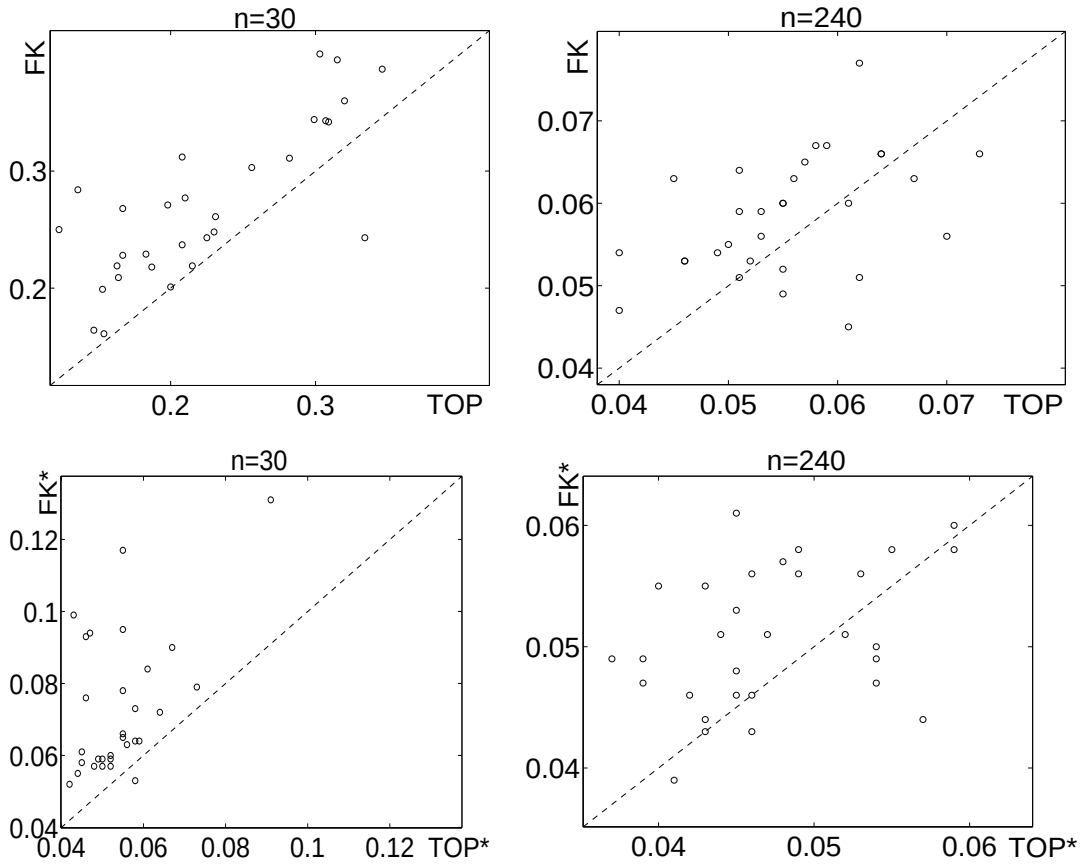

Figure 2: Comparison of error rates of SVMs with the Fisher kernel and the TOP kernel in the artificial data experiment. Every point corresponds to one of the 30 different training/validation/test sets. The upper two figures correspond to FK and TOP in Figure 1, while the lower two correspond to FK* and TOP*.

Table 1: P-values of statistical tests in the artificial data experiment, which investigate whether the error rates are significantly different or not. Two kinds of tests, t-test (denoted as T in the table) and Wilcoxson signed ranks test (i.e. WX), are used. When the difference is significant (p-value < 0.05), a single star $*$ is put beside the value. Double stars $**$ indicate that the difference is very significant (p-value < 0.01).

Methods	Test	$n = 30$	$n = 240$
TOP, FK	T	0.0090^{**}	0.12
	WX	$1.97 \times 10^{-5**}$	0.031^{*}
TOP*, FK*	T	$2.2 \times 10^{-5**}$	0.024^{*}
	WX	$2.1 \times 10^{-6**}$	0.0082^{**}

are generated from all pairs among the 4 classes. The 5th and 6th classes are not used because the number of examples is too small. Also, the 7th class is omitted because it is quite different from the others and too easy to classify. In each two-class problem, the examples are randomly divided into 25% training set, 25% validation set and 50% test set. The validation set is used for model selection.

