Dual-to-Kernel Learning with Ideals

Franz J. Király *

Martin Kreuzer [†]

Louis Theran[‡]

Abstract

In this paper, we propose a theory which unifies kernel learning and symbolic algebraic methods. We show that both worlds are inherently dual to each other, and we use this duality to combine the structure-awareness of algebraic methods with the efficiency and generality of kernels. The main idea lies in relating polynomial rings to feature space, and ideals to manifolds, then exploiting this generative-discriminative duality on kernel matrices. We illustrate this by proposing two algorithms, IPCA and AVICA, for simultaneous manifold and feature learning, and test their accuracy on synthetic and real world data.

1. Introduction

In this paper, we propose a learning theory which is the synthesis of kernel and symbolic algebraic methods, by exposing inherent dualities between them. We use this duality to combine the structure-awareness of algebraic methods with the efficiency and generality of kernels. Since their invention by Boser, Guyon and Vapnik [2, 22], kernel methods have had a fundamental impact on the fields of statistics and machine learning. The major appeal of using kernel methods for learning consists in using the kernel trick, first proposed by Aizerman, Braverman and Rozonoer [1], which allows to make otherwise costly computations in the feature space implicit and thus highly efficient for a huge variety of learning tasks - see e.g. [17, 19]. However, the major advantage of kernel methods is also their major drawback: since kernels implicitize feature space computations, the learnt model is implicit as well; in most scenarios, though kernels perform excellently, it is indeed a principal open question what it is that kernels learn - a question to which we can provide an answer through duality with ideals. On the other hand, symbolic-algebraic **methods** are inherently structural, as they yield explicit and compact representations of the data, as so-called ideals, with the major advantage of being directly interpretable. The seminal Buchberger-Möller algorithm [13] allows to transform one representation into a different, easier and sparser one. One major issue of the Buchberger-Möller algorithm is that it is numerically unstable and therefore not applicable in noisy scenarios - this has been addressed by a class of numerical algorithms surrounding the Approximate Vanishing Ideal (AVI) method [7, 16]. While these algorithms offer attractive and explicit representations, the major issue with symbolic methods preventing broad applicability is their exponential (or higher) complexity, and model selection issues - which we can considerably reduce through dual kernelization. In the intersection of symbolic algebra and kernel method, we propose general tools and two algorithms,

^{*}Department of Statistical Science, Univerity College London, and MFO f.kiraly@ucl.ac.uk

[†]Universität Passau, Martin.Kreuzer@uni-passau.de

^{*}Inst. Math., AG Diskrete Geometrie, Freie Universität Berlin, theran@math.fu-berlin.de

IPCA and AVICA, which simultaneously can learn generative information from the data manifold and discriminative features; more generally, we argue that the kernel-ideal duality translates generative and discriminative tasks in the kernel world directly to discriminative and generative tasks in the algebra world, which allows to combine the advantages of either while avoiding the disadvantages of both. We therefore expect our findings to have a considerable impact on the fields of learning, statistics, algebra, and the interaction between those.

2. Ideal-Kernel-Duality

2.1. The Polynomial Ring as Dual Kernel Space

We introduce the main objects we are relating through duality. We start by defining polynomial kernels, the main kernel-type objects involved in the duality presented here. Later we will explain how to treat general kernels. In this paper, \mathbb{K} will be one of the fields \mathbb{R} or \mathbb{C} .

Definition 2.1. Let $\theta \in (0, 1)$ be a fixed real number. Slightly different from the usual definition, we denote

by k_d the homogenous polynomial kernel function

 $k_d : \mathbb{K}^n \times \mathbb{K}^n \to \mathbb{R}, (x, y) \mapsto \theta^d \cdot \langle x, y \rangle^d$, and by $k_{\leq d}$ the inhomogenous polynomial kernel function $k_{\leq d} : \mathbb{K}^n \times \mathbb{K}^n \to \mathbb{R}, (x, y) \mapsto (\theta \cdot \langle x, y \rangle + 1)^d$.

The usual convention for the kernel function is obtained after dividing by θ^d . Since θ is chosen arbitrarily in (0, 1), no qualitative change is introduced by our convention. It is however, as we will show, the more natural one. On the algebra side, the main objects linked via the duality are vector spaces of polynomials.

Notation 2.2. We denote by $\mathbf{X} = (X_1, \dots, X_n)$ a vector of coordinate variables, by $\mathbb{K}[\mathbf{X}]_d$ the \mathbb{K} -vector space of homogeneous polynomials of degree d in \mathbf{X} , by $\mathbb{K}[\mathbf{X}]_{\leq d}$ the \mathbb{K} -vector space of all (homogeneous or inhomogeneous) polynomials of degree at most d in \mathbf{X} , by $\mathbb{K}[\mathbf{X}] = \mathbb{K}[\mathbf{X}]_0 \oplus \mathbb{K}[\mathbf{X}]_1 \oplus \cdots$ the ring of all polynomials in \mathbf{X} , and by $\mathbf{X}^{\mathbf{a}}$, for $\mathbf{a} \in \mathbb{N}^n$, the monomial $X_1^{\mathbf{a}_1} \cdots X_n^{a_n} \in \mathbb{K}[\mathbf{X}]_d$ where $d = a_1 + \cdots + a_n$.

The dimension of $\mathbb{K}[\mathbf{X}]_{\leq d}$ is $\binom{n+d}{d}$, and the dimension of $\mathbb{K}[\mathbf{X}]_d$ is $\binom{n+d-1}{d}$. The dimension of $\mathbb{K}[\mathbf{X}]$ is infinite. The ring $\mathbb{K}[\mathbf{X}]$ is dual to the vector space of kernel decision functions in the following way.

Theorem 1. Let $d \ge 0$, let $m \ge \dim \mathbb{K}[\mathbf{X}]_*$, where * can denote d or $\le d$, and let $y_1, \ldots, y_m \in \mathbb{K}^n$ be generic. Then we have $\mathbb{K}[\mathbf{X}]_* = \operatorname{span}\{k_*(y_i, \mathbf{X}), 1 \le i \le m\}$.

