Online Learning with Kernels

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Abstract—Kernel based algorithms such as support vector machines have achieved considerable success in various problems in the batch setting where all of the training data is available in advance. Support vector machines combine the so-called kernel trick with the large margin idea. There has been little use of these methods in an online setting suitable for real-time applications. In this paper we consider online learning in a Reproducing Kernel Hilbert Space. By considering classical stochastic gradient descent within a feature space, and the use of some straightforward tricks, we develop simple and computationally efficient algorithms for a wide range of problems such as classification, regression, and novelty detection.

In addition to allowing the exploitation of the kernel trick in an online setting, we examine the value of large margins for classification in the online setting with a drifting target. We derive worst case loss bounds and moreover we show the convergence of the hypothesis to the minimiser of the regularised risk functional.

We present some experimental results that support the theory as well as illustrating the power of the new algorithms for online novelty detection.

Index Terms—Reproducing Kernel Hilbert Spaces, Stochastic Gradient Descent, Large Margin Classifiers, Tracking, Novelty Detection, Condition Monitoring, Classification, Regression.

I. INTRODUCTION

ERNEL methods have proven to be successful in many batch settings (Support Vector Machines, Gaussian Processes, Regularization Networks) [1]. Whilst one can apply batch algorithms by utilising a sliding buffer [2], it would be much better to have a truely online algorithm. However the extension of kernel methods to online settings where the data arrives sequentially has proven to provide some hitherto unsolved challenges.

A. Challenges for online kernel algorithms

First, the standard online settings for linear methods are in danger of overfitting when applied to an estimator using a Hilbert Space method because of the high dimensionality of the weight vectors. This can be handled by use of regularisation (or exploitation of prior probabilities in function space if the Gaussian Process view is taken).

Second, the functional representation of classical kernel based estimators becomes more complex as the number of observations increases. The Representer Theorem [3] implies that the number of kernel functions can grow up to linearly

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The authors are with the Research School of Information Sciences and Engineering, The Australian National University. R.C. Williamson is also with National ICT Australia. with the number of observations. Depending on the loss function used [4], this will happen in practice in most cases. Thus the complexity of the estimator used in prediction increases linearly over time (in some restricted situations this can be reduced to logarithmical cost [5] or constant cost [6], yet with linear storage requirements). Clearly this is not satisfactory for genuine online applications.

Third, the training time of batch and/or incremental update algorithms typically increases superlinearly with the number of observations. Incremental update algorithms [7] attempt to overcome this problem but cannot guarantee a bound on the number of operations required per iteration. Projection methods [8] on the other hand, will ensure a limited number of updates per iteration and also keep the complexity of the estimator constant. However they can be computationally expensive since they require a matrix multiplication at each step. The size of the matrix is given by the number of kernel functions required at each step and could typically be in the hundreds in the smallest dimension.

In solving the above challenges it is highly desirable to be able to theoretically prove convergence rates and error bounds for any algorithms developed. One would want to be able to relate the performance of an online algorithm after seeing m observations to the quality that would be achieved in a batch setting. It is also desirable to be able to provide some theoretical insight in drifting target scenarios when a comparison with a batch algorithm makes little sense.

In this paper we present algorithms which deal effectively with these three challenges as well as satisfying the above desiderata.

B. Related Work

Recently several algorithms have been proposed [5], [9]– [11] which perform perceptron-like updates for classification at each step. Some algorithms work only in the noise free case, others not for moving targets, and others assume an upper bound on the complexity of the estimators. In the present paper we present a simple method which allows the use of kernel estimators for classification, regression, and novelty detection and which copes with a large number of kernel functions efficiently.

The stochastic gradient descent algorithms we propose (collectively called NORMA) differ from the tracking algorithms of Warmuth, Herbster and Auer [5], [12], [13] insofar as we do not require that the norm of the hypothesis be bounded beforehand. More importantly, we explicitly deal with the issues described earlier that arise when applying them to kernel based representations.

Concerning large margin classification (which we obtain by performing stochastic gradient descent on the soft margin loss

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function), our algorithm is most similar to Gentile's ALMA [9] and we obtain similar loss bounds to those obtained for ALMA. One of the advantages of a large margin classifier is that it allows us to track changing distributions efficiently [14].

In the context of Gaussian Processes (an alternative theoretical framework that can be used to develop kernel based algorithms), related work was presented in [8]. The key difference to our algorithm is that Csató and Opper repeatedly project on to a low-dimensional subspace, which can be computationally costly requiring as it does a matrix multiplication.

Mesterharm [15] has considered tracking arbitrary linear classifiers with a variant of Winnow [16], and Bousquet and Warmuth [17] studied tracking of a small set of experts via posterior distributions.

Finally we note that whilst not originally developed as an online algorithm, the Sequential Minimal Optimization (SMO) algorithm [18] is closely related, especially when there is no bias term in which case [19] it effectively becomes the Perceptron algorithm.

C. Outline of the Paper

In Section II we develop the idea of stochastic gradient descent in Hilbert Space. This provides the basis of our algorithms. Subsequently we show how the general form of the algorithm can be applied to problems of classification, novelty detection, and regression (Section III). Next we establish mistake bounds with moving targets for linear large margin classification algorithms in Section IV. A proof that the stochastic gradient algorithm converges to the minimum of the regularised risk functional is given in Section V, and we conclude with experimental results and a discussion in Sections VI and VII.

II. STOCHASTIC GRADIENT DESCENT IN HILBERT SPACE

We consider a problem of function estimation, where the goal is to learn a mapping $f: \mathcal{X} \to \mathbb{R}$ based on a sequence $S = ((x_1, y_1), \ldots, (x_m, y_m))$ of examples $(x_t, y_t) \in \mathcal{X} \times \mathcal{Y}$. Moreover we assume that there exists a loss function $l: \mathbb{R} \times \mathcal{Y} \to \mathbb{R}$, given by l(f(x), y), which penalises the deviation of estimates f(x) from observed labels y. Common loss functions include the soft margin loss function [20] or the logistic loss for classification and novelty detection [21], and the quadratic loss, absolute loss, Huber's robust loss [22] and the ε -insensitive loss [23] for regression. We shall discuss these in Section III.

The reason for allowing the range of f to be \mathbb{R} rather than \mathcal{Y} is that it allows for more refinement in evaluation of the learning result. For example, in *classification* with $\mathcal{Y} = \{-1, 1\}$ we could interpret $\operatorname{sgn}(f(x))$ as the prediction given by f for the class of x, and |f(x)| as the confidence in that classification. We call the output f of the learning algorithm an *hypothesis*, and denote the set of all possible hypotheses by \mathcal{H} .

We will always assume \mathcal{H} is a *reproducing kernel Hilbert* space (RKHS) [1]. This means that there exists a kernel $k: \mathcal{X} \times \mathcal{X} \to \mathbb{R}$ and a dot product $\langle \cdot, \cdot \rangle_{\mathcal{H}}$ such that

1) k has the reproducing property

$$\langle f, k(x, \cdot) \rangle_{\mathcal{H}} = f(x) \qquad \text{for } x \in \mathcal{X}$$
 (1)

2) \mathcal{H} is the closure of the span of all $k(x, \cdot)$ with $x \in \mathcal{X}$. In other words, all $f \in \mathcal{H}$ are linear combinations of kernel functions. The inner product $\langle \cdot, \cdot \rangle_{\mathcal{H}}$ induces a norm on $f \in \mathcal{H}$ in the usual way: $||f||_{\mathcal{H}} := \langle f, f \rangle_{\mathcal{H}}^{-1/2}$. An interesting special case is $\mathcal{X} = \mathbb{R}^n$ with $k(x, y) = \langle x, y \rangle$ (the normal dot-product in \mathbb{R}^n) which corresponds to learning linear functions in \mathbb{R}^n , but much more varied function classes can be learned by using different kernels.

A. Risk Functionals

In *batch learning*, it is typically assumed that all the examples are immediately available and are drawn independently from some distribution P over $\mathcal{X} \times \mathcal{Y}$. One natural measure of quality for f in that case is the *expected risk*

$$R[f, P] := E_{(x,y)\sim P}[l(f(x), y)].$$
(2)

Since P is unknown, given S drawn from P^m , a standard approach [1] is to instead minimise the *empirical risk*

$$R_{\rm emp}[f,S] := \frac{1}{m} \sum_{t=1}^{m} l(f(x_t), y_t).$$
(3)

However, minimising $R_{emp}[f]$ may lead to overfitting (complex functions that fit well on the training data but do not generalise to unseen data). One way to avoid this is to penalise complex functions by instead minimising the *regularised risk*

$$R_{\rm reg}[f,S] := R_{{\rm reg},\lambda}[f,S] := R_{\rm emp}[f] + \frac{\lambda}{2} ||f||_{\mathcal{H}}^2$$
(4)

where $\lambda > 0$ and $||f||_{\mathcal{H}} = \langle f, f \rangle_{\mathcal{H}}^{1/2}$ does indeed measure the complexity of f in a sensible way [1]. The constant λ needs to be chosen appropriately for each problem. If l has parameters (for example l_{ρ} — see later), we write $R_{\text{emp},\rho}[f, S]$ and $R_{\text{reg},\lambda,\rho}[f, S]$.