As a probabilistic model for protein sequences, we train hidden Markov models [Durbin et al., 1998] with fully connected states[10] by the Baum-Welch algorithm.[11] To construct FK and TOP kernels, the derivatives with respect to all parameters of the HMMs from both classes are included. The derivative with respect to the class prior probability is included as well: Let $q(\boldsymbol{x}, \boldsymbol{\xi})$ be the probability density function of a HMM.

[10]Several HMM models have been engineered for protein classification [Durbin et al., 1998]. However, we do not use such HMMs because the main purpose of experiment is to compare FK and TOP. Furthermore the performances achieved with plain HMM models are lower than the ones presented here using discriminative training, which is well in line with results by [Jaakkola et al., 2000].

[11]We mainly followed the implementation of [Durbin et al., 1998]. For implementation details, see [Sonnenburg, 2001].

Then, the marginal distribution is written as $p(\boldsymbol{x}|\hat{\boldsymbol{\theta}}) = \hat{\alpha}q(\boldsymbol{x}, \hat{\boldsymbol{\xi}}_{+1}) + (1-\hat{\alpha})q(\boldsymbol{x}, \hat{\boldsymbol{\xi}}_{-1})$, where α is a parameter corresponding to the class prior. The feature vector of FK consists of the following:

$$\nabla_{\boldsymbol{\xi}_s} \log p(\boldsymbol{x}|\hat{\boldsymbol{\theta}}) = P(y = s|\boldsymbol{x}, \hat{\boldsymbol{\theta}}) \nabla_{\boldsymbol{\xi}_s} \log q(\boldsymbol{x}, \hat{\boldsymbol{\xi}}_s) \qquad s \in \{-1, +1\} \tag{6.1}$$

$$\partial_\alpha \log p(\boldsymbol{x}|\hat{\boldsymbol{\theta}}) = \frac{1}{\hat{\alpha}} P(y = +1|\boldsymbol{x}, \hat{\boldsymbol{\theta}}) - \frac{1}{1-\hat{\alpha}} P(y = -1|\boldsymbol{x}, \hat{\boldsymbol{\theta}}), \tag{6.2}$$

while the feature vector of TOP includes $\nabla_{\boldsymbol{\xi}_s} v(\boldsymbol{x}, \hat{\boldsymbol{\theta}}) = s \nabla_{\boldsymbol{\xi}_s} \log q(\boldsymbol{x}, \hat{\boldsymbol{\xi}}_s)$ for $s = \pm 1$.[12] We obtained $\hat{\boldsymbol{\xi}}_{+1}$ and $\hat{\boldsymbol{\xi}}_{-1}$ from the training examples of the respective classes and set $\hat{\alpha} = \frac{1}{2}$. In the definition of the TOP kernel (4.6), we did not include any normalization of feature vectors. However, in practical situations, it is effective to normalize features for improving classification performance. Here, each feature of the TOP kernel is normalized to have mean 0 and variance 1. Also in FK, we normalized the features in the same way. Both, the TOP kernel and FK are each combined with SVMs using a bias term.

When classifying with HMMs, one observes the difference of the log-likelihoods for the two classes and discriminates by thresholding at an appropriate value. Theoretically, this threshold should be determined by the (true) class prior probability, which is typically not available. Furthermore, the estimation of the prior probability from training data often leads to poor results [Durbin et al., 1998]. To avoid this problem, the threshold is determined such that the false positive rate and the false negative rate are equal on the test set. This threshold is determined in the same way for FK-SVMs and TOP-SVMs.