Proof. Linear independence of up to dim $\mathbb{K}[\mathbf{X}]_*$ of the $k_*(y_i, \mathbf{X})$ follows from genericity of y_i . Since span $\{k_*(y_i, \mathbf{X}), 1 \le i \le m\} \subseteq \mathbb{K}[\mathbf{X}]_*$, this yields the claim.

2.2. Duality of Kernel and Ring Scalar Products

Let $d \ge 0$, and let * denote d or $\le d$. Theorem 1 implies that $\mathbb{K}[\mathbf{X}]_*$ is dual to the feature space of the kernel k_* . By passing to the limit, this implies that $\mathbb{K}[\mathbf{X}]$ contains the dual of any feature space. Explicitly, this is seen as follows: consider the usual feature map $\phi_* : \mathbb{K}^n \to \mathcal{F}_*$, where \mathcal{F}_* is the feature space. Elementary computations, such as in section 2.1 or problems 2.6.2-3 of [17], show that the feature map can be explicitly identified as $\phi_* : x \mapsto (\gamma_{\mathbf{a}} \cdot x^{\mathbf{a}} : \mathbf{a} \in \mathbb{N}^n, a_1 + \dots + a_n =$ *), with $\gamma_{\mathbf{a}} = \sqrt{\theta^d \cdot {\binom{d}{\mathbf{a}}}}$. By counting the number of distinct \mathbf{a} , we see that dim $\mathcal{F}_* = \dim \mathbb{K}[\mathbf{X}]_*$. This can be made more explicit by interpreting polynomials in $\mathbb{K}[\mathbf{X}]_*$ as elements of the dual of \mathcal{F}_* , i.e., as functions $\mathcal{F}_* \to \mathbb{K}$. Namely, for a polynomial $f \in \mathbb{K}[\mathbf{X}]_*$ with $f = \sum_{\mathbf{a} \in \mathbb{N}^n} c_{\mathbf{a}} \mathbf{X}^{\mathbf{a}}$, write $f^{\vee} := (c_{\mathbf{a}}/\gamma_{\mathbf{a}}, \mathbf{a} \in \mathbb{N}^n)$. One checks that $\langle f^{\vee}, \phi_*(p) \rangle = f(p)$ for all $p \in \mathbb{K}^n$. Thus we can identify \mathcal{F}_* with the dual polynomial ring $\mathbb{K}[\mathbf{X}]_*^{\vee}$. Since the latter is finite dimensional, it is self dual, so there is a canonical identification $\mathcal{F}_*^{\vee} \cong \mathbb{K}[\mathbf{X}]_*$.

We use this identification to transfer the canonical scalar product on \mathcal{F}_* to its dual $\mathbb{K}[\mathbf{X}]_*$ in the natural way. Namely, in order to be compatible with ϕ_* , it needs to be the unique scalar product on $\mathbb{K}[\mathbf{X}_*]$ such that, for $x, y \in \mathbb{K}^n$, the reproducing property $\langle k_*(x, \mathbf{X}), k_*(\mathbf{X}, y) \rangle = k_*(x, y)$ holds. To achieve this, the factor γ_a occurring in f^{\vee} above must be corrected for. Consequently, an explicit description of the scalar product on $\mathbb{K}[\mathbf{X}]_*$ is given as follows: Fix $d \ge 0$, and let $\mathbf{a}, \mathbf{b} \in \mathbb{N}^n$ be exponent vectors. Define $\langle \mathbf{X}^a, \mathbf{X}^b \rangle = 0$ if $\mathbf{a} \neq \mathbf{b}$, and

$$\langle \mathbf{X}^{\mathbf{a}}, \mathbf{X}^{\mathbf{a}} \rangle = \gamma_{\mathbf{a}}^{-2} = \theta^{-d} \cdot \binom{d}{\mathbf{a}}^{-1} = \theta^{-d} \cdot \frac{a_1! \cdots a_n!}{d!},\tag{1}$$

and then extend this bi- or sesquilinearly to all of $\mathbb{K}[X]$.

Theorem 1 then implies that, for $f, g \in \mathbb{K}[\mathbf{X}]_*, p \in \mathbb{K}^n$, the following equalities hold:

$$f(p) = \langle f, k_*(\mathbf{X}, p) \rangle \tag{2}$$

$$\langle fg, k_*(\mathbf{X}, p)^2 \rangle = \langle f, k_*(\mathbf{X}, p) \rangle \langle g, k_*(\mathbf{X}, p) \rangle.$$
 (3)

By applying Theorem 1 and properties of the symmetric outer product, we get an important consequence of Equation 3, namely that the scalar product is multiplicatively absorbing for orthogonality. That is, letting $f_1, f_2, g_1, g_2 \in \mathbb{K}[\mathbf{X}]$ such that $\langle f_i, g_j \rangle = 0$ for all i, j, we have

$$\left\langle f_1 f_2, \, g_1 g_2 \right\rangle = 0. \tag{4}$$

Note that in the usual convention for the polynomial kernel, similar equalities are still valid, but much less concise to express. The duality above is an algebraic analogue of the theory of reproducing kernel Hilbert spaces. The associated Hilbert space is the space of polynomial functions $f : \mathbb{K}^n \to \mathbb{K}$, which can be identified with $\mathbb{K}[\mathbf{X}]_*$ by an additional dualization; phrased in algebraic terms, by replacing the evaluation homomorphism f with the corresponding symbolic polynomial. Note that the equations 2 and 3 could also be obtained combining Riesz representation, or the reproducing property of k_* , with this identification, compare e.g. section 2.2.3 in [17].Equality 4, on the other hand, is purely obtained from algebra. The next section will also go beyond what could be reached from usual RKHS duality alone.

2.3. Ideals are Dual to Manifolds

Next we show that ideals - a classical concept in algebra - are the proper objects to dualize manifolds, in the same way as the polynomial ring dualizes feature space.

Definition 2.3. An *ideal* is a linear subspace $\mathcal{I} \subseteq \mathbb{K}[\mathbf{X}]$ which also absorbs multiplication, that is, which satisfies $f \cdot g \in \mathcal{I}$ for all $f \in \mathbb{K}[\mathbf{X}], g \in \mathcal{I}$. For $d \ge 0$, we let $\mathcal{I}_{\leq d} := \mathcal{I} \cap \mathbb{K}[\mathbf{X}]_{\leq d}$.