Since we are interested in online algorithms, which deal with one example at a time, we also define an instantaneous approximation of $R_{\text{reg},\lambda}$, the *instantaneous regularised risk* on a single example (x, y), by

$$R_{\text{inst}}[f, x, y] := R_{\text{inst}, \lambda}[f, x, y] := R_{\text{reg}, \lambda}[f, ((x, y))].$$
(5)

B. Online setting

In this paper we are interested in *online learning*, where the examples become available one by one, and it is desired that the learning algorithm produces a sequence of hypotheses $\mathbf{f} = (f_1, \ldots, f_{m+1})$. Here f_1 is some arbitrary initial hypothesis and f_i for i > 1 is the hypothesis chosen after seeing the (i-1)th example. Thus $l(f_t(x_t), y_t)$ is the loss the learning algorithm makes when it tries to predict y_t , based on x_t and the previous examples $(x_1, y_1), \ldots, (x_{t-1}, y_{t-1})$. This kind of learning framework is appropriate for real-time learning problems and is of course analogous to the usual adaptive signal processing framework [24]. We may also use an online algorithm simply as an efficient method of approximately solving a batch problem. The algorithm we propose below

can be effectively run on huge data sets on machines with limited memory.

A suitable measure of performance for online algorithms in an online setting is the *cumulative loss*

$$L_{\rm cum}[\mathbf{f}, S] = \sum_{t=1}^{m} l(f_t(x_t), y_t).$$
 (6)

(Again, if l has such as ρ , we write $L_{\text{curn},\rho}[f]$ etc.) Notice that here f_t is tested on the example (x_t, y_t) which was not available for training f_t , so if we can guarantee a low cumulative loss we are already guarding against overfitting. Regularisation can still be useful in the online setting: if the target we are learning changes over time, regularisation prevents the hypothesis from going too far in one direction, thus hopefully helping recovery when a change occurs. Furthermore, if we are interested in large margin algorithms, some kind of complexity control is needed to make the definition of the margin meaningful.

C. The General Idea of the Algorithm

The algorithms we study in this paper are classical stochastic gradient descent — they perform gradient descent with respect to the instantaneous risk. The general form of the update rule is

$$f_{t+1} := f_t - \eta_t \left. \partial_f R_{\text{inst},\lambda}[f, x_t, y_t] \right|_{f=f_t} \tag{7}$$

where for $i \in \mathbb{N}$, $f_i \in \mathcal{H}$, ∂_f is short-hand for $\partial/\partial f$ (the gradient with respect to f) and $\eta_t > 0$ is the *learning rate* which is often constant $\eta_t = \eta$. In order to evaluate the gradient, note that the evaluation functional $f \mapsto f(x_i)$ is given by (1), and therefore

$$\partial_f l(f(x_t), y_t) = l'(f(x_t), y_t)k(x_t, \cdot), \tag{8}$$

where $l'(z, y) := \partial_z l(z, y)$. Since $\partial_f ||f||_{\mathcal{H}}^2 = 2f$, the update becomes

$$f_{t+1} := (1 - \eta \lambda) f_t - \eta_t l'(f_t(x_t), y_t) k(x_t, \cdot).$$
(9)

Clearly, given $\lambda > 0$, η_t needs to satisfy $\eta_t < 1/\lambda$ for all t for the algorithm to work.

We also allow loss functions l that are only piecewise differentiable, in which case ∂ stands for subgradient. When the subgradient is not unique, we choose one arbitrarily; the choice does not make any difference either in practice or in theoretical analyses. All the loss functions we consider are convex in the first argument.

Choose a zero initial hypothesis $f_1 = 0$. For the purposes of practical computations, one can write f_t as a kernel expansion (cf. [25])

$$f_t(x) = \sum_{i=1}^{t-1} \alpha_i k(x_i, x) \qquad x \in \mathcal{X}$$
(10)

where the coefficients are updated at step t via

$$\alpha_t := -\eta_t l'(f_t(x_t), y_t) \qquad \text{for } i = t \qquad (11)$$

$$\alpha_i := (1 - \eta_t \lambda) \alpha_i \qquad \text{for } i < t. \tag{12}$$

Given: A sequence $S = ((x_i, y_i))_{i \in \mathbb{N}} \in (\mathcal{X} \times \mathcal{Y})^{\infty}$; a regularisation parameter $\lambda > 0$; a truncation parameter $\tau \in \mathbb{N}$; a learning rate $\eta \in (0, 1/\lambda)$; a piecewise differentiable convex loss function $l : \mathbb{R} \times \mathcal{Y} \to \mathbb{R}$; and a Reproducing Kernel Hilbert Space \mathcal{H} with reproducing kernel k, NORMA $_{\lambda}(S, l, k, \eta, \tau)$ outputs a sequence of hypotheses $\mathbf{f} = (f_1, f_2, \ldots) \in \mathcal{H}^{\infty}$. Initialise t := 1; $\beta_i := (1 - \lambda \eta)^i$ for $i = 0, \ldots, \tau$; Loop $f_t(\cdot) := \sum_{i=\max(1,t-\tau)}^{t-1} \alpha_i \beta_{t-i-1} k(x_i, \cdot);$ $\alpha_t := -\eta l'(f_t(x_t), y_t);$ t := t + 1;



Fig. 1. NORMA $_{\lambda}$ with constant learning rate η , exploiting the truncation approximation.

Thus, at step t the t-th coefficient may receive a non-zero value. The coefficients for earlier terms decay by a factor (which is constant for constant η_t). Notice that the cost for training at each step is not much larger than the prediction cost: once we have computed $f_t(x_t)$, α_t is obtained by the value of the derivative of l at $(f_t(x_t), y_t)$.

D. Speedups and Truncation

There are several ways of speeding up the algorithm. Instead of updating all old coefficients α_i , $i = 1, \ldots, t - 1$, one may simply cache the power series $1, (1 - \lambda \eta), (1 - \lambda \eta)^2, (1 - \lambda \eta)^3, \ldots$ and pick suitable terms as needed. This is particularly useful if the derivatives of the loss function l will only assume discrete values, say $\{-1, 0, 1\}$ as is the case when using the soft-margin type loss functions (see Section III).

Alternatively, one can also store $\tilde{\alpha}_t = (1 - \eta)^{-t} \alpha_t$ and compute $f_t(x) = (1 - \eta)^t \sum_{i=1}^{t-1} \tilde{\alpha}_i k(x_i, x_t)$, which only requires rescaling once $\tilde{\alpha}_t$ becomes too large for machine precision — this exploits the exponent in the standard floating point number representation.

A major problem with (11) and (12) is that without additional measures, the kernel expansion at time t contains t terms. Since the amount of computations required for predicting grows linearly in the size of the expansion, this is undesirable. The regularisation term helps here. At each iteration the coefficients α_i with $i \neq t$ are shrunk by $(1 - \lambda \eta)$. Thus after τ iterations the coefficient α_i will be reduced to $(1 - \lambda \eta)^{\tau} \alpha_i$. Hence one can drop small terms and incur little error as the following proposition shows.

Proposition 1 (Truncation Error) Suppose l(z, y) is a loss function satisfying $|\partial_z l(z, y)| \leq C$ for all $z \in \mathbb{R}$, $y \in \mathcal{Y}$ and k is a kernel with bounded norm $||k(x, \cdot)|| \leq X$ where $|| \cdot ||$ denotes either $|| \cdot ||_{L_{\infty}}$ or $|| \cdot ||_{\mathcal{H}}$. Let $f_{\text{trunc}} := \sum_{i=\max(1,t-\tau)}^{t-1} \alpha_i k(x_i, \cdot)$ denote the kernel expansion truncated to τ terms. The truncation error satisfies

$$\|f - f_{\text{trunc}}\| \le \sum_{i=1}^{\iota-\tau} \eta (1 - \lambda \eta)^{t-i} CX < (1 - \lambda \eta)^{\tau} CX/\lambda.$$

Obviously the approximation quality increases exponentially with the number of terms retained. The regularisation parameter λ can thus be used to control the storage requirements for the expansion. In addition, it naturally allows for distributions P(x, y) that change over time in which cases it is desirable to *forget* instances (x_i, y_i) that are much older than the average time scale of the distribution change [26].

We call our algorithm NORMA (Naive Online R_{reg} Minimisation Algorithm) and sometimes explicitly write the parameter λ : NORMA $_{\lambda}$. NORMA is summarised in Figure 1. In the applications discussed in the next section it is sometimes necessary to introduce additional parameters that need to be updated. We nevertheless refer somewhat loosely to the whole family of algorithms as NORMA.

III. APPLICATIONS

The general idea of NORMA can be applied to a wide range of problems. We utilise the standard [1] addition of the constant offset b to the function expansion, i.e. g(x) :=f(x) + b where $f \in \mathcal{H}$ and $b \in \mathbb{R}$. Hence we also update b via

$$b_{t+1} := b_t - \eta \left. \partial_b R_{\text{inst}}[g, x_t, y_t] \right|_{g=f_t+b_t}.$$

A. Classification

In (binary) classification, we have $\mathcal{Y} = \{\pm 1\}$. The most obvious loss function to use in this context is l(f(x), y) = 1 if $yf(x) \leq 0$ and l(f(x), y) = 0 otherwise. Thus, no loss is incurred if $\operatorname{sgn}(f(x))$ is the correct prediction for y; otherwise we say that f makes a *mistake* at (x, y) and charge a unit loss.