The hybrid HMM-TOP-SVM system has several model parameters: the number of HMM states, the pseudo count value [Durbin et al., 1998] and the regularization parameter C of the SVM. We determine these parameters as follows: First, the number of states and the pseudo count value are determined such that the error of the HMM on the validation set (i.e. validation error) is minimized. Based on the chosen HMM model, the parameter C is determined such that the validation error of the TOP-SVM

[12] Note, $\partial_\alpha v(\boldsymbol{x}, \hat{\boldsymbol{\theta}})$ is a constant, which does not depend on $\boldsymbol{x}$. So it is not included in the feature vector.

is minimized. Here, the number of states and the pseudo count value are chosen from $\{3, 5, 7, 10, 15, 20, 30, 40, 60\}$ and $\{10^{-10}, 10^{-7}, 10^{-5}, 10^{-4}, 10^{-3}, 10^{-2}\}$, respectively. For C, 15 equally spaced points on the log scale are taken from $[10^{-4}, 10^{1}]$. Note that the model selection is performed in the same manner for the Fisher kernel as well.

The error rates over 15 different training/validation/test divisions are shown in Figure 3 and 4. The results of statistical tests are shown in Tab. 2 as well. Compared with the plug-in estimate, the Fisher kernel performed significantly better in several settings (i.e. 1-3, 2-3, 3-4). This result partially agrees with observations in [Jaakkola & Haussler, 1999]. However, our TOP approach significantly outperforms the Fisher kernel: According to the Wilcoxson signed ranks test, the TOP kernel was significantly better in all settings. Also, the t-test judged that the difference is significant except for 1-4 and 2-4. This indicates that the TOP kernel was able to capture discriminative information better than the Fisher kernel.

Table 2: P-values of statistical tests in the protein classification experiments. Two kinds of tests, t-test (denoted as T in the table) and Wilcoxson signed ranks test (i.e. WX), are used. When the difference is significant (p-value < 0.05), a single star $*$ is put beside the value. Double stars $**$ indicate that the difference is very significant (p-value < 0.01).

Methods	Test	1-2	1-3	1-4	2-3	2-4	3-4
P, FK	T	0.95	0.14	0.78	0.0032^{**}	0.79	0.12
	WX	0.85	0.041^{*}	0.24	0.0040^{**}	0.80	0.026^{*}
P, TOP	T	0.015^{*}	$1.7 \times 10^{-8**}$	0.11	$3.0 \times 10^{-12**}$	0.059	$5.3 \times 10^{-5**}$
	WX	$4.3 \times 10^{-4**}$	$6.1 \times 10^{-5**}$	0.030^{*}	$6.1 \times 10^{-5**}$	0.035^{*}	$3.1 \times 10^{-4**}$
FK, TOP	T	0.0093^{**}	$2.2 \times 10^{-4**}$	0.21	$2.6 \times 10^{-8**}$	0.079	0.0031^{**}
	WX	$8.5 \times 10^{-4**}$	$6.1 \times 10^{-5**}$	0.048^{*}	$6.1 \times 10^{-5**}$	0.0034^{**}	$1.8 \times 10^{-4**}$