While an ideal is in general infinite dimensional as a \mathbb{K} -vector space, Hilbert's basis theorem says that all ideals admit a *finite* set of additive-multiplicative generators. As for vector spaces, such sets of generators need not be unique. An important class of ideals is given as follows.

Example 2.4. Let $S \subseteq \mathbb{K}^n$. Then the \mathbb{K} -vector space of polynomials $I(S) := \{f \in \mathbb{K}[X] : f(s) = 0 \text{ for all } s \in S\}$ is an ideal. It is called the *vanishing ideal of* S.

While *S* can be in principle any subset of \mathbb{K}^n , we will be mainly concerned with the case where *S* is a manifold. In this case, the vanishing ideal I(*S*) is the dual of the manifold *S* in the following precise sense which is an analogue to Theorem 1.

Theorem 2. Let $S \subset \mathbb{K}^n$ be a manifold. It holds that $I(S) \cap \mathbb{K}[\mathbf{X}]_* = \operatorname{span}\{k_*(s, \mathbf{X}), s \in S\}^{\perp}$.

Proof. This follows from the definition of I(S) and Equation 2.

Theorem 2 relates manifolds to ideals via kernel duality. Intuitively, it says that the manifold S corresponds to a linear subspace of feature space. This is a kernelized version of the usual algebra-geometry duality and and relates the discriminative description through decision functions $k_*(s, \mathbf{X})$ to the generative description by S.

2.4. Interpolation Space and Kernel Border Bases

In this section we reveal a further duality between certain kernel matrices and ideals. First we introduce the following notation for kernel matrices.

Notation 2.5. Let $X \in \mathbb{K}^{N \times n}$, let $Y \in \mathbb{K}^{D \times n}$, and let $x_1, \ldots, x_N, y_1, \ldots, y_D$ be the rows of X and Y, resp. For a kernel $k : \mathbb{K}^n \times \mathbb{K}^n \to \mathbb{R}$, we denote by k(X, Y) the $(N \times D)$ -matrix which has the number $k(x_i, y_i)$ as its entry in position (i, j).

The concept of an interpolation space is motivated by the duality in Theorem 2 and is the orthogonal to an ideal.

Definition 2.6. Let $S \subseteq \mathbb{K}^n$, and let $\mathcal{I} = I(S)$. The *interpolation space* of S is the vector space $\mathbb{K}[S] := \mathcal{I}^{\perp}$, where the orthogonal is taken w.r.t. the scalar product defined above. Given $d \ge 0$, we also write $K[S]_{\le d}$ for $\mathcal{I}_{\le d}^{\perp}$.

Intuitively, the interpolation space gives a canonical basis for the space of functions on S, orthogonal to those vanishing on S. It is a fixed choice of representatives for the factor ring $\mathbb{K}[\mathbf{X}]/I(S)$ usually defined in algebra. The results of the previous sections yield the following duality statements between the interpolation space and polynomial kernel matrices.

Theorem 3. Let $S \subseteq \mathbb{K}^n$, let $x_1, \ldots, x_N \in S$ be generic, and let $X \in \mathbb{K}^{N \times n}$ be the matrix which has the x_i as columns. Let $Y \in \mathbb{K}^{D \times n}$ be generic. Denote $K_d := k_{\leq d}(X, Y)$. Then the following claims hold:

- (i) rank $K_d = \min(\dim \mathbb{K}[S]_{\leq d}, N, D).$
- (ii) It holds that $k_{\leq d}(\mathbf{X}, Y)$ rowspan $K_d \subseteq \mathbb{K}[S]_{\leq d}$. Equality holds if and only if $N, D \geq \dim \mathbb{K}[S]_{\leq d}$.
- (iii) For $\alpha \in \mathbb{K}^D$, it holds that $k_{\leq d}(\mathbf{X}, Y) \cdot \alpha \in I(S)$ only if $K_d \cdot \alpha = 0$. The converse is true if and only if $N, D \geq \dim \mathbb{K}[S]_{\leq d}$.

(Notice the difference between the n-tuple of variables **X** and the data matrix *X*.)

Proof. For $d \ge 0$, we write $\tau := \dim \mathbb{K}[S]_{\le d}$. Claim (i): First assume that $N, D \ge \tau$. Theorem 2 implies that span $\{k_{\le d}(s, \mathbf{X}), s \in S\} = (I(S) \cap \mathbb{K}[\mathbf{X}]_{\le d})^{\perp} = \mathbb{K}[S]_{\le d}$. In particular, this shows dim span $\{k_{\le d}(s, \mathbf{X}), s \in S\} = \tau$. Therefore $D \ge \tau$ generic elements of the form $k_{\le d}(\mathbf{X}, y_i)$ will generate $\mathbb{K}[S]_{\le d}$, and their span will have dimension τ . By interpreting the variables in \mathbf{X} once

more as functions $\mathbb{K}^n \to \mathbb{K}^n$, we view $k_{\leq d}(\mathbf{X}, y_i)$ as a function $k_{\leq d}(., y_i) : \mathbb{K}^n \to \mathbb{R}$. Then the polynomials $k_{\leq d}(\mathbf{X}, y_i)$ span a vector space of dimension τ if and only if the functions $k_{\leq d}(., y_i)$ do that as well. By substituting $N \geq \tau$ generic arguments x_1, \ldots, x_N , we see that the vectors $k_{\leq d}(X, y_i)$ span a vector space of dimension τ . This is equivalent to rank $K_d = \tau$, proving the statement in case $N, D \geq \tau$. The general statement follows by starting with $N, D = \tau$ and removing rows and columns. Claims (ii) and (iii) follow from the fact that, if $N \geq \tau$, the vector of variables **X** in the conditions can be equivalently replaced by *X*. The case $N \lneq \tau$ follows again by removing rows and columns.