However, the mistake loss function has some drawbacks: a) it fails to take into account the margin yf(x) that can be considered a measure of confidence in the correct prediction, a non-positive margin meaning an actual mistake; b) the mistake loss is discontinuous and non-convex and thus is unsuitable for use in gradient based algorithms.

In order to deal with these drawbacks the main loss function we use here for classification is the *soft margin loss*

$$l_{\rho}(f(x), y) := \max(0, \rho - yf(x))$$
(13)

where $\rho \ge 0$ is the margin parameter. The soft margin loss $l_{\rho}(f(x), y)$ is positive if f fails to achieve a margin at least ρ on (x, y); in this case we say that f made a margin error. If f made an actual mistake, then $l_{\rho}(f(x), y) \ge \rho$.

Let σ_t be an indicator of whether f_t made a margin error on (x_t, y_t) , i.e., $\sigma_t = 1$ if $y_t f_t(x_t) \leq \rho$ and zero otherwise. Then

$$l'_{\rho}(f_t(x_t), y_t) = -\sigma_t y_t = \begin{cases} -y_t & \text{if } y_t f_t(x_t) \le \rho \\ 0 & \text{otherwise} \end{cases}$$
(14)

and the update (9) becomes

$$f_{t+1} := (1 - \eta \lambda)f_t + \eta \sigma_t y_t k(x_t, \cdot)$$
(15)

$$b_{t+1} := b_t + \eta \sigma_t y_t. \tag{16}$$

Suppose now that X > 0 is a bound such that $k(x_t, x_t) \le X^2$ holds for all t. Since $||f_1||_{\mathcal{H}} = 0$ and

$$\begin{aligned} ||f_{t+1}||_{\mathcal{H}} &\leq (1 - \eta \lambda) ||f_t||_{\mathcal{H}} + \eta ||k(x_t, \cdot)||_{\mathcal{H}} \\ &= (1 - \eta \lambda) ||f_t||_{\mathcal{H}} + \eta k(x_t, x_t)^{1/2}, \end{aligned}$$

we obtain $||f_t||_{\mathcal{H}} \leq X/\lambda$ for all t. Furthermore,

$$|f_t(x_t)| = |\langle f_t, k(x_t, \cdot) \rangle_{\mathcal{H}}| \le X^2 / \lambda.$$
(17)

Hence, when the offset parameter b is omitted (which we consider particularly in Sections IV and V), it is reasonable to require $\rho \leq X^2/\lambda$. Then the loss function becomes effectively bounded, with $l_{\rho}(f_t(x_t), y_t) \leq 2X^2/\lambda$ for all t.

The update in terms of α_i is (for i = 1, ..., t - 1)

$$(\alpha_i, \alpha_t, b) := ((1 - \eta \lambda)\alpha_i, \eta \sigma_t y_t, b + \eta \sigma_t y_t).$$
(18)

When $\rho = 0$ and $\lambda = 0$ we recover the kernel perceptron [27]. If $\rho = 0$ and $\lambda > 0$ we have a kernel perceptron with regularisation.

For *classification with the* ν -*trick* [4] we also have to take care of the margin ρ , since there (recall g(x) = f(x) + b)

$$l(g(x), y) := \max(0, \rho - yg(x)) - \nu\rho.$$
(19)

Since one can show [4] that the specific choice of λ has no influence on the estimate in ν -SV classification, we may set $\lambda = 1$ and obtain the update rule (for i = 1, ..., t - 1)

$$(\alpha_i, \alpha_t, b, \rho) := ((1-\eta)\alpha_i, \eta\sigma_t y_t, b+\eta\sigma_t y_t, \rho+\eta(\sigma_t-\nu)).$$

B. Novelty Detection

Novelty detection [21] is like classification without labels. It is useful for condition monitoring tasks such as network intrusion detection. The absence of labels y_i means the algorithm is not precisely a special case of NORMA as presented earlier, but one can derive a variant in the same spirit.

The ν -setting is most useful here as it allows one to specify an upper limit on the frequency of alerts $f(x) < \rho$. The loss function to be utilised is

$$l(f(x), x, y) := \max(0, \rho - f(x)) - \nu\rho$$

and usually [21] one uses $f \in \mathcal{H}$ rather than g = f + b where $b \in \mathbb{R}$ in order to avoid trivial solutions. The update rule is (for $i = 1, \ldots, t - 1$)

$$(\alpha_i, \alpha_t, \rho) := \begin{cases} ((1-\eta)\alpha_i, \eta, \rho + \eta(1-\nu)) & \text{if } f(x) < \rho \\ ((1-\eta)\alpha_i, 0, \rho - \eta\nu) & \text{otherwise.} \end{cases}$$
(20)

Consideration of the update for ρ shows that on average only a fraction of ν observations will be considered for updates. Thus it is necessary to store only a small fraction of the x_i s.

C. Regression

We consider the following three settings: squared loss, the ε -insensitive loss using the ν -trick, and Huber's robust loss function, i.e. trimmed mean estimators. For convenience we will only use estimates $f \in \mathcal{H}$ rather than g = f + b where $b \in \mathbb{R}$. The extension to the latter case is straightforward.

1) Squared Loss: Here $l(f(x), y) := \frac{1}{2}(y - f(x))^2$. Consequently the update equation is (for i = 1, ..., t - 1)

$$(\alpha_i, \alpha_t) := ((1 - \lambda \eta)\alpha_i, \eta(y_t - f(x_t))).$$
(21)

This means that we have to store *every* observation we make, or more precisely, the prediction error we made on the observation.

2) ε -insensitive Loss: The use of the loss function $l(f(x), y) = \max(0, |y-f(x)|-\varepsilon)$ introduces a new parameter — the width of the insensitivity zone ε . By making ε a variable of the optimisation problem we have

$$l(f(x), y) := \max(0, |y - f(x)| - \varepsilon) + \nu \varepsilon.$$

The update equations now have to be stated in terms of α_i, α_t , and ε which is allowed to change during the optimisation process. Setting $\delta_t := y_t - f(x_t)$ the updates are (for $i = 1, \ldots, t-1$)

$$\begin{aligned} &(\alpha_i, \, \alpha_t, \, \varepsilon) := \\ & \begin{cases} ((1 - \lambda \eta) \alpha_i, \, \eta \, \text{sgn} \, \delta_t, \, \varepsilon + (1 - \nu) \eta) & \text{if } |\delta_t| > \varepsilon \\ ((1 - \lambda \eta) \alpha_i, \, 0, \, \varepsilon - \eta \nu) & \text{otherwise.} \end{cases}$$

This means that every time the prediction error exceeds ε , we increase the insensitive zone by $\eta\nu$. If it is smaller than ε , the insensitive zone is decreased by $\eta(1-\nu)$.

3) Huber's Robust Loss: This loss function was proposed in [22] for robust maximum likelihood estimation among a family of unknown densities. It is given by

$$l(f(x), y) := \begin{cases} |y - f(x)| - \frac{1}{2}\sigma & \text{if } |y - f(x)| \ge \sigma \\ \frac{1}{2\sigma}(y - f(x))^2 & \text{otherwise.} \end{cases}$$
(23)

Setting $\delta_t := y_t - f(x_t)$ the updates are (for $i = 1, \dots, t-1$)

$$(\alpha_i, \alpha_t) := \begin{cases} ((1 - \eta)\alpha_i, \eta \operatorname{sgn} \delta_t) & \text{if } |\delta_t| > \sigma \\ ((1 - \eta)\alpha_i, \sigma^{-1}\delta_t) & \text{otherwise.} \end{cases}$$
(24)

Comparing (24) with (22) leads to the question of whether σ might also be adjusted adaptively. This is a desirable goal since we may not know the amount of noise present in the data. While the ν -setting allowed the formation of adaptive estimators for batch learning with the ε -insensitive loss, this goal has proven elusive for other estimators in the standard batch setting.

In the online situation, however, such an extension is quite natural (see also [28]). It is merely necessary to make σ a variable of the optimisation problem and the updates become (for i = 1, ..., t - 1)

$$\begin{aligned} &(\alpha_i, \, \alpha_t, \, \sigma) := \\ & \begin{cases} ((1-\eta)\alpha_i, \, \eta \, \text{sgn} \, \delta_t, \, \sigma + \eta(1-\nu)) & \text{if } |\delta_t| > \sigma \\ ((1-\eta)\alpha_i, \, \sigma^{-1}\delta_t, \, \sigma - \eta\nu) & \text{otherwise.} \end{cases} \end{aligned}$$

IV. MISTAKE BOUNDS FOR NON-STATIONARY TARGETS

In this section we theoretically analyse NORMA for classification with the soft margin loss with margin ρ . In the process we establish relative bounds for the soft margin loss. A detailed comparative analysis between NORMA and Gentile's ALMA [9] can be found in [14].

