Accepted for NIPS'99

SV Estimation of a Distribution's Support

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Abstract

Suppose you are given some dataset drawn from an underlying probability distribution P and you want to estimate a subset S of input space such that the probability that a test point drawn from P lies outside of S is bounded by some a priori specified $0 < \nu \leq 1$.

We propose an algorithm which approaches this problem by trying to estimate a function f which is positive on S and negative on the complement. The functional form of f is given by a kernel expansion in terms of a potentially small subset of the training data; it is regularized by controlling the length of the weight vector in an associated feature space.

The algorithm is a natural extension of the support vector algorithm to the case of unlabelled data.

1 INTRODUCTION

During recent years, a new set of kernel techniques for supervised learning has been developed [13]. Specifically, support vector (SV) algorithms for pattern recognition, regression estimation and solution of inverse problems have received considerable attention.

There have been a few attempts to transfer the idea of using kernels to compute inner products in feature spaces to the domain of unsupervised learning. The problems in that domain are, however, less precisely specified. Generally, they can be characterized as estimating *functions* of the data which tell you something interesting about the underlying distributions. For instance, kernel PCA can be characterized as computing functions which on the training data produce unit variance outputs while having minimum norm in feature space [7]. Another kernel-based unsupervised learning technique, regularized principal manifolds [11], computes functions which give a mapping onto a lower-dimensional manifold minimizing a regularized quantization error. Clustering algorithms are further examples of unsupervised learning techniques which can be kernelized [7]. An extreme point of view is that unsupervised learning is about estimating densities. Clearly, knowledge of the density of P would then allow us to solve whatever problem can be solved on the basis of the data.

The present paper addresses an easier problem: it proposes an algorithm which computes a binary function which is supposed to capture regions in input space where the probability density lives (its support), i.e. a function such that most of the data will live in the region where the function is nonzero. In doing so, it is in line with Vapnik's principle never to solve a problem which is more general than the one we actually need to solve. Moreover, it is applicable also in cases where the density of the data's distribution is not well-defined, e.g. if there are singular components.

Part of the motivation for the present work was the paper of Ben-David and Lindenbaum [1]. It turns out that there is a considerable amount of prior work in the statistical literature, but in this short version of the paper we can not fit in the details.[1] See [5] for a brief overview, and the full version of the present paper for more.

2 ALGORITHMS

We first introduce terminology and notation conventions. We consider training data $\mathbf{x}_1, \ldots, \mathbf{x}_\ell \in \mathcal{X}$, where $\ell \in \mathbb{N}$ is the number of observations, and $\mathcal{X}$ is some set. In this paper, we assume it to be a compact subset of $\mathbb{R}^N$. Let Φ be a feature map $\mathcal{X} \to F$, i.e. a map into a dot product space F such that the dot product in the image of Φ can be computed by evaluating some simple kernel [13]

$$k(\mathbf{x}, \mathbf{y}) = (\Phi(\mathbf{x}) \cdot \Phi(\mathbf{y})), \tag{1}$$

such as the Gaussian kernel

$$k(\mathbf{x}, \mathbf{y}) = e^{-\|\mathbf{x}-\mathbf{y}\|^2/c}. \tag{2}$$

Indices i and j are understood to range over $1, \ldots, \ell$ (in compact notation: $i, j \in [\ell]$). Bold face greek letters denote ℓ-dimensional vectors comprising the corresponding letters typeset in normal face.

To separate the data set from the origin, we solve the following quadratic program:

$$\begin{aligned} \min_{\mathbf{w} \in F, \boldsymbol{\xi} \in \mathbb{R}^\ell, \rho \in \mathbb{R}} \quad & \tfrac{1}{2}\|\mathbf{w}\|^2 + \tfrac{1}{\nu\ell}\textstyle\sum_i \xi_i - \rho \\ \text{subject to} \quad & (\mathbf{w} \cdot \Phi(\mathbf{x}_i)) \geq \rho - \xi_i, \;\; \xi_i \geq 0. \end{aligned} \tag{3}$$