Theorem 3 states that a large enough kernel matrix of type K(X, Y) contains all information on S, assuming the kernel degree is high enough as well. Algorithmically, it yields the important statement that, instead of size $O(\dim \mathbb{K}[\mathbf{X}]_{\leq d}) = O(n^d)$ matrices which grow exponentially in d, we have to deal with size $O(\dim \mathbb{K}[S]_{\leq d}) = O(N)$ matrices instead. These are matrices whose size is bounded from above by the number of data points. In fact, the effective size is usually even lower, depending on model complexity. We also note that claims (ii) and (iii) of Theorem 3 make statements about functions of the form $F(.) = \sum_{i=1}^{D} \alpha_i k(., y_i)$, which is a familiar form of decision functions. Since the functions in claim (ii) are part of the interpolation space of S, we call them "discriminiative features". The functions in claim (iii) vanish on S. Therefore they carry structural information about S, so we will call them "generative features". A basis of I(S) consisting of such generative features will be called a *kernel border basis*. These features will be identified by both algorithms we introduce in the subsequent section.

3. Learning with Ideals

Similar to the ubiquity of kernels, ideals enable us to address a wide variety of learning scenarios. The general motive in ideal-manifold duality is that generative features are transformed into discriminative ones and vice versa. For instance, a strategy for estimating a discriminative function in kernel learning, e.g., by kernel SVM, will be close to estimating a descriptive feature in learning a manifold via obtaining ideal generators. Conversely, estimating descriptive features such as in kernel PCA will relate to obtaining discriminative features from the interpolation space. This permits us to "dualize" techniques and to transfer the absorption property of ideals back into the kernel world, thus yielding new model selection tools and compact representations in terms of kernel degree.

3.1. Statistical Learning Theory for Ideals

The following learning approach to ideals is inspired by Vapnik's statistical learning theory. We assume that there is a *generative truth*, modelled by an unknown algebraic manifold $S \subset \mathbb{K}^n$ with vanishing ideal $\mathcal{I} = I(S)$. The sampling process produces a discrete point set $x_1, \ldots, x_N \in \mathbb{K}^n$, where $x_i = s_i + \varepsilon_i$, with $s_i \in S$ sampled from a (Hausdorff-)continuous density on S and $\varepsilon_i \in \mathbb{K}^n$ being i.i.d. centered noise of finite variance. Basic learning tasks can be expressed in this ideal-learning framework as follows:

Example 3.1 (Dimension reduction). The dimension *n* is large. The task is to estimate the true manifold S, assuming that $d \ll n$.

Example 3.2 (Regression). The variables **X** are partitioned into dependent and independent variables. The noise acts only on the dependent variables, and the task is to estimate *S*.

Example 3.3 (Classification). The generative truth S is assumed to have irreducible components S_1, \ldots, S_t . The sample *S* is given as points (x_i, ℓ_i) with labels $\ell \in [t]$. The task is to estimate the components S_i of S.

Example 3.4 (Clustering). The generative truth S is assumed to have irreducible components S_1, \ldots, S_t . The sample *S* is unlabeled, and the task is to estimate S_1, \ldots, S_t .

Measures of statistical optimality will be given after presenting our main algorithmic principle.

3.2. A New Manifold Learning Kernel PCA

Now we describe the basic idea behind computing with kernel duals. It can be applied in all of the examples above. Algorithm 1, which we term Ideal PCA, takes data x_1, \ldots, x_N , sampled with noise from a manifold S, and returns feature functions of the form $F(.) = \sum_{i=1}^{D} \alpha_i k(., y_i)$ which are labelled either generative (= part of the interpolation space) or discriminative (= part of the kernel border basis). The kernel function k is one of the polynomial kernels, but could be any kernel in principle.

Algorithm 1 IPCA Computes interpolation space and kernel border basis.

Input: data $x_1, \ldots x_N \in \mathbb{K}^n$, given as rows of an $(N \times n)$ matrix X, degree d, feature space size D, threshold ϵ .

Output: Feature functions $F_i = \sum_{j=1}^{D} \alpha_{ij} k(y_j, .)$, with labels "generative" or "discriminative" and quanta σ_i .

- 1: Sample *D* random points $y_i \in \mathbb{K}^n$; write those into a $(D \times n)$ matrix *Y*.
- 2: Compute the $N \times D$ kernel matrix K = k(X, Y) with (i, j)-th entry $k(x_i, y_j)$.
- 3: Compute the singular value decomposition $K = USV^{\top}$, $S = \text{diag}(\sigma_1, \dots, \sigma_m)$
- 4: The α_{ij} in the output are the entries of *V*; the y_j are the y_j sampled above.
- 5: For each feature F_i , assign the label "discriminative" if $\sigma_i \ge \epsilon$, otherwise "generative". Also return the σ_i .

The number *D* should be chosen sufficiently large, either as $D \ge N$, or $D \ge \dim \mathbb{K}[S]_{\le d}$, if known. In these cases, Theorem 3 guarantees convergence in the noiseless case; we will see later that this also makes IPCA (Alg. 1) a noise consistent algorithm. In the output, the discriminative features are expected to vary strongly when leaving the manifold *S*. Therefore they describe the internal structure of the data. On the other hand, the generative features are expected to almost vanish in a neighborhood of *S*. Therefore they describe the manifold itself. The singular values σ_i yield a quantitative measure. All - or some of the - features obtained from IPCA (Alg. 1) can be bulk evaluated in an efficient way: first compute the kernel matrix K = k(X, Y), then the features are obtained from the matrix $K \cdot V$. We remark again that it is not necessary to choose $D = O(n^d)$ - as it would be in symbolic methods - due to the rank guarantee in Theorem 3.

3.3. Noise Consisteny

As already said above, IPCA (Alg. 1) transfers the exact statement in Theorem 3 to the case of noisy data. We now show that IPCA does this in a beneficial way. First we want to remark that the classical concept of consistency will not be applicable here, since a manifold S which is a point can lead to the same observations as a line S if i.i.d. Gaussian noise is added to the samples.

Therefore, no algorithm can "converge" to *S* in the limit of the sample size. We argue that the proper notion of consistency in the manifold setting is *noise consistency*:

Definition 3.5. Consider the learning setup outlined in section 3.1. That is, let $\mathcal{S} \subset \mathbb{K}^n$ be manifold with ideal $\mathcal{I} = I(\mathcal{S})$, and assume that we have noisy samples $x_i = s_i + \varepsilon_i$ from \mathcal{S} . We say that an estimator $\widehat{\mathcal{S}}$ is *noise consistent* if $I(\widehat{\mathcal{S}}) =: \widehat{\mathcal{I}} \to \mathcal{I}$ as $||(\varepsilon_1, \dots, \varepsilon_n)|| \to 0$, where convergence of $\widehat{\mathcal{I}}$ is defined as convergence of all vector spaces $\widehat{\mathcal{I}}_{\leq d} \to \mathcal{I}_{\leq d}$ (possibly of different order).