A. Definitions

We consider the performance of the algorithm for a fixed sequence of observations $S := ((x_1, y_1), \ldots, (x_m, y_m))$ and study the sequence of hypotheses $\mathbf{f} = (f_1, \ldots, f_m)$, produced

by the algorithm on S. Two key quantities are the number of *mistakes*, given by

$$M(\mathbf{f}, S) := |\{ 1 \le t \le m \mid y_t f_t(x_t) \le 0 \}|, \qquad (25)$$

and the number of margin errors, given by

$$M_{\rho}(\mathbf{f}, S) := |\{ 1 \le t \le m \mid y_t f_t(x_t) \le \rho \}|.$$
(26)

Notice that margin errors are those examples on which the gradient of the soft margin loss is non-zero, so $M_{\rho}(\mathbf{f}, S)$ gives the size of the kernel expansion of final hypothesis f_{m+1} .

We use σ_t to denote whether a margin error was made at trial t, i.e., $\sigma_t = 1$ if $y_t f_t(x_t) \leq \rho$ and $\sigma_t = 0$ otherwise. Thus the soft margin loss can be written as $l_{\rho}(f_t(x_t), y_t) = \sigma_t(\rho - y_t f_t(x_t))$ and consequently $L_{\text{cum},\rho}[\mathbf{f}, S]$ denotes the total soft margin loss of the algorithm.

In our bounds we compare the performance of NORMA to the performance of function sequences $\mathbf{g} = (g_1, \ldots, g_m)$ from some *comparison class* $\mathcal{G} \subset \mathcal{H}^m$.

Notice that we often use a different margin $\mu \neq \rho$ for the comparison sequence, and σ_t always refers to the margin errors of the actual algorithm with respect to its margin ρ . We always have

$$l_{\mu}(g(x), y) \ge \mu - yg(x). \tag{27}$$

We extend the notations $M(\mathbf{g}, S)$, $M_{\mu}(\mathbf{g}, S)$, $l_{\mu}(g_t, y_t)$ and $L_{\text{cum},\mu}[\mathbf{g}, S]$ to such comparison sequences in the obvious manner.

B. A Preview

To understand the form of the bounds, consider first the case of a stationary target, with comparison against a constant sequence $\mathbf{g} = (g, \ldots, g)$. With $\rho = \lambda = 0$, our algorithm becomes the kernelised Perceptron algorithm. Assuming that some g achieves $M_{\mu}(\mathbf{g}, S) = 0$ for some $\mu > 0$, the kernelised version of the Perceptron Convergence Theorem [27], [29] gives

$$\mathcal{M}(\mathbf{f}, S) \le ||g||_{\mathcal{H}}^2 \max k(x_t, x_t)/\mu^2$$

Consider now the more general case where the sequence is not linearly separable in the feature space. Then ideally we would wish for bounds of the form

$$\mathcal{M}(\mathbf{f}, S) \le \min_{\mathbf{g} = (g, \dots, g)} \mathcal{M}(\mathbf{g}, S) + o(m),$$

which would mean that the mistake rate of the algorithm would converge to the mistake rate of the best comparison function. Unfortunately, even approximately minimising the number of mistakes over the training sequence is very difficult, so such strong bounds for simple online algorithms seem unlikely. Instead, we settle for weaker bounds of the form

$$\mathcal{M}(\mathbf{f}, S) \le \min_{\mathbf{g} = (g, \dots, g), ||g||_{\mathcal{H}} \le B} L_{\operatorname{cum}, \mu}[\mathbf{g}, S] / \mu + o(m), \quad (28)$$

where $L_{\text{cum},\mu}[\mathbf{g}, S]/\mu$ is an upper bound for $M(\mathbf{g}, S)$, and the norm bound *B* appears as a constant in the o(m) term. For earlier bounds of this form, see [30], [31].

In the non-stationary case, we consider comparison classes which are allowed to change slowly, that is

$$\begin{aligned} \mathcal{G}(B, D_1, D_2) \\ &:= \left\{ \left(g_1, \dots, g_m\right) \left| \sum_{t=1}^{m-1} ||g_t - g_{t+1}||_{\mathcal{H}} \le D_1 \right. \\ &\left. \sum_{t=1}^{m-1} ||g_t - g_{t+1}||_{\mathcal{H}}^2 \le D_2 \text{ and } ||g_t||_{\mathcal{H}} \le B \right\}. \end{aligned}$$

The parameter D_1 bounds the total distance travelled by the target. Ideally we would wish the target movement to result in an additional $O(D_1)$ term in the bounds, meaning there would be a constant cost per unit step of the target. Unfortunately, for technical reasons we also need the D_2 parameter which restricts the changes of speed of the target. The meaning of the D_2 parameter will become clearer when we state our bounds and discuss them.

Choosing the parameters is an issue in the bounds we have. The bounds depend on the choice of the learning rate and margin parameters, and the optimal choices depend on quantities (such as $\min_{\mathbf{g}} L_{\operatorname{cum},\mu}[\mathbf{g},S]$) that would not be available when the algorithm starts. In our bounds, we handle this by assuming an upper bound $K \geq \min_{\mathbf{g}} L_{\operatorname{cum},\mu}[\mathbf{g},S]$ that can be used for tuning. By substituting $K = \min_{\mathbf{g}} L_{\operatorname{cum},\mu}[\mathbf{g}, S]$, we obtain the kind of bound we discussed above; otherwise the estimate K replaces $\min_{\mathbf{g}} L_{\operatorname{cum},\mu}[\mathbf{g},S]$ in the bound. In a practical application, one would probably be best served to ignore the formal tuning results in the bounds and just tune the parameters by whatever empirical methods are preferred. Recently, online algorithms have been suggested that dynamically tune the parameters to almost optimal values as the algorithm runs [9], [32]. Applying such techniques to our analysis remains an open problem.

C. Relative Loss Bounds

Recall that the update for the case we consider is

$$f_{t+1} := (1 - \eta\lambda)f_t + \eta\sigma_t y_t k(x_t, \cdot).$$
(29)

It will be convenient to give the parameter tunings in terms of the function

$$h(x, K, C) = \sqrt{\frac{C}{K} \left(x + \frac{C}{K}\right) - \frac{C}{K}},$$
(30)

where we assume x, K and C to be positive. Notice that $0 \le h(x, K, C) \le x$ holds, and $\lim_{K \to 0+} h(x, K, C) = x/2$. Accordingly, we define h(x, 0, C) = x/2.

We start by analysing margin errors with respect to a given margin ρ .

Theorem 2 Suppose **f** is generated by (29) on a sequence S of length m. Let X > 0 and suppose that $k(x_t, x_t) \leq X^2$ for all t. Fix $K \geq 0$, B > 0, $D_1 \geq 0$ and $D_2 \geq 0$. Let

$$C = \frac{1}{4}X^{2} \left(B^{2} + B \left(\sqrt{mD_{2}} + D_{1} \right) \right)$$
(31)

and, given parameters $\mu > \rho \ge 0$, let $\eta' = 2h(\mu - \rho, K, C)/X^2$. Choose the regularisation parameter

$$\lambda = (B\eta')^{-1}\sqrt{D_2/m},\tag{32}$$

and the learning rate parameter $\eta = \eta'/(1+\eta'\lambda)$. If for some $\mathbf{g} \in \mathcal{G}(B, D_1, D_2)$, we have $L_{\operatorname{cum},\mu}[\mathbf{g}, S] \leq K$ then

$$M_{\rho}(\mathbf{f}, S) \leq \frac{K}{\mu - \rho} + \frac{2C}{(\mu - \rho)^2} + 2\left(\frac{C}{(\mu - \rho)^2}\right)^{1/2} \left(\frac{K}{\mu - \rho} + \frac{C}{(\mu - \rho)^2}\right)^{1/2}.$$

The proof can be found in Appendix A.

We now consider obtaining mistake bounds from our margin error result. The obvious method is to set $\rho = 0$, turning margin errors directly to mistakes. Interestingly, it turns out that a subtly different choice of parameters allows us to obtain the same mistake bound using a non-zero margin.

Theorem 3 Suppose **f** is generated by (29) on a sequence S of length m. Let X > 0 and suppose that $k(x_t, x_t) \leq X^2$ for all t. Fix $K, B, D_1, D_2 \geq$ and define C as in (31), and given $\mu > 0$ let $\eta' = 2r/X^2$ where $r = h(\mu, K, C)$. Choose the regularisation parameter as in (32), the learning rate $\eta = \eta'/(1 + \eta'\lambda)$, and set the margin to either $\rho = 0$ or $\rho = \mu - r$. Then for either of these margin settings, if there exists a comparison sequence $\mathbf{g} \in \mathcal{G}(B, D_1, D_2)$ such that $L_{\text{cum}, \mu}[\mathbf{g}, S] \leq K$, we have

$$\mathcal{M}(\mathbf{f}, S) \le \frac{K}{\mu} + \frac{2C}{\mu^2} + 2\left(\frac{C}{\mu^2}\right)^{1/2} \left(\frac{K}{\mu} + \frac{C}{\mu^2}\right)^{1/2}.$$

The proof of Theorem 3 is also in Appendix A.