Here, $\nu \in (0, 1]$ is a parameter whose meaning will become clear later. Since nonzero slack variables ξ_i are penalized in the objective function, we can expect that if $\mathbf{w}$ and ρ solve this problem, then the decision function

$$f(\mathbf{x}) = \mathrm{sgn}((\mathbf{w} \cdot \Phi(\mathbf{x})) - \rho) \tag{4}$$

will be positive for most examples $\mathbf{x}_i$ contained in the training set, while the SV type regularization term $\|\mathbf{w}\|$ will still be small. The actual trade-off between these two goals is controlled by ν. Using multipliers $\alpha_i, \beta_i \geq 0$, we introduce a Lagrangian $L(\mathbf{w}, \boldsymbol{\xi}, \rho, \boldsymbol{\alpha}, \boldsymbol{\beta}) = \frac{1}{2}\|\mathbf{w}\|^2 + \frac{1}{\nu\ell}\sum_i \xi_i - \rho - \sum_i \alpha_i((\mathbf{w} \cdot \Phi(\mathbf{x}_i)) - \rho + \xi_i) - \sum_i \beta_i \xi_i$, and set the derivatives by the primal variables $\mathbf{w}, \boldsymbol{\xi}, \rho$ equal to zero, yielding

$$\mathbf{w} = \sum_i \alpha_i \Phi(\mathbf{x}_i), \tag{5}$$

$$\alpha_i = \frac{1}{\nu\ell} - \beta_i \leq \frac{1}{\nu\ell}, \quad \sum_i \alpha_i = 1. \tag{6}$$

In (5), all patterns with $\alpha_i > 0$ are called Support Vectors. Together with (1), the SV expansion transforms the decision function (4) into a kernel expansion $f(\mathbf{x}) = \mathrm{sgn}\left(\sum_i \alpha_i k(\mathbf{x}_i, \mathbf{x}) - \rho\right)$. Substituting (5) - (6) into L, and using (1), we obtain the dual problem:

$$\min_{\boldsymbol{\alpha}} \frac{1}{2} \sum_{ij} \alpha_i \alpha_j k(\mathbf{x}_i, \mathbf{x}_j) \quad \text{subject to} \;\; 0 \leq \alpha_i \leq \frac{1}{\nu\ell}, \;\; \sum_i \alpha_i = 1. \tag{7}$$

[1] An extended version will soon be made available on http://svm.first.gmd.de.

One can show that at the optimum, the two inequality constraints (3) become equalities if α_i and β_i are nonzero, i.e. if $0 < \alpha_i < 1/\ell$. Therefore, we can recover ρ by exploiting that for any such α_i, the corresponding pattern $\mathbf{x}_i$ satisfies

$$\rho = (\mathbf{w} \cdot \mathbf{x}_i) = \sum_j \alpha_j k(\mathbf{x}_j, \mathbf{x}_i). \tag{8}$$

To conclude this section, we note that one can also use *balls* to describe the data in feature space, close in spirit to algorithms used in [6, 12]. Again, we try to put "most of" the data into a small ball by solving, for $\nu \in (0, 1]$,

$$\begin{aligned} \min_{R \in \mathbb{R}, \boldsymbol{\xi} \in \mathbb{R}^\ell, c \in F} \quad & \nu \cdot R^2 + \tfrac{1}{\ell} \textstyle\sum_i \xi_i \\ \text{subject to} \quad & \|\Phi(\mathbf{x}_i) - c\|^2 \leq R^2 + \xi_i, \;\; \xi_i \geq 0 \quad \text{for } i \in [\ell]. \end{aligned} \tag{9}$$

This leads to the dual

$$\min_{\boldsymbol{\alpha}} \quad \textstyle\sum_{ij} \alpha_i \alpha_j k(\mathbf{x}_i, \mathbf{x}_j) - \nu \sum_i \alpha_i k(\mathbf{x}_i, \mathbf{x}_i) \tag{10}$$

$$\text{subject to} \quad 0 \leq \alpha_i \leq \tfrac{1}{\ell}, \;\; \textstyle\sum_i \alpha_i = \nu. \tag{11}$$

For kernels $k(\mathbf{x}, \mathbf{y})$ which only depend on $\mathbf{x} - \mathbf{y}$, $k(\mathbf{x}, \mathbf{x})$ is constant. In this case, the equality constraint implies that the linear term in the dual target function is constant, and the problem (10–11) turns out to be equivalent to (7).

3 THEORY

In this section, we analyse the algorithm theoretically, starting with the uniqueness of the hyperplane (Proposition 2). We then describe the connection to pattern recognition (Proposition 3), and show that the parameter ν characterizes the fractions of SVs and outliers (Proposition 4). Following that, we give a robustness result for the soft margin (Proposition 5) and finally we briefly state error bounds (Theorem 9). (In this short version, most proofs are omitted.)