Intuitively, noise consistency is the combination of stability with respect to noise, and correctness in the noise-free case.

Theorem 4. Consider the learning setup outlined in section 3.1. That is, let $S \subset \mathbb{K}^n$ be a manifold with ideal $\mathfrak{I} = \mathrm{I}(S)$, and assume that we have noisy samples $x_i = s_i + \varepsilon_i$ from S. IPCA (Alg. 1) estimates S noise-consistently in the following sense: assume \mathfrak{I} is generated in degree d or less, let $N \ge \mathbb{K}[S]_{\le d}$, let $\widehat{\mathbb{K}[S]_{\le d}}$ be the vector space generated by the discriminative features that IPCA, with inhomogenous kernel $k = k_{\le d}$, outputs. Let $\widehat{\mathfrak{I}}$ be the ideal generated by the orthogonal complement of $\widehat{\mathbb{K}[S]_{\le d}}$. Then, $V(\widehat{\mathfrak{I}})$ is a noise consistent estimate for S.

Proof. If d = 1, this follows directly from the Eckart-Young-Theorem which implies that thresholded SVD is a noise consistent estimator for the span of a matrix. The general statement is implied as follows: by Theorem 3 and noise consistency of SVD, $\widehat{\mathbb{K}[S]}_{\leq d}$ is a noise consistent estimate for $\mathbb{K}[S]_{\leq d}$. Thus, by passing to the orthogonal complement, $\widehat{\mathcal{I}}_{\leq d}$ is a noise consistent estimate for $\mathcal{I}_{\leq d}$. Since \mathcal{I} is generated in degree d, this implies that $\widehat{\mathcal{I}}$ is a noise consistent estimate for \mathcal{I} , which implies the statement.

3.4. Informal Analysis of the Basic Method

At first glance, IPCA (Alg. 1) may seem to be another version of kernel PCA or kernel SVD. However, there is one main difference: the matrix *Y* is random. Therefore we do not work with the kernel matrix k(X,X), as usual, but with a matrix k(X,Y).

This enables us to look at the feature span of *X* from the outside, whereas the classical approach only looks at relations between *X* and *X*. More specifically, doing PCA or SVD or any method involving only k(X,X) will reveal only features *inside the data manifold*. The manifold itself - as the important generative object - will not be identified. This shortcoming has already been noticed in [12][section 3.1: "kernels can't help"], where the authors conclude that such methods are not suitable for learning generative features in an algebraic setting. The matrix k(X,Y) can be used to capture the *extrinsic structure* of the data manifold.

What happens mathematically can be exposed using a linear (and noise-free) example: take the kernel to be the linear scalar product $k = \langle ., . \rangle$. Suppose our data $x_1, ..., x_N$ come from a linear subspace $L \subseteq \mathbb{R}^n$. Then we would like to learn discriminative features, that is, features that vary among the x_i , here the principal components, and generative features, in this simple case the subspace L from which the data are sampled. Writing X as the $(N \times n)$ -matrix with the x_i as rows, the kernel matrix is the $(N \times N)$ -matrix $K = k(X,X) = XX^{\top}$. Note that this differs from the $(n \times n)$ -matrix $X^{\top}X$ which is taken in classic PCA (for centered data). Singular value decomposition of K will reveal features of X, such as the dimension of L, through the rank of K. However, rotating L together with the x_i , or embedding it into a different $\mathbb{K}^{n'}$ will leave K unchanged. Therefore the generative information on L is lost in k(X,X) since this matrix contains

only information on *X* inside *L*. On the other hand, if a random matrix $Y \in \mathbb{R}^{D \times n}$ is taken with $D \ge n$, and if $K' = k(X, Y) = XY^{\top}$ is considered, the space *L* can easily be reconstructed from the right singular vectors. Moreover, all information on k(X,X) is potentially contained as well, most easily (but impractically) by adding in the rows of *X* as rows of *Y*. This also shows that the important part of *Y* is that "orthogonal" to *X*, because it allow us to capture the *extrinsic* structure of *L*.

The case of general kernels is analogous, if we replace the scalar products above by the kernel function. The role of the y_i , which are above a basis for \mathbb{K}^n , is played by the feature vectors $\phi(y_i)$ which now span the complete feature space. The mathematical justification is given by Theorem 2 which shows that the manifold S corresponds to a proper linear subspace of the complete feature space. The interpolation space is exactly orthogonal to decision functions $k(x_i, \mathbf{X})$ with x_i a data point. Therefore k(X, X) cannot be used to say anything about the interpolation space. On the other hand, Theorem 1 says that the whole feature space is dual to decision functions of the form $k(\mathbf{X}, y_i)$, with y_i generic/random; so, k(X, Y) is the proper object which captures both features of the interpolation space - through the part of Y that is kernel orthogonal to X - and the intrinsic features of the data in X which can be obtained through k(X, X) and are recovered e.g. by kernel PCA.

3.5. The Kernel Powering Method

The IPCA algorithm (Alg. 1) provides an estimate for the interpolation space, and therefore the generative manifold S, as discussed above. However, there are two points where improvement is possible: (a) the features learnt are all of the same degree, while there may be features of different degrees. In particular, if an overly high *d* is chosen in IPCA, and if S is for instance linear, this will not be explicitly noticed. (b) The size of the approximate kernel border basis, i.e., the number of generators for I(S), when naively estimated as generators for the orthogonal of $\mathbb{K}[S]_{< d}$, grows exponentially in *d*, since dim $\mathbb{K}[\mathbf{X}]_{< d}$ does.