To gain intuition about Theorems 2 and 3, consider first the separable case K = 0 with a stationary target $(D_1 = D_2 = 0)$. In this special case, Theorem 3 gives the familiar bound from the Perceptron Convergence Theorem. Theorem 2 gives an upper bound of $X^2B^2/(\mu - \rho)^2$ margin errors. The choices given for ρ in Theorem 3 for the purpose of minimising the mistake bound are in this case $\rho = 0$ and $\rho = \mu/2$. Notice that the latter choice results in a bound of $4X^2B^2/\mu$ margin errors. More generally, if we choose $\rho = (1 - \epsilon)\mu$ for some $0 < \epsilon < 1$ and assume μ to be the largest margin for which separation is possible, we see that the algorithm achieves in $O(\epsilon^{-2})$ iterations a margin within a factor $1 - \epsilon$ of optimal. This bound is similar to that for ALMA [9], but ALMA is much more sophisticated in that it automatically tunes its parameters.

Removing the separability assumption leads to an additional K/μ term in the mistake bound, as we expected. To see the effects of the D_1 and D_2 terms, assume first that the target has constant speed: $||g_t - g_{t+1}||_{\mathcal{H}} = \delta$ for all t where $\delta > 0$ is a constant. Then $D_1 = m\delta$ and $D_2 = m\delta^2$, so $\sqrt{mD_2} = D_1$. If the speed is not constant, we always have $\sqrt{mD_2} > D_1$. An extreme case would be $||g_1 - g_2||_{\mathcal{H}} = D_1$, $g_{t+1} = g_t$ for t > 1. Then $\sqrt{mD_2} = \sqrt{mD_1}$. Thus the D_2 term increases the bound in case of changing target speed.

V. CONVERGENCE OF NORMA

A. A Preview

Next we study the performance of NORMA when it comes to minimising the regularised risk functional $R_{\text{reg}}[f, S]$, of which $R_{\text{inst}}[f, x_t, y_t]$ is the stochastic approximation at time t. We show that under some mild assumptions on the loss function,

the average instantaneous risk $(1/m) \sum_{t=1}^{m} R_{inst}[f_t, x_t, y_t]$ of the hypotheses f_t of NORMA converges towards the minimum regularised risk $\min_g R_{reg}[g, S]$ at rate $O(m^{-1/2})$. This requires no probabilistic assumptions. If the examples are i.i.d., then with high probability the expected regularised risk of the average hypothesis $(1/m) \sum_{t=1}^{m} f_t$ similarly converges towards the minimum expected risk. Convergence can also be guaranteed for the truncated version of the algorithm that keeps its kernel expansion at a sublinear size.

B. Assumptions and notation

We assume a bound X > 0 such that $k(x_t, x_t) \leq X^2$ for all t. Then for all $g \in \mathcal{H}$, $|g(x_t)| = |\langle g, k(x_t, \cdot) \rangle_{\mathcal{H}}| \leq X ||g||_{\mathcal{H}}$.

We assume that the loss function l is convex in its first argument and also satisfies for some constant c > 0 the Lipschitz condition

$$|l(z_1, y) - l(z_2, y)| \le c|z_1 - z_2|$$
(33)

for all $z_1, z_2 \in \mathbb{R}, y \in \mathcal{Y}$.

Fix now $\lambda > 0$. The hypotheses f_t produced by (9)

$$\begin{aligned} ||f_{t+1}||_{\mathcal{H}} &= ||(1-\eta_t\lambda)f_t - \eta_t l'(f(x_t), y_t)k(x_t, \cdot)||_{\mathcal{H}} \\ &\leq (1-\eta_t\lambda)||f_t||_{\mathcal{H}} + \eta_t cX, \end{aligned}$$

and since $f_1 = 0$ we have for all t the bound $||f_t||_{\mathcal{H}} \leq U$ where

$$U := \frac{cX}{\lambda}.$$
 (34)

Since $|l'(f(x_t), y_t)| \leq c$, we have $||\partial_f l(f(x_t), y_t)||_{\mathcal{H}} \leq cX$ and $||\partial_f R_{\text{inst}}[f, x_t, y_t]||_{\mathcal{H}} \leq cX + \lambda ||f||_{\mathcal{H}} \leq 2cX$ for any fsuch that $||f||_{\mathcal{H}} \leq U$.

Fix a sequence S and for $0<\epsilon<1$ define

$$\hat{g} := \operatorname*{argmin}_{g \in \mathcal{H}} R_{\mathrm{reg}}[g, S], \quad g := (1 - \epsilon)\hat{g}.$$

Considering the limit $\epsilon \to 0+$ shows that $||\hat{g}||_{\mathcal{H}} \leq U$ where U is as in (34).

C. Basic convergence bounds

We start with a simple cumulative risk bound. To achieve convergence, we use a decreasing learning rate.

Theorem 4 Fix $\lambda > 0$ and $0 < \eta < 1/\lambda$. Assume that l is convex and satisfies (33). Let the example sequence $S = ((x_t, y_t))_{t=1}^m$ be such that $k(x_t, x_t) \leq X^2$ holds for all t, and let (f_1, \ldots, f_{m+1}) be the hypothesis sequence produced by

NORMA with learning rate $\eta_t = \eta t^{-1/2}$. Then for any $g \in \mathcal{H}$ we have

$$\sum_{t=1}^{m} R_{\text{inst},\lambda}[f_t, x_t, y_t] \le m R_{\text{reg},\lambda}[g, S] + am^{1/2} + b \quad (35)$$

where $a = 2\lambda U^2(2\eta\lambda + 1/(\eta\lambda))$, $b = U^2/(2\eta)$ and U is as in (34).

The proof, given in Appendix B, is based on analysing the progress of f_t towards g at update t. The basic technique is from [33], [34], and [32] shows how to adjust the learning rate (in a much more complicated setting than we have here). Note that (35) holds in particular for $a = \hat{a}$ so

Note that (35) holds in particular for $g = \hat{g}$, so

$$\frac{1}{m} \sum_{t=1}^{m} R_{\text{inst},\lambda}[f_t, x_t, y_t] \le R_{\text{reg},\lambda}[\hat{g}, S] + O(m^{-1/2})$$

where the constants depend on X, c and the parameters of the algorithm. However, the bound does not depend on any probabilistic assumptions. If the example sequence is such that some fixed predictor g has a small regularised risk, then the average regularised risk of the on-line algorithm will also be small.

Consider now the implications of Theorem 4 to a situation in which we assume that the examples (x_t, y_t) are i.i.d. according to some fixed distribution P. The bound on the cumulative risk can be transformed into a probabilistic bound by standard methods. We assume that $k(x, x) \leq X^2$ with probability 1 for $(x, y) \sim P$. We say that the risk is bounded by L if with probability 1 we have $R_{\text{inst},\lambda}[f, x_t, y_t] \leq L$ for all t and $f \in \{\hat{g}, f_1, \ldots, f_{m+1}\}$.

As an example, consider the soft margin loss. By the preceding remarks, we can assume $||f||_{\mathcal{H}} \leq X/\lambda$. This implies $|f(x_t)| \leq X^2/\lambda$ so the interesting values of ρ satisfy $0 \leq \rho \leq X^2/\lambda$. Hence $l_{\rho}(f(x_t), y_t) \leq 2X^2/\lambda$, and we can take $L = 5X^2/(2\lambda)$. If we wish to use an offset parameter b, a bound for |b| needs to be obtained and incorporated into L. Similarly, for regression type loss functions we may need a bound for $|y_t|$.

The result of Cesa-Bianchi et al. for bounded convex loss functions [35, Theorem 2] now directly gives the following.

Corollary 5 Assume that P is a probability distribution over $\mathcal{X} \times \mathcal{Y}$ such that $k(x, x) \leq X^2$ holds with probability 1 for $(x, y) \sim P$, and let the example sequence $S = ((x_t, y_t))_{t=1}^m$ be drawn i.i.d. according to P. Fix $\lambda > 0$ and $0 < \eta < 1/\lambda$. Assume that l is convex and satisfies (33), and that the risk is bounded by L. Let $\bar{f}_m = (1/m) \sum_{t=1}^{m-1} f_t$ where f_t is the t-th hypothesis produced by NORMA with learning rate $\eta_t = \eta t^{-1/2}$. Then for any $g \in \mathcal{H}$ and $0 < \delta < 1$, and for a and b as in Theorem 4, we have

with probability at least $1 - \delta$ over random draws of S.

To apply Corollary 5, choose $g = g_*$ where

$$g_* = \operatorname*{argmin}_{f \in \mathcal{H}} \mathrm{E}_{(x,y) \sim P} R_{\mathrm{inst},\lambda}[f, x, y].$$
(36)

With high probability, $R_{\text{reg},\lambda}[g_*, S]$ will be close to $E_{(x,y)\sim P}R_{\text{inst},\lambda}[g_*, x, y]$, so with high probability $E_{(x,y)\sim P}R_{\text{inst},\lambda}[\bar{f}_m, x, y]$ will be close to the minimum expected risk.