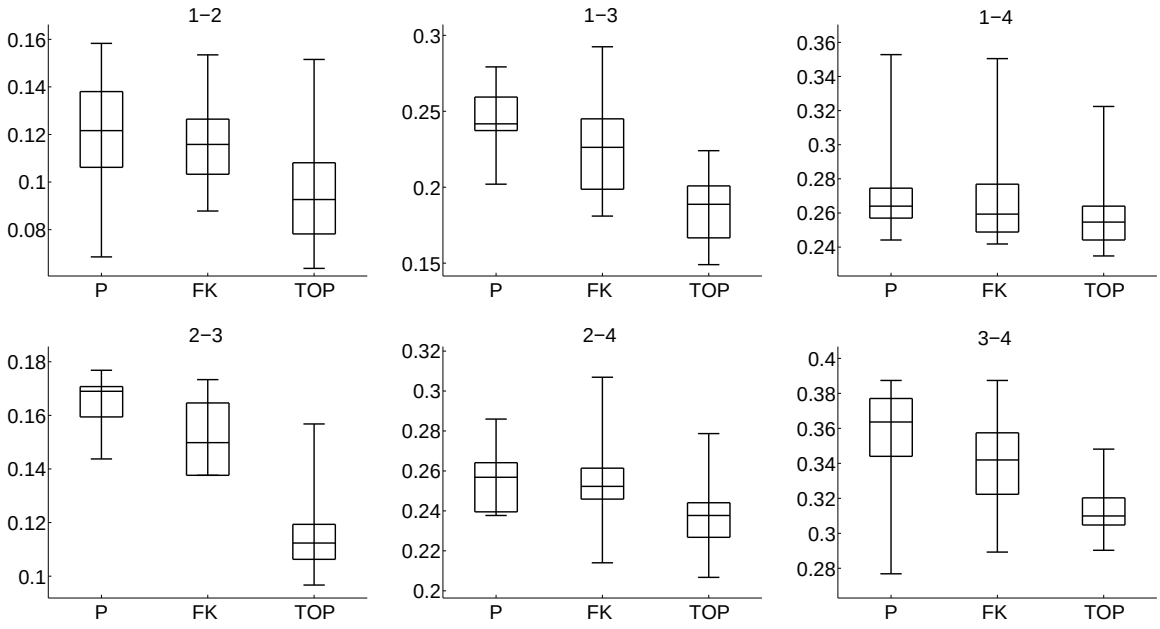

Figure 3: The error rates of SVMs with two feature extractors in the protein classification experiments. The labels 'P', 'FK', 'TOP' denote the plug-in estimate, the Fisher kernel and the TOP kernel, respectively. The title on each sub-figure shows the two protein classes used for the experiment.

7 Conclusion

In this study, we presented the new discriminative TOP kernel derived from probabilistic models. We proposed two performance measures to analyze such kernels and gave bounds and rates to gain a better insight into model dependent feature extractors from probabilistic models. Experimentally, we showed that the TOP kernel compares favorably to FK and the plug-in estimator on toy data and in a realistic protein classification experiment. Future research will focus on constructing small sample bounds for the TOP kernel to extend the validity of this work. Since other nonlinear transformations F are available for obtaining different and possibly even better features, we will furthermore consider to *learn* the nonlinear transformation F from training samples. An interesting point is that so far TOP kernels perform local linear approximations, it would be interesting to move