In the following we address these issues simultaneously by a powering-projection-strategy applied to the kernel matrix. To address (a), we increase degrees and learn features of increasing degrees step-by-step by computing entrywise-powers of the degree 1 kernel matrix, exploiting the fact that the degree d kernel matrix is the d-th power To address (b), we use the absorption property of the ideal I(S) to obtain a low number of multiplicative generators, by projecting the kernel matrix onto a low rank approximation; by Theorem 3 (iii) this corresponds to adding new elements to the kernel border basis. Powering is furthermore compatible with absorption by Equation 4. So, after powering, only new generators in higher degree will appear, and this allows us to add them sequentially to the approximate kernel border basis. Concretely, this works as follows. Start with the linear kernel matrix K_1 . Then project on a smaller rank matrix K'_1 by singular value thresholding. Next, compute K_2 as the entrywise second power $K_2 := K'_1 \otimes K_1$ and project again onto a smaller rank matrix K'_2 . In general, obtain $K_d := K'_{d-1} \otimes K_1$, then threshold. The threshold can be chosen fixed, or according to the Hilbert function of S, if that is known. In each step, we add features to the approximate kernel border basis which correspond to singular values under the threshold, but not exactly zero. This "degree greedy" strategy can be seen as a kernelization of some ideas in the AVI class of algorithms [7, 16].

3.6. Approximate Vanishing Ideal Component Analysis

We now describe an algorithm, which uses the power-projecting strategy, called Approximate Vanishing Ideal Component Analysis (AVICA). AVICA will output generative and discriminative features of various degrees, ordered by informativity. As discussed in section 3.5, the main difference to IPCA (Alg. 1) lies in the fact that the "degree greedy" strategy collects generators for the ideal of the manifold \$ with increasing degree, therefore offers a much sparser generative description of \$ than IPCA, while learning degree-ordered generators of the interpolation space as well. We present AVICA as Algorithm 2; for simplicity of reading, we first introduce notation for the projection step which is singular value thresholding:

Definition 3.6. For a matrix *K* and a threshold ϵ , we define the *thresholded SVD* to be $K = USV + U^{\perp}S^{\perp}V^{\perp}$, where the concatenations (U, U^{\perp}) and $(V, V^{\perp})^{\top}$ are the left and right singular matrices of the usual singular value decomposition, with singular values in *S* having absolute value $\geq \epsilon$, and those in S^{\perp} being $< \epsilon$.

Applied to the kernel matrix, this means, according to Theorem 3 (iii) that the features corresponding to V^{\perp} are added to the approximate kernel border basis.

Algorithm 2 AVICA Sparsely computes approximate interpolation space and kernel border basis. *Input:* data $x_1, \ldots x_N \in \mathbb{K}^n$, given as rows of an $(N \times n)$ matrix X, maximum degree *maxdeg*, threshold ϵ .

Output: Feature functions $F_i = \sum_{j=1}^{D} \alpha_{ij} k(y_j, .)$, with labels "generative" or "discriminative" and quanta q_i .

- 1: Sample random points $y_i \in \mathbb{K}^n$, $1 \le i \le D$; write those in a $(D \times n)$ matrix *Y*.
- 2: Let K_0 be the all-ones $(N \times D)$ matrix.
- 3: Compute the $N \times D$ matrix K = k(X, Y).
- 4: for d = 1, ..., maxdeg do
- 5: Set $\epsilon \leftarrow \epsilon \cdot \theta$
- 6: Set $K_d \leftarrow K_{d-1} \otimes K$ (entry-wise product)
- 7: Compute the ϵ -thresholded SVD $K_d = U_d S_d V_d + U_d^{\perp} S_d^{\perp} V_d^{\perp}.$
- 8: For each column ν of V, return a discriminative feature $F_*(.) = \sum_{j=1}^{D} \nu_j k^d(y_j, .)$.
- 9: For each column v of V^{\perp} with singular value that is not zero with machine precision, return a generative feature $F_*(.) = \sum_{j=1}^{D} v_j k^d(y_j, .)$
- 10: Also return as quantum q_* the corresponding singular values times θ^d .
- 11: $K_d \leftarrow U_d S_d V_d$
- 12: end for
- 13: Display as informativity order the generative features ascendingly by q_* , the discriminative ones descendingly.

Since AVICA computes a basis for the interpolation space in a similar way as IPCA (Alg. 1), an analogous proof shows that AVICA is a noise consistent estimator for S in the same sense. Evaluation of the features can again be done efficiently, by storing $Y, S_d, V_d, S_d^{\perp}, V_d^{\perp}$ as model parameters, then repeating the computations. Since this is sligtly more complex than in the case of IPCA, we describe this explicitly in form of Algorithm 3.

 Algorithm 3
 eval. AVICA
 Bulk evaluates features.

 Input:
 matrices $(Y, S_d, V_d, S^{\perp}, V^{\perp})$, data $x_1, \dots x_N \in \mathbb{K}^n$, given as rows of an $(N \times n)$ matrix X, maximum degree maxdeg.

 Output:
 Evaluations of all feature functions

 $F_i(x_k) = \sum_{j=1}^D \alpha_{ij} k(y_j, x_k)$.
 I:

 I:
 Let K_0 be the all-ones $(N \times D)$ matrix.

 2:
 Compute the $N \times D$ matrix K = k(X, Y).

 3:
 for $d = 1, \dots, maxdeg$ do

 4:
 Set $K_d \leftarrow K_{d-1} \otimes K$

 5:
 Return $K_d \cdot V_d$ for discriminative and $K_d \cdot V_d^{\perp}$ for generative features. Rows are indexed by k, columns by i.

 6:
 $K_d \leftarrow K_d V_d^{\top} V_d$.

3.7. AVICA for Discriminative Learning

From the discussion so far, it appears that the main advantage and novel of AVICA is learning generative features of some data manifold. However, with a minor but crucial modification, it can be adapted for discriminative supervised learning in a natural way which will allow one-vs-all or one-vs-one discrimination which is in some sense also class-generative. Namely, consider a feature $F(.) = \sum_{i=1}^{D} \alpha_i k(., y_i)$ in the kernel border basis, that is, $F(s) \approx 0$ for $s \in S$. We have said that such an F is generative, as it describes S - but it can also be viewed discriminative, distinguishing S from the "set of general points" in \mathbb{K}^n . While this is an unusual view, it is the one which generalizes well to discriminative learning: the y_i were chosen to span \mathbb{K}^n or the feature space; picking them, instead, as elements of a different manifold $S' \subsetneq \mathbb{K}^n$ will in the same way allow to distinguish S from S'. Specifically, in step 2 of AVICA (Alg. 2), replace random sampling from \mathbb{K}^n with random sampling in some $S' \supseteq S$, in order to learn to identify points in S among points in S'. To learn a one-vs-all-classifier between classes S_1, \ldots, S_k , choose $S = S_1$ and $S' = S_1 \cup \cdots \cup S_k$, then use the "generative" features, in the kernel border basis, as class discriminative.