Definition 1 *A data set*

$$\Phi(\mathbf{x}_1), \ldots, \Phi(\mathbf{x}_\ell) \tag{12}$$

is called separable if there exists some $\mathbf{w} \in F$ *such that* $(\mathbf{w} \cdot \Phi(\mathbf{x}_i)) > 0$ *for* $i \in [\ell]$.

Proposition 2 *If the data set (12) is separable, then there exists a unique* supporting hyperplane *with the properties that (1) it is closer to the origin than all data, and (2) its distance to the origin is maximal among all such hyperplanes. For any* $\rho > 0$*, it is given by* $\min_{\mathbf{w} \in F} \frac{1}{2}\|\mathbf{w}\|^2$ *subject to* $(\mathbf{w} \cdot \Phi(\mathbf{x}_i)) \geq \rho$.

Proposition 3 *(i) Suppose* $(\mathbf{w}, \rho)$ *parametrizes the supporting hyperplane for the data (12). Then* $(\mathbf{w}, 0)$ *parametrizes the optimal separating hyperplane (passing through the origin [13]) for the labelled data set* $\{(\Phi(\mathbf{x}_1), 1), \ldots, (\Phi(\mathbf{x}_\ell), 1), (-\Phi(\mathbf{x}_1), -1), \ldots, (-\Phi(\mathbf{x}_\ell), -1)\}$.
(ii) Suppose $(\mathbf{w}, 0)$ *parametrizes the optimal separating hyperplane passing through the origin for a labelled data set* $\{(\Phi(\mathbf{x}_1), y_1), \ldots, (\Phi(\mathbf{x}_\ell), y_\ell)\}$, $(y_i \in \{\pm 1\}$ *for* $i \in [\ell])$. *Suppose, moreover, that* $\mathbf{w}$ *is aligned such that* $(\mathbf{w} \cdot \Phi(\mathbf{x}_i))$ *is positive whenever* $y_i = 1$, *and that* $\rho / \|\mathbf{w}\|$ *is the margin of the optimal hyperplane. Then* $(\mathbf{w}, \rho)$ *parametrizes the supporting hyperplane for the unlabelled data set* $\{y_1 \Phi(\mathbf{x}_1), \ldots, y_\ell \Phi(\mathbf{x}_\ell)\}$.

Note that this relationship holds true also if we consider nonseparable problems. In that case, *margin errors* in binary classification (i.e. points which are either on the wrong side of the separating hyperplane or which fall inside the margin) translate into *outliers* in single-class classification, i.e. into points which fall on the wrong side of the hyperplane. Proposition 3 then holds, cum grano salis, for the training sets with margin errors and outliers, respectively, removed. The utility of Proposition 3 lies in the fact that it allows us to recycle certain results proven for binary classification [8] for use in the single-class scenario. The following, explaining the significance of the parameter ν, is such a case.

Proposition 4 *Assume the solution of (3) satisfies $\rho \neq 0$. The following statements hold:*
(i) ν is an upper bound on the fraction of outliers.
(ii) ν is a lower bound on the fraction of SVs.
(iii) Suppose the data (12) were generated independently from a distribution $P(\mathbf{x})$ which does not contain discrete components. Suppose, moreover, that the kernel is analytic and non-constant. With probability 1, asymptotically, ν equals both the fraction of SVs and the fraction of outliers.

Parts (i) and (ii) follow directly from Proposition 3 and the fact that outliers are dealt with in exactly the same way as margin errors in the optimization problem for the binary classification case [8]. (A direct proof would simply exploit the constraints that (6) imposes on the fraction of patterns that can have $\alpha_i = 1/\ell$, upper bounding the fraction of outliers, and on the fraction of patterns that must have $\alpha_i > 0$, the SVs.) Part (iii) can be proven by a uniform convergence argument showing that since the covering numbers of kernel expansions regularized by a norm in some feature space are well-behaved, the fraction of points which lie exactly on the hyperplane is asymptotically negligible [cf. 8].