D. Effects of truncation

We now consider a version where at time t the hypothesis consist of a kernel expansion of size s_t , where we allow s_t to slowly (sublinearly) increase as a function of t. Thus

$$f_t(x) = \sum_{\tau=1}^{s_t} \alpha_{t-\tau,t} k(x_{t-\tau}, x)$$

where $\alpha_{t,t'}$ is the coefficient of $k(x_t, \cdot)$ in the kernel expansion at time t'. For simplicity, we assume $s_{t+1} \in \{s_t, s_t + 1\}$ and include in the expansion even the terms where $\alpha_{t,t} = 0$. Thus at any update we add a new term to the kernel expansion; if $s_{t+1} = s_t$ we also drop the oldest previously remaining term. We can then write

$$f_{t+1} = f_t - \eta_t \partial_f R_{\text{inst}}[f, x_t, y_t]|_{f=f_t} - \Delta_f$$

where $\Delta_t = 0$ if $s_{t+1} = s_t + 1$ and $\Delta_t = \alpha_{t-s_t,t}k(x_{t-s_t}, \cdot)$ otherwise. Since $\alpha_{t,t'+1} = (1 - \eta_{t'}\lambda)\alpha_{t,t'}$, we see that the kernel expansion coefficients decay almost geometrically. However, since we also need to use a decreasing learning rate $\eta_t = \eta t^{-1/2}$, the factor $1 - \eta_t \lambda$ approaches 1. Therefore it is somewhat complicated to choose expansion sizes s_t that are not large but still guarantee that the cumulative effect of the Δ_t terms remains under control.

Theorem 6 Assume that l is convex and satisfies (33). Let the example sequence $S = ((x_t, y_t))_{t=1}^m$ be such that $k(x_t, x_t) \leq X^2$ holds for all t. Fix $\lambda > 0$, $0 < \eta < 1/\lambda$ and $0 < \epsilon < 1/2$. Then there is a value $t_0(\lambda, \eta, \epsilon)$ such that the following holds when we define $s_t = t$ for $t \leq t_0(\lambda, \eta, \epsilon)$ and $s_t = \lceil t^{1/2+\epsilon} \rceil$ for $t > t_0(\lambda, \eta, \epsilon)$. Let (f_1, \ldots, f_{m+1}) be the hypothesis sequence produced by truncated NORMA with learning rate $\eta_t = \eta t^{-1/2}$ and expansion sizes s_t . Then for any $q \in \mathcal{H}$ we have

$$\sum_{t=1}^{m} R_{\text{inst},\lambda}[f_t, x_t, y_t] \le m R_{\text{reg},\lambda}[g, S] + am^{1/2} + b \quad (37)$$

where $a = 2\lambda U^2(10\eta\lambda + 1/(\eta\lambda))$, $b = U^2/(2\eta)$ and U is as in (34).

The proof, and the definition of t_0 , is given in Appendix C. Conversion of the result to a probabilistic setting can be done as previously, although an additional step is needed to estimate how the Δ_t terms may affect the maximum norm of f_t ; we omit the details.

VI. EXPERIMENTS

The mistake bounds in Section IV are of course only worstcase upper bounds, and the constants may not be very tight. Hence we performed experiments to evaluate the performance of our stochastic gradient descent algorithms in practice.

A. Classification

Our bounds suggest that some form of regularisation is useful when the target is moving, and forcing a positive margin may give an additional benefit.

This hypothesis was tested using artificial data, where we used a mixture of 2-dimensional Gaussians for the positive examples and another for negative ones. We removed all examples that would be misclassified by the Bayes-optimal classifier (which is based on the actual distribution known to us) or are close to its decision boundary. This gave us data that were cleanly separable using a Gaussian kernel.

In order to test the ability of NORMA to deal with changing underlying distributions we carried out random changes in the parameters of the Gaussians. We used two movement schedules:

- In the *drifting* case, there is a relatively small parameter change after every ten trials.
- In the *switching* case, there is a very large parameter change after every 1000 trials.

Thus, given the form of our bounds, all other things being equal, our mistake bound would be much better in the drifting than in the switching case. In either case, we ran each algorithm for 10000 trials and cumulatively summed up the mistakes made by them.

In our experiments we compared NORMA_{λ,ρ} with ALMA [9] with p = 2 and the basic Perceptron algorithm (which is the same stochastic gradient descent with the margin ρ in the loss function (13) and weight decay parameter λ both set to zero). We also considered variants NORMA_{$\lambda,0$} and ALMA₀ where the margin ρ is fixed to zero. These algorithms are included to see whether regularisation, either by weight decay as in NORMA or by a norm bound as in ALMA, helps predicting a moving target even when we are not aiming for a large margin. We used Gaussian kernels to handle the non-linearity of the data. For these experiments, the parameters of the algorithms were tuned by hand optimally for each example distribution.

Figure 2 shows the cumulative mistake counts for the algorithms. There does not seem to be any decisive differences between the algorithms.

In particular, NORMA works quite well, also on switching data, even though our bound suggests otherwise (which is probably due to slack in the bound). In general, it does seem that using a positive margin is better than fixing the margin to zero, and regularisation even with zero margin is better than the basic Perceptron algorithm.

B. Novelty Detection

In our experiments we studied the performance of the novelty detection variant of NORMA given by (20) for various kernel parameters and values of ν .

We performed experiments on the USPS database of handwritten digits (7000 scanned images of handwritten digits at a resolution of 16×16 pixels, out of which 5000 were chosen for training and 2000 for testing purposes).

Already after one pass through the database, which took in MATLAB less than 15s on a 433MHz Celeron, the results can be used for weeding out badly written digits (cf. the left plot



Fig. 2. Mistakes made by the algorithms on drifting data (top) and on switching data (bottom).

of Figure 3). We chose $\nu = 0.01$ to allow for a fixed fraction of detected "outliers." Based on the theoretical analysis of Section V we used a decreasing learning rate with $\eta_t \propto t^{-\frac{1}{2}}$.

Figure 3 shows how the algorithm improves in its assessment of unusual observations (the first digits in the left table are still quite regular but degrade rapidly). It could therefore be used as an online data filter.

VII. DISCUSSION

We have shown how the careful application of classical stochastic gradient descent can lead to novel and practical algorithms for online learning using kernels. The use of regularisation (which is essential for capacity control when using the rich hypothesis spaces generated by kernels) allows for truncation of the basis expansion and thus computationally efficient hypotheses. We explicitly developed parameterisations of our algorithm for classification, novelty detection and regression. The algorithm is the first we are aware of for online novelty detection. Furthermore, its general form is very efficient computationally and allows the easy application of kernel methods to enormous data sets, as well, of course, to real-time online problems.

We also presented a theoretical analysis of the algorithm when applied to classification problems with soft margin ρ with the goal of understanding the advantage of securing a large margin when tracking a drifting problem. On the positive side, we have obtained theoretical bounds that give some guidance to the effects of the margin in this case. On the negative side, the bounds are not that well corroborated by the experiments we performed.

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APPENDIX

A. Proofs of Theorems 2 and 3

The following technical lemma, which is proved by a simple differentiation, is used in both proofs for choosing the optimal parameters.

Lemma 7 Given K > 0, C > 0 and $\gamma > 0$ define $f(z) = K/(\gamma - z) + C/(z(\gamma - z))$ for $0 < z < \gamma$. Then f(z) is maximised for $z = h(\gamma, K, C)$ where h is as in (30), and the maximum value is

$$f(h(\gamma, K, C)) = \frac{K}{\gamma} + \frac{2C}{\gamma^2} + 2\left(\frac{K}{\gamma} + \frac{C}{\gamma^2}\right)^{1/2} \left(\frac{C}{\gamma^2}\right)^{1/2}.$$

The main idea in the proofs is to lower bound the *progress* at update t, which we define as $||g_t - f_t||^2_{\mathcal{H}} - ||g_{t+1} - f_{t+1}||^2_{\mathcal{H}}$. For notational convenience we introduce $g_{m+1} := g_m$.

Proof of Theorem 2: Define $f'_{t+1} = f_t + \eta' \sigma_t y_t k(x_t, \cdot)$. We split the progress into three parts:

$$\begin{aligned} ||g_{t} - f_{t}||_{\mathcal{H}}^{2} - ||g_{t+1} - f_{t+1}||_{\mathcal{H}}^{2} \\ &= (||g_{t} - f_{t}||_{\mathcal{H}}^{2} - ||g_{t} - f_{t+1}'||_{\mathcal{H}}^{2}) \\ &+ (||g_{t} - f_{t+1}'||_{\mathcal{H}}^{2} - ||g_{t} - f_{t+1}||_{\mathcal{H}}^{2}) \\ &+ (||g_{t} - f_{t+1}'||_{\mathcal{H}}^{2} - ||g_{t+1} - f_{t+1}||_{\mathcal{H}}^{2}). \end{aligned}$$
(38)

By substituting the definition of f'_{t+1} , using (27) and applying $\sigma_t l_\mu(g_t(x_t), y_t) \leq l_\mu(g_t(x_t), y_t)$, we can estimate the first part of (38) as

$$\begin{aligned} ||g_{t} - f_{t}||_{\mathcal{H}}^{2} - ||g_{t} - f_{t+1}'||_{\mathcal{H}}^{2} \\ &= 2\eta' \sigma_{t} y_{t} \left\langle k(x_{t}, \cdot), g_{t} - f_{t} \right\rangle_{\mathcal{H}} - ||f_{t} - f_{t+1}'||_{\mathcal{H}}^{2} \\ &= 2\eta' \sigma_{t} y_{t} (g_{t}(x_{t}) - f_{t}(x_{t})) - \eta'^{2} \sigma_{t} k(x_{t}, x_{t}) \\ &\geq 2\eta' (\sigma_{t} \mu - l_{\mu} (g_{t}(x_{t}), y_{t})) \\ &- 2\eta' (\sigma_{t} \rho - l_{\rho} (f_{t}(x_{t}), y_{t})) - \eta'^{2} \sigma_{t} X^{2}. \end{aligned}$$
(39)