3.8. AVICA for Non-Polynomial Kernels

We would like to stress that neither IPCA (Alg. 1) nor AVICA (Alg. 2) makes a strong use of the polynomial kernel; for a general kernel, duality with a polynomial ring $\mathbb{K}[k(y_i, \mathbf{X}), 1 \le i \le D]$ takes the place of duality with the polynomial ring $\mathbb{K}[\mathbf{X}]$; the number *D* has to be taken sufficiently large for the application. Again, generative and discriminative features can be both extracted with IPCA and AVICA. The interpolation space corresponds to the usual features learnt by kernel methods, while the manifold, or ideal, yields new generative ones, depending on the kernel. For example, when taking *k* to be the Gauss kernel, AVICA will learn the *clusters themselves*, instead of separators, since the clusters correspond to manifolds in the Gauss feature space.

4. Experiments

4.1. The circle

A well-known example used to motivate discriminative kernel classification is a 2-dimensional problem, in which the classes are sampled from concentric circles. The analogous task for gen-



Figure 1: Learning a circle of radius 10 from 200 random points with $N(0, \sigma)$ noise. Blue x's are the training points. The true circle is shown in black. The green region is the [-s/10, s/10] level set of the kernel border basis element with smallest singular value *s*.

erative kernel learning is learning *one* circle from a noisy sample. Figure 1 shows that AVICA does this. In each experiment, we generate 200 uniform points on a circle of radius R = 10, centered at the origin, add $N(0, \sigma)$ and then run ≤ 2 -AVICA with threshold $2\theta \sqrt{2}\sigma^2$, which is what we expect for noise in the feature space. The width of the green region in Figure 1 is scaled by s/R, since it is proportional to length of the generator in feature space and captures the data. However, it is only there for illustrative purposes: the estimation task is to estimate the *manifold*, not the data, so what is important is not the width of the green region but that the black circle is in it.

4.2. Handwritten digits

We tested AVICA on the MNist handwritten digit recognition data set, to compare it with the AVI class algorithm in [12]. Classification was done using the discriminative method described in section 3.7; the union of all classes was subsampled to 200 data points. The class to which a test point was assigned was chosen as the minimizer of the ℓ^1 -norm of the one-vs-all-generative features. As kernels, we used the inhomogenous kernel with $\theta = 1/\sqrt{2}$, and the Gauss kernel with a width of 5000. Thresholding in AVICA was done at the logarithmic mean of the singular value spectrum. For *maxdeg* = 1, that is with purely linear features (in which case IPCA=AVICA), both methods (polynomial and Gauss) achieved an overall misclassification rate of 4.1% with an overall runtime in the order of seconds. Increasing the degree, the size of the subsample, or varying the parameters can lead to lower misclassification rates. However, it is difficult to compare these results to those of [12], since the authors do not disclose how exactly they measure runtime

or choose the threshold, therefore we refrain from more detailed comparison and conclude that IPCA and AVICA are already very fast and competitive on handwritten digits for degree 1.

5. Discussion

5.1. Duality of Generative and Discriminative Learning

Let us close out our theoretical discussion with two critical connections. The first is between our method and the by-now classical theory of discriminative learning with kernels. By our discussion on duality in section 2, we have implicitly shown the following informal "theorem":

Theorem 5. Generative learning with ideals is dual to discriminative learning with kernels; discriminative learning with ideals is dual to generative learning with kernels.

For example, in the classical discriminative scenario of the *kernel support vector machine*, the standard kernel decision function is of the form $F(.) = \sum_{i=1}^{D} \alpha_i k(., x_i)$. In the ideals setting, this is generative learning of the separating hyperplane, which is a manifold uniquely parametrized by *F*, interpreted as a polynomial and element of the *interpolation space*. In *kernel PCA*, generative features are learnt for the data; by using an analogous technique in the dual, *IPCA* learns the data manifold in a discriminative way, by separating points on the manifold (the matrix *X*) from points not on the manifold (the matrix *Y*). Moreover, the *noise consistency* guarantees that we obtain for both IPCA and AVICA are dual to *generalization bounds* that can be obtained from classical Vapnik-Chervonenkis theory.

5.2. Related Work

Finally, we briefly discuss the principal strains of related work and the ideas which are rooted there. These are, in the sequence we will discuss them: kernels, manifold learning, algebra in statistics and learning, approximate symbolic methods. Kernel methods form a broad field and have been widely studied in practical and theoretical context; a detailed overview over the field and its history can, for example, be found in the "further reading" sections of [19]. To our knowledge, there is so far no technique or result relating kernel methods to symbolic computation. The major link to existing literature is through the kernel trick [1] and the reproducing kernel hilbert space duality (see section 2.2.3 of [17]): the initial statements on algebra-kernel duality can be obtained from RKHS theory by considering polynomial functions formally as elements of the polynomial rings. Manifold learning techniques, such as principal curves [6], LLE [15], or the aforementioned kernel PCA [18] have in common that they assign an embedding of the data into low dimensional space. This corresponds to learning discriminative features. Our algorithms IPCA and AVICA also learn features which generatively describe the manifold, i.e., explicitly describe where the points lie in the high dimensional data space. As the discussion in section 3.4 explains in greater detail, these methods can be seen as an extension of kernel PCA in the sense that they do not only learn the embedding, but also the manifold. Algebraic techniques in statistics have been a recurring topic since the advent of algebraic statistics, for an overview see [4, 5, 14, 21]. However, the results in algebraic statistics are not directly applicable to a learning or data related context, since the field is predominantly concerned with understanding algebraically structured models and not estimating them from data. On the other hand, there are seemingly unrelated

scenarios where specific algebraic structures have explicitly been used for estimation and learning in particular scenarios, e.g. [8, 9, 11, 23]. A learning theory built on polynomials and ideals has been outlined in the appendix of [10]. Approximate symbolic computation techniques can be traced back to Corless et al [3] who proposed the use of singular value decomposition (SVD) for polynomial systems, and the work of Stetter [20] who pioneered a more general numerical view. The first algorithms which use SVD to estimate an approximate vanishing ideal numerically are those of Heldt et al [7], which uses border bases and a numerically stable variant of term orderings, and Sauer [16], which uses a coordinate independent degree-increasing strategy to compute homogenous bases; both algorithms can be considered as variations on the same idea set and yield an approximate version of the exact symbolic Buchberger-Möller algorithm [13]. The homogenous variant in [16] has recently reappeared under the name "Vanishing Components Analysis" [12] in the machine learning community. AVICA can be seen as a kernelization of these AVI-class algorithms: it integrates the idea of the compact order ideal/border basis representation in [7] (interpolation space/kernel border basis) with the degree-greedy strategy and homogenous coordinate independence of [16] into our kernel based algorithm through the concept of kernel-ideal-duality.