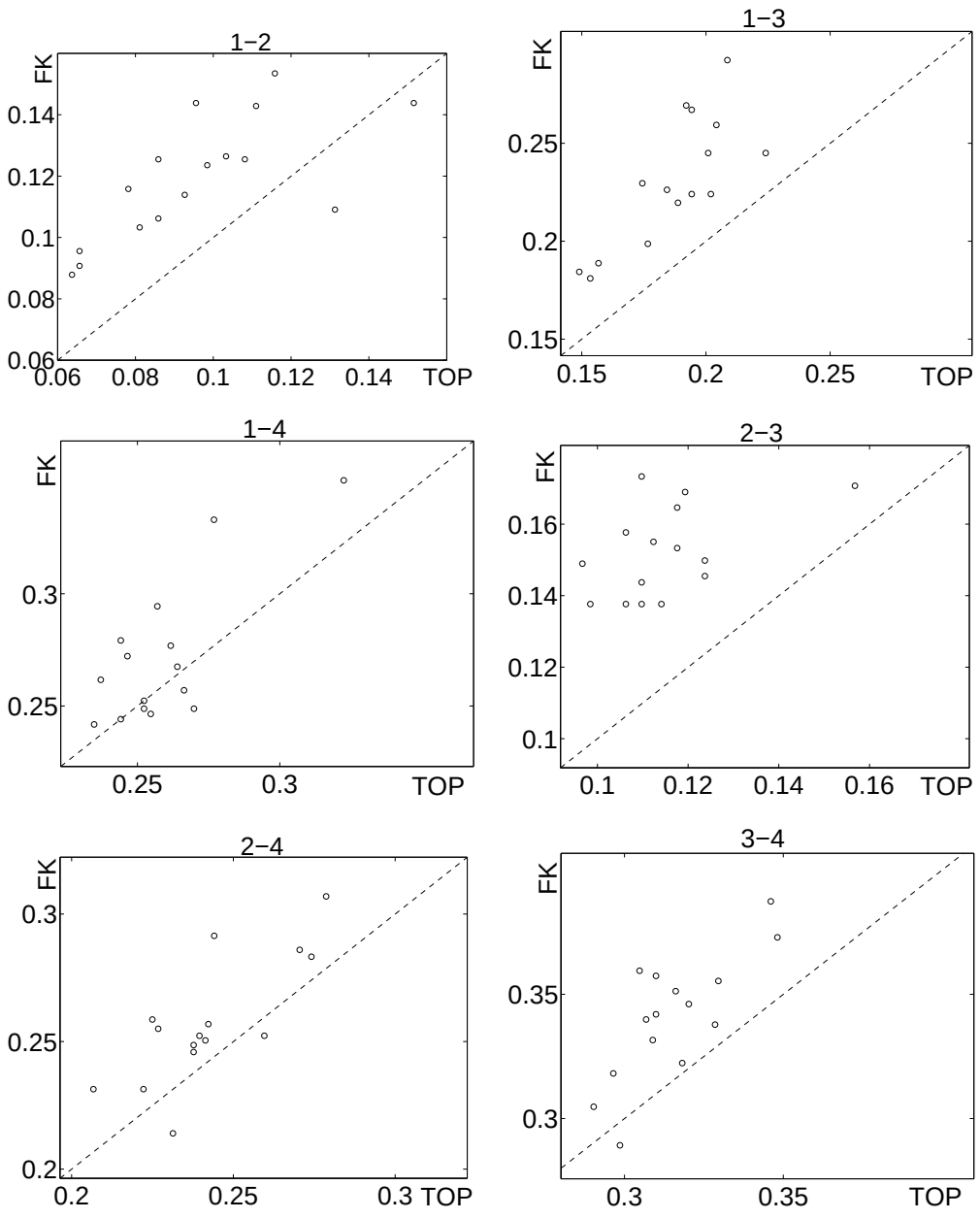

Figure 4: Comparison of the error rates of the SVMs with two feature extractors in protein classification experiments. Every point corresponds to one of the 15 different training/validation/test set splits. The title on each sub-figure shows the two protein classes used for the experiment.

in the direction of local or even global nonlinear expansions. Recently, it was reported that the Fisher kernel-based classifiers can be understood in the Bayesian framework of Maximum Entropy Discrimination [Jaakkola et al., 2000, Jaakkola et al., 1999] when the prior distribution of parameters is chosen in an appropriate way. It is therefore interesting to explore the relationship between the techniques established in this work for the TOP kernel and such Bayesian inference methods.

Acknowledgments We thank T. Tanaka, M. Sugiyama, S. -I. Amari, K. Karplus, R. Karchin, F. Sohler and A. Zien for valuable discussions. Also we acknowledge the refrees for helpful comments. Moreover, we gratefully acknowledge partial support from DFG (JA 379/9-1 and 9-2, MU 987/1-1) and travel grants from EU (Neurocolt II). Thanks also to the anonymous referees for their valuable comments and suggestions that lead to a strong improvement of this work.

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A Derivatives with respect to HMM parameters

We will illustrate how to compute derivatives of the likelihood with respect to HMM parameters [Rabiner, 1989, Durbin et al., 1998]. Let n and m be the number of states and the number of symbols in the alphabet of HMM, respectively. Typically, HMM has the following parameters:

- $\boldsymbol{a} \in \mathbb{R}^{n \times n}$: the transition matrix, i.e. a_{ij} denotes the probability of a transition from state i to j.
- $\boldsymbol{b} \in \mathbb{R}^{n \times m}$ the emission matrix, i.e. b_{ik} denotes the probability of emitting symbol k in state i.
- $\boldsymbol{p} \in \mathbb{R}^{n}$: the initial state distribution, i.e. p_i denotes the probability of the HMM to start in state i.
- $\boldsymbol{q} \in \mathbb{R}^{n}$: the terminal/end state distribution, i.e. q_i denotes the probability of the HMM to terminate in state i.