Proposition 5 *Local movements of outliers parallel to $\mathbf{w}$ do not change the hyperplane.*

Proof Suppose $\mathbf{z}_o := \Phi(\mathbf{x}_o)$ is an outlier, i.e. $\xi_o > 0$, hence by the KKT conditions [e.g. 2] $\alpha_o = 1/\ell$. Transforming it into $\mathbf{z}'_o := \mathbf{z}_o + \delta \cdot \mathbf{w}$, where $|\delta| < \xi_o/\|\mathbf{w}\|$, leads to a slack which is still nonzero, i.e. $\xi'_o > 0$, hence we still have $\alpha_o = 1/\ell$. Therefore, $\boldsymbol{\alpha}' = \boldsymbol{\alpha}$ is still feasible, as is the primal solution $(\mathbf{w}', \boldsymbol{\xi}', \rho')$. Here, we use $\xi'_i = \xi_i$ for $i \neq o$, $\mathbf{w}' = \mathbf{w} + \delta \cdot \alpha_o \mathbf{w}$, and ρ' as computed from (8). Finally, the KKT conditions are still satisfied, as still $\alpha'_o = 1/\ell$. Thus [2, e.g.], $\boldsymbol{\alpha}$ is still the optimal solution. ∎

We now move on to the subject of generalization. Our goal is to bound the probability that a novel point drawn from the same underlying distribution lies outside of the estimated region by a certain margin. We start by introducing a common tool for measuring the capacity of a class $\mathcal{F}$ of functions that map $\mathcal{X}$ to $\mathbb{R}$.

Definition 6 *Let (X, d) be a pseudo-metric space, let A be a subset of X and $\epsilon > 0$. A set $B \subseteq X$ is an* ϵ-cover *for A if, for every $a \in A$, there exists $b \in B$ such that $d(a, b) \leq \epsilon$. The* ϵ-covering number *of A, $\mathcal{N}_d(\epsilon, A)$, is the minimal cardinality of an ϵ-cover for A (if there is no such finite cover then it is defined to be ∞). The cover is called proper if $B \subseteq A$.*

The idea is that B should be finite but approximate all of A with respect to the pseudometric d. We will use the l^∞ distance over a finite sample $\mathbf{X} = (\mathbf{x}_1, \ldots, \mathbf{x}_\ell)$ for the pseudo-metric in the space of functions, $d_{\mathbf{X}}(f, g) = \max_{i \in [\ell]} |f(\mathbf{x}_i) - g(\mathbf{x}_i)|$. Let $\mathcal{N}(\epsilon, \mathcal{F}, \ell) = \max_{\mathbf{X} \in \mathcal{X}^\ell} \mathcal{N}_{d_{\mathbf{X}}}(\epsilon, \mathcal{F})$. Below, logarithms are to base 2.

Theorem 7 *Consider any distribution P on $\mathcal{X}$ and any $\theta \in \mathbb{R}$. Suppose $\mathbf{x}_1, \ldots, \mathbf{x}_\ell$ are generated i.i.d. from P. Then with probability $1 - \delta$ over such an ℓ-sample, if we find $f \in \mathcal{F}$ such that $f(\mathbf{x}_i) \geq \theta + \gamma$ for all $i \in [\ell]$*

$$P\{\mathbf{x} : f(\mathbf{x}) < \theta - \gamma\} \leq \tfrac{2}{\ell}(k + \log \tfrac{2\ell}{\delta}),$$

where $k = \lceil \log \mathcal{N}(\gamma, \mathcal{F}, 2\ell) \rceil$.

The basis of the proof is [9, Lemma 3.9].

We now consider the possibility that for a small number of points $f(\mathbf{x}_i)$ fails to exceed $\theta + \gamma$. This corresponds to having a non-zero slack variable ξ_i in the algorithm, where we take $\theta + \gamma = \rho/\|\mathbf{w}\|$ and use the class of linear functions in feature space in the application of the theorem. There are well-known bounds for the log covering numbers of this class. We first introduce notation for the size of the shortfall in $f(\mathbf{x})$.