For the second part of (38), we have

$$\begin{aligned} ||g_t - f'_{t+1}||_{\mathcal{H}}^2 - ||g_t - f_{t+1}||_{\mathcal{H}}^2 \\ &= ||f_{t+1} - f'_{t+1}||_{\mathcal{H}}^2 + 2\left\langle f'_{t+1} - f_{t+1}, f_{t+1} - g_t \right\rangle_{\mathcal{H}}. \end{aligned}$$

Since $f'_{t+1} - f_{t+1} = \eta \lambda f'_{t+1} = \eta \lambda f_{t+1}/(1 - \eta \lambda)$, we have

$$||f_{t+1} - f'_{t+1}||_{\mathcal{H}}^2 = \left(\frac{\eta\lambda}{1 - \eta\lambda}\right)^2 ||f_{t+1}||_{\mathcal{H}}^2$$



Fig. 3. Results of online novelty detection after one pass through the USPS database. The learning problem is to discover (online) novel patterns. We used Gaussian RBF kernels with width $2\sigma^2 = 0.5d = 128$ and $\nu = 0.01$. The learning rate was $\frac{1}{\sqrt{t}}$. Left: the first 50 patterns which incurred a margin error — it can be seen that the algorithm at first finds even well formed digits novel, but later only finds unusually written ones; *Middle:* the 50 worst patterns according to $f(x) - \rho$ on the training set — they are mostly badly written digits, *Right:* the 50 worst patterns on an unseen test set.

and

$$\left\langle f_{t+1}' - f_{t+1}, f_{t+1} - g_t \right\rangle_{\mathcal{H}} = \frac{\eta \lambda}{1 - \eta \lambda} \left(\left(||f_{t+1}||_{\mathcal{H}}^2 - \langle f_{t+1}, g_t \rangle_{\mathcal{H}} \right) \right).$$

Hence, recalling the definition of η , we get

$$\begin{aligned} ||g_{t} - f_{t+1}'||_{\mathcal{H}}^{2} - ||g_{t} - f_{t+1}||_{\mathcal{H}}^{2} \\ &= \left(2\eta'\lambda + \eta'^{2}\lambda^{2}\right)||f_{t+1}||_{\mathcal{H}}^{2} - 2\eta'\lambda \langle f_{t+1}, g_{t} \rangle_{\mathcal{H}} (40) \end{aligned}$$

For the third part of (38) we have

$$\begin{aligned} ||g_t - f_{t+1}||_{\mathcal{H}}^2 - ||g_{t+1} - f_{t+1}||_{\mathcal{H}}^2 \\ &= ||g_t||_{\mathcal{H}}^2 - ||g_{t+1}||_{\mathcal{H}}^2 + 2\langle g_{t+1} - g_t, f_{t+1}\rangle_{\mathcal{H}}. \end{aligned}$$
(41)

Substituting (39), (40) and (41) into (38) gives us

$$\begin{aligned} ||g_{t} - f_{t}||_{\mathcal{H}}^{2} - ||g_{t+1} - f_{t+1}||_{\mathcal{H}}^{2} \\ \geq & 2\eta'(\sigma_{t}\mu - l_{\mu}(g_{t}(x_{t}), y_{t})) \\ & - 2\eta'(\sigma_{t}\rho - l_{\rho}(f_{t}(x_{t}), y_{t})) \\ & - \eta'^{2}\sigma_{t}X^{2} \\ & + ||g_{t}||_{\mathcal{H}}^{2} - ||g_{t+1}||_{\mathcal{H}}^{2} + H[f_{t+1}] \end{aligned}$$
(42)

where

$$H[f] = (2\eta'\lambda + \eta'^2\lambda^2) ||f||_{\mathcal{H}}^2 - 2\eta'\lambda \langle f, g_t \rangle_{\mathcal{H}} + 2 \langle g_{t+1} - g_t, f \rangle_{\mathcal{H}}.$$

To bound $H[f_{t+1}]$ from below, we write

$$H[f] = a||f||_{\mathcal{H}}^2 - 2\langle r, f \rangle_{\mathcal{H}} = a||f - r/a||_{\mathcal{H}}^2 - ||r||_{\mathcal{H}}^2/a$$

where $a = 2\eta'\lambda + \eta'^2\lambda^2$ and $r = (1 + \eta'\lambda)g_t - g_{t+1}$. Hence,

$$H[f_{t+1}] \geq -||r||_{\mathcal{H}}^{2}/a \\\geq -\frac{1}{2\eta'\lambda + \eta'^{2}\lambda^{2}} \left(||g_{t} - g_{t+1}||_{\mathcal{H}} + \eta'\lambda||g_{t}||_{\mathcal{H}}\right)^{2} \\= -\frac{1}{2 + \eta'\lambda} \left(\frac{||g_{t} - g_{t+1}||_{\mathcal{H}}^{2}}{\eta'\lambda} + 2||g_{t} - g_{t+1}||_{\mathcal{H}}||g_{t}||_{\mathcal{H}} + \eta'\lambda||g_{t}||_{\mathcal{H}}^{2}\right) (43)$$

Since $-1/(2 + \eta' \lambda) > -1/2$, (42) and (43) give

$$\begin{aligned} ||g_{t} - f_{t}||_{\mathcal{H}}^{2} - ||g_{t+1} - f_{t+1}||_{\mathcal{H}}^{2} \\ \geq & -2\eta'(\sigma_{t}\rho - l_{\rho}(f_{t}(x_{t}), y_{t})) \\ & + 2\eta'(\sigma_{t}\mu - l_{\mu}(g_{t}(x_{t}), y_{t})) \\ & - \eta'^{2}\sigma_{t}X^{2} + ||g_{t}||_{\mathcal{H}}^{2} - ||g_{t+1}||_{\mathcal{H}}^{2} \\ & - \frac{1}{2} \left(\frac{||g_{t+1} - g_{t}||_{\mathcal{H}}^{2}}{\eta'\lambda} \\ & + 2||g_{t}||_{\mathcal{H}}||g_{t+1} - g_{t}||_{\mathcal{H}} + \eta'\lambda||g_{t}||_{\mathcal{H}}^{2} \right). (44) \end{aligned}$$

By summing (44) over t = 1, ..., m and using the assumption that $\mathbf{g} \in \mathcal{G}(B, D_1, D_2)$ we obtain

$$||g_{1} - f_{1}||_{\mathcal{H}}^{2} - ||g_{m+1} - f_{m+1}||_{\mathcal{H}}^{2} \\ \geq 2\eta' L_{\operatorname{cum},\rho}[\mathbf{f}, S] - 2\eta' L_{\operatorname{cum},\mu}[\mathbf{g}, S] \\ + \eta' M_{\rho}(\mathbf{f}, S) \left(2\mu - 2\rho - \eta' X^{2}\right) \\ + ||g_{1}||_{\mathcal{H}}^{2} - ||g_{m+1}||_{\mathcal{H}}^{2} \\ - \frac{1}{2} \left(\frac{D_{2}}{\eta' \lambda} + 2BD_{1} + m\eta' \lambda B^{2}\right).$$
(45)

Now λ appears only in (45) as a subexpression $Q(\eta'\lambda)$ where $Q(z) = -\frac{D_2}{z} - zmB^2$. Since the function Q(z) is maximised for $z = \sqrt{D_2/(mB^2)}$, we choose λ as in (32) which gives $Q(\eta'\lambda) = -2B\sqrt{mD_2}$. We assume $f_1 = 0$, so $||g_1 - f_1||_{\mathcal{H}}^2 - ||g_{m+1} - f_{m+1}||_{\mathcal{H}}^2 \leq ||g_1||_{\mathcal{H}}^2$. By moving some terms around and estimating $||g_{m+1}||_{\mathcal{H}} \leq B$ and $L_{\text{cum},\mu}[\mathbf{g}, S] \leq K$ we get

$$L_{\text{cum},\rho}[\mathbf{f}, S] + M_{\rho}(\mathbf{f}, S) \left(\mu - \rho - \eta' X^{2}/2\right) \\ \leq K + \frac{B^{2} + B(\sqrt{mD_{2}} + D_{1})}{2\eta'}.$$
(46)

To get a bound for margin errors, notice that the value η' given in the theorem satisfies $\mu - \rho - \eta' X^2 > 0$. We make the trivial estimate $L_{\text{cum},\rho}[\mathbf{f}, S] \ge 0$, which gives us

$$M_{\rho}(\mathbf{f}, S) \leq \frac{K}{\mu - \rho - \eta' X^{2}/2} \\ + \frac{B^{2} + B(\sqrt{mD_{2}} + D_{1})}{2\eta'(\mu - \rho - \eta' X^{2}/2)}$$

The bound follows by applying Lemma 7 with $\gamma = \mu - \rho$ and $z = \eta' X^2/2$.