Let us define $\boldsymbol{\lambda} = \{\boldsymbol{a}, \boldsymbol{b}, \boldsymbol{p}, \boldsymbol{q}\}$ for convenience. Let $\boldsymbol{o}$ denote an observed sequence of length T,

$$\boldsymbol{o} = (o_0, \cdots, o_{T-1}),\ 1 \leq o_i \leq m.$$

Then, the probability that the sequence $\boldsymbol{o}$ is generated by the HMM is described as

$$\Pr[\boldsymbol{o}|\boldsymbol{\lambda}] = \sum_{\boldsymbol{s}} p_{s_0} b_{s_0 o_0} \left(\prod_{t=0}^{T-2} a_{s_t s_{t+1}} b_{s_{t+1} o_{t+1}} \right) q_{s_{T-1}}, \tag{A.1}$$

where $\sum_{\boldsymbol{s}}$ denotes the sum over all possible state sequences $s_0, \cdots, s_{T-1}$: $\sum_{\boldsymbol{s}} = \sum_{s_0=1}^{n} \cdots \sum_{s_{T-1}=1}^{n}$. We will describe the derivative of $\Pr[\boldsymbol{o}|\boldsymbol{\lambda}]$ with respect to $\boldsymbol{\lambda}$ using forward and backward variables, where the forward variable α_t^i is defined as

$$\alpha_t^i := \Pr[o_0, o_1, \ldots, o_t, s_t = i|\boldsymbol{\lambda}]$$

and the backward variable β_t^i is described as

$$\beta_t^i := \Pr[o_{t+1}, o_{t+2}, \ldots, o_{T-1}|s_t = i, \boldsymbol{\lambda}].$$

These variables are efficiently computed by the standard forward-backward algorithm [Durbin et al., 1998]. Then the derivatives with respect to parameters are obtained as follows:

$$\frac{\partial \Pr[\boldsymbol{o}|\boldsymbol{\lambda}]}{\partial p_k} = b_{k\, o_0} \beta_0^k \tag{A.2}$$

$$\frac{\partial \Pr[\boldsymbol{o}|\boldsymbol{\lambda}]}{\partial q_k} = \alpha_{T-1}^k \tag{A.3}$$

$$\frac{\partial \Pr[\boldsymbol{o}|\boldsymbol{\lambda}]}{\partial a_{kl}} = \sum_{t=0}^{T-2} \alpha_t^k b_{l\, o_{t+1}} \beta_{t+1}^l \tag{A.4}$$

$$\frac{\partial \Pr[\boldsymbol{o}|\boldsymbol{\lambda}]}{\partial b_{kl}} = \sum_{t=0}^{T-1} I(o_t = l) \frac{\alpha_t^k \beta_t^k}{b_{k o_t}} \tag{A.5}$$

where $I(o_t = l) = 1$ if $o_t = l$ and 0 otherwise. The parameters in standard HMMs must satisfy the stochasticity conditions, i.e.

$$\sum_{j=1}^{n} a_{ij} = 1,\ \sum_{j=1}^{m} b_{ij} = 1,\ \sum_{j=1}^{n} p_j = 1,\ \sum_{j=1}^{n} q_j = 1.$$

For computations of FK and TOP, we use the derivatives with respect to unconstrained parameters $\boldsymbol{\lambda}'$ as in [Jaakkola et al., 2000]. These unconstrained parameters are related to the original ones as

$$p_i = p'_i / \sum_{j=1}^{n} p'_j,$$

where other parameters a'_{ij}, b'_{ij}, q'_i have the same relations (formulas not shown for brevity). By the chain rule, the derivative with respect to p'_i at the point $p'_i = p_i$ is obtained as

$$\frac{\partial \Pr[\boldsymbol{o}|\boldsymbol{\lambda}]}{\partial p'_i} = \frac{\partial \Pr[\boldsymbol{o}|\boldsymbol{\lambda}]}{\partial p_i} - \sum_{j=1}^{n} p_j \frac{\partial \Pr[\boldsymbol{o}|\boldsymbol{\lambda}]}{\partial p_j}. \tag{A.6}$$

The derivatives with respect to other unconstrained parameters can be obtained in the same way.