Definition 8 *Let f be a real valued function on a space $\mathcal{X}$. Fix $\theta \in \mathbb{R}$. For $\mathbf{x} \in \mathcal{X}$ we denote by $d(\mathbf{x}, f, \gamma)$ the quantity $d(\mathbf{x}, f, \gamma) = \max\{0, \theta + \gamma - f(\mathbf{x})\}$. Similarly for a training sequence $\mathbf{X}$, we define $D(\mathbf{X}, f, \gamma) = \sqrt{\sum_{\mathbf{x} \in \mathbf{X}} d(\mathbf{x}, f, \gamma)^2}$.*

Theorem 9 *Fix $\theta \in \mathbb{R}$. Consider a fixed but unknown probability distribution P on the input space $\mathcal{X}$ and a class of real valued functions $\mathcal{F}$ with range $[a, b]$. Then with probability $1 - \delta$ over randomly drawn training sequences $\mathbf{X}$ of size ℓ, for all $\gamma > 0$ and any $f \in \mathcal{F}$,*

$$P\left\{\mathbf{x}\colon f(\mathbf{x}) < \theta - \gamma \text{ and } \mathbf{x} \notin \mathbf{X}\right\} \le \tfrac{2}{\ell}\left(k + \log \tfrac{4\ell}{\delta}\right),$$

where $k = \left\lceil \log \mathcal{N}(\gamma/2, \mathcal{F}, 2\ell) + \frac{64 D(\mathbf{X}, f, \gamma)^2}{\gamma^2} \log\left(\frac{e\ell(b-a)\gamma}{8D(\mathbf{X}, f, \gamma)^2}\right) \log\left(\frac{32\ell(b-a)^2}{\gamma^2}\right) \right\rceil$.

The proof is based on similar proofs for the classification case in [10, Theorem 3]. The theorem bounds the probability of a new training point falling in the region for which $f(\mathbf{x})$ has value less than $\theta - \gamma$, this being the complement of the estimate for the support of the distribution. In the algorithm described in this paper, one would use the hyperplane shifted by 2γ towards the origin to define the region. Note that there is no restriction placed on the class of functions though these functions could be probability density functions.

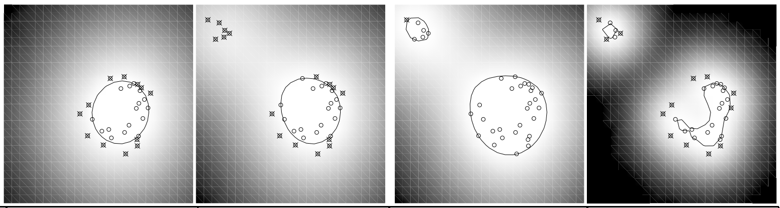
The choice of γ gives a trade-off between the size of the region over which the bound holds (increasing γ increases the size of the region) and the size of the probability ϵ (increasing γ decreases the size of the log covering numbers).

The result shows that we can bound the probability of points falling outside the region of estimated support by a quantity involving the ratio of the log covering numbers (which can be bounded by the fat shattering dimension at scale proportional to γ) and the number of training examples, plus a factor involving the 2-norm of the slack variables. A similar bound can also be made in terms of the 1-norm of the slack variables, which is the form which appears in the optimization performed by the algorithm.

The result is significantly stronger than related results given in Ben-David and Lindenbaum [1], since their bound involves the square root of the ratio of the Pollard dimension (the fat shattering dimension when γ tends to 0) and the number of training examples.

4 EXPERIMENTS AND DISCUSSION

We briefly illustrate the approach on artificial and real-world data. Figure 1 displays 2-D toy examples, and shows how the parameter settings influence the solution. Figure 2 shows a plot of the outputs $(\mathbf{w} \cdot \Phi(\mathbf{x}))$ on training and test set of the US postal service database of handwritten digits. The database contains 9298 digit images of size 16×16, 2007 of which are used as a test set. We fed our algorithm, using a Gaussian kernel of width 0.5 (a typical value for SVMs, cf. [6]), with the training instances of digit 0 only. Testing was done on both digit 0 and on all other digits. As shown in figure 2, $\nu = 0.5$ leads to *zero* false positives (i.e. even though the learning machines has not seen any non-0s during training, it correctly identifies all non-0s as such), while still recognizing 44% of the digits 0 in the test set. Higher recognition rates can be achieved using smaller values of ν: for 0.05, we get 91% correct recognition of digits 0 in the test set, while the false positive rate is still fairly moderate at 7%. While these first results are necessarily incomplete, they still convey an idea of the potential utility of the proposed algorithm.