5.3. Conclusion and Outlook

In this paper, we have exposed an intricate duality between kernels and commutative algebra, between ideals and manifolds, between kernel methods and symbolic algebraic methods, between generative and discriminative learning. We have outlined how a statistical learning theory in this new ideal-kernel-duality setting can be obtained, and we have described how the duality can be exploited in general for learning explicit, generative structures with kernels. We have demonstrated, theoretically and competitively on real-world-data, how the duality can be used to construct a novel type of algorithm, AVICA, which simultaneously extracts discriminative and generative components from the data.

In the light of this, the whole field of statistical data analysis and machine learning stands open to a plethora of new methods following this conceptual regime.

Acknowledgments

LT is supported by the European Research Council under the European Union's Seventh Framework Programme (FP7/2007-2013) / ERC grant agreement no 247029- SDModels. This research was carried out at MFO, supported by FK's Oberwolfach Leibniz Fellowship.

References

- [1] Mark A. Aizerman, Emmanuel M. Braverman, and Lev I. Rozonoer. Theoretical foundations of the potential function method in pattern recognition learning. In *Automation and Remote Control*, number 25 in Automation and Remote Control, pages 821–837, 1964.
- [2] Bernhard E. Boser, Isabelle M. Guyon, and Vladimir N. Vapnik. A training algorithm for optimal margin classifiers. In *Proceedings of the 5th Annual ACM Workshop on Computational Learning Theory*, pages 144–152. ACM Press, 1992.

- [3] Robert M. Corless, Patrizia M. Gianni, Barry M. Trager, and Steven M. Watt. The singular value decomposition for polynomial systems. *Proc. ISSAC '95*, pages 195–207, 1995.
- [4] Mathias Drton, Bernd Sturmfels, and Seth Sullivant. *Lectures on Algebraic Statistics*. Oberwolfach Seminars. Birkhauser Basel, 2010. ISBN 9783764389048.
- [5] Paolo Gibilisco, Eva Riccomagno, Maria Piera Rogantin, and Henry P. Wynn. *Algebraic and Geometric Methods in Statistics*. Cambridge University Press, 2010.
- [6] Trevor Hastie. Principal curves and surfaces. Technical report, DTIC Document, 1984.
- [7] Daniel Heldt, Martin Kreuzer, Sebastian Pokutta, and Hennie Poulisse. Approximate computation of zero-dimensional polynomial ideals. *Journal of Symbolic Computation*, 44(11): 1566 – 1591, 2009.
- [8] Franz J Király and Louis Theran. Error-minimizing estimates and universal entry-wise error bounds for low-rank matrix completion. In *Neural Information Processing Systems 2013*, 2013.
- [9] Franz Johannes Király, Paul von Bünau, Frank Meinecke, Duncan Blythe, and Klaus-Robert Müller. Algebraic geometric comparison of probability distributions. *Journal of Machine Learning Research*, 13(Mar):855–903, 2012.
- [10] Franz Johannes Király, Paul von Bünau, Jan Saputra Müller, Duncan Blythe, Frank Meinecke, and Klaus-Robert Müller. Regression for sets of polynomial equations. *JMLR Workshop and Conference Proceedings*, 22:628–637, 2012.
- [11] Risi Kondor. *Group Theoretical Methods in Machine Learning*. PhD thesis, Columbia University, 2008.
- [12] Roi Livni, David Lehavi, Sagi Schein, Hila Nachliely, Shai Shalev-Shwartz, and Amir Globerson. Vanishing component analysis. In *Proceedings of the 30th International Conference on Machine Learning (ICML-13)*, pages 597–605, 2013.
- [13] H Michael Möller and Bruno Buchberger. The construction of multivariate polynomials with preassigned zeros. In *Computer algebra*, pages 24–31. Springer, 1982.
- [14] Giovanni Pistone, Eva Riccomagno, and Henry P Wynn. *Algebraic statistics: Computational commutative algebra in statistics.* CRC Press, 2002.
- [15] Sam T Roweis and Lawrence K Saul. Nonlinear dimensionality reduction by locally linear embedding. *Science*, 290(5500):2323–2326, 2000.
- [16] Tomas Sauer. Approximate varieties, approximate ideals and dimension reduction. *Numerical Algorithms*, 45(1-4):295–313, 2007.
- [17] Bernhard Schölkopf and Alexander J Smola. *Learning with kernels*. MIT Press, 2002.
- [18] Bernhard Schölkopf, Alexander Smola, and Klaus-Robert Müller. Nonlinear component analysis as a kernel eigenvalue problem. *Neural computation*, 10(5):1299–1319, 1998.

- [19] John Shawe-Taylor and Nello Cristianini. *Kernel Methods for Pattern Analysis*. Cambridge University Press, New York, NY, USA, 2004.
- [20] Hans J. Stetter. *Numerical polynomial algebra*. Society for Industrial and Applied Mathematics, 2004.
- [21] Bernd Sturmfels. Solving Systems of Polynomial Equations, volume 97 of CBMS Regional Conferences Series. Amer. Math. Soc., Providence, Rhode Island, 2002.
- [22] Vladimir N. Vapnik. *The Nature of Statistical Learning Theory*. Springer-Verlag New York, Inc., New York, NY, USA, 1995.
- [23] René Vidal, Yi Ma, and Sastry Shankar. Generalized principal component analysis (GPCA). *IEEE Transactions on Pattern Analysis and Machine Intelligence*, 27(12), 2005.