Proof of Theorem 3: The claim for $\rho = 0$ follows directly from Theorem 2. For non-zero ρ , we take (46) as our starting point. We choose $\eta' = 2(\mu - \rho)/X^2$, so the term with $M_{\rho}(\mathbf{f}, S)$ vanishes and we get

$$L_{\operatorname{cum},\rho}[\mathbf{f},S] \le K + \frac{X^2(B^2 + B(\sqrt{mD_2} + D_1))}{4(\mu - \rho)}.$$
 (47)

Since $L_{\operatorname{cum},\rho}[\mathbf{f},S] \ge \rho \mathcal{M}(\mathbf{f},S)$, this implies

$$M(\mathbf{f}, S) \le \frac{K}{\rho} + \frac{X^2 (B^2 + B(\sqrt{mD_2} + D_1))}{4\rho(\mu - \rho)}.$$
 (48)

The claim follows from Lemma 7 with $\gamma = \mu$ and $z = \mu - \rho$.

B. Proof of Theorem 4

Without loss of generality we can assume $g = \hat{g}$, and in t/4, we have $\eta_r \leq 2\eta_t$, so particular $||g||_{\mathcal{H}} \leq U$. First notice that

$$\begin{aligned} ||f_{t} - g||_{\mathcal{H}}^{2} - ||f_{t+1} - g||_{\mathcal{H}}^{2} \\ &= -||f_{t+1} - f_{t}||_{\mathcal{H}}^{2} - 2\langle f_{t+1} - f_{t}, f_{t} - g \rangle_{\mathcal{H}} \\ &= -\eta_{t}^{2} ||\partial_{f} R_{\text{inst}}[f, x_{t}, y_{t}]|_{f=f_{t}} ||_{\mathcal{H}} \\ &+ 2\eta_{t} \langle \partial_{f} R_{\text{inst}}[f, x_{t}, y_{t}]|_{f=f_{t}}, f_{t} - g \rangle_{\mathcal{H}} \\ &\geq -4\eta_{t}^{2} c^{2} X^{2} \\ &- 2\eta_{t} (R_{\text{inst}}[g, x_{t}, y_{t}] - R_{\text{inst}}[f_{t}, x_{t}, y_{t}]) \end{aligned}$$
(49)

where we used the Lipschitz property of l and the convexity of R_{inst} in its first argument. This leads to

$$\begin{aligned} \frac{1}{\eta_t} ||f_t - g||_{\mathcal{H}}^2 &- \frac{1}{\eta_{t+1}} ||f_{t+1} - g||_{\mathcal{H}}^2 \\ &= \frac{1}{\eta_t} \left(||f_t - g||_{\mathcal{H}}^2 - ||f_{t+1} - g||_{\mathcal{H}}^2 \right) \\ &+ \left(\frac{1}{\eta_t} - \frac{1}{\eta_{t+1}} \right) ||f_{t+1} - g||_{\mathcal{H}}^2 \\ &\ge -4\eta_t c^2 X^2 - 2R_{\text{inst}}[g, x_t, y_t] + 2R_{\text{inst}}[f_t, x_t, y_t] \\ &+ 4U^2 \left(\frac{1}{\eta_t} - \frac{1}{\eta_{t+1}} \right) \end{aligned}$$

since $||f_{t+1} - g||_{\mathcal{H}} \leq 2U$. By summing over $t = 1, \ldots, m + d$ 1, and noticing that some terms telescope and $\sum_{t=1}^{m} \eta_t \leq$ $2\eta m^{1/2}$, we get

$$\frac{||f_1 - g||_{\mathcal{H}}^2}{\eta} - \frac{||f_{m+1} - g||_{\mathcal{H}}^2}{\eta_{m+1}}$$

$$\geq -8\eta c^2 X^2 m^{1/2} - 2\sum_{t=1}^m R_{\text{inst}}[g, x_t, y_t]$$

$$+ 2\sum_{t=1}^m R_{\text{inst}}[f_t, x_t, y_t] + 4U^2 \left(\frac{1}{\eta} - \frac{(m+1)^{1/2}}{\eta}\right)$$

The claim now follows by rearranging terms and estimating $||f_1-g||_{\mathcal{H}} \leq U, ||f_{m+1}-g||_{\mathcal{H}}^2 \geq 0 \text{ and } (m+1)^{1/2} - 1 \leq m^{1/2}.$

C. Proof of Theorem 6

First, let us define $t_0(\lambda, \eta, \epsilon)$ to be the smallest possible such that the following hold for all $t \ge t_0(\lambda, \eta, \epsilon)$:

- $\eta \lambda t^{-1/2} \le 1$,
- $\exp(-\eta\lambda t^{\epsilon}) \leq \eta\lambda t^{-1/2}$ and $\lceil t^{1/2+\epsilon} \rceil \leq 3t/4.$

We use this to estimate $||\Delta_t||_{\mathcal{H}}$. If $s_{t+1} = t+1$, then clearly $\Delta_t = 0$, so we consider the case $t \ge t_0(\lambda, \eta, \epsilon)$. Let $r = t - s_t$, so $||\Delta_t||_{\mathcal{H}} \leq X|\alpha_{r,t}|$. We have $|\alpha_{r,r}| \leq \eta_r c$, and $|\alpha_{r,r+\tau+1}| =$ $(1-\eta_{r+\tau}\lambda)|\alpha_{r,r+\tau}| \leq (1-\eta_t\lambda)|\alpha_{r,r+\tau}|$ for $\tau = 0,\ldots,s_t-1$. Hence

$$|\alpha_{r,t}| \leq \eta_r c (1 - \eta_t \lambda)^{s_t} \leq \eta_r c \left(\left(1 - \frac{\eta \lambda}{t^{1/2}} \right)^{t^{1/2}} \right)^{t^*}.$$

Since $\eta \lambda / t^{1/2} \leq 1$, we have

$$\left(1 - \frac{\eta\lambda}{t^{1/2}}\right)^{\frac{t^{1/2}}{\eta\lambda}} \le \exp(-1),$$

so $|\alpha_{r,t}| \leq \eta_r c \exp(-\eta \lambda t^{\epsilon}) \leq \eta_r c \eta \lambda t^{-1/2}$. Finally, since $r \geq$

$$||\Delta_t||_{\mathcal{H}} \le 2\eta_t^2 \lambda c X.$$

In particular, we have $||\Delta_t||_{\mathcal{H}} \leq 2\eta_t c X$, so

$$\begin{aligned} ||f_{t+1}||_{\mathcal{H}} &\leq (1 - \eta_t \lambda) ||f_t||_{\mathcal{H}} \\ &+ \eta_t |l'(f_t(x_t, y))||k(x_t, \cdot)||_{\mathcal{H}} + ||\Delta_t||_{\mathcal{H}} \\ &\leq (1 - \eta_t \lambda) ||f_t||_{\mathcal{H}} + 3\eta_t c X. \end{aligned}$$

Since $f_1 = 0$, we get $||f_t||_{\mathcal{H}} \leq 3cX/\lambda$. Again, without loss of generality we can assume $g = \hat{g}$ and thus in particular $||f_t - g||_{\mathcal{H}} \le 4cX/\lambda.$

To estimate the progress at trial t, let $\tilde{f}_{t+1} = f_{t+1} + \Delta_t$ be the new hypothesis before truncation. We write

$$\begin{aligned} ||f_t - g||_{\mathcal{H}}^2 - ||f_{t+1} - g||_{\mathcal{H}}^2 \\ &= ||f_t - g||_{\mathcal{H}}^2 - ||\tilde{f}_{t+1} - g||_{\mathcal{H}}^2 \\ &+ ||\tilde{f}_{t+1} - g||_{\mathcal{H}}^2 - ||f_{t+1} - g||_{\mathcal{H}}^2. \end{aligned}$$
(50)

To estimate (51) we write

$$\begin{aligned} |f_{t+1} - g||_{\mathcal{H}}^2 &- ||f_{t+1} - g||_{\mathcal{H}}^2 \\ &= ||(\tilde{f}_{t+1} - f_{t+1}) + (f_{t+1} - g)||_{\mathcal{H}}^2 - ||f_{t+1} - g||_{\mathcal{H}}^2 \\ &= 2 \langle \Delta_t, f_{t+1} - g \rangle_{\mathcal{H}} + ||\Delta_t||_{\mathcal{H}}^2 \\ &\geq -2||\Delta_t||_{\mathcal{H}}||f_{t+1} - g||_{\mathcal{H}} \\ &\geq -16\eta_t^2 c^2 X^2. \end{aligned}$$

By combining this with the estimate (49) for (50) we get

$$||f_t - g||_{\mathcal{H}}^2 - ||f_{t+1} - g||_{\mathcal{H}}^2$$

$$\geq -20\eta_t^2 c^2 X^2 - 2\eta_t (R_{\text{inst}}[g, x_t, y_t] - R_{\text{inst}}[f_t, x_t, y_t]);$$

notice the similarity to (49). The rest follows as in the proof of Theorem 4.

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