ν, width c	0.5, 0.5	0.5, 0.5	0.1, 0.5	0.5, 0.1
frac. SVs/OLs	0.54, 0.43	0.59, 0.47	0.24, 0.03	0.65, 0.38
margin $\rho/\|\|\mathbf{w}\|\|$	0.84	0.70	0.62	0.48

Figure 1: *First two pictures:* A single-class SVM applied to two toy problems; $\nu = c = 0.5$, domain: $[-1, 1]^2$. Note how in both cases, at least a fraction of ν of all examples is in the estimated region (cf. table). The large value of ν causes the additional data points in the upper left corner to have almost no influence on the decision function. For smaller values of ν, such as 0.1 *(third picture)*, the points cannot be ignored anymore. Alternatively, one can force the algorithm to take these 'outliers' into account by changing the kernel width (2): in the *fourth picture*, using $c = 0.1, \nu = 0.5$, the data is effectively analyzed on a different length scale which leads the algorithm to consider the outliers as meaningful points.

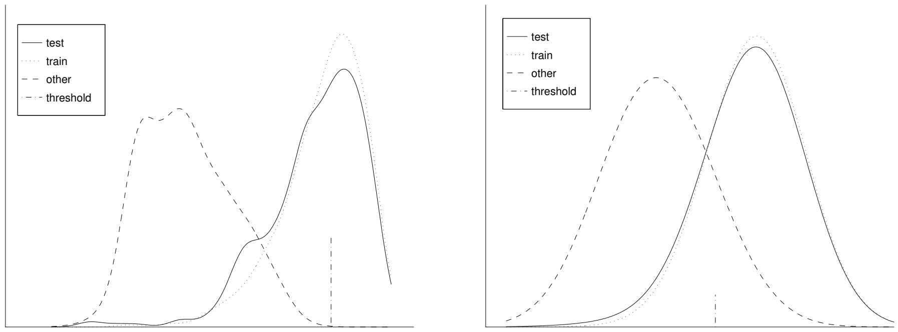


Figure 2: Experiments on the US postal service OCR dataset. Recognizer for digit 0; output histogram for the exemplars of 0 in the training/test set, and on test exemplars of other digits. For $\nu = 50\%$ *(left)*, we get 50% SVs and 49% outliers (consistent with Proposition 4); for $\nu = 5\%$ *(right)*, we get 6% and 4%, respectively. The threshold ρ is marked in the graphs.

The main inspiration for our approach stems from the earliest work of Vapnik and collaborators [15, 14]. In the sixties, they proposed an algorithm for characterizing a set of unlabelled data points by separating it from the origin using a hyperplane. However, they quickly moved on to two-class classification problems, both in terms of algorithms and in terms of the theoretical development of statistical learning theory which originated in those days.

From an algorithmic point of view, we can identify two weaknesses of the original approach which may have caused research in this direction to stop for more than three decades. Firstly, the original algorithm in [14] was limited to linear decision rules in input space, secondly, there was no way of dealing with outliers. In conjunction, these restrictions are indeed severe — a generic dataset need not be separable from the origin by a hyperplane.

The two modifications that we have incorporated dispose of these shortcomings. First, the kernel trick allows for a much larger class of functions by nonlinearly mapping into a high-dimensional feature space, and thereby increases the chances of a separation from the origin being possible. In particular, using a Gaussian kernel (2), such a separation always exists: to see this, note that $k > 0$, thus all dot products between mapped patterns are positive, implying that all patterns lie inside the same orthant. Moreover, since $k(\mathbf{x}, \mathbf{x}) = 1$ for all $\mathbf{x}$, they all have unit length. Hence they are separable. The second modification directly allows for the possibility of outliers. We have incorporated this 'softness' of the decision rule using the ν-trick [8] and thus obtained a direct handle on the fraction of outliers.

We believe that our approach, proposing a concrete algorithm with well-behaved computational complexity (convex quadratic programming) for a problem that so far has mainly been studied from a theoretical point of view [e.g. 5, 3], has abundant practical applications, such as condition monitoring [4], marketing [1], or information retrieval. To turn the algorithm into an easy-to-use black-box method for practicioners, questions like the selection of kernel parameters (such as the width of a Gaussian kernel) have to be tackled. It is our expectation that the theoretical results which we have only briefly outlined in this paper will provide a solid foundation for this formidable task.

Acknowledgement. This work was supported by the ARC and the DFG (# Ja 379/9-1). Thanks to C. Schnörr and N. Oliver for helpful discussions.

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